Second International Workshop on Harmonic Oscillators

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Organizing Institution

CIFMA   Centro Internacional de Física y Matemáticas Aplicadas, AC

Supporting Institutions

UNAM   Universidad Nacional Autónoma de México, *incl.:*

CIC   Coordinación de la Investigación Científica

DGAPA   Dirección General de Asuntos del Personal Académico

DGIA   Dirección General de Intercambio Académico

ICN   Instituto de Ciencias Nucleares

IF   Instituto de Física

FC   Facultad de Ciencias

IIMAS   Instituto de Investigaciones er   ¬das y en Sistemas

FUNED   Fundación Mexicana par   la Ciencia, AC

CLAF   Centro Latino Ame·

IAMP   International A·

ISF   Internationa·'

NASA   Nationa¹

Preface

The Second International Workshop on **Harmonic Oscillators** was held at the Hotel Hacienda Cocoyoc from March 23 to 25, 1994. The Workshop gathered 67 participants; there were 10 invited lectures, 30 plenary oral presentations, 15 posters, and plenty of discussion divided into the five sessions of this volume.

The Organizing Committee was asked by the chairmen of several Mexican funding agencies what exactly was meant by *harmonic oscillators*, and for what purpose the new research could be useful. **Osciladores Armónicos** —as we explained— is a code name for a family of mathematical models based on the theory of Lie algebras and groups, with applications in a growing range of physical theories and technologies: molecular, atomic, nuclear and particle physics; quantum optics and communication theory. Yet it is true that the Workshop —and these Proceedings— are not by/for front-line industrial soldiers, but by/for strategic planners in the staff room, where academic curiosity should be quite welcome. While in México we have no dearth of academic excelence (with tradition precisely in harmonic oscillators), local industry has yet to train the infantry to translate *applicable* science into *applied* research.

The Harmonic Oscillators II Workshop was funded and organized through the **Centro Internacional de Física y Matemáticas Aplicadas** (CIFMA). It is intended that CIFMA develop in México the manifold activities pioneered by the International Centre for Theoretical Physics, in Trieste, with special attention to the perceived scientific and technological needs and strong points of this country and the Latin American region. The Cuernavaca center adds to the existing networks initiated by the Centro Latino Americano de Física, in Brazil, and the Centro Internacional de Física, in Colombia. Through the great generosity of the Moshinsky family it was possible to announce at the Workshop Dinner that CIFMA is starting construction of it own installations at the campus of the National and State universities in Cuernavaca. It was very encouraging for our travails to see that our guests remarked the meeting's research atmosphere more than the excelent weather.

Indeed, on a lighter note, Professor Roy Glauber declared he was on a secret fact-finding mission for the US Congress, to see if after the NAFTA agreement all the harmonic oscillators would be rushing South (— *with a giant sucking sound*, as KBW recalling RP's one-time one-liner remarked) due to better conditions. Yes, they were. We see the motion as harmonic.

Professor Young S. Kim touched a sensitive chord in physics when convening the very successful first Harmonic Oscillators meeting at the College Park campus of the University of Maryland (March 25–28, 1992). [Proceedings: NASA Conference Publication 3197 (1993), Ed. by D. Han, Y.S. Kim and W.W. Zachary.] An informal harmonic oscillators 'network' now exists that is strengthened with these Proceedings. The Speakers of the Second Workshop will act as a Standing Committee for further meetings. It is now up to the local organizers of the Third Workshop to provide an attractive program for the Harmonic Oscillators community to gather again.

Timely technical help for the composition of this volume is gratefully acknowledged to Natig M. Atakishiyev, Mesuma K. Atakishiyeva, and Guillermo Krötzsch, at IIMAS–UNAM in Cuernavaca.

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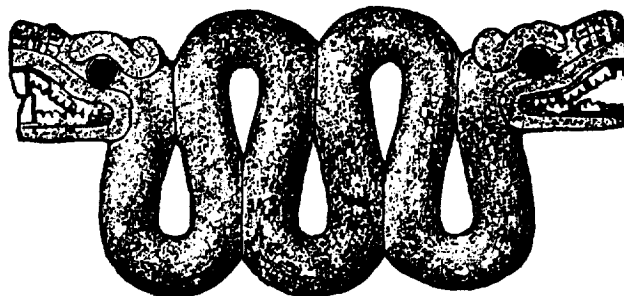
ALGEBRAIC THEORY OF MOLECULES

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Abstract

An algebraic formulation of quantum mechanics is presented. In this formulation, operators of interest are expanded onto elements of an algebra, $\mathcal{G}$. For bound state problems in ν dimensions the algebra $\mathcal{G}$ is taken to be $U(\nu + 1)$. Applications to the structure of molecules are presented.

1 Introduction

The development of new experimental techniques is giving rise to a wealth of information on complex systems. This information needs to be understood in terms of theoretical models which can, on one side, describe the observations and, on the other side, make predictions for other experiments. In view of the accuracy of the experiments, one needs new and more accurate mathematical models. For quantum mechanical problems, a natural framework is provided by the Schrödinger equation. In complex systems, the direct solution of the multiparticle Schrödinger equation becomes rather difficult and one many seek alternative methods. In this note, an alternative method, called algebraic theory, will be introduced and discussed briefly. The method will then be applied to the study of the structure of molecules. Problems of current interest in this field are, among others, the substitution of atoms in a large molecule leading to a lowering of symmetry, the polymerization process in which dimers, trimers, ... are formed from the original molecule, the study of new molecules, such as the cage fullerene molecules, C_{60}; ..., and, particularly important, the study of molecules at high excitation energy. An example of the latter will be presented.

2 Algebraic Theory

The logic scheme of algebraic theory is as follows:

<div align="center">

Quantum mechanical problem

$\Downarrow$

Algebraic Structure

</div>

$$\left\{ \begin{array}{l} \text{Lie Algebras} \\ \text{Graded Lie Algebras} \\ \text{Infinite Dimensinal Lie Algebras (Kac-Moody)} \\ \text{q-Deformed Lie Algebras (Hopf)} \\ \cdots \end{array} \right.$$

$$\Downarrow$$

Observables

$$\left\{ \begin{array}{l} \text{Spectra} \\ \text{Transitions} \\ \cdots \end{array} \right.$$

$$\Downarrow$$

Experiment

In the first step, all quantum mechanical operators of interest are mapped onto the elements of an algebra, $\mathcal{G}$. For example, the Hamiltonian operator is written as

$$H = E_o + \sum_\alpha \epsilon_\alpha G_\alpha + \sum_{\alpha\beta} u_{\alpha\beta} G_\alpha G_\beta + \ldots \quad , \quad G_\alpha \epsilon \mathcal{G} \quad . \tag{1}$$

The algebra $\mathcal{G}$ is called the spectrum generating algebra (SGA) and H is in the enveloping algebra of $\mathcal{G}$.

In some cases, it may happen that the Hamiltonian H contains only certain elements of $\mathcal{G}$, the invariant Casimir operators of $\mathcal{G}$ and of one of its subalgebra chains, $\mathcal{G} \supset \mathcal{G}' \supset \mathcal{G}'' \supset \ldots$,

$$H = f(C_i) \quad . \tag{2}$$

This case, called a dynamic symmetry, plays a special role in algebraic theory, since then the eigenvalues of H can be obtained in closed analytic form in terms of the quantum numbers characterizing the representations of $\mathcal{G} \supset \mathcal{G}' \supset \ldots$.

Dynamic symmetries and spectrum generating algebras have been used in various contexts for more than 30 years [1]. As a result of the systematic investigation and use in the context of nuclear and molecular physics, initiated with the introduction of the interacting boson model [2] in 1974 and of the vibron model [3] in 1981, it has become clear that all quantum mechanical problems in ν space dimensions can be mapped onto the algebra $U(\nu + 1)$ and all its states assigned to the totally symmetric representation [N] of $U(\nu + 1)$[4]. Examples of this mapping are given in the following section.

3   One dimensional problems

To begin with, consider the single case of one space dimension, $\nu = 1$. A trivial application of algebraic theory is provided here by the harmonic oscillator. The Schrödinger (differential) equation

$$H = \frac{1}{2} \left(-\frac{d^2}{dx^2} + x^2 \right) \quad , \quad H\psi_n = E\psi_m \tag{3}$$

with eigenvalues $E_n = (n + \frac{1}{2})$, and eigenfunctions

$$u_n(x) = \left[\pi^{\frac{1}{2}} 2^n n! \right]^{-\frac{1}{2}} \left(x - \frac{d}{dx} \right)^n e^{-\frac{1}{2} x^2} \tag{4}$$

(the Hermite polynomials), can be mapped into

$$H = \left(a^\dagger a + \frac{1}{2} \right) \quad , \tag{5}$$

with the same eigenvalues $E_m = (n + \frac{1}{2})$ and eigenstates

$$| n > = (n!)^{-\frac{1}{2}} (a^\dagger)^n | 0 > \quad . \tag{6}$$
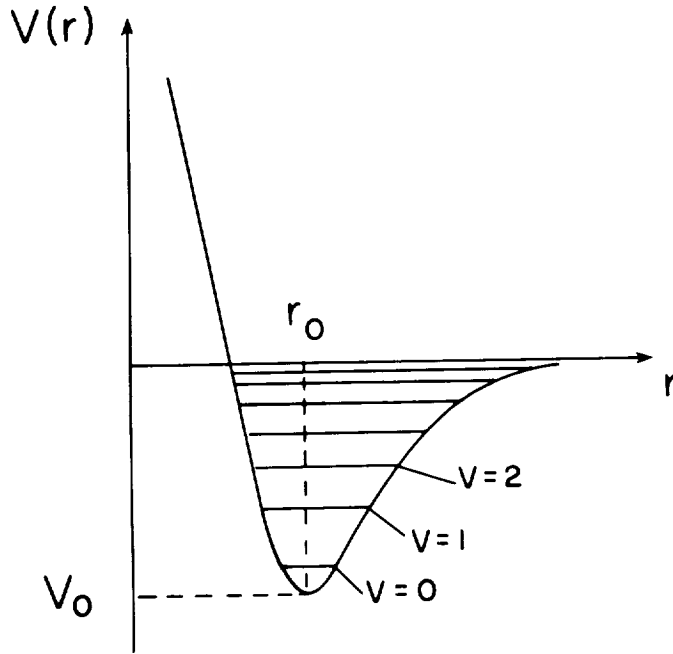
FIG. 1. The Morse potential V(r).

Here

$$a = \frac{1}{\sqrt{2}} \left(x + \frac{d}{dx} \right) \quad , \quad a^\dagger = \frac{1}{\sqrt{2}} \left(x - \frac{d}{dx} \right) \quad ; \quad [a, a^\dagger] = 1 \quad . \tag{7}$$

The algebra is

$$H(2) = a, a^\dagger, 1, a^\dagger a \quad , \tag{8}$$

called the Heisenberg, quantum mechanical or oscillator algebras [5]. The mapping produces a great simplification both in the evaluation of the matrix elements of operators which are integrals in the differential formulation

$$I_{nn'} = \int_{-\infty}^{\infty} u_{n'}(x) f\left(x, \frac{d}{dx}\right) u_n(x) dx \quad , \tag{9}$$

and algebraic functions in the algebraic formulation

$$I_{nn'} = < n' \mid f(a, a^\dagger) \mid n > \quad . \tag{10}$$

A slightly more complicated problem is provided by the anharmonic Morse oscillator [6], Fig.1. The Schrödinger equation with

$$H = -\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} + V(x) \, , \; V(x) = D[1 - exp(-\beta x)]^2 \quad , \tag{11}$$

with eigenfunctions

$$\begin{aligned}
\psi_v(x) &= N_s z^{\eta-v} e^{-\frac{z}{2}+\frac{1}{2}x\beta} L_v^{2\eta-2v-1}(z) \\
z &= 2\eta e^{-\beta x} \, , \; \eta = \frac{1}{\hbar\beta}\sqrt{2\mu D} \, , v = 0, 1, \ldots, \eta - \frac{1}{2} \, ,
\end{aligned} \tag{12}$$

and eigenenergies

$$E(v) = 2\hbar\beta\sqrt{\frac{D}{2\mu}}(v + \frac{1}{2}) - \frac{1}{2}\frac{\hbar^2\beta^2}{\mu}(v + \frac{1}{2})^2 \tag{13}$$

can be mapped onto the algebra $\mathcal{G} = U(2)$ with elements F_+, F_-, F_0, N and corresponds to the dynamic symmetry $U(2) \supset 0(2)$ of this algebra. The Hamiltonian is

$$H = AC \quad , \quad C = F_0^2 - N^2 \tag{14}$$

with eigenenergies

$$E(m) = A(m^2 - N^2); \; m = N, N - 2, \ldots, \, 1 \, or \, 0 \; (N = odd \, or \, even) \, . \tag{15}$$

The eigenvalues can be brought into the standard vibrational form introducing $v = (N - m)/2$,

$$E(v) = -4A(Nv - v^2); \; v = 0, 1, \ldots, \, \frac{N}{2} \, or \, \frac{N}{2} - \frac{1}{2}(N = even \, or \, odd) \, . \tag{16}$$

With some small changes this is seen to correspond to Eq.(13). The eigenstates can be written as $\mid N, v >$ and observables calculated as

$$< N, v' \mid \hat{T}(G) \mid N, v > \quad , \tag{17}$$

where $\hat{T}$ (G) is the appropriate operator built from the elements of $\mathcal{G}$. By making use of the algebraic method, all results of the anharmonic Morse oscillator can be found easily. (Note that in

the association of the Morse oscillator with $U(2) \supset O(2)$ only the positive branch of $O(2), m \geq 0$, has been used.)

As a third simple case, consider the anharmonic Pöshl-Teller oscillator

$$V(x) = -\frac{D}{cosh^2 \alpha x} \quad . \tag{18}$$

This potential can also be associated with $U(2) \supset O(2)$ and Hamiltonian [7]

$$H = AC \tag{19}$$

with eigenvalaues

$$E(v) = -4A(Nv - v^2) \tag{20}$$

One can see from (16) and (20) that the Morse and Pöshl-Teller potentials have the same bound state spectrum (isospectral potentials). (This statement is not true in $\nu = 2, 3, \dots$ dimensions.) The Morse and Pöshl-Teller potentials in 1 dim belong to a class of potentials called exactly solvable since their eigenvalues can be written in explicit analytic form. All exactly solvable potentials in 1 dim have been classified.

The overall algebraic structure of 1 dim problems can be written as

$$\begin{array}{l} U(2) \quad \supset O(2) \approx U(1) \quad , \\ \Downarrow c \\ H(2) \quad \supset O(2) \approx U(1) \quad . \end{array} \tag{21}$$

In this equation, the arrow with a c denotes a contraction of the algebra of U(2). (In addition to the contraction $U(2) \vec{c} H(2)$, there is another one $U(2) \vec{c} E(2)$, where $E(2)$ is the Euclidean algebra not discussed here.)

4 Multidimensional problems

In more than one dimension, the connection between the Schrödinger equation and the corresponding algebraic equation is not so straightforward, with the only exception of the harmonic oscillator and Coulomb problem. It is here that algebraic methods are particularly useful, since by formulating directly the problem in an algebraic framework one can construct the spectrum and calculate observables without reference to a specific form of the potential. The algebraic structure of three dimensional problems can be written as [4],[8]

$$\begin{array}{llll} & U(3) \quad \supset \quad O(3) \quad \supset \quad O(2) & & (I) \\ & \nearrow & & \\ U(4) & & & \\ & \searrow & & & (22) \\ & O(4) \quad \supset \quad O(3) \quad \supset \quad O(2) & & (II) \\ c \Downarrow & & & \\ H(4) \quad \supset \quad U(3) \quad \supset \quad O(3) \quad \supset \quad O(2) & & (III) \end{array}$$

The chain (I) corresponds to Schrödinger problems with Pöschl-Teller-like potentials, the chain (II) corresponds to Morse-like potentials, while the chain (III) corresponds to the harmonic oscillator in 3 dim.

In general, in ν dim one has

$$
\begin{array}{lll}
 & U(\nu) & \supset \ \ldots \\
 & \nearrow & \\
U(\nu+1) & \rightarrow \ \ldots & \\
 & \searrow & \\
c \Downarrow & O(\nu+1) & \supset \ \ldots \\
H(\nu+1) & \supset \quad U(\nu) & \supset \ \ldots
\end{array}
\tag{23}
$$

where now additional chains may appear in the reduction of $U(\nu+1)$. The five dimensional case, $\nu = 5$, has been extensively investigated in the context of nuclear physics [9]

5 Algebraic Theory of Large Molecules

The algebraic approach of Sect. 2 can be used to study molecular structure. For reasons that will be mentioned in the subsequent section, it is convenient to separate large molecules from small molecules (large here means molecules with more than 4 atoms). In large molecules each degree of freedom, x,y,z, is quantized with $U(2)$ and the total spectrum generating algebra is taken to be $\mathcal{G} = \sum_i \oplus U_i(2)$ [10]. A calculation of spectral properties proceeds then as follows: In step 1, all atoms are numbered, $\mathcal{N}$; in step 2, three coordinates are assigned to each atom for a total of $3\mathcal{N}$; in step 3, each coordinate is quantized with $U(2) \supset O(2)$, thus being treated as an anharmonic oscillator; in step 4, the oscillators are coupled with Hamiltonians

$$
H = \sum_{i=1}^{3\mathcal{N}} h_i + \sum_{i \geq j=1}^{3\mathcal{N}} w_{ij} \quad .
\tag{24}
$$

The structure of the Hamiltonian (24), when written in terms of the elements of the algebra $\mathcal{G}$ is

$$
h_i = \epsilon_{oi} + A_i(\hat{F}_{oi} - N_i)^2 \quad , w_{ij} = \lambda_{ij}(\hat{F}_{+i}\hat{F}_{-j} + \hat{F}_{-i}\hat{F}_{+j})
\tag{25}
$$

The h_i terms are diagonal in the basis $U_i(2) \supset O_i(2)$ characterized by the quantum numbers $|N_i, v_i >$ discussed in Sect. 3, while the w_{ij} are given in Ref. [10],[11]. In the final step 5, the spurious species corresponding to overall rotations and vibrations, are identified and removed by diagonalizing the Hamiltonian

$$
H' = H + \lambda \mathcal{P} \quad ,
\tag{26}
$$

where $\mathcal{P}$ is a projection operator into the spurious species and λ is taken to be a large number such that the spurious species are moved to a large energy. The removal of the spurious species

6

leaves $3\mathcal{N} - 6$ non spurious vibrations. This procedure produces the vibrational spectrum of the molecule.
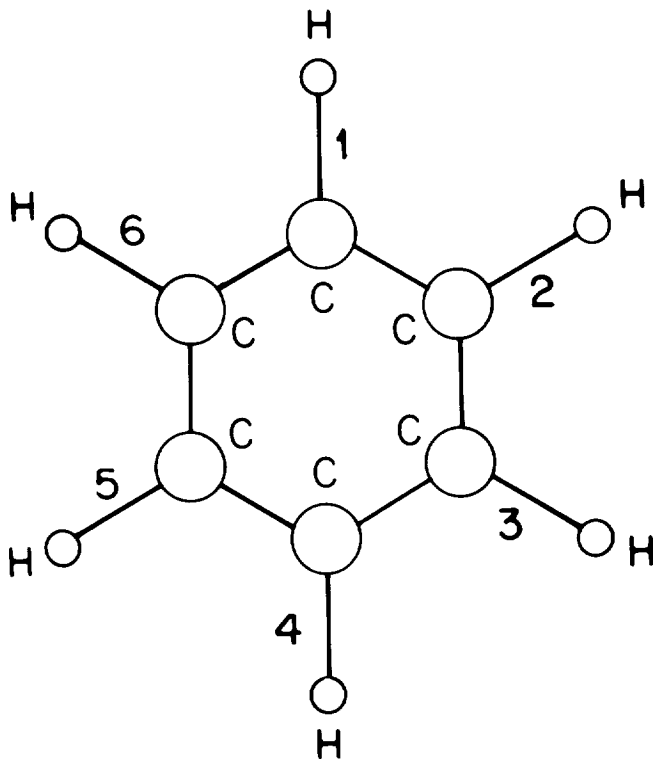
FIG. 2. Schematic representation of benzene (C_6H_6).

In a similar way one can compute intensities of transitions. There are two types of transitions of importance in molecules, infrared (IR) and Raman (R) transitions. For infrared transitions, the appropriate operator is a vector. Each component x,y,z of this vector is written in terms of elements of $\mathcal{G}$, i.e.

$$\hat{T}_x = \sum_{i=1}^{3\mathcal{N}} \alpha_{i,x} \hat{t}_i \quad , \quad \hat{t}_i = e^{-\beta_i(\hat{F}_{+i}+\hat{F}_{-i})} \quad , \quad \ldots \quad \cdot \tag{27}$$

The matrix elements of the operator (27) (and $\hat{T}_y$, $\hat{T}_z$) are then evaluated algebraically. For Raman transitions, the appropriate operator is a symmetric quadrupole tensor. The six components of this tensor, $x^2, y^2, z^2, xy, xz, yz$, are also written in terms of $\mathcal{G}$ and their matrix elements evaluated algebraically.

As an example of vibrational analysis of large molecules, consider the case of benzene, C_6H_6. The benzene molecule has the geometric structure shown in Fig. 2. A problem which arises in large molecules is that of the discrete symmetry of the molecule. In the case of benzene, the

appropriate symmetry is $\mathcal{D}_{6h}$. The discrete symmetries of molecules can be simply implemented in the algebraic framework. For example, consider the six stretching vibrations of the hydrogen atoms in benzene. All hydrogen atoms are equivalent. The Hamiltonian (24) which describes those vibrations

$$H = \sum_{i=1}^{6} A_i C_i + \sum_{i \leq j=1}^{6} \lambda_{ij} M_{ij} , \qquad (28)$$

where C_i and M_{ij} are a short-hand notation for the terms in (25), must be such that one cannot distinguish the equivalent atoms. Thus, all A_i's must be equal, $A_i = A$. In the interaction term, there are three contributions, first, second and third neighbor interactions. These too must be equal, $\lambda_{ij}^{(I)} = \lambda^{(I)}, \lambda_{ij}^{(II)} = \lambda^{(II)}$ and $\lambda_{ij}^{(III)} = \lambda^{(III)}$. The Hamiltonian H thus becomes

$$H = AC + \lambda^{(I)} S^{(I)} + \lambda^{(II)} S^{(II)} + \lambda^{(III)} S^{(III)} , \qquad (29)$$

and is characterized by a smaller set of parameters. The operators $C, S^{(I)}, S^{(II)}, S^{(III)}$ are appropriate linear combinations of the C_i's and M_{ij}'s. A corollary of the algebraic method is that certain linear combinations of the operators M_{ij} are symmetry adapter operators of $\mathcal{D}_{6h}$ and the irreducible representations of $\mathcal{D}_{6h}$ are obtained automatically by diagonalizing them [10],[12].

Using the algebraic method discussed above it has been possible to study the complete spectroscopy of benzene [13]. This molecule has 12 atoms and thus 36 degrees of freedom, 6 of which are spurious. The 30 non spurious species are shown in Table I.

TABLE I: Coordinates and symmetry species of benzene.

Coordinates	Number	Species	Spurious
CH stretch	6	$E_{2g} + B_{1u} + E_{1u} + A_{1g}$	
CC stretch	6	$A_{1g} + B_{2u} + E_{1u} + E_{2g}$	
CH in plane bend	6	$E_{1u} + B_{2u} + E_{2g} + A_{2g}$	
CH out of plane bend	6	$A_{2u} + B_{2g} + E_{1g} + E_{2u}$	
CC in plane bend	3+3	$B_{1u} + E_{2g}$	$A_{1g} + E_{1u}$
CC out of plane bend	3+3	$B_{2g} + E_{2g}$	$A_{1u} + E_{1g}$

The calculation describes the observed vibrational states not only in the low excitation energy region, fundamental vibrations, but also in the high excitation energy region, overtones. An example is shown in Fig. 3. This region cannot be described in the harmonic approximation and thus the use of algebraic methods based on the anharmonic Morse or Pöschl-Teller oscillators are

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crucial for an accurate description of the observed spectra.
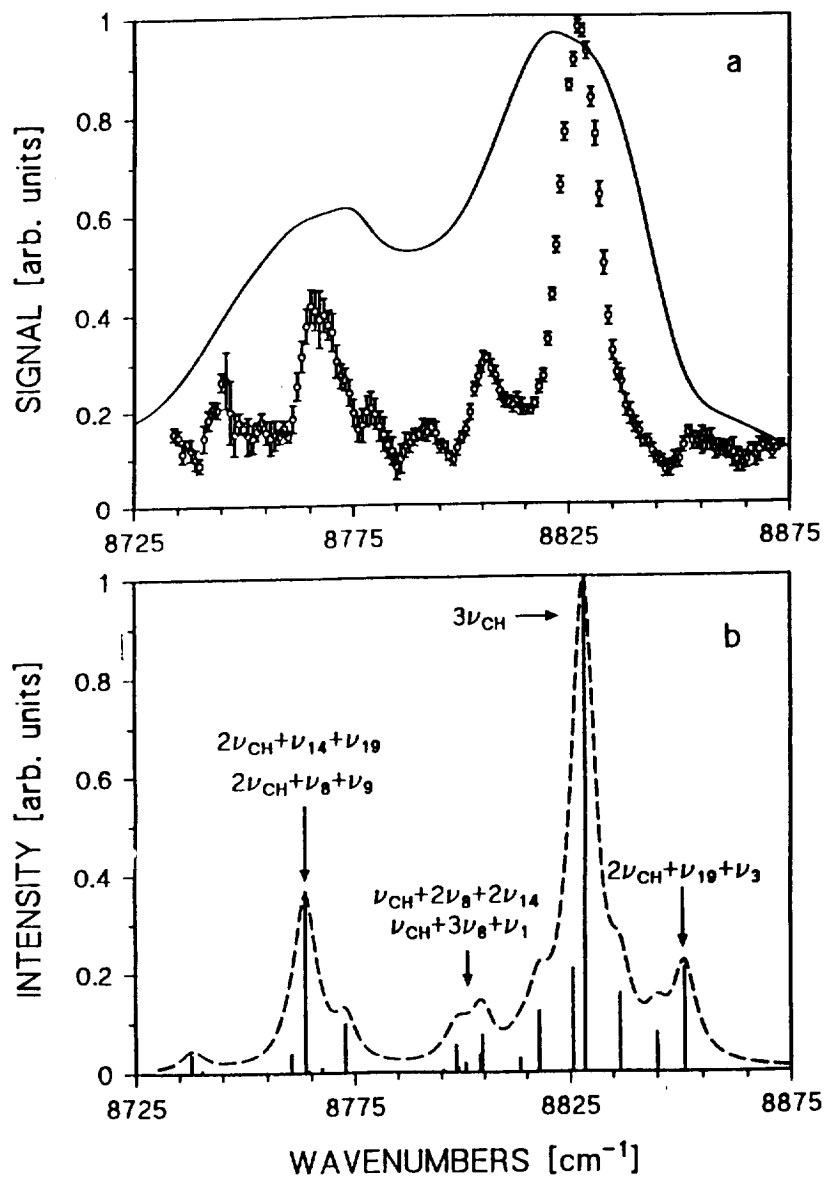
FIG. 3. (a) Opto-thermal spectrum in the region of the $\Delta v = 3$ overtone of the stretching CH mode of benzene. The full-line is a low-resolution experiment. (b) The spectrum calculated by means of algebraic theory. From Ref.[14].

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6   Algebraic Theory of Small Molecules

For molecules with a number of atoms less or equal to four, it is possible to quantize each vector degree of freedom, $\vec{r} \equiv (x,y,z)$, directly in terms of $U(4)$. When quantized in this way both rotations and vibrations are simultaneously included.
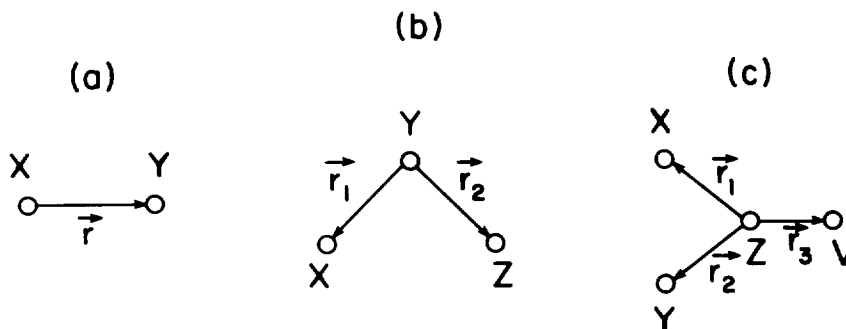
FIG. 4. Bond variables for small molecules.

It is also convenient to treat as vector variables the bond degrees of freedom, Fig.4, rather than the coordinates of the individual atoms, thus avoiding the problem of spurious states. The quantization scheme is thus here $\mathcal{G} = \sum_i \oplus U_i(4)$. This scheme has been extensively used to treat diatomic molecules with $U(4)$, triatomic molecules with $U(4) \oplus U(4)$ [15] and four atomic molecules with $U(4) \oplus U(4) \oplus U(4)$ [16]. It has also been possible recently to study high order interactions such as rotation-vibration couplings.

7   Conclusions

Algebraic methods have been used in recent years in the study of molecular structure. When applied to this system, algebraic theory offers two main advantages: (i) The use of Lie algebras to describe the interaction (Morse, Pöschl-Teller, ...) allows one to extend the traditional harmonic analysis to anharmonic analysis. One can thus deal easily with highly excited states of molecules where anharmonicities play a crucial role (a subject of current experimental interest especially in connection with intramolecular relaxation and energy transfer.) (ii) The use of algebraic operators to couple the individual modes of a molecule allows one to construct symmetry adapted states in a simple way. One can thus deal with complex molecules where discrete symmetries play a crucial role.

The algebraic method can be used in molecules in two ways:

A) With rotation and vibrations treated separately. In this case the spectrum generating algebra is

$$\begin{aligned}
\mathcal{G} &= \mathcal{G}_{ROT} \oplus \mathcal{G}_{VIB} \\
\mathcal{G}_{VIB} &= \sum_i \oplus U_i(2) \quad .
\end{aligned} \tag{30}$$

B) With rotations and vibrations treated simultaneously. In this case the spectrum generating algebra is

$$\mathcal{G} = \sum_i \oplus U_i(4) \quad . \tag{31}$$

The latter case is more complete, but more difficult to treat than the former, since one has to deal with the Racah algebra of U(4).

In view of its simplicity, the method is particularly well suited for a study of complex systems such as macromolecules, clusters, polymers, ... Work in this direction is in progress. An account of the algebraic theory of molecules is given in Ref.[17] and the mathematical formalism of Sects. 5 and 6 is reviewed in Ref.[18].

Acknowledgements

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EXACT, E = 0, CLASSICAL AND QUANTUM SOLUTIONS
FOR GENERAL POWER-LAW OSCILLATORS

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Abstract

For zero energy, $E = 0$, we derive exact, classical and quantum solutions for *all* power-law oscillators with potentials $V(r) = -\gamma/r^\nu$, $\gamma > 0$ and $-\infty < \nu < \infty$. When the angular momentum is non-zero, these solutions lead to the classical orbits $\rho(t) = [\cos \mu(\varphi(t) - \varphi_0(t))]^{1/\mu}$, with $\mu = \nu/2 - 1 \neq 0$. For $\nu > 2$, the orbits are bound and go through the origin. We calculate the periods and precessions of these bound orbits, and graph a number of specific examples. The unbound orbits are also discussed in detail. Quantum mechanically, this system is also exactly solvable. We find that when $\nu > 2$ the solutions are normalizable (bound), as in the classical case. Further, there are normalizable discrete, yet *unbound*, states. They correspond to unbound classical particles which reach infinity in a finite time. Finally, the number of space dimensions of the system can determine whether or not an $E = 0$ state is bound. These and other interesting comparisons to the classical system will be discussed.

1 Introduction

This all really started in Moscow, in 1992. That is where I met my colleague, Jamil Daboul, at the Second International Workshop on Squeezed States and Uncertainty Relations. It was held at the Conference Center-Hotel that the Russian Academy of Sciences uses. Late at night Jamil and I would get into sessions on life, physics, women, politics – you know, the usual stuff – while we drank his scotch.

The physics came around to musings about why certain problems can be solved exactly while others cannot, and the symmetries associated with such problems. There is a "folk-theorem" I often think of, which certainly is not exact but also certainly is intriguing. This theorem declares that if you can solve (or not solve) something classically the same is true quantum mechanically, and *visa versa*.

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Things stood there until Jamil visited me last year, and we took things up again. While wondering about the role of the Runge-Lenz vector in potential systems, a number of small observations started us down the line: a) the classical orbit for the attractive $-\gamma/r^4$ potential with centripetal potential barrier can be solved exactly; b) this type of quantum system is usually only discussed for $E \neq 0$; c) for $E = 0$, both the classical and quantum equations are simpler. Eventually we found out that *all* potentials of the form:

$$V(r) = -\frac{\gamma}{r^\nu} = -\frac{\gamma}{r^{2\mu+2}} \; , \qquad \gamma > 0 \; , \qquad -\infty < \nu < \infty \; , \tag{1}$$

can be solved exactly, both classically and quantum mechanically, for zero binding energy, $E = 0$. – In what follows, it will be useful to switch back and forth between the variables ν and μ related by

$$\mu = (\nu - 2)/2, \qquad \nu = 2(\mu + 1) \; . \tag{2}$$

Therefore, contrary to the usual scenario of solving a particular potential for all energies, one could solve an infinite system of potentials for a particular energy. The physics that came out was most amusing. In this piece I will report on this work. For further details you can consult a letter on the new results for the quantum system [1], as well as longer articles on the classical and quantum physics involved [2, 3].

In Section 2 I will demonstrate the solution to the classical problem. Section 3 contains amusing specific examples of some of the classical trajectories. The quantum solution will be given in Section 4. Section 5 contains interesting aspects of the quantum solutions, and then I give a brief closing comment.

Before continuing, I wish to further parametrize the power-law potentials as

$$V(r) \equiv -\frac{\gamma}{r^\nu} \equiv -\mathcal{E}_0 \frac{g^2}{\rho^\nu} = -\frac{L_0^2}{2ma^2} \frac{g^2}{\rho^\nu} \; , \qquad \rho \equiv r/a \; . \tag{3}$$

The dimensional coupling constant, γ, is more useful in classical physics. The dimensionless coupling constant, g^2, is more useful in quantum physics. Note, in particular, that the constant L_0 becomes $\hbar$ in quantum physics. Finally, the "effective potential," including the angular-momentum barrier, is

$$U(L,r) = \frac{L^2}{2mr^2} - \frac{\gamma}{r^\nu} \; . \tag{4}$$

2 Classical Solution

Let us now obtain the classical solution. By substituting the angular-momentum conservation condition

$$\dot{\varphi} = L/(mr^2) \tag{5}$$

into the energy conservation condition

$$E - V = \frac{m}{2}\dot{\varphi}^2 \left[\left(\frac{dr}{d\varphi}\right)^2 + r^2 \right] \; , \tag{6}$$

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one obtains

$$\left(\frac{dr}{d\varphi}\right)^2 + r^2 = \frac{2m(E-V)r^4}{L^2} . \tag{7}$$

This is essentially a first-order differential equation, which could be formally integrated. However, for $E = 0$, it is much more efficient to solve Eq. (7) directly. Converting to the dimensionless variable $\rho = r/a$ and substituting V into Eq. (7), we obtain

$$\left(\frac{d\rho}{d\varphi}\right)^2 + \rho^2 = \rho^{(4-\nu)} = \rho^{(2-2\mu)}. \tag{8}$$

For $\nu = 4$ the right-hand side of this equation is unity, so the solution is a cosine. This is the circular orbit $\rho = \cos\varphi$ which we will discuss in the next section. Guided by this we multiply Eq. (8) by $\rho^{2\mu-2}$ to yield

$$\left(\rho^{\mu-1}\frac{d\rho}{d\varphi}\right)^2 + \rho^{2\mu} = \left(\frac{d\rho^\mu}{\mu d\varphi}\right)^2 + (\rho^\mu)^2 = 1 . \tag{9}$$

Now, ρ^μ satisfies the differential equation for the trigonometric functions. Therefore, the *general* solution of Eq. (9) is given by

$$\rho^\mu = \cos \mu(\varphi - \varphi_0) = \cos\left[\frac{\nu-2}{2}(\varphi - \varphi_0)\right] , \tag{10}$$

or

$$\rho = [\cos \mu (\varphi - \varphi_0)]^{1/\mu} = \left[\cos\left(\frac{\nu-2}{2}(\varphi - \varphi_0)\right)\right]^{\frac{2}{\nu-2}} . \tag{11}$$

The phase, φ_0, is the integration constant.

Actually, for bound trajectories, which are the case for $\nu > 2$, the angle φ and the phase φ_0 both change value at the origin. There a particle is both at the end of a particular orbit (which starts and ends at the origin) and also at the beginning of the next orbit. φ changes value because of the use of polar coordinates and φ_0 does because of the singular nature of the potentials. One has to be careful in matching solutions for bound orbits, and I refer you to Ref. [2] for the details. For now just note that this problem can be taken care of, and we set $\varphi_0 = 0$ for the first orbit.

3 Classical Trajectories

3.1 Bound trajectories: $2 < \nu$ or $1 < \mu$

For $2 < \nu$ or $1 < \mu$, the trajectories go out of and back in to the origin in a finite amount of time. The reason for this is that the dynamic potential dominates at the origin, but the centripetal barrier dominates at a finite distance. The effective potential then asymptotes to zero from above as $r \to \infty$. This is shown in Figure 1.

These bound orbits have an opening angle at the origin of

$$\Phi_\nu = \frac{2\pi}{\nu-2} = \frac{\pi}{\mu} . \tag{12}$$

15
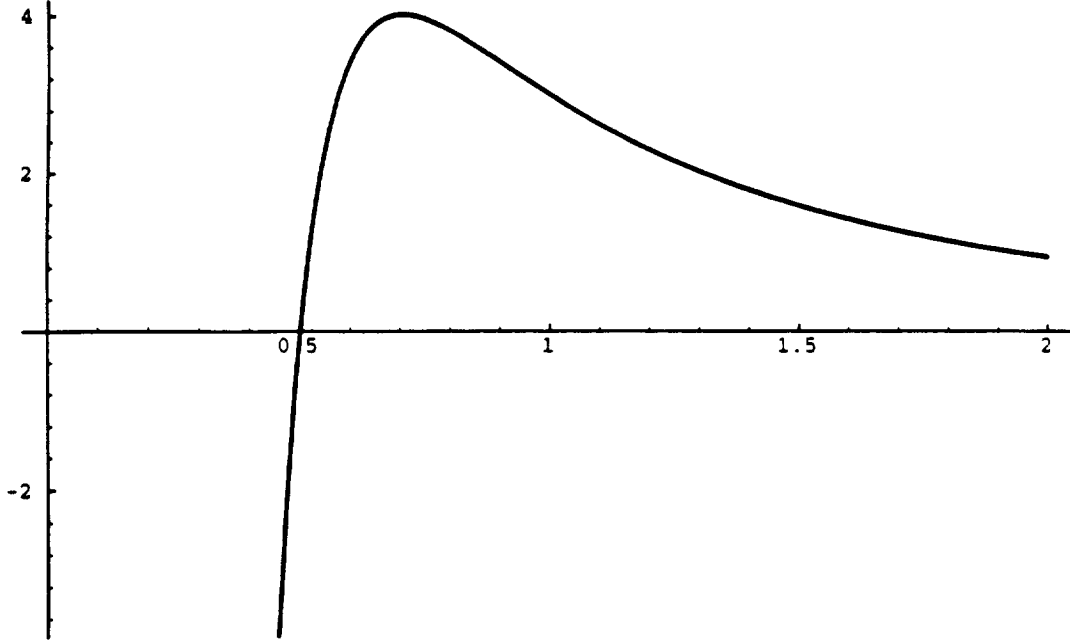
FIG. 1. The effective potential obtained from Eq. (4) for $\nu = 4$ in units of $\mathcal{E}_0/2$, as a function of $\rho = r/a$. The form is $U(\rho) = 4/\rho^2 - 1/\rho^4$.

The precession per orbit is

$$P_\nu = \left(\frac{1}{\mu} - 1\right)\pi = \left(\frac{4 - \nu}{\nu - 2}\right)\pi , \tag{13}$$

which means that if ν is a rational fraction, the trajectory will close after a finite number of orbits. The classical period of an orbit is

$$\tau_\nu = \left[\frac{ma^2}{L}\right]\frac{\sqrt{\pi}}{|\mu|}\frac{\Gamma(b)}{\Gamma(b + 1/2)} , \qquad b \equiv \frac{1}{\mu} + \frac{1}{2} = \frac{\nu + 2}{2\nu - 4} > 0 . \tag{14}$$

(Once again, see Ref. [2] for details.)

Starting with very large ν, the first orbit describes a very thin petal. The second orbit precesses by almost $-\pi$, being a thin petal almost on the opposite side of the first orbit. As ν gets smaller, the petals become larger and the precession per orbit becomes smaller.

For example, the $\nu = 8$ case, has three petals. Here a petal is $\pi/3$ wide and the precession per orbit is $-2\pi/3$. Thus, there are three orbits before the trajectory closes. Note that here the three petals in a closed trajectory cover only half of the opening angle from the origin. We show this in Figure 2.

The case $\nu = 6$ is very interesting. The width of a petal is $\pi/2$ and the precession is $-\pi/2$ per orbit. Here, the width of a petal and the precession are exactly such that there is no overlap and also no "empty angles." It takes four orbits to close a trajectory. This is shown in Figure 3. We see that the physical solution consists of two perpendicular lemniscates (figure-eight curves composed of two opposite petals).

16
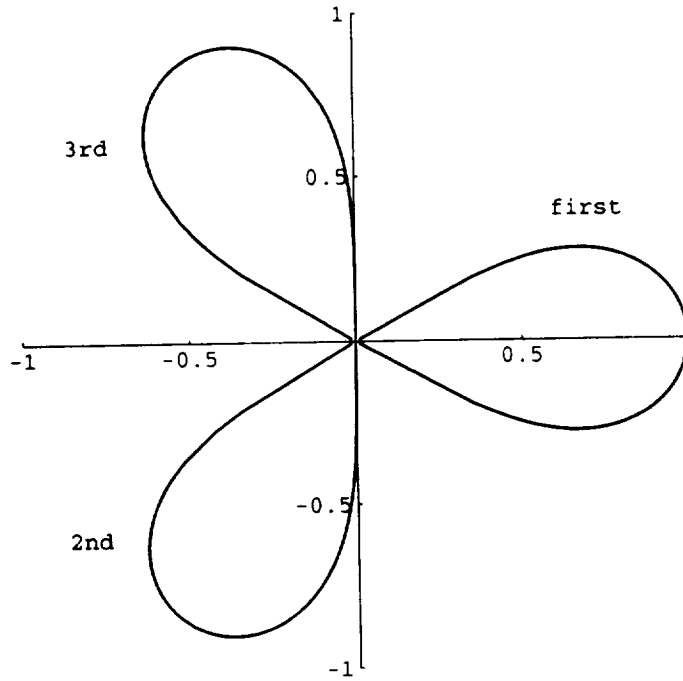
FIG. 2. The first three orbits for $\nu = 8$. Each orbit is precessed $-2\pi/3$ from the previous one, so that by the end of the 3rd orbit, the trajectory closes. In this, and later orbits, we show cartesian coordinates for orientation.
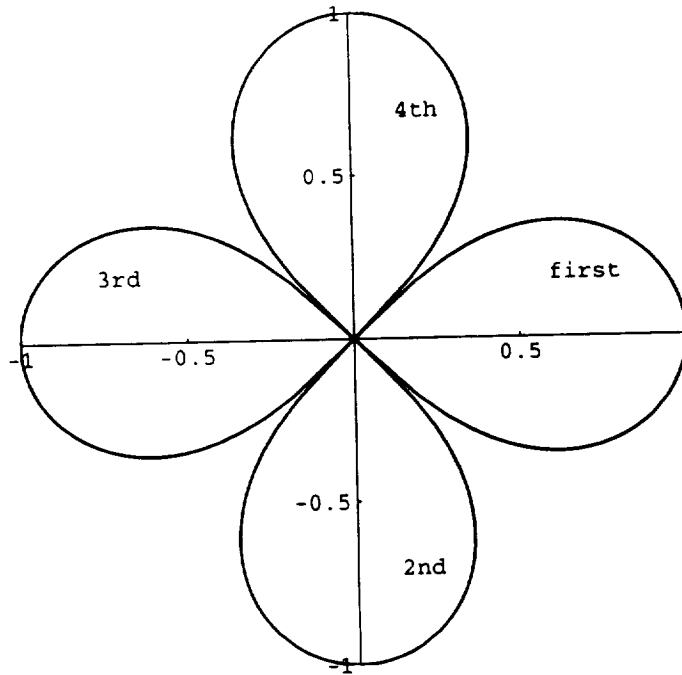
FIG. 3. The first four orbits for $\nu = 6$. Each orbit is precessed $-\pi/2$ from the previous one, so that by the end of the 4th orbit, the trajectory closes.

17
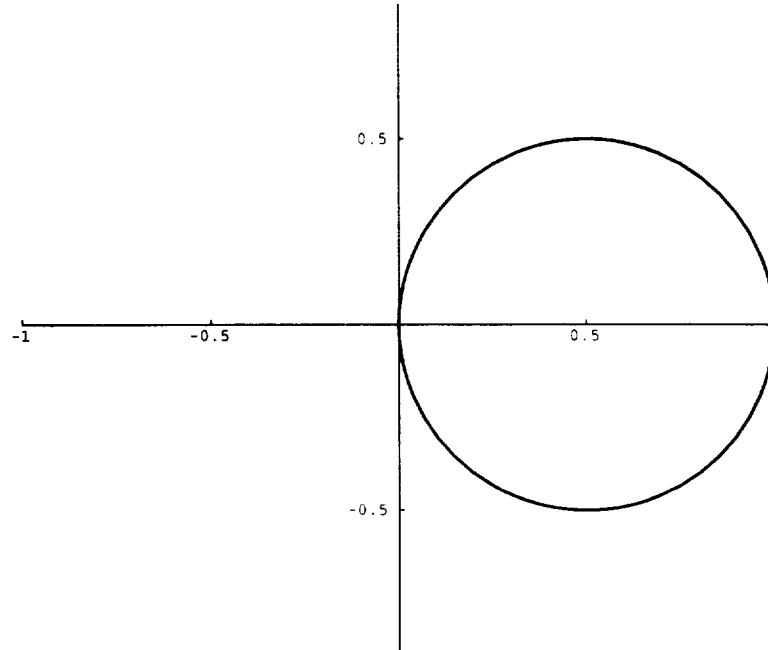
FIG. 4. The orbit for $\nu = 4$. It is a circle, and repeats itself continually.
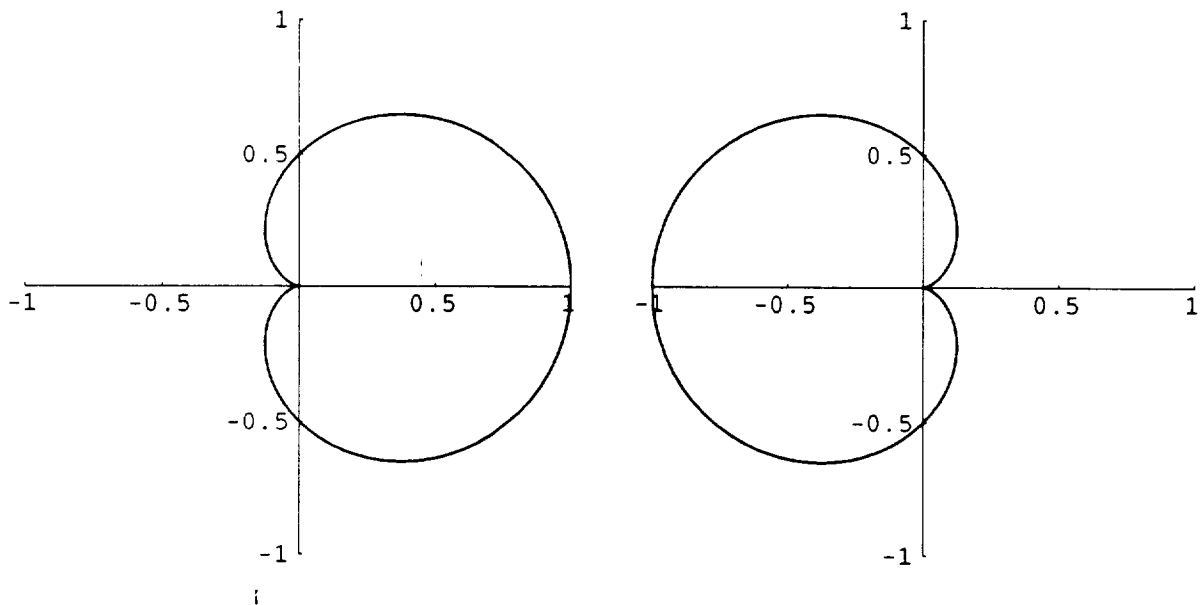
FIG 5. The first two orbits for $\nu = 3$. Each orbit is precessed π from the previous one, so that by the end of the 2nd orbit, the trajectory closes.

When we reach $\nu = 4$, the petals have widened so much that they form a circle. The circle starts at the origin, travels symmetrically about the positive x-axis, and returns to the origin. The precession is zero, so the orbit continually repeats itself. In Figure 4 we show this orbit.

As ν becomes less than 4, we can think of a petal obtaining a width greater than π, i.e., an orbit consists of two spirals, one out and one in, at opposite ends of the orbit.

Consider the special case $\nu = 3$. The width of the double-spiral orbit is still given by the formula for Φ_ν, and is 2π. Therefore, the first orbit begins and ends towards the negative x-axis. The precession is π, so the trajectory closes after two orbits. We show this case in Figure 5.

As ν approaches 2. the spirals become tighter and tighter and the precession (now clockwise) becomes larger. In fact, the spirals' angular variation as well as the orbit's precession both become infinite in magnitude as ν approaches 2.

3.2   Unbound trajectories: $\nu \leq 2$ or $\mu \leq 0$

When ν reaches 2, there is a singular change. First, the double spiral becomes infinite in angular width. But also, the joining of the two sides of the double spiral at $\rho = 1$ and $\varphi = 0$ breaks down. It is as if a tightly-wound double spring broke. The ends spiral out to infinity. This special case is a Cotes' (infinite) spiral. It takes an infinite time to reach infinity from the origin.

When the potential parameter ν just leaves that of the infinite spiral, that is, when one barely has $\nu < 2$ or $\mu < 0$, there is another change. Although the two ends of the entire trajectory still reach to infinity and the spirals in and out almost have infinite angular widths, the distance of closest approach jumps from $\rho = 0$ to $\rho = 1$.

As the value of ν decreases, the value of the angular width of the trajectory, now given by $\Phi_\nu = \pi/|\mu|$, also decreases accordingly. By the time $\nu = 1$, the angular width has decreased to 2π. Eventually it becomes less than π, meaning the orbit comes in and out in the same half plane. This happens for $\nu < 0$, i.e., when the force becomes repulsive.

When $0 < \nu < 2$, the repulsive centripetal barrier dominates at small r whereas the attractive potential $V = -\gamma/r^\nu$ dominates at large r. A typical shape is familiar from the Kepler problem. Therefore, for $0 < \nu < 2$, the $E = 0$ classical orbits are all unbounded. The distance, a, now has a completely different interpretation. It is now the distance of closest approach. Even so, the formal solution (10) remains valid for negative values of μ.

As a first example consider the case $\nu = 3/2$ or $\mu = -1/4$. This orbit has a total angular width of 4π. It is shown in the two drawings of Figure 6. The large-scale first drawing shows the trajectory coming in from the top, performing some gyration, and going out at the bottom. The small-scale second drawing shows the trajectory winding around twice near the origin, with the distance of closest approach being one.

A second example is the exact Kepler potential, $\nu = 1$ or $\mu = -1/2$. Eq. (10) gives

$$\rho^{-1/2} = \cos\varphi/2 \ , \tag{15}$$

so that

$$\frac{1}{\rho} = (\cos\varphi/2)^2 = \frac{1 + \cos\varphi}{2} \ . \tag{16}$$

This is the famous parabolic orbit for the Kepler problem with $E = 0$. This orbit is shown in the first drawing of Figure 7. The parabola yields an angular width of 2π, as it should.
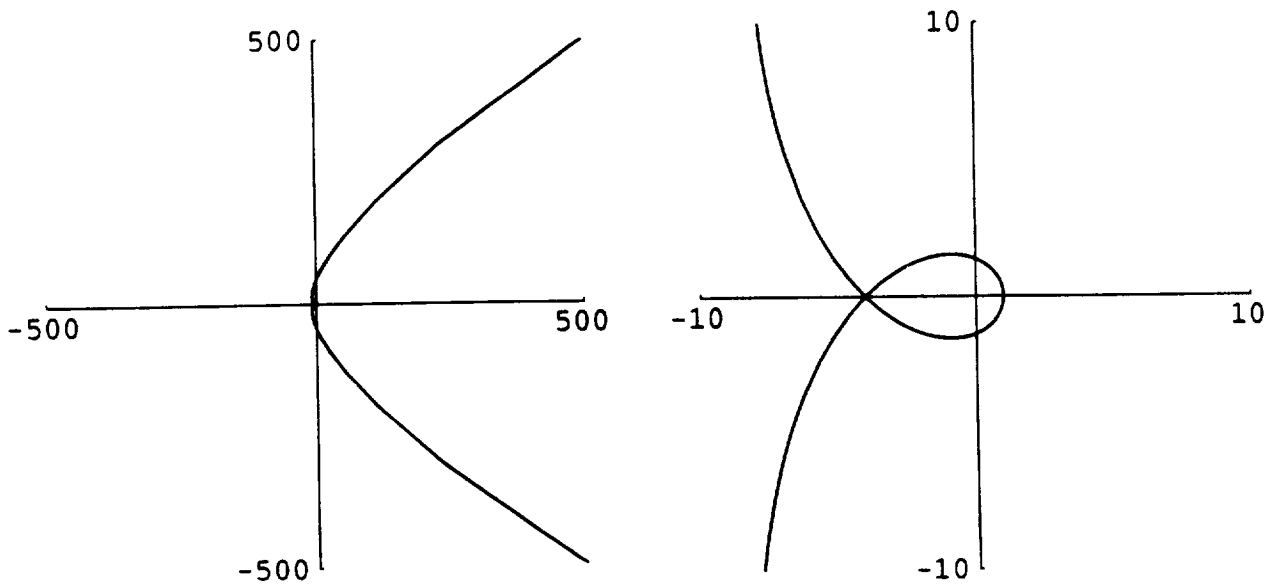
FIG. 6. A large-scale view, and a small-scale view near the origin, of the trajectory for $\nu = 3/2$.
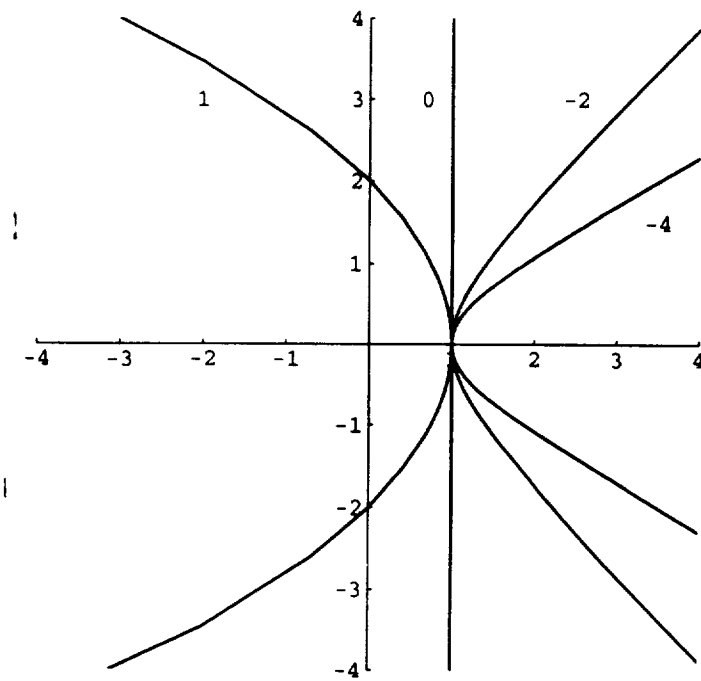
FIG 7. From left to right, he trajectories for the cases i) $\nu = 1$, ii) $\nu = 0$, iii) $\nu = -2$, and iv) $\nu = -4$. The curves are labeled by the numbers ν.

If we formally set $\nu = 0$ in the expression (3), we get a negative constant potential $V(r) = -\gamma$. Therefore, in this case the force vanishes and we have a free particle. Its orbit must be a straight line. However, Eq. (8) shows that one still has the same type of solution, Eq. (11). Here it is

$$\rho = [\cos \varphi]^{-1} , \qquad x = r \cos \varphi = a . \tag{17}$$

This is the equation for a vertical straight line that crosses the x-axis at $x = a$, as required by the initial conditions. This orbit is shown in the second drawing Figure 7, it subtending an angular width of π from the origin.

For $\nu < 0$ or $\mu < -1$ the potentials $V(r)$ in Eq. (3) are repulsive and negative-valued for all $r > 0$, with $V(r)$ going to $-\infty$ at large distances. Since both the potential, $V(r)$, and the centripetal potential decrease monotonically, the effective potential has no minima or maxima. Even so, for $E = 0$ these unbounded orbits behave qualitatively like those for $0 \leq \nu < 2$. The quantity a now labels the distance of closest approach and the solutions are given by the same expression (10), which is also valid for all $\mu < 0$:

$$\rho = [\cos \mu\varphi]^{1/\mu} = [\cos |\mu|\varphi]^{-1/|\mu|} , \qquad \mu < 0 . \tag{18}$$

The most famous special case of these potentials is the "inverted" harmonic-oscillator potential, with $\nu = \mu = -2$. The orbit is given by $\rho = [\cos 2\varphi]^{-1/2}$, so that

$$1 = \frac{r^2}{a^2} \cos 2\varphi = \frac{r^2}{a^2}(\cos^2 \varphi - \sin^2 \varphi) = \frac{x^2}{a^2} - \frac{y^2}{a^2} . \tag{19}$$

Thus, the trajectory is a special hyperbolic orbit, whose minor and major axes are equal, $b^2 = a^2$. We show this orbit as the third drawing in Figure 7. Now the angular width has decreased to $\pi/2$.

As the last case, we consider the orbit for $\nu = -4$ or $\mu = -3$. This orbit is shown in the last drawing of Figure 7. The orbit subtends an angle of $\pi/3$, again as it should. One sees that as ν becomes more and more negative, the orbits will become narrower and narrower. This is just as in the bound case, where the petals became narrower and narrower as ν became more and more positive.

4   Quantum Solution

Consider the radial Schrödinger equation with angular-momentum quantum number l:

$$ER_l = \left[-\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} \right) + V(r) \right] R_l . \tag{20}$$

This Schrödinger equation is exactly solvable for the potential of Eq. (3) for all $E = 0$ and all $-\infty < \nu < \infty$. To see this, set $E = 0$ in Eq. (20), change variables to ρ, and then multiply by $-\rho^2$. One finds

$$0 = \left[\rho^2 \frac{d^2}{d\rho^2} + 2\rho \frac{d}{d\rho} - l(l+1) + \frac{g^2}{\rho^{2\mu}} \right] R_l(r) . \tag{21}$$

21

This is a well-known differential equation of mathematical physics. For $\nu \neq 2$ or $\mu \neq 0$, the solution can be directly given as

$$R_l(r) = \frac{1}{\rho^{1/2}} \mathbf{J}_{\left(\frac{2l+1}{|\nu-2|}\right)} \left(\frac{2g}{|\nu-2|\rho^{\left(\frac{\nu-2}{2}\right)}} \right) = \frac{1}{\rho^{1/2}} \mathbf{J}_{\left(\frac{l+1/2}{|\mu|}\right)} \left(\frac{g}{|\mu|\rho^\mu} \right) , \quad \mu \neq 0 . \tag{22}$$

One actually has to be careful about when an absolute value of μ is called for in the labels of the solution, and whether the J Bessel functions are called for vs. the Y function. These details are given in Ref. [3].

5 Properties of the Quantum Solution

5.1 Normalizable bound states: $2 < \nu$ or $1 < \mu$

The normalization constants for the wave functions would have to be of the form

$$N_l^{-2} = \int_0^\infty \frac{r^2 dr}{\rho} \mathbf{J}^2_{\left(\frac{l+1/2}{|\mu|}\right)} \left(\frac{g}{|\mu|\rho^\mu} \right) . \tag{23}$$

Changing variables first from r to ρ and then from ρ to $z = g/(|\mu|\rho^\mu)$, and being careful about the limits of integration for all μ, one obtains

$$N_l^{-2} = \frac{a^3}{|\mu|} \left(\frac{g}{|\mu|} \right)^{2/\mu} I_l , \tag{24}$$

where

$$I_l = \int_0^\infty \frac{dz}{z^{(1+2/\mu)}} \mathbf{J}^2_{\left(\frac{l+1/2}{|\mu|}\right)}(z) . \tag{25}$$

This integral is convergent and given by

$$I_l = \frac{1}{2\pi^{1/2}} \frac{\Gamma\left(\frac{1}{2} + \frac{1}{\mu}\right)}{\Gamma\left(1 + \frac{1}{\mu}\right)} \frac{\Gamma\left(\frac{l+1/2}{|\mu|} - \frac{1}{\mu}\right)}{\Gamma\left(1 + \frac{l+1/2}{|\mu|} + \frac{1}{\mu}\right)} , \tag{26}$$

if the following two conditions are satisfied:

$$\frac{2l+1}{|\mu|} + 1 > \frac{2}{\mu} + 1 > 0 . \tag{27}$$

Eqs. (26) and (27) lead to two sets of normalizable states. The first is when

$$\mu > 0 \quad \text{or} \quad \nu > 2 , \qquad l > 1/2 . \tag{28}$$

These are ordinary bound states and result because the effective potential asymptotes to zero from above, as in Figure 1. In this case, for $E = 0$, the wave function can reach infinity only by tunneling through an infinite forbidden region. That takes forever, and so the state is bound.

Note that the condition on l in Eq. (28) is the minimum nonzero angular momentum allowed in quantum mechanics, $l_{min} = 1$. This agrees with the classical orbit solution which is bound for any nonzero angular momentum. Also, the above $E = 0$ solutions exist for all $g^2 > 0$, and not just for discrete values of the coupling constant.

5.2 Free states: $-2 \leq \nu \leq 2$ or $-2 \leq \mu \leq 0$

For $-2 \leq \nu \leq 2$ or $-2 \leq \mu \leq 0$ and $l \geq 1$ (as well as the solutions with $l = 0$ and $0 < \mu$ or $2 < \nu$) the solutions are free, continuum solutions. This is in analogy to the classical case, where the trajectories are normal and free.

5.3 Unbound yet normalizable states: $\nu < -2$ or $\mu < -2$

There is another class of normalizable solutions which is quite surprising. For any l and all $\nu < -2$ or $\mu < -2$, one can verify that the conditions of Eq. (27) are also satisfied. Thus, even though one here has a repulsive potential that falls off faster than the inverse-harmonic oscillator and the states are *not* bound, the solutions are *normalizable*!

The corresponding classical solutions yield infinite orbits, for which the particle needs only a finite time to reach infinity [2]. But it is known that a classical potential which yields trajectories with a finite travel time to infinity also yields a discrete spectrum in the quantum case. This discrete spectrum is obtained by imposing particular boundary conditions on the solutions, which defines a self-adjoint extension of the Hamiltonian. (See Ref. [1].)

5.4 Bound states in arbitrary dimensions

One can easily generalize the problem of the last section to arbitrary D space dimensions. Doing so yields another surprising physical result.

To obtain the D-dimensional analogue of Eq. (21), one simply has to replace 2ρ by $(D-1)\rho$ and $l(l+1)$ by $l(l+D-2)$. The solutions follow similarly as

$$
\begin{aligned}
R_{l,D} &= \frac{1}{\rho^{D/2-1}} \mathbf{J}_{\left(\frac{2l+D-2}{|\nu-2|}\right)} \left(\frac{2g}{|\nu-2|\rho^{\left(\frac{\nu-2}{2}\right)}} \right) \\
&= \frac{1}{\rho^{D/2-1}} \mathbf{J}_{\left(\frac{l+D/2-1}{|\mu|}\right)} \left(\frac{g}{|\mu|\rho^{\mu}} \right) .
\end{aligned}
\tag{29}
$$

To find out which states are now normalizable one first has to change the integration measure from $r^2 dr$ to $r^{D-1} dr$ and then continue as before. The end result is that if the wave functions are normalizable, the normalization constant is given by

$$
N_{l,D}^{-2} = \frac{a^D}{|\mu|} \left(\frac{g}{|\mu|} \right)^{2/\mu} I_{l,D} ,
\tag{30}
$$

where

$$
I_{l,D} = \frac{1}{2\pi^{1/2}} \frac{\Gamma\left(\frac{1}{2} + \frac{1}{\mu}\right)}{\Gamma\left(1 + \frac{1}{\mu}\right)} \frac{\Gamma\left(\frac{l+D/2-1}{|\mu|} - \frac{1}{\mu}\right)}{\Gamma\left(1 + \frac{l+D/2-1}{|\mu|} + \frac{1}{\mu}\right)} ,
\tag{31}
$$

which is defined and convergent for

$$
\frac{2l+D-2}{|\mu|} + 1 > \frac{2}{\mu} + 1 > 0 .
\tag{32}
$$

This yields the surprising result that there are bound states for all $\nu > 2$ or $\mu > 0$ when $l > 2 - D/2$. Explicitly this means that the minimum allowed l for there to be zero-energy bound states are:

$$
\begin{aligned}
D = 2 \,, \quad l_{min} &= 2 \,, \\
D = 3 \,, \quad l_{min} &= 1 \,, \\
D = 4 \,, \quad l_{min} &= 1 \,, \\
D > 4 \,, \quad l_{min} &= 0 \,.
\end{aligned}
\tag{33}
$$

This effect of dimensions is purely quantum mechanical, and exists for all central potentials. Classically, the number of dimensions involved in a central potential problem has no intrinsic effect on the dynamics. The orbit remains in two dimensions, and the problem is decided by the form of the effective potential, U, which contains only the angular momentum barrier and the dynamical potential.

In quantum mechanics there are two places where an effect of dimension appears. The first is in the factor $l(l + D + 2)$ of the angular-momentum barrier. The second is more fundamental. It is due to the operator

$$
U_{qm} = -\frac{(D - 1)}{\rho} \frac{d}{d\rho} \,.
\tag{34}
$$

This is a new contribution to the "effective potential," and can be calculated [1]. The end result is that given in Eq. (33).

The dimensional effect produces what amounts to an additional centrifugal barrier which can bind the wave function at the threshold, even though the expectation value of the angular momentum vanishes.

6   Closing Comment

I hope you have found this discussion of anharmonic power potentials entertaining and enlightening. Jamil and I certainly have. The intuition obtained into the workings and relationships between classical and quantum physics has been delightful to us, to say the least.

Thank you very much.

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ALGEBRAIC APPROACH TO THE VIBRATIONAL EXCITATIONS IN METHANE

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Abstract

We present a description of the vibrational excitations of methane by means of an algebraic analysis of a model of coupled anharmonic oscillators.

1   Introduction

Consider an AB_4-like tetrahedral molecule and suppose we are interested in describing its vibrational degrees of freedom. This can be accomplished either in the framework of an integro-differential scheme or by means of an algebraic approach. The former constitutes the traditional method, which consists in parametrizing the Hamiltonian in terms of internal coordinates [1], where the potential is modeled in terms of force field constants that can be obtained from theoretical calculations or from fits to spectroscopic data [2]. On the other hand, the algebraic approach represents an alternative to the traditional methods based on the use of Lie algebras to represent the interactions [3]. The algebra used to describe the vibrational degrees of freedom is not unique. Michelot and Leroy, for example, use a unitary group $U(n)$ as the dynamical group of the system with $n - 1$ vibrational degrees of freedom [4], while Iachello and Oss introduce an $SU(2)$ algebra for each atomic degree of freedom [5]. In this work we carry out a complete description of the vibrational excitations of tetrahedral molecules by assigning a $U(2)$ algebra to each interatomic potential.

2   Algebraic Model

The model is based on the isomorphism of the $U(2)$ algebra with a one-dimensional Morse oscillator, whose eigenstates may be put into a one to one correspondence with a set of $U(2) \supset O(2)$ states, characterized by the quantum numbers $|[N], m >$, as long as the value of m is restricted to be non-negative. In this space the Morse Hamiltonian takes the simple form $\hat{\mathcal{H}} =$

$A\hat{C}_{2O(2)}$, where A and N are related to the Morse potential parameters and $\hat{C}_{2O(2)}$ corresponds to the square of the $O(2)$ invariant operator [3].
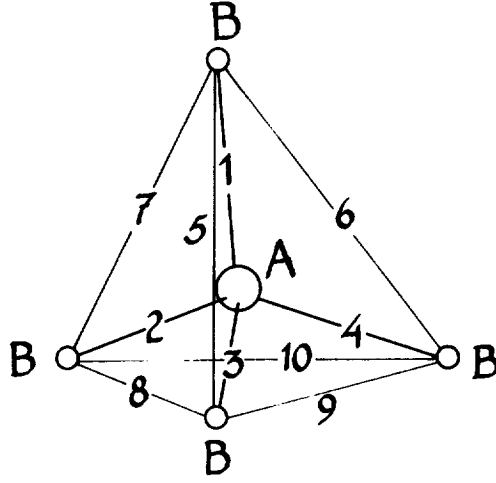
FIG. 1. Assignment of the $U^i(2)$ algebras to tetrahedral molecules.

For the description of a tetrahedral molecule we assign a $U^i(2)$ algebra to each interaction present, as shown in Fig. 1. The first four algebras have been chosen to correspond to the $A - B$ interactions, while the other six represent the $B - B$ couplings. The molecular dynamical group is then given by the product $U^1(2) \times \ldots \times U^{10}(2)$, and the most general Hamiltonian, up to two body interactions, conserving the total number of quanta and invariant under the tetrahedral group T_d, can be written as

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}^S + \hat{\mathcal{H}}^B + \hat{V}^{S-B} \quad . \tag{1}$$

The term $\hat{\mathcal{H}}^S$ describes the stretching degrees of freedom and has the form

$$\hat{\mathcal{H}}^S = A_1 \sum_{i=1}^{4} \hat{C}_{2O^i(2)} + B_{12} \sum_{i=1}^{3} \sum_{j=i+1}^{4} C_{2O^{ij}(2)} + \lambda_{12} \sum_{i=1}^{3} \sum_{j=i+1}^{4} \hat{\mathcal{M}}_{ij} \quad ,$$

while $\hat{\mathcal{H}}^B$ is the bending contribution, given by

$$\hat{\mathcal{H}}^B = A_5 \sum_{i=5}^{10} \hat{C}_{O^i(2)} + B_{5,6} \left\{ \sum_{j=6}^{9} \sum_{i=5,10} \hat{C}_{2O^{ij}(2)} + \sum_{j=7,9} \sum_{i=6,8} \hat{C}_{2O^{ij}(2)} \right\}$$

$$+ B_{5,10} \left\{ \hat{C}_{2O^{5,10}(2)} + \hat{C}_{2O^{6,8}(2)} + \hat{C}_{2O^{7,9}(2)} \right\}$$

$$+ \lambda_{5,6} \left\{ \sum_{j=6}^{9} \sum_{i=5,10} \hat{\mathcal{M}}_{ij} + \sum_{j=7,9} \sum_{i=6,8} \hat{\mathcal{M}}_{ij} \right\}$$

$$+ \lambda_{5,10} \left\{ \hat{\mathcal{M}}_{5,10} + \hat{\mathcal{M}}_{6,8} + \hat{\mathcal{M}}_{7,9} \right\} \quad .$$

The last operator, $\hat{V}_f^{S-B}$, represents the stretching-bending interactions, which will be neglected as a first approximation. In these expressions $\hat{C}_{2O^{ij}(2)}$ corresponds to the $O^{ij}(2)$ Casimir invariant, while $\hat{\mathcal{M}}_{ij}$ is the Majorana operator, which is related to the $U^{ij}(2)$ Casimir operator [3].

The simplest basis to diagonalize the Hamiltonian is the one associated to the local-mode chain [3]

$$U^{(1)}(2) \times \ldots \times U^{(4)}(2) \times U^{(5)}(2) \times \ldots \times U^{(10)}(2) \supset O^{(1)}(2) \times \ldots \times O^{(10)}(2) \supset O(2)$$

$$\downarrow \quad\quad \downarrow \quad\quad \downarrow \quad\quad\quad \downarrow \quad\quad \downarrow \quad\quad\quad \downarrow \quad\quad \downarrow \tag{2}$$

$$|[N_1] \,, \quad \ldots \quad [N_1] \quad\quad [N_2] \,, \quad \ldots \,, \quad\quad [N_2] \quad v_1\,, \quad \ldots \,, \quad v_{10}; \quad\quad V > \,,$$

where below each group we have indicated the quantum numbers characterizing the eigenvalue of the corresponding invariant operator. The two boson numbers N_1 and N_2, are related to the two sets of physical modes (stretching and bending). The quantum numbers v_i correspond to the number of phonons in each oscillator ($v_i = \frac{N_i}{2} - m_i$), while $V = \sum_{i=1}^{10} v_i$.

A simple analysis of an AB_4 tetrahedral molecule [6] shows that it presents 9 vibrational degrees of freedom, four of them corresponding to the fundamental stretching modes ($A_1 \oplus F_2$) and the other five to the fundamental bending modes ($E \oplus F_2$). Comparing this result with the local basis (2), we deduce that an unphysical bending mode is present in the algebraic formalism. We thus proceed to eliminate this spurious state both from the Hamiltonian and the basis.

To accomplish this goal we first transform, for the one phonon case, the local basis to a normal one, which carries the irreducible representations (irreps) of the T_d group. With this change of basis we obtain the decomposition $A_1 \oplus F_2$ for the stretches and $A_1 \oplus E \oplus F_2$ for the bends. From this result we readily identify the A_1 bending mode as the spurious state. We now eliminate this spurious state from the space and proceed to construct the higher phonon basis from the physical one-phonon set by means of the coupling coefficients $C(\;;\;)$

$$^{V_1+V_2}\Psi_\gamma^\Gamma = \sum_{\gamma_1 \gamma_2} C(\Gamma_1\Gamma_2\Gamma;\gamma_1\gamma_2\gamma) \; ^{V_1}\Psi_{\gamma_1}^{\Gamma_1} \; ^{V_2}\Psi_{\gamma_2}^{\Gamma_2} \,, \tag{3}$$

where Γ and γ label the irreps of T_d and its components, respectively.

To eliminate the spurious contributions from the Hamiltonian we demand its null expectation value with respect to the one-phonon spurious functions [7]

$$< \, ^1\Psi_{\text{bending}}^{A_1} \, |\hat{\mathcal{H}}| \, ^1\Psi_{\text{bending}}^{A_1} \, > = 0 \,, \tag{4}$$

which leads to a constraint

$$4(1 - N_2)A_5 + 16(1 - 2N_2)B_{5,6} + 4(1 - 2N_2)B_{5,10} = 0$$

between the interaction parameters.

The vibrational energies are obtained by diagonalizing the Hamiltonian (1) with respect to the normal basis (3), constructed from the projected one-phonon functions (A_1, F_2)—stretching and (E, F_2)— bending, taking into account the constraint (4).

TABLE I. Experimental [2,6,9] and calculated energies (cm^{-1}) for methane.

V	Normal label	Γ	Expt.	Calc.
1	ν_4	F_2	1310.0	1303.7
	ν_2	E	1533.0	1520.4
	ν_1	A_1	2916.5	2918.4
	ν_3	F_2	3019.4	3027.2
2	$2\nu_4$	A_1		2474.5
		E		2476.4
		F_2	2614.0	2610.5
	$\nu_2 + \nu_4$	F_1		2827.2
		F_2	2830.4	2841.5
	$2\nu_2$	A_1		3003.7
		E		3026.3
	$\nu_1 + \nu_4$	F_2	4223.0	4222.0
	$\nu_3 + \nu_4$	A_1		4330.9
		E		4330.9
		F_1		4330.9
		F_2	4319.0	4330.9
	$\nu_2 + \nu_3$	F_1		4547.7
		F_2	4549.0	4547.7
	$\nu_1 + \nu_2$	E		4438.8
	$2\nu_1$	A_1		5788.0
	$\nu_1 + \nu_3$	F_2	5861.0	5856.7
	$2\nu_3$	A_1		5974.4
		F_2	6004.7	6014.5
		E		6047.7
3	$3\nu_4$	F_2		3624.3
		F_1		3778.3
		F_2		3779.4
		A_1		3920.4
	$\nu_2 + 2\nu_4$	A_1		3925.7
		E		3935.6
		E		3987.9
		A_2		4017.6
		F_2	4123.0	4123.9
		F_1		4260.4
	$2\nu_2 + \nu_4$	F_1		4425.5
		F_2		4317.4
		F_2		4387.6

V	Normal label	Γ	Expt.	Calc.
3	$\nu_1 + \nu_2 + \nu_4$	F_1		5745.6
		F_2	5775.0	5759.9
		A_2		5854.4
		E		5854.4
		F_1		5854.4
	$\nu_2 + \nu_3 + \nu_4$	F_2		5854.4
		A_1		5868.7
		E		5868.7
		F_1		5868.7
		F_2	5861.0	5868.7
	$\nu_1 + 2\nu_2$	A_1		5922.0
		E		5944.7
	$2\nu_2 + \nu_3$	F_2		6030.9
		F_1		6053.5
		F_2		6053.5
	$2\nu_1 + \nu_4$	F_2		7091.7
	$\nu_1 + \nu_3 + \nu_4$	A_1		7160.4
		E		7160.4
		F_1		7160.4
		F_2		7160.4
	$2\nu_3 + \nu_4$	F_2		7278.1
		E		7308.4
		A_1		7318.2
		F_1		7318.2
		F_2		7318.2
		F_2		7351.4
		F_1		7351.4
	$2\nu_1 + \nu_2$	E		7318.2
	$\nu_1 + \nu_2 + \nu_3$	F_1		7377.1
		F_2		7377.1
	$\nu_2 + 2\nu_3$	E		7494.8
		F_1		7534.9
		F_2	7514.0	7534.9
		E		7568.1
		A_2		7568.1
		A_1		7568.1
	$3\nu_1$	A_1		8581.1

V	Normal label	Γ	Expt.	Calc.	V	Normal label	Γ	Expt.	Calc.
		A_1		4495.3	$2\nu_1 + \nu_3$		F_2	8604.0	8603.0
	$3\nu_2$	E		4510.9			A_1		8725.5
		A_2		4575.7	$\nu_1 + 2\nu_3$		F_2	8807	8794.1
		A_1		5392.8			E		8838.5
$\nu_1 + 2\nu_4$		E		5394.7			F_2	8900.0	8910.0
		F_2		5501.7	$3\nu_3$		F_1		8944.8
		F_1		5503.6			A_1		8982.1
		F_2		5503.6			F_2	9045.0	9034.5
		F_2		5528.8					
$\nu_3 + 2\nu_4$		F_2		5637.7					
		A_1		5637.7					
		E		5637.7					
		F_1		5637.7					

3 Methane

In this section we apply this algebraic approach to describe the vibrational levels of methane. According to the Hamiltonian (1) the number of parameters is eight, plus the boson numbers N_1 and N_2. The vibron number N_1 can be fixed from the anharmonicity of the $C - H$ bond, while for the bending vibrations we have taken N_2 from the $H - H$ interaction in H_2O given in reference [8]. From these considerations, the number of free parameters is seven, taking into account the constraint (4).

TABLE II. Parameters of the Hamiltonian obtained in the least square fitting (cm^{-1}). The numbers of bosons are taken to be $N_1=43$ and $N_2=28$.

Stretching			Bending					rms
A_1	B_{12}	λ_{12}	A_5	$B_{5,6}$	$B_{5,10}$	$\lambda_{5,6}$	$\lambda_{5,10}$	
-13.2125	-0.6850	0.6328	35.4844	2.6492	-28.0164	9.0501	5.1799	12.16

The Hamiltonian (1) is diagonalized in the normal basis, built by repeated couplings of the form (3). Since by construction this basis is symmetry adapted, the Hamiltonian matrix separates into blocks corresponding to the irreps of T_d. In Table I we present the least square fit for methane up to three quanta. Following Herzberg's notation [6], the four fundamental energies for A_1, F_2 (stretching) and E, F_2 (bending) have been denoted by ν_1, ν_3, ν_2 and ν_4, respectively. The final parameters are given in Table II. The model in its simplest form (without

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including the V^{B-S} interaction or higher order terms) seems to provide a good description of 19 experimental energy levels with an *rms* deviation of 12.16 cm^{-1}.

4 Conclusions

We have presented a new method, which applied to an algebraic model of coupled anharmonic oscillators is able to describe the complete vibrational spectrum of polyatomic molecules. We emphasize that the method systematically incorporates group theoretical techniques which simplify the diagonalization of the Hamiltonian and provide a clear methodological procedure that can be applied to other molecules [10]. Although we have used the model in its simplest form, it can be improved in the following ways: a) Inclusion of the stretching-bending interactions $\hat{V}^{S-B}$, (b) Introduction in the Hamiltonian of higher order terms and (c) Addition of interactions which do not conserve the total number of quanta.

Acknowledgments

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ALGEBRAIC DESCRIPTION OF ATOM-MOLECULE INTERACTIONS

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Abstract

We describe a new method based on algebraic techniques, which leads to a model of atom-diatom collisions.

1   Introduction

One-dimensional atom-molecule collisions have been studied using a combination of differential and algebraic techniques in conjunction with time evolution operator methods for a variety of molecular potentials [1]. For three-dimensional systems, however, one needs to resort to a number of computational integro-differential techniques to describe such interactions [2,3]. In recent papers we have proposed an algebraic framework based on the vibron model [4], that leads to a three-dimensional scheme for such interactions [5], which starts from a $U(4) \times U(4)$ description of three-atomic molecules. We then apply a coherent state method to one of the $U(4)$'s, thus extracting a coordinate dependence for the interaction between one of the atoms and the remaining diatom, while the latter is still described algebraically. The resulting Hamiltonian is formally analogous to the ones used in one dimension [1] and can be solved in principle in the interaction picture [5]. This is a difficult task, however, particularly with respect to assessing the different degrees of approximation involved. For this reason we consider here a one-dimensional version of our model based on a $U(2) \times U(2)$ dynamical algebra, which is simpler to analyze and already incorporates much of the complexity of the full three-dimensional model.

2   One-Dimensional Model

In our one dimensional model, the stretching vibrations of triatomic molecules are described in terms of the dynamical algebra

$$U_1(2) \times U_2(2) \tag{1}$$

by means of the Hamiltonian

$$\hat{H} = E_0(N_1, N_2) + A J_{z_1}^2 + B J_{z_2}^2 + C \hat{J}_{z_1} \hat{J}_{z_2} + D \hat{J}_1 \cdot \hat{J}_2 + \dots, \tag{2}$$

where $\hat{J}_{x_i}$, $\hat{J}_{y_i}$ and $\hat{J}_{z_i}$ are the $SU_i(2)$ generators and $\hat{N}_i$ the (fixed) total boson number associated to $U_i(2)$. The dots at the end of (2) indicate that we may also need other combinations of generators, such as $\hat{J}_{y_1} \cdot \hat{J}_{y_2}$. Such Hamiltonians are well suited to describe stretching vibrations, due to the connection that can be established between the $U(2)$ algebra and the one-dimensional Morse oscillator Schrödinger equation [6]. We now introduce the coherent state basis associated to bond number 2 [7],

$$|[N]r> = \frac{1}{\sqrt{N!(1+r^2)^N}} (s^\dagger + rt^\dagger)^N |0> , \tag{3}$$

where $s^\dagger$, $t^\dagger$ are two scalar boson creation operators through which the $U(2)$ algebras are realized [6]. Computing the expectation value of (2) in the basis (3) and carrying out the coordinate transformation

$$r = \sqrt{\frac{e^{-bx/a_0}}{2 - e^{-bx/a_0}}} , \tag{4}$$

we arrive at a Hamiltonian of the form

$$H = \hat{H}_0 + \hat{V}_1 + \hat{V}_2 + \hat{V}_3 , \tag{5}$$

where

$$\hat{H}_0 = A \hat{J}_{z_1}^2 , \tag{6a}$$

$$\hat{V}_1 = -\hat{\alpha} e^{-bx/2a_0}(2 - e^{-bx/a_0})^{1/2} , \tag{6b}$$

$$\hat{V}_2 = -\beta(2e^{-bx/a_0} - e^{-2bx_0/a_0}) , \tag{6c}$$

$$\hat{V}_3 = \hat{\gamma} e^{-bx/a_0} , \tag{6d}$$

and

$$\hat{\alpha} = -\frac{1}{2}(C + D) N \hat{J}_{z_1} , \tag{7a}$$

$$\beta = -\frac{1}{4} B N (N - 1) , \tag{7b}$$

$$\hat{\gamma} = -\frac{1}{2} D N \hat{J}_{y_1} . \tag{7c}$$

The potentials (6b) and (6c) generalize the typical interactions of exponential form (6d) used in previous works [1]. For collision energies high compared with the vibrational excitations, we may "freeze" the molecular coordinates and substitute $\hat{J}_{z_1}$ and $\hat{J}_{y_1}$ in (7a) and (7c) by their

expectation values in the $|jm>$ basis, leading to a well defined potential for which we evaluate classical trajectories, associated to a classical Lagrangian of the form

$$L = \frac{\mu}{2}\dot{x}^2 + V_1(x) + V_2(x) + V_3(x) \ . \tag{8}$$

Substituting these trajectories $x(t)$ back into (5) then leads to a time-dependent potential of the form

$$\hat{V}(t) = V_1(t)\hat{J}_{z_1} + V_2(t) + V_3(t)\hat{J}_{y_1} + V_4(t)\hat{J}_{x_1} \ , \tag{9}$$

where $V_i(t)$ are obtained from (6), except for $V_4(t)$, which is identically zero.

We now use the interaction scheme, which is appropriate to determine time-dependent solutions for Hamiltonians of the form $\hat{H} = \hat{H}_0 + \hat{V}(t)$, as in (5). The evolution operator in this scheme satisfies the equation

$$i\hbar\frac{\partial\hat{U}(t)}{\partial t} = \hat{V}_{int}\hat{U}(t) \ , \tag{10}$$

where

$$\hat{V}_{int}(t) = e^{i\hbar\hat{H}_0(t-t_1)}\hat{V}(t)e^{-i\hbar\hat{H}_0(t-t_1)} \ . \tag{11}$$

A great simplification arises when $\hat{V}_{int}$ is a linear combination of a closed algebra. For the particular case of $SU(2)$, $U(t_1,t)$ can be expressed in the form

$$\hat{U}(t) = e^{-i/\hbar g_1(t)\hat{J}_x}e^{-i/\hbar g_2(t)\hat{J}_y}e^{-i/\hbar g_3(t)\hat{J}_z}e^{-i/\hbar g_4(t)} \ . \tag{12}$$

If this is the case, substitution of (12) into (10) gives rise to differential equations for $g_i(t)$ in terms of the (known) potentials $V_i(t)$. Once $\hat{U}(t_1,t)$ is known, the scattering matrix is defined in terms of it as

$$\hat{S} = \hat{U}(-\infty,\infty) \ , \tag{13}$$

i.e., the transition probabilities can be obtained through

$$P(|jm> \to |jm'>) = |<jm|\hat{S}|jm'>|^2$$
$$= |\sum_{rm_2} e^{-i\beta_1 r}d^j_{rm'}(-\pi/2)d^j_{rm_2}(-\pi/2)d^j_{m_2m}(\beta_2)|^2 \ , \tag{14}$$

where $\beta_i = g_i(-\infty,\infty)/\hbar$ and the d-functions are the usual Jacobi functions appearing in the definition of Wigner's D-functions [8].

3 Calculations

The main stumbling block for the evaluation of the evolution opperator is the calculation of $\hat{V}_{int}(t)$ through (11). We proceed to discuss briefly some approximations to carry out this task.

a) Sudden Approximation

In the sudden approximation, the interaction time is considered to be very short. A Taylor expansion of (11) along t_1 leads to

$$\hat{V}_{int}(t) = V(t) + \frac{i}{\hbar}[\hat{H}_0, V(t)]V(t - t_1) + \ldots \tag{15}$$

which at zeroth order gives $\hat{V}_{int}(t) = V(t)$. This represents an approximation where all dynamical information of the molecular potential is lost in equation (10). We may then solve for the classical trajectories using (12), in some cases analytically, which generalize results known previously for the exponential interaction (6d) [9]. In this limit we are able to exactly reproduce the analysis of Levine and Wulfman [10,11] and extend them to the more general interactions in (6). We omit these results here for lack of space and refer the reader to reference [9].

b) Averaging Techniques for $\hat{V}_{int}(t)$

Since we are interested in comparing our algebraic methods with quantum mechanical *ab initio* calculations (when these are available), we should improve the evaluation of $\tilde{V}_{int}$ so as to introduce the dynamical effects of the molecular potential. The sudden approximation of the previous subsection fails to account for the fine properties required. Fortunately, a quantum mechanical calculation for the transition probabilities in the scattering of an atom from a one-dimensional Morse oscillator has been presented by Clark and Dickinson [12], so we may gauge our approximations by comparing with their results. Returning to eq. (11), we substitute (6a) and make use of the commutation relations

$$[J_z^2, \ \hat{J}_y] = -\hat{J}_y - 2i\hat{J}_z\hat{J}_x \ , $$
$$[J_z^2, \ \hat{J}_x] = -\hat{J}_x + 2i\hat{J}_z\hat{J}_y \ . \tag{16}$$

After some algebra we find the expression

$$\hat{V}_{int}(t) = \left[\frac{-i}{2\sin(x_0\omega_0 t)} \left(-\cos(2x_0\omega_0 t\hat{J}_z)\hat{J}_y + \hat{J}_y \cos(2x_0\omega_0 t\hat{J}_z) \right) \right.$$
$$\left. + \frac{1}{2\sin(x_0\omega_0 t)} \left(-\cos(2x_0\omega_0 t\hat{J}_z)\hat{J}_y + \hat{J}_y \cos(2x_0\omega_0 t\hat{J}_z) \right) \right] V_3(t)$$
$$+ V_1(t)\hat{J}_{z_1} + V_2(t) \ , \tag{17}$$

where $x_0\omega_0$ is the standard anharmonicity parameter, which can be expressed in terms of the Morse potential parameter through $x_0\omega_0 = \frac{-A}{\hbar}$. The problem with eq. (17) is that it no longer satisfies being linear in the $SU(2)$ generators, so (12) is not valid. To deal with this problem, we proceed as follows. We apply $\hat{V}_{int}(t)$ to a Morse eigenfunction $|jm>$ and insert a complete set of states $\sum_\mu |j\mu><j\mu|$ to the resulting expression. Taking into account the selection rules for $\hat{J}_y$, which imply, $\mu = m \pm 1$, we find a state-dependent potential:

$$\hat{V}_m(t) = \left(\frac{\cos(2x_0\omega_0 tm)}{\cos(x_0\omega_0 t)}V_3(t) + \frac{\cos(2x_0\omega_0 t(m+1))}{\cos(x_0\omega_0 t)}V_3(t)|jm+1><jm+1| \right.$$
$$\left. + \frac{\cos(2x_0\omega_0 t(m-1))}{\cos(x_0\omega_0 t)}V_3(t)|jm-1><jm-1| \right) \hat{J}_y + V_1(t)\hat{J}_z + V_2(t) \ . \tag{18}$$

The m-dependent cosine functions, however, are practically the same for small values of the phonon number $v = j - m$ (large m values), so we can simplify (18) by averaging the excitation to the two possible states $\mu = m \pm 1$, so we arrive at the simple m-dependent potential

$$\hat{V}_m(t) = (\cos(2x_0\omega_0 tm)\cos(x_0\omega_0 t)V_3(t)\hat{J}_y$$
$$+ V_1(t)\hat{J}_z + V_2(t) \ , \tag{19}$$

which is linear in the $SU(2)$ generators, so (12) is valid. Since we are interested in comparing our approach with the calculations of ref. [12] where only $V_3(t) \neq 0$, the potential (19) simplifies further and only $\hat{J}_y$ remains. The evolution operator is then given by

$$\hat{U}_m(t) = e^{-ig_2(m,t)\hat{J}_y/\hbar} \ , \tag{20}$$

where

$$\dot{g}_2(m,t) = V_3\cos(x_0\omega_0 t)\cos(2x_0\omega_0 mt) \ . \tag{21}$$

The differential equation for the evolution operator then lead to exactly solvable forms for the classical trajectories and to the asymptotic value of $g_2(m,t)$ (see below (14))

$$\beta_2(m) = \frac{E}{\hbar}\int_{-\infty}^{\infty}\cos(x_0\omega_0 t)\cos(2mx_0\omega_0)\,\mathrm{sech}^2\left(\sqrt{\frac{E}{2\mu}}\frac{t}{a_0}\right)dt \tag{22}$$

where E is the collision energy. From (14) this leads to the simple expression for the transition probabilities

$$P(|jm> \rightarrow |jm'>) = d^j_{m,m'}(\beta_2(m')) \ , \tag{23}$$

where

$$\beta_2(m') = \frac{\mu\omega_0\pi a_0^2}{b^2\hbar}\left[\frac{(2m'-1)x_0}{\sinh((2m'-1)x_0 k_0)} + \frac{(2m'+1)x_0}{\sinh((2m'+1)x_0 k_0)}\right] \ , \tag{24}$$

with $k_0 = \frac{\omega_0 a_0 \pi}{b}\sqrt{\frac{\mu}{2E}}$. In Table I we compare the results of our calculation, using (23), (24), with those of Clark ahd

TABLE I. Comparison between the algebraic model and the Clark-Dickinson Model[12]

Energy ($\hbar\omega_0$ /2 units): 16

Final state	Initial State = 0		Initial State = 1	
	Clark-Dickinson Probability	Model Probability	Clark-Dickinson Probability	Model Probability
1	0.245000	0.157837		
2	3.38000E(-02)	1.45652E(-02)	0.318000	0.253196
3	2.72000E(-03)	8.65153E(-04)	5.72000E(-02)	3.62444E(-02)
4	1.61000E(-04)	3.71652E(-05)	5.16000E(-03)	2.86219E(-03)

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| | 5 | 7.44000E(-06) | 1.22993E(-06) | 3.24000E(-04) | 1.50963E(-04) |

Energy ($\hbar\omega_0/2$ units): 12

	Initial State = 0		Initial State = 1	
Final state	Clark-Dickinson Probability	Model Probability	Clark-Dickinson Probability	Model Probability
1	0.129000	0.124019		
2	6.65000E(-03)	8.57432E(-03)	0.167000	0.208828
3	1.49000E(-04)	3.81572E(-04)	8.41000E(-03)	2.19917E(-02)
4	1.48000E(-06)	1.22807E(-05)	1.38000E(-04)	1.28983E(-03)
5	4.95000E(-09)	3.04486E(-07)	7.01000E(-07)	5.07090E(-05)

Energy ($\hbar\omega_0/2$ units): 10

	Initial State = 0		Initial State = 1	
1	7.39000E(-02)	0.105782		
2	1.66000E(-03)	6.09133E(-03)	8.15000E(-02)	0.182403
3	1.17000E(-05)	2.25776E(-04)	1.22000E(-03)	1.58582E(-02)
4	1.95000E(-08)	6.05219E(-06)	5.12000E(-06)	7.71373E(-04)
5	0.	1.24982E(-07)	2.95000E(-10)	2.51949E(-05)

Energy ($\hbar\omega_0/2$ units): 8

	Initial State = 0		Initial State = 1	
1	3.15000E(-02)	8.66178E(-02)		
2	1.85000E(-04)	3.98810E(-03)	2.28000E(-02)	0.152903
3	1.18000E(-07)	1.18193E(-04)	3.07000E(-05)	1.05375E(-02)
4	0.	2.53330E(-06)	1.37000E(-11)	4.08112E(-04)
5	0.	4.18294E(-08)	0.	1.06318E(-05)

Energy ($\hbar\omega_0/2$ units): 6

	Initial State = 0		Initial State = 1	
1	7.31000E(-03)	6.64920E(-02)		
2	2.30000E(-06)	2.29488E(-03)	1.25000E(-03)	0.120126
3	0.	5.09821E(-05)	0.	6.15327E(-03)
4	0.	8.19113E(-07)	0.	1.77900E(-04)

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| 5 | 0. | 1.01384E(-08) | 0. | 3.46550E(-06) |

Dickinson [12] for different collision energies and for two different initial states. Although our results differ from the exact ones, particularly for higher final states where the probabilities are very small, the general trend is reproduced remarkably well, taking into account our semiclassical method.

4 Conclusions

The algebraic model seems to provide an attractive alternative to integro-differential techniques for the description of atom-molecule collisions. The approximation methods developed for the one-dimensional test model can be readily extended to the three dimensional case and applied to real systems [2,3]. We are currently exploring the generalization of these techniques to include reaction channels, which would represent an important development because of the relevance of these processed in atmospheric interactions [13].

Acknowledgments

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FIBONACCI CHAIN POLYNOMIALS: IDENTITIES FROM SELF-SIMILARITY

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Abstract

Fibonacci chains are special diatomic, harmonic chains with uniform nearest neighbour interaction and two kinds of atoms (mass-ratio r) arranged according to the self-similar binary Fibonacci sequence $ABAABABA...$, which is obtained by repeated substitution of $A \to AB$ and $B \to A$.

The implications of the self-similarity of this sequence for the associated orthogonal polynomial systems which govern these Fibonacci chains with fixed mass-ratio r are studied.

1 Introduction

Fibonacci chains are linear diatomic chains with nearest neighbour harmonic interaction of uniform strength κ and the two masses (ratio $r = m_1/m_0$) follow the pattern of the binary sequence $\{h(n)\}_1^\infty$ obtained by repeated substitutions σ in the following way.

$$\sigma(1) = 10 \quad , \quad \sigma(0) = 1 \quad , \tag{1}$$

starting with 0. By definition $\sigma(uv) = \sigma(u)\sigma(v)$ for any two strings u and v. $\sigma^n(0) \equiv H_n$ is a string of length $|H_n| = F_{n+1}$, where $F_n = F_{n-1} + F_{n-2}$, $n = 2, 3, ...$, $F_0 = 0$, $F_1 = 1$ are the Fibonacci numbers. $h(n)$ is defined to be the n'th entry of the half-infinite string $H_\infty := lim_{n \to \infty} H_n$. E.g. $H_5 = \sigma^5(0) = 10110101$, $h(1) = 1$, $h(2) = 0$, etc. (1) is called the Fibonacci substitution rule, and the masses of the half-infinite chain are taken to be

$$m_n = m_{h(n)} \quad , \quad n = 1, 2, ... \tag{2}$$

This sequence $\{h(n)\}_1^\infty$ is self-similar because the string H_∞ satisfies $\sigma(H_\infty) = H_\infty$. Aperiodicity follows from this invariance, or fixed point, property. (This sequence is in fact also quasiperiodic, but this does not concern us here.)

Chains of this type have been considered as models of binary alloys [1]. For instance, one may consider chains with an elementary unit determined by the first N members of the $\{h(n)\}$ sequence and repeat it periodically, using certain boundary conditions. This then corresponds to $(AB)^\infty$ chains for $N = 2$, $(ABA)^\infty$ chains for $N = 3$, etc.

The dual of such chains (with equal masses but two spring constants κ_0 and κ_1 following the pattern of the Fibonacci substitution sequence) are related to one-dimensional quasicrystals [2]. One can also make contact to artificially manufactured superlattices [3].

Originally such Fibonacci chains were considered as models for the study of the regime in between periodic and random structures.[4, 5].

The purpose of this work is to write down the identities which are satisfied by the characteristic polynomials of these Fibonacci chains due to the self-similarity of the substituion sequence $\{h(n)\}$ which determines the pattern of the masses of the oscillators. These identities will be expressed in terms of the 2×2 transfer matrices M_n which are unimodular and real. The matrix elements are given by the characteristic polynomials $\{S_n^{(r)}(x)\}$, where r is the mass-ratio of the two types of atoms and x is a normalized frequency squared ($x \equiv \omega^2/2\omega_0^2$, $\omega_0^2 = \kappa/m_0$). The zeros of $S_N^{(r)}(x)$ determine the eigenfrequencies of finite Fibonacci chains with N atoms and both ends fixed. One also encounters so-called first associated polynomials $\{\hat{S}_n^{(r)}(x)\}$. They correspond to a right shift by one unit in the substitution sequence. Hence, the zeros of $\hat{S}_N^{(r)}(x)$ produce the eigenfrequencies of chains with masses $m_{h(2)} = m_0, ..., m_{h(N+1)}$. Both r−families of polynomials generalize Chebyshev's $\{S_n(y)\}$ polynomials ($S_{-1} = 0$, $S_0 = 1$, $S_n = yS_{n-1} - S_{n-2}$) to two variables with the identification

$$S_n^{(1)}(x) = \hat{S}_n^{(1)}(x) = S_n(2(1-x)) . \tag{3}$$

They constitute, for fixed mass-ratio r, systems of orthogonal polynomials and have been studied in some detail in refs.[6, 7, 8, 9].

2 Fibonacci Chain Polynomials

For the Fibonacci chains $(\kappa, m_{h(n)})$ defined in *section 1* the equation of motion for longitudinal, time-stationary vibrations $q_n(t) = q_n\, exp\,(i\omega t)$ are

$$q_{n+1} + q_{n-1} - Y(n)q_n = 0 , \quad n = 1, 2, ... \tag{4}$$

with

$$Y(n) \equiv 2(1 - \omega^2/(2\omega_n^2)) , \quad \omega_n^2 \equiv \kappa/m_{h(n)} . \tag{5}$$

We use the two variables $r \equiv m_1/m_0$ and $x \equiv \omega^2/(2\omega_0^2)$. We put $Y(n) = Y$ if $h(n) = 1$ and $Y(n) = y$ if $h(n) = 0$. Hence

$$Y = 2(1 - rx) , \quad y = 2(1 - x) . \tag{6}$$

The equations of motion are rewritten with the help of the $SL(2, \mathbf{R})$ transfer matrix R_n:

$$\begin{pmatrix} q_{n+1} \\ q_n \end{pmatrix} = R_n \begin{pmatrix} q_n \\ q_{n-1} \end{pmatrix} := \begin{pmatrix} Y(n) & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} q_n \\ q_{n-1} \end{pmatrix} . \tag{7}$$

R_n is either R_1 or R_0 depending on the $Y(n)$ value, *i.e* $R_n = R_{h(n)}$. For the half-sided infinite chains considered here iteration leads to

$$\begin{pmatrix} q_{n+1} \\ q_n \end{pmatrix} = R_n R_{n-1} \cdots R_1 \begin{pmatrix} q_1 \\ q_0 \end{pmatrix} =: M_n \begin{pmatrix} q_1 \\ q_0 \end{pmatrix} , \tag{8}$$

with the inputs q_1 and q_0 (the mass at site number 0 is irrelevant). M_n is real and unimodular. The recursion $M_n = R_n M_{n-1}$ with input $M_1 = R_1$ leads to

$$M_n = \begin{pmatrix} S_n & -\hat{S}_{n-1} \\ S_{n-1} & -\hat{S}_{n-2} \end{pmatrix} , \tag{9}$$

where the recursion formulae for the generalized two-variable Chebyshev polynomials are

$$S_n = Y(n)S_{n-1} - S_{n-2} \quad , \quad S_{-1} = 0, \quad S_0 = 1 \quad , \tag{10}$$

$$\hat{S}_n = Y(n+1)\hat{S}_{n-1} - \hat{S}_{n-2} \quad , \quad \hat{S}_{-1} = 0, \quad \hat{S}_0 = 1 \quad . \tag{11}$$

These polynomials generate certain combinatorial numbers [10]. The meaning of these numbers can be understood if one uses the intimate connection of the Fibonacci substitution sequence with Wythoff's A and B sequences

$$A(n) = n + \sum_{k=1}^{n-1} h(k) \quad , \quad B(n) = n + A(n) . \tag{12}$$

These sequences $\{A(n)\}_1^\infty$ and $\{B(n)\}_1^\infty$ cover the positive integers in a complementary way: every number $N > 0$ is either an $A-$ or a $B-$number. For an $A-$number n $(i.e.\ n = A(m)$ for some $m)$ $h(n) = 1$, and for a $B-$number n $(i.e\ n = B(m)$ for some $m)$ $h(n) = 0$. Wythoff's sequences are a special case of Beatty sequences: $A(n) = \lfloor n\varphi \rfloor$, $B(n) = \lfloor n\varphi^2 \rfloor$, with $\varphi^2 = \varphi + 1$, $\varphi > 0$, the golden mean.

The characteristic polynomials $\{S_n^{(r)}(x)\}$, obtained from $\{S_n(Y,y)\}$ by replacement of Y and y according to eq.(6), constitute, for fixed mass-ratio r, a system of orthogonal polynomials. $\{\hat{S}_n^{(r)}(x)\}$ are the first-associated orthogonal polynomials.

3 Self-Similarity Identities

The string, or 'word', H_∞ defined in *section 1* is invariant under the inverse substitution σ^{-1}, with $\sigma^{-1}(1) = 0$, $\sigma^{-1}(10) = 1$. This is equivalent to the self-similarity of the sequence $\{h(n)\}_1^\infty$ which is shown in the FIG.
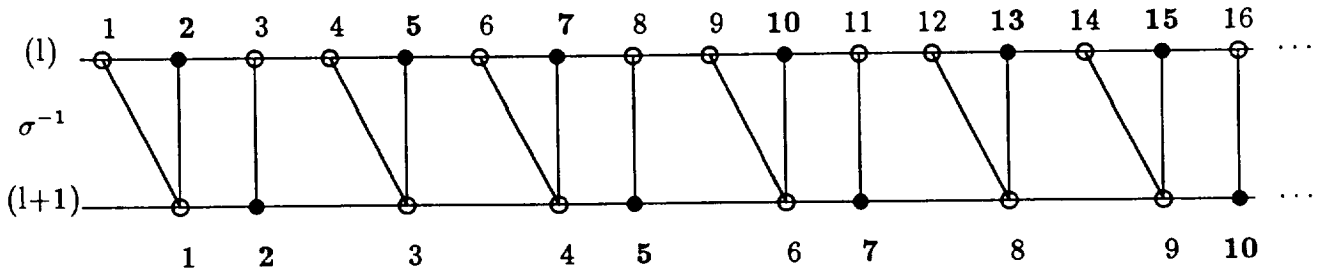

FIG. Self-similarity of the sequence $\{h(n)\}_1^\infty$. Circles stand for the value 1 (A-numbers n), and disks stand for the value 0 (B-numbers n). $\sigma^{-1}(10) = 1$, $\sigma^{-1}(1) = 0$. Level (l) is mapped to level $(l+1)$ by σ^{-1}.

The upper level, called (l) in the FIG., shows the numbers marked as $A-$ and $B-$numbers. The $h(n)$ value is 1 or 0, denoted by a circle or disk, respectively. When the substitution σ^{-1} is applied one reaches the next higher level, called ($l+1$) in the FIG., on which the same sequence is reproduced. Let the position of the $n's$ number at level (l) be $x_n^{(l)}$ for $l = 0, 1, ...$. Level $l = 0$ is assumed to correspond to the original sequence. Then one finds for $p \in \mathbb{N_0} \equiv \mathbb{N} \cup \{0\}$

$$x_{A(p)}^{(l+1)} = x_{B(p)}^{(l)} \ , \tag{13}$$

$$x_{B(p)}^{(l+1)} = x_{AB(p)}^{(l)} \ , \tag{14}$$

where $AB(p)$ stands for the composition $A(B(p))$ of Wythoff's sequences. $E.g.$ The number $A(4) = 6$ at level ($l+1$) occurs in the FIG. at the same position as $B(4) = 10$ at level (l), or $B(2) = 5$ at level ($l+1$) corresponds to $AB(2) = A(5) = 8$ at level (l).
Iteration, depending on the parity of the level number, leads to

$$x_{A(p)}^{(2k+1)} = x_{B^{k+1}(p)}^{(0)} \quad , \quad x_{A(p)}^{(2k)} = x_{AB^k(p)}^{(0)} \ , \tag{15}$$

$$x_{B(p)}^{(2k+1)} = x_{AB^{k+1}(p)}^{(0)} \quad , \quad x_{B(p)}^{(2k)} = x_{B^{k+1}(p)}^{(0)} \ . \tag{16}$$

Consider the level ($l+1$) transfer matrix

$$M_n^{(l+1)} = R_{h(n)}^{(l+1)} \cdots R_{h(1)}^{(l+1)} \ , \tag{17}$$

satisfying the recursion relation

$$R_1^{(l+1)} = R_0^{(l)} R_1^{(l)} \quad , \quad R_0^{(0)} \equiv R_0 = \begin{pmatrix} y & -1 \\ 1 & 0 \end{pmatrix} \ , \tag{18}$$

$$R_0^{(l+1)} = R_1^{(l)} \quad , \quad R_1^{(0)} \equiv R_1 = \begin{pmatrix} Y & -1 \\ 1 & 0 \end{pmatrix} \ . \tag{19}$$

Iteration leads , with $M_n \equiv M_n^{(0)}$, to

$$R_1^{(l+1)} = M_{F_{(l+3)}} \quad , \quad R_0^{(l+1)} = M_{F_{(l+2)}} \ , \tag{20}$$

with the Fibonacci numbers F_n.
Due to (15) and (16) one has

$$M_{A(p)}^{(2k+1)} = M_{B^{k+1}(p)} \quad , \quad M_{A(p)}^{(2k)} = M_{AB^k(p)} \ , \tag{21}$$

$$M_{B(p)}^{(2k+1)} = M_{AB^{k+1}(p)} \quad , \quad M_{B(p)}^{(2k)} = M_{B^{k+1}(p)} \ . \tag{22}$$

The recursion at each level is

$$M_n^{(l+1)} = R_{h(n)}^{(l+1)} M_{n-1}^{(l+1)} \quad , \quad M_1^{(l+1)} = R_1^{(l+1)} \ . \tag{23}$$

Combining iteration and recursion, in a systematic way, leads to transfer matrix identities for level (0), $i.e.$ for the original matrices M_n of eq. (8). One finds alltogether six families of such

identities, depending on the parity of the level one starts with and the specification of the index. These identities are, for $m \in \mathbf{N}$ and $k \in \mathbf{N}$,

$$
\begin{array}{rll}
(I) & M_{B^{k+1}(m)} & = & M_{F_{2k+1}} \, M_{AB^k A(m)} \ , \\
(IIa) & M_{B^k A(A(m)+1)} & = & M_{F_{2k+1}} \, M_{B^{k+1}(m)} \ , \\
(IIb) & M_{B^k A(B(m)+1)} & = & M_{F_{2k+1}} \, M_{AB^{k+1}(m)} \ , \\
(III) & M_{AB^k(m)} & = & M_{F_{2k}} \, M_{B^k A(m)} \ , \\
(IVa) & M_{AB^k A(A(m)+1)} & = & M_{F_{2(k+1)}} \, M_{AB^{k+1}(m)} \ , \\
(IVb) & M_{AB^k A(B(m)+1)} & = & M_{F_{2(k+1)}} \, M_{B^{k+2}(m)} \ .
\end{array} \tag{24}
$$

(I), (IIa), (IIb) and (III) result from odd levels $l = 2k + 1$, with n put $AB(m)$, $AA(A(m) + 1)$, $AA(B(m) + 1)$ and $B(m)$, respectively. (III), (IVa) and (IVb) result from even levels $l = 2k$, with n put $B(m)$, $A(A(m) + 1)$ and $A(B(m) + 1)$, respectively.

E.g. (I) and (III) produce for $m = 1$, due to $A(1) = 1$, $B^{k+1}(1) = F_{2k+3}$ and $AB^k(1) = F_{2(k+1)}$, identities which are the well-known recursion formula for transfer matrices with neighbouring Fibonacci number indices

$$
M_{F_{n+1}} = M_{F_{n-1}} \, M_{F_n} \ . \tag{25}
$$

Not all eqs.(24) are independent. *E.g.* if one puts $m = B(p) + 1$ in (I), replaces k by $k + 1$ and combines it with eqs. (IVb), with $k \to k - 1$ and $m \to p$, one finds eqs. (IIa), due to the identiy $B(p) + 1 = A(A(p) + 1)$ and eq.(25) for even n. However, eqs.(IIa) provide identities for $M_{B^k A(p)}$ which complement those obtained from eqs. (IIb).

It is possible to combine (I) of eq.(24) with (III) specialized to $m \to A(m)$ and use (I) again with $k \to k - 1$ and $m \to A^2(m)$. Continuing this process one finds for $k \in \mathbf{N}$ and $m \in \mathbf{N}$

$$
\begin{array}{rll}
(I') & M_{B^{k+1}(m)} & = & M_{F_{2k+1}} \, M_{F_{2k}} \cdots M_{F_2} \, M_{BA^{2k}(m)} \\
(III') & M_{AB^k(m)} & = & M_{F_{2k}} \, M_{F_{2k-1}} \cdots M_{F_2} \, M_{BA^{2k-1}(m)}
\end{array} \tag{26}
$$

(I) and (III) in (24) can be replaced by both eqs. (26), and the other eqs. of (24) can be rewritten using (26).

The sum of the indices of the transfer matrices on the *r.h.s.* of eqs.(24) and (26) have to match the index of the *l.h.s.* This fact produces families of identities among iterated Wythoff A and B sequences. A detailed investigation of these Wythoff composites identities will be given elsewhere. All of these identities can be rederived as corollaries of a new theorem relating two seemingly different unique number systems: the Wythoff- and the Zeckendorf- (or Fibonacci-) representations.

The transfer matrix identities (24) are equivalent to those for their matrix elements, *i.e.* the characteristic polynomials $\{S_n(Y, y)\}$ and $\{\hat{S}_n(Y, y)\}$. In order to derive them one rewrites the indices of all matrix elements as Wythoff composites. Consider, for example, (I). For the elements of $M_{B^{k+1}(m)}$ one employs the simple identities $B^{k+1}(m) - 1 = B(B^k(m)) - 1 = A^2 B^k(m)$ and $B^{k+1}(m) - 2 = ABAB^{k-1}(m)$. The last identity can be proved for $m = A(p)$ and $m = B(p)$ separately. On the *r.h.s.* of (I) one rewrites the indices of the matrix elements with the help of the identities $F_{2k+1} = B^k(1)$, $F_{2k+1} - 1 = A^2 B^{k-1}(1)$, $F_{2k+1} - 2 = ABAB^{k-2}(1)$ for $k = 2, 3, \ldots$, and $F_3 - 2 = 0$. Moreover, $AB^k A(m) - 1 = BAB^{k-1} A(m)$, $AB^k A(m) - 2 = A^3 B^{k-1} A(m)$.

Finally, (I) decomposes into the following four sets of eqs.

$$(I,(1,1)) \qquad S_{B^{k+1}(m)} = S_{B^k(1)} S_{AB^kA(m)} - \hat{S}_{A^2B^{k-1}(1)} S_{BAB^{k-1}A(m)} \ ,$$

$$(I,(1,2)) \qquad \hat{S}_{A^2B^k(m)} = S_{B^k(1)} \hat{S}_{BAB^{k-1}A(m)} - \hat{S}_{A^2B^{k-1}(1)} \hat{S}_{A^3B^{k-1}A(m)} \ ,$$

$$(I,(2,1)) \qquad S_{A^2B^k(m)} = S_{A^2B^{k-1}(1)} S_{AB^kA(m)} - \hat{S}_{ABAB^{k-2}(1)} S_{BAB^{k-1}A(m)} \ , \qquad (27)$$

$$(I,(2,2)) \qquad \hat{S}_{ABAB^{k-1}(m)} = S_{A^2B^{k-1}(1)} \hat{S}_{BAB^{k-1}A(m)} - \hat{S}_{ABAB^{k-2}(1)} \hat{S}_{A^3B^{k-1}A(m)} \ .$$

The last two sets of eqs. hold only for $k = 2, 3, \dots$. For $k = 1$ one has

$$S_{A^2B(m)} = Y \, S_{ABA(m)} - S_{BAA(m)} \ ,$$
$$\hat{S}_{ABA(m)} = Y \, \hat{S}_{BAA(m)} - \hat{S}_{A^4(m)} \ . \qquad (28)$$

The other eqs. in (24) decompose in a similar way. The arguments of the polynomials is always (Y, y), which can be replaced using eq.(6).
This concludes the derivation of the self-similarity eqs. for the Fibonacci chain polynomials. It is clear that further work is needed in order to extract from this gamut of eqs. information pertaining to chain properties, like structure of spectra and displacements.

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A SUPERSYMMETRIC FAMILY OF HARMONIC OSCILLATORS
SIMULATING H-BONDS IN DNA

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Abstract

We test an isospectral potential from harmonic oscillator simulating H-bond interation in DNA macromolecules.

1 Introduction

In the context of Supersymmetric Quantum Mechanics (SQM), several new potentials have been generated from shape invariant potentials[1] . In particular, with reference to the harmonic oscillator[2-4]. However, to date, none of these new potentials have been applied to real physical systems.

Peyrard and Bishop[5] have introduced a theoretical treatment of DNA. In this model, starting from the classical Hamiltonian and using the transfer integral operator, the partition functions follow from the eigenvalues of a Schrödinger-type equation.

We intend, in this communication, to demonstrate the feasability of using a new potential generated from the harmonic oscillator in the Schrödinger-type equation to describe H-bonds in DNA.

2 SQM

In SQM the nilpotent operators Q and Q^+ satisfy the algebra[6]

$$\{Q,Q^+\} = H_{SS};Q^2 = Q^{+2} = 0 \tag{1}$$

which can be realized in a usual matrix form. In this case, the supersymmetric Halmitonian H_{SS} consists of two partners H_+ and H_- which can be factorized in $H_+ = a^+a^-$ and $H_- = a^- a^+$ (where a^+ and a^- are bosonic operators), and they have the same spectra except for the ground state, where only H_+ has an eigenvalue equal to zero $E_+ = 0$. The eigenfunctions of H_+ and H_- are related to one another by: $\Psi_+ = a^+ \Psi_-$ and $\Psi_- = a^- \Psi_+$, where the bosonic operators are defined by:

$$a^\pm = \{\mp \frac{d}{dx} + W(x)\}. \tag{2}$$

Redefining the operators $a^\pm$, it is possible to obtain a family of Hamiltonians as shown by Sukumar[7] , or the isoespectral potentials[2-4] . In this second case defining new operators:

$$A^\pm = \mp \frac{d}{dx} + F(x) \tag{3}$$

and imposing $H_- = A^- A^+$ yields a general form to get $F(x)$. The new Hamiltonian is written as

$$\tilde{H}_+ = A^- A^+ - 2 \frac{d}{dx} F(x) \tag{4}$$

and the eigenfunctions of the new Hamiltonian are related to the original Hamiltonian ones . The missing ground state is obtained from $A^- \Psi_{+0} = 0$.

As an example, consider the original potential to be the harmonic oscillador, $V(x)=x^2$. It then follows[1-4] :

$$\tilde{H}_+ = -\frac{d^2}{dx^2} + x^2 - 1 - 2 \frac{d}{dx} \frac{\exp(-x^2)}{\Gamma + \int_0^x \exp(-z^2)dz} \tag{5}$$

$$\Psi_{+,0} = \exp\{-x^2 + \int_0^x \frac{\exp(-z^2)dz}{\Gamma + \int_0^z \exp(-y^2)dy}\}. \tag{6}$$

3 DNA Model

Bishop & Peyrard's DNA model includes two degrees of freedom (u_n, v_n) corresponding to displacements of the bases from their equilibrium positions along the direction of the H-bonds connecting them. A harmonic coupling due to the stacking interactions between neighboring bases is also assumed with the same coupling constant (k) for the two strands. Each base has the mass m.

The Hamiltonian for this model is

$$H = \sum_n \{\frac{p_n^2}{2m} + \frac{k}{2}(x_n - x_{n-1})^2 + \frac{q_n^2}{2m} + \frac{k}{2}(y_n - y_{n-1})^2 + V(y_n)\}, \tag{7}$$

where $x_n = (u_n + v_n)/\sqrt{2}$, $y_n = (u_n - v_n)/\sqrt{2}$, $p_n = m\dot{x}_n$, $q_n = m\dot{y}_n$ and $V(y_n)$ is the potential for the hydrogen bonds. Using the transfer integral operators to solve configuration integral energy the classical partition function can be obtained.

The temperature of denaturation of DNA can be monitored through the mean stretching $<y_n>$ of the H-bond. Considering the limit of large N, only the ground state will be important, and

$$< y >=< \Phi_0(y)|y|\Phi_0(y) >= \int \Phi_0^2(y)y\,dy, \tag{8}$$

where $\Phi_0(y)$ is the ground state eigenfunction of a Schrödinger-type equation:

$$\{-\frac{1}{2\beta^2 k}\frac{d^2}{dy^2} + V(y)\}\Phi_i(y) = \{\varepsilon_i + \frac{1}{2\beta}\ln\frac{2\pi}{\beta k}\}\Phi_i(y). \tag{9}$$

It is important to note the mean value $< y >$ depends on the form of the eigenfunction $\Phi_0(y)$.

4 H-bond Potential

The Morse potential is usually used to simulate the H-bonds in DNA. However, we suggest here that the potential generated from the harmonic oscillator using the superalgebra can also be used. This potential has the form:

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which can be realized in a usual matrix form. In this case, the supersymmetric Halmitonian H_{SS} consists of two partners H_+ and H_- which can be factorized in $H_+ = a^+ a^-$ and $H_- = a^- a^+$ (where a^+ and a^- are bosonic operators), and they have the same spectra except for the ground state, where only H_+ has an eigenvalue equal to zero $E_+ = 0$. The eigenfunctions of H_+ and H_- are related to one another by: $\Psi_+ = a^+ \Psi_-$ and $\Psi_- = a^- \Psi_+$, where the bosonic operators are defined by:

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and imposing $H_- = A^- A^+$ yields a general form to get $F(x)$. The new Hamiltonian is written as

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$$\Psi_{+,0} = \exp\{-x^2 + \int_0^x \frac{\exp(-z^2) dz}{\Gamma + \int_0^z \exp(-y^2) dy}\} . \tag{6}$$

3 DNA Model

Acknowledgements

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MOLECULAR VIBRATIONAL STATES DURING A COLLISION

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Abstract

Alternative algebraic techniques to approximate a given Hamiltonian by a harmonic oscillator are described both for time-independent and time-dependent systems. We apply them to the description of a one dimensional atom-diatom collision. From the resulting evolution operator, we evaluate vibrational transition probabilities as well as other time-dependent properties. As expected, the ground vibrational state becomes a squeezed state during the collision.

1 INTRODUCTION

Let us consider the problem of translation-vibration energy transfer in a colinear collision between an atom A and a diatomic molecule BC. The system is described by a Hamiltonian H

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{V}_S(x, t),$$

with the molecule modeled by a Morse Hamiltonian

$$\mathcal{H}_0 = \frac{p^2}{2m} + D(e^{-Ax} - 1)^2$$

and we use a semiclassical approach [1] to construct an effective time-dependent interaction $\mathcal{V}_S$ between the particle and the molecule.

A harmonic Hamiltonian is usually related to $\mathcal{H}_0$ just by making a Taylor series expansion of the potential around $x = 0$ and keeping up to second order terms. However, as we shall show here, this is not necessarily the best harmonic approximation to the Morse Hamiltonian.

In this work, we analyze the time evolution of several physical observables during the collision. To that end, we obtain an approximate time evolution operator by algebraic means. The resulting vibrational transition probabilities are compared with results obtained by other authors [2]. We also evaluate the occupancy of the ground state and the dispersion of the relative position and momentum of the atoms in the diatomic molecule during the collision.

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2 ALGEBRAIC TECHNIQUES

As usual in this type of problem, we shall work in the interaction picture where the behavior of the free molecule is separated from that of the total system. The observables $\mathcal{O}$ evolve in time according to

$$\mathcal{O}_I(t) = \mathcal{U}_0^\dagger \mathcal{O} \mathcal{U}_0, \tag{1}$$

where $\mathcal{U}_0$ is the time evolution operator corresponding to the Hamiltonian $\mathcal{H}_0$, while the time evolution of states is determined by the operator $\mathcal{U}_I$ associated with the interaction picture Hamiltonian

$$\mathcal{H}_I(t) = e^{i\mathcal{H}_0(t-t_0)/\hbar} \mathcal{V}_S(x,t) e^{-i\mathcal{H}_0(t-t_0)/\hbar}. \tag{2}$$

For both time evolution operators we shall make a harmonic approximation described in the following paragraphs.

a) On the harmonic approximation to the Morse Hamiltonian.

The harmonic approximation to the Morse Hamiltonian is usually carried out by just considering the second order Taylor series expansion to the Morse potential

$$D(e^{-Ax} - 1)^2 \approx DA^2 x^2. \tag{3}$$

Let us consider the introduction of creation and annihilation operators with arbitrary scale parameter α and a translation parameter d:

$$a = \frac{1}{\sqrt{2}}\left(\alpha x + \frac{i}{\alpha}p\right) - d \tag{4}$$

and

$$a^\dagger = \frac{1}{\sqrt{2}}\left(\alpha x - \frac{i}{\alpha}p\right) - d. \tag{5}$$

The usual commutation relation still holds and the position and momentum operators are given by

$$\dot{x} = \frac{1}{\sqrt{2}\alpha}(a + a^\dagger + 2d) \qquad p = \frac{\alpha}{\sqrt{2}i}(a - a^\dagger). \tag{6}$$

In terms of a and $a^\dagger$ the Morse Hamiltonian can be written as

$$\mathcal{H}_0 = \sum_{i,j=0}^{\infty} G_{ij} a^{\dagger i} a^j \tag{7}$$

as can be easily shown using the fact

$$e^{\alpha(a+a^\dagger)} = e^{\alpha a^\dagger} e^{\alpha a} e^{-\frac{1}{2}\alpha^2}. \tag{8}$$

The coefficient G_{00} can be interpreted as an estimate of the ground state energy on the harmonic basis determined by the scale parameter α and the traslation parameter d. Invoking the variational principle we choose them such that

$$\frac{\partial G_{00}}{\partial d}\Big|_{d=d_0} = 0 \tag{9}$$

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and

$$\frac{\partial G_{00}}{\partial \alpha}\Big|_{\alpha=\alpha_0} = 0. \tag{10}$$

By direct evaluation of these derivatives it can be shown that the variational conditions are equivalent to the diagonalization of the approximate Hamiltonian

$$H_0 = \sum_{0 \leq i+j \leq 2} G_{ij} a^{\dagger^i} a^j \tag{11}$$

taking it to a form similar to the one of a harmonic oscillator

$$H_0 = G_{11} a^\dagger a + G_{00}, \tag{12}$$

but with a variationally optimized G_{00}.

b) Nonperturbative approximate solution for the time-dependent interaction Hamiltonian.
In many scattering problems, a perturbative technique is applied to obtain the major effects of the collision on the state of the system. In the case of a collision between an atom and a diatom, even-though transition probabilities may be small, perturbative results differ significantly from exact numerical results. Besides, as is well known, there are several successful nonperturbative methods to deal with the parametric harmonic oscillator model. Taking this into account, harmonic approximations to the time-dependent interaction between an atom and a diatom have been studied [3] [4]. In this section, we describe an iterative procedure which has proven to take advantage of this fact in an optimized way [6]. This method has been applied to the calculation of vibrational transition probabilities when the molecule is described by the usual harmonic oscillator derived from a Morse potential.

Once the time-independent Hamiltonian $\mathcal{H}_0$ has been approximated by the harmonic Hamiltonian H_0 the evolution operator is simply

$$\mathcal{U}_0 = e^{-i/\hbar G_{00} t} e^{-i/\hbar G_{11} t a^\dagger a} \tag{13}$$

thus, the interaction Hamiltonian $\mathcal{H}_I(t)$, can be easily written in terms of the creation and anihilation operators a and $a^\dagger$

$$\mathcal{H}_I(t) = \sum_{i,j} \Phi_{ij}^{(0)}(t) a^{\dagger^i} a^j \tag{14}$$

with the coefficients $\Phi_{ij}^{(0)}$ simple functions of time. Solving this problem corresponds to find an evolution operator $\mathcal{U}_I(t)$ solution of the equation

$$i\hbar \partial_t \mathcal{U}_I = \mathcal{H}_I \mathcal{U}_I, \tag{15}$$

with the initial condition $\mathcal{U}_I(t_0, t_0) = \mathcal{I}$.

In analogy with the time-independent problem we split $\mathcal{H}_I$ as a sum of two terms [6]

$$\mathcal{H}_I = \mathcal{H}_{I_0}^{(I)} + \mathcal{H}_{I_0}^{(II)} \tag{16}$$

with

$$\mathcal{H}_{I_0}^{(I)} = \sum_{0 \leq i+j \leq 2} \Phi_{ij}^{(0)}(t) a^{\dagger^i} a^j \tag{17}$$

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and

$$\mathcal{H}_{I_0}^{(II)} = \sum_{3 \leq i+j} \Phi_{ij}^{(0)}(t) a^{\dagger i} a^j. \tag{18}$$

Accordingly, the time evolution operator will be a product,

$$\mathcal{U}_I = \mathcal{U}_{I_0}^{(I)} \mathcal{U}_{I_0}^{(II)} \tag{19}$$

with $\mathcal{U}_{I_0}^{(I)}$ such that

$$i\hbar \partial_t \mathcal{U}_{I_0}^{(I)} = \mathcal{H}_{I_0}^{(I)} \mathcal{U}_{I_0}^{(I)} \qquad \mathcal{U}_{I_0}^{(I)}(t_0, t_0) = \mathcal{I}, \tag{20}$$

and $\mathcal{U}_{I_0}^{(II)}$ an analogous solution for the effective Hamiltonian

$$\mathcal{H}_{I_1} = \mathcal{U}_{I_0}^{(I)\dagger} \mathcal{H}_{I_0}^{(II)} \mathcal{U}_{I_0}^{(I)}. \tag{21}$$

Due to the fact that the operators contained in $\mathcal{H}_{I_0}^{(I)}$ form a finite Lie algebra, the evolution operator $\mathcal{U}_{I_0}^{(I)}$ can be expressed as a product of exponentials [7]

$$\mathcal{U}_{I_0}^{(I)} = \prod_{0 \leq i+j \leq 2} e^{-\beta_{ij}^{(0)} a^{\dagger i} a^j} \tag{22}$$

where the complex functions $\beta_{ij}^{(0)}(t)$ satisfy a set of coupled, first order differential equations which can be solved numerically. With this expression for $\mathcal{U}_{I_0}^{(I)}$ we can construct the Hamiltonian $\mathcal{H}_{I_1}$. It again comprises a part which forms a finite Lie algebra and a part which does not. The time evolution operator $\mathcal{U}_{I_0}^{(II)}$ is then again written as the product of two evolution operators and we can proceed in a completely analogous manner as before. The evolution operator obtained after k-iterations $\mathcal{U}_{I_k}$ would correspond to the product

$$\mathcal{U}_{I_k} = U_{I_0}^{(I)} ... U_{I_k}^{(I)}. \tag{23}$$

To approximate $\mathcal{U}_I$ by $\mathcal{U}_{I_k}$ corresponds to neglect the Hamiltonian $\mathcal{H}_{I_k}^{(II)}$ with respect to $\mathcal{H}_{I_k}^{(I)}$. We call this the time-dependent iterative Bogolubov transformation (TDITB) method in analogy with its quite efficient time-independent counterpart [8].

3 AN EXAMPLE

Let us consider, a colinear collision of an H_2 molecule with an H_e atom. For the H_2 molecule the parameters of the Morse potential are taken to be $A = 0.183385$ and $D = 2.33509$ so that comparison with the results of [2] can be done. To study how efficient is the TDITB method, consider first the H_2 molecule modeled by the *usual* harmonic oscillator. In Table I we show the transition probability from the ground to the first excited vibrational state for several values of the collision energy $E = NE_0$, $E_0 = \hbar\omega$ with ω as given by Secrest and Johnson [5] and for different levels of approximation [6].

TABLE I. Transition probabilities using a harmonic oscillator representing the diatomic molecule and one (P_{01}) or two (P_{02}) iterations for the time-dependent interaction. Results are shown for comparaison with the Basis Set (BS) and Exact Quantum Harmonic (UHA) of [5].

$E/\hbar\omega$	P_{01}	P_{02}	BS	UHA
4	9.20(-4)	9.73(-4)	9.84(-4)	7.20(-4)
6	3.50(-2)	3.76(-2)	3.89(-2)	2.95(-2)
8	1.38(-1)	1.47(-1)	1.55(-1)	1.33(-1)
10	2.61(-1)	2.73(-1)	2.87(-1)	2.92(-1)
12	3.45(-1)	3.49(-1)	3.59(-1)	4.28(-1)
16	3.44(-1)	3.29(-1)	2.96(-1)	4.07(-1)

The results obtained with a basis set expansion (BS) are *exact* numerical results within the semiclassical approximation. We also show in the table the exact quantum results of [5] (UHA). The transition probabilities using the TDITB method after one (P_{01}) or two transformations (P_{02}) are also reported. That is , P_{01} corresponds to approximating the time evolution operator in the interaction picture by

$$\mathcal{U}_I = \mathcal{U}_{I_0}$$

with $\mathcal{U}_{I_0}$ the operator which evolves according to the Hamiltonian $\mathcal{H}_{I_0}^{(I)}$. Meanwhile P_{02} corresponds to

$$\mathcal{U}_I = \mathcal{U}_{I_0}^{(I)} \mathcal{U}_{I_1}^{(I)}. \tag{24}$$

In the procedure for finding $\mathcal{U}_{I_0}^{(I)}$ and $\mathcal{U}_{I_1}^{(I)}$,up to quartic, $0 \le i + j \le 4$, terms were kept.

Notice that for all the energies considered the transitions obtained after two transformations are closer to the (BS) results than those obtained after one transformation. We also see that if we compare our approximations with the exact quantum results (UHA) then for some energies the first iteration gives closer results than the second one. However this fact may be misleading since in our case the exact results are those obtained in the semiclassical approximation. Because the difference between the results obtained after two transformations and the exact ones is very small we did not pursue these transformations further. We believe that this example shows clearly that our method deals quite efficently with the time-dependent anharmonicities.

Now, consider the H_2 molecule modeled by the alternative harmonic oscillator defined using the variationaly optimized displacement and scale parameters. In this case $d_0 = 0.17$ while α_0 differs from the usual α in less than two percent. In Table II, we show the results obtained for the transition probabilities from the lowest three states for several values of the collision energy. This table also shows the transition probabilities obtained numerically for the exact Morse potential (MP)[2] and the usual harmonic approximation (UHA)[5]. These results do not comprise the semiclassical approximation for the atom-molecule interaction and use is made of the full exponential function.

TABLE II. Transition probabilities using the modified harmonic oscillator for different energies and transitions. The upper value corresponds to Exact Quantum Morse Results (MP), the next corresponds to our's and the last to (UHA).

$E/\hbar\omega$	$\cdot P$(0-1)	P(1-2)	P(0-2)	P(1-3)	P(2-3)	P(0-3)
6	7.31(-3)	1.25(-3)	2.30(-6)			
	2.00(-2)	2.75(-4)	1.44(-6)			
	2.95(-2)	1.42(-3)	1.07(-5)			
10	7.39(-2)	8.15(-2)	1.66(-3)	1.22(-3)	5.47(-2)	1.17(-5)
	2.07(-1)	1.62(-1)	1.22(-2)	2.16(-3)	4.25(-2)	7.04(-5)
	2.92(-1)	2.17(-1)	2.25(-2)	5.39(-3)	7.70(-2)	2.31(-4)
16	2.45(-1)	3.18(-1)	3.38(-2)	5.72(-2)	3.34(-1)	2.72(-3)
	3.13(-1)	1.92(-1)	1.57(-1)	1.72(-1)	2.07(-1)	3.30(-2)
	4.07(-1)	1.56(-1)	3.30(-1)	2.85(-1)	1.89(-1)	9.88(-2)

We observe that our results are in general in better agreement with the exact quantal (MP) results than the (UHA). If we compare P_{02} in Table I with the corresponding results in Table II we see a large difference between them and this is due entirely to the slight change in frequency that we have done defining the frequency of the transformed oscillator. Though the difference in frequencies is rather small the differences in the values of the transition probabilities are rather large, for example, for a collision energy $E/\hbar\omega = 4$ we go from $P_{02} = 9.73 \times 10^{-4}$ to 2.51×10^{-4} which is very close to the (MP) value of 2.46×10^{-4}. This is an indication of the quality of the approximation made for the Morse oscillator.

Once we have constructed the matrix elements of the time evolution operator, we can calculate the survival probability, that is, the probability for the molecule to remain in the initial state. We have done that from a time long before the collision takes place up to a time where the collision is over.

We see that the collision lasts the order of 1.5 time units ($t_{col} \approx 3 \times 10^{-14}$sec); the permanency probability is one long before the collision begins and starts to decrese around $t_0 = -0.75$ time units reaching an asymptotic value at approximately $t_{as} = 1$ time units. The frequency of the H_2 oscillator is $\omega_{H_2} = 8.054 \times 10^{14}$/sec and the corresponding period is of the order of $T_{H_2} \approx 3/2t_{col}$ so that the molecule is able to make a couple of oscillations before the collision is over. From this figure it becomes evident why a perturbative treatment of the problem may lead to wrong results. Although the asymptotic transition probability may be small, in a short interval around $t = 0$ the state of the molecule highly differs from the initial state.

In the interaction picture, the creation-annihilation operators can be written in the form

$$a(t) = d_1(t)a^\dagger + d_2(t)a + d_3(t)$$

where $d_i(t)$ are funtions of the time, and we have used the fact that the set of operators appearing in the time evolution operators is closed under the operation of commutation. We can now consider the time evolution of the expectation value of the momentum $< p >$, the coordinate $< x >$ and the dispersions Δx and Δp using the expressions for the momentum and the coordinate operators in terms of the creation-annihilation operators.
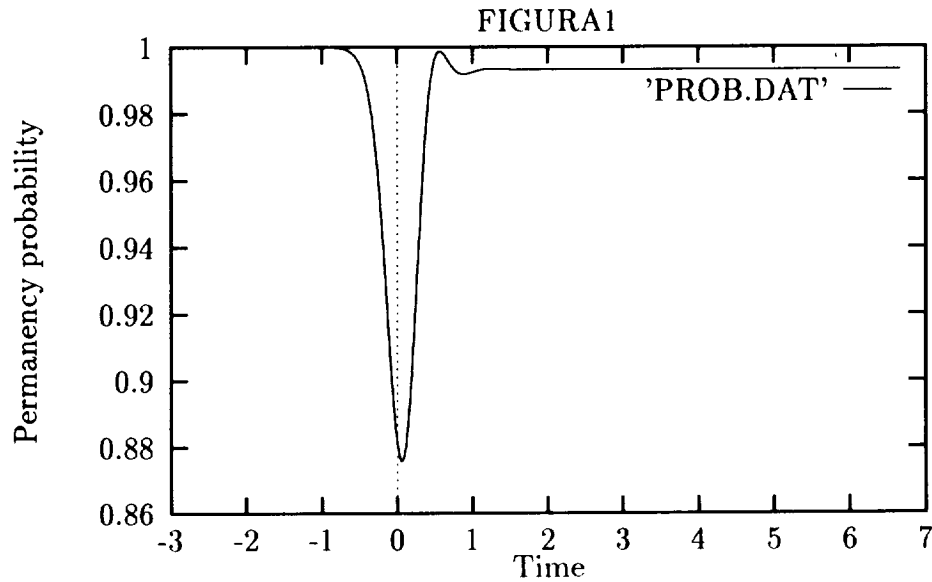
FIGURA1

Figure 1: Time dependent survival probability for the ground state of an H_2 molecule colliding with a He atom for a collision energy $E = 4\hbar\omega$.

It can be seen in figure 2 that, when the atom is far apart from the molecule, the average value of the position operator in the ground state is zero as it should since we are dealing with an effective harmonic oscillator.

As the atom approaches the molecule, this one recedes, taking also negative values of the momentum, when $t \approx 0$ the momentum changes sign and the average value of the position initiates an increase towards the origin. Since the collision time is larger than the frequency of oscillation, the projectile is hit again and the oscillator's momentum changes sign, the position does not reach the origin and moves away from the origin. After that, the projectile leaves the range of the interaction and the molecule is left in an excited state as indicated by the oscillatory behavior of the position and momentum operators around the zero value.
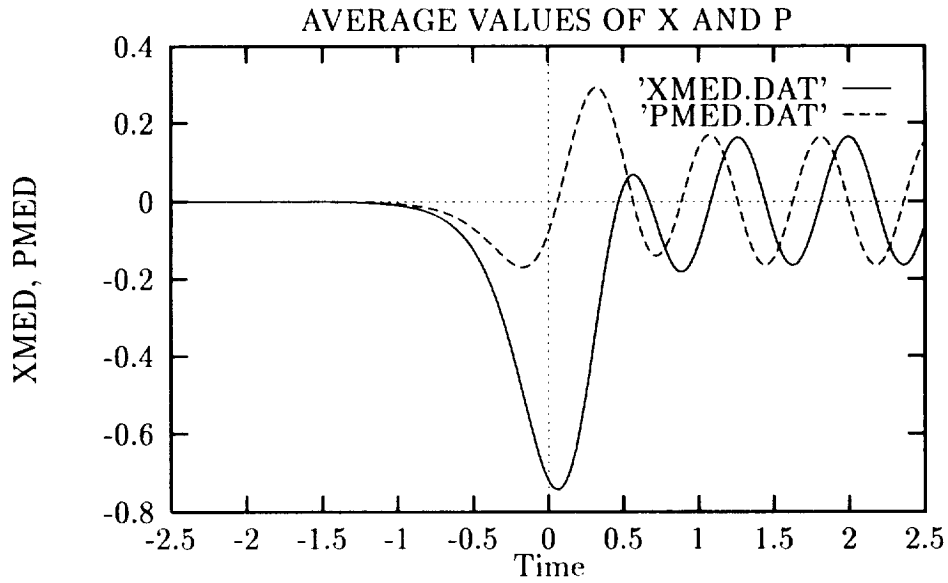
Figure 2: Time evolution of the average values of **P** (squares) and **X** (continous line) as the collision takes place.

Finally, in figure 3 we see that, since we begin with a minimum uncertainty state the dispersion in each coordinate is $\sqrt{1/2}$ and it remains being a minimum uncertainty state during the collision because we are dealing with an harmonic oscillator.

However, due to the time dependence of the parameters defining the oscillator, we can see that there is squeezing in the dispersions which become more pronounced as the energy increases. Notice that as the projectile approaches the molecule, the dispersion in the momentum decreases while that of the coordinate increases in such a way as to keep their product constant. The squeezing of the dispersion reaches its peak value at the time of the collision (t=0). The presence of squeezing is to be expected since the time dependence of the creation-annihilation operators which define our harmonic oscillator has the form of a generalized Bogoliubov transformation. Not long ago it was shown that states of light with nonclassical properties can be generated if the frequency of the harmonic oscillator is swept as a function of time [12]. In that work, the authors dealt with a simple time dependence for the frequency of the oscillator in order to obtain exact analytical results. As we have shown here, the presence of these nonclassical properties is due to the time dependence of the frequency irrespective of the functional form used to describe it.

4 CONCLUSIONS

In this work we have shown that a suitable harmonic approximation for the description of an anharmonic potential like, for instance, the Morse potential, can yield very good results when one is looking for properties like the transition probabilities between the vibrational states of the oscillator. We found that a slight change in the parameters defining the oscillator with respect to
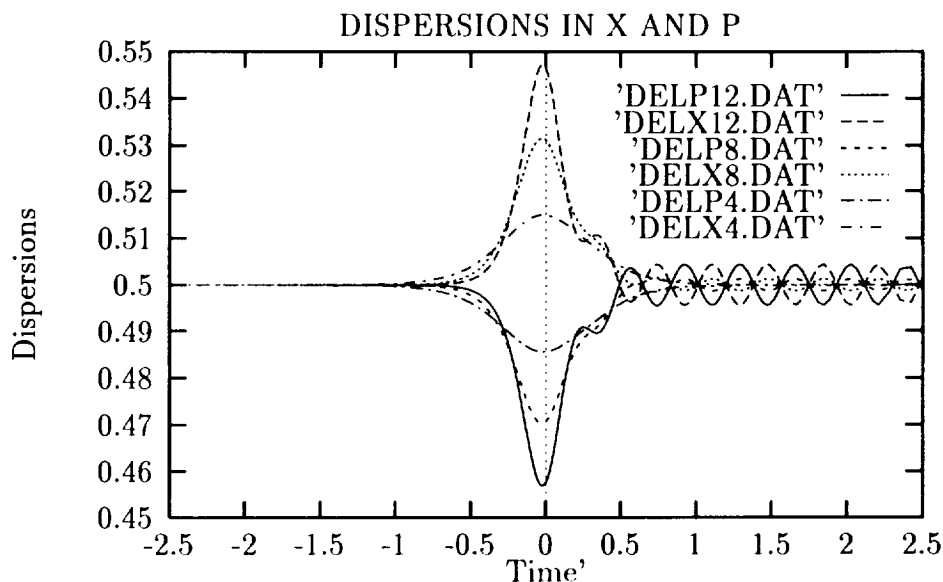
Figure 3: Time evolution of the dispersion of the coordinate and momentum values for the ground state of the molecule during the collision for E=4$\hbar\omega$ (thin lines) and E=12$\hbar\omega$ (thik lines).

their original values, when no optimization is made, can have a great importance for the evaluation of transition probabilities. However, when we evaluate the dispersions and the average values of the position and momentum operators we get essentially the same results for the oscillator before and after the optimization, this leads us to believe that the non classical behavior that we have found, like the squeezing, is a property of the system and not of the particular model we are using for its description.

The method we have used can be taken as a starting point for more accurate calculations when anharmonic potentials are studied. Here, we are searching for the *best* harmonic potential to mimic the anharmonic one and at least part of the information coming from the anharmonic part of the potential is accounted for with the use of the generalized Bogoliubov transformations.

Acknowledgements

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QUANTUM FIELD BETWEEN MOVING MIRRORS:
A THREE DIMENSIONAL EXAMPLE

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Abstract

The scalar quantum field between uniformily moving plates in three dimensional space is studied. Field equations for Dirichlet boundary conditions are solved exactly. Comparison of the resulting wavefunctions with their instantaneous static counterpart is performed via Bogolubov coefficients. Unlike the one dimensional problem, "particle" creation as well as squeezing may occur. The time dependent Casimir energy is also evaluated.

1 Introduction.

During the last twenty five years, much effort has been devoted to the understanding of quantum phenomena in systems under the influence of external conditions. In particular, Moore [1] initiated the study of the quantization of the electromagnetic field in a cavity with perfectly reflecting movable boundaries. Nowadays, it is recognized that this kind of system has several interesting nonclassical properties. Among them, there is the possibility of producing a nonadiabatic distortion of vacuum state leading to a modification of the field (Casimir) energy [2], along with the "creation" of photons [3]. It is also possible to obtain nonclassical statistical properties of the photons inside such a cavity: squeezing [4] and nonthermal distributions [5] are expected.

In order to avoid technical complications, most investigations of the field between moving plates have been restricted to the one dimensional case. However, it is not obvious whether all the results can be extrapolated to the three dimensional space. In this article, we study the quantum mechanics of a scalar massless field propagating between two plates which approach or recede each other with constant speed. The main results which follow are that the boundary conditions on the moving plates produce squeezed states and a nonzero vacuum expectation value of the particle number operator. These effects vanish in the one dimensional case [6]. The nonstationary Casimir energy is also evaluated.

2 Quantum field between the plates

Consider two parallel plates which are moving with a constant relative velocity. The natural coordinates for this problem are

$$t = \tau \cosh \zeta, \quad z = \tau \sinh \zeta, \tag{1}$$

where z and t are the Minkowski coordinates. Taking $-\infty < \tau, \zeta < \infty$, the Milne coordinates cover the entire past and future quadrants of the (z, τ) plane.

The equation for a massless scalar field ψ is:

$$\Box\psi \equiv -\frac{1}{\tau}\frac{\partial}{\partial\tau}\left(\tau\frac{\partial}{\partial\tau}\psi\right) + \left[\frac{1}{\tau^2}\frac{\partial^2}{\partial\zeta^2} + \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right]\psi = 0. \tag{2}$$

Now, the world-line of each plate can be taken as $\zeta = \pm\zeta_0$, where ζ_0 is the speed of each plate as seen in their center of velocity frame. Dirichlet boundary conditions on the plates take the simple form $\psi(\pm\zeta_0) = 0$. (It is also straightforward to impose Neumann boundary conditions.) It will be convenient to normalize the field in a box with fixed walls with separation a and b in the x and y directions

The general solution of the wave equation with the above boundary conditions can be decomposed as the product of a function of ζ and τ, and a plane wave solution propagating in the $\mathbf{r} \equiv \{x, y\}$ plane with wave vector $\mathbf{k} \equiv \pi\{n_x/a, n_y/b\}$. Explicitly,

$$\psi_{n,\mathbf{k}} = N_\psi \sin(k_x x)\, \sin(k_y y) \sin\left[\nu(\zeta + \zeta_0)\right] H_{i\nu}^{(j)}(k\tau), \tag{3}$$

where

$$N_{\psi\pm} = \left(\frac{\pi}{ab\zeta_0}\right)^{1/2} e^{\pm\nu\pi/2}. \tag{4}$$

is a normalization factor, $H_{i\nu}^{(j)}$ are the standard Hankel functions ($j = 1, 2$), $k \equiv |\mathbf{k}|$, and we have defined $\nu \equiv n\pi/2\zeta_0$, n being a positive integer. In the future region, $t > 0$, $H_{i\nu}^{(2)}$ and $H_{i\nu}^{(1)}$ correspond to modes of positive and negative frequency respectively, while the opposite is true in the past region, $t < 0$ (see, e. g.: [7][8]). We will denote the positive (negative) frequency modes by ψ^+ (ψ^-).

At this point, we note that the field between plates separated a *fixed* distance L is given by

$$\phi_{n,\mathbf{k}} = N_\phi e^{i(\mathbf{k}\mathbf{r}-\omega t)} \sin\left[\frac{n\pi}{L}(z + L/2)\right], \tag{5}$$

where $\omega = [\mathbf{k}^2 + (n\pi/L)^2]^{1/2}$ and the normalization coefficient is now

$$N_\phi = \left(\frac{4}{\omega abL}\right)^{1/2} \tag{6}$$

This coefficient follows from the scalar product in Minkowski coordinates:

$$(\phi_1, \phi_2)_{Ins} \equiv -i \int_{-L/2}^{L/2} dz \int dy\, dx(\phi_1^*\frac{\partial\phi_2}{\partial t} - \phi_2\frac{\partial\phi_1^*}{\partial t}), \tag{7}$$

where the subindex Ins refers to the instantaneous frame: the integration is taken over the volume enclosed by the fixed box at an arbitrary time t.

Hereafter, the field modes between moving plates will be called dynamical modes, whereas the modes between fixed plates will be called instantaneous modes. The crucial point is that between moving plates, the positive frequency modes of the dynamical field are a sum of both positive and

negative frequency modes of the instantaneous field between fixed plates. In general, any field mode ϕ_n can be expanded in terms of ψ_m as

$$\psi_m = \sum_n \alpha_{mn}\phi_n + \sum_n \beta_{mn}\phi_n^*, \tag{8}$$

where α_{mn} and β_{mn} are the Bogolubov coefficients, and the indices m and n describe the set of all parameters characterizing the modes. In the particular case we are interested in, take ϕ and ψ as the wave functions describing the fields between fixed and moving plates respectively. More precisely, consider a pair of plates of fixed separation $L = 2t \tanh \zeta_0$ which coincides instantaneously at Minkowski time t with a pair of plates moving with relative speed $v = \tanh(2\zeta_0)$ (Fig. 1). Now, the Bogolubov coefficients can be calculated taking the scalar product between the ψ_m and ϕ_n modes over the hypersurface $t = const.$ between the plates, (Note that for definitiveness we are considering the future region $t > 0$ where the plates are separating but it is straighforward to adapt the analysis to the past region.) Thus,

$$\alpha_{m,n,\mathbf{k},\mathbf{k}'} = (\phi_{n,\mathbf{k}}^+, \psi_{m,\mathbf{k}'}^+)_{Ins} \tag{9}$$

and

$$\beta_{m,n,\mathbf{k},\mathbf{k}'} = (\phi_{n,\mathbf{k}}^-, \psi_{m,\mathbf{k}'}^+)_{Ins}. \tag{10}$$

The integration involved in Eqs. (9) and (10) is to be performed over the hypersurface $t = const.$ bounded by the plates with separation $L = 2t \tanh \zeta_0$, with t interpreted as a parameter. At this point, we note that in any practical case, the velocities of the plates are non relativistic, that is $\zeta_0 \ll 1$. This permits to make a convenient approximation which, together with the change of variables $z = t \tanh \zeta$, simplifies Eq. (9) to the form:

$$\alpha_{m,n,\mathbf{k},\mathbf{k}'} \simeq i\frac{ab}{4}N_\phi N_\psi \delta_{\mathbf{k}\mathbf{k}'}\delta_{m,n}\zeta_0\, t \left[\frac{d}{dt}H_{i\nu}^{(2)}(kt) - i\omega H_{i\nu}^{(2)}(kt)\right]e^{i\omega t} \tag{11}$$

with an analogous equation for β. In this nonrelativistic approximation, it is very convenient to use the asymptotic forms of the Hankel functions which are valid for indices with large magnitudes[10]:

$$H_{i\nu}^{(2)}(kt) \simeq \sqrt{2/\pi}(\nu^2 + k^2 t^2)^{-1/4}$$
$$\exp\left[-\nu\pi/2 - i(\nu^2 + k^2 t^2)^{1/2} + i\nu \text{Arsh}(\nu/kt) - i\pi/4\right]. \tag{12}$$

It finally follows that the Bogolubov coefficients can be approximated as

$$\alpha_{m,n,\mathbf{k},\mathbf{k}'} \simeq \delta_{\mathbf{k}\mathbf{k}'}\,\delta_{m,n}\left[1 + \frac{-i(kt)^2}{4[\nu^2 + (kt)^2]^{3/2}}\right]e^{-\pi i/4 + i\nu \text{Arsh}(\nu/kt)} \tag{13}$$

and

$$\beta_{m,n,\mathbf{k},\mathbf{k}'} \simeq \delta_{\mathbf{k}\mathbf{k}'}\,\delta_{m,n}\left[\frac{i(kt)^2}{4[\nu^2 + (kt)^2]^{3/2}}\right]e^{-\pi i/4 - 2i[\nu^2 + (kt)^2]^{1/2} + i\nu \text{Arsh}(\nu/kt)}. \tag{14}$$

It is also worth mentioning that in the case when there are no plates, the β coefficient turns out to be null when evaluated as a scalar product over the entire $\tau = const.$ hyperplane (the interested reader can check this point using the standard properties of the Hankel functions). This implies

that the Milne vacuum is equivalent to the Minkowski vacuum (see ref.[8] for a discussion of this point).

However, unlike the one dimensional case, the coefficient β is not null when the field is rectricted between the moving plates; thus the Fock space defined by the dynamical modes $\{\psi_{nk}\}$ is nontrivialy related to the instantaneous Fock space specified by the fixed modes $\{\phi_{nk}\}$. which, in principle, can be interpreted as the number of particles "created" by the motion of the plates; this point will be further discussed in the next section.

In particular, the dynamical vacuum state $|0>_{Dyn}$ has a nonzero expectation value of the number of "instantaneous" particles. Thus, the dynamical vacuum is a nontrivial distortion of the instantaneous vacuum state $|0>_{Ins}$. Explicitly, the "particle" number density is given by the distribution function

$$P_{\mathbf{k},n} = \sum_{\mathbf{k},n} |\beta_{\mathbf{k},n}|^2 = \frac{(kt)^4}{16[\nu^2 + (kt)^2]^3}, \tag{15}$$

Notice, however, that the real character of this particles is intrinsically related to its measurability.

The Bogolubov coefficients also relate coherent and squeezed sates. A state which is originally coherent according to a instantaneous configuration of the plates becomes a squeezed state with variances [2]:

$$\left\{ \begin{array}{c} \sigma_{x_i,x_j} \\ \sigma_{p_i,p_j} \end{array} \right\} = \frac{1}{2}\delta_{ij} + \text{Re}\sum_n \left[\beta_{ni}^*\beta_{nj} \pm \frac{1}{2}(\alpha_{ni}\beta_{nj}^* + \alpha_{nj}\beta_{ni}^*) \right] \delta_{ij} ,$$

and

$$\sigma_{x_i,p_j} = \text{Im}\sum_n \left[\beta_{ni}^*\beta_{nj} + \frac{1}{2}(\alpha_{ni}\beta_{nj}^* + \alpha_{nj}\beta_{ni}^*) \right] . \tag{16}$$

In our problem i denotes the set of variables $\mathbf{k}, n$. So that,

$$\left\{ \begin{array}{c} \sigma_{x_i,x_j} \\ \sigma_{p_i,p_j} \end{array} \right\} = \frac{1}{2}\delta_{ij} + \delta_{ij}\frac{(kt)^4}{16[\nu^2 + (kt)^2]^3}\left\{1 \mp \cos(2[\nu^2 + (kt)^2]^{1/2})\right\}$$

$$\pm \delta_{ij}\frac{(kt)^2}{4[\nu^2 + (kt)^2]^{3/2}} \sin(2[\nu^2 + (kt)^2]^{1/2}) \tag{17}$$

and

$$\sigma_{x_i,p_j} = - \delta_{ij}\frac{(kt)^4}{16[\nu^2 + (kt)^2]^3} \sin(2[\nu^2 + (kt)^2]^{1/2})$$

$$- \delta_{ij}\frac{(kt)^2}{4[\nu^2 + (kt)^2]^{3/2}} \cos(2[\nu^2 + (kt)^2]^{1/2}) . \tag{18}$$

Thus, the squeezed ellipse in phase space rotates with its ellipticity vanishing as an inverse power of time.

3   Casimir effect

Boundary conditions in any given system may alter its ground state. A well known example in quantum field theory is Casimir effect, i.e., the attractive force between two infinite conducting

plates in otherwise empty space. A direct consequence of the existence of Casimir forces is that mantaining even uniform relative motion of a pair of conducting plates requires external forces. It is also expected that the Casimir energy for nonstationary boundaries differs from the stationary case. In fact, one could think that the creation of particles with distribution (4.3) or the squeezing (4.5) of originally coherent states take place at the expense of the Casimir energy between the plates [2]. Notice, however, that such an interpretation is not obvious because the distribution of particles (4.3) diverges when integrated over all momenta. This is a consequence of dealing with idealized conducting plates.

The energy density for our nonstationary problem is given by [11]

$$\epsilon = \frac{1}{\pi} \int_0^\infty d\omega \omega^2 [\tilde{D}^+(\omega, \tau) + \tilde{D}^-(\omega, \tau)] \tag{19}$$

where $\tilde{D}^\pm$ denotes the Fourier transform of Wightman $D^\pm$ functions:

$$\tilde{D}^\pm(\omega, \tau) = \int_{-\infty}^\infty d\sigma e^{i\omega\sigma} D^\pm(\tau + \frac{1}{2}\sigma, \tau - \frac{1}{2}\sigma) \tag{20}$$

$$D^\pm(\tau + \frac{1}{2}\sigma, \tau - \frac{1}{2}\sigma) =_{Dyn} < 0|\psi(\tau \pm \frac{1}{2}\sigma, x, y, \zeta)\psi(\tau \mp \frac{1}{2}\sigma, x, y, \zeta)|0 >_{Dyn} \tag{21}$$

The free Wightman function in Milne coordinates is given by

$$D_F^\pm(x, x') = -\frac{1}{4\pi^2} \frac{1}{-\tau^2 - \tau'^2 + 2\tau\tau' \cosh(\zeta \pm \zeta') + (y - y')^2 + (x - x')^2} \tag{22}$$

The boundary conditions in our problem can be easily imposed by image method. So that, for two infinite plates

$$D^\pm(x, x') = -\frac{1}{4\pi^2} \sum_{n=-\infty}^\infty \frac{1}{-\tau^2 - \tau'^2 + 2\tau\tau' \cosh(\zeta \pm \zeta' - 4\zeta_0 n) + (y - y')^2 + (x - x')^2} \tag{23}$$

The energy of the field between plates per unit area is

$$E = \frac{1}{ab} \int_{-\zeta_0}^{\zeta_0} d\zeta \, \tau \, \epsilon \tag{24}$$

When performing the ζ integration two different contributions in the energy density arise. The first one has terms independent of the ζ_0 value. It is formed by the D^+ term and by the zero mode term of D^-. The Fourier tranform of the latter is the well known $\omega/2$ which gives rise to infinite vacuum expectation value in free space. The second kind of terms correspond to the Casimir energy per unit area, which is explicitely given by

$$E_C = -\frac{1}{4\pi^2} \frac{\zeta_0}{(2\tau)^3} \left[\sum_n \frac{1}{sh^4(2n\zeta_0)} + \sum_n \frac{1}{sh^2(2n\zeta_0)} \right]. \tag{25}$$

In the nonrelativistic limit:

$$E_C \simeq -\frac{1}{4\pi^2} \frac{\zeta_0}{(2\tau)^3} \left[\sum_n \frac{1}{(2\zeta_0 n)^4} + \sum_n \frac{1}{(2\zeta_0 n)^2} \right]. \tag{26}$$

and the instantaneous separation of the plates is

$$L \simeq 2\tau\zeta_0 - \frac{1}{3}\tau\zeta_0^3 \tag{27}$$

Thus, we recover the static Casimir energy and find the first order correction due to the movement of the plates.

4 Concluding remarks

From the results obtained above, it is clear that the three dimensional case contains many features which are not present in one dimension. Roughly speaking, the one dimensional case corresponds to the limit $k = 0$ of our formulas, that is, when there are no modes propagating parallel to the plates.

The first thing to notice is that there is a squeezing of quantum states between the moving plates, although with peculiar oscillating variances.

The other important result concerns the possibilty of creating "photons". If one believes the standard interpretation of particle number (see, e. g. [3]), the motion of the plates creates new particles with a distribution function given by Eq. (4.3). This interpretation is *qualitatively* consistent with the change in Casimir energy due to the movement of the plates. In fact, whether real particles are created is a question which can be settled only when an operational definition of particle is given, for instance in terms of the interaction of the field with a well defined detector, e.g. an atom.

The results presented here are still preliminary since we have analized only a scalar field. The case of an electromagnetic field will be studied in a forthcoming publication. We expect that by considering a more realistic field, several problems will become clearer. Among them, the detectability of "created" particles by an incoming atom originally in an ordinary stationary state. In any case, the problem seems to be sufficiently rich to deserve further considerations.

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Coherent State Constructions of Bases for
Some Physically Relevant Group Chains:

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Abstract

Rotor coherent state constructions are given for the Wigner supermultiplet $SU(4) \supset$ $SU(2) \times SU(2)$ and for the special irreducible representations [N0] of the $SO(5) \supset SO(3) \supset SO(2)$ group chain in exact parallel with the rotor coherent state construction for the $SU(3) \supset$ $SO(3) \supset SO(2)$ case given by Rowe, LeBlanc, and Repka. Matrix elements of the coherent state realizations of the group generators are given in all cases by very simple expressions in terms of angular momentum Wigner coefficients involving intrinsic projection labels K. The $\mathcal{K}$-matrix technique of vector coherent state theory is used to effectively elevate these K labels to the status of good quantum numbers. Analytic expressions are given for the $(\mathcal{K}\mathcal{K}^\dagger)$-matrices for many of the more important irreducible representations.

1 Introduction

In the past few years two types of coherent state constructions have been widely used to give very explicit matrix representations of many higher rank symmetry groups. In both, the irreducible representations of a larger group are constructed by an induction process from the irreducible representations of a simpler subgroup, hopefully with completely known Wigner-Racah calculus. In the more widely used first type of vector coherent state construction, [1], [2], [3], state vectors are mapped onto states of a multi-dimensional harmonic oscillator through a set of Bargmann variables, z. This VCS construction has been widely used for many of the mathematically natural group chains such as U(n) $\supset$ U(n-1) x U(1) $\supset$ U(n-2) x U(1) $\supset$... for which the subgroup chain gives a complete labelling of the state vectors. In the more recent second type of coherent state construction rotor expansions are used which are particularly effective for many of the physically relevant group chains for which an SO(3) or SU(2) subgroup related to a physically meaningful angular momentum is the important subgroup in the group chain.

In this talk I want to focus on three group chains with particular relevance for nuclear structure problems: 1) The SU(3) $\supset$ SO(3) $\supset$ SO(2) chain of the 3-dimensional harmonic oscillator of the nuclear shell model with good orbital angular momentum; 2) The SU(4) $\supset$ SU(2) x SU(2) Wigner supermultiplet with good spin and isospin needed to complement the orbital functions of 1); and finally, the SO(5) $\supset$ SO(3) $\supset$ SO(2) chain needed e.g. for the 5-dimensional harmonic oscillator of the quadrupole phonon states of the Bohr-Mottelson collective model or for two of the important symmetry group chains of the interacting boson model of Iachello and Arima, [4]. Like all physically relevant group chains, all three suffer from a missing label problem. For all of them many solutions have been proposed for this problem, some of them highly practical, others quite elegant or numerically feasible; see e.g. the pioneering work of Moskinsky [5], [6], [7]. It is the purpose of this presentation to try to convince you that the new rotor coherent state constructions give a very elegant yet also very systematic and practical solution to the missing label problem. Moreover the solution is essentially exactly the same for all three examples.

2 The Rotor Coherent State Expansion for the SU(3) $\supset$ SO(3) Case

For the SU(3) scheme in a basis of good orbital angular momentum a coherent state rotor expansion has recently been given by Rowe, LeBlanc, and Repka, [8]. This construction is closely parallel to the seminal work of Elliott [9], [10], [11] in which an angular momentum projection label, K, the projection of the orbital angular momentum onto an intrinsic or body-fixed z'-axis is used in place of the missing quantum number in the SU(3) $\supset$ SO(3) $\supset$ SO(2) scheme. Only a brief synopsis of this work will be given, the details of the derivations being reserved for the second example.

In the rotor coherent state construction for SU(3) an arbitrary state vector, $|\Psi>$, is transformed into its coherent state wave function, $\Psi(\Omega)$,

$$\Psi(\Omega) = \langle \phi_{(\lambda\mu)}|R(\Omega)|\Psi \rangle \tag{1}$$

where $|\phi_{(\lambda\mu)}>$ is the highest weight state in the SU(3) $\supset$ SU(2) x U(1) scheme. Here R(Ω) is a

standard rotation operator

$$R(\Omega) = e^{i\alpha L_z} e^{i\beta L_y} e^{i\gamma L_z} \tag{2}$$

where α, β, γ are Euler angles, L_i are space-fixed components of the orbital angular momentum operator, and where the scalar product is defined in terms of the standard angular measure

$$\int d\Omega = \int \int \int d\alpha \sin\beta d\beta d\gamma \tag{3}$$

(Note, however, that the conventions for the $R(\Omega)$ of ref [8] are somewhat different from the most widely used nuclear physics conventions [12].) If $|\Psi>$ is expanded in angular momentum eigenvectors $|\nu;LM>$, where ν is shorthand for all additional quantum numbers, these angular momentum base vectors are mapped into their coherent state realizations

$$\begin{aligned}
\Psi_{\nu;LM}(\Omega) &= \langle \phi_{(\lambda\mu)}|R(\Omega)|\nu; LM\rangle \\
&= \sum_K \langle \phi_{(\lambda\mu)}|\nu; LK\rangle D^L_{KM}(\Omega) \\
&= \sum_K c_K \sqrt{\frac{2L+1}{8\pi^2}} D^L_{KM}(\Omega).
\end{aligned} \tag{4}$$

That is, angular momentum eigenstates are mapped into a basis of (normalized) D-functions which form a simple orthonormal set with respect to the rotational measure of eq. (3). The symmetries of the c_K are such that the *symmetrized, orthonormal* rotor basis

$$\sqrt{\frac{(2L+1)}{16\pi^2(1+\delta_{K0})}}\{D^L_{KM}(\Omega) + (-1)^{\lambda+\mu+L}D^L_{-KM}(\Omega)\} \tag{5}$$

is most convenient. Operators, **O**, are then mapped into their coherent state realizations, $\Gamma(\mathbf{O})$, through

$$\Gamma(\mathbf{O})\Psi(\Omega) = \langle \phi_{(\lambda\mu)}|R(\Omega)\mathbf{O}|\Psi\rangle. \tag{6}$$

It will of course be convenient to express all operators in terms of spherical tensors of rank, r, such that

$$\begin{aligned}
\Gamma(O^r_m)\Psi(\Omega) &= \langle \phi_{(\lambda\mu)}|R(\Omega)O^r_m|\Psi\rangle \\
&= \langle \phi_{(\lambda\mu)}|R(\Omega)O^r_m R(\Omega)^{-1}R(\Omega)|\Psi\rangle \\
&= \sum_k D^r_{km}(\Omega)\langle \phi_{(\lambda\mu)}|O^r_k R(\Omega)|\Psi\rangle.
\end{aligned} \tag{7}$$

The SU(3) group generators are the 3 components of the orbital angular momentum operators, L^1_m, and the 5 components of the Elliott ($\lambda\mu$-preserving) quadrupole operator, Q^2_m. The rotor realizations $\Gamma(L^1_m)$ are given in terms of their usual Euler angle realizations

$$\Gamma(L_0) = \frac{1}{i}\frac{\partial}{\partial\gamma}, \qquad \Gamma(L_\pm) = e^{\pm i\gamma}\{i\cot\beta\frac{\partial}{\partial\gamma} \pm \frac{\partial}{\partial\beta}\}, \tag{8}$$

where $\Gamma(L_0)$ has eigenvalue M, while $\Gamma(L_+)$, $(\Gamma(L_-))$ are standard M-raising, (lowering) operators. Eq. (7) shows that we need both the standard (right-action) rotor realizations of operators, O^r_m, as well as their left-action version which will be denoted by a $\bar{\Gamma}$,

$$\bar{\Gamma}(O^r_k)\Psi(\Omega) = \langle \phi_{(\lambda\mu)}|O^r_k R(\Omega)|\Psi\rangle. \tag{9}$$

The latter can be evaluated from the left action of the operator on the SU(3) highest weight state. For the angular momentum generators

$$\bar{\Gamma}(L_k^1)\Psi_{\nu;LM}(\Omega) = \langle\phi_{(\lambda\mu)}|L_k^1 R(\Omega)|\nu;LM\rangle$$

$$= \sum_K D_{KM}^L(\Omega)\langle\phi_{(\lambda\mu)}|L_k^1|\nu;LK\rangle$$

$$= \sum_K D_{KM}^L(\Omega)\sqrt{L(L+1)}\langle LK1k|L(K+k)\rangle\langle\phi_{(\lambda\mu)}|\nu;L(K+k)\rangle$$

$$= \sum_K D_{(K-k)M}^L(\Omega)\sqrt{L(L+1)}\langle L(K-k)1k|LK\rangle\langle\phi_{(\lambda\mu)}|\nu;LK\rangle, \tag{10}$$

so that $\bar{\Gamma}(L_+)$, $(\bar{\Gamma}(L_-))$ are now K-lowering, (raising) operators, a well known property of the intrinsic (body-fixed) components of angular momentum operators. The $\bar{\Gamma}(L_k)$ can therefore be given in terms of their Euler angle realizations through the well known rotor expressions for intrinsic components,

$$\bar{\Gamma}(L_0) = \frac{1}{i}\frac{\partial}{\partial\alpha}; \qquad \bar{\Gamma}(L_\pm) = e^{\mp i\alpha}\left\{\frac{i}{\sin\beta}\frac{\partial}{\partial\gamma} - i\cot\beta\frac{\partial}{\partial\alpha} \pm \frac{\partial}{\partial\beta}\right\}; \tag{11}$$

where $\bar{\Gamma}(L_0)$ has the simple eigenvalue K. The coherent state realizations of the quadrupole operator as given by Rowe, LeBlanc, and Repka [4] are

$$\Gamma(Q_m^2) = (2\lambda + \mu + 3)D_{0m}^2(\Omega) - \frac{1}{2}[\mathbf{L}^2, D_{0m}^2(\Omega)]$$

$$+\sqrt{\tfrac{3}{2}}\{D_{2m}^2(\Omega)(\mu - \bar{\Gamma}(L_0)) + D_{-2m}^2(\Omega)(\mu + \bar{\Gamma}(L_0))\}, \tag{12}$$

i.e., these are expressed in terms of the very simple operators, $\mathbf{L}^2$, $\bar{\Gamma}(L_0)$, and simple D-functions. The well-known matrix elements of these D-functions in the orthonormal rotor basis of eq. (5) at once lead to the (standard) angular-momentum reduced matrix elements

$$\langle K; L'||\Gamma(Q^2)||K; L\rangle = \sqrt{(2L+1)}\{\langle LK20|L'K\rangle[(2\lambda + \mu + 3)$$

$$-\tfrac{1}{2}L'(L'+1) + \tfrac{1}{2}L(L+1)] + \delta_{K1}\langle L12-2|L'1\rangle\sqrt{\tfrac{3}{2}}(-1)^{L+\lambda+1}(\mu+1),\} \tag{13}$$

$$\langle(K\pm2); L'||\Gamma(Q^2)||K; L\rangle = \sqrt{(2L+1)}\langle LK2\pm2|L'(K\pm2)\rangle\sqrt{\tfrac{3}{2}}(\mu \mp K)\sigma_{KK'}, \tag{14}$$

with $\sigma_{KK'} = \sqrt{2}$ for either K or $K' = 0$, and $\sigma_{KK'} = 1$ otherwise. The simplicity of this result is negated partly by the fact that the $\Gamma(Q_m^2)$ are nonunitary realizations of these operators. In order to translate the above nonhermitian matrix elements into the hermitian matrix elements of Q_m^2 in ordinary Hilbert space, the nonunitary realizations, $\Gamma(\mathbf{O})$, of coherent state constructions is converted to a unitary realization $\gamma(\mathbf{O})$ via the $\mathcal{K}$-operator equation

$$\gamma(\mathbf{O}) = \mathcal{K}^{-1}\Gamma(\mathbf{O})\mathcal{K}. \tag{15}$$

Matrix elements of the $\mathcal{K}$ and $\mathcal{K}^{-1}$ operators can then be used to convert the nonhermitian matrix elements of $\Gamma(\mathbf{O})$ to hermitian form $\gamma(\mathbf{O})$ and hence directly to hermitian form in ordinary Hilbert space. Thus

$$\langle\nu'; L'||Q^2||\nu; L\rangle = \sum_{K,K'}(\mathcal{K}^{-1}(L'))_{\nu'K'}\langle K'; L'||\Gamma(Q^2)||K; L\rangle(\mathcal{K}(L))_{K\nu} \tag{16}$$

C-2 .

where the new quantum numbers, ν, are defined through the eigenvalues of the hermitian matrix $(\mathcal{K}\mathcal{K}^\dagger)$ which can be calculated in coherent state theory by simple recursion techniques through the known matrix elements of the group generators $\Gamma(Q^2)$. The $(\mathcal{K}\mathcal{K}^\dagger)_{KK'}$ matrix elements, moreover, can be given in simple analytic form [13] as functions of λ, μ, and L. As a simple example, the $(\mathcal{K}\mathcal{K}^\dagger)$ matrix for the irreducible representations $(\lambda 2)$ with λ-L = even is 2-dimensional, with K=2 or 0, in the basis of eq. (5), with

$$
\begin{aligned}
(\mathcal{K}\mathcal{K}^\dagger)_{22} &= \tfrac{1}{2}[2(\lambda + 3)^2 - L(L + 1)]C \\
(\mathcal{K}\mathcal{K}^\dagger)_{00} &= [2(\lambda + 2)^2 - L(L + 1)]C \\
(\mathcal{K}\mathcal{K}^\dagger)_{20} &= \sqrt{\tfrac{1}{2}(L - 1)L(L + 1)(L + 2)}C,
\end{aligned}
\tag{17}
$$

with

$$
C = N/(\lambda + 2 - L)!!(\lambda + L + 3)!!,
\tag{18}
$$

with

$$
N = \frac{(\lambda - 1)!!(\lambda + 4)!!}{2(\lambda + 3)} \quad for \quad \lambda = odd; \qquad N = \frac{\lambda!!(\lambda + 3)!!}{2(\lambda + 2)} \quad for \quad \lambda = even,
\tag{19}
$$

where $\lambda!! = \lambda (\lambda\text{-}2) \ldots 2$ (or 1). The $(\mathcal{K}\mathcal{K}^\dagger)$-matrix can be converted into the needed matrix elements of $\mathcal{K}$ and $\mathcal{K}^{-1}$ through the unitary matrix, U, which diagonalizes the hermitian matrix $\mathcal{K}\mathcal{K}^\dagger$

$$
(U(\mathcal{K}\mathcal{K}^\dagger)U^\dagger)_{\nu'\nu} = \Lambda_\nu \delta_{\nu'\nu}
\tag{20}
$$

with

$$
(\mathcal{K})_{K\nu} = U_{K\nu}^\dagger \sqrt{\Lambda_\nu}; \qquad (\mathcal{K}^{-1})_{\nu K} = \frac{1}{\sqrt{\Lambda_\nu}}U_{\nu K}
\tag{21}
$$

defined for all states ν with non zero eigenvalue, Λ_ν. Note, that a zero eigenvalue Λ_ν signals a forbidden state. The matrix of eq. (17), e.g., has one zero eigenvalue for $L = \lambda + 2$; so that there is but a single allowed state for this maximum L-value. For $L > (\lambda+2)$ the matrix elements of $\Gamma(Q^2)$ insure that all matrix elements of $\mathcal{K}\mathcal{K}^\dagger$ are zero. The $\mathcal{K}$-matrix technique of coherent state theory thus effectively converts the Elliott K-projection label to the status of a good quantum number.

It should, however, be stressed that the coherent state construction outlined here is very closely related to the Elliott angular momentum projection technique [10]. The matrix elements of Q_m^2 in the form of eqs. 13) and 14) have essentially been given by Elliott in ref. [10]. Except for an overall normalization, (see eq. (19), which is related to the fact that the 1-dimensional $(\mathcal{K}\mathcal{K}^\dagger)$ for the minimum L-value of 0 (or 1) is chosen to be unity in the coherent state construction), the $(\mathcal{K}\mathcal{K}^\dagger)$-matrix elements are given by the overlap matrix of Elliott (see e.g., eq. (A.3) for $A(KLK')$ of ref. [11]; and the specific analytic functions given by Vergados for the lower μ-values in table 2A of ref. [14]).

What then are the advantages of the coherent state rotor construction? By mapping the SU(3) angular momentum eigenstates onto the orthonormal basis, eq. (5), of the rotor expansion the construction of matrix elements is split into two clearly separated simple steps: In step 1, matrix elements of $\Gamma(O)$ are given very simply in the orthonormal rotor basis where K defines the

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orthonormal states. In step 2, which is the unitarization process, K is converted to the quantum number ν in ordinary Hilbert space. By relating ν to the non-zero eigenvalues of $(\mathcal{K}\mathcal{K}^\dagger)$ an essentially author-independent choice can be made for the quantum number ν. Although some numerical work is required in the determination of the U-matrix elements which diagonalize the multi-dimensional $(\mathcal{K}\mathcal{K}^\dagger)$-matrices; no arbitrary choices are made in a Gram-Schmidt orthonormalization process, as in the Vergados basis [14], which is an attempt to make the Hilbert space quantum number, (the κ of ref. ([14]), as close as possible to the Elliott projection label K. (In this connection, it is interesting to note that both κ and ν tend to pure K-values in the limit $\lambda \gg L$ as a glance at the special example of eq. (17) will verify.

3   A Double Rotor Coherent State Expansion for the Wigner Supermultiplet SU(4) ⊃ SU(2) x SU(2).

A complete labelling scheme for the Wigner supermultiplet has been achieved by Draayer [15] who used the Elliott angular momentum projection technique to augment the spin and isospin quantum numbers (SM_S), (TM_T) with the projection labels K_S and K_T. In order to calculate the generator matrix elements and SU(4) reduced Wigner coefficients in this fully labelled but nonorthogonal basis, however, Draayer first calculates the transformation coefficients to the canonical fully specified orthonormal U(4) ⊃ U(3) ⊃ U(2) ⊃ U(1) basis, leading to a somewhat laborious calculational algorithm. This example therefore will fully illustrate the power of the rotor coherent state construction which leads in a very simple and direct way to the desired results.

The supermultiplet scheme is based on the four spin-charge states of a single nucleon, $|m_s m_t\rangle$, with nucleon, $|m_s\ m_t >$, with

$$
\begin{aligned}
|a\rangle &= |+\tfrac{1}{2} +\tfrac{1}{2}>, & |b\rangle &= |-\tfrac{1}{2} -\tfrac{1}{2}>, \\
|c\rangle &= |+\tfrac{1}{2} -\tfrac{1}{2}>, & |d\rangle &= |-\tfrac{1}{2} +\tfrac{1}{2}> .
\end{aligned}
\tag{22}
$$

To gain the most convenient double rotor expansion it will be useful to define the basis states $|i\rangle$, $i = 1,\ldots,4$, by

$$
\begin{aligned}
|a\rangle &= \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle), & |b\rangle &= \frac{1}{\sqrt{2}}(-|1\rangle + |2\rangle), \\
|c\rangle &= \frac{1}{\sqrt{2}}(|3\rangle + |4\rangle), & |d\rangle &= \frac{1}{\sqrt{2}}(-|3\rangle + |4\rangle),
\end{aligned}
\tag{23}
$$

and define the 15 supermultiplet generators [17], **S**,**T**, and **E** $= \sigma\tau$ in terms of U(4) generators, C_{ij},

$$
C_{ij} = \sum_\alpha a^\dagger_{\alpha i} a_{\alpha j}, \qquad i,j = 1,\ldots,4
\tag{24}
$$

where i,j give the spin, isospin quantum numbers and α stands for all additional (orbital) quantum numbers needed to specify the single nucleon creation and annihilation operators. In terms of the C_{ij} the generators are

$$
S_0 = \tfrac{1}{2}(C_{12} + C_{21} + C_{34} + C_{43})
$$

$$
\begin{aligned}
S_+ &= \tfrac{1}{2}(-C_{13} - C_{23} + C_{14} + C_{24} - C_{31} + C_{32} - C_{41} + C_{42}) \\
S_- &= \tfrac{1}{2}(-C_{31} - C_{32} + C_{41} + C_{42} - C_{13} + C_{23} - C_{14} + C_{24}) \\
T_0 &= \tfrac{1}{2}(C_{12} + C_{21} - C_{34} - C_{43}) \\
T_+ &= \tfrac{1}{2}(C_{13} + C_{23} + C_{14} + C_{24} + C_{31} - C_{32} - C_{41} + C_{42}) \\
T_- &= \tfrac{1}{2}(C_{31} + C_{32} + C_{41} + C_{42} + C_{13} - C_{23} - C_{14} + C_{24}) \\
E_{00} &= \tfrac{1}{2}(C_{11} + C_{22} - C_{33} - C_{44}) \\
E_{10} &= \tfrac{1}{2\sqrt{2}}(C_{13} + C_{23} - C_{14} - C_{24} - C_{31} + C_{32} - C_{41} + C_{42}), \\
E_{-10} &= \tfrac{1}{2\sqrt{2}}(-C_{31} - C_{32} + C_{41} + C_{42} + C_{13} - C_{23} + C_{14} - C_{24}), \\
E_{01} &= \tfrac{1}{2\sqrt{2}}(-C_{13} - C_{23} - C_{14} - C_{24} + C_{31} - C_{32} + C_{42} - C_{41}), \\
E_{0-1} &= \tfrac{1}{2\sqrt{2}}(C_{31} + C_{32} + C_{41} + C_{42} - C_{13} + C_{23} - C_{24} + C_{14}), \\
E_{11} &= \tfrac{1}{2}(-C_{11} + C_{22} + C_{12} - C_{21}), \\
E_{-1-1} &= \tfrac{1}{2}(-C_{11} + C_{22} - C_{12} + C_{21}), \\
E_{1-1} &= \tfrac{1}{2}(C_{33} - C_{44} - C_{34} + C_{43}), \\
E_{-11} &= \tfrac{1}{2}(C_{33} - C_{44} + C_{34} - C_{43}).
\end{aligned}
\tag{25}
$$

The SU(4) irreducible representations are labelled by 4-rowed Young tableaux partition labels $[f_1, f_2, f_3, f_4]$, by the SU(4) labels $\{\lambda_1, \lambda_2, \lambda_3\}$, or by the Wigner supermultiplet (or standard Cartan SO(6) labels (P, P', P'')), with

$$
\begin{aligned}
\lambda_1 &= f_1 - f_2, \qquad \lambda_2 = f_2 - f_3, \qquad \lambda_3 = f_3 - f_4, \\
P &= \tfrac{1}{2}(\lambda_1 + 2\lambda_2 + \lambda_3), \quad P' = \tfrac{1}{2}(\lambda_1 + \lambda_3), \quad P'' = \tfrac{1}{2}(\lambda_1 - \lambda_3).
\end{aligned}
\tag{26}
$$

These characterize the highest weight state $|\phi\rangle$ with

$$
\begin{aligned}
C_{ij}|\phi\rangle &= 0 \quad \text{for} \quad i < j \\
C_{11}|\phi\rangle &= (\lambda_1 + \lambda_2 + \lambda_3)|\phi>, \qquad C_{22}|\phi\rangle = (\lambda_2 + \lambda_3)|\phi>, \\
C_{33}|\phi\rangle &= \lambda_3|\phi\rangle, \qquad C_{44}|\phi >= 0.
\end{aligned}
\tag{27}
$$

The double rotor expansion uses the double rotation operator $R(\Omega) \equiv R(\Omega_S)R(\Omega_T)$, with Euler angles $\alpha_S, \beta_S, \gamma_S \equiv \Omega_S$ and $\alpha_T, \beta_T, \gamma_T \equiv \Omega_T$ in the spin and isospin space. Draayer [15] has shown that the set of states, $\{R(\Omega)|\phi\rangle\}$, obtained by rotation of the highest weight state through all possible angles $\alpha_S, \ldots, \gamma_T$ span the full SU(4) space. Arbitrary state vectors $|\Psi\rangle$ in this space are now tranformed into their coherent state realizations with coherent state wave function

$$
\Psi(\Omega) = \langle \phi | R(\Omega) | \Psi \rangle.
\tag{28}
$$

A state $|\alpha S M_S T M_T\rangle$ with definite spin and isospin quantum numbers is represented by

$$
\begin{aligned}
\Psi_{\alpha S M_S T M_T}(\Omega) &= \langle \phi | R(\Omega) | \alpha S M_S T M_T \rangle = \\
&\sum_{K_S, K_T} \langle \phi | \alpha S K_S T K_T \rangle D^S_{K_S M_S}(\Omega_S) D^T_{K_T M_T}(\Omega_T).
\end{aligned}
\tag{29}
$$

Draayer [15] has shown that the SU(4) irreducible representations $[f_1, f_2, f_3, f_4] \equiv \{\lambda_1 \lambda_2 \lambda_3\}$ are spanned by the double rotor wave functions with K_S, K_T-values restricted by

$$
\begin{aligned}
(K_S + K_T) &= \pm \lambda_1, \pm(\lambda_1 - 2), \pm(\lambda_1 - 4), \ldots, 0(or \pm 1), \\
(K_S - K_T) &= \pm \lambda_3, \pm(\lambda_3 - 2), \pm(\lambda_3 - 4), \ldots, 0(or \pm 1).
\end{aligned}
\tag{30}
$$

Again, it will be useful to introduce symmetrized combinations of the D-functions. The double rotor coherent state wave functions are then spanned by the symmetrized (normalized) double rotor functions

$$
\frac{1}{8\pi^2} \left[\frac{(2S+1)(2T+1)}{2(1 + \delta_{K_S 0} \delta_{K_T 0})} \right]^{\frac{1}{2}}
$$
$$
\times \{ D^S_{K_S M_S}(\Omega_S) D^T_{K_T M_T}(\Omega_T) + (-1)^{\lambda_2 + \lambda_3 + S + T} D^S_{-K_S M_S}(\Omega_S) D^T_{-K_T M_T}(\Omega_T) \}, \tag{31}
$$

and it will therefore be sufficient to choose $K_S \geq 0$, and for $K_S = 0 : K_T \geq 0$. The requirement $S \geq |K_S|, T \geq |K_T|$ together with the structure of the $\mathcal{K}\mathcal{K}^\dagger$-matrices will determine the multiplicity of a given S, T value. For states with low values of $S + T$, for which the eigenvalues of $\mathcal{K}\mathcal{K}^\dagger$ are all nonzero (no redundant states), the number of occurrences of a given S, T will be determined by the number of possible K_S, K_T combinations. States with the maximum possible value of $S + T = \lambda_1 + \lambda_2 + \lambda_3 = f_1 - f_4$, and with $S(\text{or } T) \geq \frac{1}{2}(\lambda_1 + \lambda_3)$, always have an occurrence of 1. For these S, T-values the $\mathcal{K}\mathcal{K}^\dagger$ matrix always has only a single nonzero eigenvalue giving only a single nonredundant or physically allowed state. In general, the states with $S + T \geq \lambda_2 + 2$ will have $\mathcal{K}\mathcal{K}^\dagger$-matrices with some zero eigenvalues and hence some physically forbidden states. Table 1 gives a specific example, the possible S, T-values for the irreducible representation [8620] with $\{\lambda_1 \lambda_2 \lambda_3\} = \{242\}$. In this case there are five possible symmetrized states of the type of eq. (31), with $K_S K_T = 20, 11, 1 - 1, 02$, and 00. Note that states with $K_S K_T = 00$ must have $S + T =$ even since $\lambda_2 + \lambda_3 =$ even. States with both S and $T \geq 2$ can thus have a 5-fold occurrence for $S + T =$ even and a 4-fold occurrence for $S + T =$ odd. The maximum $S + T$-value is 8 in this case. States with $S + T = 8$, $S(\text{or } T) \geq 2$, are all single as indicated in the first column of the table. The $\mathcal{K}\mathcal{K}^\dagger$-matrix for this case has four eigenvalues of 0. In addition, it can be shown that the $\mathcal{K}\mathcal{K}^\dagger$-matrices for states with $S + T = 7$ have two eigenvalues of 0, thus reducing the possible number of physical states by two, while states with $S + T = 6$ lead to $\mathcal{K}\mathcal{K}^\dagger$-matrices with one eigenvalue of 0 reducing the possible number of physical states by one.

In the VCS rotor expansion operators, $\mathbf{O}$, are transformed into their VCS realizations, $\Gamma(\mathbf{O})$, through $\mathbf{O}|\Psi\rangle \to \Gamma(\mathbf{O})\Psi(\Omega)$, with (cf. eq. (6)),

$$
\Gamma(\mathbf{O})\Psi(\Omega) = \langle \phi | R(\Omega) \mathbf{O} | \Psi \rangle. \tag{32}
$$

The SU(4) generators, $\mathbf{O} = \mathbf{S}, \mathbf{T}, \mathbf{E}$ are again of greatest interest. Again, both the left and right realizations of $\mathbf{S}$ and $\mathbf{T}$ can be expressed in terms of the Euler angles $\alpha_S, \beta_S, \gamma_S$ and $\alpha_T, \beta_T, \gamma_T$ as in eqs. (8) and (11). Now $\Gamma(S_0)$ has the simple eigenvalue M_S whereas $\bar{\Gamma}(S_0)$ has eigenvalue K_S; while $\Gamma(S_+), (\Gamma(S_-)$ are M_S-raising, (lowering) operators, whereas $\bar{\Gamma}(S_+), (\bar{\Gamma}(S_-))$ are K_S-lowering, (raising) operators; with similar properties for the $\Gamma(\mathbf{T})$ and $\bar{\Gamma}(\mathbf{T})$.

The generators $\mathbf{E}$ can be transformed into left-action operators via

$$
\begin{aligned}
\Gamma(E_{m_S m_T})\Psi(\Omega) &= \langle\phi|R(\Omega)E_{m_S m_T}|\Psi\rangle \\
&= \langle\phi|(R(\Omega)E_{m_S m_T}R^{-1}(\Omega))R(\Omega)|\Psi\rangle \\
&= \sum_{k_S k_T} \langle\phi|E_{k_S k_T}R(\Omega)|\Psi\rangle D^1_{k_S m_S}(\Omega_S)D^1_{k_T m_T}(\Omega_T).
\end{aligned}
\tag{33}
$$

Using the properties of the highest weight state, eq. (27), and the specific expressions of the generators, eqs. (25), it can be seen that

$$
\begin{aligned}
\langle\phi|E_{00} &= \tfrac{1}{2}(\lambda_1 + 2\lambda_2 + \lambda_3)\langle\phi|, \\
\langle\phi|E_{\pm10} &= -\tfrac{1}{\sqrt{2}}\langle\phi|S_\pm, \qquad \langle\phi|E_{0\pm1} = -\tfrac{1}{\sqrt{2}}\langle\phi|T_\pm, \\
\langle\phi|E_{\pm1\pm1} &= \tfrac{1}{2}\langle\phi|(-\lambda_1 \pm S_0 \pm T_0), \qquad \langle\phi|E_{\pm1\mp1} = \tfrac{1}{2}\langle\phi|(\lambda_3 \mp S_0 \pm T_0)).
\end{aligned}
\tag{34}
$$

At this stage the usefulness of the transformation (22) can be appreciated. Although it seemingly complicates the relations of the group generators in terms of the C_{ij}, it can now be seen that the transformation (22) makes it possible to express the operators $E_{k_S k_T}$ in their left actions on the single highest weight state into equivalent left actions of components of $\mathbf{S}$ or $\mathbf{T}$ or the Cartan generators C_{ii}. The relations (34) lead to

$$
\begin{aligned}
\Gamma(E_{m_S m_T})\Psi(\Omega) = \{ &\tfrac{1}{2}(\lambda_1 + 2\lambda_2 + \lambda_3)D^1_{0m_S}(\Omega_S)D^1_{0m_T}(\Omega_T) \\
-&\tfrac{1}{\sqrt{2}}[D^1_{1m_S}(\Omega_S)\bar{\Gamma}(S_+) + D^1_{-1m_S}(\Omega_S)\bar{\Gamma}(S_-)]D^1_{0m_T}(\Omega_T) \\
-&\tfrac{1}{\sqrt{2}}D^1_{0m_S}(\Omega_S)[D^1_{1m_T}(\Omega_T)\bar{\Gamma}(T_+) + D^1_{-1m_T}(\Omega_T)\bar{\Gamma}(T_-)] \\
+&\tfrac{1}{2}D^1_{1m_S}(\Omega_S)D^1_{1m_T}(\Omega_T)(-\lambda_1 + \bar{\Gamma}(S_0) + \bar{\Gamma}(T_0)) \\
+&\tfrac{1}{2}D^1_{-1m_S}(\Omega_S)D^1_{-1m_T}(\Omega_T)(-\lambda_1 - \bar{\Gamma}(S_0) - \bar{\Gamma}(T_0)) \\
+&\tfrac{1}{2}D^1_{1m_S}(\Omega_S)D^1_{-1m_T}(\Omega_T)(\lambda_3 - \bar{\Gamma}(S_0) + \bar{\Gamma}(T_0)) \\
+&\tfrac{1}{2}D^1_{-1m_S}(\Omega_S)D^1_{1m_T}(\Omega_T)(\lambda_3 + \bar{\Gamma}(S_0) - \bar{\Gamma}(T_0))\}\langle\phi|R(\Omega)|\Psi\rangle.
\end{aligned}
\tag{35}
$$

Finally, using the identity

$$
[\mathbf{S}^2, D^1_{0m_S}(\Omega_S)] = \sqrt{2}(D^1_{1m_S}(\Omega_S)\bar{\Gamma}(S_+) + D^1_{-1m_S}(\Omega_S)\bar{\Gamma}(S_-)) + 2D^1_{0m_S}(\Omega_S),
\tag{36}
$$

and the similar relation for the isospin operators, we obtain

$$
\begin{aligned}
\Gamma(E_{m_S m_T}) = \{ &\tfrac{1}{2}(\lambda_1 + 2\lambda_2 + \lambda_3) + 2\}D^1_{0m_S}(\Omega_S)D^1_{0m_T}(\Omega_T) \\
-&\tfrac{1}{2}\{[\mathbf{S}^2, D^1_{0m_S}(\Omega_S)]D^1_{0m_T}(\Omega_T) + D^1_{0m_S}(\Omega_S)[\mathbf{T}^2, D^1_{0m_T}(\Omega_T)]\} \\
+&\tfrac{1}{2}D^1_{1m_S}(\Omega_S)D^1_{1m_T}(\Omega_T)(-\lambda_1 + \bar{\Gamma}(S_0) + \bar{\Gamma}(T_0)) \\
+&\tfrac{1}{2}D^1_{-1m_S}(\Omega_S)D^1_{-1m_T}(\Omega_T)(-\lambda_1 - \bar{\Gamma}(S_0) - \bar{\Gamma}(T_0)) \\
+&\tfrac{1}{2}D^1_{1m_S}(\Omega_S)D^1_{-1m_T}(\Omega_T)(\lambda_3 - \bar{\Gamma}(S_0) + \bar{\Gamma}(T_0)) \\
+&\tfrac{1}{2}D^1_{-1m_S}(\Omega_S)D^1_{1m_T}(\Omega_T)(\lambda_3 + \bar{\Gamma}(S_0) - \bar{\Gamma}(T_0)).
\end{aligned}
\tag{37}
$$

This is the analogue of eq. (12). Using the symmetrized (normalized) rotor basis states of eq. (31) the standard S and T-space rotational measure, and a standard definition of a spin, isospin reduced

double-barred matrix element, together with the well-known triple D-function integrals, we obtain (for the general $K_S K_T$ case with $K_S + K_T > 1$) the result

$$\langle K_S K_T; S'T' || \Gamma(E) || K_S K_T; ST \rangle$$
$$= [(2S+1)(2T+1)]^{\frac{1}{2}} \langle S K_S 10 | S'; K_S \rangle \langle T K_T 10 | T' K_T \rangle$$
$$\times \{ \tfrac{1}{2}(\lambda_1 + 2\lambda_2 + \lambda_3) + 2 - \tfrac{1}{2}S'(S'+1) + \tfrac{1}{2}S(S+1) - \tfrac{1}{2}T'(T'+1) + \tfrac{1}{2}T(T+1) \},$$
$$\langle (K_S \pm 1)(K_T \pm 1); S'T' || \Gamma(E) || K_S K_T; ST \rangle$$
$$= \tfrac{1}{2}[(2S+1)(2T+1)]^{\frac{1}{2}} \langle S K_S 1 \pm 1 | S'(K_S \pm 1) \rangle \langle T K_T 1 \pm 1 | T'(K_T \pm 1) \rangle (-\lambda_1 \pm K_S \pm K_T),$$
$$\langle (K_S \pm 1)(K_T \mp 1); S'T' || \Gamma(E) || K_S K_T; ST \rangle$$
$$= \tfrac{1}{2}[(2S+1)(2T+1)]^{\frac{1}{2}} \langle S K_S 1 \pm 1 | S'(K_S \pm 1) \rangle \langle T K_T 1 \mp 1 | T'(K_T \mp 1) \rangle (\lambda_3 \mp K_S \pm K_T). \quad (38)$$

The special cases $K_S K_T = \tfrac{1}{2} \tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2}; 10$ and 01 will again require additional terms, (the analogues of the special case K = 1 for eq. (13)). The details can be found in ref. [16]. As for the SU(3) case, the reduced matrix elements of the $\Gamma(E)$ are given by very simple expressions involving ordinary spin (S) and isospin (T) Wigner coefficients with projection labels K_S and K_T. Since the $\Gamma(E)$ are nonunitary realizations of the generators **E** these first have to be translated to unitary form via the $\mathcal{K}$-operators through the analogs of eq. (15) and (16). The $(\mathcal{K}\mathcal{K}^\dagger)$-matrix elements are now calculated most easily through recursion relations such as

$$\sum_{K'_{S_2} K'_{T_2}} (\mathcal{K}\mathcal{K}^\dagger(S', T'))_{K'_{S_1} K'_{T_1}; K'_{S_2} K'_{T_2}} \langle K_{S_2} K_{T_2}; ST || \Gamma(E) || K'_{S_2} K'_{T_2}; S'T' \rangle (-1)^{S+T-S'-T'}$$
$$= \sum_{K_{S_1} K_{T_1}} \langle K'_{S_1} K'_{T_1}; S'T' || \Gamma(E) || K_{S_1} K_{T_1}; ST \rangle (\mathcal{K}\mathcal{K}^\dagger(S,T))_{K_{S_1} K_{T_1}; K_{S_2} K_{T_2}} \quad (39)$$

If the quantum numbers $(\lambda_1 + \lambda_3)$ - are not too large, the dimensions of the $(\mathcal{K}\mathcal{K}^\dagger)$ matrices will be of manageable size so that analytic expressions can be given for the matrix elements as functions of S, T, and the SU(4) quantum numbers. As a special example, the irreducible representation $[f_1 f_2 f_3 f_4] = [y+2, y, 0, 0] = \{\lambda_1 \lambda_2 \lambda_3\} = \{2y0\}$ has the simple $(\mathcal{K}\mathcal{K}^\dagger)$-matrix elements

$$\begin{aligned}
(\mathcal{K}\mathcal{K}^\dagger(S,T))_{11,11} &= \tfrac{1}{2}[(y+3)(y+4) - S(S+1) - T(T+1)]\mathrm{CF}, \\
(\mathcal{K}\mathcal{K}^\dagger(S,T))_{00,00} &= [(y+3)(y+2) - S(S+1) - T(T+1)]\mathrm{CF}, \\
(\mathcal{K}\mathcal{K}^\dagger(S,T))_{11,00} &= -[2S(S+1)T(T+1)]^{\frac{1}{2}}\mathrm{CF}, \quad (40)
\end{aligned}$$

with common factor given by

$$\mathrm{CF} = \frac{\mathrm{Num}}{(y+4+S+T)!!(y+2-S-T)!!(y+3+S-T)!!(y+3-S+T)!!}, \quad (41)$$

with Num given by

$$\begin{aligned}
\mathrm{Num} &= (y+4)!!y!!(y+3)!!(y+1)!! & \text{for } y = \text{even}, \\
&= (y+5)!!(y-1)!!(y+2)!!(y+2)!! & \text{for } y = \text{odd}. \quad (42)
\end{aligned}$$

Similar $(\mathcal{K}\mathcal{K}^\dagger)$-matrix elements are given in ref. [16] for most of the important SU(4) irreducible representations.

For the Wigner supermultiplet therefore, as for the SU(3) $\supset$ SO(3) scheme, the matrix elements of double (spin and isospin-space) spherical tensor operators, (not necessarily group generators), can be evaluated by a simple two-step process. By mapping the SU(4) states of good spin and isospin onto the symmetrized orthonormal basis states of the double rotor coherent state expansion, very simple expressions are gained for the reduced matrix elements of the $\Gamma(O^{r_S r_T})$. By converting the nonunitary $\Gamma(O^{r_S r_T})$ to unitary form via the $\mathcal{K}$-matrix technique, these can then be converted to standard Hilbert space matrix elements in which the labels $K_S K_T$ are replaced with the quantum numbers ν which enumerate the nonzero eigenvalues Λ_ν, of the $(\mathcal{K}\mathcal{K}^\dagger)$-matrix. These Λ_ν again give an author-independent meaning to the quantum numbers, ν, where now

$$\langle \nu'; S'T'||O^{r_S r_T}||\nu, ST\rangle = \sum_{K_S K_T} \sum_{K'_S K'_T} (\mathcal{K}^{-1})_{\nu', K'_S K'_T} \langle K'_S K'_T; S'T'||\Gamma(O^{r_S r_T})||K_S K_T; ST\rangle (\mathcal{K})_{K_S K_T, \nu}$$

(43)

The $\mathcal{K}$-matrix thus effectively elevates the Draayer (Elliott-type) projection labels K_S, K_T to the status of good quantum numbers.

4 A Rotor Coherent State Expansion for the SO(5) $\supset$ SO(3) Chain

Very recently, Rowe [18] has also given a vector coherent state rotor realization for the special irreducible representations [N0] and [NN] of SO(5). With a slight change of emphasis [19] this rotor construction can be put into exact parallel with that used for the SU(3) $\supset$ SO(3) and SU(4) $\supset$ SU(2) x SU(2) group chains. In the SO(5) basis of good orbital angular momentum, $|[N_1 N_2], ..., ..., LM\rangle$, there are two missing quantum numbers, in contrast to the mathematically natural basis $| [N_1 N_2] sm_s tm_t\rangle$ which exploits the local isomorphism between SO(5) and Sp(4) and labels the states with the quantum numbers of the SU(2) x SU(2) subgroup generated by two angular momentum generators s and t (not to be confused with the spin and isospin of the last section). For this reason it will be convenient to express the group generators in the Sp(4) notation in terms of the particle creation and annihilation operators for a family of spin-$\frac{3}{2}$ particles with states m $= + \frac{3}{2}, + \frac{1}{2}, - \frac{1}{2}, - \frac{3}{2}$ to be denoted by labels a, b, c, d, respectively. In order to generate the rotor states in terms of a single intrinsic (maximal weight) state, it will be convenient to make a rotation in the m $= + \frac{3}{2}, - \frac{3}{2}$ subspace, viz.

$$
\begin{aligned}
|a\rangle &= \tfrac{1}{\sqrt{2}}(|1\rangle + |4\rangle), & |b\rangle &= |2\rangle,, \\
|d\rangle &= \tfrac{1}{\sqrt{2}}(-|1\rangle + |4\rangle), & |c\rangle &= |3\rangle;
\end{aligned}
$$

(44)

where this will achieve the same purpose as the analagous eq. (23).

Since the totally symmetric SO(5) irreducible representations, [N0], are of greatest interest in nuclear physics applications, we will focus on this case. The rotor coherent state can now again be given in terms of a single intrinsic state $|\phi\rangle$ via $\langle\phi|R(\Omega|\Psi\rangle$. For the totally symmetric irreps,

[N0], $|\phi\rangle$ is now chosen such that

$$\left\{ \begin{array}{l} \frac{1}{2}(C_{11} - C_{44}) \\ \frac{1}{2}(C_{22} - C_{33}) \end{array} \right\} |\phi\rangle = \left\{ \begin{array}{l} +s_{max} \\ -s_{max} \end{array} \right\} |\phi\rangle = \left\{ \begin{array}{l} +\frac{1}{2}N \\ -\frac{1}{2}N \end{array} \right\} |\phi\rangle \tag{45}$$

with

$$\left\{ \begin{array}{l} C_{14} \\ C_{32} \end{array} \right\} |\phi\rangle = 0; \quad \left\{ \begin{array}{l} (C_{12} + C_{34}) \\ (C_{13} - C_{24}) \\ (C_{31} - C_{42}) \end{array} \right\} |\phi\rangle = 0. \tag{46}$$

The group generators are now given by the orbital angular momentum vector **L**, (a spherical tensor of rank 1), and the 7 components of a spherical tensor of rank 3, O_m^3. Eqs. (45) and (46) assure that the left action of these octupole generators can be replaced by operators $\bar{\Gamma}(L_k)$. In particular,

$$\begin{aligned}
\langle\phi|O_0 &= -\langle\phi|(\tfrac{L_0}{3} + \tfrac{5}{3}N), \\
\langle\phi|O_{-1} &= \tfrac{\sqrt{3}}{2}\langle\phi|L_-, \qquad \langle\phi|O_{+1} = \tfrac{1}{\sqrt{3}}\langle\phi|L_+, \\
\langle\phi|O_{+2} &= 0, \qquad\qquad \langle\phi|O_{-2} = -\sqrt{\tfrac{5}{6}}\langle\phi|L_+, \\
\langle\phi|O_{+3} &= \tfrac{\sqrt{5}}{3}\langle\phi|(L_0 - N), \langle\phi|O_{-3} = \tfrac{\sqrt{5}}{3}\langle\phi|(L_0 + 2N),
\end{aligned} \tag{47}$$

leads to an expression for $\Gamma(O_m)$ in terms of the $\bar{\Gamma}(L_k)$ and $D_{km}^3(\Omega)$. Analogs of eq. (36) lead to the simplest form for $\Gamma(O_m)$

$$\begin{aligned}
\Gamma(O_m) &= -D_{0m}^3(\Omega)(\tfrac{1}{3}\bar{\Gamma}(L_0) + \tfrac{5}{3}N + 2) + \tfrac{1}{6}[\mathbf{L}^2, D_{0m}^3] \\
&\quad + \tfrac{1}{2\sqrt{3}}D_{-1m}^3(\Omega)\bar{\Gamma}(L_-) + \tfrac{\sqrt{5}}{3}D_{+3m}^3(\Omega)(\bar{\Gamma}(L_0) - N) \\
&\quad + \sqrt{5}D_{-3m}^3(\Omega)(-\tfrac{2}{3}\bar{\Gamma}(L_0) + \tfrac{2}{3}N + 2) - \tfrac{\sqrt{5}}{6}[\mathbf{L}^2, D_{-3m}^3].
\end{aligned} \tag{48}$$

Note the parallels between this expression and the comparable eqs. (12) and (37) of sections 2 and 3; but also note that in this case it was now not possible to eliminate both $\bar{\Gamma}(L_-)$ and $\bar{\Gamma}(L_+)$. However, the K-raising matrix element of $\bar{\Gamma}(L_-)$ in combination with the K-lowering of the $D_{-1m}^3(\Omega)$ operator leads to a simple contribution to the matrix element diagonal in K in the rotor basis, $D_{KM}^L(\Omega)$. The $\Gamma(O_m)$ of eq. (48) thus lead to very simple matrix elements in the rotor basis with $K' = K$, $K + 3$, and K - 3. Williams and Pursey [20] have shown that the allowed K sequences for the irreps [N0] are the following (with n = integer)

For N = 3n   K=   ..., -6, -3, 0, +3, +6, +9, ...
For N = 3n+1   K=   ..., -8, -5, -2, +1, +4, +7, ...
For N = 3n+2   K=   ..., -7, -4, -1, +2, +5, +8, ...

Starting with the simplest state for [N0] = [10], with L = 2, with the normalized rotor state

$$\sqrt{\frac{5}{16\pi^2}}\{D_{+1M}^2(\Omega) + D_{-2,M}^2(\Omega)\}, \tag{49}$$

totally symmetric rotor states for N > 1 can be built up from simple products of D-functions.

In such a basis the reduced matrix elements of the $\Gamma(O_m^3)$ of eq. (48) are again given by very simple expressions involving ordinary Wigner coefficients with projection labels K. The $\mathcal{K}$-matrix technique of coherent state theory can again be used to convert these to the status of good quantum numbers, ν, through the eigenvalues Λ_ν of the $\mathcal{K}\mathcal{K}^\dagger$-matrix.

Table 1: The Possible ST-values for the Irrep. [8620]

```
                    (60)¹
          (61)¹            (50)¹
(62)¹            (51)³            (40)²
          (52)²            (41)³            (30)¹
(53)¹            (42)⁴            (31)⁴            (20)²
          (43)²            (32)⁴            (21)³
(44)¹            (33)⁴            (22)⁵            (11)³    (00)¹
          (34)²            (23)⁴            (12)³
(35)¹            (24)⁴            (13)⁴            (02)²
          (25)²            (14)³            (03)¹
(26)¹            (15)³            (04)²
          (16)¹            (05)¹
                    (06)¹
   ↑         ↑         ↑
   4         2         1
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The numbers below the arrows give the number of zeros of the $(\mathcal{K}\mathcal{K}^\dagger)$-matrices in the columns indicated by the arrows.

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HARMONIC OSCILLATOR REPRESENTATION IN THE THEORY OF SCATTERING AND NUCLEAR REACTIONS

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Abstract

The following questions, concerning to the application of the harmonic oscillator representation (HOR) in the theory of scattering and reactions, are discussed: the formulation of the scattering theory in HOR; exact solutions of the free motion Schroedinger equation in HOR; separable expansion of the short range potentials and the calculation of the phase shifts; "isolated states" as generalization of the Wigner-von Neumann bound states embedded in continuum; a nuclear coupled channel problem in HOR; the description of true three body scattering in HOR. As an illustration the soft dipole mode in the ^{11}Li nucleus is considered in a frame of the ^{9}Li+n+n cluster model with taking into account of three body continuum effects.

1 Introduction

Usually harmonic oscillator wave functions are used for the description of bound states of quantum systems that belong to the discrete spectrum [1]. In this talk the application of the harmonic oscillator (HO) basis to the solution of the scattering problem, i.e. in *continuum*, will be discussed.

This line of investigations was begun in Refs. [2] (see also the papers cited there) and independently in the papers of Kiev [3] and Moscow [4] groups. The similar approach, also connected with an application of the HO basis to the scattering problem, was developed by the Hungarian group [5].

In order to illustrate the essence of the approach to the scattering problem in the harmonic oscillator basis, we shall consider at first the simplest problem of the scattering of a single particle by the central potential $V(r)$ [4]. Thus, we come to the Schroedinger equation

$$\left(\frac{P^2}{2m} + V(r)\right)\psi_{lm}(\mathbf{r}) = \varepsilon\psi_{lm}(\mathbf{r}) .$$

(1)

Its solution $\psi_{lm}(\mathbf{r}) = R_l(r)Y_{lm}(\Omega)$ will be sought in the form of an expansion in the eigenfunctions of the harmonic oscillator

$$R_l(r) = \sum_{n=0}^{\infty} C_{nl}R_{nl}(r)$$

(2)

where

$$R_e(r) = (-1)^n \left(\frac{2n!}{\Gamma(n+l+\frac{3}{2})} \right)^{1/2} r^l L_n^{l+1/2}(r^2) e^{-r^2/2} \tag{3}$$

is the radial wave function of three-dimensional harmonic oscillator. This wave function corresponds to the eigenvalues of the oscillator energy $E_n^{osc} = (2n + l + 3/2)\hbar\omega$ [1]. The value $r_o = (\hbar/m\omega)^{1/2}$ is selected as a length scale in relations (1) and (2). Here ω is the oscillator frequency; the energy $\varepsilon = q^2/2$ is measured in units $\hbar\omega$; the wave vector k is expressed in units r_0^{-1}, $q = kr_0$ is the dimensionless momentum. Substituting expansion (2) in (1) and multiplying (1) scalarly by $R_{nl}Y_{lm}$, we obtain the following equation determining the wave function ψ_{lm} in the harmonic oscillator representation (HOR):

$$\sum_{n'}(H_{nn'} - \delta_{nn'}\varepsilon)C_{n'l} = 0 \ , \quad n = 0, 1, 2, \dots \ . \tag{4}$$

Here, $H = T + V$ and only the following matrix elements of the kinetic energy operator $T = P^2/2$ are nonvanishing:

$$T_{nn-1} = -\frac{1}{2} \left[\ n\left(n+l+\frac{1}{2}\right) \ \right]^{1/2} \ ,$$

$$T_{nn} = \frac{1}{2} \left(2n + l + \frac{3}{2}\right) \ , \tag{5}$$

$$T_{nn+1} = -\frac{1}{2} \left[\ (n+1)\left(n+l+\frac{3}{2}\right) \ \right]^{1/2} \ .$$

As to behaviour of the coefficient C_{nl} for $n \geq N$, their asymptotics are similar to the asymptotic of the wave function in the coordinate representation [3] if r is substituted by $2n^{1/2}r_0$:

$$C_{nl} \sim 2n^{1/4}\psi_{lm}(2\sqrt{n}r_0) \ , \quad n \to \infty \ . \tag{6}$$

this result can be obtained if the WKB expression for the oscillator function $R_{nl}(r)$ is substituted in the expression for the coefficients

$$C_{nl} = < \psi_{nlm}(\mathbf{r})|\psi_{lm}(\mathbf{r}) > \tag{7}$$

and the integral (7) is calculated by the stationary phase method. The result (6) follows also from the fact that the finite-difference equation

$$-\left[\ n\left(n+l+\frac{1}{2}\right) \ \right]^{1/2} C_{n-1l} + \left(2n + l + \frac{3}{2} - q^2\right) C_{nl}$$

$$-\left[\ (n+1)\left(n+l+\frac{3}{2}\right) \ \right]^{1/2} C_{n+1l} + 2\sum_{n'} < nl|V|n'l > C_{n'l} = 0 \tag{8}$$

in the limit $n \gg \nu = l/2 + 3/4$ can be replaced by the following second-order differential equation [4]:

$$X_l'' - \frac{l(l+1)}{x^2}X_l - \int_0^\infty V(x,x')\sqrt{xx'}X_l(x')dx + q^2 X_l = 0 .$$ (9)

Here $x = 2(n+\nu)^{1/2}$, $X_l(x) = x^{1/2}C_{nl}$. The Eq. (9) should be solved at the boundary condition

$$X_l(2\sqrt{\nu-1}) = 0 .$$ (10)

Thus, in the asymptotic limit for large n, the wave function of our system X_l for the partal wave with angular momentum l in the HOR obeys the conventional Schroedinger equation with nonlocal potential

$$V(x,x')\sqrt{xx'} \simeq 2 < nl|V|n'l > [(n+\nu)(n'+\nu)]^{1/4}$$ (11)

where the value $2(n+\nu)^{1/2}r_0$ plays the role of "coordinate". In actual calculations, the potential matrix has to be cut off by the condition $V_{nn'} = 0$, if n or (and) $n' > N$. Then a set of equations (4) can be splitted in two parts:

$$a) \; n \le N \; , \; \sum_{n'=0}^{N}(H_{nn'} - \varepsilon\delta_{nn'})C_{n'l} = -\delta_{nN}T_{NN+1}C_{N+1l} ,$$ (12a)

$$b) \; n \ge N+1 \; , \; T_{nn-1}C_{n-1l} + (T_{nn} - \varepsilon)C_{nl} + T_{nn+1}C_{n+1l} = 0 .$$ (12b)

Thus, the coefficients C_{nl} with $n > N$ obey the equation of free motion (12b) or, in the asymptotic limit of continuous n, the Schroedinger equation of free motion

$$X_l'' - \frac{l(l+1)}{x^2}X_l + q^2 X_l = 0 .$$

It means that the condition

$$C_{nl} \sim 2n^{1/4}e^{-2\sqrt{n}k}$$ (13a)

(where $\varepsilon = -k^2/2$ is the binding energy) must be satitfied for the bound states. The coefficients C_{nl} for the scattering problem have the following asymptotic behaviour:

$$C_{nl} \sim 2n^{1/4}\sin(2q\sqrt{n} - l\pi/2 + \delta_l)$$ (13b)

where $\varepsilon = q^2/2$. According to Eq.(6) the phase shift δ_l in Eq. (13b) coincides with the standard phase shift of the wave function in coordinate spase. For the decaying resonance states, we get (see in [3]):

$$C_{nl} \sim 2n^{1/4}e^{2iq\sqrt{n}} .$$ (13c)

If the calculations are made up to sufficiently high values of $N \gg 1$ it is possible to use the asymptotic expressions (13) [3] . At modest N it is necessary to use the exact, rather than approximate, solution for the equation of free motion (12b) which was found in Refs. [2, 4] in order to calculate the binding energy, the scattering phases etc. Before considering the solution for the equation of free motion, we shall note that the solution for the set (12) is equivalent to the

solution for the Schroedinger equation with Hamiltonian $H = T + V^N$ containing the many-term separable potential

$$V^N = \sum_{n,n'}^{N} < nl|V|n'l > |nl >< n'l|$$ (14)

with harmonic oscillator formactors. The technique of solving such an equation in the frame of the momentum representation was described in [5, 6]. Here we shall describe an alternative method for solving the same problem in HOR.

2 Solution for the equation of free motion in the harmonic oscillator representation

Consider first the case of positive energy $\varepsilon = q^2/2 > 0$. The Schroedinger equation of free motion in the coordinate space has two linear-independent solutions (regular and irregular) [4]:

$$R_l^{reg} = j_l(kr) \sim \frac{1}{kr} \sin(kr - \frac{l\pi}{2}) \ ,$$

$$R_l^{irreg} = n_l(kr) \sim \frac{1}{kr} \cos(kr - \frac{l\pi}{2}) \ .$$ (15)

In accordance with this, the finite difference equation of free motion (12b) will have also two fundamental solutions in the HOR [4] namely the regular solution

$$C_{nl}^{reg}(q) = \left(\frac{2\Gamma(n + l + \frac{3}{2})}{\Gamma(n + 1)} \right)^{1/2} \frac{q^l}{\Gamma(l + \frac{3}{2})} e^{-q^2/2} M(-n, l + \frac{3}{2}; q^2) =$$

$$= (-1)^n R_{nl}(q) \sim \frac{2^{3/2}}{\pi^{1/2}} n^{1/4} j_l(2\sqrt{n}q)$$ (16)

satisfying the boundary condition (6) $C_{-1l}^{reg} = 0$, and the irregular solution

$$C_{nl}^{irreg}(q) = \left(\frac{2\Gamma(n + 1)}{\Gamma(n + l + \frac{3}{2})} \right)^{1/2} \frac{(-1)^l q^{-l-1}}{\Gamma(-l + \frac{1}{2})} e^{-q^2/2} M(-n - l - \frac{1}{2}, -l + \frac{1}{2}; q^2) =$$

$$\sim \frac{2^{3/2}}{\pi^{1/2}} n^{1/4} n_l(2\sqrt{n}q)$$ (17)

which is singular at the point $n = -1$.

The Casorati determinant K_{nl} for these two solutions which plays the same role for the difference equations as the Wronskian for the differential equations [7] is of the form:

$$K_{nl} = T_{n+1n} \begin{vmatrix} C_{nl}^{reg} & C_{nl}^{irreg} \\ C_{n+1l}^{reg} & C_{n+1l}^{irreg} \end{vmatrix} = \frac{-1}{\pi q} \ .$$ (18)

Since $K_{nl} \neq 0$ for any values of n and l, the expressions (16) and (17) constitute the fundamental set of solutions for equation (12b). An arbitrary solution for (12b) may be presented as a linear

combination of fundamental solutions. In particular, the solution for the set (12) for $n \geq N$ must be of the form

$$C_{nl}(q) = \cos \delta_l C_{nl}^{reg}(q) + \sin \delta_l C_{nl}^{irreg}(q) \tag{19}$$

whence it follows that

$$\tan \delta_l = -\frac{C_{nl}C_{n+1l}^{reg} - C_{n+1l}C_{nl}^{reg}}{C_{nl}C_{n+1l}^{irreg} - C_{n+1l}C_{nl}^{irreg}} . \tag{20}$$

The equivalent pair of fundamental solutions for the free motion equation has the asymptotic form of the type of Hankel functions

$$C_{nl}^{\pm}(q) = C_{nl}^{irreg}(q) \pm i C_{nl}^{reg}(q) . \tag{21}$$

These solutions are useful for the calculation of the S-matrix and analyzing the decaying Gamov states. If we are interested in bound states ($\varepsilon = -k^2/2, q = ik$) the solution for the equation of free motion with a corresponding asymptotic

$$C_{nl}^{bound}(k) = i^l \left[C_{nl}^{irreg}(ik) + i C_{nl}^{reg}(ik) \right] \tag{22}$$

must be used. The numerical values of solutions (16), (17) can be obtained by using the book [8], where the function $M(a, b; z)$ is tabulated. Similarly to the regular and irregular solutions of the free motion Schroedinger equation the functions C_{nl}^{reg} and C_{nl}^{irreg} are oscillating functions of n and the period of oscillations decreases with increasing energy ε.

3   The solution of the scattering problem in HOR

Consider now the solution for set (12). It follows from equations (12) that the coefficient C_{nl} for $n \geq N + 1$ obey the equation of free motion with an appropriate asymptotic, i.e. $C_{nl} = C_{nl}^{0}$, where C_{nl}^{0} is the solution for the equation of free motion with asymptotic (19), (21) or (22). The coefficients $C_{nl}(n \geq N+1)$ form the "external" part of the wave function in HOR. The coefficients $C_{nl}(n \leq N)$ belong to the "internal" part of this function. The equation

$$C_{Nl}^{intern} = C_{Nl}^{extern} \tag{23}$$

plays a role of "fitting" condition of "internal" and "external" parts of the wave function. The r.h.s. of this equation has one of the form (19), (21) or (22). Into the left hand side of Eq. (23) the solution of the set (12a) must be substituted. The last one can be found in the following manner [2]. At first we shall diagonalize the truncated Hamiltonian matrix $||H_{nn'}||$ using the unitary transformation Γ, i.e. turn from C_{nl} to the new coefficients

$$C_{\lambda l}' = \sum_{n=0}^{N} \Gamma_{\lambda n} C_{nl} , \quad \lambda = 0, 1, ..., N . \tag{24}$$

As a result of this transformation, equation (12a) takes the form

$$(E_\lambda - \varepsilon) C_{\lambda l}' = -\Gamma_{\lambda N} T_{NN+1} C_{N+1l} , \quad \lambda = 0, 1, ..., N$$

i.e.

$$C'_{\lambda l} = -\frac{\Gamma_{\lambda N} T_{NN+1}}{E_\lambda - \varepsilon} C_{N+1l} \tag{25a}$$

and

$$C_{nl} = -\sum_{\lambda=0}^{N} \frac{\Gamma^*_{\lambda n} \Gamma_{\lambda N}}{E_\lambda - \varepsilon} T_{NN+1} C_{N+1l} \tag{25b}$$

where E_λ - is the eigenvalues of the matrix $||H_{nn'}||$ $(n, n' \leq N)$.

Substituting the "internal" solution (25b) at $n = N$ into Eq. (23) we obtain

$$P_{NN+1} \, C^0_{N+1l} = -C^0_{Nl}, \quad P_{nN+1} = \sum_{\lambda=0}^{N} \frac{\Gamma^*_{\lambda n} \Gamma_{\lambda N}}{E_\lambda - \varepsilon} T_{NN+1} \ . \tag{26}$$

If we deal with bound states of Gamov resonances, C^0_{nl} and C^0_{N+1l} are the known functions of energy (see (21) and (22)). In such cases the condition (26) is the transcendent equation which may be used to find the energies ε_i of the bound or resonant states. For the scattering problem, we get in accordance with (19):

$$C^0_{Nl} = C^{reg}_{Nl} + \tan \delta_l \, C^{irreg}_{Nl} \ ,$$

$$C^0_{N+1l} = C^{reg}_{N+1l} + \tan \delta_l \, C^{irreg}_{N+1l} \ . \tag{27}$$

Substituting these expressions in (26), we find in accordance with Refs. [2]:

$$\tan \delta_l = -\frac{C^{reg}_{Nl} + P_{NN+1} \, C^{reg}_{N+1l}}{C^{irreg}_{Nl} + P_{NN+1} \, C^{irreg}_{N+1l}} \ . \tag{28}$$

It can be seen now that the scattering phase *at an arbitrary energy* ε can be obtained by diagonalizing the Hamiltonian matrix $||H_{nn'}||$ $(n, n' \leq N)$ but *one time*.

In agreement with the Ritz variational principle, the negative eigenvalues $E_\lambda < 0$ of the Hamiltonian matrix $||H_{nn'}||$ $(n, n' \leq N)$ may be treated as approximate values of the energies of discrete levels of a particle in the studied potential. In this case the approximation accuracy improves with increasing the size of the matrix N. The question arises, what is the sense of the matrix positive eigenvalues and of the respective wave functions? The question was answered in works [2, 4, 9] as follows. In the limit $\varepsilon \to E_\lambda$ expression (28) takes on the form

$$\tan \delta_l \, (E_\lambda) = -\frac{C^{reg}_{N+1l}}{C^{irreg}_{N+1l}} \ . \tag{29}$$

By comparing this result with formula (19) we get the coefficient $C^{reg}_{N+1l}(E_\lambda) = 0$ for E_λ. Thus, by diagonalizing the Hamiltonian matrix $||H_{nn'}||$ $(n, n' \leq N)$, we find the solutions for equations (12) in the region of the continuum at such discrete energies $E_\lambda > 0$ which correspond to the vanishing of the HOR$_\iota$ wave function $C_{nl}(E_\lambda)$ at the point $n = N + 1$. The scattering phase can be calculated at such energies using simple formula (29). In the asymptotic limit of high N, the diagonalization of the Hamiltonian matrix on the cutoff basis $n \leq N$ means the solution for the Schroedinger equation (9) with the additional condition $X_l(b) = 0$, where $b = 2(N + \nu)^{1/2}$, i.e. when the system is placed within a rigid box of radius b. In this case the energy spectrum

for equation (9) gets discrete and the energy of any level becomes a function of the position of the boundary point $b = 2[(N + \nu)\hbar/m\omega]^{1/2}$. The condition $X_l(b) = 0$ is nothing other than the equation for the P-matrix poles in the system of radius b described by the Schroedinger equation (9) [10]. Thus the eigenvalues E_λ of the Hamiltonian matrix $\|H_{nn'}\|$ are poles of the discrete analogue of the P-matrix. The important point is a convergency of this approach. The practical calculations [3, 4] show that for rather smooth potentials $V(r)$ it is sufficent to use a number of terms $N \sim 20 - 30$ in the expansion (2) in order to calculate phase shifts and other scattering characteristics in reasonable accuracy.Therefore the using of HOR, or J-matrix approach [2], is a rather effective and practicable method for the study of continuum problems. Some additional example of application of this method will be discussed in section 6.

4   Multichannel case

Let us consider the case of two open (binary, spinless) channel for simplicity. The wave function has the form of a column

$$\psi(r) = \begin{pmatrix} \psi_1(r) \\ \psi_2(r) \end{pmatrix} \tag{30}$$

and the Hamiltonian is the operator matrix of a size 2×2:

$$H = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} . \tag{31}$$

Let us assume that the wave function of the entrance channel $\psi_1(r)$ is characterized by the following asymptotic behaviour

$$\psi_1(r) \sim (e^{-ik_1 r} - S_{11} e^{ik_1 r})/r \tag{32a}$$

while in the second channel only the outgoing wave presents

$$\psi_2(r) \sim - \left((v_1/v_2)^{1/2} S_{21} e^{ik_2 r} \right) /r . \tag{32b}$$

The transition into n-representation consists in the expansion of both channel wave functions

$$\psi_1(r) = \sum_n C_{1n} |n, r_{01} > ,$$

$$\psi_2(r) = \sum_m C_{2m} |m, r_{02} > , \tag{33}$$

in terms of harmonic oscillator wave functions $|n, r_{01} >$, $|m, r_{02} >$ with a unique frequency $\hbar\omega$ while the linear scale parameters $r_{0i} = (\hbar/\mu_i\omega)^{1/2}$ can be different for the channels 1 and 2 if the reduced masses μ_1 and μ_2 of two fragments in these channels are different. Assuming that it is possible to restrict ourselves to a truncated matrix of the potential energy

$$V_{1n,1n'} \ (0 \le n, n' \le N_1), \quad V_{2m,2m'} \ (0 \le m, m' \le N_2),$$

$$V_{1n,2m}, \ V_{2m,1n} \ (0 \le n \le N_1, 0 \le m \le N_2)$$

(generally speaking $N_1 \neq N_2$) we obtain the following set of equations for C_{1n}, C_{2m} coefficients instead of Eqs., (12), (23), (27)

$$(H - E)C = -TC^0 \ ,$$

$$C_{1N_1} = C^0_{1N_1} \ , \quad C_{2N_2} = C^0_{2N_2} \ ,$$

$$C^0_{1n} = C^-_{1n} - S_{11}C^+_{1n} \ , n \geq N_1 \ ,$$

$$C^0_{2m} = -(q_2/q_1)^{1/2}S_{21}C^+_{2m} \ , \quad m \geq N_2 \ . \tag{34}$$

Here C is a column of $N_1 + N_2 + 2$ coefficients $C_{10}C_{11}...C_{1N_1}C_{20}...C_{2N_2}$, H is the matrix of Hamiltonian in a truncated basis $|n, r_{01} >, |m, r_{02} > (n \leq N_1, m \leq N_2)$. The column TC contains only two nonvanishing elements, namely $T_{N_1,N_1+1}C^0_{1N_1+1}$ in the $N_1 + 1$-th row and $T_{N_2N_2+1}C^0_{2N_2+1}$ in the last row. The functions $C^\pm_{ik} = C^{reg}_{ik} \pm iC^{irreg}_{ik}$ are the same ones as in Eq. (21). As it was shown in Ref. [2, 11] the asymptotic of the function $\psi^\pm = \sum_{n=0}^\infty C^\pm_n |n >$ is of the form $k \ exp(\pm ikr)$ for $\to \infty$. This fact and the difference of r_{0i} in various channels are the origin of the factor $(q_2/q_1)^{1/2}$ in Eq. (34) instead of the usual velocities ratio $(v_2/v_1)^{1/2}$ in Eq. (32). Solving the Eq. (34) similarly to Eq. (12) we obtain the following results instead of Eq. (26)

$$C_{1N_1} = C^-_{1N_1} - S_{11}C^+_{1N_1} = P_{11}(C^-_{1N_1+1} - S_{11}C^+_{1N_1+1})+$$

$$+P_{12}\left(-(q_2/q_1)^{1/2}S_{21}C^+_{2N_2+1}\right) \ ,$$

$$C_{2N_2} = -S_{21}C^+_{2N_2}(q_2/q_1)^{1/2} = P_{21}\left(C^-_{1N_1+1} - S_{11}C^+_{1N_1+1}+\right.$$

$$\left.+P_{22}\left(-(q_2/q_1)^{1/2}S_{21}C^+_{2N_2+1}\right)\right) \tag{35}$$

where

$$P_{ij} = \sum_\lambda \frac{\Gamma_{\lambda N_i}\Gamma_{\lambda N_j}}{E_\lambda - E}T_{N_jN_j+1} \ .$$

E_λ is the eigenvalue of the truncated matrix H, $(\Gamma_{\lambda 0}...\Gamma_{\lambda N_1}...\Gamma_{\lambda N_2})$ is the corresponding eigenvector of this matrix.

The relations (35) should be considered as the equations for elements of the S-matrix. The solutions of these equations are of the form

$$S_{11} = \frac{1}{D}\left[(C^-_{1N_1} + P_{11}C^-_{1N_1+1})(C^-_{2N_2} + P_{22}C^-_{2N_2+1}) - P_{21}P_{12}C^-_{1N_1+1}C^-_{2N_2+1}\right]$$

$$S_{21} = \frac{1}{D}\frac{2iP_{12}P_{21}}{\sqrt{\pi q_1 q_2}} \ , \tag{36}$$

$$D = \left[(C^+_{1N_1} + P_{11}C^+_{1N_1+1})(C^+_{2N_2} + P_{22}C^+_{2N_2+1}) - P_{12}P_{21}C^+_{1N_1+1}C^+_{2N_2+1}\right] \ .$$

Here the property of the Casorati determinant

$$T_{NN+1}\begin{vmatrix} C^-_N & C^+_N \\ C^-_{N+1} & C^+_{N+1} \end{vmatrix} = \frac{2i}{\pi q}$$

was used. The elements S_{22}, S_{12} of the S-matrix can be obtained from (36) by substitution of indices 1 and 2. Obviously the S-matrix is symmetrical in accordance with the time reflection

symmetry of the Hamiltonian. As in the previous section, the eigenvalues E_λ are the poles of the discrete analogue of the P-matrix.

The eigenfunctions $\psi_\lambda = \sum_n \Gamma_{\lambda n} |n>$ are discrete analogs of "primitives" (in terms of the paper [10]).

The expressions (36) allow us to find the numerical values of the S-matrix elements and then to calculate the cross-sections of elastic scattering and reactions

$$\sigma_{el} = \frac{\pi}{k_1^2} |S_{11} - 1|^2 , \tag{37}$$

$$\sigma_r = \frac{\pi}{k_1^2} |S_{21}'|^2 , \tag{38}$$

the differential cross-sections, various polarization characteristics (taking into account the spin degree of freedom) etc. If we want to describe the reaction with three-four fragments in the final states it is necessary to extend the above developed formalism, which is valid only for two body (binary) channels, to three, four body collisions.

5 The description of "true" many body scattering in a hyperspherical HOR

We restrict ourselves by the case of the so called "true" many body scattering (TMBS) when the wave function of an A body system is in the asymptotic region of the form

$$\psi_K(\rho, \Omega) = \delta_{K\gamma, K_0\gamma_0} e^{-ik\rho} Y_{K_0\gamma_0}(\Omega) - \sum_{K'\gamma'} S_{K'\gamma', K_0\gamma_0} e^{ik\rho} Y_{K'\gamma'}(\Omega) , \quad \rho \to \infty . \tag{39}$$

$\rho^2 = \sum_{i=1}^A (\mathbf{r}_i - \mathbf{R})^2$ is a global radius in $3(A-1)$ dimensional space, the angles Ω are hyperspherical coordinates in this space. $\mathbf{R}$ is the center-of-mass of the system, $Y_{K\gamma}(\Omega)$ is a hyperspherical harmonic with a global momentum K, γ substitutes all the rest quantum numbers labelling this harmonic. The approximation taking into account only the contribution of TMBS is valid if there is a "democracy" in the A body system i.e. there is no pair of particles with dominating interaction between them in comparison with the rest of the interactions. The TMBS - approximation is applicable to a lot of processes of three, four body decay of light nuclei and hypernuclei [17] (for example disintegration $^{12}C \to 3\alpha$ etc.).

For the description of TMBS we shall use the expansion of the A-body wave function $\psi(\vec{r}_1...\vec{r}_A)$ in terms of A-1 body oscillator wave function (the center of mass variable $\mathbf{R}$ is excluded)

$$|nK\gamma> = R_{nK}(\rho) Y_{K\gamma}(\Omega) \tag{40}$$

depending on hyperspherical coordinates ρ, Ω:

$$\psi = \sum_{nK\gamma} < nK\gamma|\psi > |nK\gamma > . \tag{41}$$

Further consideration is totally parallel to sections 1-4 and we represent the result in very short form. Instead of Eq. (3) we have for the many body case

$$R_{NK}(\rho) = \rho^{-(3A-4)/2} \phi_n^{\mathcal{L}}(\rho) , \tag{42}$$

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$$\phi_n^\mathcal{L}(\rho) = (-1)^n \sqrt{\frac{2n!}{\Gamma(n + \mathcal{L} + \frac{3}{2})}} \rho^{\mathcal{L}+1} e^{-\rho^2/2} L_n^{\mathcal{L}+1/2}(\rho^2) \tag{43}$$

$\mathcal{L} = K + (3A - 6)/2$, ρ is taken in units of r_0. The Eq. (4) takes on the form

$$\sum_{n'K'\gamma'} < nK\gamma|H - E|n'K'\gamma' >< n'K'\gamma'|\psi >= 0 . \tag{44}$$

The kinetic term T in the Hamiltonian $H = T + V$ is diagonal in the quantum numbers K and γ. As for the main quantum number, n, the matrix is three diagonal with respect to n and its matrix elements coincide with Eq. (5) except for substitution of l by $\mathcal{L}$. We also truncate the matrix of potential energy $V = \sum_{i<j}^A V_{ij}$ to $n \leq N$, $K \leq K_{max}$. Then for $n \geq N$ the expansion coefficients $< nK\gamma|\psi >\equiv C_{nl}$ obey the three-term recurrent relation similar to Eq. (12b)

$$\sqrt{n(n + \mathcal{L} + \frac{1}{2})} < n - 1K\gamma|\psi > - \left(2n + \mathcal{L} + \frac{3}{2} - q^2\right) < nK\gamma|\psi > +$$

$$\sqrt{(n + 1)(n + \mathcal{L} + \frac{1}{2})} < n + 1K\gamma|\psi >= 0 , \quad q = \sqrt{2E} . \tag{45}$$

This difference equation has two fundamental solutions

$$C_{n\mathcal{L}}^{reg} = \sqrt{\frac{2n!}{\Gamma(n + \mathcal{L} + \frac{3}{2})}} q^{\mathcal{L}+1} e^{-q^2/2} L_n^{\mathcal{L}+1/2}(q^2) \tag{46}$$

and

$$C_{n\mathcal{L}}^{irreg} = -\frac{2q}{\pi C_{0\mathcal{L}}^{reg}(q)} v.p. \int_0^\infty \frac{C_{0\mathcal{L}}^{reg}(q')C_{n\mathcal{L}}^{reg}(q')}{q^2 - q'^2} dq' \tag{47}$$

or the equivalent pair of solutions

$$C_{n\mathcal{L}}^\pm = -\frac{2q}{\pi C_{0\mathcal{L}}^{reg}(q)} \int_0^\infty \frac{C_{0\mathcal{L}}^{reg}(q')C_{nl}^{reg}(q')}{q^2 - q'^2 \pm i0} dq' . \tag{48}$$

The problem of TMBS is similar to the multichannel problem described in section 4. Thus the wave function (39) with ingoing wave in some channel $K_0\gamma_0$ and outgoing waves in each channels $K'\gamma'$ under consideration takes on the form at $n > N$ (in principle the truncation boundary N may be different in the various channels $K\gamma$):

$$< nK\gamma|\psi >= \delta_{K\gamma,K_0\gamma_0}C_{n\mathcal{L}}^-(q) - \sum_{K'\gamma'} S_{K\gamma,K'\gamma'}C_{n\mathcal{L}'}^+(q) . \tag{49}$$

In analogy with Eq. (36) we can obtain

$$S = A^{-1}B \tag{50}$$

where

$$(A)_{K'\gamma',K\gamma} = P_{K'\gamma',K\gamma}C_{N+1\mathcal{L}}^+(q) - \delta_{K\gamma,K'\gamma'}C_{N\mathcal{L}}^+(q) ,$$

$$(B)_{K'\gamma',K\gamma} = P_{K'\gamma',K\gamma}C_{N+1\mathcal{L}}^-(q) - \delta_{K\gamma,K'\gamma'}C_{N\mathcal{L}}^-(q) , \tag{51}$$

$$P_{K\gamma,K'\gamma'} = \sum_\lambda \frac{< NK\gamma|\lambda >< \lambda|NK'\gamma' >}{E - E_\lambda} T_{NK',N+1K'} \; .$$

E_λ and $< NK\gamma|\lambda >$ are eigenvalues and eigenvector components of the truncated Hamoltónian matrix $< nK\gamma|H|n'K'\gamma' > (n, n' \leq N)$. The poles of the S-matrix (i.e. bound states and Gamov resonance states) can be found from the equation

$$det\ A = 0 \; . \tag{52}$$

Thus we have all expressions that are necessary for the construction of the wave function for few body states belonging to continuum or discrete spectrum in the frame of TMBS approximation.

6 Soft dipole mode in ^{11}Li and three body continuum

In order to demonstrate the effectiveness of the HOR in an analysis of concrete nuclear processes the calculations of the properties of the low energy E1 excitations in the ^{11}Li nucleus were done. The remarkable feature of this nucleus is a presence of a large neutron halo formed by two neutrons weakly bound with the ^{9}Li core. In this connection the following model was used for the description of this nucleus.

6.1 The model

It was assumed that the ^{11}Li ground and continuum states can be interpreted in the framework of the three-body cluster structure ^{9}Li$+n + n$.

1) The cluster ^{9}Li is supposed to be structureless and the excitations of its internal degrees of freedom are not considered.

2) We don't account for non-central components of the interaction between two valence neutrons and between valence neutron and the cluster ^{9}Li. Therefore, the wave function can be characterized by the three-body orbital angular momentum L, spin $S = 3/2$, total angular momentum J and its projection M.

3) The states with the total spin of the valence neutron pair $S = 0$ are only considered, and the ground state three-body orbital angular momentum is supposed to be equal to zero: $L = 0$.

4) n-^{9}Li interaction is described by the shallow potential of Johansen et al [13]. NN-interaction is described by the Gaussian potential [13].

5) Only democratic decay channels are allowed for.

The wave function of the system ^{9}Li$+n + n$, $\psi_{JM}(\mathbf{x}, \mathbf{y})$, is expanded in three-body hyperspherical functions, $\Phi^{l_x l_y J M}(\hat{\Omega})$ (including the internal wave function of ^{9}Li with a spin $S = 3/2$)

$$\psi_{JM}(\mathbf{x}, \mathbf{y}) = \sum_{K l_x l_y} \psi^{(J)}_{K l_x l_y}(\rho)\, \Phi^{l_x l_y J M}_K(\hat{\rho}) \; , \tag{53}$$

where K is hypermomentum, l_x and l_y are the angular momenta corresponding to the Jacobi coordinates

$$\mathbf{x} = \sqrt{\frac{m\omega}{2\hbar}}(\mathbf{r}_1 - \mathbf{r}_2)\,, \qquad \mathbf{y} = \sqrt{\frac{18\,m\omega}{11\ \hbar}}(\frac{\mathbf{r}_1 + \mathbf{r}_2}{2} - \mathbf{r}_3)\,, \tag{54}$$

respectively, m is the neutron mass, $\mathbf{r}_i$ are coordinates of the valence neutrons ($i = 1,2$) and the cluster ^{9}Li ($i = 3$), $\rho = (\mathbf{x}^2 + \mathbf{y}^2)^{1/2}$ is a three-body hyperradius.

In the c. m. frame the Hamiltonian is of the form:

$$H = T + V_{12} + V_{13} + V_{23} \,, \tag{55}$$

where T is the three-body relative motion kinetic energy operator, and V_{ij} are the two-body potentials. For the radial wave functions $\psi^{(J)}_{K\,l_x l_y}(\rho)$ we have the usual set of the K-harmonic method coupled equations (see, e.g., [12]). The equations are solved by expanding the radial wave function.

$$\psi^{(J)}_{K\,l_x l_y}(\rho) = \sum_{n=0}^{\infty} D^{(J)}_{n\,K\,l_x l_y}(E)\ \varphi_{n\,K}(\rho)\,, \tag{56}$$

in the six-dimensional harmonic oscillator eigenfunctions. To calculate the bound state energy, i.e. to locate the corresponding S-matrix pole, one should solve the nonlinear equation [11]

$$\det A^{(+)} = 0 \,, \tag{57}$$

where the matrix A is given by the Eq. (51).

For the continuum spectrum states we calculate S-matrix for any positive energy E using (50)

The interactions of the valence neutrons with each other and with the cluster ^{9}Li are described by the potentials $V_{12}(r_{12})$ and $V_{13}(r_{13}) = V_{23}(r_{23})$, respectively. We use the following parametrization of the potentials [13]:

$$V_{ij}(r) = V^{(1)}_{ij} \exp\left[-(r/b^{(1)}_{ij})^2\right] + V^{(2)}_{ij} \exp\left[-(r/b^{(1)}_{ij})^2\right],$$

$$V^{(1)}_{12} = -31 \text{ MeV}, \qquad V^{(2)}_{12} = 0, \qquad b^{(1)}_{12} = 1.8 \text{ fm};$$

$$V^{(1)}_{13} = -7 \text{ MeV}, \qquad V^{(2)}_{13} = -1 \text{ MeV}, \qquad b^{(1)}_{13} = 2.4 \text{ fm}, \qquad b^{(2)}_{13} = 3.0 \text{ fm}.$$

In the external asymptotic region $n \geq N$ we consequently allow for channels Γ characterized by $K = K_{min}, K_{min} + 2, \ldots$ (K_{min} is the minimal possible value of K for a given J) until the convergence for all physical properties under consideration is achieved. The convergence is found to be very good, and the allowance for the decay channels with $K > K_{min} + 2$ do not yield any visual variation of the results. So, we consider in the external asymptotic region $n > N$ the channels with $K \leq K_{min} + 2$ only. Note, that components with all possible values of $K \leq N$ are accounted for in the calculation of the wave function in the inner region $n \leq N$.

The parameter $\hbar\omega$ is set to be equal to 7.1 MeV in our calculations. This value corresponds approximately to the minimum of ground state energy E_0.

6.2 The ground state

The results for the ^{11}Li ground state for different values of the truncation parameter N are presented in the table 1. The variational ground state energies, $E_0^{(d)}$, obtained by the pure diagonalization of the truncated Hamiltonian matrix are listed in the second column, while the J-matrix results, E_0, which are the solutions of the eq. (57), are listed in the third column. It is seen, that by locating the S-matrix pole using eq. (57) that is equivalent to the allowance for the

Table 1: ^{11}Li ground state properties (see text for details).

Truncation boundary N	Ground state energy, MeV		Neutron halo mean square radius $< r^2 >_{11}^{1/2}$, fm	
	$E_0^{(d)}$	E_0	$< r^2 >_{11}^{1/2\ (d)}$	$< r^2 >_{11}^{1/2}$
12	-0.012	-0.150	2.83	3.31
16	-0.116	-0.199	2.91	3.29
20	-0.171	-0.225	2.98	3.31
24	-0.202	-0.240	3.04	3.32
Experiment	-0.247±0.080		3.16±0.11	

long asymptotic tail of the wave function, we improve essentially the convergence for the binding energy.

The results presented in the table 1 have been obtained using Lanczos smoothing of the three-body potential energy matrix [5, 14].

The ^{11}Li r.m.s. radius, $< r^2 >_{11}^{1/2}$, can be calculated by the following equation:

$$< r^2 >_{11} = \frac{9}{11} < r^2 >_9 + \frac{\hbar}{11\, m\, \omega} < \rho^2 > , \qquad (58)$$

where $< r^2 >_9^{1/2}$ is the ^{9}Li r.m.s. radius and the mean square value of the hyperradius, $< \rho^2 >$, can be easily calculated using the ground state wave function. The values of $< r^2 >^{1/2\ (d)}$ and $< r^2 >^{1/2}$ obtained by the pure diagonalization of the truncated Hamiltonian matrix and with the allowance for the asymptotic tail of the wave function, respectively, are presented in the 4-th and the 5-th columns of the table 1.

It is seen that in calculation of the ground state, the allowance for the wave function asymptotics is very important for a weakly-bound system like ^{11}Li. The terms of expansion (56) with the number of total oscillator quanta $N \simeq 100$ that cannot be obtained in the usual oscillator-basis variational calculations, play an essential role in the description of the transverse momentum distribution, r.m.s. radius, etc. The convergence of $< r^2 >^{1/2}$, transverse momentum distribution and other properties of the wave function in the full J-matrix calculation is rather good. Nevertheless, it is seen that the r.m.s. radius converges to a value that is somewhat larger than the experimental one, and the calculated transverse momentum distribution appeares narrower than the experimental one. These shortcomings can be overcome by the adjustment of n-^{9}Li potential. We have not aimed to fit the potential to the ^{11}Li properties, we have just take its parameters from ref. [13].

6.3 The soft dipole mode

The dipole transition operator in our model is of the form

$$\mathcal{M}(E1\,\mu) = -\frac{N_v Z}{A}\, e\, y\, Y_{1\mu}(\hat{y}) , \qquad (59)$$

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where e is the proton charge, $A = 11$, $Z = 3$ and the number of valence neutrons, $N_v = 2$. The operator (59) corresponds to the excitation of the three-body cluster modes only. The excitation energy of the first excited state of ^{9}Li is relatively high ($\sim$4 MeV). So, low-energy $E1$-transitions correspond to the excitation of the cluster degrees of freedom only and should be described by the operator (59).
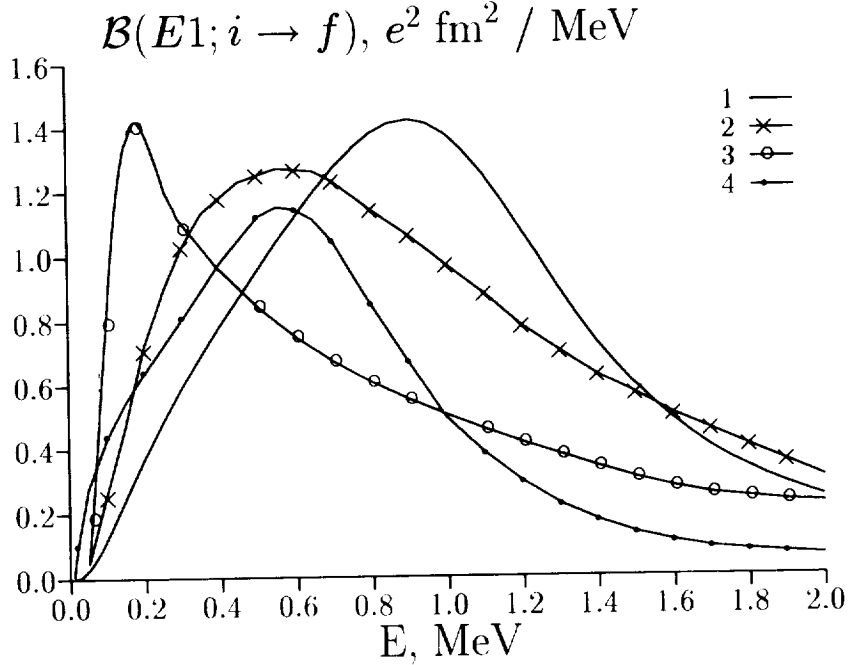

Figure 1: Comparison of our results for $\mathcal{B}(E1; g.s. \rightarrow continuum)$ in ^{11}Li with results of other authors. 1 — this work (J-matrix method), 2 — ref. [15]., 3 — ref. [16], 4 — experimental data parametrization of ref. [17].

The cluster reduced probability of the $E1$-transition, $\mathcal{B}(E1;\ E_f - E_0)$, associated with the operator (59), is displayed on the figure 1.

This figure shows the comparison of the results of our calculations of cluster $\mathcal{B}(E1;\ E_f - E_0)$ with the parametrization of experimental data of ref. [17]. The agreement is reasonable. The form of the $\mathcal{B}(E1;\ E_f - E_0)$ peak is well reproduced, the discrepancy in the position of the $\mathcal{B}(E1;\ E_f - E_0)$ maximum is supposed to be eliminated by the adjustment of the potentials. The results of the $\mathcal{B}(E1;\ E_f - E_0)$ calculations of refs. [15, 16] are also depicted. All these colculations give a low energy peak which can be associated with the soft dipole mode.

The soft dipole mode exhausts about 90% of the cluster sum rule (EWSR) associated with the operator (59). The contribution from the soft dipole mode to the total EWSR is relatively small. In the vicinity of the sharp $\mathcal{B}(E1;\ E_f - E_0)$ maximum at the excitation energy $E \approx$1-2 MeV only $\sim$8% fraction of the total EWSR is exhausted. Nevertheless, the account for the soft dipole mode results in an essential increase of the electromagnetic dissociation cross section of 0.8 GeV/nucleon ^{11}Li beams on Pb and Cu targets. Using the sums of the ^{11}Li and target nucleus charge radii as impact parameter we obtain for the electromagnetic dissociation cross sections the values of 0.966 barn for the Pb target and 0.132 barn for the Cu target; the corresponding experimental values

are 0.890 ± 0.110 barn and 0.21 ± 0.04 barn, respectively [18]. $E0$- and $E2$-transitions give only 1.2% contribution in the cross sections.

Thuse, it is shown, that cluster model ^{9}Li+n+n yields a good description of the ground state properties and $E1$-transitions in the ^{11}Li nucleus. The HOR may be used successfully in the studies of weakly-bound systems with long-tailed wave functions, e.g., in the study of neutron halo properties. For both bound and continuum states the correct account of the wave function asymptotics in the framework of the oscillator representation of scattering theory is very important in such studies. Low-energy $E1$-transitions in ^{11}Li are of the cluster nature. The widths and the position of resonant states calculated in the democratic decay approximation are in a reasonable agreement with experiment.

Appendix. Isolated States. The scattering problem with nonlocal separable potential V^N can display some peculiarities which we explain here using a simple example when the Hamiltonian H is approximated by the matrix of a size 2×2 (i.e. $N = 1$). In specific situation when $T_{01} = -V_{01}$, i.e. the nondiagonal matrix elements of the kinetic and potential energies cancellate each other $H_{01} = 0$, we obtain that the Harmonic oscillator wave function $R_{00}(r)$ is an eigenfunction of this Hamiltonian corresponding to the eigenvalue $E_0 = T_{00} + V_{00}$. If $E_0 > 0$ we find an example of the bound state embedded in continuum [19]. It is clear that the eigenfunction $R_{00}(r)$ is not connected with the rest basis states $R_{n0}(r)$. Thus it is isolated from continuum states and can be called an *isolated states*. The phase shift $\delta_0(k)$ displays a narrow resonance near energy E_0 at small value of h_{01}. It transforms into the resonance of zero width when $H_{01} \to 0$.

Acknowledgments

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GEOMETRICAL INTERPRETATION
FOR THE
$SU(3)$ OUTER MULTIPLICITY LABEL

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Abstract

A geometrical interpretation for the outer multiplicity ρ that occurs in a reduction of the product of two $SU(3)$ representations, $(\lambda_\pi, \mu_\pi) \times (\lambda_\nu, \mu_\nu) \to \sum_\rho (\lambda, \mu)_\rho$, is introduced. This coupling of proton (π) and neutron (ν) representations arises, for example, in both boson and fermion descriptions of heavy deformed nuclei. Attributing a geometry to the coupling raises the possibility of introducing a simple interaction that provides a physically meaningful way for distinguishing multiple occurrences of (λ, μ) values that can arise in such products.

1   Introduction

The objective of our program in nuclear structure physics has been to bridge the gap that exists between collective and shell-model descriptions of observed nuclear phenomena. Progress has been slow because of the difficulty in making realistic shell-model calculations, at least when measured against the background of the success of simpler collective models. Algebraic shell-model theories come closest to realizing this objective. Regarding the latter, there are two basic types of algebraic theories: those based on a boson description of the dynamics, such as the Interacting Boson Model (IBM) [1], and those which treat the nucleons as fermions.

The first and most familiar algebraic fermion model is the Elliott $SU(3)$ scheme. It is known to work well for light ($A \leq 28$) nuclei [2]. Another is the $Sp(3, R)$ (denoted $Sp(6, R)$ sometimes) or symplectic model which is a natural multi-$\hbar\omega$ extension of the Elliott scheme [3]. For heavier systems ($A \geq 150$) there are currently two algebraic models being employed: the so-called Fermion Dynamical Symmetry Model (FDSM) which identifies s and d fermion pair operators that form an algebra which closes under commutation (the $SO(8)$ group for the $n = 4$ shell and $Sp(6)$ for $n = 5$ and $n = 6$, which has $SU(3)$ as a subgroup) and gives a possible microscopic interpretation of the IBM [4], and the pseudo-$SU(3)$ model and its pseudo-symplectic extension which builds on the concept of good pseudo-spin symmetry in heavy nuclei [5, 6, 7].

The common algebraic structure in these theories is the $SU(3)$ group. This is understandable because the angular momentum L and the deformation generating quadrupole operator Q – when restricted to a single major oscillator shell – are generators of $SU(3)$. In particular, large irreducible representations (irreps) of $SU(3)$ correspond to configurations of constant deformation. In

the next section we expand on the $SU(3)$ - rotor connection, and in so doing establish a basis for the geometrical picture of the $SU(3)$ outer multiplicity that is presented in the subsequent section. While no proofs are given, it should be clear from the discussion that the proposed scheme has potentially far reaching consequences regarding a physically motivated interpretation of the outer multiplicity whenever there is an applicable group contraction-expansion procedure, which is $SU(3) \leftrightarrow T_5 \wedge SO(3)$ in the present case. Here $T_5 \wedge SO(3)$ is the symmetry group of the rotor.

2 $SU(3)$ - Rotor Connection

A geometrical interpretation for $SU(3)$ can be achieved by looking at a shell-model interpretation of collective quadrupole motion as depicted in terms of a triaxial quantum rotor. The trick that we apply is to first express the Hamiltonian for the rotor in a frame-independent form because that expression can then be rewritten in terms of its corresponding microscopic operators. The rotor is a particularly elegant example because this prescription is easy to apply and leads immediately to the sought after shell-model representation. Furthermore, the operators that enter into the expression have historical significance, dating back to Racah's pioneering work on the $SU(3) \supset SO(3)$ symmetry group [8]. Since the argument is illustrative it bears repeating, but in an abbreviated form. A more complete description can be found in the book by Casten [9].

The triaxial rotor Hamiltonian is given by

$$H_{ROT} = A_1 I_1^2 + A_2 I_2^2 + A_3 I_3^2 \tag{1}$$

where I_α ($\alpha = 1, 2, 3$) is the projection of the total angular momentum on the α-th body-fixed symmetry axis and A_α is the corresponding inertia parameter: $A_\alpha = 1/(2\mathcal{J}_\alpha)$ where $\mathcal{J}_\alpha$ is the moment of inertia about the α-th principal axis. This familiar principal-axis form can be rewritten in a frame-independent representation by introducing three special scalar operators:

$$L^2 = \sum_\alpha L_\alpha L_\alpha = \sum_\alpha I_\alpha^2,$$

$$X_3^c = \sum_{\alpha,\beta} L_\alpha Q_{\alpha\beta}^c L_\beta = \sum_\alpha \lambda_\alpha I_\alpha^2,$$

$$X_4^c = \sum_{\alpha,\beta,\gamma} L_\alpha Q_{\alpha\beta}^c Q_{\beta\gamma}^c L_\gamma = \sum_\alpha \lambda_\alpha^2 I_\alpha^2. \tag{2}$$

The L_α and $Q_{\alpha\beta}^c$ in this equation are Cartesian forms for the total angular momentum and collective quadrupole operators, respectively. (The superscript c appended to the Q denotes the *collective* quadrupole operator which has non-vanishing matrix elements between major shells ($n' = n$, $n \pm 2$), in contrast with the *algebraic* quadrupole operators, $Q_{\alpha\beta}^a$, which have non-vanishing matrix elements only within a major shell, $n' = n$.) The last expression given for each scalar in eq.(2) is the form these operators take in the body-fixed, principal-axis system where the eigenvalues of the $Q_{\alpha\beta}^c$ are presumed to be sharp: $\langle Q_{\alpha\beta}^c \rangle = \lambda_\alpha \delta_{\alpha,\beta}$. These equations can be inverted to yield the I_α^2 in terms of L^2, X_3^c, and X_4^c:

$$I_\alpha^2 = \left[(\lambda_1 \lambda_2 \lambda_3)L^2 + (\lambda_\alpha^2)X_3^c + (\lambda_\alpha)X_4^c \right]/D_\alpha \text{ where } D_\alpha \equiv 2\lambda_\alpha^3 + \lambda_1 \lambda_2 \lambda_3. \tag{3}$$

Substituting this result for the I_α^2 into eq.(1) yields

$$H_{ROT} = aL^2 + bX_3^c + cX_4^c ; \tag{4}$$

where a, b and c depend on the inertia parameters and the eigenvalues of $Q_{\alpha\beta}^c$:

$$a = \sum_\alpha a_\alpha A_\alpha , \quad b = \sum_\alpha b_\alpha A_\alpha , \quad c = \sum_\alpha c_\alpha A_\alpha , \tag{5}$$

$$a_\alpha = \frac{\lambda_\beta \lambda_\gamma}{2\lambda_\alpha^2 + \lambda_\beta \lambda_\gamma} , \quad b_\alpha = \frac{\lambda_\alpha}{2\lambda_\alpha^2 + \lambda_\beta \lambda_\gamma} , \quad c_\alpha = \frac{1}{2\lambda_\alpha^2 + \lambda_\beta \lambda_\gamma}$$

where $\alpha \neq \beta \neq \gamma \neq \alpha$.

A shell-model image of the rotor Hamiltonian can be obtained by substituting single-particle forms for the collective L_α and $Q_{\alpha\beta}^c$ operators: $L_\alpha = \sum_i l_\alpha(i)$ and $Q_{\alpha\beta}^c = \sum_i q_{\alpha\beta}^c(i)$. However, this ignores the shell structure and the fermion character of the many-body system. It is important to remember that while the L_α have non-vanishing matrix elements only within a major oscillator shell, the $Q_{\alpha\beta}^c$ couple shells differing by two quanta ($n' = n, n \pm 2$). Indeed, the off-diagonal ($n' = n \pm 2$) couplings are about equal in magnitude to the diagonal ($n' = n$) ones. It follows from this that operators like $Q^c \cdot Q^c$ and the X_3^c and X_4^c (even if used only as residual interactions) can destroy the shell structure. This catastrophe can be avoided easily by simply setting all off-diagonal couplings between major shells to zero, an action which corresponds to replacing the $Q_{\alpha\beta}^c$ operators by their algebraic counterparts, $Q_{\alpha\beta}^a$. Elliott was the first person to recognize that the $Q_{\alpha\beta}^a$ operators, along with the L_α, generate $SU(3)$, the symmetry algebra of the isotropic harmonic oscillator Hamiltonian. The appropriate shell-model image of the rotor Hamiltonian, eqs.(1) and (4), is thus given by

$$H_{SU3} = H_0 + aL^2 + bX_3^c + cX_4^c, \tag{6}$$

where H_0 is the harmonic oscillator Hamiltonian.

Shell-model values for the λ_α are required to complete the mapping. This follows by equating invariants of the two theories, a very natural thing to do since constants of the motion relate to the important physics, which in turn should be independent of the particular description. Because $SU(3)$ is a rank two group it has two invariants: C_2 with eigenvalue $[\lambda^2 + \lambda\mu + \mu^2 + 3(\lambda + \mu)]$, and C_3 with eigenvalue $[(\lambda - \mu)(\lambda + 2\mu + 3)(2\lambda + \mu + 3)/2]$, where λ and μ are $SU(3)$ representation labels with $(\lambda + \mu)$ and μ, respectively, specifying the number of boxes in the first and second rows in a standard Young diagram labeling of irreps of the $SU(3)$ group. Note that C_2 is of degree two in the generators of $SU(3)$ while C_3 is of degree three. The symmetry group of the rotor $[T_5 \wedge SO(3)]$ also has two invariants: traces of the square $\{\text{Trace}[(Q_2)^2]\}$ and cube $\{\text{Trace}[(Q_2)^3]\}$ of the collective quadrupole matrix. The eigenvalues of these two invariant operator forms are $\lambda_1^2 + \lambda_2^2 + \lambda_3^2 \to (k\beta)^2$ and $\lambda_1\lambda_2\lambda_3 \to (k\beta)^3 \cos(3\gamma)$, respectively, where (β, γ) are the shape variables of the collective model and $k^2 = \frac{5}{9\pi}(A\bar{r}^2)^2$. The requirement of a linear correspondence between these two sets of invariants leads to the following relations,

$$\lambda_1 = -(\lambda - \mu)/3, \quad \lambda_2 = -(\lambda + 2\mu + 3)/3, \quad \lambda_3 = +(2\lambda + \mu + 3)/3. \tag{7}$$

This correspondence, in turn, sets up a direct relationship between the (β, γ) shape variables of the collective model and the (λ, μ) irrep labels of $SU(3)$,

$$\beta^2 = \frac{4\pi}{5(A\bar{r}^2)^2} \left[\lambda^2 + \lambda\mu + \mu^2 + 3(\lambda + \mu) + 3\right], \quad \gamma = \tan^{-1}\left(\frac{\sqrt{3}(\mu + 1)}{2\lambda + \mu + 3}\right) . \tag{8}$$

Since λ and μ are positive integers, this translates into a regular grid when superimposed on a traditional (β, γ) plot, with β the radius vector and γ the azimuthal angle:

$$k\beta_x = k\beta \cos(\gamma) = \frac{2\lambda + \mu + 3}{3}, \quad k\beta_y = k\beta \sin(\gamma) = \frac{\mu + 1}{\sqrt{3}}. \tag{9}$$

Each (λ, μ)-irrep corresponds to a unique value for the (β, γ)-pair. In the limit of large (λ, μ) values the constant $+3$ factor in λ_2 and λ_3 can be dropped and in so doing one arrives at the asymptotic results [3]. The $+3$ and $+1$ factors in β^2 and γ as well as those in β_x and β_y also disappear in this limit.

3 $SU(3)$ - Outer Mulitiplicity

Having established the $SU(3)$ - rotor connection, it is instructive to push the $(\beta, \gamma) \leftrightarrow (\lambda, \mu)$ connection to a consideration of a coupled double-rotor picture which is commonly used to describe heavy nuclei in a collective model framework, see Figure 1 ahead, with one rotor representing the protons (π) and another the neutrons (ν). This associates physics with the $SU(3)$ coupling picture and, as we will see in greater detail later, it also leads naturally to a geometrical interpretation for the $SU(3)$ outer multiplicity label. This picture also suggests a natural way for parameterizing the proton-neutron interaction in terms of the geometry of this simple scheme, for example, one with final states of the same (λ, μ) but different multiplicity energetically separated from one another due to a simple interaction that senses the relative orientation of the parent proton-neutron configurations. We will return to this matter after making the geometrical picture quantitative for the special case of prolate proton-neutron ($\pi - \nu$) parent configurations.

To get a feeling for the proposed scheme, consider the special case of prolate $\pi - \nu$ factors ($\gamma_\pi = 0$ and $\gamma_\nu = 0$) in the parent configuration. In this case it is sufficient to introduce a single angle θ which measures the relative orientation of the principal axes of the two distributions; rotations about either the proton or neutron symmetry axis effect no change, only rotations about an axis that is perpendicular to the plane defined by the principal axes are distinguishable. (The scissors mode used to describe B(M1) strengths gets its name from this simple picture ... θ measures the angle between the two blades of the scissors. Also note that the Exclusion Principle, which applies because the nucleons are considered to be fermions, is not violated by the coupling because the two distributions are made up of different particle types.) For $\theta = 0^o$ the two axially symmetric ellipsoids overlap maximally (aligned principal axes) whereas when $\theta = 90^o$ the principal axes are perpendicular to one another and the resulting overlap is a minimum.

The (β, γ) value of the product can be determined once β_π, β_ν and θ are specified. Recall that β and γ are determined respectively by the trace of the square and cube of the quadrupole matrix, see eq.(8), and that the quadrupole matrix of the joint distribution is just the sum of the separate proton and neutron distributions, with the second (Q_ν) rotated by an angle θ relative to the first (Q_π): $Q = Q_\pi + RQ_\nu R^{-1}$ where $R = \exp(i\theta \cdot \hat{n})$ and $\hat{n}$ points in the direction of $\hat{n}_\pi \times \hat{n}_\nu$ with $\hat{n}_\pi$ and $\hat{n}_\nu$ defined to be unit vectors that point respectively along the proton and neutron symmetry axes. Or vice-versa, given β_ν, β_π and (β, γ) one can clearly deduce the relative orientation angle θ. This construction corresponds to the $(\lambda_\pi, \mu_\pi = 0) \otimes (\lambda_\nu, \mu_\nu = 0) \rightarrow \sum \oplus (\lambda, \mu)$ coupling in the $SU(3)$ case which is known to be simply reducible, that is, each of the allowed (λ, μ) irreps in the product $[(\lambda, \mu) = (\lambda_\pi + \lambda_\nu, 0), (\lambda_\pi + \lambda_\nu - 2, 1), (\lambda_\pi + \lambda_\nu - 4, 2), \ldots, (\lambda_> - \lambda_<, \lambda_<)$, where

$\lambda_> = \max(\lambda_\pi, \lambda_\nu)$ and $\lambda_< = \min(\lambda_\pi, \lambda_\nu)$], occurs once and only once. Arguing by analogy with the collective model picture, it is relatively easy to see that a discrete orientation angle θ_n can be associated with the $(\lambda_\pi + \lambda_\nu - 2n, n)$ irrep in the product $(\lambda_\pi, \mu_\pi = 0) \otimes (\lambda_\nu, \mu_\nu = 0)$ where n is an integer given by $n = 0$ $(\theta = 0^o \to \|)$, $1, \ldots, \min(\lambda_\pi, \lambda_\nu)$ $(\theta = 90^o \to \bot)$.
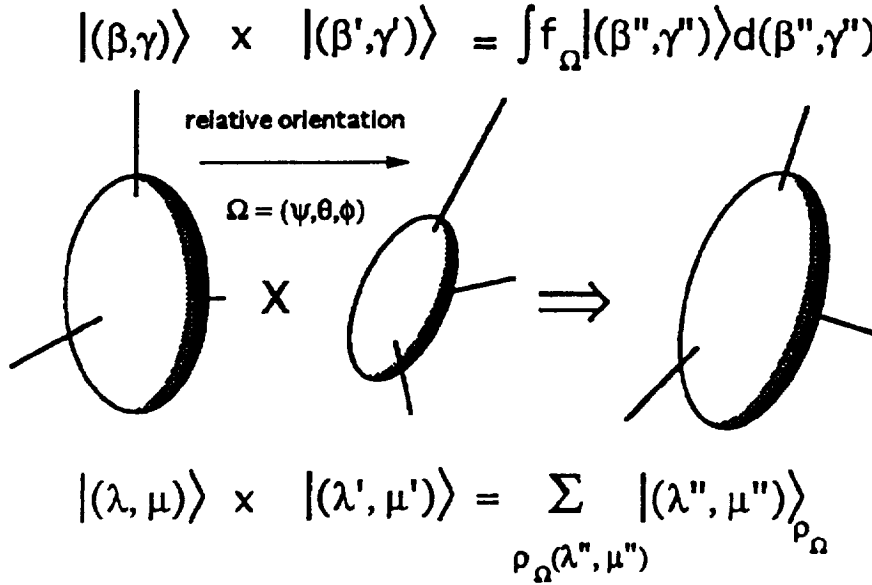

Figure 1: Schematic representation for the expansion of a product of two quadrupole mass distributions in terms of other quadrupole mass distributions. The upper product is for triaxial quantum rotors, which are characterized by the (β, γ) shape variables of the collective model and have a $[T_5 \wedge SO(3)]$ symmetry; the lower coupling is for (λ, μ) irreps of $SU(3)$. The overlap function f_Ω is the inner product $\langle (\beta'', \gamma'') | (\beta, \gamma); (\beta', \gamma') \rangle_\Omega$ where $\Omega = (\psi, \theta, \phi)$ specifies the Euler angles giving the relative orientation of the principal axes of the unprimed $(|(\beta, \gamma)\rangle)$ and primed $(|(\beta', \gamma')\rangle)$ systems. In the $SU(3)$ case, the decomposition is a sum of $SU(3)$ irreps with integer multiplicity ρ which can be determined by the Littlewood rules for coupling Young diagrams. The multiplicity ρ_Ω, like f_Ω, can be related to the number of distinguishable orientations of the two initial distributions that yield the final one.

Finding an expression for θ_n in terms of $(\lambda_\pi, \mu_\pi = 0)$, $(\lambda_\nu, \mu_\nu = 0)$, and the final (λ, μ) illustrates a prescription that can also be applied to the case of general shapes when the μ values of the factors $(\mu_\alpha \neq 0; \alpha = \pi, \nu)$ are non-zero. First of all note that the various (λ, μ) values that enter determine the eigenvalues of the corresponding quadrupole matrix, see eq.(7). It follows from this that an analytic form for θ_n can be derived by requiring that the roots of the characteristic

equations for $Q_\pi + RQ_\nu R^{-1}$ and Q coincide: $|Q_\pi + RQ_\nu R^{-1}| \Leftrightarrow |Q|$. The solution to the set of equations that this condition generates, yields the following general result for θ_n as a function of λ_π and λ_ν:

$$\theta_n = \sin^{-1}([n(\lambda_\pi + \lambda_\nu - n)/(\lambda_\pi \lambda_\nu)]^{1/2}), \tag{10}$$

where the integer index $n = 0, 1, \ldots, \min(\lambda_\pi, \lambda_\nu) = \lambda_<$. Although this expression is symmetric in λ_π and λ_ν and goes respectively to 0^o and 90^o for $n = 0$ and $n = \lambda_<$ as required, it has no other obvious symmetry properties, and in particular, note that the allowed θ values are not distributed symmetrically about the $\theta = 45^o$ plane, a result that is related to the occurrence of the square root in the argument of the inverse sine function.

When one of the two factor distributions is triaxial ($\gamma_\pi \neq 0$ and $\gamma_\nu = 0$ or $\gamma_\pi = 0$ and $\gamma_\nu \neq 0$) the situation is only slightly more complicated. In this case two angles rather than one are required to specify the relative orientation of the two distributions: θ as introduced above to specify the relative orientation of the major axes, and another angle φ that specifies the rotation of the minor axes of the triaxial shape relative to an axis that is perpendicular to the plane defined by the principal axes of the two factor distributions. Only values of θ and φ that lie between 0^o and 90^o lead to distinguishable configurations. In the $SU(3)$ case this construction corresponds to the $(\lambda_\pi, \mu_\pi) \otimes (\lambda_\nu, \mu_\nu) \to \sum \oplus (\lambda, \mu)$ coupling, where $\mu_\pi \neq 0$ and $\mu_\nu = 0$ or $\mu_\pi = 0$ and $\mu_\nu \neq 0$, respectively. While this $SU(3)$ coupling is more complicated than the previous case, it remains simply reducible, that is, each of the allowed (λ, μ) irreps in the product occurs just one time. However, because one of the two μ values is now nonzero, the pattern of allowed final (λ, μ) values is considerably richer than in the previous case: $(\lambda, \mu) = (\lambda_\pi + \lambda_\nu, \mu_>), (\lambda_\pi + \lambda_\nu - 2, \mu_> + 1), \ldots,$ $(\lambda_\pi + \lambda_\nu - 1, \mu_> - 1), (\lambda_\pi + \lambda_\nu - 3, \mu_>), \ldots, (\lambda_\pi + \lambda_\nu - 2, \mu_> - 2), (\lambda_\pi + \lambda_\nu - 4, \mu_> - 1), \ldots,$ where $\mu_> = \max(\mu_\pi, \mu_\nu)$. The general result, $(\lambda_\pi, \mu_\pi) \otimes (\lambda_\nu, \mu_\nu) \to \sum_{m,n} \oplus (\lambda_\pi + \lambda_\nu - 2n - m, \mu_> + n - m)$, requires one additional non-negative integer (m) that specifies the number of completed (three box) columns in the final Young diagram.

In general one must deal with two triaxial shapes ($\gamma_\pi \neq 0$ and $\gamma_\nu \neq 0$) and the corresponding product distribution: $(\beta_\pi, \gamma_\pi) \times (\beta_\nu, \gamma_\nu) \to (\beta, \gamma)$. The geometrical interpretation is considerably more complicated in this case because three Euler angles (φ, θ, ϕ) are required to specify the relative orientation of the factor distributions. For $(\varphi, \theta, \phi) = (0^o, 0^o, 0^o)$ the major and minor axes of the sub-distributions coincide (maximum alignment) whereas if $(\varphi, \theta, \phi) = (0^o, 90^o, 0^o)$ the semi-axes (y) remain aligned but the major (z) and minor (x) axes of the two systems are perpendicular to one another, etc. In the corresponding $SU(3)$ case the allowed product configurations are again determined by the Littlewood Rules but now for the coupling of two two-rowed Young diagrams. There is a need for three $(\varphi, \theta, \phi) \leftrightarrow (m, n, \rho)$ rather than one [prolate shapes: $(\theta) \leftrightarrow (n)$] or two [one prolate and one triaxial shape: $(\theta, \phi) \leftrightarrow (m, n)$] quantum labels in this general case: $(\lambda_\pi, \mu_\pi) \otimes (\lambda_\nu, \mu_\nu) \to (\lambda_\pi + \lambda_\mu + m, \mu_\pi + \mu_\nu + n)_\rho$, where ρ is a non-negative integer index $(\rho = 1, 2, \ldots, \rho_{max})$ labeling distinct occurrences of the same (λ, μ) in the $(\lambda_\pi, \mu_\pi) \otimes (\lambda_\nu, \mu_\nu)$ product. Working backwards, it should also be clear that the $(\beta, \gamma) \leftrightarrow (\lambda, \mu)$ correspondence can be used to give a geometrical interpretation to the abstract group theoretical concept of the outer multiplicity – at least for the $SU(3)$ case – which has up until now escaped a simple physical interpretation. Specifically, the multiplicity ρ, together with m and n, can be considered to be a measure of the relative orientation of the two factor distributions. In this way the first $(\rho = 1)$ occurrence of (λ, μ) corresponds to a parent configuration oriented with one set of angles $(\varphi_1, \theta_1, \phi_1)$ while the second $(\rho = 2)$ solution corresponds to another set $(\varphi_2, \theta_2, \phi_2)$, and so on.

If $\rho_{max} = 1$, the corresponding (λ, μ) distribution can only be realized in one way. With this interpretation in hand the evaluation of reduced matrix elements and especially $SU(3)$ coupling and recoupling coefficients should be revisited, looking for asymptotic solutions that exploit the geometrical concept of overlapping ellipsoidal mass distributions.

It is instructive to view the relationship between the rotor and $SU(3)$ theories at a more fundamental level. This can be achieved by comparing the algebras of their symmetry groups. The symmetry group of the quantum rotor is the semi-direct product $T_5 \wedge SO(3)$ where T_5 is generated by the five independent components of the (spherical) collective quadrupole operator (Q_μ^c) and $SO(3)$ is generated by the angular momentum operators (L_μ). The generators of $SU(3)$, on the other hand, are the Q_μ^a [see the discussion following eq.(1)] and the L_μ operators. If Q^x denotes a generic quadrupole operator, the commutation relations of the L_μ and the Q_μ^x are

$$
\begin{aligned}
[L_\mu, L_\nu] &= -\sqrt{2} < 1\mu, 1\nu | 1, \mu + \nu > L_{\mu+\nu} , \\
[L_\mu, Q_\nu^x] &= -\sqrt{6} < 1\mu, 2\nu | 2, \mu + \nu > Q_{\mu+\nu}^x , \\
\left[Q_\mu^x, Q_\nu^x \right] &= c < 2\mu, 2\nu | 1, \mu + \nu > L_{\mu+\nu} ,
\end{aligned}
\tag{11}
$$

where $c = 0$ for $T_5 \wedge SO(3)$, $(Q^x = Q^c)$, $c = +3\sqrt{10}$ for $SU(3)$ $(Q^x = Q^a)$, and $c = -3\sqrt{10}$ for a heretofore not mentioned group $Sl(3,R)$ $[Q^x = Q^b \sim (x_i p_j + p_j x_i)]$ which is associated with shear degrees of freedom. In eq.(11) the $< -, -|- >$ symbol denotes an ordinary $SO(3)$ Clebsch-Gordan coefficient. [All three of these groups, $T_5 \wedge SO(3)$, $SU(3)$, and $Sl(3, R)$, are subgroups of the symplectic group $Sp(3,R)$.] From these commutation relations it is easy to see how the $SU(3)$ algebra reduces to that of $T_5 \wedge SO(3)$: if Q^a is divided by the square root of the second order invariant of $SU(3)$ $(Q^a \leftarrow Q^a/\sqrt{C_2}$ where by definition the invariant $C_2 = (Q^a \cdot Q^a + 3L^2)/4$ commutes with the Q^a and L_μ operators), the first and second commutators in eq.(11) remain unchanged, while the $L_{\mu+\nu}$ on the right-hand-side of the third goes over into $L_{\mu+\nu}/C_2$ and for low L values in large $SU(3)$ irreps, $L_{\mu+\nu}/C_2 \to 0$. This renormalization of the Q^a operator is a group contraction process and the arguments presented show the $SU(3)$ algebra reduces to the algebra of $T_5 \wedge SO(3)$ in the contraction limit, and consequently, the $SU(3)$ theory reduces to that of the quantum rotor. Differences between observables of the two theories occur because $SU(3)$ is a compact group with finite dimensional irreps while $T_5 \wedge SO(3)$ is non-compact with infinite dimensional representations. Band termination and a fall-off in B(E2) strengths are examples.

4 Conclusion

A geometrical interpretation for the outer multiplicity ρ that occurs in a reduction of the product of two $SU(3)$ representations, $(\lambda_\pi, \mu_\pi) \times (\lambda_\nu, \mu_\nu) \to \sum_\rho (\lambda, \mu)_\rho$, has been introduced. This structure arises, for example, in the coupling of proton (π) and neutron (ν) representations that occur in both boson and fermion descriptions of heavy deformed (rare earth and actinide) nuclei. Attributing a geometry to the proton-neutron coupling, raises the possibility of introducing a simple phenomenological interaction that provides a physically meaningful way for distinguishing among different (λ, μ) and multiple occurrences of the same (λ, μ) values that arise, for example, when coupling deformed proton and neutron configurations in heavy deformed nuclei.

Acknowledgments

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Boson Mapping Techniques applied to Constant Gauge Fields in QCD

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Abstract

Pairs of coordinates and derivatives of the constant gluon modes are mapped to new gluon-pair fields and their derivatives. Applying this mapping to the Hamiltonian of constant gluon fields results for large coupling constants into an effective Hamiltonian which separates into a one describing a scalar field and another one for a field with spin two. The ground state is dominated by pairs of gluons coupled to color and spin zero with slight admixtures of color zero and spin two pairs. As color group we used SU(2).

1   Introduction

In this contribution we report on a possible non- perturbative treatment of Quantum- Chromo-Dynamics (QCD). As the color group we use SU(2). We further restrict to gluons only because due to their larger color charge, compared to quarks and anti- quarks, they will dominate at low energy , e.g., in the vacuum state. As has been indicated by several previous contributions [1, 2] the coupling to color and spin zero pairs are dominating the low energy structure of QCD, at least in perturbative calculations. This leads to assume that pair correlations play an important role in the lowest energy state (the vacuum) and that boson mapping techniques may help to make more transparent the physical structure. Combined with many body techniques of nuclear physics this can represent a possibility to solve non-perturbatively QCD. The method presented in this contribution can, e.g., be applied to the Hamiltonian as proposed in ref. [3]. There the complete Hilbert space in a finite universe (radius of several fm) is mapped to a model space of constants modes only. The non- constant modes are taken perturbatively into account, leading to renormalized interaction constants.

In section 2 we discuss the boson mapping after having introduced the Hamiltonian of constant modes. Furthermore, we give the result of the mapped effective Hamiltonian in the limit of large coupling constant g. Finally in section 3 conclusions are given and future applications are mentioned.

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2 A Boson Mapping of Pair Fields

Confinement properties of QCD are considered to be related to the infrared limit (large wave lengths) of the QCD. Therefore, in order to get a first idea one may just restrict to constant modes of gluons, i.e. the vector fields A_{ia} are approximated by constant fields denoted by c_{ia}. Here i is the space and a the color index, both ranging from 1 to 3 (in SU(2)- color the gluons are in the color T=1 representation). With this the Hamiltonian of gluonic QCD aquires the form[4]

$$\hat{H} = -\frac{1}{2}\sum_{ia}\frac{\partial^2}{\partial C_{ia}\partial C_{ia}} + \frac{1}{4}g^2[(\sum_{la}C_{ia}C_{ia})^2 - \sum_{ij}(\sum_a C_{ia}C_{ja})(\sum_b C_{ib}C_{jb})] \tag{1}$$

where g is the coupling constant. If the non constant modes are included perturbatively higher terms will appear but the general pair structure, pairwise coupling to color zero (contraction over the indices a or b), remains. In equ. (1), having contracted over the color index, only spin zero and two pairs appear and therefore suggests to apply a boson mapping to the paired expressions. One often redefines $C_{ia} \rightarrow g^{-\frac{1}{3}}C_{ia}$ which as a result produces an overall factor $g^{\frac{2}{3}}$ in front of the Hamiltonian.

Normally boson mappings are related to boson creation and annihilation operators. For an excellent review see ref.[5]. One distinguishes between two types of boson mappings: (i) the Dyson (D) and the (ii) Holstein- Primakoff mapping (HP). The first one results into a non- hermitian Hamiltonian and the latter into a hermitian one. Both are equivalent and the problem is well defined but of course the HP gives a more pleasent hermitian structure of the Hamiltonian. Instead of using boson creation and annihilation operators we will use coordinates C_{ia} and derivatives $P^{ia} = \frac{\partial}{\partial C_{ia}}$ (for convnience we will use cartesian components, i.e. $P^{ia} = P_{ia}$). The reason for this is the more simpler and transparent structure of the Hamiltonian which would be very complicate in terms of the creation and annihilation operators. First we will give the Dyson mapping which is completely analog to the one using creation and annihilation operators. Then we go from there to the HP mapping **which will be very different** to the one in terms of creation and annihilation operators!

The boson- pair mapping is given by

$$
\begin{aligned}
(\sum_a C_{ia}C_{ja})_D &= q_{ij} \\
(\sum_a P_{ia}P_{ja})_D &= \frac{1}{2}\sum_{k,k'}(p_{k'i}q_{k'k}p_{kj} + p_{kj}q_{kk'}p_{k'i}) - p_{ij} \\
(\sum_a C_{ia}P_{ja} + \frac{3}{2}\delta_{ij})_D &= \sum_k q_{ik}p_{kj} + \frac{3}{2}\delta_{ij}
\end{aligned}
\tag{2}
$$

with

$$[p_{ij}, q_{nm}] = \delta_{in}\delta_{jm} + \delta_{im}\delta_{jn} \tag{3}$$

In equation (2) the index D refers to "Dyson mapping". As can be seen the pair of derivatives does not preserve their hermitian structure under the D- mapping. Also the operator in the last line, which is introduced in order to obtain a closed algebra and is anti- hermitian in the original

space, does also not preserve the anti- hermitian property in the mapped space. The q_{ij} and p_{ij} are not yet normalized as can be seen from equ. (3).

That the hermitian properties are not preserved has to do with an additional assumption, namely that the volume element is of the simple form $d\mathbf{q}$ ($=\prod_{i \leq j} q_{ij}$). However, if one assumes a more complicate volume element $d\mathbf{q} K^2(\mathbf{q})$ (in the argument of K the notation $\mathbf{q}$ refers to the dependence on all q_{ij}) we can choose then $K(\mathbf{q})$ such that all hermitian properties are conserved. In order to recover the simple volume element we have to redefine all operators of equ. (2) (denoted now collectively by $\hat{O}$) and the wave functions Ψ by

$$
\begin{aligned}
(\hat{O})_{HP} &= K(\mathbf{q})(\hat{O})_D K^{-1}(\mathbf{q}) \\
(\Psi)_{HP} &= K(\mathbf{q})(\psi)_D
\end{aligned}
\tag{4}
$$

where the index HP now refers to the Holstein- Primakoff mapping.

The difference to the HP mapping using creation and annihilation operators becomes obvious when one remembers that in the latter the K is an operator depending on the Casimir operators of the unitary group U(3)[5, 6] (the generators are given in the last line of equ. (2) when C_{ia} is substituted by a creation and P_{ia} by an annihilation operator) while in our proposal the K is a function in the coordinates q_{ij} only. The equivalent in the other case would be a function in pairs of creation operators. Besides this essential difference the HP mapping results always into a non-polynomial function in the operators, except this does not represent a difficulty when we deal with coordinates. Even if the function K is complicate we always can integrate numerically!

In order to determine the function K we require that the anti- hermitian property of ($\sum_a C_{ia} P_{ia} + \frac{3}{2} \delta_{ij}$) is preserved, i.e.

$$
(K(\mathbf{q})(\sum_a C_{ia} P_{ja} + \frac{3}{2} \delta_{ij})_D K^{-1}(\mathbf{q}))^\dagger = -K(\mathbf{q})(\sum_a C_{ia} P_{ja} + \frac{3}{2} \delta_{ij})_D K^{-1}(\mathbf{q})
\tag{5}
$$

which results into the condition

$$
\begin{aligned}
\sum_{ik}(q_{ik} p_{ki} K(\mathbf{q})) &= -\frac{3}{2} K(\mathbf{q}) \\
\sum_k (q_{ik} p_{kj} K(\mathbf{q})) &= 0 \quad , for \quad i \neq j
\end{aligned}
\tag{6}
$$

This implies that $K(\mathbf{q})$ is a spin scalar and K^{-4} a sum of monomials of order 3 (note that $\sum_{ik}(q_{ik} p_{ki} q_{nn}) = 2q_{nn}$).

Because of lack of space we cannot go into details here but merely give a rough description of the results. The detailed analysis is given elsewhere[7]. The $K(\mathbf{q})$ is a function in the pair coordinates q_{ij}. Instead of using decoupled indices we can introduce coordinates of a given spin, i.e. $q_m^{[l]}$ with $l = 0, 2$. The exact dependence is obtained by using a linear combination of all possible monomials of order three with total spin zero. After that we made a change of variables by transforming $q_m^{[2]}$ to an intrinsic system very similar to what is done in the collective model of a nucleus where one transforms from the deformation quadrupole coordinate (which has also angular momentum 2) to a system where the quadrupole operator is diagonal[8]. Also here appear

some kind of "deformation" coordinates β and γ. The physical interpretation is that they describe the deformation (distribution) of the wave function in coordinate space. Also we have transformed the coordinate $q_0^{[0]}$ to $\sqrt{2}q_0^{[0]} = q + \sqrt{2}\beta cos(\gamma + \frac{\pi}{3})$. With this we obtain the final expression of the exact mapping of the Hamiltonian. However, this expression appears complicate at first sight. It gets more transparent when one developes around the minimum values of the potential. One finds that in lowest order the Hamiltonian can be separated in a sum of a pure q and $q_m^{[2]}$ dependent part:

$$
\hat{H}_q \doteq 2\sqrt{\frac{2}{3}}g^{\frac{2}{3}} \left\{ -\frac{d}{dq}q\frac{d}{dq} + \frac{9}{4q} + \frac{1}{2}\sqrt{\frac{3}{2}}q^2 \right\}
$$

$$
\hat{H}_\beta = 2\sqrt{5}g^{\frac{2}{3}} \left\{ -[\frac{d}{dq^{[2]}} \times \frac{d}{dq^{[2]}}]_0^{[0]} + \frac{1}{2\sqrt{5}}\beta^2[4cos^2(\gamma + \frac{\pi}{3}) + \frac{1}{2}] \right\} \qquad (7)
$$

where the square bracket with the cross ($\times$) inbetween means standart angular momentum couling. This result is only a good approximation when the coupling constant is large! Nevertheless we can construct a basis of functions with which we can also diagonalize the general expression. The interesting part of the above result is that we have a Hamiltonian in q which has a minimum in its potential for values of $q \neq 0$! This has as a consequence that the ground state will contain a q-condensate. The Hamiltonian in β is just an anharmonic oscillator, i.e., the ground state will contain small admixtures in the spin two pair. Within a rough approximation, and taking into account the relation of q with $q_0^{[0]}$ and β, γ, we can state that within the model of constant modes in QCD the vacuum state is dominated by a spin and color zero condensate.

3 Conclusions

We have applied a boson mapping technique to the model of constant modes of QCD. Instead of using creation and annihilation operators we used coordinates and derivatives. The non- hermitian Dyson mapping works very similar to the standart boson mapping[5, 6]. However, going from there to the Holstein- Primakoff mapping is quite different! The mapped Hamiltonian of the model of constant modes separates for large coupling constant into a part depending on q (essential the spin and color zero gluon pair) and the other depending on the color zero and spin two gluon pair. The spin zero part shows a minimum in the potential at values different from zero and thus produces a spin and color zero condensate for the vacuum state. The spin two part is an anharmonic oscillator and indicates slight admixtures of those bosons to the vacuum state. For large coupling constant the Hamiltonian separates into a sum of a pure (q, p) and a pure $(q_m^{[2]}, p_m^{[2]})$ depending part.

The model used is of course very simple. Nevertheless, using the more realistic Hamiltonian of ref.[3] the principal qualitative results will not change. This contribution has to be seen as a further step towards the non- perturbative description of QCD. The detailed analysis of the results presented here are given in ref.[7].

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A POSSIBLE GENERALIZATION OF THE HARMONIC OSCILLATOR POTENTIAL

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Abstract

A four-parameter potential is analyzed, which contains the three-dimensional harmonic oscillator as a special case. This potential is exactly solvable and retains several characteristics of the harmonic oscillator, and also of the Coulomb problem. The possibility of similar generalizations of other potentials is also pointed out.

1 Introduction

Searching for exact solutions of the Schrödinger equation has been an interesting challenge since the early period of quantum mechanics. This classic area has gained new momentum from the recent introduction of supersymmetric quantum mechanics (SUSYQM) [1], which relates pairs of essentially isospectral potentials to each other by means of (super)algebraic manipulations. (See, for example [2] for a recent review on SUSYQM, and [3] and references for its relation to other methods of analyzing isospectral potentials.) This new approach helped to view old problems from a new angle, and allowed unified, systematic treatment of previously unrelated results. New solutions of the Schrödinger equation have been described and classified, together with already known ones. The most well-known potentials have been shown to have the property of shape invariance [4], a concept introduced in SUSYQM. Much less is known, however, about the more general Natanzon potentials [5], which are, in principle, solvable, nevertheless their practical use is hindered by their complicated mathematical structure. The techniques inspired by SUSYQM allow a straightforward generalization of the simplest shape-invariant potentials, while avoiding most of the mathematical complications characterizing the general Natanzon potentials.

Here I discuss a potential which can be considered the simultaneous generalization of the three-dimensional harmonic oscillator and Coulomb potentials: these two shape-invariant potentials can be obtained from it by tuning one of its four parameters. Its Coulomb limit has already been described [6], and here I discuss its connection with the harmonic oscillator. In contrast with other anharmonic oscillators, this potential converges to a finite value in the $r \to \infty$ limit. It also inherited several characteristics from its two "parent potentials", which may enable its applications to physical problems, where deviations from these two fundamental potentials are relevant.

In Section 2. I give a brief account of a simple procedure which can be used to derive exactly solvable potentials. Section 3. contains the main results of this contribution, while in Section 4. a summary is given and directions towards futher investigations are pointed out.

2 Transformations of the Schrödinger Equation

Here I describe an old method of solving the Schrödinger equation to demonstrate how a wide range of solvable potentials can be derived in a relatively straightforward way. Originally this procedure was used [7] to derive only some well–known potentials, but it can be shown that the general Natanzon potentials can also be derived from it. This procedure was also connected to the formalism of SUSYQM [8].

The solutions of the one–dimensional Schrödinger equation (with $\hbar = 2m = 1$)

$$\frac{d^2\Psi}{dx^2} + (E - V(x))\Psi(x) = 0 \qquad (1)$$

are generally written as

$$\Psi(x) = f(x)F(g(x)), \qquad (2)$$

where $F(g)$ is a special function which satisfies a second–order differential equation

$$\frac{d^2F}{dg^2} + Q(g)\frac{dF}{dg} + R(g)F(g) = 0. \qquad (3)$$

Here $Q(g)$ and $R(g)$ are well–known for any specified special function $F(g)$, while $f(x)$ and $g(x)$ are some functions to be determined. Substituting (2) in (1) and comparing the results with (3) we arrive at the following expression [8] after some straightforward algebra:

$$E - V(x) = \frac{g'''(x)}{2g'(x)} - \frac{3}{4}\left(\frac{g''(x)}{g'(x)}\right)^2 + (g'(x))^2 \left(R(g(x)) - \frac{1}{2}\frac{dQ(g)}{dg} - \frac{1}{4}Q^2(g(x))\right). \qquad (4)$$

Eq. (4) relates the only undetermined function $g(x)$ to the difference of the energy E and the potential $V(x)$. Observing that the energy term E on the left–handside of Eq. (4) represents a constant, the authors of Ref. [7] equated certain terms of the right–handside with a constant to account for it. This results simple differential equations for $g(x)$. The authors in Ref. [7] applied this method to the hypergeometric and confluent hypergeometric function and obtained the solutions of some simple potentials.

Considering the particular example of the confluent hypergeometric function $F(-n, \beta; g(x))$ and introducing the simple $g(x) = \rho h(x)$ substitution we get

$$\begin{aligned} E_n - V(x) &= \frac{h'''(x)}{2h'(x)} - \frac{3}{4}\left(\frac{h''(x)}{h'(x)}\right)^2 \\ &+ \frac{(h'(x))^2}{h(x)}\rho\left(n + \frac{\beta}{2}\right) - (h'(x))^2\frac{\rho^2}{4} + \frac{(h'(x))^2}{(h(x))^2}\frac{\beta}{2}\left(1 - \frac{\beta}{2}\right). \end{aligned} \qquad (5)$$

Identifying one of the last three terms on the right–hand side of Eq. (5) with a constant, the three shape–invariant potentials of the confluent hypergeometric case, the three–dimensional harmonic oscillator, the Coulomb problem and the Morse potential, are recovered. These potentials appear in the radial Schrödinger equation, therefore in what follows I shall replace x with r.

3   Generalization of the Harmonic Oscillator Potential

A straightforward way of generalizing the simplest possible solvable potentials to more general ones is identifying combinations of several terms on the right-hand side of (5) with a constant. This procedure recovers the Natanzon confluent potentials [5], the solutions of which contain confluent hypergeometric functions. The most general six–parameter version of these potentials can be obtained by considering the combination of all three terms on the right–hand side of (5), which explicitly contain parameters, however, the technical difficulties increase considerably in this case. The problem remains relatively easy to handle if we take the combination of two such terms only. Considering the differential equation

$$(h'(x))^2 \left(1 + \frac{\theta}{h(x)}\right) = C \tag{6}$$

corresponds to "mixing" the harmonic oscillator and the Coulomb potentials: $\theta \to 0$ recovers the latter one [6], while $\theta \to \infty$ combined with $C = \tilde{C}\theta$ yields the former one. (See Eq. (5)). The Coulomb limit has been discussed in detail in Ref. [6], and here we focus on the harmonic oscillator limit. The potential described here and in Ref. [6] is essentially the same for any finite value of θ, nevertheless, it is more convenient to use different notations when we discuss its connection to the two limiting case. In order to make the formalism of the two limits compatible with each other, here we follow the notations of Ref. [6] as closely as possible.

As described in [6], the differential equation (6) can be solved explicitly for the inverse $r(h)$ function only:

$$r = \tilde{C}^{-1/2} \left(\theta^{1/2} \tanh^{-1}\left(\left(\frac{h}{h+\theta}\right)^{1/2}\right) + \left(h\left(1 + \frac{h}{\theta}\right)\right)^{1/2}\right). \tag{7}$$

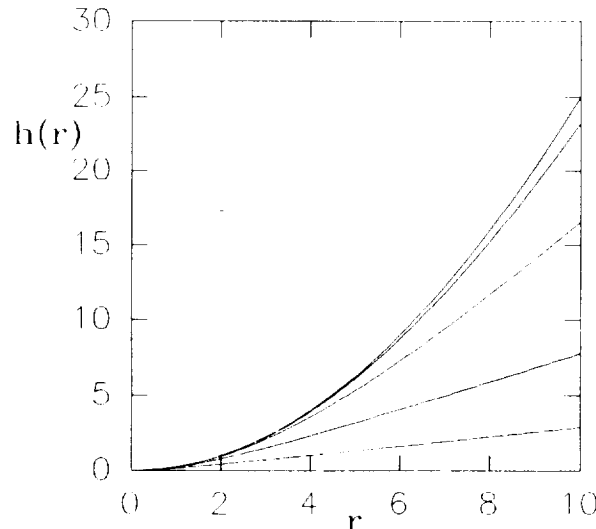This function, of course, can be used to determine $h(r)$ as well to any desired accuracy.

FIG. 1. The $h(r)$ function defined by Eq. (7), displayed for $\theta = 0.1, 1, 10, 100, \infty$ and $\tilde{C} = 1$. (Curves lying higher correspond to higher value of θ.)

We have plotted $h(r)$ in Fig. 1. for several values of the parameter θ. As discussed in Ref. [6], $h(r)$ can be approximated by $\tilde{C}r^2/4$ near the origin, and asymptotically follows $h(r) \to (\tilde{C}\theta)^{1/2}r$ in the $r \to \infty$ limit, which correspond to the $h(r)$ functions characterizing the harmonic oscillator and Coulomb problems, respectively. (See e.g. Ref. [8].) The range of the transition between these two regions is governed by the θ parameter: it moves towards larger values of r as θ increases (see Fig. 1.), and disappears completely in the $\theta \to \infty$ (harmonic oscillator) limit.

Substituting $h(r)$ into (5) and removing the n-dependence from the potential terms by introducing the constant

$$\widetilde{D} = \frac{\rho^2}{4} + \frac{\rho}{\theta}\left(n + \frac{\beta}{2}\right) \tag{8}$$

(which amounts to a specific choice of $\rho \equiv \rho_n$,) we arrive at the following potential

$$V(r) = \tilde{C}\widetilde{D}\frac{h(r)}{1 + \frac{h(r)}{\theta}} + \left(\beta - \frac{3}{2}\right)\left(\beta - \frac{1}{2}\right)\frac{\tilde{C}}{4h(r)\left(1 + \frac{h(r)}{\theta}\right)} - \frac{3\tilde{C}}{16\theta\left(1 + \frac{h(r)}{\theta}\right)^2} + \frac{5\tilde{C}}{16\theta\left(1 + \frac{h(r)}{\theta}\right)^3} \tag{9}$$

and energy eigenvalues

$$E_n = \tilde{C}(2n + \beta)\left(\left(\frac{1}{\theta^2}\left(n + \frac{\beta}{2}\right)^2 + \widetilde{D}\right)^{1/2} - \frac{1}{\theta}\left(n + \frac{\beta}{2}\right)\right). \tag{10}$$

These formulas differ from the corresponding ones in Ref. [6] only in a shift of the energy scale and in the usage of slightly different parameters. The changes reflect the difference between the Coulomb and harmonic oscillator limits of the general problem containing both potentials as a special case. These differences, however, do not essentially influence the form of the wavefunctions:

$$\Psi_n(r) = \frac{\tilde{C}^{1/4}\rho_n^{\frac{\beta+1}{2}}}{\Gamma(\beta)}\left(\frac{\Gamma(n+\beta)}{n!((\beta + 2n)\theta^{-1} + \rho_n)}\right)^{1/2}$$
$$\times(1 + h(r)/\theta)^{1/4}(h(r))^{\frac{2\beta-1}{4}}\exp\left(-\frac{\rho_n}{2}h(r)\right)F(-n, \beta; \rho_n h(r)). \tag{11}$$

(Here and in Eq. (10) n denotes the number of nodes in the radial wavefunction.)

As we can expect from (6), these formulas reduce to the corresponding ones for the harmonic oscillator in the $\theta \to \infty$ limit, if we introduce the notation $\omega = \tilde{C}\widetilde{D}^{1/2}$ and $l = \beta - 3/2$. In particular, the two last terms in (9) vanish and the first and second terms transform into the harmonic oscillator and centrifugal terms, respectively. We have displayed $V(r)$ and the position of some of the lowest-lying energy eigenvalues in Fig. 2. for some values of parameter θ. As it can be seen there, the oscillator character of the potential strenghtens with increasing θ. $V(r)$ is oscillator-like near the origin, and approximates the Coulomb potential (with $Ze^2 = \tilde{C}^{1/2}\widetilde{D}\theta^{3/2}$) for large r. The domain of oscillator-like behavior expands with increasing θ: this is related to the structure of $h(r)$ discussed previously. (See also Fig. 1.) Also, the energy spectrum is oscillator-like for small values of n, and Coulomb-like for large n: E_n converges to $E_{n\to\infty} = V(r \to \infty) = \tilde{C}\widetilde{D}\theta$. See Ref. [6] for a more detailed description of $V(r)$ in terms of powers of r.
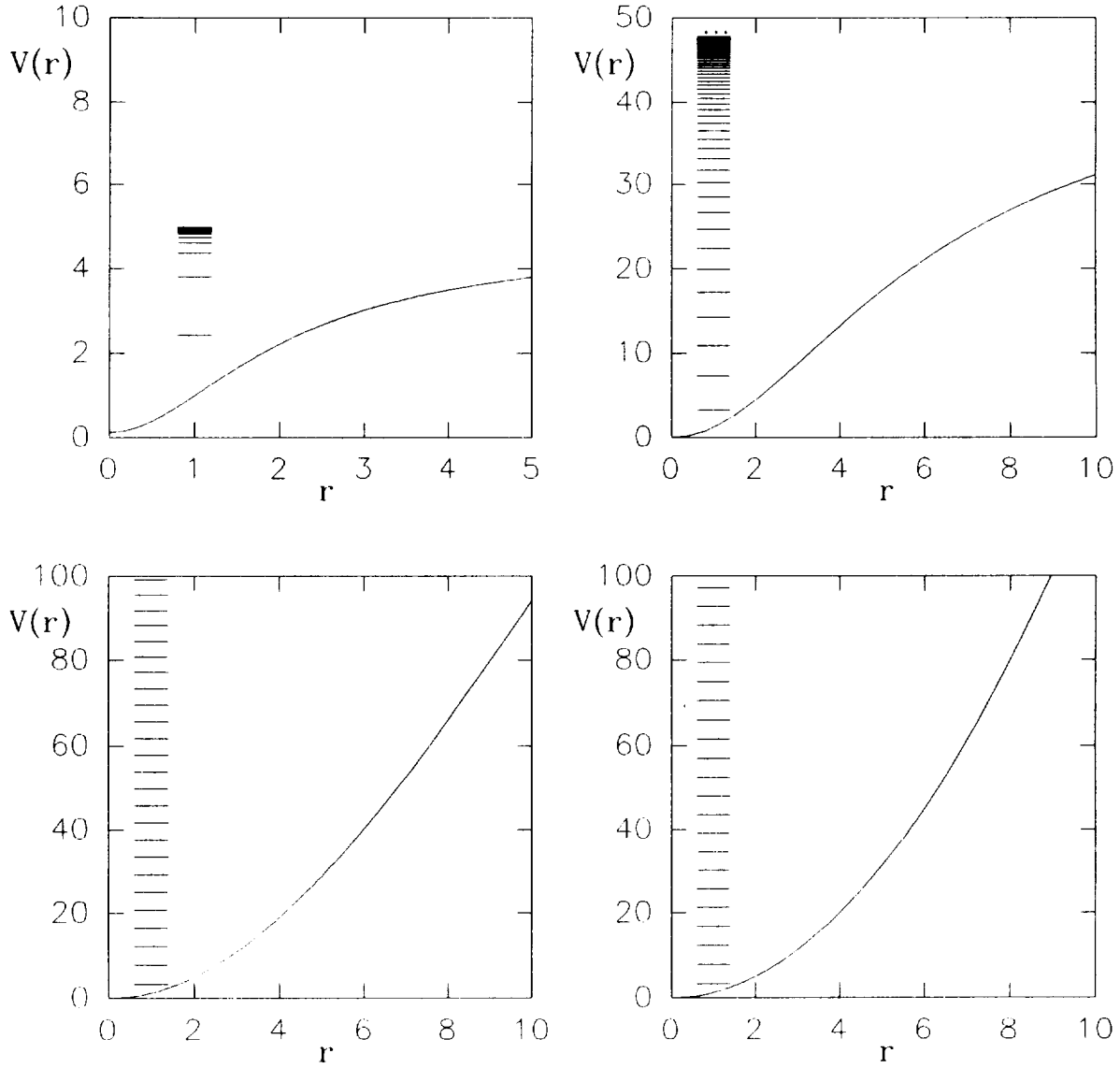
FIG. 2. Potential $V(r)$ in Eq. (9) displayed together with the lowest–lying energy levels for $\theta = 1$, 10, 100 and ∞. The other parameters are $\widetilde{C} = 1$, $\widetilde{D} = 5$ and $\beta = 1.5$ in all cases. $V(r \to \infty) = \widetilde{C}\widetilde{D}\theta$ in each case.

Similarly to the Coulomb limit discussed in [6], this potential can be rewritten into the sum of a central, centrifugal and l–dependent part:

$$V(r) = V_0(r) + V_l(r) + \frac{l(l+1)}{r^2}, \tag{12}$$

where

$$V_0(r) = \tilde{C}\tilde{D}\frac{h(r)}{1 + h(r)/\theta} - \frac{3\tilde{C}}{16\theta(1 + h(r)/\theta)^2} + \frac{5\tilde{C}}{16\theta(1 + h(r)/\theta)^3},$$ (13)

and

$$V_l(r) = \frac{l(l + 1)}{r^2}\left(\frac{\tilde{C}r^2}{4h(r)(1 + h(r)/\theta)} - 1\right) \equiv \frac{l(l + 1)}{r^2}v(r).$$ (14)

The definition of l is, however, different in the two limits: $l = \beta/2 - 1$ for the Coulomb [6], and $l = \beta - 3/2$ for the oscillator limit. (Fig. 2. displays potentials with $l = 0$ only.) Also in contrast with the Coulomb limit, $v(r)$ in Eq. (14) does not vanish for large values of r, rather it goes to the value $-3/4$. This, again, is the consequence of the asymptotical Coulomb–like character of $V(r)$.

It is remarkable, that E_n depends on the combination $2n + \beta$ only (i.e. on $2n + l + 3/2$ in the oscillator limit), therefore the generalized harmonic oscillator potential has a degeneracy pattern similar to that of the harmonic oscillator. In other words, the terms representing the anharmonicity do not remove the degeneracy of the energy levels.

This generalization of the harmonic oscillator potential could be applied to physical problems, where an attractive Coulomb potential is distorted by an oscillator–like potential component for small values of r. This is the case, for example, for a finite, homogenous, spherical charge distribution, but in that case the resulting potential can strictly be separated into two domains, where it *exactly* follows r^2-like and r^{-1}-like behavour. The potential discussed here can be considered a deviation from this simple model problem. An example for a similar situation is discussed in Ref. [9] in connection with a potential experienced by electrons in certain crystal environments.

Finally, there are some other potentials occupying a similar intermediate position between the simple shape–invariant potentials and the general Natanzon potentials. Some of these, like the Woods–Saxon [10] and Ginocchio [11] potentials have been found earlier, while some others, the "PIII" [12] potential and those in Refs. [13,14,15] have been identified only recently, mainly in SUSYQM–related studies. See Ref. [6] for more details.

4 Summary

Here I have analyzed a four–parameter potential, which contains both the harmonic oscillator and the Coulomb potential as special cases. I have interpreted this potential as the generalization of the harmonic oscillator potential, and have established that it is a special admixture of a long–range attractive Coulomb term, and an oscillator–like term near the origin. This is also reflected in the structure of the energy spectrum.

Exact analytical solution of the radial Schrödinger equation can be obtained for any partial wave, however, an angular–momentum–dependent term appears for $l \neq 0$. A remarkable finding is that the anharmonicity appearing in the general form of the potential does not remove the degeneracy of the energy levels.

Similar generalizations of the harmonic oscillator and other well–known potentials are also possible by considering further simple differential equations similar to that in Eq. (6). These subclasses of the Natanzon potentials seem to be suitable for applications, because they have

more flexible shape than the simplest solvable potentials, but may still remain relatively simple to handle mathematically.

Acknowledgments

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AN ALGEBRAIC CLUSTER MODEL BASED ON THE HARMONIC OSCILLATOR BASIS

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Abstract

We discuss the semimicroscopic algebraic cluster model introduced recently, in which the internal structure of the nuclear clusters is described by the harmonic oscillator shell model, while their relative motion is accounted for by the Vibron model. The algebraic formulation of the model makes extensive use of techniques associated with harmonic oscillators and their symmetry group, $SU(3)$. The model is applied to some cluster systems and is found to reproduce important characteristics of nuclei in the sd-shell region. An approximate $SU(3)$ dynamical symmetry is also found to hold for the $^{12}C + {}^{12}C$ system.

1 Introduction

The harmonic oscillator and the $SU(3)$ group have proven to be invaluable tools of nuclear physics. (See, e.g. Ref. [1].) These concepts can be used to describe complex physical systems in a relatively straightforward way by utilizing the advantages of the group theoretical description. The harmonic oscillator picture has been found to be a suitable approach to various nuclear excitations, which sometimes could also be related to each other in terms of it.

Clustering can be considered a special collective excitation of certain nuclei. The structure of these (mainly light) nuclei can be interpreted in terms of a picture based on the relative motion of two (or more) nuclear clusters. In order to describe these nuclear systems cluster models have to take into account the relative motion, as well as the internal structure of the clusters. These models generally differ in their basic model assumptions, mathematical formulation and, consequently, also in the range of their applicability. Microscopic cluster models apply effective two-nucleon forces and rigorously take into account the effect of the Pauli principle by using antisymmetrized wavefunctions. However, fully microscopic calculations may turn out to be prohibitively difficult for a large number of realistic cluster systems. Phenomenologic cluster models, which are based on less strict model assumptions may have a wider range of applicability, and are generally used to describe a large amount of experimental data in a systematic way. Semimicroscopic cluster models utilize the advantageous sides of microscopic and phenomenologic models by combining the microscopic (antisymmetrized) basis with phenomenologic cluster-cluster interactions. This allows calculations in a wider range of nuclei without forgetting about the fermionic nature of the nucleons, i.e. without abandoning the Pauli principle.

From the technical point of view, most of the cluster models apply the geometric description, i.e. they use (nucleon-nucleon or cluster-cluster) potentials and work in the geometric space, while

some others prefer the algebraic description in terms of creation and annihilation operators and the second quantized formalism. Harmonic oscillators appear in a natural way in both approaches and offer a convenient way of interrelating them.

Recently we have intoduced a semimicroscopic algebraic cluster model [2,3] which makes extensive use of the harmonic oscillator picture in describing the relative motion as well as the internal structure of the clusters. In the first applications of the model we tested its ability of reproducing certain features of realistic cluster systems and tried to estimate the validity of the harmonic oscillator picture it is based on.

2   The Semimicroscopic Algebraic Cluster Model

Our earlier attempts of describing various nuclear cluster systems in terms of a pheonomenologic cluster model, the Vibron model [4] and its extensions have revealed [5,6] that these models can not distinguish between Pauli–forbidden and allowed states: complete forbidden shells can be excluded by a simple rule, the Wildermuth condition, but no such distinction can be made within allowed shells. These studies, however, have also pointed out the importance of the $SU(3)$ group as a possible of tool combining the relative motion and the internal structure of the clusters. This group appears in a special limit of the Vibron model accounting for the relative motion sector, and it can also be used to describe the internal excitations of the individual clusters. These preliminaries have paved the way to the introduction of the semimicroscopic algebraic cluster model [2,3].

In this model the internal structure of a cluster is described in terms of the $SU(3)$ (harmonic oscillator) shell model [7], therefore its wavefunction is characterized by the $U_C^{ST}(4) \otimes U_C(3)$ symmetry, where C refers to cluster, and $U^{ST}(4)$ is Wigner's spin-isospin group [8]. The relative motion of the clusters is accounted for by the vibron model with $U_R(4)$ group structure [4]. The representation labels of the group chain

$$U_{C_1}^{ST}(4) \otimes U_{C_1}(3) \otimes U_{C_2}^{ST}(4) \otimes U_{C_2}(3) \otimes U_R(4)$$
$$\supset U_C^{ST}(4) \otimes U_C(3) \otimes U_R(3) \supset U_C^S(2) \otimes U(3)$$
$$\supset U_C^S(2) \otimes O(3) \supset U(2) \supset O(2) \tag{1}$$

provide us with the quantum numbers for the basis states of a two-cluster system. From this set we have to skip those states, which are Pauli forbidden, or which correspond to spurious excitations of the center of mass. A simple recipe for eliminating these states is applying a matching requirement between the quantum numbers of the shell model basis of the whole nucleus and its cluster model basis [2,3]. This recipe is based on the connection between the harmonic oscillator shell model and harmonic oscillator cluster model [10]. This procedure corresponds to a special truncation of the extensive shell model basis in the sense, that only those states survive, which are Pauli–allowed, and are relevant to the cluster structure under study.

When the internal structure of each cluster is described by a single $U_C^{ST}(4) \otimes U_C(3)$ representation, then the physical operators of the system can be obtained in terms of the generators of the $U_{C_1}^{ST}(4) \otimes U_{C_1}(3) \otimes U_{C_2}^{ST}(4) \otimes U_{C_2}(3) \otimes U_R(4)$ group. In such a case the description is algebraically closed, i.e. the matrix elements can be deduced by means of group theoretical techniques. In the

limiting case when the Hamiltonian is given by the invariant operators of (1), then the eigenvalue problem has an analytical solution, and a $U(3)$ dynamical symmetry is said to hold.

The problem can be simplified further if one or both of the clusters are even–even nuclei (i.e. they consist of even number of protons and neutrons). In this case the clusters are said to be $U_C^{ST}(4)$ scalars, furthermore, if the clusters are closed shell nuclei, then they are also $U_C(3)$ scalars. In this case these groups and the quantum numbers associated with them do not appear explicitly in the formulas. In Ref. [3] the formalism is presented in detail for the $U_C(3) \otimes U_R(4)$ and $U_{C_1}(3) \otimes U_{C_2}(3) \otimes U_R(4)$ models, as well as for the restricted $U_C^{ST}(4) \otimes U_C(3) \otimes U_R(4)$ model. In this latter case the restriction implies that only spin and isospin free interactions and a single $U_C^{ST}(4)$ representation are considered. If both of the clusters are $U_C^{ST}(4)$ and $U_C(3)$ scalars, the model reduces to that of the simple vibron model with a basis truncation corresponding to the Wildermuth condition [5].

Here we give a brief account of the $U_C(3) \otimes U_R(4)$ model, which is able to describe two-cluster systems in which one of the clusters is a closed-shell nucleus (e.g. ^4He, ^{16}O, or ^{40}Ca), while the other one is an even–even nucleus. In this simple case the basis states can be labeled without explicit reference to the $U^{ST}(4)$ group, (unless some higher excitations of the non–closed-shell nucleus are also considered), and the cluster model basis states are characterized by the representation labels of the group chain:

$$U_C(3) \otimes U_R(4) \supset U_C(3) \otimes U_R(3) \supset SU_C(3) \otimes SU_R(3) \supset SU(3) \supset O(3) \supset O(2)$$
$$|[n_1^C, n_2^C, n_3^C], [N, 0, 0, 0], \quad [n_\pi, 0, 0,], \ (\lambda_C, \mu_C) \ , \ (n_\pi, 0) \ , \ (\lambda, \mu), K_L, L \quad , \ M \ ).$$

(2)

The irreducible representations (λ, μ) of $SU(3)$ are obtained by taking the outer product of $(\lambda_C, \mu_C) \otimes (n_\pi, 0)$. N stands for the maximal number of the excitation quanta assigned to the relative motion, and it determines the size of the model space. The angular momentum content of a (λ, μ) representation is given by the usual relations of the Elliott model [7]. For technical reasons, however, it is more convenient to use the orthonormal $SU(3)$ basis of Draayer and Akiyama [11], rather than the Elliott basis, which is not orthogonal. The parity of the basis states is determined by the parity assigned to the relative motion: $P_R = (-1)^{n_\pi}$. (The internal states of the non–$U(3)$–scalar cluster carry positive parity $P_C = (-1)^{n_1^C + n_2^C + n_3^C}$, unless major shell excitations of the clusters are also considered.)

The coupled wavefunction can be expressed in terms of $SU(3) \supset O(3)$ Wigner coefficients:

$$|(\lambda_C, \mu_C), N(n_\pi, 0); (\lambda, \mu)\chi LM\rangle$$
$$= \sum_{\chi_C L_C M_C} \sum_{L_R M_R} \langle (\lambda_C, \mu_C)\chi_C L_C M_C; N(n_\pi, 0)L_R M_R|(\lambda, \mu)\chi LM \rangle$$
$$\times |(\lambda_C, \mu_C)\chi_C L_C M_C\rangle |N(n_\pi, 0)L_R M_R\rangle.$$

(3)

The physical operators can be constructed from the generators of the groups present in group chain (2). In particular, the most general form of the Hamiltonian can be obtained in terms of a series expansion of these generators. In the simplest case, however, when we use the $SU(3)$ dynamical symmetry approximation, and consider only one $U_C(3)$ representation to describe the structure of the non–closed-shell even–even cluster, the energy eigenvalues can be obtained in a closed form:

$$E = \epsilon + \gamma n_\pi + \delta n_\pi^2 + \eta C_2(\lambda, \mu) + \beta L(L + 1).$$

(4)

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In this approximation the energy levels can easily be assigned to rotational bands labeled by the quantum numbers $n_\pi(\lambda,\mu)\chi$. (See Eqs. (3) and (4).) Bands following an approximate rotational pattern usually appear in the energy spectrum of nuclear cluster systems.

The electromagnetic transition operators are also constructed from the group generators, which automatically implies selection rules in the dynamical symmetry approximation. The electric quadrupole transition operator, for example, is written as the sum of the rank-2 generators of the $U_C(3)$ and the $U_R(3)$ groups:

$$T^{(E2)} = q_R Q_R^{(2)} + q_C Q_C^{(2)}. \tag{5}$$

The matrix elements of the operators with the basis states (3) are calculated using tensor algebraic techniques [12].

The formulation of the $U_{C_1}(3) \otimes U_{C_2}(3) \otimes U_R(4)$ and $U_C^{ST}(4) \otimes U_C(3) \otimes U_R(4)$ models can be done via a straightforward generalization of the results presented here. These models can also be used away from the $SU(3)$ dynamical symmetry limit: in this case the diagonalization of the Hamiltonian becomes necessary. Although the interactions applied in this approach are phenomenological ones, they can be related to the effective two-nucleon forces, due to the use of the microscopic $SU(3)$ cluster model basis. See Ref. [13] for the details.

3   Applications

The applications of the semimicroscopic algebraic cluster model have been carried out so far within the $SU(3)$ dynamical symmetry approximation. This approximation allows exact analytical expression of the energy eigenvalues and electromagnetic transition rates in terms of reduced matrix elements, Clebsch–Gordan coefficients, etc. obtained from the algebraic description. Its validity, and also that of the underlying oscillator picture can be estimated from the comparison of the results with the corresponding experimental data.

As an illustrative example we present here the description of the $T = 0$ states of the ^{24}Mg nucleus in terms of a $^{12}C + ^{12}C$ cluster model [14]. The structure of this nucleus has been studied carefully via various reactions both in the ground-state region and in the ragion of molecular resonances observed in $^{12}C + ^{12}C$ heavy ion collisions. These experiments have resulted a large amount of experimental information on the structure of the ^{24}Mg nucleus. Most of the theoretical investigations have focused only on one of the two regions mentioned above, and relatively little effort has been put into their simultaneous investigation.

Our aim was to give a unified description of these two domains in terms of the $U_{C_1}(3) \otimes U_{C_2}(3) \otimes U_R(4)$ model. In this description the internal structure of the ^{12}C clusters is accounted for by the $(\lambda_C,\mu_C) = (0,4)$ $U_C(3)$ representation, which corresponds to an oblate deformation in the geometric picture. We have analyzed about 150 experimental levels in the energy range of 0 to 40 MeV (see Fig. 1.), and nearly 100 electric quadrupole transition probability data in our study, which is a more complete account of the energy spectrum and $E2$ transitions of the ^{24}Mg nucleus than any previous model calculation. We have displayed the $B(E2)$ values for the in-band transitions in Table 1. Our results for interband $E2$ transitions are also satisfactory. The fact that most of the transitions forbidden by the selection rules due to the $SU(3)$ dynamical symmetry have very weak experimental counterparts seems to indicate that the $SU(3)$ dynamical symmetry approach is a realistic approximation of the actual physical situation here. The model

was able to describe the general features of the moleular resonance spectrum as well. $E2$ transition probabilities calculated for in–band transitions within this region were significantly smaller than most of the corresponding results of other models. The example of the ^{12}C + ^{12}C system demonstrated that a large number of experimental data, including the ground–state region as well as the highly excited molecular resonances can be reconciled in terms of relatively straightforward calculations, which is one of the major advantages of the semimicroscopic algebraic cluster model.
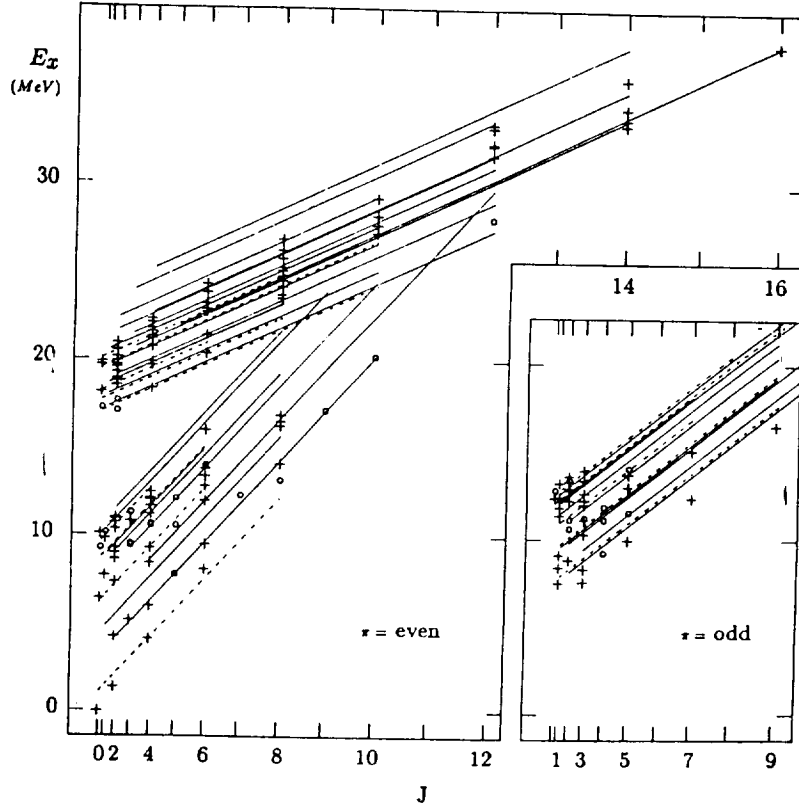

FIG. 1. Positive- and negative-parity T = 0 energy levels of the ^{24}Mg nucleus displayed separately in rotational diagram form [14]. Circles (o) stand for states with uncertain J^{π} assignment. The lines denote the position of the calculated model bands. (Dashed lines indicate bands with χ = 0, which contain only every second possible J value.)

Similar conclusions have been drawn from another application of the model to the ^{14}C + α system in terms of the restricted $U_C^{ST}(3) \otimes U_C(3) \otimes U_R(4)$ model, describing the T = 1 states of the ^{18}O nucleus [15]. Being a considerably less complex nuclear system than ^{12}C + ^{12}C, this example also allowed comparison of our results with those of microscopic calculations. We have found strong correlation between these two data sets, which seems to indicate, that the semimicroscopic algebraic cluster model approximates certain microscopic features reasonably well.

The model has been applied in other areas of nuclear physics as well, where the cluster picture may be relevant. In particular, the link between superdeformed and cluster states of α-like ($N = Z = even$) nuclei has been discussed [16]; the allowed and forbidden binary fission modes

of ground–state–like configurations in sd–shell nuclei have been studied [17]; and the possibility of describing exotic cluster radioactivity has been pointed out via the example of ^{210}Pb + ^{14}C clusterization of the ^{224}Ra nucleus [18]. In this latter case the model has to be adapted to heavy nuclei by introducing the pseudo-$SU(3)$ scheme.

TABLE I. In–band transitions for the ^{24}Mg nucleus. See Ref. [14] for the sources of the experimental data. The quantum numbers $n_\pi(\lambda,\mu)\chi$ assigned to the bands are also displayed.

$J_i^\pi(E_{xi})$	$J_f^\pi(E_xf)$	$B(E2)_{Exp}$	$B(E2)_{Th}$	$n_\pi(\lambda,\mu)\chi$
$2^+(1.37)$	$0^+(0.0)$	21.0 ± 0.4^a	21.0^a	$12(8,4)0$
$4^+(4.12)$	$2^+(1.37)$	37.8 ± 3.0	28.0	
$6^+(8.11)$	$4^+(4.12)$	38 ± 13	27.1	
$8^+(13.21)$	$6^+(8.11)$	30 ± 14	23.1	
$3^+(5.24)$	$2^+(4.24)$	38.0 ± 5.5	37.5	$12(8,4)2$
$4^+(6.01)$	$2^+(4.24)$	18.7 ± 2.4	11.4	
$5^+(7.81)$	$3^+(5.24)$	35.0 ± 4.9	17.5	
$5^+(7.81)$	$4^+(6.01)$	24 ± 10	19.5	
$6^+(9.53)$	$4^+(6.01)$	18 ± 8	18.0	
$7^+(12.35)$	$5^+(7.81)$	21 ± 14	19.7	
$8^+(14.15)$	$6^+(9.53)$	9.1 ± 2.4	13.7	
$2^+(8.65)$	$0^+(6.43)$	14.0 ± 4.3	12.4	$12(6,2)0$
$6^+(12.86)$	$4^+(9.30)$	11.2 ± 2.1	12.2	
$5^-(10.03)$	$3^-(8.36)$	20^{+8}_{-5}	34.7	$13(9,4)0$
$7^-(12.44)$	$5^-(10.03)$	51 ± 10	32.3	
$5^-(13.06)$	$3^-(10.33)$	22 ± 4	28.1	$13(8,3)1$
$4^-(9.30)$	$3^-(7.62)$	29 ± 6	35.1	$13(8,3)3$
$5^-(11.60)$	$3^-(7.62)$	4.6 ± 1.4	7.3	
$5^-(11.60)$	$4^-(9.30)$	37 ± 11	31.8	

^{a} Used to fit model parameters.

4 Summary and Outlook

We have discussed the new semimicroscopic algebraic cluster model, in which a harmonic oscillator picture is used to account for the internal structure and the relative motion of nuclear clusters. The model combines a microscopic harmonic oscillator basis with phenomenologic interactions formulated in algebraic terms. Its first applications to realistic nuclear systems have shown, that it is able to describe a large amount of experimental data in a coherent way, and also seems to reproduce certain microscopic effects reasonably well. The $SU(3)$ dynamical symmetry limit of the model was found to be a realistic approximation for several sd–shell nuclei.

The model can be developed further along several lines. First, the treatment of cluster systems with arbitrary open–shell structure can be considered by introducing spin and isospin degrees of freedom. The formalism of the model can also be extended to incorporate several internal configurations, including major shell excitations. Furthermore, by considering symmetry breaking terms in the Hamiltonian a more realistic description of nuclei can be given, relaxing, for example the selection rules imposed by the $SU(3)$ dynamical symmetry.

Acknowledgments

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HARMONIC OSCILLATOR IN QUANTUM ROTATIONAL SPECTRA: MOLECULES AND NUCLEI

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Abstract

The mapping of a rotational dynamics on a harmonic oscillator one is considered. The method is used for studying the stabilization of the rigid top rotation around the intermediate moment of inertia axis by orbiting particle.

1   Introduction

The quantum rotation is a specific type of excitation of microscopic system: hadrons, nuclei, molecules, and even atoms. The rotational excitations of molecules and nuclei have been studied in more detail. Electronic excitations are much higher than vibrational ones for most so-called "normal" molecules. Therefore they may be described adequately in the Born-Oppenheimer approximation. There is no analog of the Born-Oppenheimer approximation for atomic nuclei. Yet the occurrence of the rotational bands with strong (nearly 100 single particles) E2-transitions between neighboring states shows the existence of the collective rotation. All nucleons participate cooperatively into this collective motion with internal degrees of freedom being frozen completely or partly. The rotational excitations are grouped into rotational bands having states characterized in simplest case of a rigid axially-symmetric top by the energy ($\hbar = 1$)

$$E = I(I+1)/2\Im, \tag{1}$$

and quantum number I of the total angular momentum. $\Im$ is a moment of inertia. A simplest non-axial system is a rigid asymmetric top with the Hamiltonian

$$H = A_1 I_1^2 + A_2 I_2^2 + A_3 I_3^2, \tag{2}$$

where I_α are the projections of the total angular momentum operator on the BFF (body-fixed frame) axes $\alpha = 1, 2, 3$. The rotational constants $A_\alpha = 1/(2\Im_\alpha)$ depend on the principal moments of inertia $\Im_\alpha$. The rotational band of an asymmetric top consists of rotational multiplets, i.e., of the levels with the same value of the quantum number I. Besides I, these levels are characterized by the irreducible representations of the group $D_2 = \{1, \Re_1, \Re_2, \Re_3\}$, which contains the identity operator and three 180° rotations around the BFF axes $\Re_\alpha(\pi) = exp(-i\pi I_\alpha)$. The irreducible representations of D_2 are labeled a_1, a_2, b_1, b_2. They correspond to the eigenvalues $r_\alpha = \pm 1$ of the operators $\Re_\alpha$. The subscripts 1 and 2 label even and odd symmetry levels with respect to the $\Re_2$ rotation, a and b label even and odd symmetry levels with respect to the $\Re_3$ rotation. Note that $r_1 r_2 r_3 = 1$ is true for each four representations.

Different methods are used to solve the Hamiltonian (2). As the first step we will calculate the classical rotation energy E as the function defined in the system phase space (a rotational energy surface). The phase space of a rotational motion is formed by three Euler angles ϕ, ϑ, ψ and three conjugated momenta $p_\phi, p_\vartheta, p_\psi$. The absolute value of the angular momentum I and its projection $I_z = p_\phi$ on the z-axis of the space-fixed frame are the integrals of motion. It is suitable to do the canonical transformation [1] to new conjugated variables I and q_I, I_z and q_z, I_3 and q. Since q_I and q_z are cyclic variables, the phase space of a rotational motion is two-dimensional. It is convenient to map it on the surface of the sphere of the I radius with a center in the origin of the BFF. The point on the sphere with coordinates θ and φ determines the orientation of the vector $\mathbf{I}$ in the BFF. The canonical transformation enables us to relate the conjugated variables I_3 and q to the angles θ and φ. For $I_z = q_I = 0$ and an arbitrary q, we have $\cos\theta = I_3/I$, $\varphi = \frac{\pi}{2} - q$. Thus, the trajectories of the tip of $\mathbf{I}$ on the phase sphere are classical trajectories of the system in its rotational phase space. When the rotational energy is close to $A_1 I^2$ or $A_3 I^2$, where A_1 and A_3 correspond to the smallest or the largest moment of inertia, the classical trajectories are small ellipses around axes 1 or 3. They represent precession motion around these axes. The trajectories close to axis 2 with the intermediate moment of inertia are unclosed. They represent unstable motion. A small deviation from this axis takes a top away from it.

2 Precession motion

Let us begin with classical precession. It is described by the Euler equations

$$\dot{I}_\alpha = \{H, \ I_\alpha\}, \ \alpha = 1, 2, 3, \tag{3}$$

for the projections of the vector $\mathbf{I}$ on the BFF axes. In this equation $\{\ldots\}$ are the Poisson brackets. Let us introduce the classical concept of stationary rotation axis defined by the three equations $\{H, \ I_{0\alpha}\} = 0$. The stationary states $\mathbf{I}_0$ are identical with the fixed points of the energy surface. There are three stationary axes coinciding with the principal axes of a rigid top. For small precession around axis 1 ($I_1 \approx I$; $I_2, I_3 \ll I$) Eqs. (3) have the form

$$\dot{I}_2 = -(A_3 - A_1)I I_3,$$
$$\dot{I}_3 = (A_2 - A_1)I I_2. \tag{4}$$

They describe a harmonic oscillation motion

$$I_2(t) = i_0\sqrt{A_3/A_1 - 1} \cos\omega_{11}t, \ \ I_3(t) = -i_0\sqrt{A_2/A_1 - 1} \sin\omega_{11}t, \tag{5}$$

with small amplitude i_0 and frequency

$$\omega_{11} = 2I\sqrt{(A_2 - A_1)(A_3 - A_1)}. \tag{6}$$

In the BFF, the $\mathbf{I}$ vector precess around axis 1 and, in the laboratory frame, the top precess around the angular momentum $\mathbf{I}$. It follows from the stability condition $\omega^2 > 0$ that the precession motion around the axis with the smallest or the largest moment of inertia is stable and around the axis with the intermediate one is unstable.

To obtain the energy level structure of a rotational band corresponding to a precession motion one must quantize this motion. It can be done by different methods.

Holstein-Primakoff Representation of Angular Momentum Operators. The method developed by Marshalek for a quantized rotator [2] is based on the one boson realization of angular momentum operators [3]

$$I_1 = I - b^+b, \quad I_+ = I_2 + iI_3 = b^+\sqrt{2I - b^+b} = (I_-)^+,\tag{7}$$

in the space of wavefunctions

$$\varphi_{I\nu} = \sum_{K=-I}^{I} a_{K\nu} \frac{(b^+)^{I-K}}{[(I-K)!]^{1/2}} \mid 0\rangle,\tag{8}$$

where ν is the quantum number of a state in a rotational multiplet. The state $\mid 0\rangle$ corresponding to $K = I$ is a vacuum state of the boson creation and annihilation operators b^+, b. For describing precession motion we expand the square-root operator in I_+ and I_- in the series of a small quantity $\hat{n}/I$, where $\hat{n} = b^+b$ is the boson number operator. In the harmonic approximation $(n \ll I)$, the Hamiltonian (2) is quadratic in boson operators

$$H = A_1 I^2 + \frac{I}{2}(A_2 + A_3) + I(A_2 + A_3 - 2A_1)b^+b + \frac{I}{2}(A_2 + A_3)(b^+b + bb).\tag{9}$$

The Hamiltonian (9) can be diagonalized by a canonical transformation

$$b = u\beta + v\beta^+, \quad \mid u \mid^2 - \mid v \mid^2 = 1,\tag{10}$$

to new boson operators β and β^+. The energy of the lowest levels is given by

$$E_{In} = A_1 I(I+1) + \omega_{11}(n + 1/2), \quad n = 0, 1, 2, \ldots .\tag{11}$$

The quantum number n describes the precession motion. For the state with $n = 0$ the wave function

$$\varphi_{I0} = \mid u \mid^{-1/2} \exp\left(\frac{v}{2u}b^+b^+\right) \mid 0\rangle,\tag{12}$$

localizes near rotational axis 1. It corresponds to the sharply localized orientation of the angular momentum **I** along the positive direction of axis 1. Eq. (12) is not the eigenfunction of D_2 symmetries. Thus, the harmonic approximation is a "symmetry-breaking approximation." Being a linear theory it cannot describe tunneling the vector **I** through a potential barrier separating two degenerate minima.

Bargmann Representation [4]. Let us consider the complex variable

$$\zeta = x + iy = e^{i\varphi} \cot \frac{\theta}{2},\tag{13}$$

which is the stereographic projection of a point on the phase sphere with polar angles θ and φ on the plane passing through the south pole. As shown in Ref. [5], it is possible to construct the $SU(2)$ group representation in the space of the polynomials

$$\varphi(\zeta) = \sum_{K=-I}^{I} a_K \zeta^{I+K}.\tag{14}$$

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The angular momentum operators in this representation have the form

$$I_1 = I\zeta + \frac{1}{2}(1 - \zeta^2)\frac{d}{d\zeta}, \quad I_2 = -iI\zeta + \frac{i}{2}(1 + \zeta^2)\frac{d}{d\zeta}, \quad I_3 = -I + \zeta\frac{d}{d\zeta}. \tag{15}$$

Many problems in nuclear and molecular physics can be treated by this approach [6]. With the operators (15), the Schrödinger equation for a top is reduced to the Heine equation [7]. To describe for example the precession motion around axis 3 we should consider the approximation $|\zeta| \ll 1$.

Approximate Solution of Reccurence Relations. This method is based on the approximation of recurrence relations by a second-order differential equation for high-I values [8]. The eigenfunction of the Hamiltonian (2) can be written in the form

$$\Psi_{IM\nu} = \sum_{K=-I}^{I} a_{IK\nu} D_{MK}^I(\vartheta), \tag{16}$$

where M and K are the quantum numbers of the operators I_z and I_3 respectively. D_{MK}^I is the Wigner function depending on the Euler angles ϑ. For the coefficients $a_{IK\nu}$, the three-term recurrence relation is obtained

$$P_K a_{I,K-2,\nu} + (H_{KK} - E_{I\nu})a_{IK\nu} + P_{K+2}a_{I,K+2,\nu} = 0, \tag{17}$$

where

$$H_K = H_{KK} = \frac{1}{2}(A_1 + A_2) + \frac{1}{2}(2A_3 - A_1 - A_2)K^2,$$
$$P_K = H_{KK-2} = \frac{1}{4}(A_1 - A_2)[(I - K + 2)(I + K - 1)(I - K + 1)(I + K)]^{1/2}. \tag{18}$$

By using the small parameter $\delta = [I(I + 1)]^{-1/2}$ let us introduce the continuous variable $k = K\delta$. We will treat the coefficients P and H as the smooth functions of this variable. As a result, the recurrence relation (17) may be rewritten in the form of the Schrödinger equation

$$I(I + 1)\mathbf{H}a_{I\nu}(k) = E_{I\nu}a_{I\nu}(k), \tag{19}$$

with the Hamiltonian

$$\mathbf{H} = [P(k + 2\delta) + P(k)]\cos 2\hat{p}\delta + i[P(k + 2\delta) - P(k)]\sin 2\hat{p}\delta + H(k), \tag{20}$$

where $\hat{p} = -id/dk$ is the canonically conjugated momentum to the coordinate k.

In the harmonic approximation $K \ll I$, Eq. (19) is reduced to the second-order differential equation

$$\frac{d^2 a_{I\nu}}{dK^2} + 2m[E - A_1 I(I + 1) - V(K)]a_{I\nu} = 0, \tag{21}$$

in the space of quantum numbers K. The equation describes the motion of the angular momentum I with effective mass $m = 1/[2(A_2 - A_1)I(I+1)]$ in potential $V(K) = (A_3 - A_1)K^2$. This harmonic oscillator has the energy spectrum (11) and the wave function

$$a_{In} = \left[\frac{2}{2^n n!}\sqrt{\frac{2w}{\pi(2I + 1)}}\right]^{1/2} H_n\left(K\sqrt{\frac{2w}{2I + 1}}\right)\exp\left(-\frac{wK^2}{2I + 1}\right), \tag{22}$$

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where $w = [(A_3 - A_1)/(A_2 - A_1)]^{1/2}$, and H_n is the Hermite polynomial. We have again a sharp localized state with broken symmetry.

The rotational dynamics of real many-body systems is more complicated than that of a rigid top because of the centrifugal and Coriolis forces. However the harmonic approximation can be used in this chase to understand the physical nature of the phenomenon under study. The example is bifurcations in quantum rotational spectra considered in Ref. [9]. In the next section we consider another problem having a bearing on a precessional motion.

3 Precession Motion around Intermediate Moment of Inertia Axis

As we proved above, the rotation of a rigid top around the intermediate axis is unstable. This is not a case if a system has additional degrees of freedom apart from rotational ones. We are going to consider a particle coupled with an asymmetric rigid top. This is the situation of one-electron Rydberg states in triatomic molecules, such as H_2O [10], and rotational bands in odd deformed nuclei [11].

The Born-Oppenheimer approximation breaks down in the molecular Rydberg spectra. As the total angular momentum I increases, the rotational levels pass from Hund's case (a) or (b) (the strong-coupling scheme), where the electronic splitting is large compared with the rotational one, to the Hund's case (d) (the weak-coupling scheme), where it is small. The model of an isolated j-complex is widely used for the description of the transition from strong to weak coupling in nuclear [11] and molecular [12] physics. This approximation is valid if coupling the states of a j-complex with other Rydberg states is small compared to the Coriolis coupling. The assumption means that one-particle angular momentum $\mathbf{j}$ is an integral of motion. As I increases, the momentum $\mathbf{j}$ decouples from the molecular ion core and couples to the axis of rotation with the maximal moment of inertia.

Let us consider the effective Hamiltonian describing the two degrees of freedom: rotational and one-particle. The rotational part of the Hamiltonian is the kinetic energy of a rigid top. We will use the self-consistent field approximation for describing one-particle motion. The non-spherical part of this field can be written in terms of the particle multipole momenta $q_{\lambda\mu}(\mathbf{r})$ as follows: $V = \sum_{\lambda\mu} Q_{\lambda\mu} q_{\lambda\mu}(\mathbf{r})$, where λ-values are even for the reflection symmetric field. For an isolated j-complex, the one-particle part of the Hamiltonian can be expressed in terms of the spherical tensor operators $T_{\lambda\mu}(\mathbf{j})$. Thus, the effective Hamiltonian of the system for an isolated j-complex is algebraic with symmetry $SU(2) \otimes SU(2)$. We consider this Hamiltonian in the quadrupole approximation when the components of mean field V with $\lambda > 2$ are smaller than the ones with $\lambda = 2$. It is convenient to write the Hamiltonian in the coordinate system fixed by the principal inertia axes:

$$H = \sum_\alpha [A_\alpha (I_\alpha - j_\alpha)^2 + g_\alpha j_\alpha^2], \tag{23}$$

where $g_1 = -g_2 = (g_0 \sin\gamma)/\sqrt{3}$, $g_3 = g_0 \cos\gamma$ $(-\infty < g_0 < +\infty,\ 0° < \gamma < 60°)$ are the parameters of the quadroupole part of the self-consistent field, which is diagonal in the considered frame. In

classical mechanics, the system dynamics is described by the equations of motion:

$$\dot{I}_\alpha = -2\epsilon_{\alpha\beta\gamma}A_\beta(I_\beta - j_\beta)I_\gamma$$
$$\dot{j}_\alpha = 2\epsilon_{\alpha\beta\gamma}[-A_\beta(I_\beta - j_\beta) + g_\beta l_\beta]j_\gamma, \tag{24}$$

where repeated indexes are summed.

The stationary state $\mathbf{I_0}$ and $\mathbf{j_0}$ of Eqs. (24) is determined by the eight algebraic equations since the two integrals of motion $\mathbf{I}^2$ and $\mathbf{j}^2$ exist. Therefore, the stationary state with an arbitrary orientation does not exist. There are two types of stationary states of Eqs. (24), corresponding to the lowest level of the rotational multiplets. The three aligned states S_α: $I_\alpha = I, j_\alpha = j, \alpha = 1, 2, 3$ with the energy

$$E_\alpha = A_\alpha(I - j)^2 + g_\alpha j^2, \tag{25}$$

have the parallel vectors $\mathbf{I_0}$ and $\mathbf{j_0}$ aligned along axis α. In the three plane stationary states $S_{\alpha\beta}$, these vectors are placed in the $(\alpha\beta)$-plane. As I increases the sequence of stationary states S_α and $S_{\alpha\beta}$ with the minimal energy for given I leads to the aligned state with the maximal moment of inertia. The transition from aligned state S_α to plane one $S_{\alpha\beta}$ is accompanied by the bifurcation of the C_{2v}-type [9] at the critical angular momentum

$$I_{\alpha\beta} = j\left\{1 + \frac{g_\alpha - g_\beta}{2A_\alpha} + \left[\left(\frac{g_\alpha - g_\beta}{2A_\alpha}\right)^2 - \frac{(g_\alpha - g_\beta)A_\beta}{A_\alpha(A_\alpha - A_\beta)}\right]^{\frac{1}{2}}\right\}. \tag{26}$$

The index α denotes the axis from which the angular momenta $\mathbf{I_0}$ and $\mathbf{j_0}$ decouple, while index β denotes the axis to which they approach. Both indexes $(\alpha\beta)$ denote the plane, in which these vectors move for $j < I_{\alpha\beta} < I < I_{\beta\alpha}$. Another pair of critical momenta determines the similar bifurcation points in the region $I < j$. The expression for these values is the same as Eq. (26) except the sign before a square root. We will consider below only the region $I > j$ in the case when $A_1 < A_2 < A_3$, $g_0 > 0$.

The precessional motion near the stable stationary state is described by linearized set of Eqs. (24). Four linear differential equations describe two normal modes corresponding to the small harmonic oscillations of vectors $\mathbf{I}$ and $\mathbf{j}$. The frequencies of these modes are obtained as the roots of a biquadratic equation. We begin our consideration with the precession near the S_1-state in the weak-coupling limit $A_\alpha I >> g_\alpha j$. To simplify expressions let us use assumption $I >> j$. The precessional mode with smaller frequency ω_{11} (6) represents the precession of the vectors $\mathbf{I}$ and $\mathbf{j}$ with different amplitudes. While the $\mathbf{I}$ vector circumscribes according to Eqs. (5) an elliptical cone around axis 1 with the amplitude i_0, the amplitude of the $\mathbf{j}$ vector is j/I times smaller that of the $\mathbf{I}$ one. Thus, this mode involves the precession of core angular momentum vector $\mathbf{R} = \mathbf{I} - \mathbf{j}$, which coincides, in considered approximation, to rigid top precession. Another normal mode with the frequency $\omega_{12} = 2IA_1$, which is equal to the core angular velocity around axis 1, involves the uniform rotation of the angular momentum vectors around this axis with identical amplitudes:

$$I_2(t) = j_2(t) = i_0 \cos\omega_{12}t, \quad I_3(t) = j_3(t) = i_0 \sin\omega_{12}t. \tag{27}$$

Consequently the momentum $\mathbf{R}$ does not participate in this motion.

Now we consider precession near the stationary state S_2, corresponding to the central axis. An orbiting particle stabilizes this state due to the anisotropic (quadrupole) interaction with a top.

The small values of $(A_2 - A_1)/A_2$ favors stability of the aligned state S_2 lowering its energy E_2 relative to E_1 (see Eq.(25)). To clarify the physical picture we will use the approximations $I >> j$ and $(A_2 - A_1)/A_1 << 1$ in describing precessional motion. The smaller frequency

$$\omega_{21} = 2 \left[(A_2 - A_1)(A_3 - A_2)(I_{21}^2 - I^2) \right]^{1/2} \tag{28}$$

vanishes at the critical momentum I_{21} (26). The time-dependence of the angular momentum components for this mode is defined by

$$\begin{aligned} I_1(t) &= i_0 \left[A_3/A_2 - 1 \right]^{1/2} \cos \omega_{21} t, \\ I_3(t) &= -i_0 [(A_2/A_1 - 1)(I_{21}^2/I^2 - 1)]^{1/2} \sin \omega_{21} t, \end{aligned} \tag{29}$$

and $\mathbf{j}(t) = (j/I)\mathbf{I}(t)$. The interpretation of this result is straightforward. Since the amplitude of the $\mathbf{j}$-vector is small compared to that of the $\mathbf{I}$ ones, the considered mode represents the precession of the core angular momentum $\mathbf{R}$ similar to the rigid top precession (5). Yet unlike the latter, the tips of vectors $\mathbf{I}$ and $\mathbf{j}$ move on elliptic orbits stretched along axis 1 if the angular momentum I is close to I_{21}. This is just a consequence of the bifurcation, which shifts the angular momentum vectors into the (12)-plane. For another normal mode of frequency $\omega_{22} = 2IA_2$, the time-dependence of angular momentum components has the same form as in Eq. (27).

Thus, we have shown that the precession motion around the axis with intermediate moment of inertia is possible for a system consisting of a particle anisotropically coupled with an asymmetric top. The isolated j-complex approximation is used in considering this phenomenon. To examine it one can solve the classical equation of motion for a particle coupled with an asymmetric top without this restriction. The equations involve two different time scales: fast particle motion and slow core rotational motion. After averaging on the fast motion, one can obtain the closed set of nine equations for components of $\mathbf{I}$ and particle angular and quadrupole momenta. The averaged equations can describe the stabilization phenomenon and the precession around intermediate axis. This insight into the problem reveals the close relationship of our stabilization effect with that of the Kapitza pendulum [13]. Another intriguing analogy is the new discovery in planetary science where it has been shown recently [14] that the Moon stabilizes the chaotic wobble of the Earth's rotational axis, which is unstable due to orbital coupling with other planets. Thus, without the Moon, large variations in obliquity resulting from the chaotic wobble might have driven dramatic changes in the Earth's climate. There are two fundamental distinctions of our problem from considered above: we deal with the *isolated and quantum* system.

The above found precessional frequencies are associated with the splitting between the lowest levels of a multiplet. To obtain this result one must quantize the precession motion. It can be done by using the Holstein-Primakoff representation. The result for lowest multiplet levels corresponding to the stationary state S_α is

$$E_{In} = E_\alpha(I) + \omega_{\alpha 1}(n_1 + 1/2) + \omega_{\alpha 2}(n_2 + 1/2) \tag{30}$$

where E_α is given by Eq. (25), and n_1 and n_2 are the numbers of bosons in corresponding mode. The boson operators b_k^+ and b_k connect the odd and even with respect to the C_2^α-transformation states inside a rotational multiplet. Consider, for example, the precession around axis 1 in the weak-coupling limit. In this approximation, any rotational multiplet (I-multiplet) consists of R-multiplets with the quantum numbers $R = I - j + m, \quad m = 0, 1, ..., 2j$. The levels in R-multiplets

with the same quantum number R but different I are degenerated. The frequency (6) describing the precession of the **R**-vector is equal to the splitting between the lowest levels a_1 and b_1 (or a_2 and b_2) in a R-multiplet. Another frequency $\omega_{12} = 2IA_1$ is equal to the splitting between the lowest levels of adjacent R-multiplets belonging to the same I-multiplet. The situation for the precession around the intermediate axis is more complicated. According to the precessional approximation, the lowest states of a multiplet involve two groups of roughly equidistant levels, which are described by Eq. (30). But a smaller frequency vanishes in a critical point and the precessional approximation becomes inappropriate in this region. This means the redistribution of multiplet levels, which provides a method for the identification of the intermediate axis precession in an experiment.

Acknowledgments

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GALACTIC OSCILLATOR SYMMETRY

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Abstract

Riemann ellipsoids model rotating galaxies when the galactic velocity field is a linear function of the Cartesian coordinates of the galactic masses. In nuclear physics, the kinetic energy in the linear velocity field approximation is known as the collective kinetic energy. But, the linear approximation neglects intrinsic degrees of freedom associated with nonlinear velocity fields. To remove this limitation, the theory of symplectic dynamical symmetry is developed for classical systems. A classical phase space for a self-gravitating symplectic system is a co-adjoint orbit of the noncompact group Sp(3,R). The degenerate co-adjoint orbit is the 12 dimensional homogeneous space Sp(3,R)/U(3), where the maximal compact subgroup U(3) is the symmetry group of the harmonic oscillator. The Hamiltonian equations of motion on each orbit form a Lax system $\dot{X} = [X, F]$, where X and F are elements of the symplectic Lie algebra. The elements of the matrix X are the generators of the symplectic Lie algebra, viz., the one-body collective quadratic functions of the positions and momenta of the galactic masses. The matrix F is composed from the self-gravitating potential energy, the angular velocity, and the hydostatic pressure. Solutions to the Hamiltonian dynamical system on Sp(3,R)/U(3) are given by symplectic isospectral deformations. The Casimirs of Sp(3,R), equal to the traces of powers of X, are conserved quantities.

1 Riemann Ellipsoids

A remarkably unified picture of rotating systems is attained by adopting an algebraic perspective. Classical rotating bodies such as galaxies (period=10^{15}s), stars (10^6s), and fluid droplets (1s), and quantum rotating nuclei (10^{-20}s) may be described in terms of a single subgroup GCM(3) (for general collective motion in 3 dimensions) of the noncompact symplectic Lie group Sp(3,R). In classical physics, the GCM(3) theory is identical to the Riemann ellipsoidal model [1, 2, 3].

A Riemann ellipsoid is a uniform density fluid with an ellipsoidal boundary whose velocity field is a linear function of the inertial frame Cartesian position coordinates $\vec{X}$. The isodensity surfaces of elliptical galaxies are very nearly ellipsoidal [4]. Linear velocity fields $\vec{U}^L$ (the superscript L indicates a laboratory inertial frame quantity) span the dynamical continuum from rigid rotation, $\vec{U}^L(\vec{X}) = \vec{\omega}^L \times \vec{X}$, to irrotational flow, $\vec{\nabla} \times \vec{U}^L = 0$. Thus, Riemann ellipsoids can model a wide class of rotating systems.

The principal aim of this paper is to present the classical symplectic model with particular emphasis upon its relationship with the Riemann ellipsoidal model [5]. But first the Riemann model and its equivalence to the algebraic GCM(3) theory will be reviewed. To describe a linear velocity field, the dynamical group GCM(3) contains the general linear group GL(3,R) as a subgroup. In

addition, to characterize the size, deformation, and orientation of an ellipsoid, the GCM(3) Lie algebra includes the inertia tensor.

There are several advantages to adopting the powerful dynamical group method. First, the Euler fluid equations of motion for a Riemann ellipsoid can be proven to form a Hamiltonian dynamical system [3, 6]. A Riemann ellipsoid phase space is a co-adjoint orbit of GCM(3), and its Poisson bracket is inherited from the Lie algebra structure of GCM(3). Moreover, this Hamiltonian system is a special Lax pair system [7]. Second, the group method is not restricted to continuum fluids. GCM(3) dynamical symmetry applies equally well to discrete systems of particles. Third, GCM(3) dynamical symmetry also applies to some quantum rotating bodies. For example, the Bohr-Mottelson irrotational surface wave model of collective rotational and vibrational states forms an irreducible unitary representation of GCM(3) [8, 9, 10]. Finally, GCM(3) symmetry suggests a natural extension to symplectic Sp(3,R) dynamical symmetry [11]. The latter replaces the collective kinetic energy of the GCM(3) theory by its exact microscopic expression.

The hydrodynamic Riemann ellipsoidal model provides a physical interpretation to the abstract GCM(3) theory: The length C of the Kelvin circulation vector, a constant of the motion for a frictionless, homoentropic fluid flow, is the Casimir invariant for GCM(3) [6].

The velocity fields of rigid rotors and irrotational droplets have very different Kelvin circulation vectors $\vec{C}$. Suppose the rotating system has an ellipsoidal boundary with semi-axes lengths a_k. The inertial frame Kelvin circulation vector, projected onto the kth body-fixed axis, is defined as the line integral of the velocity field $\vec{U}$ around the boundary of the ellipse D_k in the $i - j$ principal plane for i, j, k cyclic. According to Stoke's theorem, these line integrals equal the surface integrals of the curl of the velocity field,

$$C_k = \frac{M}{5\pi} \oint_{\partial D_k} \vec{U} \cdot d\vec{l} = \frac{M}{5\pi} \iint_{D_k} \vec{\nabla} \times \vec{U} \cdot d\vec{S}, \tag{1}$$

where $\vec{U}$ denotes the projection of the inertial frame velocity field onto the body-fixed axes, and M is the fluid's mass.

By definition, the curl of the velocity field of an irrotational droplet is zero, and, hence, the Kelvin circulation of an irrotational fluid vanishes, $\vec{C} = 0$. For a rigid rotor velocity field, $\vec{\nabla} \times \vec{U} = 2\vec{\omega}$. Because $\pi a_i a_j$ is the area of the ellipse D_k, the rigid rotor circulation components equal $C_k = (2M/5)a_i a_j \omega_k$. For a general linear velocity field, the curl is a constant vectorfield $\vec{\nabla} \times \vec{U} = \vec{\zeta} + 2\vec{\omega}$, where $\vec{\zeta}$ is called the uniform vorticity. As the uniform vorticity ranges continuously from zero to the negative of twice the angular velocity, the complete Riemann sequence from rigid rotation to irrotational flow is traversed.

2   GCM(3) Dynamical Symmetry

The symplectic algebra Sp(3,R) consists of the inertia, virial momentum, and kinetic tensors [11]:

$$\begin{aligned}
Q_{ij}^{\mathrm{L}} &= \sum m_\alpha X_{\alpha i} X_{\alpha j}, \\
N_{ij}^{\mathrm{L}} &= \sum X_{\alpha i} P_{\alpha j}, \\
T_{ij}^{\mathrm{L}} &= \sum m_\alpha^{-1} P_{\alpha i} P_{\alpha j},
\end{aligned} \tag{2}$$

where the sums are carried over the particle index $\alpha = 1, \ldots, A$, m_α denotes the mass of particle α, and $\vec{X}_\alpha$, $\vec{P}_\alpha$ are the inertial frame vector Cartesian position and momentum of particle α. In fluid dynamics, the sums over particles are replaced by integrals over the density distribution, e.g., $Q_{ij}^{\mathrm{L}} = \int \rho(X) X_i X_j d^3 X$. The Poisson brackets close to form the symplectic algebra:

$$
\begin{aligned}
\left\{ N_{ij}^{\mathrm{L}}, N_{kl}^{\mathrm{L}} \right\} &= \delta_{il} N_{kj}^{\mathrm{L}} - \delta_{jk} N_{il}^{\mathrm{L}}, \\
\left\{ Q_{ij}^{\mathrm{L}}, Q_{kl}^{\mathrm{L}} \right\} &= 0, \\
\left\{ Q_{ij}^{\mathrm{L}}, N_{kl}^{\mathrm{L}} \right\} &= \delta_{il} Q_{jk}^{\mathrm{L}} + \delta_{jl} Q_{ik}^{\mathrm{L}} \\
\left\{ T_{ij}^{\mathrm{L}}, T_{kl}^{\mathrm{L}} \right\} &= 0, \\
\left\{ N_{ij}^{\mathrm{L}}, T_{kl}^{\mathrm{L}} \right\} &= \delta_{il} T_{jk}^{\mathrm{L}} + \delta_{ik} T_{jl}^{\mathrm{L}} \\
\left\{ Q_{ij}^{\mathrm{L}}, T_{kl}^{\mathrm{L}} \right\} &= \delta_{ik} N_{jl}^{\mathrm{L}} + \delta_{il} N_{jk}^{\mathrm{L}} + \delta_{jk} N_{il}^{\mathrm{L}} + \delta_{jl} N_{ik}^{\mathrm{L}}.
\end{aligned}
$$

The general collective motion GCM(3) subalgebra includes only the inertia tensor Q_{ij}^{L} and the virial momentum tensor N_{ij}^{L}. The rotational ROT(3) subalgebra is spanned by just the inertia tensor and the antisymmetric part of the viral momentum tensor, viz., the angular momentum $L_k^{\mathrm{L}} = \epsilon_{ijk} N_{ij}^{\mathrm{L}}$. The Lie algebra GL(3,R) of the general linear group is generated by the virial momentum tensor, and the Lie algebra SO(3) of the rotation group is generated by the angular momentum. The inertia tensor generates a 6 dimensional R^6 abelian Lie algebra. GCM(3) and ROT(3) are semidirect sum Lie algebras of the abelian ideal R^6 with GL(3,R) and SO(3), respectively.

In the principal axis frame, the inertia tensor Q is, by definition, diagonal, and its eigenvalues are proportional to the squared axis lengths a_i^2 of the inertia ellipsoid.

Although the exact kinetic tensor T_{ij} is not an element of GCM(3), its linear velocity field value, the collective kinetic tensor, is a function of the algebra generators, [12] $t = {}^t N \cdot Q^{-1} \cdot N$. The Kelvin circulation of a linear velocity field may be expressed in terms of the GCM(3) generators as $C_k = \epsilon_{kij}(Q^{-1/2} \cdot N \cdot Q^{1/2})_{ij}$.

Time evolution in the classical collective models based upon ROT(3), GCM(3), and Sp(3,R) is governed by Hamiltonian dynamics of a special type known as a Lax system. Consider first the simple case of ROT(3) for which the dynamics corresponds to Euler rigid body rotation. If the inertia ellipsoid is rotating with an angular velocity $\Omega_{ij} = \epsilon_{ijk}\omega_k$ and $L_{ij} = N_{ij} - N_{ji}$ is the angular momentum tensor, then Hamiltonian dynamics is given by

$$
\dot{L} = [\Omega, L]. \tag{3}
$$

In terms of vectors, this equation is the familiar law $\dot{\vec{L}} = -\vec{\omega} \times \vec{L}$ that determines the precession of the angular momentum vector in the body-fixed frame.

A matrix equation of the form $\dot{X} = [F, X]$ is called a Lax equation and $X - F$ are referred to as a Lax pair [13, 14]. A useful property of any Lax equation is that the trace of any power of X is conserved. Let I_p denote the trace of the pth power of the matrix X.

$$
I_p = \frac{1}{p} \mathrm{Tr}(X)^p. \tag{4}
$$

For any Lax equation, it is evident that every I_p is a constant of the motion,

$$\dot{I}_p = \text{Tr}\left(X^{p-1} \cdot \dot{X}\right) = \text{Tr}\left(X^{p-1} \cdot [F, X]\right) = \text{Tr}\left(X^{p-1}FX - X^pF\right) = 0. \tag{5}$$

In the case of the Euler equation, $I_2 = -\vec{L} \cdot \vec{L}$ is the negative of the squared length of the angular momentum vector. If p is odd, then I_p is zero. If $p > 2$ is even, then I_p is a function of the squared length of the angular momentum vector. Thus, there is only one independent invariant among the Lax invariants.

Suppose that $X(t)$ is a solution to the Lax equation, $\dot{X} = [F, X]$, corresponding to the initial condition $X = X_0$. If $g(t)$ is a smooth curve of invertible matrices satisfying the matrix differential equation $\dot{g} = F \cdot g$ with the initial condition $g = I$, then the solution to the Lax equation is just the isospectral deformation,

$$X(t) = g(t) \cdot X_0 \cdot g(t)^{-1}. \tag{6}$$

This is proven using the identity $dg^{-1}/dt = -g^{-1}\dot{g}g^{-1}$. If Ω is constant, the matrix differential equation $\dot{g} = \Omega \cdot g$ for the Euler equation has the unique solution $g(t) = \exp(\Omega t)$ for the initial condition $g(0) = I$. Thus, $g(t)$ is a curve in the rotation group SO(3), and the isospectral deformation $L(t) = g(t)L_0 g(t)^{-1}$ describes explicitly the precession of the angular momentum in the body-fixed frame resulting from the rotation $g(t)$ of the intrinsic frame relative to the laboratory frame. Because of the choice of initial conditions for g, L_0 represents the constant angular momentum vector in the inertial laboratory frame.

To present the time evolution for Riemann ellipsoids as a Lax system, suppose the potential energy in the body-fixed frame $V = V(a_1, a_2, a_3)$ is a smooth function of the axes lengths. For a star or galaxy, V is the attractive gravitational self- energy. For a nucleus, V may be approximated by the sum of the attractive surface energy and the repulsive Coulomb energy. Define the Chandrasekhar potential energy tensor W in the rotating frame to be the diagonal matrix,

$$W_{ij} = -\delta_{ij}a_i\frac{\partial V}{\partial a_i}, \tag{7}$$

and, to impose a constraint to constant volume, define the pressure tensor $\Pi = pv$ to be the product of the hydrostatic pressure p times the ellipsoid's volume $v = 4\pi a_1 a_2 a_3/3$. Hamiltonian dynamics for Riemann ellipsoids is given as follows [7]:

Theorem. If the inertia ellipsoid is rotating with an angular velocity $\Omega_{ij} = \epsilon_{ijk}\omega_k$, then the Riemann ellipsoid Hamiltonian dynamical system is equivalent to the Lax system, $\dot{X} = [F, X]$, where the 6×6 real matrices X and F in the body-fixed frame are given by

$$X = \begin{pmatrix} N & -Q \\ t & -{}^tN \end{pmatrix}, \quad F = \begin{pmatrix} \Omega & I \\ (W + \Pi) \cdot Q^{-1} & \Omega \end{pmatrix}. \tag{8}$$

The quadratic Lax invariant equals the negative of the squared length of the Kelvin circulation vector, $I_2 = \text{Tr}(N^2 - t \cdot Q) = -C'^2$. The higher order Lax invariants are either zero (odd powers) or are functions of the circulation vector's squared length.

The phase space for a Riemann ellipsoid obeying the Lax equation is a co-adjoint orbit of GCM(3):

Theorem. Each Riemann ellipsoid orbit is diffeomorphic to some coset space of GCM(3). The coset depends upon the value of the circulation C:

$$\mathcal{O}_C = \begin{cases} GCM(3)/SO(2) \cong R^{12} \times S_2, & C \neq 0, \quad \dim = 14 \\ GCM(3)/SO(3) \cong R^{12}, & C = 0, \quad \dim = 12 \end{cases} \tag{9}$$

The degenerate orbit is diffeomorphic to 12-dimensional Euclidean space. This irrotational flow phase space, coordinatized by $\alpha_{2\mu}, \pi_{2\mu}, \alpha_0, \pi_0$ for the quadrupole and monopole degrees of freedom, was quantized by A. Bohr. The generic orbits $C \neq 0$ were undiscovered for many years because the significant role of Lie groups in this problem was not appreciated by the Copenhagen school. The generic orbits are diffeomorphic to the Cartesian product $R^{12} \times S_2$ of Euclidean space with the two-dimensional sphere. The topology of the sphere forces the circulation to be quantized to integer multiples of $\hbar$ in a way parallel to the usual angular momentum quantization. Thus, the spectrum of the squared length of the quantum circulation operator is quantized to $C(C + 1)\hbar^2$, where C is a nonnegative integer.

3   Sp(3,R) Dynamical Symmetry

Classical symplectic Sp(3,R) time evolution in the rotating frame is given by the Lax equation, $\dot{X} = [F, X]$, if, in the Lax matrix X, the linear approximation t to the kinetic energy is replaced by its exact expression T. In this way, the restriction to linear velocity fields of the Riemann GCM(3) model is removed in the symplectic Sp(3,R) theory.

The symplectic conservation laws are provided by the Lax invariants I_p. The quadratic Casmir invariant of the symplectic algebra is the quadratic Lax invariant, $C^{(2)} = \text{Tr}(N^2 - Q \cdot T)$. Note that for a linear velocity field, the quadratic symplectic invariant simplifies to the negative of the squared length of the Kelvin circulation vector. The odd order invariants vanish. The quartic symplectic Casimir invariant is the quartic Lax invariant,

$$C^{(4)} = \text{Tr}\left[(NQ - Q^t N)(TN - {}^t NT)\right] - 1/2\,\text{Tr}\left[(N^2 - QT)^2\right]. \tag{10}$$

There is only one more independent Casimir and Lax invariant $C^{(6)} = I_6$; the higher order invariants are functionally dependent upon the three independent Casimirs $C^{(p)} = I_p$ for $p = 2, 4, 6$.

Since the matrices X and F are elements of the symplectic Lie algebra, the following theorem may be proved:

Theorem. Every solution to the classical symplectic Lax system is given by a isospectral transformation $g(t) \in$ Sp(3,R) applied to the initial state

$$X(t) = g(t) \cdot X_0 \cdot g(t)^{-1}, \tag{11}$$

where X_0 and X are elements of the symplectic Lie algebra sp(3,R). The group element $g(t)$ is a solution to the matrix differential equation $\dot{g} = Fg$ with the initial condition $g = I$ if and only if X is a solution to the Lax equation with the initial condition $X = X_0$.

Consider the co-adjoint orbit of the symplectic group through the point X,

$$\mathcal{O}_X = \left\{ g \cdot X \cdot g^{-1} \mid g \in \mathrm{Sp}(3, \mathrm{R}) \right\}. \tag{12}$$

The co-adjoint orbit is regarded as a surface in the Euclidean symplectic dual space, $sp(3, R)^*$. A manifold that intersect each co-adjoint orbit exactly once is called a "transversal." A transversal $\mathcal{T}$ for the symplectic co-adjoint group action is provided by a three-dimensional surface [15, 16]

$$\mathcal{T} = \left\{ \hat{S} = \begin{pmatrix} 0 & -S \\ S & 0 \end{pmatrix} \in sp(3, R)^* \mid S = \mathrm{diag}(s_1, s_2, s_3) \right\}. \tag{13}$$

Transversal points correspond to elementary systems for which the virial momentum tensor vanishes, $N = 0$, and the inertia and kinetic tensors are equal and diagonal, $Q = T = S$. Since the inertia and kinetic tensors are positive-definite, the physically relevant transversal consists of only those points for which S is positive-definite, $s_i > 0$.

An orbit of the transversal point $\hat{S} \in \mathcal{T}$ is diffeomorphic to a coset space of the symplectic group modulo the isotropy subgroup. These isotropy subgroups may be proven to be subgroups of the unitary group,

$$U(3) \simeq \left\{ \begin{pmatrix} U & -V \\ V & U \end{pmatrix} \in Sp(3, R) \mid U + iV \in U(3) \right\}, \tag{14}$$

and, thereby, the coset spaces are given explicitly as follows [15, 16, 5]:

Theorem. The symplectic phase spaces are diffeomorphic to coset spaces of Sp(3,R):

$$\mathcal{O}_S = \begin{cases} Sp(3, R)/[U(1) \times U(1) \times U(1)], & s_i \text{ distinct}, & \dim = 18 \\ Sp(3, R)/[U(2) \times U(1)], & s_1 = s_2 \neq s_3, & \dim = 16 \\ Sp(3, R)/U(3), & s_1 = s_2 = s_3, & \dim = 12 \end{cases} \tag{15}$$

The degenerate orbit $Sp(3,R)/U(3)$ is diffeomorphic to the complex Siegel half-plane. In future work, the dynamical system on the Siegel half-plane will be reported.

Acknowledgments

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SHAPES AND STABILITY OF
ALGEBRAIC NUCLEAR MODELS [1]

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Abstract

A generalization of the procedure to study shapes and stability of algebraic nuclear models introduced by Gilmore is presented. One calculates the expectation value of the hamiltonian with respect to the coherent states of the algebraic structure of the system. Then equilibrium configurations of the resulting energy surface, which depends in general on state variables and a set of parameters, are classified through the Catastrophe theory. For one and two-body interactions in the hamiltonian of the interacting boson model-1, the critical points are organized through the Cusp catastrophe. As an example, we apply this *Separatrix* to describe the energy surfaces associated to the Rutenium and Samarium isotopes.

1 Introduction

The geometry of algebraic nuclear models can be studied by means of the time-dependent variational principle [1], [2]. This formalism provides us with a classical limit of the nuclear model, in particular we are mainly concerned with the static properties of the hamiltonian function (energy surface) associated to the considered algebraic nuclear model. In general these hamiltonian functions depend on state variables and a set of parameters, then the appropriate mathematical tool to determine the most general behaviour of their equilibrium configurations is the Catastrophe formalism [3].

A connection between the interacting boson model-1(IBM-1) [4] and the geometrical approach of Bohr-Mottelson [5] was done by expressing the IBM-1 hamiltonian in terms of shape variables. This can be achieved by means of the intrinsic boson states defined by [6] or by the corresponding coherent states [2]. Analysis of shape and phase transitions in this model have been done by [7], [8]. In this work we apply the procedure introduced in Ref. [2] to the interacting boson model, but for the general hamiltonian of one and two-body central interactions involving s and d bosons [4] and determining its associated *Separatrix*. We show that the equilibrium configurations can be

classified through the Cusp catastrophe, this means that two parameters are enough to describe the most general energy surface. Therefore this analysis generalize those presented previously [4], in which only transitions between pairs of exact $SU(5)$, $O(6)$ and $SU(3)$ symmetries are considered. In the last decade, effective hamiltonians of the IBM-1 have been used to describe energy spectra and transition probabilities of chains of isotopes and isotones [9], [10]. In particular, the effective hamiltonians for Ru [11] and Sm [12] isotopes were determined, *i.e.*, the best choice of the parameters of the general IBM-1 hamiltonian that reproduced the corresponding experimental data. Using these effective hamiltonians we construct their energy surfaces and show that their critical points follow a curve in the parameters space organized by the Cusp *Separatrix*. This let us to know: i) How many equilibrium configurations yield the system and ii) If the behaviour of the model around the critical points may or may not be approximated by an harmonic oscillator.

In the Second Section we review how the energy surfaces can be determined considering a hamiltonian constructed in terms of the generators of a Heisenberg-Weyl algebra. In the Third Section a brief summary of the IBM-1 is presented. In the Fourth Section, an analysis of the shape and stability of the most general energy surfaces of the IBM-1 is made, also the curves associated to the Ru and Sm isotopes are plotted in the parameters space. Finally some remarks are indicated in the last section.

2   Energy Surfaces of Algebraic Models

The energy surfaces (ES) of algebraic models can be determined by means of the coherent states of the associated algebraic structure of the hamiltonian. As an example, a hamiltonian written in terms of the generators of a Heisenberg-Weyl algebra is considered, *i.e.*,

$$H = c_0 \, b^\dagger b + c_2 \, (b^{\dagger 2} + b^2) + c_1 \, (b^\dagger + b) \,, \tag{1}$$

where the operators $b^\dagger$ and b satisfy standard creation and annihilation commutation relations. Although this hamiltonian can be solved analytically by means of a Bogoliubov transformation, we use it to illustrate the procedure to construct the coherent states and the ES of an algebraic model.

The coherent state is defined by the action of the raising generator on the vacuum state [1]

$$|\alpha\rangle = \exp(\alpha^* \, b^\dagger)|0\rangle \,. \tag{2}$$

The Baker-Campbell-Hausdorff formulas can be used to calculate the overlap of two coherent states and the coherent state representation of the creation and annihilation boson operators

$$\langle \alpha' | \alpha \rangle = \exp\left(\alpha' \alpha^*\right) \,, \tag{3}$$

$$\langle \alpha | b = \frac{\partial}{\partial \alpha} \langle \alpha | \,, \qquad \langle \alpha | b^\dagger = \alpha \langle \alpha | \,. \tag{4}$$

Then the energy surface is given by

$$E(\alpha) = \lim_{\alpha' \to \alpha} \frac{\langle \alpha' | H | \alpha \rangle}{\langle \alpha' | \alpha \rangle} \,. \tag{5}$$

Substituting the expressions (1), (3) and (4) into the previous one, one gets the result

$$E(\rho) = (c_0 + 2c_2)\rho^2 + 2c_1\rho , \tag{6}$$

where the reality condition $\alpha = \alpha^* = \rho$ was also used.

3 The Interacting Boson Model

In 1975 this model [4] was introduced to describe collective properties of even-even nuclei far from closed shells through the interactions between two kinds of bosons, one with angular momentum $L = 0$ (the s-boson) and another with angular momentum $L = 2$ (the d-boson). The six possible boson states give rise to a $U(6)$ group structure. The bosons represent pairs of fermions, the s-boson reflects the strong pairing attraction of identical nucleons whereas the d-boson is a result of the weaker $J = 2^+$ attraction [4]. Therefore nuclei are pictured as systems of s and d bosons, whose number is equal to half the number of the valence nucleons, the core being considered inert. When a shell is more than half full, hole-pairs are counted instead of particle-pairs.

The most general one and two body hamiltonian that conserves the total number of bosons is

$$
\begin{aligned}
H_{IBM} &= \varepsilon_s\, N_s + \varepsilon_d\, N_d + \sum_{L=0,2,4} \frac{c_L}{2} \sqrt{2L+1}\, [[d^\dagger \times d^\dagger]^{[L]} \times [\tilde{d} \times \tilde{d}]^{[L]}]^{[0]} \\
&+ \frac{v_0}{\sqrt{2}} \left([[d^\dagger \times d^\dagger]^{[2]} \times \tilde{d}]^{[0]} s + s^\dagger\, [d^\dagger \times [\tilde{d} \times \tilde{d}]^{[2]}]^{[0]} \right) \\
&+ \frac{v_2}{2} \left([[d^\dagger \times d^\dagger]^{[0]} s^2 + s^{\dagger 2} [\tilde{d} \times \tilde{d}]^{[0]} \right) \\
&+ \sqrt{5} u_0\, s^\dagger s\, [d^\dagger \times \tilde{d}]^{[0]} + u_2\, s^{\dagger 2} s^2 ,
\end{aligned}
\tag{7}
$$

where the sets of boson operators s, $s^\dagger$ and $d_\mu^\dagger$, d_μ satisfy the following, different from zero, commutators

$$\left[s, s^\dagger\right] = 1 , \qquad \left[d_\mu, d_{\mu'}^\dagger\right] = \delta_{\mu,\mu'} . \tag{8}$$

Now, we construct the coherent state of a six dimensional harmonic oscillator, following the procedure indicated in the previous section. However in this case the associated group is compact and then we restrict the exponential to only one term of the Taylor series expansion,

$$|N, \vec{\alpha}\rangle = A_N (s^\dagger + \sum_\mu \alpha_\mu d_\mu^\dagger)^N |0\rangle , \tag{9}$$

where A_N is the normalization constant. Evaluating the corresponding Eq.(5) one arrives to the formulae for the energy surface of the model [8], i.e.,

$$E(\beta, \gamma) = N\epsilon \frac{\beta^2}{(1+\beta^2)} + \frac{N(N-1)}{(1+\beta^2)^2}\, (a_1\beta^4 + a_2\beta^3 \cos 3\gamma + a_3\beta^2 + u_2) , \tag{10}$$

where it was used that the laboratory variables α_μ can be expressed in terms of two intrinsic parameters β and γ plus three Euler angles. Besides as the energy surface is a rotational invariant

all the dependence in the Euler angles disappear. The parameters a_1, a_2, a_3, and ϵ of the Eq.(10) are combinations of those that appear in the IBM-1 hamiltonian (7)

$$a_1 = \frac{c_0}{10} + \frac{c_2}{7} + \frac{9c_4}{35} , \tag{11}$$

$$a_2 = -\sqrt{\frac{8}{35}} v_0 , \tag{12}$$

$$a_3 = -\frac{2}{\sqrt{5}} v_2 + u_0 , \tag{13}$$

$$\epsilon = \epsilon_d - \epsilon_s . \tag{14}$$

4   Shapes and Stability of Energy Surfaces

The energy surfaces define functions of state variables and a set of parameters, and the Catastrophe theory is used to analize their equilibrium configurations. This formalism let us organize all the possible shapes of the ES into well defined separated regions of the parameters space.

To illustrate how this is done, we consider the potential energy surfaces (PES) of the simplest version of the Generalized Collective Model [5], $i.e.$,

$$V(\beta,\gamma; C_2, C_3) = \beta^4 - C_3 \beta^3 cos3\gamma + C_2 \beta^2 . \tag{15}$$

The equilibrium or critical points are determined by solving the equation $\nabla V(\beta,\gamma) = 0$. The results are given by $(0,0)$ and (β_0, γ_0), with

$$\beta_0 = \frac{3C_3 \pm \sqrt{9C_3^2 - 32C_2}}{8} , \quad \gamma_0 = 0, \pi/3 . \tag{16}$$

The set of degenerated critical points defines a locus in the parameters space which is called the *Separatrix*. This can be obtained through the determinant of the Hessian matrix or by other procedures, in this case it is immediate that the critical points are double degenerated if the parameters satisfy the expressions

$$9 C_3^2 - 32 C_2 = 0 , \tag{17}$$

$$C_2 = 0 , \quad C_3 \neq 0 . \tag{18}$$

For the expression (17) the critical points are localized in $\beta_0 = 3C_3/8$ while for (18) in $\beta_0 = 0$. Besides, it is straight to prove that if $C_2 = 0$ and $C_3 = 0$ the critical point is triple degenerated and localized at $\beta_0 = 0$. The *Separatrix* of the system is shown in Fig.1. It divides the space in regions each characterizing a typical shape yield by the model. By means of the transformation $\beta = y + C_3/4$ the *Separatrix* is taken to the canonical form of the Cusp catastrophe.

Now we study the equilibrium configurations of the energy surface associated to the IBM-1, which is given in Eq.(10). Then we calculate the critical points by taking the derivatives with respect to β and γ variables. It is straightforward to see that the critical points correspond only to $\gamma = 0$ (prolate case) or $\gamma = \pi/3$ (oblate case). Therefore we can restrict to the prolate case,

without losing generality. The energy surface (10), with $\gamma = 0$, can be re-written in terms of the following parameters

$$r_1 = -\frac{2u_2(N-1) - (N-1)a_3 - \epsilon}{2a_1(N-1) - (N-1)a_3 + \epsilon} , \tag{19}$$

$$r_2 = -\frac{2a_2(N-1)}{2a_1(N-1) - (N-1)a_3 + \epsilon} , \tag{20}$$

and it takes the form

$$E(\beta) = \frac{1}{(1+\beta^2)^2} \left\{ \beta^4 + r_1\beta^2(\beta^2 + 2) - r_2\beta^3 \right\} , \tag{21}$$

where $E(\beta) = E(\beta, \gamma = 0)/N - \epsilon_s - u_2(N-1)$. One has to notice that the oblate case can be regained by interchanging r_2 by $-r_2$ or equivalently a_2 by $-a_2$.
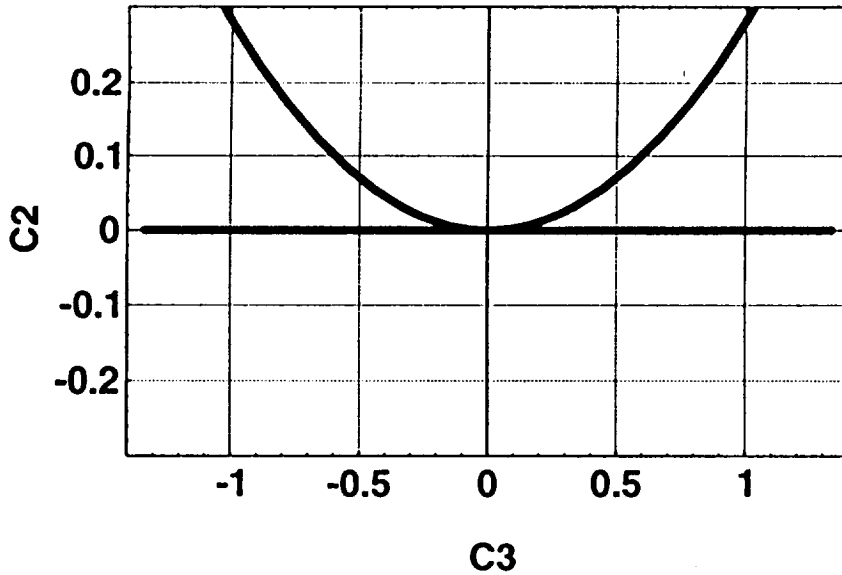
FIG. 1. Separatrix for the Bohr Mottelson Hamiltonian

To find the extrema in β of the Eq.(21) one needs to solve the equation

$$\beta \left(r_2\beta^3 + 4\beta^2 - 3r_2\beta + 4r_1 \right) = 0 . \tag{22}$$

From this expression, one determines the locus in the parameters space (r_2, r_1) of degenerated critical points. Then the Separatrix of the model is defined by the curves

$$r_1 = \pm\frac{(16 + 9r_2^2)^{3/2}}{54r_2^2} - \frac{32}{27r_2^2} - 1 , \tag{23}$$

$$r_1 = 0 . \tag{24}$$

This Separatrix is shown in Fig.2 and it corresponds to the Cusp catastrophq although it does not has the canonical form.
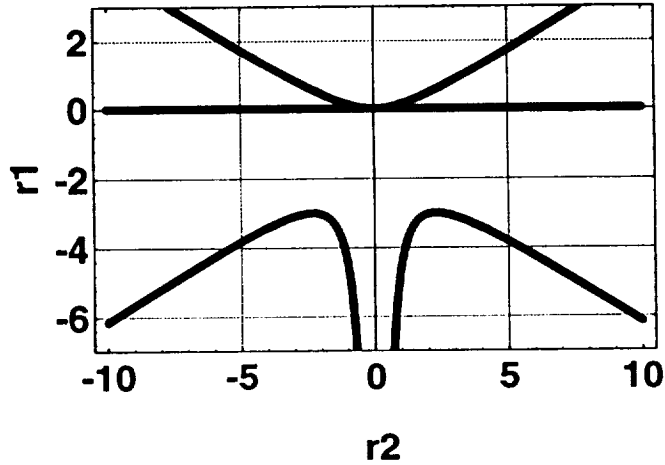
FIG. 2. Separatrix for the IBM-1 Hamiltonian

Now we applied the results to find the shapes and stability of the Ru and Sm isotopes. For the Ru case, one has the number of valence protons pairs, $N_\pi = 3$. As we consider isotopes with a mass number varying from $A = 98 - 110$, the corresponding number of neutron bosons runs from $N_\nu = 2$ to $N_\nu = 8$. Thus the size of the space in the IBM-1 is determined by the total number of bosons, which is the sum of the numbers of proton and neutron bosons. In the Sm case, one has the number of proton bosons, $N_\pi = 6$, and as we take into account $A = 148 - 160$, the number of neutron bosons runs from $N_\nu = 2$ to $N_\nu = 8$. An analysis of their energy spectra and electromagnetic transitions using the hamiltonian (7) is made in [11] and [12]. For both isotope chains, the parameters used are presented in the first eight columns of Table I. Substituting these parameters into the equations (11) to (13) we get the values of a_1, a_2 and a_3. These are given in the last three columns of Table I, by means of which one can easily construct the corresponding energy surface of each nucleus.

To find the region of the $Separatrix$, Fig. 2, where the different isotopes are localized one calculates the parameters r_1 and r_2 through the equations (19) and (20), as functions of the total number of bosons. For the Ru, one gets the expressions

$$r_1 = \frac{990.2 + 146.2(N - 1)}{990.2 + 40.2(N - 1)} \ , \qquad r_2 = 0 \ , \tag{25}$$

while for the Sm isotopes the parameters are

$$r_1 = \frac{2171.2 + 258.3\,(N - 1)}{2171.2 + 151.2\,(N - 1)} \ , \qquad r_2 = \frac{86\,(N - 1)}{2175 - 151\,(N - 1)} \ . \tag{26}$$

The localization of the points (25) and (26) are shown in Fig. 3 and Fig 4, respectively.

TABLE I. Parameters, in KeV units, used to describe the Ru and Sm isotope chains

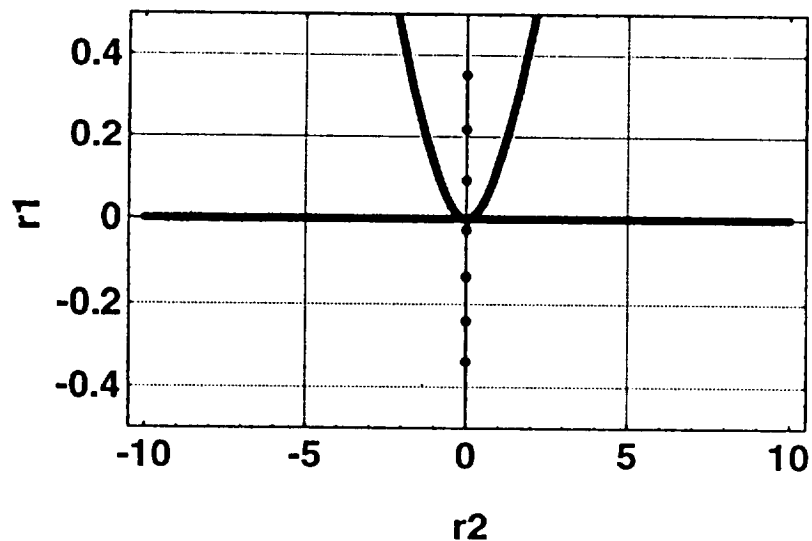|	ϵ	c_0	c_2	c_4	u_0	u_2	v_0	v_2	a_1	a_2	a_3
Ru	990.2	-185.4	-77.4	-.0.4	-53.0	23.3	0	-52.1	-29.7	0	-52.1
Sm	2170.6	-613.7	-318.8	-377.6	227.4	0.4	89.9	-33.0	-204.1	-43.0	-256.9

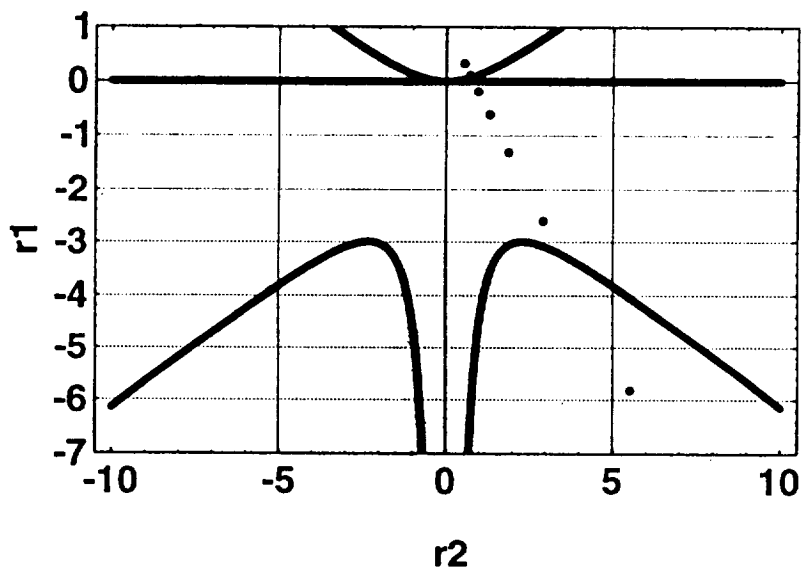FIG. 3. Plot of the points (25) associated to the Ru isotopes chain.

FIG. 4. Plot of the points (26) associated to the Sm isotopes chain.

5 Conclusions

For the Bohr-Mottelson model the yielded shapes and equilibrium configurations are classified by the *Separatrix* of Fig.1. One can identify four regions: (i) Above the parabola, the PES have one minimum at $\beta = 0$. ii) Between the parabola and the C_2 axis, in the PES appear additionally a second minimum at $\beta \neq 0$. iii) Below the C_3 axis the PES have two mimima at $\beta \neq 0$ and

the maximum occurs at $\beta = 0$. The PES around these critical points can be approximated by an harmonic oscillator. iv) On the locus of points that define the *Separatrix*, we have shape transitions and in the vecinity of the critical points (16) the PES cannot be approximated by quadratic functions. It is important to remark that the PES have a mirror symmetry along the C_3 axis, which physically represents transitions from prolate to oblate shapes.

For the IBM-1 hamiltonian one gets (see Fig. 2): (i) For positive values of r_1 one has two regions, above the curve the ES present one minimum at $\beta = 0$ and below the curve they have a second minumum at $\beta \neq 0$. ii) For negative values of r_1 one has again two regions, above the curve the ES are built with two minima at $\beta \neq 0$ and a maximum at $\beta = 0$ and below of it, the ES have one mimimum point at $\beta \neq 0$ and a maximum at $\beta = 0$. For the critical points mentioned above the energy surfaces can be approximated by an harmonic oscillator. iii) Finally on the *Separatrix*, there are shape transitions, and in the vecinity of their critical points the ES cannot be approximated by quadratic functions. It is important to remark that these ES have also a mirror symmetry along the r_2 axis, representing transitions from prolate to oblate shapes.

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A RAMANUJAN-TYPE MEASURE FOR THE ASKEY-WILSON POLYNOMIALS

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Abstract

A Ramanujan-type representation for the Askey-Wilson q-beta integral, admitting the transformation $q \to q^{-1}$, is obtained. Orthogonality of the Askey-Wilson polynomials with respect to a measure, entering into this representation, is proved. A simple way of evaluating the Askey-Wilson q-beta integral is also given.

1 Introduction.

The Askey-Wilson polynomials $p_n(x; a, b, c, d|q)$ [1], which have already become classical, represent a five-parameter system of polynomials. They satisfy the orthogonality relation

$$\int_{-1}^{1} p_m(x; a, b, c, d|q)\, p_n(x; a, b, c, d|q)\, w(x; a, b, c, d|q)\, dx = \delta_{mn} I_n(a, b, c, d|q) \tag{1.1}$$

with respect to the absolutely continuous measure $d\alpha(x) = w(x)dx$, with the weight function

$$w(x; a, b, c, d|q) = \frac{1}{\sin\theta} \frac{h(\cos 2\theta, 1; q)}{\prod_{v=a,b,c,d} h(\cos\theta, v; q)}, \quad x = \cos\theta, \tag{1.2}$$

$$h(a, b; q) = \prod_{j=0}^{\infty}(1 - 2abq^j + b^2 q^{2j}).$$

As special and limiting cases, the Askey-Wilson polynomials contain many known systems of polynomials (see, for example, [2]). In particular, the choice of the parameters $a = -b = \sqrt{\beta}$, $c = -d = \sqrt{q\beta}$, leads to the continuous q-ultraspherical polynomials $C_n(x; \beta|q)$ [3], i.e.,

$$p_n(x; \sqrt{\beta}, -\sqrt{\beta}, \sqrt{q\beta}, -\sqrt{q\beta}|q) = \frac{(\beta^2; q)_{2n}(q; q)_n}{(\beta, \beta^2; q)_n} C_n(x; \beta|q), \tag{1.3}$$

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where we have used the standard notation of the theory of q-special functions

$$(a;q)_n = \prod_{j=0}^{n-1}(1 - aq^j), \qquad (a_1,...,a_k;q)_n = \prod_{j=1}^{k}(a_j;q)_n. \qquad (1.4)$$

In turn, from $C_n(x;\beta|q)$ one can obtain the continuous q-Hermite polynomials $H_n(x|q) = (q;q)_n C_n(x;0|q)$, the Gegenbauer (ultraspherical) polynomials $C_n^\lambda(x) = \lim_{q\to 1} C_n(x;q^\lambda|q)$, and also the Chebyshev polynomials of the first and second kinds, $T_n(x)$ and $U_n(x)$, by taking the limit $\beta \to 1$ or by putting $\beta = q$ in $C_n(x;\beta|q)$, respectively.

The key ingredient of the original proof of the orthogonality (1.1), which led to the discovery of the Askey-Wilson system of polynomials (see the discussion of this point in [4]), was the evaluation of the Askey-Wilson q-beta integral:

$$I_0(a,b,c,d|q) \equiv \int_{-1}^{1} w(x;a,b,c,d|q)dx = \frac{2\pi(abcd;q)_\infty}{(q,ab,ac,ad,bc,bd,cd;q)_\infty},$$

$$(1.5)$$

$$max_{v=a,b,c,d}|v| < 1, \quad |q| < 1.$$

The integral (1.5) has acquired its name because in a special case, when the parameters $a = q^{\alpha+1/2}$, $b = -q^{\beta+1/2}$, and $c = -d = q^{1/2}$, the $q \to 1^-$ limit of $I_0(a,b,c,d|q)$ is the beta function (or Euler's integral of the first kind)

$$\int_{-1}^{1}(1-x)^\alpha(1+x)^\beta dx = 2^{\alpha+\beta+1}B(\alpha+1,\beta+1) = 2^{\alpha+\beta+1}\frac{\Gamma(\alpha+1)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+2)}. \qquad (1.6)$$

A nonstandard form of the orthogonality on the full real line for the continuous q-Hermite polynomials $H_n(\sin\kappa x|q)$, $q = \exp(-2\kappa^2)$, was considered in [5]. It turned out that if one uses the modular transformation and the periodicity property of the ϑ-function appearing in the weight function for these polynomials, the finite interval of orthogonality can be transformed into an infinite one. This technique is of interest both from a mathematical point of view and from the point of view of possible applications in theoretical physics, beginning with a number of problems, related with q-oscillators (see the review [6]).

The purpose of this article is to discuss the applicability of this idea to the more general case, i.e. to the Askey-Wilson q-beta integral (1.5) [7, 8]. To simplify consideration it will be assumed in Sections 2-4 that $|v| < 1$, $v = a,b,c,d$, and that the parameter $q = \exp(-2\kappa^2)$ satisfies the requirement $0 < q < 1$. The possibility of extending these results to other values of the parameters is discussed in Section 5.

2 A Ramanujan-type representation for the q-beta integral.

From the point of view of symmetry the parametrization $x = \sin\varphi$ is most convenient; it corresponds to the change of variable $\theta = \frac{\pi}{2} - \varphi$, $-\frac{\pi}{2} \leq \varphi \leq \frac{\pi}{2}$ in formula (1.2). Consequently, the left

side of (1.5) is equal to

$$I_0(a, b, c, d|q) = \int_{-\pi/2}^{\pi/2} \frac{h(-\cos 2\varphi, 1; q)}{\prod_{v=a,d,c,d} h(\sin\varphi, v; q)} \, d\varphi .$$ (2.1)

Comparison of the numerator

$$h(-\cos 2\varphi, 1; q) = \prod_{j=0}^{\infty}(1 + 2q^j \cos 2\varphi + q^{2j})$$

of the integral (2.1) with Jacobi's expression for the theta-function $\vartheta_2(z, q) \equiv \vartheta_2(z|\tau)$, $q = \exp(\pi i\tau)$ as an infinite product [9]

$$\vartheta_2(z, q) = 2q^{1/4}(q^2; q^2)_\infty \cos z \prod_{j=1}^{\infty}(1 + 2q^{2j} \cos 2z + q^{4j}),$$ (2.2)

shows that

$$h(-\cos 2\varphi, 1; q) = \frac{2\cos\varphi}{q^{1/8}(q; q)_\infty} \vartheta_2(\varphi, q^{1/2})$$ (2.3)

and therefore

$$I_0(a, b, c, d|q) = \frac{2}{q^{1/8}(q; q)_\infty} \int_{-\pi/2}^{\pi/2} \frac{\vartheta_2(\varphi, q^{1/2}) \cos\varphi}{\prod_{v=a,b,c,d} h(\sin\varphi, v; q)} \, d\varphi .$$ (2.4)

With the aid of the modular transformation [9]

$$\vartheta_2(z|\tau) = \frac{\exp\left(-\frac{iz^2}{\pi\tau}\right)}{(-i\tau)^{\frac{1}{2}}} \vartheta_4(z\tau^{-1}|-\tau^{-1}), \qquad \tau = \frac{i\kappa^2}{\pi},$$ (2.5)

and the change of variable $\varphi = \kappa x$, the integral (2.4) can be written as

$$I_0(a, b, c, d|q) = \frac{2\sqrt{\pi}}{q^{1/8}(q; q)_\infty} \int_{-\pi/2\kappa}^{\pi/2\kappa} \frac{\vartheta_4\left(\frac{\pi i}{\kappa}x, e^{-\pi^2/\kappa^2}\right) e^{-x^2} \cos\kappa x}{\prod_{v=a,b,c,d} h(\sin\kappa x, v; q)} \, dx.$$ (2.6)

Using the expansion

$$\vartheta_4(z, q) = \sum_{k=-\infty}^{\infty}(-1)^k q^{k^2} e^{2ikz}$$ (2.7)

and taking into account the uniform convergence of the series (2.7) in any bounded domain of values of z [9], we substitute (2.7) into (2.6) and integrate this series termwise, i.e.,

$$I_0(a, b, c, d|q) = \frac{2\sqrt{\pi}}{q^{1/8}(q; q)_\infty} \sum_{k=-\infty}^{\infty}(-1)^k \int_{-\pi/2\kappa}^{\pi/2\kappa} \frac{e^{-(x+\pi/\kappa k)^2} \cos\kappa x \, dx}{\prod_{v=a,b,c,d} h(\sin\kappa x, v; q)}.$$ (2.8)

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The change of variable $x_k = x + \frac{\pi}{\kappa}k$, $x_k^{min} = \frac{\pi}{\kappa}(k - \frac{1}{2}) \leq x_k \leq \frac{\pi}{\kappa}(k + \frac{1}{2}) = x_k^{max}$ and an account for the relation $x_{k-1}^{max} = x_k^{min}$ allows to sum the right-hand side of (2.8) with respect to k and represent (2.8) in the form

$$I_0(a,b,c,d|q) = \frac{2\sqrt{\pi}}{q^{1/8}(q;q)_\infty} \tilde{I}_0(a,b,c,d|q) = \frac{2\sqrt{\pi}}{q^{1/8}(q;q)_\infty} \int_{-\infty}^{\infty} \frac{e^{-x^2}\cos\kappa x \, dx}{\prod_{v=a,b,c,d} h(\sin\kappa x, v; q)}. \qquad (2.9)$$

Thus, combining formulas (1.5) and (2.9) yields the following representation for the Askey-Wilson q-beta integral [7]

$$\tilde{I}_0(a,b,c,d|q) \equiv \int_{-\infty}^{\infty} \rho(\kappa x; a,b,c,d|q) e^{-x^2}\cos\kappa x \, dx = \frac{\sqrt{\pi}q^{\frac{1}{8}}(abcd;q)_\infty}{(ab,ac,ad,bc,bd,cd;q)_\infty}, \qquad (2.10)$$

where, in accordance with the definition (1.2),

$$\rho(x; a,b,c,d|q) = \prod_{v=a,b,c,d} h^{-1}(\sin x, v; q) = \prod_{v=a,b,c,d} e_q(ive^{-ix})e_q(-ive^{ix}), \qquad (2.11)$$

and $e_q(z) = (z;q)_\infty^{-1}$ is the q-exponential function [2].

We note that each factor $h^{-1}(\sin\kappa x, v; q)$, $v = a,b,c,d$, in the integrand (2.10) is represented as

$$h^{-1}(\sin\kappa x, v; q) = \sum_{n=0}^{\infty}(iv)^n \sum_{k=0}^{n} \frac{(-1)^k \exp[-i(n-2k)\kappa x]}{(q;q)_k(q;q)_{n-k}}, \qquad (2.12)$$

if one uses the generating function for the continuous q-Hermite polynomials $H_n(x|q)$

$$(te^{i\theta}, te^{-i\theta}; q)_\infty^{-1} = \sum_{n=0}^{\infty} \frac{H_n(\cos\theta|q)}{(q;q)_n}t^n \qquad |t| < 1, \qquad (2.13)$$

and their explicit representation [2]

$$H_n(\cos\theta|q) = \sum_{k=0}^{n} \begin{bmatrix} n \\ k \end{bmatrix}_q e^{i(n-2k)\theta}, \qquad (2.14)$$

where the symbol $\begin{bmatrix} n \\ k \end{bmatrix}_q$ denotes the q-binomial coefficient [2]. Therefore the integration over x in (2.10) is reduced to the Fourier transformation formula for the ground state of the linear harmonic oscillator

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp(-x^2/2 + ixy)dx = \exp(-y^2/2). \qquad (2.15)$$

An explicit evaluation of the nonstandard form of the Askey-Wilson q-beta integral (2.10) will be discussed in greater detail in Section 4.

As mentioned above, the weight function (1.2) with the parameters $a = -b = \beta^{1/2}$, $c = -d = aq^{1/2}$, corresponds to the continuous q-ultraspherical polynomials $C_n(x; \beta|q)$. The relations [2]

$$(a;q)_\infty = (a, aq; q^2)_\infty, \qquad (a, -a; q)_\infty = (a^2; q^2)_\infty,$$

enable the representation (2.10) for this particular case to be simplified to

$$\int_{-\infty}^{\infty} \frac{\exp\left(-x^2 + i\kappa x\right)dx}{(-\beta\exp\left(2i\kappa x\right), -\beta\exp\left(-2i\kappa x\right); q)_\infty} = \frac{\sqrt{\pi}q^{1/8}(\beta, q\beta; q)_\infty}{(\beta^2; q)_\infty}. \tag{2.16}$$

If one compares (2.16) with the Ramanujan integral ($q = \exp\left(-2k^2\right)$, $|q| < 1$) [10, 11]

$$\int_{-\infty}^{\infty} e^{-x^2 + 2mx} e_q(aq^{1/2}e^{2ikx}) e_q(bq^{1/2}e^{-2ikx})\, dx = \frac{\sqrt{\pi}e^{m^2}}{(qab; q)_\infty} E_q(aqe^{2imk}) E_q(bqe^{-2imk}), \tag{2.17}$$

it is easy to verify that (2.16) agrees with (2.17) if one sets $2m = ik = i\kappa$ and $a = b = -\beta q^{1/2}$.

3 Orthogonality of the Askey-Wilson polynomials with respect to the measure $\rho(\kappa x; a, b, c, d|q)$.

A direct proof of the orthogonality for the Askey-Wilson polynomials

$$\int_{-\infty}^{\infty} p_m(\sin\kappa x; a, b, c, d|q) p_n(\sin\kappa x; a, b, c, d|q)\rho(\kappa x; a, b, c, d|q) \exp\left(-x^2\right) \cos\kappa x\, dx =$$

$$= \delta_{mn}\tilde{I}_n(a, b, c, d|q) \tag{3.1}$$

with respect to the weight function appearing in the nonstandard integral representation (2.10), is analogous to the proof of eigenfunctions orthogonality for the Sturm-Liouville differential equation [12] . Indeed, the difference differentiation formula for the Askey-Wilson polynomials [1]

$$\sin\kappa\partial_x\, p_n(\sin\kappa x; a, b, c, d|q) = \tag{3.2}$$

$$= q^{-n/2}(1 - q^n)(1 - abcdq^{n-1})\, \cos\kappa x\, p_{n-1}(\sin\kappa x; aq^{1/2}, bq^{1/2}, cq^{1/2}, dq^{1/2}|q)$$

provides a lowering operator for these polynomials. To find a raising operator one can use the relation

$$w(\sin\varphi; a, b, c, d|q) = \frac{2\vartheta_2(\varphi, q^{1/2})}{q^{1/8}(q; q)_\infty}\, \rho(\varphi; a, b, c, d|q), \tag{3.3}$$

which follows from (1.2), (2.3) and (2.11), and write the difference equation for the Askey-Wilson polynomials [1] in the form

$$\sin\kappa\partial_x\left[\frac{\vartheta_2(\kappa x, q^{1/2})}{\cos\kappa x}\rho(\kappa x; aq^{1/2}, bq^{1/2}, cq^{1/2}, dq^{1/2}|q)\sin\kappa\partial_x p_n(\sin\kappa x; a, b, c, d|q)\right] =$$

$$\tag{3.4}$$

$$= (1 - q^{-n})(1 - abcdq^{n-1})\cos\kappa x\, \vartheta_2(\kappa x, q^{1/2})\rho(\kappa x; a, b, c, d|q)\, p_n(\sin\kappa x; a, b, c, d|q).$$

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Now, using the difference differentiation formula (3.2) in the left-hand side of (3.4) and the periodicity property of the ϑ_2-function [9],

$$\vartheta_2(z \pm \pi\tau, q) = q^{-1} \exp\left(\mp 2iz\right)\vartheta_2(z, q), \qquad q = \exp\left(\pi i\tau\right), \tag{3.5}$$

we arrive at the raising operator

$$(\sin 2\kappa x \cos \kappa\partial_x - \cos 2\kappa x \sin \kappa\partial_x)\rho(\kappa x; aq^{1/2}, bq^{1/2}, cq^{1/2}, dq^{1/2}|q)$$

$$p_{n-1}(\sin \kappa x; aq^{1/2}, bq^{1/2}, cq^{1/2}, dq^{1/2}|q) = q^{\frac{1-n}{2}} \cos \kappa x\, \rho(\kappa x; a, b, c, d|q)p_n(\sin \kappa x; a, b, c, d|q). \tag{3.6}$$

We are now in a position to give a direct proof of the orthogonality relation (3.1). We multiply both sides of the equality (3.6) by $p_m(\sin \kappa x; a, b, c, d|q) \exp\left(-x^2\right)$ and integrate in x over the full real line. As a result we obtain in the right-hand side,

$$q^{\frac{1-n}{2}} \int_{-\infty}^{\infty} p_m(\sin \kappa x; a, b, c, d|q)\, p_n(\sin \kappa x; a, b, c, d, |q)\, \rho(\kappa x; a, b, c, d|q)\, e^{-x^2} \cos \kappa x\, dx \equiv$$

$$q^{\frac{1-n}{2}} I_{mn}(a, b, c, d|q). \tag{3.7}$$

The left-hand side

$$\int_{-\infty}^{\infty} dx p_m(\sin \kappa x; a, b, c, d|q)e^{-x^2}(\sin 2\kappa x \cos \kappa\partial_x - \cos 2\kappa x \sin \kappa\partial_x)$$

$$\tag{3.8}$$

$$\rho(\kappa x; aq^{1/2}, bq^{1/2}, cq^{1/2}, dq^{1/2}|q)\, p_{n-1}(\sin \kappa x; aq^{1/2}, bq^{1/2}, cq^{1/2}, dq^{1/2}|q),$$

can be integrated by parts with the aid of (3.2) and the evident relations

$$\int_{-\infty}^{\infty} dx f(x) \cos \kappa\partial_x \varphi(x) = \int_{-\infty}^{\infty} dx\, \varphi(x) \cos \kappa\partial_x f(x),$$

$$\tag{3.9}$$

$$\int_{-\infty}^{\infty} dx f(x) \sin \kappa\partial_x \varphi(x) = -\int_{-\infty}^{\infty} dx\, \varphi(x) \sin \kappa\partial_x f(x),$$

which apply to (3.8) because the function $\rho(\kappa z; aq^{1/2}, bq^{1/2}, cq^{1/2}, dq^{1/2}|q)$ has no singularities inside of the strip $-\kappa \leq y \leq \kappa$, $-\infty < x < \infty$ in the complex plane $z = x + iy$. This leads to

$$q^{\frac{1-m}{2}}(1 - q^m)(1 - abcdq^{m-1})I_{m-1n-1}(aq^{1/2}, bq^{1/2}, cq^{1/2}, dq^{1/2}|q). \tag{3.10}$$

Equating the right-hand (3.7) and left-hand (3.10) sides thus yields

$$q^{\frac{m-n}{2}} I_{mn}(a, b, c, d|q) = (1 - q^m)(1 - abcdq^{m-1})I_{m-1n-1}(aq^{1/2}, bq^{1/2}, cq^{1/2}, dq^{1/2}|q). \tag{3.11}$$

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We now interchange m and n in (3.11) and take into account that the integral $I_{mn}(a,b,c,d|q)$ is symmetric in m and n due to the definition (3.7), *i.e.*,

$$q^{\frac{n-m}{2}} I_{mn}(a,b,c,d|q) = (1 - q^n)(1 - abcdq^{n-1})I_{m-1n-1}(aq^{1/2}, bq^{1/2}, cq^{1/2}, dq^{1/2}|q). \qquad (3.11')$$

Finally, multiplying both sides of (3.11) by $(1 - q^n)(1 - abcdq^{n-1})$ and of (3.11') by $(1 - q^m)(1 - abcdq^{m-1})$ and subtracting the second expression from the first, we get

$$(q^{\frac{m-n}{2}} - q^{\frac{n-m}{2}})(1 - abcdq^{m+n-1})I_{mn}(a,b,c,d|q) = 0. \qquad (3.12)$$

From (3.12) it follows that $I_{mn}(a,b,c,d|q) = \delta_{mn}\tilde{I}_n(a,b,c,d|q)$, confirming the orthogonality (3.1) of the Askey-Wilson polynomials for $m \neq n$ [8].

We note that as special and limiting cases, (3.1) contains the orthogonality relations for other known sets of polynomials, such as the continuous q-ultraspherical polynomials $C_n(x; \beta|q)$, the continuous q-Hermite polynomials $H_n(x; q) = (q; q)_n C_n(x; 0|q)$ (the corresponding special case of (3.1), when the all parameters a, b, c, d are equal to zero, is considered in [5]), the Chebyshev polynomials of the first and second kinds, $T_n(x)$ and $U_n(x)$, and so on.

4 Evaluation of the integrals $\tilde{I}_n(a,b,c,d|q)$.

Iterating the recurrence relation

$$\tilde{I}_n(a,b,c,d|q) = (1 - q^n)(1 - abcdq^{n-1})\tilde{I}_{n-1}(aq^{1/2}, bq^{1/2}, cq^{1/2}, dq^{1/2}|q), \qquad (4.1)$$

which follows from (3.11) or (3.11') when $m = n$, allows to express the normalization integrals $\tilde{I}_n(a,b,c,d|q)$, $n = 1, 2, ...$, through a known value of the Askey-Wilson q-beta integral $\tilde{I}_0(a,b,c,d|q)$, i.e.

$$\tilde{I}_n(a,b,c,d|q) = \frac{(q, ab, ac, ad, bc, bd, cd; q)_n}{(1 - abcdq^{2n-1})(abcd; q)_{n-1}} \tilde{I}_0(a,b,c,d|q). \qquad (4.2)$$

It only remains to evaluate the integral $\tilde{I}_0(a,b,c,d|q)$ itself. To this end, having defined the symmetrical $\rho_+(x)$ and antisymmetrical $\rho_-(x)$ combinations with respect to the inversion $x \rightarrow -x$,

$$\rho_{\pm}(x; a,b,c,d|q) = \tfrac{1}{2}[\rho(x; a,b,c,d|q) \pm \rho(-x; a,b,c,d|q)], \qquad (4.3)$$

it is convenient to rewrite (2.10) as

$$\tilde{I}_0(a,b,c,d|q) = \int\limits_{-\infty}^{\infty} dx \exp\left(-x^2 + i\kappa x\right)\rho_+(\kappa x; a,b,c,d|q). \qquad (4.4)$$

Let us carry out the replacements $v \rightarrow v\sqrt{q}$, $v = a, b, c, d$, and the subsequent shift of the variable of integration $x \rightarrow x + i\kappa$ in (4.4). (We remind that the function $\rho(\kappa z; aq^{1/2}, bq^{1/2}, cq^{1/2}, dq^{1/2}|q)$ does not have singularities in the strip $-\kappa \leq y \leq \kappa$, $-\infty < x < \infty$ of the complex plane $z = x + iy$). Then, taking into account that in accordance with the definitions (1.2) and (2.11)

$$\rho(\kappa(x + i\kappa); aq^{1/2}, bq^{1/2}, cq^{1/2}, dq^{1/2}|q) = \rho(\kappa x; a,b,c,d|q) \prod_{v=a,b,c,d} (1 + iv \exp(i\kappa x)), \qquad (4.5)$$

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we obtain

$$\tilde{I}_0(aq^{1/2}, bq^{1/2}, cq^{1/2}, dq^{1/2}|q) = (1 - s_2)\tilde{I}_0(a, b, c, d|q) +$$

(4.6)

$$+ s_4 \int_{-\infty}^{\infty} dx \exp\left(-x^2 + 3i\kappa x\right)\rho_+(\kappa x; a, b, c, d|q) - is_3 \int_{-\infty}^{\infty} dx \exp\left(-x^2 + 2i\kappa x\right)\rho_-(\kappa x; a, b, c, d|q),$$

where

$$s_2 = ab + ac + ad + bc + bd + cd,$$

(4.7)

$$s_3 = abc + abd + acd + bcd, \quad s_4 = abcd.$$

It remains only to express the second and third integrals in the right-hand side of (4.6) in terms of $\tilde{I}_0(a, b, c, d|q)$. To that end one can use the $n = 1$ case of (3.6)

$$(\sin 2\kappa x \cos \kappa \partial_x - \cos 2\kappa x \sin \kappa \partial_x)\rho(\kappa x; aq^{1/2}, bq^{1/2}, cq^{1/2}, dq^{1/2}|q) =$$

(4.8)

$$= [(1 - s_4)\sin 2\kappa x + (s_3 - s_1)\cos \kappa x]\rho(\kappa x; a, b, c, d|q),$$

taking into account that $p_0(x; a, b, c, d|q) = 1$, $p_1(x; a, b, c, d|q) = 2(1 - s_4)x + s_3 - s_1$ and $s_1 = a + b + c + d$. The symmetrization of (4.8) leads to the relations

$$(\sin 2\kappa x \cos \kappa \partial_x - \cos 2\kappa x \sin \kappa \partial_x)\rho_{\pm}(\kappa x; aq^{1/2}, bq^{1/2}, c\,q^{1/2}, d\,q^{1/2}|q) =$$

(4.9)

$$= (1 - s_4)\sin 2\kappa x\, \rho_{\pm}(\kappa x; a, b, c, d|q) + (s_3 - s_1)\cos \kappa x\, \rho_{\mp}(\kappa x; a, b, c, d|q).$$

Multiplying both sides of the equality (4.9) for the antisymmetrical combination $\rho_-(\kappa x)$ by $\exp(-x^2)$ and integrating over the variable x yields

$$(1 - s_4) \int_{-\infty}^{\infty} dx \exp\left(-x^2 + 2i\kappa x\right)\rho_-(\kappa x; a, b, c, d|q) = i(s_1 - s_3)\tilde{I}_0(a, b, c, d|q). \qquad (4.10)$$

Now we multiply both sides of (4.9) for $\rho_+(\kappa x; aq^{1/2}, bq^{1/2}, cq^{1/2}, dq^{1/2}|q)$ by $\exp\left(-x^2 + i\kappa x\right)$ and integrate over x. Using (4.10), the result can be written as

$$\int_{-\infty}^{\infty} dx \exp(-x^2 + 3i\kappa x)\rho_+(\kappa x; a, b, c, d|q) =$$

(4.11)

$$= \left[1 - \frac{(s_3 - s_1)^2}{(1 - s_4)^2}\right] \tilde{I}_0(a, b, c, d|q) - \frac{1 - q}{1 - s_4} \tilde{I}_0(aq^{1/2}, bq^{1/2}, cq^{1/2}, dq^{1/2}|q).$$

Substituting (4.10) and (4.11) into (4.6), we find

$$(1 - abcd)(1 - qabcd)\, \tilde{I}_0(aq^{1/2}, bq^{1/2}, cq^{1/2}, dq^{1/2}|q) =$$

$$\text{(4.12)}$$

$$= (1 - ab)(1 - ac)(1 - ad)(1 - bc)(1 - bd)(1 - cd)\, \tilde{I}_0(a, b, c, d|q).$$

Since $0 < q < 1$, by iterating equation (4.12) one can express the Askey-Wilson q-beta integral (2.10) with arbitrary parameters in terms of its value for vanishing parameters a, b, c, d, $i.e.$,

$$\tilde{I}_0(a, b, c, d|q) = \frac{(abcd; q)_\infty}{(ab, ac, ad, bc, bd, cd; q)_\infty}\, \tilde{I}_0(0, 0, 0, 0|q). \qquad \text{(4.13)}$$

The value of $\tilde{I}_0(0, 0, 0, 0|q)$ is easily found from (2.10) and (3.1) with the aid of the Fourier transformation formula (2.15) for the quadratically decreasing exponential function, $i.e.$,

$$\tilde{I}_0(0, 0, 0, 0|q) = \int_{-\infty}^{\infty} dx \exp\left(-x^2 + i\kappa x\right) = \sqrt{\pi} q^{1/8}. \qquad \text{(4.14)}$$

Combining formulas (4.13) and (4.14) leads to

$$\tilde{I}_0(a, b, c, d|q) = \frac{\sqrt{\pi} q^{1/8}(abcd; q)_\infty}{(ab, ac, ad, bc, bd, cd; q)_\infty}, \qquad \text{(4.15)}$$

which is the known value of the Askey-Wilson q-beta integral [1]

$$I_0(a, b, c, d|q) = \frac{2\sqrt{\pi}}{q^{1/8}(q; q)_\infty} \tilde{I}_0(a, b, c, d|q) = \frac{2\pi(abcd; q)_\infty}{(q, ab, ac, ad, bc, bd, cd; q)_\infty}. \qquad \text{(4.15')}$$

Substituting (4.15) into (4.2), we finally obtain the explicit form for the normalization integral

$$\tilde{I}_n(a, d, c, d|q) = \frac{\sqrt{\pi} q^{1/8}(q; q)_n(abcdq^{n-1}; q)_\infty}{(1 - abcdq^{2n-1})(abq^n, acq^n, adq^n, bcq^n, bdq^n, cdq^n; q)_\infty}. \qquad \text{(4.16)}$$

The complications arising in the evaluation of the standard form of the Askey-Wilson q-beta integral (1.5) can be illustrated by the following short quotation from reference [4]: "This was surprisingly hard, and it has taken over five years before relatively simple ways of evaluating this integral were found".

5 The transformation $q \to q^{-1}$.

It is necessary to emphasize that the nonstandard orthogonality relation (3.1) admits the transformation $q \to q^{-1}$ [7, 8]. The standard form of the Askey-Willson integral (1.5) does not in general have this property. Even in the simplest case of vanishing parameters a, b, c and d, which corresponds to the continuous q-Hermite polynomials $H_n(x|q)$, the definition of a weight function for the system of polynomials $h_n(x; q) = i^{-n} H_n(ix|q^{-1})$ requires a special analysis [13, 14].

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Since

$$(z; q^{-1})_\infty = (qz; q)_\infty^{-1}, \qquad (5.1)$$

the change $q \to q^{-1}$ (i.e. $\kappa \to i\kappa$) in the function $\rho(\kappa x; a, b, c, d|q)$ appearing in (2.10) and (3.1), transforms it into

$$\rho(i\kappa x; a, b, c, d|q^{-1}) = \prod_{v=a,b,c,d} (ivqe^{\kappa x}, -ivqe^{-\kappa x}; q)_\infty = \prod_{v=a,b,c,d} E_q(ivqe^{-\kappa x}) E_q(-ivqe^{\kappa x}), \qquad (5.2)$$

where $E_q(z) = e_q^{-1}(-z) = (-z; q)_\infty$ [2]. Therefore, under the transformation $q \to q^{-1}$, the orthogonality relation (3.1) for the Askey-Wilson polynomials with the parameter $q < 1$ converts into the following orthogonality relation for the Askey-Wilson polynomials with $q > 1$:

$$\int_{-\infty}^{\infty} p_m(i\sinh\kappa x; a, b, c, d|q^{-1}) \, p_n(i\sinh\kappa x; a, b, c, d|q^{-1}) \, \rho(i\kappa x; a, b, c, d|q^{-1}) \, e^{-x^2} \cosh\kappa x \, dx =$$

$$\delta_{mn} \tilde{I}_n(a, b, c, d|q^{-1}) \qquad (5.3)$$

The explicit form of $\tilde{I}_n(a, b, c, d|q^{-1})$ is readily obtained from (4.16), upon making use of the formulas (5.1) and $(a; q^{-1})_n = (a^{-1}; q)_n (-a)^n q^{-n(n-1)/2}$ [2].

On the other hand, with the aid of the explicit representation for the Askey-Wilson polynomials [1, 2]

$$p_n(\sin\varphi; a, b, c, d|q) = (ab, ac, ad; q)_n \, a^{-n} \, {}_4\phi_3 \left[\begin{matrix} q^{-n}, abcdq^{n-1}, iae^{i\varphi}, -iae^{-i\varphi} \\ ab, ac, ad \end{matrix} ; q, q \right] \qquad (5.4)$$

and the inversion formula (with respect to the transformation $q \to q^{-1}$) for the basic hypergeometric series ${}_4\phi_3$ (see [2], p.21, exercise 1.4(i)), it is easy to show that

$$p_n(x; a, b, c, d|q^{-1}) = (-1)^n (abcd)^n \, q^{-\frac{3}{2}n(n-1)} \, p_n(x; a^{-1}, b^{-1}, c^{-1}, d^{-1}|q). \qquad (5.5)$$

Consequently, from (5.3) and (5.5) it follows the orthogonality relation

$$\int_{-\infty}^{\infty} p_m(i\sinh\kappa x; a^{-1}, b^{-1}, c^{-1}, d^{-1}|q) p_n(i\sinh\kappa x; a^{-1}, b^{-1}, c^{-1}, d^{-1}|q) \rho(i\kappa x; a, b, c, d|q^{-1}) *$$

$$\qquad (5.6)$$

$$e^{-x^2} \cosh\kappa x \, dx = \frac{(q, 1/ab, 1/ac, 1/ad, 1/bc, 1/bd, 1/cd; q)_n}{(1 - q^{2n-1}/abcd)(1/abcd; q)_{n-1}} \tilde{I}_0(a, b, c, d|q^{-1}) \delta_{mn}$$

for the Askey-Wilson polynomials with the parameters $|v| > 1, v = a, b, c, d$ and $0 < q < 1$. The value of the integral $\tilde{I}_0(a, b, c, d|q^{-1})$ is simple to obtain from (4.15) by means of the formula (5.1).

6 Concluding remarks.

The orthogonality relations (3.1) and (5.6) are bound to be related by the Fourier transformation for the Askey-Wilson functions, analogous to the well-known transformation for the harmonic oscillator wave functions $H_n(x)\exp(-x^2/2)$ (or Hermite functions in the terminology of mathematicians [15, 16]) connecting the coordinate and momentum realizations in quantum mechanics. It should be interesting to compare this Fourier transformation with the q-transformations, that reproduce the Askey-Wilson polynomials [17, 18]. For the q-Hermite functions $H_n(\sin \kappa x|q)\exp(-x^2/2)$, $q = \exp(-2\kappa^2)$, which are the simplest case of the Askey-Wilson functions with vanishing parameters a, b, c, and d, such Fourier transformation has the form [5]

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \exp(ixy - x^2/2)H_n(\sin \kappa x|q)dx = i^n q^{n^2/4}h_n(\sinh \kappa y|q)\exp(-y^2/2).$$

The general case needs to be analyzed in greater detail.

7 Acknowledgments.

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C-3.

NONCLASSICAL LIGHT IN INTERFEROMETRIC MEASUREMENTS

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Abstract

It is shown that the even and odd coherent light and other nonclassical states of light like superposition of coherent states with different phases may replace the squeezed light in interferometric gravitational wave detector to increase its sensitivity.

1 Introduction

The problem of detecting gravitational wave has been a subject of interest for many years [1]. Specially the quantum sensitivity of Michelson interferometric gravitational wave detection (GWD) has been discussed by Caves [2]. In Michelson interferometer, the light from an input laser beam splits through a 50-50 beam splitter (BS), bounces back and forth between two end mirrors of interferometer and recombines again at the BS. The intensity at one or both output ports of the interferometer provides informations about the difference between the two displacements of the end mirrors. The quantum mechanical treatment of the system shows that the vacuum fluctuations enter in to the interferometer from the unused port and result in a limit on the optimum power of the input laser, which comes out to be quite large and of no experimental interest. Caves [2] suggested that by squeezing the vacuum, the optimum power of the laser can be reduced considerably. Squeezed states [3] of an electromagnetic field are non-classical states in which the quantum fluctuations in one quadrature can be reduced below the standard quantum limit at the expanse of the increased fluctuations in the other quadrature such that the Heisenberg uncertainty principle remains valid.

It is also interesting to try to use the other non-classical light in the place of squeezed light and study its effect on the better sensitivity of the interferometer in GWD. The different superpositions of coherent states because of their non-classical nature are of our particular interest. Yurke and Stoler [4], have predicted that a coherent state propagating in a dispersive medium evolves into a superposition of two coherent states 180^0 out of phase. Another type of superposition of coherent states, namely, even and odd coherent states was introduced by Dodonov, Malkin, and Man'ko

[5]. Even coherent states are closely related to the squeezed vacuum states because they too are the superposition of even number of photons but with different coefficients. The non-classical properties of Yurke-Stoler coherent states and even and odd coherent states have been discussed in [6]. In Refs.[7] -[10], different theoretical possibilities regarding the generations of even and odd coherent states have been discussed. The properties of even and odd coherent states as a representatives of a set of nonclassical light states have been considered recently by Nieto and Truax [11].

In the following sections we will study the effects of the non-classical light on the optimal power of the input laser for interferometric GWD. The most general analysis of non-classical states in interferometry was done by Yurke, McCall and Klauder [12]. We will following the approach adopted by Ansari et al.[13], in which the noise error can be expressed as a product of two factors with tensorial-like structure, each of the factors being related to the geometry of an interferometer and light states correspondingly.

2 Nonclassical Light

In this section we will briefly discuss the properties of three types of superposition of coherent states, Yurke-Stoler coherent states (YS), even (ECS) and odd (OCS) coherent states.

2.1 Even and Odd Coherent States

The even and odd coherent states may be defined in the form [5]

$$| \beta_{\pm} > = N_{\pm}(| \beta > \pm | -\beta >),$$ (1)

where + sign is for ECS and − sign is for OCS. $| \beta >$ is a coherent state and the normalizing constants $N_{\pm}$ are

$$N_+ = \frac{e^{|\beta|^2/2}}{2\sqrt{\cosh | \beta |^2}},$$

$$N_- = \frac{e^{|\beta|^2/2}}{2\sqrt{\sinh | \beta |^2}}.$$ (2)

Also from Eq.(1), we can define the relations

$$a | \beta_+ > = \beta\sqrt{\tanh | \beta |^2} | \beta_- >,$$

$$a | \beta_- > = \beta\sqrt{\coth | \beta |^2} | \beta_+ > .$$ (3)

With the help of above equations we can easily evaluate the expectation values of first and higher order moments of annihilation and creation operators of even and odd coherent states. For example,

$$< a >_+ = < \beta_+ | a | \beta_+ > = \beta\sqrt{\tanh | \beta |^2} < \beta_+ | \beta_- > = 0,$$ (4)

as even and odd coherent states are orthogonal states. Similarly,

$$
\begin{aligned}
< a^\dagger a >_+ &= |\beta|^2 \, tanh \, |\beta|^2, \\
< a^\dagger a >_- &= |\beta|^2 \, coth \, |\beta|^2, \\
< a^2 >_\pm &= \beta^2, \\
< a^{\dagger 2} >_\pm &= \beta^{*2}.
\end{aligned}
\tag{5}
$$

2.2 Yurke-Stoler Coherent States

Yurke-Stoler (YS) coherent states are defined as [4],[6]

$$
|\beta>_{YS} = \frac{1}{\sqrt{2}}(|\beta> + e^{i\pi/2}|-\beta>).
\tag{6}
$$

In terms of number states these states can be defined as

$$
|\beta>_{YS} = \frac{e^{-|\beta|^2/2}}{\sqrt{2}} \sum_{n=0}^{\infty} \frac{\beta^n}{\sqrt{n!}} (1 + i(-1)^n) |n>.
\tag{7}
$$

The first order moments of YS coherent states are not equal to zero as in the case of ECS or OCS

$$
< a >_{YS} = -i\beta e^{-2|\beta|^2},
\tag{8}
$$

and second order moments are

$$
\begin{aligned}
< a^\dagger a >_{YS} &= |\beta|^2, \\
< a^2 >_{YS} &= \beta^2.
\end{aligned}
\tag{9}
$$

We will use different first and second order moments as given in Eqs.(4-9) in the following section, when we will discuss the important role played by nonclassical light for GWD.

3 Michelson Interferometer for GWD

Michelson interferometer is a two arms device at the end of which two mirrors are attached to strings, thus behaving as two pendula. The positions of the mirrors are controlled by the joint action of the restoring force and the radiation pressure [14]. We will suppose that in all process the dissipative and active effects are negligible and the conservation of energy is ensured.

There are two input field modes described by the operators $(a_i, a_i^\dagger)$ at the two ports of the interferometer. At the end mirrors M_i, the fields are defined by $(b_i, b_i^\dagger)$. The output fields at the two ports P_i are described by $(c_i, c_i^\dagger)$. The input fields are related with the fields at the mirrors through the relations

$$
\begin{aligned}
b &= Va, \\
b^\dagger &= a^\dagger V,
\end{aligned}
\tag{10}
$$

where

$$a = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix},$$

$$b = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix},$$

$$a^\dagger = \begin{pmatrix} a_1^\dagger & a_2^\dagger \end{pmatrix},$$

$$b^\dagger = \begin{pmatrix} b_1^\dagger & b_2^\dagger \end{pmatrix}. \tag{11}$$

Also

$$V = \Phi K, \tag{12}$$

with

$$\Phi = \begin{pmatrix} e^{i\phi_1} & 0 \\ 0 & e^{i\phi_2} \end{pmatrix},$$

$$K = \begin{pmatrix} \zeta_1 & \xi_2 \\ \xi_1 & \zeta_2 \end{pmatrix}. \tag{13}$$

In Eq.(13) ζ and ξ are the complex transitivity and reflectivity parameters of the BS arbitrarily oriented for the i-th field mode respectively and ϕC_i is the phase distance between BS and M_i.

The relations between the input field and the output fields at the two interferometric ports are of the form

$$c = Ua,$$

$$c^\dagger = a^\dagger U^\dagger \tag{14}$$

with

$$U = -K^T \Phi^2 K = -V^T V, \tag{15}$$

where $-$ sign in Eq.(15) corresponds to the phase change on reflection at the mirrors. Thus from the above equations we can define the relations between different fields by including all the informations about influence of the BS and the end mirrors M_i.

3.1 Sources of Noise

The accuracy with which the difference in displacement z can be measured is limited by the Heisenberg uncertainty principle. Following [2], we have two sources of errors namely radiation pressure error and photon counting noise. The standard quantum limit for a Michelson interferometer can be obtained by balancing these two sources of error. Radiation pressure error (PR) is due to the pressure exerted by the field on the mirrors and the photon counting noise (PC) is due to the fluctuations in the number of photons in the input field. So,

$$\Delta z = \sqrt{(\Delta z_{RP})^2 + (\Delta z_{PC})^2}, \tag{16}$$

where

$$(\Delta z_{RP})^2 = \sigma_{RP}^2 \left(\frac{\hbar \omega \tau}{mc}\right)^2,$$

$$(\Delta Z_{PC})^2 = \sigma_{PC}^2 \left(\frac{\partial(c^\dagger \sigma_3 c)}{\partial(\phi_2 - \phi_1)}\right)^{-2}. \tag{17}$$

Also

$$\sigma_{RP}^2 = <(b^\dagger \sigma_3 b)^2> - <b^\dagger \sigma_3 b>^2,$$

$$\sigma_{PC}^2 = <(c^\dagger \sigma_3 c)^2> - <c^\dagger \sigma_3 c>^2. \tag{18}$$

In Eq.(17), τ is the observation time and m is the mass of the end mirrors. Here we consider that BS is attached to a large mass M ($M >> m$), which remained fixed during the observation time. By using Eqs.(10-15), we can write

$$\sigma_{RP}^2 = (V^\dagger \sigma_3 V)_{ik}(V^\dagger \sigma_3 V)_{mn} T_{ikmn},$$

$$\sigma_{PC}^2 = (U^\dagger \sigma_3 U)_{ik}(U^\dagger \sigma_3 U)_{mn} T_{ikmn}, \tag{19}$$

with the summation over the repeated indices taken from 1 to 2 and

$$T_{ikmn} = <a_i^\dagger a_k a_m^\dagger a_n> - <a_i^\dagger a_k><a_m^\dagger a_n>. \tag{20}$$

Eq.(20) allows us to study the use of different field modes from the input port. By using Eqs.(16-20), we can write

$$\Delta z = X_{ikmn} T_{ikmn} \qquad (ikmn = 1, 2), \tag{21}$$

where X_{ikmn} contains the geometrical and physical properties of the interferometer.

If we consider a 50-50 ideally thin BS which introduces a phase difference of $\pi/2$ between the reflected and the transmitted waves, then from Eq.(10) and (13), we can write

$$V^\dagger \sigma_3 V = \begin{pmatrix} o & i \\ -i & o \end{pmatrix} \tag{22}$$

and

$$U^\dagger \sigma_3 U = \begin{pmatrix} -\cos\phi & -\sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix}, \tag{23}$$

where $\phi = \phi_2 - \phi_1$. Also if the interferometer is operated in the dark fringe, then two arms of the interferometer can be adjusted such that $\phi = (2n + 1)\pi/2$. For dark fringe operation we get

$$X_{1212} = X_{2121} = -A^2 + B^2,$$

$$X_{1221} = X_{2112} = A^2 + B^2. \tag{24}$$

Also

$$A = \left(\frac{\hbar \omega \tau}{mc}\right),$$

$$B = \left(\frac{\partial I}{\partial Z}\right)^{-1} \tag{25}$$

and

$$I = <c^\dagger \sigma_3 c>,$$
$$Z = \phi\frac{c}{2\omega}. \tag{26}$$

The variable Z corresponds to the difference between the displacement of two end mirrors with respect to their mean position due to radiation pressure exerted by the input laser.

(i)   The corresponding field contributions can be found from Eq.(20). If we consider that the input field at port P_1 is a coherent light and from the second port is in even or odd coherent states, then the two fields are anticorrelated and the states of these fields can be written as

$$|\psi>=|\alpha,\beta_\pm>. \tag{27}$$

For the case of even coherent light we can write the coefficients T_{ikmn} as

$$
\begin{aligned}
T_{1111} &= \alpha^2 \\
T_{1122} &= 0 \\
T_{1212} &= \alpha^2 \mid \beta \mid^2 e^{2i\theta_1} \\
T_{1221} &= \alpha^2 \mid \beta \mid^2 tanh \mid \beta \mid^2 + \alpha^2 \\
T_{2112} &= \alpha^2 \mid \beta \mid^2 tanh \mid \beta \mid^2 + \mid \beta \mid^2 tanh \mid \beta \mid^2 \\
T_{2121} &= \alpha^2 \mid \beta \mid^2 e^{-2i\theta_1} \\
T_{2211} &= 0 \\
T_{2222} &= \mid \beta \mid^4 - \mid \beta \mid^4 tanh^2 \mid \beta \mid^2 + \mid \beta \mid^2 tanh \mid \beta \mid^2,
\end{aligned}
\tag{28}
$$

where θ_1 is the phase of β and we have consider α to be real. Also for OCS we will get the same expressions as in the above equation except $tanh \mid \beta \mid^2$ should be replace by $coth \mid \beta \mid^2$.

(ii)   For the case of Yurke-Stoler coherent states from the second port and the coherent state from the first port we can define the states as

$$|\psi>=|\alpha,\beta_{YS}>, \tag{29}$$

and the new expressions for T_{ikmn} are

$$
\begin{aligned}
T_{1111} &= \alpha^2 \\
T_{1122} &= 0 \\
T_{1212} &= \alpha^2 \mid \beta \mid^2 e^{2i\theta_2}(1 + e^{-4|\beta|^2}) \\
T_{1221} &= \alpha^2 \left[\mid \beta \mid^2 \left(1 - e^{-4|\beta|^2}\right) + 1\right] \\
T_{2112} &= \mid \beta \mid^2 \left[\alpha^2 \left(1 - e^{-4|\beta|^2}\right) + 1\right] \\
T_{2121} &= \alpha^2 \mid \beta \mid^2 e^{-2i\theta_2}(1 + e^{-4|\beta|^2}) \\
T_{2211} &= 0 \\
T_{2222} &= \mid \beta \mid^2,
\end{aligned}
\tag{30}
$$

where θ_2 is the phase of β in the case of YS coherent states. A comparison of Eqs.(29) and (31) shows the difference between different order correlations between the two types of the input fields from port P_2.

3.2 Optimum Input Laser Power

The general expression for $(\Delta z)^2$ by using Eqs.(21) and (25) becomes

$$(\Delta z)^2 = A^2(T_{1221} + T_{2112} - T_{1212} - T_{2121}) + B^2(T_{1221} + T_{2112} + T_{1212} + T_{2121}). \tag{31}$$

Minimizing the total error with respect to α^2 gives optimal value of α^2 (coherent field intensity from port P_1). In the presence of ordinary vacuum fluctuations from the second port, the optimum intensity of the input laser becomes [2]

$$(\alpha_{opt}^2)^o = \frac{mc^2}{2\hbar\omega^2\tau}. \tag{32}$$

Caves [2] showed that the optimal laser intensity can be reduced considerably if we squeezed the vacuum from the second port. We will analyze the situation when the squeezed vacuum is replaced by the nonclassical light as discussed before.

In the first case, we will study the effect of even and odd coherent states on the optimum value of α^2. Under the condition of $\alpha^2 >>| \beta |^2 \tanh | \beta |^2$, we get

$$(\alpha_{opt}^2)^{ev} = \sqrt{\frac{2 | \beta |^2 \tanh | \beta |^2 + 2 | \beta |^2 \cos 2\theta_1 + 1}{2 | \beta |^2 \tanh | \beta |^2 - 2 | \beta |^2 \cos 2\theta_1 + 1}}(\alpha_{opt}^2)^o, \tag{33}$$

and for OCS

$$(\alpha_{opt}^2)^{od} = \sqrt{\frac{2 | \beta |^2 \coth | \beta |^2 + 2 | \beta |^2 \cos 2\theta_1 + 1}{2 | \beta |^2 \coth | \beta |^2 - 2 | \beta |^2 \cos 2\theta_1 + 1}}(\alpha_{opt}^2)^o. \tag{34}$$

Thus for $\theta_1 = \pi/2$ and under the limit $1 <<| \beta |^2<< \alpha^2$, we get

$$(\alpha_{opt}^2)^{ev} = \frac{(\alpha_{opt}^2)^o}{2 | \beta |}. \tag{35}$$

Eq. (35) allows us an alternative way to reduce the optimum input laser power or to increase the sensitivity of interferometer by using even or odd coherent states from the second port of the interferoeter. As $| \beta |>>1$, from Eq.(35), we predict that the optimum value of the input laser intensity can be reduced considerably if we apply even or odd coherent state from the second port.

When we apply Yurke-Stoler coherent states and for the choices of $\alpha^2 >>| \beta |^2$ and $\theta_2 = \pi/2$, we get the relation

$$(\alpha_{opt}^2)^{YS} = \sqrt{\frac{-2 | \beta |^2 e^{-4|\beta|^2} + 1}{4 | \beta |^2 + 1}}(\alpha_{opt}^2)^o. \tag{36}$$

Also in the limit of $1 <<| \beta |^2<< \alpha^2$, we will get the same expression as we get in the case of ECS or OCS, i.e.,

$$(\alpha_{opt}^2)^{YS} = \frac{(\alpha_{opt}^2)^o}{2 | \beta |}. \tag{37}$$

Eqs.(35) and (37) show that we get the same expressions for the optimum power of input laser for large $| \beta |$. Thus we predict an important property of the superposition of coherent states that differet superpositions of coherent states may play an important role in reducing the optimum power of input laser. In other words by applying these coherent states, better quantum sensitivity of interferometer can be achieved as compare to no field contribution from the second port.

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Non-Noetherian Symmetries for Oscillators
in Classical Mechanics and in Field Theory

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Abstract

Infinitely many new conservation laws both for free fields as well as for test fields evolving on a given gravitational background are presented. The conserved currents are constructed using the field theoretical counterpart of a recently discovered non-Noetherian symmetry which gives rise to a new way of solving the classical small oscillations problem. Several examples are discussed.

1 Introduction

Noether's theorem plays a fundamental role in field theory [1]. Besides Noetherian symmetries there are, however, other kinds of symmetry transformations for the field equations which, loosely speaking, do not preserve the variational principle, i.e., they do not satisfy Noether's theorem [2,3,4]. They are non-Noetherian symmetries. Noether theorem gives rise to a conservation law associated to each Noetherian symmetry transformation of a system. On the other hand, non-Noetherian symmetries provide several (and sometimes infinitely many) conservation laws associated to one transformation [3,4,5,6]. In some instances one non-Noetherian symmetry transformation provides enough information to solve completely an n degrees of freedom problem [4]. In order to be more precise let us turn our attention to the small oscillations problem in classical mechanics. The Lagrangian is

$$L = \frac{1}{2}T_{ij}\dot{q}^i\dot{q}^j - \frac{1}{2}V_{ij}q^iq^j \quad i,j = 1,2,....,n \tag{1}$$

with

$$T_{ij} = T_{ji} \ , \qquad V_{ij} = V_{ji} \tag{2}$$

and

$$\det \frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j} = \det T_{ij} \neq 0 \tag{3}$$

Consider the transformation

$$q'^i = q^i + \delta q^i, \quad t' = t \tag{4}$$

with

$$\delta q^i = \epsilon (T^{-1}V)^i_j q^j \tag{5}$$

It is straightforward to prove that (4)-(5) is a non–Noetherian symmetry transformation for Lagrangian (1) as it maps the space of solutions of its equations of motion into itself (for details, see [4]). As it is well known, energy is conserved for Lagrangian (1) and therefore

$$H_0 = \frac{1}{2}T_{ij}\dot{q}^i\dot{q}^j + \frac{1}{2}V_{ij}q^iq^j \tag{6}$$

is a constant of motion. It may be easily proved [2,3,4] that the deformation δH_0 of H_0 along a symmetry transformation δq^i,

$$\delta H_0 = \frac{\partial H_0}{\partial q^i}\delta q^i + \frac{\partial H_0}{\partial \dot{q}^i}\frac{\bar{d}}{dt}(\delta q^i) \tag{7}$$

is also a constant of motion. Thus, we get for the symmetry transformation given by Eqs. (4)-(5) that

$$H_1 = \frac{1}{2}V_{ij}\dot{q}^i\dot{q}^j + \frac{1}{2}(VT^{-1}V)_{ij}q^iq^j \tag{8}$$

is a constant of motion. Deforming H_1, so on and so forth we get that, in general,

$$H_s = \frac{1}{2}((VT^{-1})^{s-1}V)_{ij}\dot{q}^i\dot{q}^j + \frac{1}{2}((VT^{-1})^sV)_{ij}q^iq^j \tag{9}$$

is a constant of motion for $s \geq 1$. At most n of these constants of motion are functionally independent due to the Cayley-Hamilton theorem. Note that this restriction dissappears in field theory. Furthermore, it may be proved that all these constants are in involution. In the next sections we will obtain the counterpart of these results for different examples in field theory.

2 Free Scalar Field

Consider the scalar field Lagrangian [7]

$$\mathcal{L} = \frac{1}{2}\partial_\mu\varphi\partial^\mu\varphi - \frac{1}{2}\mathrm{m}^2\varphi^2 \tag{10}$$

where $\varphi = \varphi(x^\mu)$ is a real scalar field. The equation of motion is

$$\partial_\mu\partial^\mu\varphi + \mathrm{m}^2\varphi = 0 \tag{11}$$

which written in detail reads

$$\frac{\partial^2\varphi}{\partial t^2} = (\nabla^2 - \mathrm{m}^2)\varphi \tag{12}$$

Consider the transformation

$$\delta_1\varphi = \epsilon(\nabla^2 - \mathrm{m}^2)\varphi \equiv \epsilon D\varphi \tag{13}$$

It is straightforward to prove that $\delta_1\varphi$ satisfies Eq. (12) , i.e.,

$$\frac{\partial^2}{\partial t^2}\delta_1\varphi = \mathrm{D}\delta_1\varphi \tag{14}$$

Therefore, if φ is a solution of Eq. (12), then, φ' given by

$$\varphi' = \varphi + \delta_1\varphi \tag{15}$$

also solves it. The energy-momentum tensor $\mathrm{T}^{\mu\nu}_{(0)}$

$$\mathrm{T}^{\mu\nu}_{(0)} = \varphi^{,\mu}\varphi^{,\nu} - \eta^{\mu\nu}\mathcal{L} \tag{16}$$

is conserved for the scalar field. It is easy to prove that its first deformation given by

$$\mathrm{T}^{\mu\nu}_{(1)} = \frac{1}{2}\left[\varphi^{,\mu}(\mathrm{D}\varphi)^{,\nu} + \varphi^{,\nu}(\mathrm{D}\varphi)^{,\mu} - \eta^{\mu\nu}(\varphi^{,\alpha}(\mathrm{D}\varphi)_{,\alpha} - \mathrm{m}^2\varphi\mathrm{D}\varphi)\right], \tag{17}$$

is also conserved (the factor $\frac{1}{2}$ has been introduced for convenience). The transformations

$$\delta_n\varphi = \epsilon\,\mathrm{D}^n\varphi \quad n = 1, 2, ... \tag{18}$$

are also symmetry transformations for Eq. (11). Therefore, in general,

$$\mathrm{T}^{\mu\nu}_{(n)} = \frac{1}{2}\left[\varphi^{,\mu}(\mathrm{D}^n\varphi)^{,\nu} + \varphi^{,\nu}(\mathrm{D}^n\varphi)^{,\mu} - \eta^{\mu\nu}(\varphi^{,\alpha}(\mathrm{D}^n\varphi)_{,\alpha} - \mathrm{m}^2\varphi\mathrm{D}^n\varphi)\right], \tag{19}$$

is conserved for any n, as it can be readily checked. To understand the physical meaning of $\mathrm{T}^{\mu\nu}_{(n)}$ it is interesting to consider its expression in terms of the Fourier transform of $\varphi(x)$. The solution $\varphi(x)$ of Eq. (11) may be written in terms of $\varphi(k)$ as

$$\varphi(x) = \frac{1}{(2\pi)^{3/2}}\int \mathrm{d}^4k\,\delta(k^2 - \mathrm{m}^2)\theta(k^0)(e^{ikx}\varphi(k) + e^{-ikx}\varphi^*(k)) \tag{20}$$

where $kx = k_\mu x^\mu$ and the star denotes complex conjugation, then one gets that the energy is

$$\mathrm{P}^0_{(0)} = \int \mathrm{d}^3x\,\mathrm{T}^{00}_{(0)} = \int \mathrm{d}^3k\,k^0\,\varphi^*(\vec{k})\varphi(\vec{k}) \tag{21}$$

where $\varphi(\vec{k}) = (2k^0)^{-1/2}\varphi(k)$, with $k^0 = +\sqrt{\vec{k}^2 + m^2}$ and

$$\mathrm{P}^0_{(n)} = \int \mathrm{d}^3x\,\mathrm{T}^{00}_{(n)} = (-1)^n\int \mathrm{d}^3k\,(k^0)^{2n+1}\,\varphi^*(\vec{k})\varphi(\vec{k}) \tag{22}$$

which is a result very similar to the one obtained for the small oscillations problem [4]. We have, therefore obtained infinitely many conservation laws for the free scalar field. Of course, getting infinitely many conserved quantities for the free scalar field is no surprise since the general solution to the problem has been known for a long time. The purpose of discussing the free scalar field is to get a better understanding of the meaning of the non-Noetherian charges, in the next section we will obtain similar conservation laws for a test scalar field evolving on a given static gravitational background which constitutes a more powerful result.

3 Test Scalar Field on a Static Gravitational Background

Consider the Lagrangian

$$\mathcal{L} = \frac{1}{2}\sqrt{-g}(g^{\mu\nu}\partial_\mu\varphi\partial_\nu\varphi - \mathrm{m}^2\varphi^2) \tag{23}$$

where the gravitational field is described by the static metric $g_{\mu\nu}$, with determinant g, which satisfies

$$\frac{\partial g_{\mu\nu}}{\partial x^0} = 0 \tag{24}$$

and

$$g_{0i} = 0 \tag{25}$$

and g is the determinant of the metric. The equation of motion for the scalar field is

$$\partial_\mu(\sqrt{-g}g^{\mu\nu}\partial_\nu\varphi) + \sqrt{-g}\mathrm{m}^2\varphi = 0 \tag{26}$$

or, in full detail

$$\ddot{\varphi} = \frac{-g_{00}}{\sqrt{-g}}\partial_i(\sqrt{-g}g^{ij}\partial_j\varphi) - \mathrm{m}^2 g_{00}\varphi \tag{27}$$

where $\dot{\varphi} = \partial\varphi/\partial x^0$. The Lagrangian is time independent

$$\frac{\partial\mathcal{L}}{\partial x^0} = 0 \tag{28}$$

and therefore energy is conserved

$$\partial_\mu \mathrm{T}^\mu_{(0)0} = 0 \tag{29}$$

with

$$\mathrm{T}^\mu_{(0)0} = \frac{\sqrt{-g}}{2}\left(2g^{\mu\lambda}\partial_\lambda\varphi\dot{\varphi} - \delta^\mu_0(g^{\alpha\beta}\partial_\alpha\varphi\partial_\beta\varphi - \mathrm{m}^2\varphi^2)\right) \tag{30}$$

Again we may prove that

$$\delta_1\varphi = \epsilon\,\mathcal{D}\varphi \tag{31}$$

is a symmetry transformation for Eq. (27) with

$$\mathcal{D} \equiv \frac{-g_{00}}{\sqrt{-g}}\partial_i(\sqrt{-g}g^{ij}\partial_j) - \mathrm{m}^2 g_{00} \tag{32}$$

Therefore, we find that

$$\mathrm{T}^\mu_{(n)0} = \frac{\sqrt{-g}}{2}\left(g^{\mu\lambda}\dot{\varphi}\partial_\lambda\mathcal{D}^n\varphi + g^{\mu\lambda}\partial_\lambda\varphi\mathcal{D}^n\dot{\varphi} - \delta^\mu_0(g^{\alpha\beta}\partial_\alpha\varphi\partial_\beta\mathcal{D}^n\varphi - \mathrm{m}^2\varphi\mathcal{D}^n\varphi)\right) \tag{33}$$

is conserved for any n as it can be readily checked. We have thus found infinitely many independent new conservation laws for a scalar field evolving on a static gravitational background. Note that the general solution for Eq. (27) on a Schwarzschild background metric is not known at present.
Consider the Schwarzschild metric [8]

$$g_{\mu\nu} = \mathrm{diag}(1 - \frac{2M}{r}, \frac{-1}{1 - \frac{2M}{r}}, -r^2, -r^2\sin^2\theta) \tag{34}$$

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in units such that G=c=1. In this case,

$$\mathcal{D} = \frac{e^\lambda}{r^2 \sin\theta} \left(\frac{\partial}{\partial r}(r^2 \sin\theta e^\lambda \frac{\partial}{\partial r}) + \frac{\partial}{\partial \theta}(\sin\theta \frac{\partial}{\partial \theta}) + \frac{1}{\sin\theta} \frac{\partial^2}{\partial \phi^2} - m^2 r^2 \sin\theta \right) \tag{35}$$

with $e^\lambda = 1 - 2M/r$. We get that

$$T^0_{(0)0} = \frac{r^2 \sin\theta}{2}(e^{-\lambda}(\dot{\varphi})^2 + e^\lambda(\varphi_{,r})^2 + \frac{1}{r^2}(\varphi_{,\theta})^2 + \frac{1}{r^2 \sin^2\theta}(\varphi_{,\phi})^2 + m^2\varphi^2) \tag{36}$$

and

$$T^0_{(n)0} = \frac{r^2 \sin\theta}{2} \left(e^{-\lambda}\dot{\varphi}\mathcal{D}^n\dot{\varphi} + e^\lambda\varphi_{,r}(\mathcal{D}^n\varphi)_{,r} + \frac{1}{r^2}\varphi_{,\theta}(\mathcal{D}^n\varphi)_{,\theta} + \right.$$

$$\left. + \frac{1}{r^2\sin^2\theta}\varphi_{,\phi}(\mathcal{D}^n\varphi)_{,\phi} + m^2\varphi\mathcal{D}^n\varphi \right) \tag{37}$$

are conserved for all n. Thus we have infinitely many new conservation laws for the scalar field evolving on a gravitational background. In regard to the convergence of the integrals which define the conserved charges associated to $T^0_{(n)0}$, it is straightforward to realize that $\mathcal{D}^n\varphi$ behaves no worse than φ in the limit $r \to \infty$, for the massive case, while it vanishes faster than φ for the massless case. In other words, the new conserved charges behave (at worst) in the same fashion as the usual conserved energy does (and much better in the massless case). This fact may be explicitly verified for the particular case of a massless scalar field of angular momentum and frequency equal to 0. The explicit solution to Eq. (27) is [9]

$$\varphi(r) = \ln(1 - \frac{2M}{r}) \tag{38}$$

as it can be readily verified. From Eq. (37) we have that T^0_0 and $T^0_{(1)0}$ behave as r^{-2} and r^{-5}. For $n > 1$, $T^0_{(n)0}$ converges faster than r^{-5} when $r \to \infty$.
As another example, consider the following metric [10]

$$g_{\mu\nu} = \text{diag}(r^{2\alpha}, -\beta, -r^2, -r^2\sin^2\theta) \tag{39}$$

which has been considered as a model for galactic dark matter dynamics. In Eq. (38) α and β are constants with $\alpha = 2(\gamma - 1)/\gamma$ and $\beta = (\gamma^2 + 4\gamma - 4)/\gamma$, where $2 > \gamma > 1$. The Klein-Gordon equation for a massless scalar field evolving on this metric is separable and its solutions are known [11]. The radial part of $\varphi(x^\mu)$ is

$$R(r) = r^{\frac{2-3\gamma}{2\gamma}}(AJ_\nu(\omega z) + BN_\nu(\omega z)) \tag{40}$$

where $J_\nu(x)$ and $N_\nu(x)$ are the Bessel and Neumann functions, ω is the frequency and

$$\nu^2 = \frac{(3\gamma - 2)^2/4 + l(l + 1)(\gamma^2 + 4\gamma - 4)}{(2 - \gamma)^2} \quad , \quad z = \frac{\sqrt{(\gamma^2 + 4\gamma - 4)}}{2 - \gamma}r^{\frac{2-\gamma}{\gamma}} \tag{41}$$

Since the metric (38) satisfies Eqs. (24) and (25) we have that (36) and (37) are conserved. The interesting fact in this case, is that if one studies the asymptotic behaviour of solution (39), one finds that $T^0_{\ 0}$ and $T^0_{(n)0}$ when $r \to \infty$ behave as

$$T^0_{\ 0} \approx \frac{1}{r^\alpha} \ , \qquad T^0_{(n)0} \approx \frac{1}{r^{2n(1-\alpha)+\alpha}} \tag{42}$$

Since $1 > \alpha > 0$ this implies that $2n(1 - \alpha) + \alpha > 1$ for $n \geq 1$. It is straightforward to realize that the conserved charge associated to $T^0_{\ 0}$ diverges, while the ones linked to $T^0_{(n)0}$ do exist, for $n \geq 1$. Of course the metric is not asymptotically flat, so there is no Poincaré invariance (at infinity). Nevertheless the new conservation laws provide relevant information for the problem at hand.

4 Non–Linear Systems: Burgers Equation

The results we have presented above hold, in general, for linear differential systems. Nevertheless, there are some physically relevant non–linear equations to which our findings may be applied. Burgers equation is one such example. It has been known for some time [12,13] that (the non–linear) Burgers equation may be, in fact, related to a linear equation, which is, of course, tractable using our method. Therefore, even though in an indirect way, we will use our methods to deal with physically relevant non–linear evolution equations. These results may prove, in the future, to be applicable to other non–linear systems.

Consider the linear equation

$$u_t + u_{xx} = 0, \tag{43}$$

for the field $u(x,t)$. Here, u_t means partial differentiation of the field u with respect to t, and similarly for the other suffixes. Define the new field $v(x,t)$ by the transformation

$$v \equiv \frac{u_x}{u}. \tag{44}$$

It is a straightforward matter to prove that v satisfies Burgers equation

$$v_t + v_{xx} + (v^2)_x = 0. \tag{45}$$

We have already seen a general algorithm to generate symmetry transformations for linear differential equations. We find that δu defined by

$$\delta u = u_{xxxx}, \tag{46}$$

is a symmetry transformation for Eq. (43). A symmetry transformation δv based on (46) can now be found for Burgers equation (45),

$$\delta v = (v^4 + 6v^2 v_x + 4v v_{xx} + 3v_x^2 + v_{xxx})_x. \tag{47}$$

Of course, simpler transformations can also be constructed, but they will usually produce vanishing deformations of the conserved quantities already obtained.

We are not aware of the existence of a Lagrangian for Eq. (43) by itself, i.e., without considering it together with its time reversed counterpart, in which case the construction of the Lagrangian is trivial. Under these considerations, all the symmetry transformations presented in this Section are non–Noetherian.

5 Summary and Conclusions

We have presented non–Noetherian symmetry transformations for oscillators in classical mechanics as well as in field theory which give rise to many conservation laws by deformation of a given conserved quantity. For the classical mechanical case, the symmetry transformation produced enough constants of the motion to completely solve the small oscillations problem. In the case of field theory, we have found infinitely many conserved quantities even for fields interacting with a given background gravitational field. In some cases, this procedure can be extended to physically relevant non–linear equations such as Burgers equation. These results may also be helpful to deal with Eckhaus equation [13]. The method presented here could be used as an alternative way to diagonalize matrices using the procedure described in the classical mechanical case [4], and it also affords a different procedure to deal with differential equations such as the kind which give rise to special functions, for instance. Finally, we should mention that the results presented in this note may be generalized to include electromagnetic like forces linear in the velocities for the classical mechanical oscillators and the corresponding changes can be introduced in the partial differential equations for the field oscillators.

Acknowledgments

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COVARIANT DEFORMED OSCILLATOR ALGEBRAS

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Abstract

The general form and associativity conditions of deformed oscillator algebras are reviewed. It is shown how the latter can be fulfilled in terms of a solution of the Yang-Baxter equation when this solution has three distinct eigenvalues and satisfies a Birman-Wenzl-Murakami condition. As an example, an $SU_q(n) \times SU_q(m)$-covariant q-bosonic algebra is discussed in some details.

1   Introduction

Since the advent of quantum groups and q-algebras (see e.g. [1] and references quoted therein), much attention has been paid to deformations of the algebras of bosonic and fermionic creation and annihilation operators [2]–[6]. Different deformations of the latter arise depending on which property of the undeformed operators is preserved.

In the simple case of the $su(2)$ Lie algebra, two pairs of bosonic creation and annihilation operators $a_i^\dagger$, a_i, $i = 1, 2$, give rise to the Jordan-Schwinger realization

$$J_+ = a_1^\dagger a_2, \qquad J_- = a_2^\dagger a_1, \qquad J_0 = \tfrac{1}{2}(N_1 - N_2), \tag{1}$$

where $N_i = a_i^\dagger a_i$, $i = 1, 2$, are number operators. In addition, the creation operators $a_1^\dagger$, $a_2^\dagger$ (as well as the modified annihilation operators $\tilde{a}_1 = a_2$, $\tilde{a}_2 = -a_1$) are the components $+1/2$ and $-1/2$ of an $su(2)$ spinor, respectively. When extending these two properties to the corresponding q-algebra $su_q(2)$ (where q is real and positive), one gets two different sets of q-bosonic operators.

On the one hand, those first considered by Biedenharn [2], Macfarlane [3], Sun and Fu [4], give rise to a Jordan-Schwinger realization of $su_q(2)$ of the same type as (1), where $a_i^\dagger$, a_i, $i = 1, 2$, now satisfy the relations

$$a_i a_i^\dagger - q^{\pm 1} a_i^\dagger a_i = q^{\mp N_i}, \tag{2}$$

while operators with different indices do still commute, and $a_i^\dagger a_i = [N_i]_q \equiv (q^{N_i} - q^{-N_i})/(q - q^{-1})$. However, the operators $a_1^\dagger$, $a_2^\dagger$ do not transform any more under a definite representation of the algebra.

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On the other hand, the operators $A_i^\dagger$, A_i, $i = 1, 2$, introduced by Pusz and Woronowicz [5], satisfy different relations

$$\begin{aligned}
A_i^\dagger A_j^\dagger - q^{-1} A_j^\dagger A_i^\dagger &= A_i A_j - q A_j A_i = 0, \qquad i < j, \\
A_i A_j^\dagger - q A_j^\dagger A_i &= 0, \qquad i \neq j, \\
A_i A_i^\dagger - q^2 A_i^\dagger A_i &= I + (q^2 - 1) \sum_{j=1}^{i-1} A_j^\dagger A_j,
\end{aligned} \tag{3}$$

where the two modes are not independent any more. As a result of this coupling, the operators $A_1^\dagger$, $A_2^\dagger$ (as well as $\tilde{A}_1 = q^{1/2} A_2$, $\tilde{A}_2 = -q^{-1/2} A_1$) are the components $+1/2$ and $-1/2$ of an $su_q(2)$ spinor respectively, but yield an $su_q(2)$ realization that is substantially more complicated than (1). The algebra (3) has also important covariance properties under the quantum group $SU_q(2)$, dual to $su_q(2)$.

The present communication is concerned with the construction of covariant deformed oscillator algebras that generalize the Pusz-Woronowicz algebra for other quantum groups than $SU_q(2)$ (or more generally $SU_q(n)$). The method used will be based on an R-matrix approach similar to that applied in noncommutative differential geometry [7,8]. In Sec. 2, after reviewing the general form and associativity conditions of deformed oscillator algebras, we will show how to fulfil the latter in terms of a solution of the Yang-Baxter equation with three distinct eigenvalues. The example of an $SU_q(n) \times SU_q(m)$-covariant q-bosonic algebra $\mathcal{A}_q(n, m)$ will be treated in some details in Sec. 3. Finally, in Sec. 4, an alternative derivation of the same algebra, based upon the q-algebra $u_q(n) + u_q(m)$ will be presented.

2 Deformed Oscillator Algebras

Let us consider the complex algebras generated by I, $A_i^\dagger$ $A_i = (A_i^\dagger)^\dagger$, $i = 1, \ldots, N$, subject to the relations [9,10]

$$\begin{aligned}
A_i^\dagger A_j^\dagger &= X_{ij,kl} A_k^\dagger A_l^\dagger, \\
A_i A_j &= X_{ji,lk}^* A_k A_l, \\
A_i A_j^\dagger &= \delta_{ij} + Z_{jl,ik} A_k^\dagger A_l,
\end{aligned} \tag{4}$$

where X and Z are some complex $N^2 \times N^2$ matrices, and there are summations over dummy indices. As a consequence of the Hermiticity properties of the generators, X^* is the complex conjugate of X, and Z is a Hermitian matrix.

For these algebras to be associative, it is sufficient to require the braid transposition schemes for triples of generators. The braid scheme for $A_i^\dagger A_j^\dagger A_k^\dagger$ yields the condition

$$X_{ij,ab} X_{bk,cz} X_{ac,xy} = X_{jk,ab} X_{ia,xc} X_{cb,yz}, \tag{5}$$

i.e., in compact tensor notation, the Yang-Baxter equation for X (in the "braid" version)

$$X_{12} X_{23} X_{12} = X_{23} X_{12} X_{23}. \tag{6}$$

Similarly, for $A_i A_j^\dagger A_k^\dagger$, one gets the two conditions

$$\delta_{ji}\delta_{kx} - X_{jk,ix} + Z_{jk,ix} - X_{jk,ab}Z_{ab,ix} = 0, \tag{7}$$

and

$$Z_{kz,ac}Z_{ja,ib}X_{bc,xy} = X_{jk,ab}Z_{bz,cy}Z_{ac,ix}, \tag{8}$$

which may be written in compact form as

$$(I_{12} - X_{12})(I_{12} + Z_{12}) = 0, \tag{9}$$

and

$$Z_{23}Z_{12}X_{23} = X_{12}Z_{23}Z_{12}. \tag{10}$$

From the Hermiticity properties of the generators, it follows that the remaining two triple products $A_i A_j A_k$ and $A_i A_j A_k^\dagger$ will be associative if $A_i^\dagger A_j^\dagger A_k^\dagger$ and $A_i A_j^\dagger A_k^\dagger$ are so. Hence, eqs. (6), (9), and (10) are the only associativity conditions of algebra (4).

Let now R be any $N^2 \times N^2$ solution of the Yang-Baxter equation

$$R_{12}R_{13}R_{23} = R_{23}R_{13}R_{12}. \tag{11}$$

Then the corresponding braid matrix $\hat{R} = \tau R$, where τ is the twist operator (i.e., $\tau_{ij,kl} = \delta_{il}\delta_{jk}$), satisfies an equation similar to (6).

If $\hat{R}$ has three distinct eigenvalues λ_α, $\alpha = 1, 2, 3$, and satisfies a Birman-Wenzl-Murakami (BWM) condition[2]

$$(\hat{R} - \lambda_1 I)(\hat{R} - \lambda_2 I)(\hat{R} - \lambda_3 I) = 0, \tag{12}$$

then with each eigenspace of $\hat{R}$, one can associate two solutions of the set of associativity conditions (6), (9), and (10). In terms of the projector

$$\mathcal{P}_\alpha = \prod_{\beta \neq \alpha} \frac{(\hat{R} - \lambda_\beta I)}{(\lambda_\alpha - \lambda_\beta)} \tag{13}$$

onto the eigenspace corresponding to the eigenvalue λ_α, these two solutions can be written as

$$I - X \simeq \mathcal{P}_\alpha \qquad \text{and} \qquad Z = -\lambda_\alpha^{-1}\hat{R} \quad \text{or} \quad Z = -\lambda_\alpha \hat{R}^{-1}. \tag{14}$$

Considering for instance $Z = -\lambda_\alpha^{-1}\hat{R}$ leads to the following deformed oscillator algebra (written in compact tensor form)

$$A_2^\dagger A_1^\dagger = S A_1^\dagger A_2^\dagger, \qquad A_1 A_2 = S^* A_2 A_1, \qquad A_1 A_2^\dagger = I_{12} - \lambda_\alpha^{-1} R^{t_1} A_2^\dagger A_1, \tag{15}$$

where $S = \tau X$ is found from (13) and (14), and t_1 means transposition with respect to the first space in the tensor product.

Several examples of such deformed oscillator algebras have been worked out so far [9]–[11]. In all cases, the solution of the Yang-Baxter equation that has been considered is the fundamental R-matrix of some classical quantum group. In such circumstances, the deformed oscillator algebras

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[2]The $SU_q(n)$-covariant algebra constructed by Pusz and Woronowicz [5] corresponds to the simpler case where $\hat{R}$ has only two distinct eigenvalues, and satisfies a Hecke condition (see Sec. 3).

are left invariant under the transformations induced by the quantum group. The construction presented here is not restricted however to such a choice, and any solution of (11) and (12) might actually be used. In a similar way, deformed oscillator algebras differing from that of Pusz-Woronowicz have been built by considering non-standard solutions of the Yang-Baxter equation and the Hecke condition [12].

The algebras constructed in refs. [9]–[11] include both standard and non-standard ones. The former [9,10] are either of q-bosonic or q-fermionic type, meaning that whenever $q \rightarrow 1$, they go over smoothly into ordinary bosonic or fermionic algebras, respectively. The latter [11], on the contrary, do not have such a smooth behaviour, but share instead some features with the quon algebra [13]. In the next section, we shall consider in more details a covariant q-bosonic algebra generalizing that of Pusz-Woronowicz.

3 An $SU_q(n) \times SU_q(m)$-Covariant q-Bosonic Algebra

The $SU_q(n)$ quantum group [1] is a complex associative algebra generated by I and the noncommutative elements T_{ij}, $i, j = 1, \ldots, n$ of an $n \times n$ matrix T, subject to the relations

$$RT_1T_2 = T_2T_1R, \qquad \det_q T = 1, \tag{16}$$

and the *-involution condition

$$T^* = (T^{-1})^t, \tag{17}$$

with q real. In (16), $\det_q$ denotes the quantum determinant, and R is the fundamental R-matrix associated with the A_{n-1} series of Lie algebras,

$$R = q \sum_{i=1}^{n} e_{ii} \otimes e_{ii} + \sum_{\substack{i,j=1 \\ i \neq j}}^{n} e_{ii} \otimes e_{jj} + (q - q^{-1}) \sum_{\substack{i,j=1 \\ i<j}}^{n} e_{ij} \otimes e_{ji}, \tag{18}$$

where $(e_{ij})_{kl} = \delta_{ik}\delta_{jl}$. The coproduct, counit and antipode are defined by

$$\Delta(T) = T_1 \dot\otimes T_2, \qquad \epsilon(T) = 1, \qquad S(T) = T^{-1}, \tag{19}$$

where $\Delta(T_{ij}) = T_{ik} \otimes T_{kj}$.

The braid matrix $\hat{R}$, corresponding to (18), is a real symmetric matrix with two distinct eigenvalues, q and $-q^{-1}$. Their respective multiplicities are $\frac{1}{2}n(n+1)$ and $\frac{1}{2}n(n-1)$, i.e., the dimensions of the symmetric and antisymmetric irreps $[2\,\dot{0}]_n$ and $[1^2\dot{0}]_n$ of $SU_q(n)$. The $\hat{R}$-matrix satisfies the Hecke condition

$$(\hat{R} - qI)(\hat{R} + q^{-1}I) = 0. \tag{20}$$

Similar relations are valid for $SU_q(m)$. Its generators and fundamental R-matrix will be denoted by $\mathcal{T}_{st}$, $s, t = 1, \ldots, m$, and $\mathcal{R}$, respectively, to distinguish them from the corresponding quantities for $SU_q(n)$. Note that T_{ij} and $\mathcal{T}_{st}$ are assumed to commute with one another.

For the product $SU_q(n) \times SU_q(m)$, one can introduce a "large" R-matrix, $\boldsymbol{R} = q^{-1}R\mathcal{R}$, of dimension $(nm)^2 \times (nm)^2$ [10]. Its matrix elements are defined by

$$\boldsymbol{R}_{(is)(jt),(ku)(lv)} = q^{-1}R_{ij,kl}\mathcal{R}_{st,uv}. \tag{21}$$

From the properties of the two "small" braid matrices $\hat{R}$ and $\hat{\mathcal{R}}$, it follows that $\hat{\hat{R}} = q^{-1}\hat{R}\hat{\mathcal{R}}$ has three distinct eigenvalues q, $-q^{-1}$, and q^{-3}, with respective multiplicities corresponding to the dimensions of the representations $[2\,0]_n[2\,0]_m$, $[2\,0]_n[1^2 0]_m + [1^2 0]_n[2\,0]_m$, and $[1^2 0]_n[1^2 0]_m$ of $SU_q(n) \times SU_q(m)$, and satisfies the BWM condition (12).

By applying the results of the previous section to the antisymmetric (reducible) eigenspace of $\hat{\hat{R}}$ associated with the eigenvalue $-q^{-1}$, one gets a deformed oscillator algebra of type (15), which will be denoted by $\mathcal{A}_q(n, m)$, and whose defining relations are [10]

$$A_2^\dagger A_1^\dagger = S A_1^\dagger A_2^\dagger, \qquad A_2 A_1 = A_1 A_2 S, \qquad A_2 A_1^\dagger = I_{21} + q R^{t_1} A_1^\dagger A_2, \tag{22}$$

where

$$S = \tau(I - (q + q^{-1})\mathcal{P}_A), \qquad \mathcal{P}_A = \frac{(\hat{\hat{R}} - qI)(\hat{\hat{R}} - q^{-3}I)}{(q + q^{-1})(q^{-1} + q^{-3})}, \tag{23}$$

and the creation and annihilation operators $A_{is}^\dagger$, A_{is} now have two indices, $i = 1, 2, \ldots, n$, and $s = 1, 2, \ldots, m$. Whenever $q \to 1$, R and S go over into I, so that (22) becomes an ordinary bosonic algebra.

The defining relations (22) of the q-bosonic algebra $\mathcal{A}_q(n, m)$ may be rewritten in terms of the two "small" R-matrices as

$$R A_1^\dagger A_2^\dagger = A_2^\dagger A_1^\dagger \mathcal{R}, \qquad R A_2 A_1 = A_1 A_2 \mathcal{R}, \qquad A_2 A_1^\dagger = I_{21} \mathcal{I}_{21} + R^{t_1} \mathcal{R}^{t_1} A_1^\dagger A_2, \tag{24}$$

or, in a more explicit form, as

$$\begin{aligned}
R_{ij,kl} A_{ks}^\dagger A_{lt}^\dagger &= A_{jv}^\dagger A_{iu}^\dagger \mathcal{R}_{uv,st}, \\
R_{ij,kl} A_{lt} A_{ks} &= A_{iu} A_{jv} \mathcal{R}_{uv,st}, \\
A_{is} A_{jt}^\dagger &= \delta_{ij}\delta_{st} + R_{ki,jl}\mathcal{R}_{us,tv} A_{ku}^\dagger A_{lv}.
\end{aligned} \tag{25}$$

Let us consider the map $\varphi : \mathcal{A}_q(n, m) \to \mathcal{A}_q(n, m) \otimes (SU_q(n) \times SU_q(m))$, defined by

$$\begin{aligned}
A_{is}^{\prime\dagger} &= \varphi(A_{is}^\dagger) = A_{jt}^\dagger T_{ji} \mathcal{T}_{ts}, \\
A_{is}^\prime &= \varphi(A_{is}) = A_{jt} T_{ji}^* \mathcal{T}_{ts}^* = T_{ij}^{-1} \mathcal{T}_{st}^{-1} A_{jt},
\end{aligned} \tag{26}$$

where the elements T_{ij} and $\mathcal{T}_{st}$ of $SU_q(n) \times SU_q(m)$ are assumed to commute with $A_{is}^\dagger$ and A_{is}. As a consequence of (16) and its counterpart for $SU_q(m)$, this map leaves the defining relations (25) of $\mathcal{A}_q(n, m)$ invariant. Hence, the latter is an $SU_q(n) \times SU_q(m)$-covariant algebra.

In the next section, an important part will be played by the modified annihilation operators

$$\tilde{A}_{is} = A_{jt}C_{ji}\mathcal{C}_{ts}, \qquad C_{ji} = (-1)^{n-j}q^{-(n-2j+1)/2}\delta_{j,i'}, \qquad \mathcal{C}_{ts} = (-1)^{m-t}q^{-(m-2t+1)/2}\delta_{t,s'}, \tag{27}$$

where $i' \equiv n + 1 - i$, $s' \equiv m + 1 - s$. Eq. (24) can be rewritten in terms of $A_{is}^\dagger$, $\tilde{A}_{is}$ as

$$R A_1^\dagger A_2^\dagger = A_2^\dagger A_1^\dagger \mathcal{R}, \qquad R \tilde{A}_1 \tilde{A}_2 = \tilde{A}_2 \tilde{A}_1 \mathcal{R}, \qquad \tilde{A}_2 A_1^\dagger = C_{12}\mathcal{C}_{12} + q^2 A_1^\dagger \tilde{A}_2 \tilde{R}^{-1} \tilde{\mathcal{R}}^{-1}, \tag{28}$$

where $\tilde{R}$ is defined by

$$\tilde{R} = \sum_{i=1}^n e_{ii} \otimes e_{i'i'} + q \sum_{\substack{i,j=1 \\ i \neq j'}}^n e_{ii} \otimes e_{jj} + (q - q^{-1}) \sum_{\substack{i,j=1 \\ i < j}}^n (-q)^{i-j+1} e_{ij} \otimes e_{i'j'}, \tag{29}$$

and a similar definition holds for $\tilde{\mathcal{R}}$. Under map φ of eq. (26), $\tilde{A}_{is}$ is transformed into

$$\tilde{A}'_{is} = \varphi(\tilde{A}_{is}) = \tilde{A}_{jt}\tilde{T}_{ji}\tilde{T}_{ts}, \qquad \hat{T} \equiv C^{-1}(T^{-1})^t C, \qquad \tilde{T} \equiv \mathcal{C}^{-1}(\mathcal{T}^{-1})^t \mathcal{C}. \tag{30}$$

Finally, combining eqs. (18) and (25) yields the detailed form of the $\mathcal{A}_q(n, m)$ defining relations

$$\begin{aligned}
A_{is}^\dagger A_{it}^\dagger - q^{-1} A_{it}^\dagger A_{is}^\dagger &= 0, & s < t, \\
A_{is}^\dagger A_{js}^\dagger - q^{-1} A_{js}^\dagger A_{is}^\dagger &= 0, & i < j, \\
A_{is}^\dagger A_{jt}^\dagger - A_{jt}^\dagger A_{is}^\dagger &= 0, & i > j, \quad s < t, \\
A_{is}^\dagger A_{jt}^\dagger - A_{jt}^\dagger A_{is}^\dagger &= -(q - q^{-1}) A_{js}^\dagger A_{it}^\dagger, & i < j, \quad s < t,
\end{aligned} \tag{31}$$

and

$$\begin{aligned}
A_{is} A_{jt}^\dagger - A_{jt}^\dagger A_{is} &= 0, & i \neq j, \quad s \neq t, \\
A_{is} A_{js}^\dagger - q A_{js}^\dagger A_{is} &= (q - q^{-1}) \sum_{t=1}^{s-1} A_{jt}^\dagger A_{it}, & i \neq j, \\
A_{is} A_{it}^\dagger - q A_{it}^\dagger A_{is} &= (q - q^{-1}) \sum_{j=1}^{i-1} A_{jt}^\dagger A_{js}, & s \neq t, \\
A_{is} A_{is}^\dagger - q^2 A_{is}^\dagger A_{is} &= I + (q^2 - 1)\Big(\sum_{j=1}^{i-1} A_{js}^\dagger A_{js} + \sum_{t=1}^{s-1} A_{it}^\dagger A_{it} \\
&\quad - (q^{-2} - 1) \sum_{j=1}^{i-1}\sum_{t=1}^{s-1} A_{jt}^\dagger A_{jt}\Big),
\end{aligned} \tag{32}$$

together with the Hermitian conjugates of (31). Whenever $m = 1$, substituting $A_i^\dagger$, A_i for $A_{i1}^\dagger$, A_{i1} in (31) and (32) yields the Pusz-Woronowicz relations (3) for arbitrary n values. Hence, the covariant q-bosonic algebra $\mathcal{A}_q(n, m)$ is a generalization of that of Pusz-Woronowicz for values of m greater than 1.

4 Alternative Derivation in Terms of $u_q(n) + u_q(m)$

An alternative approach to the construction of covariant deformed oscillator algebras, based upon q-algebras, has been developed elsewhere [14,15]. In the case of the algebra $\mathcal{A}_q(n, m)$ introduced in the previous section, one considers the q-algebra $u_q(n) + u_q(m)$. The Cartan-Chevalley generators of $u_q(n)$ are denoted by $E_{ii} = (E_{ii})^t$, $i = 1, 2, \ldots, n$, $E_{i,i+1}$, $E_{i+1,i} = (E_{i,i+1})^t$, $i = 1, 2, \ldots, n - 1$, and satisfy the commutation relations

$$\begin{aligned}
[E_{ii}, E_{jj}] &= 0, & [E_{ii}, E_{j,j+1}] &= (\delta_{ij} - \delta_{i,j+1}) E_{j,j+1}, \\
[E_{ii}, E_{j+1,j}] &= (\delta_{i,j+1} - \delta_{ij}) E_{j+1,j}, & [E_{i,i+1}, E_{j+1,j}] &= \delta_{ij}[H_i]_q,
\end{aligned} \tag{33}$$

together with the quadratic and cubic q-Serre relations. In (33), $H_i \equiv E_{ii} - E_{i+1,i+1}$. The algebra is endowed with a Hopf algebra structure with coproduct Δ, counit ϵ, and antipode S, defined by

$$\Delta(E_{ii}) = E_{ii} \otimes I + I \otimes E_{ii}, \qquad \Delta(E_{i,i+1}) = E_{i,i+1} \otimes q^{H_i/2} + q^{-H_i/2} \otimes E_{i,i+1},$$

$$\Delta(E_{i+1,i}) = E_{i+1,i} \otimes q^{H_i/2} + q^{-H_i/2} \otimes E_{i+1,i}, \tag{34}$$

$$\epsilon(E_{ii}) = \epsilon(E_{i,i+1}) = \epsilon(E_{i+1,i}) = 0, \tag{35}$$

$$S(E_{ii}) = -E_{ii}, \qquad S(E_{i,i+1}) = -qE_{i,i+1}, \qquad S(E_{i+1,i}) = -q^{-1}E_{i+1,i}. \tag{36}$$

The Cartan-Chevalley generators of $u_q(m)$ are denoted by $\mathcal{E}_{ss}$, $s = 1, 2, \ldots, m$, $\mathcal{E}_{s,s+1}$, $\mathcal{E}_{s+1,s}$, $s = 1, 2, \ldots, m-1$, and satisfy relations similar to (33)–(36), while commuting with the generators of $u_q(n)$.

In the approach based upon $u_q(n)+u_q(m)$, the q-bosonic creation operators $A_{is}^\dagger$, $i = 1, 2, \ldots, n$, $s = 1, 2, \ldots, m$, belonging to $\mathcal{A}_q(n,m)$, are defined as the components of a double irreducible tensor $T^{[1\dot{0}]_n[1\dot{0}]_m}$ with respect to this q-algebra. This means that they fulfil the relations

$$E_{jj}(A_{is}^\dagger) = \delta_{ji}A_{is}^\dagger, \qquad E_{j,j+1}(A_{is}^\dagger) = \delta_{j,i-1}A_{i-1,s}^\dagger, \qquad E_{j+1,j}(A_{is}^\dagger) = \delta_{ji}A_{i+1,s}^\dagger, \tag{37}$$

$$\mathcal{E}_{tt}(A_{is}^\dagger) = \delta_{ts}A_{is}^\dagger, \qquad \mathcal{E}_{t,t+1}(A_{is}^\dagger) = \delta_{t,s-1}A_{i,s-1}^\dagger, \qquad \mathcal{E}_{t+1,t}(A_{is}^\dagger) = \delta_{ts}A_{i,s+1}^\dagger, \tag{38}$$

where, for any $u_q(n) + u_q(m)$ generator X, $X(A_{is}^\dagger)$ denotes the quantum adjoint action $X(A_{is}^\dagger) = \sum_r X_r^1 A_{is}^\dagger S(X_r^2)$, with $\Delta(X) = \sum_r X_r^1 \otimes X_r^2$. The modified annihilation operators $\tilde{A}_{is}$, $i = 1, 2, \ldots, n$, $s = 1, 2, \ldots, m$, of eq. (27), are similarly defined as the components of a double irreducible tensor $T^{[\dot{0}-1]_n[\dot{0}-1]_m}$ with respect to $u_q(n) + u_q(m)$, and satisfy the relations

$$E_{jj}(\tilde{A}_{is}) = -\delta_{ji'}\tilde{A}_{is}, \qquad E_{j,j+1}(\tilde{A}_{is}) = \delta_{ji'}\tilde{A}_{i-1,s}, \qquad E_{j+1,j}(\tilde{A}_{is}) = \delta_{j,i'-1}\tilde{A}_{i+1,s}, \tag{39}$$

$$\mathcal{E}_{tt}(\tilde{A}_{is}) = -\delta_{ts'}\tilde{A}_{is}, \qquad \mathcal{E}_{t,t+1}(\tilde{A}_{is}) = \delta_{ts'}\tilde{A}_{i,s-1}, \qquad \mathcal{E}_{t+1,t}(\tilde{A}_{is}) = \delta_{t,s'-1}\tilde{A}_{i,s+1}. \tag{40}$$

The operators $A_{is}^\dagger$ and $\tilde{A}_{is}$ can be explicitly written down in terms of m independent copies of the Pusz-Woronowicz operators [14]. By using such expressions and exploiting the tensorial character of the operators, it is straightforward to prove that their q-commutation relations are given in coupled form by

$$[A^\dagger, A^\dagger]^{[2\dot{0}]_n[1^2\dot{0}]_m} = [A^\dagger, A^\dagger]^{[1^2\dot{0}]_n[2\dot{0}]_m} = [\tilde{A}, \tilde{A}]^{[\dot{0}-2]_n[\dot{0}(-1)^2]_m} = [\tilde{A}, \tilde{A}]^{[\dot{0}(-1)^2]_n[\dot{0}-2]_m} = 0,$$

$$[\tilde{A}, A^\dagger]^{[1\dot{0}-1]_n[1\dot{0}-1]_m} = [\tilde{A}, A^\dagger]_{q^m}^{[1\dot{0}-1]_n[\dot{0}]_m} = [\tilde{A}, A^\dagger]_{q^n}^{[\dot{0}]_n[1\dot{0}-1]_m} = 0, \tag{41}$$

$$[\tilde{A}, A^\dagger]_{q^{n+m}}^{[\dot{0}]_n[\dot{0}]_m} = \sqrt{[n]_q[m]_q},$$

where, for simplicity's sake, the row labels of the coupled $u_q(n) + u_q(m)$ irreps have been dropped. In (41), the coupled q-commutator of two double irreducible tensors $T^{[\lambda_1]_n[\lambda_2]_m}$ and $U^{[\lambda_1']_n[\lambda_2']_m}$ is defined by [14]

$$\left[T^{[\lambda_1]_n[\lambda_2]_m}, U^{[\lambda_1']_n[\lambda_2']_m}\right]_{(M_1)_n(M_2)_m q^\alpha}^{[\Lambda_1]_n[\Lambda_2]_m}$$

$$= \left[T^{[\lambda_1]_n[\lambda_2]_m} \times U^{[\lambda_1']_n[\lambda_2']_m}\right]_{(M_1)_n(M_2)_m}^{[\Lambda_1]_n[\Lambda_2]_m} - (-1)^\epsilon q^\alpha \left[U^{[\lambda_1']_n[\lambda_2']_m} \times T^{[\lambda_1]_n[\lambda_2]_m}\right]_{(M_1)_n(M_2)_m}^{[\Lambda_1]_n[\Lambda_2]_m}. \tag{42}$$

Here

$$\epsilon = \phi([\lambda_1]_n) + \phi([\lambda_1']_n) - \phi([\Lambda_1]_n) + \phi([\lambda_2]_m) + \phi([\lambda_2']_m) - \phi([\Lambda_2]_m),$$

$$\phi([\lambda_1]_n) = \frac{1}{2}\sum_{i=1}^n (n+1-2i)\lambda_{1i}, \qquad \phi([\lambda_2]_m) = \frac{1}{2}\sum_{s=1}^m (m+1-2s)\lambda_{2s}, \tag{43}$$

and

$$\left[T^{[\lambda_1]_n[\lambda_2]_m} \times U^{[\lambda_1']_n[\lambda_2']_m}\right]_{(M_1)_n(M_2)_m}^{[\Lambda_1]_n[\Lambda_2]_m}$$

$$= \sum_{(\mu_1)_n(\mu_2)_m(\mu_1')_n\mu_2')_m} \langle[\lambda_1]_n(\mu_1)_n,[\lambda_1']_n(\mu_1')_n|[\Lambda_1]_n(M_1)_n\rangle_q \langle[\lambda_2]_m(\mu_2)_m,[\lambda_2']_m(\mu_2')_m|[\Lambda_2]_m(M_2)_m\rangle_q$$

$$\times T^{[\lambda_1]_n[\lambda_2]_m}_{(\mu_1)_n(\mu_2)_m} U^{[\lambda_1']_n[\lambda_2']_m}_{(\mu_1')_n(\mu_2')_m}, \tag{44}$$

where $\langle\,,\,|\,\rangle_q$ denotes a $u_q(n)$ or $u_q(m)$ Wigner coefficient.

By using the values of the latter, eq. (41) can be written in an explicit form [14]. The resulting relations coincide with eqs. (31) and (32), thereby proving the equivalence of the two constructions of $\mathcal{A}_q(n,m)$ based upon $SU_q(n) \times SU_q(m)$ and $u_q(n) + u_q(m)$, respectively.

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LOCALIZATION IN DEFORMED QUANTUM MECHANICS

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Abstract

In this talk it is shown that in one version of q-algebras there exists states -a subset of the coherent states- that have negligible dispersion in energy, position and momentum.

1 General remarks

This talk is devoted to the construction of localized states in deformed quantum mechanics. These states will be exhibited explicitly. A localized state is defined as one whose dispersion vanishes or that is at least near zero. To start with I will say that the version of q-algebras [1, 2, 3, 4, 5] that will be used in the sequel is $AA^\dagger - qA^\dagger A = I$ where $q : 0 \to 1$. The operators A and $A^\dagger$ are realized as operators on a space of analytic functions of a complex variable z as follows

$$Af(z) = \frac{f(z) - f(qz)}{(1-q)z} \equiv Df(z) \tag{1}$$

$$A^\dagger f(z) = zf(z) \tag{2}$$

The space of functions -denoted H_q- has an inner product (f,g) defined by [10, 1, 4] see also [6, 9, 7, 8]

$$(f,g) = \int D^2 z f^*(z) m(|z|^2) g(z) = \pi^{-1} \int_0^{[\infty]} D(|z|^2) \int_0^{2\pi} d\phi f^*(z) m(|z|^2) g(z) \tag{3}$$

where the kernel $m(|z|^2)$ is fixed by the requirement that A has to be the hermitian conjugate of $A^\dagger$. The explicit form of the kernel $m(|z|^2)$ is

$$m(|z|^2) = \frac{1}{exp_q(q|z|^2)} \tag{4}$$

where the deformed exponential $exp_q(z)$ is defined as the solution to the equation $Df(z) = f(z)$ and has the explicit expression

$$exp_q(z) = \sum_{n=0}^\infty \frac{z^n}{[n]!} \tag{5}$$

The box symbol $[n]$ is defined as $[n] = \frac{1-q^n}{1-q}$; the special value with $n = \infty$ is given by $[\infty] = \frac{1}{1-q}$ and the deformed factorial is defined as $[n]! = [1] \cdots [n]$ and $[1]! = 1$. At this point it is convenient to remark that the form of the box symbol is intimately related to the particular version of the q-algebra that is being used while the realization 1 and 2 is not. See [11].

Under the inner product 3 the set of functions $u_n(z) = \frac{z^n}{[n]!^{\frac{1}{2}}}, n = 0, \ldots, \infty$ are orthonormal. It is clear that $u_n(z)$ is an eigenfunction of the operator $z\frac{d}{dz}$ with eigenvalue n; in fact $z\frac{d}{dz}$ is the number operator. To each function $u_n(z)$ there corresponds a ket $\mid n >$ which is an eigenket of the number operator. As a further remark, it is clear from the definition of the deformed exponential function that its series expansion converges in a finite region of the complex z-plane; this region is defined by $\mid z \mid < [\infty]$.

2 Coherent states

Coherent states are defined as eigenfunctions of the anihilation operator. Each function will be labelled with a complex number β so that the function $f_\beta(z)$ represents the coherent state $\mid \beta >$ in the ket notation. The explicit expression for the coherent state $f_\beta(z)$ is

$$f_\beta(z) = C(\beta)exp_q(\beta z) = C(\beta) \sum_{n=0}^{\infty} \frac{\beta^n u_n(z)}{[n]!^{\frac{1}{2}}} \tag{6}$$

where the normalization constant $C(\beta)$ is given by

$$C(\beta)^2 = \frac{1}{exp_q(\mid \beta \mid^2)} \tag{7}$$

The set of all coherent states is overcomplete as seen by the fact that the functions $f_\beta(z)$ are not orthogonal to one another and that a resolution of the identity can be constructed with them. This construction requires that the identity be resolved both in terms of the orthonormal set of functions $u_n(z)$ defined above and in terms of coherent states. This leads to the equation

$$I = \sum_0^{\infty} u_n^*(z)u_n(z) = \int D^2\beta M(\mid \beta \mid^2)f^*(z)f(z) \tag{8}$$

where the kernel $M(\mid \beta \mid^2)$ is obtained by requiring that the above equation be satisfied. Its explicit expression is [5]

$$M(\mid \beta \mid^2) = \frac{exp_q(\mid \beta \mid^2)}{exp_q(q \mid \beta \mid^2)} \tag{9}$$

At this point it is convenient to reconsider the convergence question. The coherent states are constructed so as to be normalized. This implies that the region in the β -complex plane allowed for the label of the coherent states is $\mid \beta \mid^2 < [\infty]$. The same upper bound is found for $\mid z \mid^2$ to have a convergent power series. As a result it is found that the functions that belong to the Hilbert space H_q are analytic in a finite region of the complex z-plane. This region extends to the whole complex z-plane when q goes to 1 and reduces to the unit circle when q goes to zero.

3 Localization

To study localization two hermitian operators Q and P will be introduced in such a way that their relation to the creation and anihilation operators A and $A^\dagger$ resembles closely the relation valid for q=1. Then Q and P are written in the form [12]

$$Q = sA + s^*A^\dagger, P = rA + r^*A^\dagger \tag{10}$$

From the commutation relations for A and $A^\dagger$ it is found that Q and P satisfy

$$[Q, P] = (rs^* - r^*s)[1 + (q-1)A^\dagger A] \tag{11}$$

which reduces to the usual commutation relation for the position and momentum operators when q=1 after a particular selection of the constants r and s that appear in equation (10). This justifies calling Q the deformed position operator and P the deformed momentum operator.

From the commutation relation equation(11) for Q and P it follows the uncertainty relation

$$(\Delta Q)^2_f(\Delta P)^2_f \geq \frac{|< [Q, P] >_f|^2}{4} \tag{12}$$

In equation (12) $(\Delta Q)^2_f = < Q^2 >_f - < Q >^2_f$ and $< Q >_f = (f, Qf)$; f is any function in H_q. Now the expectation values and dispersions will be computed using the coherent state basis (that means that $f(z)$ is taken as $f_\beta(z)$). The results are

$$(\Delta Q)^2_\beta = | s |^2 [1 + (q-1) | \beta |^2] \tag{13}$$

$$(\Delta P)^2_\beta = | r |^2 [1 + (q-1) | \beta |^2] \tag{14}$$

$$< PQ >_\beta - < QP >_\beta = (rs^* - r^*s)[1 + (q-1) | \beta |^2] \tag{15}$$

From these results it follows that, unlike the non-deformed (q=1) case, the uncertainties depend on the label β of the particular coherent state used to compute them. Notice that if q=1 then all uncertainties are constant. The fact that the uncertainties depend on β is the crucial result to exhibit localization; in fact, if $| \beta |^2$ has a value near $\frac{1}{1-q}$ which is an annulus near the boundary of the convergence region then all uncertainties in equations(13), ('14) and (15) are negligible. So those coherent states whose labels are near the boundary show localization according to the definition stated above. Moreover, near the boundary the operators Q and P are commuting, at least in the weak sense that $< PQ >_\beta - < QP >_\beta$ tends to 0. Those coherent states that are localized behave as classical states in a much closer way than the usual (q=1) coherent states which exhibit minimum non-vanishing uncertainty. The deformed coherent states are in this sense a better answer to the original Schroedinger question of finding those states that resemble classical states than the ordinary coherent states.

Now I will show that the deformed coherent states are minimum uncertainty states and that they can be generated by the action of a shifting operator acting on the vacuum. To start with, the right-hand side of 12 (T denotes the right-hand side of 11) is found to be

$$|< T >_\beta|^2 = | r |^2| s |^2 [2 - exp2i(\phi_r - \phi_s) - exp2i(\phi_s - \phi_r)][1 + (q-1) | \beta |^2] \tag{16}$$

which tends to zero when $\mid \beta \mid^2$ tends to $\frac{1}{1-q}$; in the above equation ϕ_r and ϕ_s denote the phases of the complex numbers r and s, respectively. If $exp2i(\phi_r - \phi_s) = -1$ then the equality sign is valid in equation (12) so that for any fixed value of β the corresponding coherent state has minimum uncertainty; on the other hand, if the boundary of the convergence region is approached both sides of 12 tend to zero.

4 Shifting operator

Next, turn to the shifting operator. Notice that the function $f_\beta(z)$ representing the coherent state labelled by β can be written

$$f_\beta(z) = C(\beta)exp_q(\beta A^\dagger)f_0(z) \tag{17}$$

where $f_0(z) = 1$ represents the vacuum state. Then

$$f_\beta = C(\beta)D_q(A, A^\dagger; \beta)f_0 \tag{18}$$

where

$$D_q(A, A^\dagger; \beta) = exp_q(\beta A^\dagger)\frac{1}{exp_q(\beta^* A)} \tag{19}$$

$D_q(A, A^\dagger; \beta)$ is the shifting operator. It follows that $D_q^{-1} \neq D_q^\dagger$ so that D_q is non-unitary. The action of $D_q(A, A^\dagger; \beta)$ on $f_0(z)$ generates unnormalized coherent states; that is why the factor $C(\beta)$ appears in an explicit way. Finally, it is easy to verify that $D_q(A, A^\dagger; \beta)$ satisfies

$$D_q(A, A^\dagger; \beta)AD_q^{-1}(A, A^\dagger; \beta) = \frac{exp_q(\beta A^\dagger)}{exp_q(q\beta A^\dagger)}[A - \beta I] \tag{20}$$

which gives the usual result when $q = 1$. For labels α , β and γ

$$D_q(A, A^\dagger; \alpha)D_q(A, A^\dagger; \beta) \neq D_q(A, A^\dagger; \gamma) \tag{21}$$

5 Hamiltonian

The last point concerns the hamiltonian of the system. This is constructed from the commutation relation for Q and P and has the form

$$h_q = AA^\dagger + A^\dagger A = \frac{Q^2}{2 \mid s \mid^2} + \frac{P^2}{s \mid r \mid^2} \tag{22}$$

whose uncertainty is

$$(\Delta h_q)_\beta^2 = \mid \beta \mid^2 [1 + (q - 1) \mid \beta \mid^2] \tag{23}$$

which tends to zero when $\mid \beta \mid^2$ approaches $\frac{1}{1-q}$. This is another indication that the system described by the coherent states near the boundary of the convergence region resembles a classical system.

To summarize: when $\mid \beta \mid^2$ is near $\frac{1}{1-q}$ then $(\Delta Q)_\beta^2$, $(\Delta P)_\beta^2$, $(\Delta h_q)_\beta^2$ and $< PQ >_\beta - < QP >_\beta$ all tend to zero. This corresponds closely to the behavior of a classical system.

Acknowledgments

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Noisy bases in Hilbert space: A new class of thermal coherent states and their properties

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Abstract

Coherent mixed states (or thermal coherent states) associated with the displaced harmonic oscillator at finite temperature, are introduced as a "random" (or "thermal" or "noisy") basis in Hilbert space. A resolution of the identity for these states is proved and used to generalise the usual coherent state formalism for the finite temperature case. The Bargmann representation of an operator is introduced and its relation to the P and Q representations, is studied. Generalised P and Q representations for the finite temperature case are also considered and several interesting relations among them are derived.

1. Introduction

Coherent states have played an important role in various areas of physics. They provide a non-orthonormal, over-complete basis in the Hilbert space, which however is very useful in many problems. In spite of the non-orthonormal nature of this basis, the resolution of the identity makes it practically usable in the sense that it can be used for the expansion of an arbitrary state in the coherent state basis.

In a previous publication [1] we have considered a generalisation of the ordinary coherent states into the so-called "coherent mixed states" or "thermal coherent states". They describe displaced harmonic oscillators at finite temperature T; or alternatively, mixtures of coherent states in thermal noise [2]. In contrast to the various types of coherent states considered in the literature which are pure states, our coherent mixed states are, as the name indicates, mixed states in general; and they are pure states only in the special case of zero temperature. They can be considered as a "noisy" or "random" basis in the Hilbert space. We prove that there exists a resolution of the identity for these states, and this makes possible an expansion of an arbitrary state in the coherent mixed state basis. The Q and P representations which are usually defined in terms of ordinary coherent states are generalised within our formalism.

The purpose of this paper is to expand our previous work and express it within the Bargmann representation [3]. This representation makes possible

the exploitation of the powerful theory of analytic functions in the complex plane, within a quantum mechanical context. In section 2, we define the coherent mixed states in the Bargmann representation. For example, we derive a transformation which connects the Bargmann representation with the usual x- an p- representations. We also explain how an operator can be expressed in a differential form or in an integral form (i.e. as the kernel of an integral) in the Bargmann formalism. In section 3 we explain how our mixed coherent states can be considered as a "random" or "noisy" basis in the Hilbert space. In section 4 we explain the relation between the Bargmann representation of on operator and its P, Q, W (Wigner) representations. In section 5 we introduce generalised (finite temperature) P and Q representations and examine various relations among them. Known results [4, 5, 6] on P and Q representations are in this section generalised for the finite temperature P and Q representations. We conclude in section 6 with a discussion of our results.

2. Displaced oscillator at finite temperature in the Bargmann representation

We consider the Glauber coherent states

$$|z> = D (z) |0> = \exp \left[- \tfrac{1}{2} |z|^2 \right] \sum_{N=0}^{\infty} z^N (N!)^{-\tfrac{1}{2}} |N>$$

$$D (z) = \exp [za^+ - z^*a]; \quad [a,a^+] = I \tag{1}$$

$$<z|z'> = \exp \left[-\tfrac{1}{2}|z|^2 - \tfrac{1}{2}|z'|^2 + z^*z' \right]$$

We introduce the Bargmann analytic representation by considering an arbitrary state

$$|f> = \sum_{N=0}^{\infty} f_N |N> = \sum_{N=0}^{\infty} f_N (N!)^{-\tfrac{1}{2}} (a^+)^N |0>$$

$$\sum_{N=0}^{\infty} |f_N|^2 = 1 \tag{2}$$

$$<f^*| = \left(|f^*> \right)^+ = \sum_{N=0}^{\infty} f_N <N|$$

and representing it with the analytical function

$$|f> \longrightarrow f_B (z) = F_B (|f>;z = \exp \left[\tfrac{1}{2}|z|^2 \right] <z^*|f> = \sum_{N=0}^{\infty} f_N \cdot z^N (N!)^{-\tfrac{1}{2}} \tag{3}$$

Using the resolution of the identity

$$\int \frac{d^2z}{\pi} |z> <z| = I; \quad d^2z = d(Rez) \, d (Imz) = \frac{1}{2i} dzdz^* \tag{4}$$

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we easily prove that the scalar product of two states $|f>$, $|g>$ can be expressed as

$$<f^*|g> = \int f_B (z) \, g_B (z^*) \, \exp (-|z|^2) \, \frac{d^2z}{\pi} \tag{5}$$

The creation and annihilation operators are represented as

$$a \longrightarrow \frac{d}{dz} \tag{6}$$

$$a^+ \longrightarrow z$$

As an example we consider the coherent states $|A>$ and the number eigenstates $|N>$ which in the Bargmann representation are represented by the analytical functions:

$$|A> \longrightarrow F_B (|A>;z) = \exp \left[- \tfrac{1}{2} |A|^2 + Az \right] \tag{7}$$

$$|N> \longrightarrow F_B (|N>;z) = z^N (N!)^{-\tfrac{1}{2}}$$

We next introduce transformations that connect the Bargmann representation with the usual position and momentum representations denoted here with the indices x,p correspondingly

$$f_x (z_R) = \pi^{-3/4} \exp \left[- \tfrac{1}{2} z_R^2 \right] \int_\infty^\infty dz_I \, \exp (-z_I^2) \, f_B (2^{\tfrac{1}{2}}z) \tag{8}$$

$$f_p (z_I) = \pi^{-3/4} \exp \left[- \tfrac{1}{2} z_I^2 \right] \int_\infty^\infty dz_R \, \exp (-z_R^2) \, f_B (2^{\tfrac{1}{2}}z^*) \tag{9}$$

where $z_R = \mathrm{Re}z$ and $z_I = \mathrm{Im}z$. The proof is based on equ (3) and the integral representations of the Hermite Polynomials:

$$H_N (x) = 2^N \pi^{-\tfrac{1}{2}} \int_\infty^\infty (x + it)^N \exp (-t^2) \, dt \tag{10}$$

An operator θ

$$\theta = \sum \theta_{NM} |N> <M| \tag{11}$$

can be represented by the analytic function of two variables:

$$\theta \longrightarrow \theta_B (z_1,z_2^\dagger) = B (\theta;z_1,z_2^*) = \exp \left[\tfrac{1}{2}|z_1|^2 + \tfrac{1}{2}|z_2|^2 \right] <z_1^*|\theta|z_2^*>$$

$$= \sum_{N,M} \theta_{NM} z_1^N (z_2^*)^M \left[(N!)(M!) \right]^{-\frac{1}{2}} \tag{12}$$

We refer to this as the B-representation. It provides an "integral" representation of an operator in the Bargmann formalism. The operator is here represented by a kernel of an integral. The action of this operator on the (arbitrary) state $|f\rangle$ of equ (2) can be described by the integral

$$\theta|f\rangle \longrightarrow \int B\ (\theta;z_1,z'^*)\ f_B\ (z')\ \exp\ (-|z'|^2)\ \frac{d^2 z'}{\pi} \tag{13}$$

The B - representation of the product of two operators is given by

$$B\ (\theta_1 \theta_2;z_1,z_2^*) = \int B\ (\theta_1;z_1,z_3^*)\ B\ (\theta_2;z_3,z_2^*)\ \exp\ (-|z_3|^2)\ \frac{d^2 z_3}{\pi} \tag{14}$$

The creation and annihilation operators (already given in equ (6)) are here represented by the functions:

$$B\ (a;z_1,z_2*) = z_2^*\ \exp\ (z_1 z_2^*)$$

$$B\ (a^+;z_1,z_2^*) = z_1\ \exp\ (z_1 z_2^*) \tag{15}$$

The representations of equ (15) are consistent with these of equ (6). Indeed

$$\int z_2^*\ \exp\ (z_1 z_2^*)\ \exp\ (-|z_2|^2)\ f\ (z_2)\ \frac{d^2 z_2}{\pi} = \frac{d}{dz_1}\ f_B(z_1)$$

$$\int z_1\ \exp\ (z_1 z_2^*)\ \exp\ (-|z_2|^2)\ f\ (z_2)\ \frac{d^2 z_2}{\pi} = z_1 f_B(z_1) \tag{16}$$

Both equations can be proved using the fact that $f(z)$ is a holomorphic function therefore

$$\frac{1}{2\pi i}\ \int \frac{f(z_2)}{z_2 - z_1}\ dz_2 = f_B(z_1) \tag{17}$$

Where the integral is taken around some suitable contour enclosing the point z_1 in an anticlockwise direction. Note that the trace of an operator can be expressed as

$$\mathrm{Tr}(\theta) = \int \frac{d^2 z}{\pi}\ \exp\ (-|z|^2)\ B\ (\theta;z,z^*) \tag{18}$$

and that the trace of the product of two operators can be expressed as:

$$\text{Tr} \ (\Theta_1 \Theta_2) = \int B \ (\Theta_1; z_1, z_2{}^*) \ B \ (\Theta_2; z_2, z_1{}^*) \ \exp \ (-|z_1|^2 - |z_2|^2)$$

$$\frac{d^2 z_1}{\pi} \ \frac{d^2 z_2}{\pi} \qquad (19)$$

For later use we mention that the unit operator I is represented by the function

$$B \ (I; z_1, z_2{}^*) = \exp \ (z_1 z_2{}^*) \qquad (20)$$

and that the displacement operator is represented by the function

$$B \ (D(A); z_1, z_2{}^*) = \exp \ \left[-\tfrac{1}{2}|A|^2 - A^* z_2{}^* + z_1 A + z_1 z_2{}^* \right] \qquad (21)$$

A density matrix ρ with eigenvalues p_N, eigenstates $|e^{(N)}\rangle$ and matrix elements with respect to the number eigenstates p_{NM}

$$\rho = \sum \ p_N \ |e^{(N)}\rangle \ \langle e^{(N)}| = \sum p_{NM} |N\rangle \langle M|$$

$$0 \leq p_N \leq 1$$

$$\sum p_N = 1 \qquad (22)$$

can be represented by the analytical function of two variables (equ (12)):

$$\rho_B(z_1, z_2{}^*) = \exp \ \left[\tfrac{1}{2}|z_1|^2 + \tfrac{1}{2}|z_2|^2 \right] \ \langle z_1{}^*|\rho|z_2{}^*\rangle \qquad (23)$$

$$= \sum \ p_N \ e^{(N)}{}_B \ (z_1) \left[e^{(N)}{}_B \ (z_2) \right]^* = \sum \ p_{NM} \ (z_1)^N (z_2{}^*)^M \left[(N!)(M!) \right]^{-\tfrac{1}{2}}$$

The displaced oscillator of finite temperature is represented by the density matrix ($k_B = h = \omega = 1$):

$$\rho(A; \beta) = D(A) \ \exp \ [-\beta a^+ a] D^+ \ (A) \ (1 - e^{-\beta})$$

$$= \exp \ \left[-\beta(a^+ - A^*)(a - A) \right] \ (1 - e^{-\beta})$$

where β is the inverse temperature. We can easily prove that in limit $\beta \longrightarrow \infty$ ($T \longrightarrow o$)

$$\lim_{\beta \longrightarrow \infty} \rho \ (A; \beta) = |A\rangle \langle A| \qquad (25)$$

The Bargmann representation of this density matrix can be found from equ (23). We prove:

$$\rho_B(A; \beta; z_1, z_2{}^*) = (1 - e^{-\beta})$$

$$x \exp \left[(1 - e^{-\beta}) (A^* z_2{}^* + z_1 A - |A|^2) + z_1 z_2{}^* e^{-\beta} \right] \qquad (26)$$

3. Mixed states as "noisy bases" in Hilbert space:

The simplest type of basis in a Hilbert space is the orthonormal $\{|u_N\rangle\}$ for which

$$\pi_N = |u_N\rangle \langle u_N| \qquad (27)$$

$$\pi_N \pi_M = \delta_{NM} \pi_N \qquad (28)$$

$$\sum \pi_N = 1 \qquad (29)$$

The π_N are orthonormal projection operators. Equ (29) is important for two reasons. First, it is a proof of the completeness of the basis. And second, it can be used to expand an arbitrary state $|s\rangle$ as:

$$|s\rangle = \sum s_N |u_N\rangle \qquad (30)$$

$$s_N = \langle u_N|s\rangle \qquad (31)$$

This second point is very important from a practical point of view, because for some bases we might have an abstract proof of completeness, but not a resolution of the identity like (29); and then we do not know how to use this basis, in practice.

Another type of basis is provided by the coherent states, which is overcomplete and non-orthonormal:

$$\pi(A) = |A\rangle \langle A| | \qquad (32)$$

$$\pi^2(A) = \pi(A) \qquad (33)$$

$$\int \frac{d^2A}{\pi} \pi(A) = 1 \qquad (34)$$

The $\pi(A)$ are still projection operators (describing pure states); but in this case they are non-orthonormal. And yet, the resolution of the identity (34) allows us to express an arbitrary state $|s\rangle$ as

$$|s\rangle = \int \frac{d^2A}{\pi} s(A) |A\rangle \qquad (35)$$

$$s(A) = \langle A|s\rangle \qquad (36)$$

Our proposal in this and in our previous work [1] is to use a set of mixed states as a basis in a Hilbert space. A mixed state described by a

density matrix ρ with eigenstates $|e_N\rangle$ and eigenvalues p_N

$$\rho = \sum_{N=0}^{\infty} p_N |e_N\rangle \langle e_N|, \qquad (37)$$

$$\sum_{N=0}^{\infty} p_N = 1; \quad 0 \leq p_N \leq 1, \qquad (38)$$

represents a set of states $\{|e_N\rangle\}$ with a probability distribution $\{p_N\}$. Therefore the idea of using mixed states as a basis replaces the "fixed" veetors which are usually used, in a basis with "noisy vectors" (i.e. "random vectors").

The basis used in this paper is the set of all density matrices $\rho(A;\beta)$ of equ (24) for all complex values A and fixed (but arbitrary) value of β. In this case equ (37) becomes

$$\rho(A;\beta) = \sum p_N(\beta) |N;A\rangle \langle N;A| \qquad (39)$$

$$|N;A\rangle = D(A)|N\rangle \qquad (40)$$

$$p_N(\beta) = \left[1 - \exp(-\beta)\right] \exp(-\beta N) \qquad (41)$$

We have proved in [1] that the $\rho(A;\beta)$ obey the resolution of the identity

$$\int \frac{d^2 A}{\pi} \rho(A;\beta) = I \qquad (42)$$

This is a significant relation for our purposes because it can be used to expand an arbitrary state $|s\rangle$ as

$$|s\rangle = \int \frac{d^2 A}{\pi} \rho(A,\beta)|s\rangle \qquad (43)$$

The density matrices $\rho(A;\beta)$ have been expressed in the Bargmann representation in equ (26). The resolution of the identity (42) can be written in the Bargmann representation as:

$$\int \rho_B(A;\beta;z_1,z_2{}^*)\frac{d^2 A}{\pi} = \exp(z_1 z_2{}^*) \qquad (44)$$

where as explained in equ (18) the right hand side is the unit operator in this formalism.

4. **B- representation and its relationship to P, Q, W representations:**

There has been a lot of discussion in the literature (reviewed in [4, 5, 6]) on the Q, P and Weyl representations and the relationships among them. The purpose of this section is to examine the relationship of the

B-representation with the others; and also to present some basic material which will be used in the next section, where all these quantities will be generalised into their finite temperature equivalents.

The Q and P representations of an operator θ are defined as

$$Q\ (\theta;A) = <A|\theta|A> \tag{45}$$

$$\theta = \int P(\theta;A)\pi(A)\frac{d^2A}{\pi} \tag{46}$$

where the $\pi(A)$ have been defined in (32).

The Q and P-representations are related with the Bargmann representation of equ (12) as follows:

$$Q(\theta;z) = \left[\exp\ (-|z|^2)B(\theta;z^*,z)\right] \tag{47}$$

$$P(\theta;A) = \exp\ (|A|^2)\int\frac{d^2z}{\pi}\ B(\theta;\ -z^*,z)\ \exp\ (Az^* - A^*z)\Bigg] \tag{48}$$

Equ (47) can be easily proved with the use of the definition (12); equ (48) is similar to the result given by Mehta [7].

We introduce the notation $\tilde{f}(w)$ for the two-dimensional Fourier transform of the function f(z) defined as:

$$\tilde{f}(w) = \int d^2z\ \exp\ \left[i(w_R z_R + w_I z_I)\right]f(z) \tag{49}$$

where the indices R,I indicate the real and imaginary parts correspondingly. We can prove the following relations that express the Bargmann representation in terms of the P and Q representations:

$$B(\theta;z_1,z_2^*) = \int P\ (\theta;z)\ \exp\ (zz_1 + z^*z_2^* - |z|^2)\ \frac{d^2z}{\pi} \tag{50}$$

$$B(\theta;z_1,z_2^*) = e^{z_1z_2^*}\int\frac{d^2w}{(2\pi)^2}\tilde{Q}\ (\theta;w)\ \exp\ \left[-\ i\tfrac{1}{2}(wz_1 + w^*z_2^*)\right] \tag{51}$$

We next use the relation

$$\int\frac{d^2A}{\pi}\ f\ (A^*,A)\ k\ \exp\ (-k|A - B|^2) = \exp\ \left[\frac{1}{4k}\ \Delta_B\right]\ f\ (B^*,B)$$

$$\Delta_B = 4\ \frac{\partial^2}{\partial B\partial B^*}\ ,k>0 \tag{52}$$

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which can be proved with a Fourier transform of both sides. Δ_B is the Laplacian in a two-dimensional space.

We next consider the Wigner function corresponding to an operator θ.

$$\theta_W (A) = Tr \left[\theta D(A) \right] \tag{53}$$

It is known [4] that

$$\theta = \int \frac{d^2 A}{\pi} \; Tr \left[D^+(A) \theta \right] \; D(A) = \int \frac{d^2 A}{\pi} \; \theta_W (-A) \; D (A) \tag{54}$$

For a density matrix ρ the definition (53) leads to the more familiar expression

$$\rho_W (A) = Tr \left[\rho D(A) \right] = \int dx < -2^{-\frac{1}{2}} A_R + x \; |\rho| 2^{-\frac{1}{2}} A_R + x > \exp \left[i \; x \; (2^{\frac{1}{2}} A_I) \right] \tag{55}$$

It is convenient for later purposes to make a trivial change of variables

from A to $\frac{1}{2}iw$ and denote the resulting function by $\tilde{W}(\theta;w)$

$$\tilde{W} (\theta;w) = \pi Tr \left[\theta D(\tfrac{1}{2}iw) \right] = \pi \theta_W(\tfrac{1}{2}iw) \tag{56}$$

We shall also use its Fourier transform $W(z;\theta)$ defined as the inverse of the transform given in equ (36). Using equs (54), (21) we prove:

$$B(\theta;z_1,z_2{}^*) = \int \frac{d^2 A}{\pi^2} \; \tilde{W} (\theta;2iA) \; \exp \left[-\tfrac{1}{2}|A|^2 + Az_1 - A^* z_2{}^* + z_1 z_2{}^* \right] \tag{57}$$

Using equs (19), (21), (56) we prove the inverse of this transform:

$$\tilde{W} (\theta;2iA) = \frac{1}{\pi} \int d^2 z_1 \; d^2 z_2 \; B (\theta;z_1,z_2{}^*)$$

$$\exp \left[-\tfrac{1}{2}|A|^2 - |z_1,|^2 - |z_2|^2 - A^* z^*{}_1 + z_2 A + z_2 z_1{}^* \right] \tag{58}$$

5. Generalized P and Q representations for finite temperature

The formalism of P and Q representations is based on coherent states. Although they form an overcomplete basis, it is the fact that a resolution of the identity (equ(4)) is available, that makes them practically usable. The density matrices $\rho(A;\beta)$ provide a generalization of the coherent states and they also obey the resolution of the identity (42). It seems therefore natural to define generalized P and Q representations based on $\rho(A;B)$. More

specifically we introduce:

$$Q\ (\Theta;A;\beta)\ =\ \mathrm{Tr}\ \left[\rho(A;\beta)\Theta\right] \tag{59}$$

$$\Theta\ =\ \int\frac{d^2A}{\pi}\ \rho\ (A;\beta)\ P\ (\Theta;A;\beta) \tag{60}$$

It is clear from equ (25) that in the limit $T\longrightarrow 0$ ($\beta\longrightarrow\infty$) they reduce to the ordinary Q and P representations.

From equs (59), (60) we easily get

$$Q\ (\Theta;A;\beta)\ =\ \int\frac{d^2B}{\pi}\ P(\Theta,B;\beta')\ \mathrm{Tr}\ \left[\rho(B,\beta')\ \rho\ (A,\beta)\right] \tag{61}$$

We next show

$$\mathrm{Tr}\ \left[\rho(B,\beta')\ \rho\ (A,\beta)\right]\ =\ 2\ \left[g(\beta,\beta')\right]^{-1}\ \exp\ \left[-2\ \frac{1}{g(\beta,\beta')}\ |A\text{-}B|^2\right] \tag{62}$$

where

$$g(\beta,\beta')\ =\ \frac{\sinh\ [\tfrac{1}{2}\ (\beta\ +\ \beta')]}{\sinh\ (\tfrac{1}{2}\ \beta)\ \sinh\ (\tfrac{1}{2}\ \beta')} \tag{63}$$

Combining equs (61), (62), (63) and taking into account equ (52) we get:

$$Q\ (\Theta;z;\beta)\ =\ \exp\ \left[\frac{1}{8}\ g\ (\beta,\beta')\ \Delta_z\right]\ P\ (\Theta;z;\beta') \tag{64}$$

Fourier transform of this equation gives

$$\tilde{Q}\ (\Theta;w;\beta)\ =\ \exp\ \left[-\ \frac{1}{8}\ g\ (\beta,\beta')\ |w|^2\right]\ \tilde{P}\ (\Theta;w;\beta') \tag{65}$$

In the special case $\beta\ =\ \beta'$ equs (63), (64), (65) give

$$g\ (\beta,\beta)\ =\ 2\ \coth\ (\tfrac{1}{2}\beta) \tag{66}$$

$$Q\ (\Theta;z;\beta)\ =\ \exp\ \left[\tfrac{1}{4}\ \coth\ (\tfrac{1}{2}\beta)\ \Delta_z\right]\ P\ (\Theta;z;\beta) \tag{67}$$

$$\tilde{Q}\ (\Theta;w;\beta)\ =\ \exp\ \left[-\tfrac{1}{4}\ \coth\ (\tfrac{1}{2}\beta)\ |w|^2\right]\ \tilde{P}\ (\Theta;w;\beta) \tag{68}$$

In the zero temperature limit

$$\lim\ g\ (\beta,\beta)\ =\ 2 \tag{69}$$

$\beta \longrightarrow \infty$

and equs (67), (68) reduce to

$$Q(\theta;z) = \exp(\tfrac{1}{4}\Delta_z) P(\theta_{;z})$$ (70)

$$\tilde{Q}(\theta;w) = \exp(-\tfrac{1}{4}|w|^2) \tilde{P}(\theta;w)$$ (71)

Equs (70), (71) are known in the literature [4, 5, 6]. Our contribution is to generalize them into equs (64), (65).

We next relate the P and Q representations to the Wigner function introduced in the previous section. Using equs (54), (55), (59), (60) we prove

$$Q(\theta;A;\beta) = \int \frac{d^2B}{(2\pi)^2} \tilde{W}(\theta;B) \exp\left[-\frac{1}{8}|B|^2 \coth(\tfrac{1}{2}\beta)\right]$$

$$x \exp\left[-i(A_R B_R + A_I B_I)\right] = \exp\left[\frac{1}{8}\coth(\tfrac{1}{2}\beta)\Delta_A\right] W(\theta;A)$$ (72)

$$P(\theta;A;\beta) = \int \frac{d^2B}{(2\pi)^2} \tilde{W}(\theta;B) \exp\left[\frac{1}{8}|B|^2 \coth(\tfrac{1}{2}\beta)\right] x$$

$$x \exp\left[-i(A_R B_R + A_I B_I)\right] = \exp\left[-\frac{1}{8}\coth(\tfrac{1}{2}\beta)\Delta_A\right] W(\theta;A)$$ (73)

Note that from equs (72), (73) we can derive equ (67). The expressions (72), (73) are identical, apart from a minus sign. In this sense the Q-representation can be considered as the analytic continuation of the P-representation at "negative temperatures". In the zero temperature limit ($\beta \longrightarrow \infty$) the above equations reduce to

$$Q(\theta;A) = \exp\left[\frac{1}{8}\Delta_A\right] W(\theta;A)$$ (74)

$$P(\theta;A) = \exp\left[-\frac{1}{8}\Delta_A\right] W(\theta;A)$$ (75)

6. Conclusions

Generalizations of the original coherent states are usually based on replacing the Weyl group with another one (e.g. SU(2), SU(1,1) etc.). All these coherent states are pure states. In this paper and in ref [1] we have studied coherent mixed states associated with the displaced oscillator at finite temperature. We have shown that these states can be viewed as consisting a "random" (or "noisy" or "thermal") basis in the Hilbert Space. The fact that we were able to prove a resolution of the identity for these states, makes them practically usable.

All the calculations in this paper have been presented in the Bargmann

representation. Relations between the Bargmann and the P, Q representations of an operator have been studied. A generalization of the P and Q representations for the finite temperature case, has been proposed and various relations among them have been studied.

From a practical point of view our coherent mixed states can be used for the description of coherent signals in thermal noise. There is a lot of activity in this area [8] and our work provides theoretical support to such studies.

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GEOMETRIC PHASES, EVOLUTION LOOPS AND GENERALIZED OSCILLATOR POTENTIALS

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Abstract

The geometric phases for dynamical processes where the evolution operator becomes the identity (evolution loops) are studied. The case of time–independent Hamiltonians with equally spaced energy levels is considered; special emphasis is made on the potentials having the same spectrum as the harmonic oscillator potential (the generalized oscillator potentials) and their recently found coherent states.

1 Introduction

Departing from Berry's work [1], a *geometric phase* β has been associated to the cyclic evolution of a vector state $|\psi(t)\rangle$, i.e., $|\psi(\tau)\rangle = e^{i\phi}|\psi(0)\rangle$, where τ is the period, $\langle\psi(t)|\psi(t)\rangle = 1$, and $\phi \in \mathbf{R}$. For a non–relativistic system with Hamiltonian $H(t)$, β takes the form [2]:

$$\beta = \phi + i \int_0^\tau \langle\psi(t)|\frac{d}{dt}|\psi(t)\rangle dt = \phi + \hbar^{-1}\int_0^\tau \langle\psi(t)|H(t)|\psi(t)\rangle dt. \tag{1}$$

The geometric phase describes some curvature effects arising on the projective space $\mathcal{P}$ associated to the system's Hilbert space $\mathcal{H}$: β turns out to be the holonomy of the horizontal lifting of the closed trajectory $|\psi(t)\rangle\langle\psi(t)| \in \mathcal{P}$ to $\mathcal{H}$.

Eq.(1) is valid for *any* cyclic evolution, regardless of whether or not it is induced by a time–dependent Hamiltonian. There is a widespread believing, however, that β becomes non–null just when the Hamiltonian inducing the cyclic evolution is time–dependent. This could be understood if one realizes the great influence of Berry's article; so one could think of Eq.(1) as applied to the cyclic evolutions of the eigenstates of a cyclic $H(t)$ changing adiabatically in time [1]. Making use of this idea, $\beta = 0$ for the eigenstates of a time–independent Hamiltonian H. In this paper we are going to show that for any H having at least two bounded states there are a lot of cyclic evolutions for which $\beta \neq 0$.

On the other hand, some developments in the analysis of the dynamics of a quantum system led to the concept of *evolution loop* (EL) [3, 4]. An evolution loop is a specific dynamical process, induced by time–dependent [3, 4] or time–independent Hamiltonians [5], whose evolution operator becomes the identity **1** (modulo phase) for a certain time $\tau > 0$ (the loop period):

$$U(\tau) = e^{i\phi}\mathbf{1}, \tag{2}$$

where $U(0) = 1$. The EL is interesting because, if perturbed by some additional external fields, it can induce any unitary transformation of $\mathcal{H}$ as the result of the small precessions of the distorted loop [6]. There is, moreover, an obvious interelation between the evolution loops and the geometric phases.

2 Geometric phases and evolution loops

In this work, we restrict the discussion to systems with a time–independent Hamiltonian whose evolution operator performs an evolution loop. The main property of these systems is that *any* state evolves cyclically from $t = 0$ until $t = \tau$:

$$|\psi(\tau)\rangle = e^{i\phi}|\psi(0)\rangle. \tag{3}$$

According to (1), $|\psi(t)\rangle$ will have associated, in general, a non-null geometric phase. Indeed, because $U(t) = e^{-iHt/\hbar}$ commutes with H we have:

$$\beta = \phi + \hbar^{-1}\int_0^\tau \langle\psi(0)|U^\dagger(t)HU(t)|\psi(0)\rangle dt = \phi + \hbar^{-1}\tau\langle H\rangle, \tag{4}$$

where $\langle H\rangle = \langle\psi(0)|H|\psi(0)\rangle$. In terms of the basis $\{|E_m\rangle\}$ of eigenstates of H, $|\psi(0)\rangle = \sum_m c_m|E_m\rangle$ with $c_m = \langle E_m|\psi(0)\rangle$, and Eq.(4) becomes:

$$\beta = \phi + \hbar^{-1}\tau\sum_m |c_m|^2 E_m. \tag{5}$$

There are some interesting systems whose time–independent Hamiltonian induces evolution loops (see, e.g., [7, 5, 8, 9]). We will illustrate this assertion with the simplest generic case. Suppose that H has an equally spaced spectrum of the form:

$$E_n = E_0 + n\Delta E, \tag{6}$$

where ΔE is the level's spacing, E_0 is the ground state energy and $n = 0, 1, \cdots, N$, being N either finite or infinite. The evolution operator reads:

$$U(t) = \sum_{n=0}^N e^{-iE_n t/\hbar}|E_n\rangle\langle E_n|. \tag{7}$$

As can be seen, an evolution loop is present at $\tau = 2\pi\hbar/\Delta E$:

$$U(\tau) = \sum_{n=0}^N e^{-i2\pi(E_0 + n\Delta E)/\Delta E}|E_n\rangle\langle E_n| = e^{-i2\pi E_0/\Delta E}\mathbf{1}. \tag{8}$$

By comparing with (2), $\phi = -2\pi E_0/\Delta E$, and according with (4-5) the geometric phase for the cyclic state $|\psi(t)\rangle$ is:

$$\beta = 2\pi\frac{(\langle H\rangle - E_0)}{\Delta E} = 2\pi\sum_{n=1}^N n|c_n|^2 \geq 0. \tag{9}$$

By restricting β (modulo 2π) to the interval $[0, 2\pi)$ one can interpret (9) in the following way: β measures the energy excess in dimensionless units of $\langle H \rangle$ with respect to its nearest energy level E_k (see Fig.1).
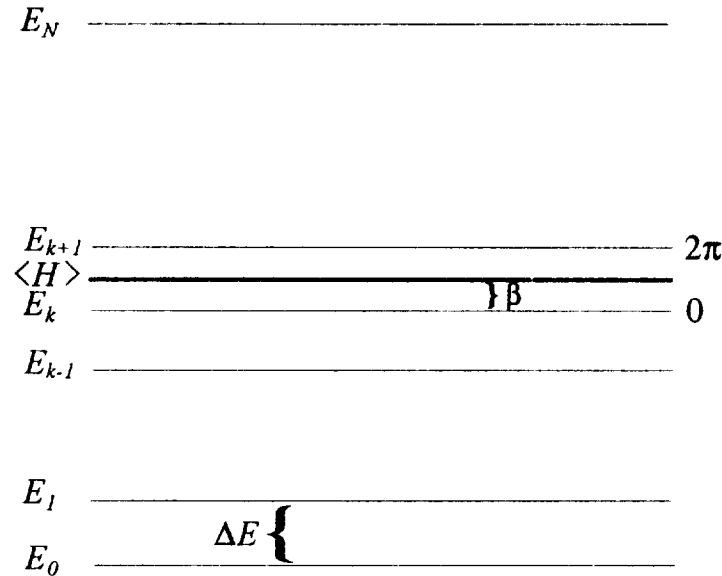

FIG. 1. Schematic representation of the $N + 1$ energy levels and the geometric phase for a system with equally spaced spectrum.

Suppose now that, due to some physical reasons, we are faced with a situation involving just two energy levels of H. Restricting considerations to the subspace $\mathcal{E}_2$ generated by the two eigenstates $|E_0\rangle$ and $|E_1\rangle$ it can be shown that the evolution operator performs an evolution loop. Formulae (6-9) are valid in this situation with $N = 1$ and $\tau = 2\pi\hbar/\Delta E$. In particular, (9) becomes $\beta = 2\pi|c_1|^2$, where c_1 is the component along $|E_1\rangle$. As there are an infinite number of linear combinations $c_0|E_0\rangle + c_1|E_1\rangle$ such that $|c_0|^2 + |c_1|^2 = 1$, $c_0 \neq 0$ and $c_1 \neq 1$, we have shown the following: for any H having at least two bounded states there are an infinity of cyclic evolutions for which $\beta \neq 0$ (see also [10]).

Other examples for which formulae (6-9) can be applied are the following: a spin-j system interacting with a constant homogeneous magnetic field $\mathbf{B}$; the harmonic oscillator potential and all the Hamiltonians having the same spectrum as the harmonic oscillator (generalized oscillators). Next, we will derive the geometric phases for a family of generalized oscillator Hamiltonians.

3 The generalized oscillator potentials

The simplest method to derive a family of generalized oscillator potentials was introduced by Mielnik by means of a modification of the well known factorization method [11]. Consider the

classical factorization of the harmonic oscillator Hamiltonian in dimensionless coordinates $m = \omega = \hbar = 1$:

$$H = \frac{1}{2}\left(-\frac{d^2}{dx^2} + x^2\right), \quad aa^\dagger = H + \frac{1}{2}, \quad a^\dagger a = H - \frac{1}{2}, \tag{10}$$

where $a = (d/dx + x)/\sqrt{2}$, and $a^\dagger = (-d/dx + x)/\sqrt{2}$ are the ordinary ladder operators with $[a, a^\dagger] = 1$. The eigenfunctions and eigenvalues of the harmonic oscillator can be constructed using the relations

$$Ha^\dagger = a^\dagger(H + 1), \quad Ha = a(H - 1). \tag{11}$$

The ground state $\psi_0(x)$ has eigenvalue $E_0 = 1/2$ and satisfies $a\psi_0(x) = 0 \Rightarrow \psi_0(x) \propto e^{-x^2/2}$, while the $\psi_n(x)$'s associated to $E_n = n + 1/2$ are:

$$\psi_n(x) = \frac{(a^\dagger)^n}{\sqrt{n!}}\psi_0(x). \tag{12}$$

The *generalized* factorization method [11] consists in looking for more general operators

$$b = \frac{1}{\sqrt{2}}\left(\frac{d}{dx} + \beta(x)\right), \quad b^\dagger = \frac{1}{\sqrt{2}}\left(-\frac{d}{dx} + \beta(x)\right), \tag{13}$$

satisfying just one of relations (10):

$$bb^\dagger = H + \frac{1}{2}. \tag{14}$$

Hence, the unknown function $\beta(x)$ obeys the Riccati equation

$$\beta' + \beta^2 = 1 + x^2, \tag{15}$$

whose general solution is

$$\beta(x) = x + \frac{e^{-x^2}}{\lambda + \int_0^x e^{-y^2}dy}, \quad \lambda \in \mathbf{R}. \tag{16}$$

Now, the point is that $b^\dagger b$ is not related with the harmonic oscillator Hamiltonian, but it leads to a new operator H_λ:

$$b^\dagger b = H_\lambda - \frac{1}{2}, \tag{17}$$

where

$$H_\lambda = -\frac{1}{2}\frac{d^2}{dx^2} + V_\lambda(x), \tag{18}$$

with

$$V_\lambda(x) = \frac{x^2}{2} - \frac{d}{dx}\left(\frac{e^{-x^2}}{\lambda + \int_0^x e^{-y^2}dy}\right) = \left(x + \frac{e^{-x^2}}{\lambda + \int_0^x e^{-y^2}dy}\right)^2 - \frac{x^2}{2}, \quad |\lambda| > \sqrt{\pi}/2. \tag{19}$$

The relationships analogous to (11) provide now the way to obtaining the eigenfunctions and eigenvalues of H_λ:

$$H_\lambda b^\dagger = b^\dagger(H + 1), \quad Hb = b(H_\lambda - 1). \tag{20}$$

Hence, the states $\theta_n(x) = b^\dagger \psi_{n-1}(x)/\sqrt{n}$, $n = 1, 2, \cdots$ form an orthonormal set of eigenfunctions of H_λ with eigenvalues $E_n = n + 1/2$. However, $\{\theta_n(x), \ n = 1, 2, \cdots\}$ is not a basis of $L^2(\mathbf{R})$. There is a missing vector $\theta_0(x)$, orthogonal to $\theta_n(x), n = 1, 2, \cdots$. It turns out to be an eigenfunction of H_λ with eigenvalue $E_0 = 1/2$ satisfying $b\theta_0(x) = 0$, and taking the form:

$$\theta_0(x) \propto \exp\left(-\int_0^x \beta(y)dy\right). \tag{21}$$

The set $\{\theta_n(x), \ n = 0, 1, 2, \cdots\}$ forms an orthonormal basis in $L^2(\mathbf{R})$; then $\{H_\lambda : |\lambda| > \sqrt{\pi}/2\}$ is a family of Hamiltonians distinct of the harmonic oscillator one but having exactly the same spectrum as the oscillator. In the limit $|\lambda| \to \infty$, the harmonic oscillator potential is recovered, $V_\lambda(x) \to x^2/2$.

We return now to our original subject. Due to the kind of spectrum of H_λ, relations (6–9) involving the evolution loops and the geometric phases can be applied here with $E_0 = 1/2$, $\Delta E = 1$, $\tau = 2\pi$, $\phi = -\pi$ and $N = \infty$. In particular, $\beta = 2\pi(\langle H_\lambda \rangle - 1/2)$, and when applied to the cyclic states $\{\theta_n(x), n = 0, 1, 2 \cdots\}$ we recover again $\beta = 2n\pi$. Is there any other set of generic states for which we can evaluate explicitly the geometric phase?

The answer turns out positive if we consider the recently found coherent states of H_λ (the generalized coherent states GCS) [12]. Let's denote them as $|z\rangle$ with $z \in \mathbf{C}$. The annihilation and creation operators of the system can be identified as:

$$A = b^\dagger ab, \qquad A^\dagger = b^\dagger a^\dagger b. \tag{22}$$

Define now $|z\rangle$ by $A|z\rangle = z|z\rangle$. A direct calculation leads to:

$$|z\rangle = \frac{1}{\sqrt{{}_0F_2(1, 2; |z|^2)}} \sum_{n=0}^{\infty} \frac{z^n}{n!\sqrt{(n+1)!}} |\theta_{n+1}\rangle, \tag{23}$$

where $|\theta_n\rangle$ represents to $\theta_n(x)$ and ${}_0F_2(1, 2; y)$ is a generalized hypergeometric function [13]. Each $z \neq 0$ is a non–degenerate eigenvalue. However, $z = 0$ is a double degenerate eigenvalue of A with eigenvectors $|\theta_0\rangle$ and $|z = 0\rangle = |\theta_1\rangle$. It is possible to find a measure in the complex plane such that $\{|\theta_0\rangle, |z\rangle\}$ is complete in $\mathcal{H}$.

To evaluate the geometric phase β_{GCS}, $\langle z|H_\lambda|z\rangle$ is needed. A direct calculation leads to:

$$\langle H_\lambda \rangle = \langle z|H_\lambda|z\rangle = 1/2 + \frac{{}_0F_2(1, 1; |z|^2)}{{}_0F_2(1, 2; |z|^2)}. \tag{24}$$

Finally:

$$\beta_{GCS} = 2\pi \frac{{}_0F_2(1, 1; |z|^2)}{{}_0F_2(1, 2; |z|^2)}. \tag{25}$$

The behaviour of β_{GCS}, is shown in Fig.2. Notice that β_{GCS} is independent of λ. Moreover, its behaviour is quite different compared with the standard coherent state (SCS) of the harmonic oscillator for which $\beta_{SCS} = 2\pi|z|^2$ (see Fig.2). The difference rests on the fact that the GCS do not tend to the SCS when $\lambda \to \infty$ and $A_\infty \equiv \lim_{\gamma \to \infty} A = a^\dagger a^2 \neq a$ even though $V_\lambda(x) \to x^2/2$ in this limit.
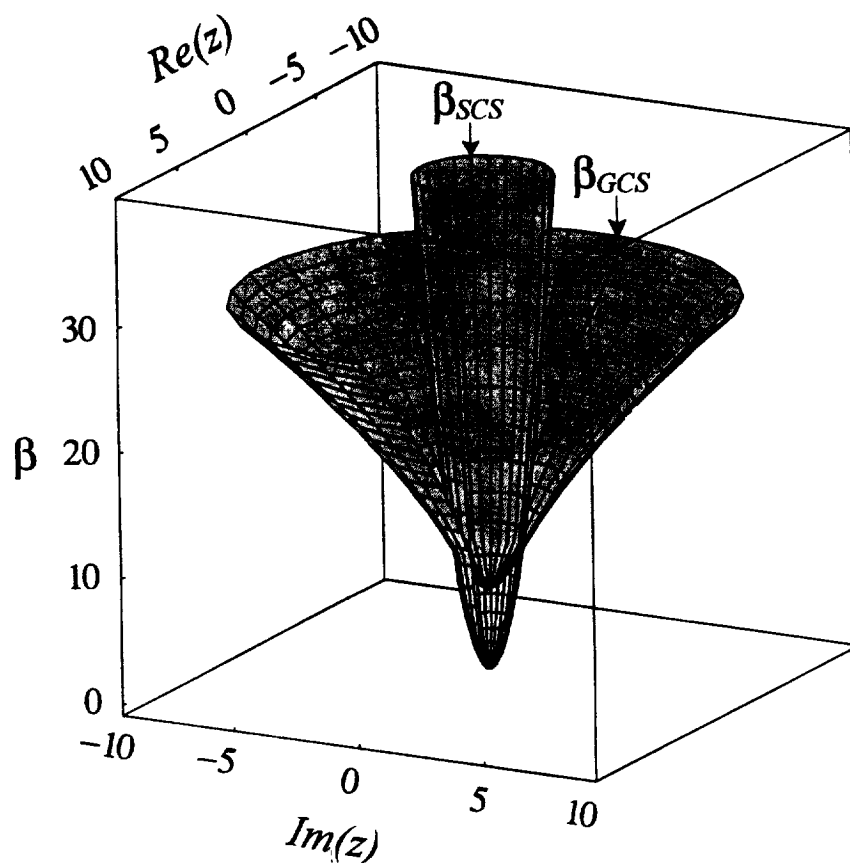
FIG. 2. The geometric phases versus z for the standard coherent states of the harmonic oscillator (β_{SCS}) and the coherent states of the generalized oscillator (β_{GCS}).

Acknowledgments

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COHERENT STATES FOR A GENERALIZATION
OF THE HARMONIC OSCILLATOR

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Abstract

Coherent states for a family of isospectral oscillator Hamiltonians are derived from a suitable choice of annihilation and creation operators. The Fock-Bargmann representation is also obtained.

1 Generalized Oscillator

Let us consider the harmonic oscillator Hamiltonian and its annihilation and creation operators

$$H = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2, \quad a = \frac{1}{\sqrt{2}}\left(\frac{d}{dx} + x\right), \quad a^\dagger = \frac{1}{\sqrt{2}}\left(-\frac{d}{dx} + x\right), \quad [a, a^\dagger] = 1. \tag{1}$$

We obviously have $a^\dagger a = H - \frac{1}{2}$, $aa^\dagger = H + \frac{1}{2}$, $Ha^\dagger = a^\dagger(H + 1)$ and $Ha = a(H - 1)$. The eigenstates verify

$$|\psi_n\rangle = \frac{(a^\dagger)^n|\psi_0\rangle}{\sqrt{n!}}; \quad a^\dagger|\psi_n\rangle = \sqrt{n+1}\,|\psi_{n+1}\rangle, \quad a|\psi_n\rangle = \sqrt{n}\,|\psi_{n-1}\rangle. \tag{2}$$

In his paper of 1984, Mielnik [1] (see also [2]) looked for operators b and $b^\dagger$ such that $bb^\dagger = H + \frac{1}{2}$ and taking the following form:

$$b = \frac{1}{\sqrt{2}}\left(\frac{d}{dx} + \beta(x)\right), \quad b^\dagger = \frac{1}{\sqrt{2}}\left(-\frac{d}{dx} + \beta(x)\right). \tag{3}$$

Hence, $\beta(x)$ must verify the Riccati equation

$$\beta' + \beta^2 = 1 + x^2, \quad \text{whose general solution is} \quad \beta(x) = x + \frac{e^{-x^2}}{\lambda + \int_0^x e^{-y^2}dy}, \quad \lambda \in \mathbf{R}. \tag{4}$$

The inverted product of the new operators is not related to the oscillator Hamiltonian, but gives a one-parametric family of operators:

$$H_\lambda = b^\dagger b + \frac{1}{2} = -\frac{1}{2}\frac{d^2}{dx^2} + V_\lambda(x) = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{x^2}{2} - \frac{d}{dx}\left[\frac{e^{-x^2}}{\lambda + \int_0^x e^{-y^2}dy}\right]. \tag{5}$$
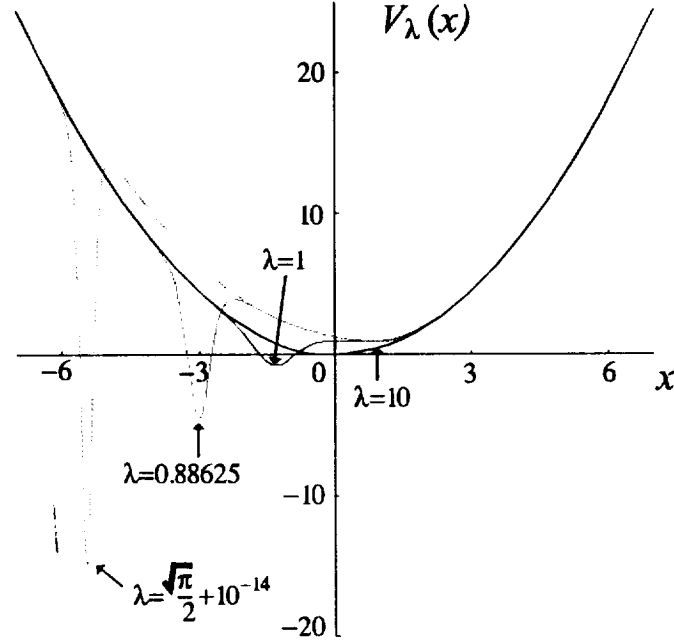

FIG. 1. The potentials $V_\lambda(x)$ associated to H_λ.

The operator $b^\dagger$ connects H and H_λ: $H_\lambda b^\dagger = b^\dagger(H + 1)$. Therefore, the normalized eigenstates and eigenvalues of H_λ are

$$|\theta_n\rangle = \frac{b^\dagger|\psi_{n-1}\rangle}{\sqrt{n}}, \qquad E_n = n + \frac{1}{2}, \qquad n = 1, 2, \ldots \tag{6}$$

They do not generate all $L^2(\mathbf{R})$. There is a missing vector $|\theta_0\rangle$ verifying $b|\theta_0\rangle = 0$ and given by

$$\theta_0(x) = \frac{C_0 e^{-x^2/2}}{\lambda + \int_0^x e^{-y^2}dy}. \tag{7}$$

It is an eigenvector of H_λ with eigenvalue $1/2$; then H_λ is a Hamiltonian with spectrum equal to that of the harmonic oscillator. The annihilation and creation operators for H_λ can be chosen

$$A = b^\dagger ab, \qquad A^\dagger = b^\dagger a^\dagger b. \tag{8}$$

2 New Coherent States

It is well-known that there are several non-equivalent definitions of coherent states [3, 4]. One of the possibilities is to look for eigenstates of an annihilation operator. We have seen that A is such an operator. Hence, the states $|z\rangle$ we are looking for must verify

$$A|z\rangle = z|z\rangle, \qquad |z\rangle = \sum_{n=0}^{\infty} a_n|\theta_n\rangle. \tag{9}$$

After normalizing, we get

$$|z\rangle = \frac{1}{\sqrt{{}_0F_2(1,2;|z|^2)}} \sum_{n=0}^{\infty} \frac{z^n}{n!\sqrt{(n+1)!}} |\theta_{n+1}\rangle, \tag{10}$$

where the generalized hypergeometric function is defined as [5]

$$_0F_2(\alpha,\beta;x) = \sum_{n=0}^{\infty} \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+n)\Gamma(\beta+n)} \frac{x^n}{n!}. \tag{11}$$

We see that $z = 0$ is a doubly degenerated eigenvalue for A, with eigenvectors $|0\rangle \equiv |\theta_1\rangle$ and $|\theta_0\rangle$. We analyze now the overcompleteness. The resolution of the identity must take the form

$$I_{\mathcal{H}} = |\theta_0\rangle\langle\theta_0| + \int |z\rangle\langle z| d\mu(z), \tag{12}$$

where the measure $d\mu(z)$ can be determined as in [6] (see [7] for details). This measure is positive and non-singular. Some other interesting results are the form of the reproducing kernel $\langle z|z'\rangle$

$$\langle z|z'\rangle = \frac{{}_0F_2(1,2;\bar{z}z')}{\sqrt{{}_0F_2(1,2;|z|^2)\,{}_0F_2(1,2;|z'|^2)}}, \tag{13}$$

the dynamical evolution of the coherent states

$$U(t)|z\rangle = \frac{1}{\sqrt{{}_0F_2(1,2,|z|^2)}} \sum_{n=0}^{\infty} \frac{z^n}{n!\sqrt{(n+1)!}} e^{-itH_\lambda}|\theta_{n+1}\rangle = e^{-i3t/2}|e^{-it}z\rangle, \tag{14}$$

and the expected value of the Hamiltonian H_λ in a coherent state

$$\langle z|H_\lambda|z\rangle = \frac{{}_0F_2(1,1;|z|^2)}{{}_0F_2(1,2;|z|^2)} + \frac{1}{2}. \tag{15}$$

3 The harmonic oscillator limit

Notice that H_λ tends to the harmonic oscillator Hamiltonian when $|\lambda| \to \infty$. Let us consider this limit to see if there is a relationship between the coherent states we have computed and the

harmonic oscillator ones. In the limit, $\beta(x) \to x$; therefore, $b \to a$ and $b^\dagger \to a^\dagger$. Then, we get $|\theta_n\rangle \to |\psi_n\rangle$. Nevertheless, $A \to A_o = a^\dagger a^2$; as a consequence, the coherent states (10) become

$$|z\rangle_o \equiv \lim_{|\lambda| \to \infty} |z\rangle = \frac{1}{\sqrt{{}_0F_2(1,2;|z|^2)}} \sum_{n=0}^{\infty} \frac{z^n}{n!\sqrt{(n+1)!}} |\psi_{n+1}\rangle, \tag{16}$$

which are not the usual coherent states. For $|z\rangle$ it is difficult to compute the expectation values of the position and momentum operators, but for $|z\rangle_o$ the problem can be easily solved using

$$\hat{x} = \frac{1}{\sqrt{2}}(a^\dagger + a), \qquad \hat{p} = \frac{i}{\sqrt{2}}(a^\dagger - a). \tag{17}$$

For the position operator we get

$$_o\langle z|\hat{x}|z\rangle_o = \frac{z + \bar{z}}{\sqrt{2}} \frac{{}_0F_2(2,2;|z|^2)}{{}_0F_2(1,2;|z|^2)}; \tag{18}$$

$$_o\langle z|\hat{x}^2|z\rangle_o = \frac{1}{2\,{}_0F_2(1,2;|z|^2)} \left(3\,{}_0F_2(1,2;|z|^2) + \frac{(z + \bar{z})^2}{2}{}_0F_2(2,3;|z|^2)\right). \tag{19}$$

For the momentum operator we obtain similar results. The uncertainty product is then

$$(\Delta\hat{x})(\Delta\hat{p}) = \sqrt{\left(\frac{3}{2}\right)^2 + \frac{3}{2}|z|^2 \varrho(|z|) + [\text{Re}(z)\text{Im}(z)\varrho(|z|)]^2}, \tag{20}$$

where

$$\varrho(|z|) = \frac{{}_0F_2(1,2;|z|^2){}_0F_2(2,3;|z|^2) - 2[{}_0F_2(2,2;|z|^2)]^2}{[{}_0F_2(1,2;|z|^2)]^2}. \tag{21}$$

A plot of $(\Delta\hat{x})(\Delta\hat{p})$ is shown in Figure 2. It can be rigorously proved that $1/2 \le (\Delta\hat{x})(\Delta\hat{p}) \le 3/2$.
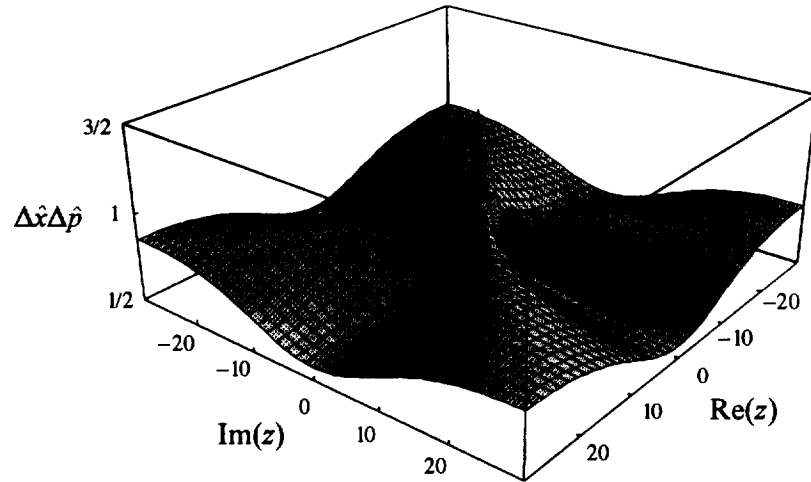

FIG. 2. The uncertainty product $(\Delta\hat{x})(\Delta\hat{p})$ as a function of z.

4 The Fock-Bargmann representation

For the harmonic oscillator it is possible to find a realization of the Hilbert space in terms of entire functions [4, 8]. The same is true for the coherent states of the Lie algebra $su(1,1)$ [6, 9]. We will show next that we can construct a similar realization for the problem under study. The Hilbert space $\mathcal{H}$ is generated by the basis vectors $\{|\theta_0\rangle, |\theta_1\rangle, |\theta_2\rangle, \ldots\}$; the state $|\theta_0\rangle$ is isolated from the others, in the sense that it is an atypical coherent state. Let us call $\mathcal{H}_0$ the one-dimensional subspace generated by $|\theta_0\rangle$ and $\mathcal{H}_1$ the Hilbert space generated by $\{|\theta_1\rangle, |\theta_2\rangle, \ldots\}$, so that $\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1$. From now on, we are going to concentrate on $\mathcal{H}_1$. A vector $|g\rangle \in \mathcal{H}_1$, is

$$|g\rangle = \sum_{m=1}^{\infty} c_m |\theta_m\rangle \in \mathcal{H}_1; \qquad c_m = \langle\theta_m|g\rangle; \qquad \langle g|g\rangle = \sum_{m=1}^{\infty} |c_m|^2 < \infty. \qquad (22)$$

Using (10)

$$\langle z|g\rangle = \frac{1}{\sqrt{{}_0F_2(1,2;|z|^2)}} \sum_{n=0}^{\infty} \frac{\bar{z}^n}{n!\sqrt{(n+1)!}} \langle\theta_{n+1}|g\rangle. \qquad (23)$$

A realization of $\mathcal{H}_1$ as a space $\mathcal{F}$ of entire analytic functions is obtained by associating to every $|g\rangle \in \mathcal{H}_1$ the entire function

$$g(z) = \sum_{n=0}^{\infty} \frac{\langle\theta_{n+1}|g\rangle}{n!\sqrt{(n+1)!}} z^n; \qquad \langle z|g\rangle = \frac{g(\bar{z})}{\sqrt{{}_0F_2(1,2;|z|^2)}}. \qquad (24)$$

From the relation $|g(z)| \leq \|g\|\sqrt{{}_0F_2(1,2;|z|^2)}$, $\forall g(z) \in \mathcal{F}$ (issued from the Schwarz inequality), we can show that $g(z)$ is an entire function of order $2/3$ and type $3/2$ (see [7]). This characterizes completely the space $\mathcal{F}$ (the usual coherent states are related to the Segal-Bargmann space of entire functions of growth $(1/2,2)$). In particular, the entire function corresponding to a coherent state $|\alpha\rangle$ is

$$\alpha(z) = \frac{{}_0F_2(1,2;\alpha z)}{\sqrt{{}_0F_2(1,2;|\alpha|^2)}}. \qquad (25)$$

The functions

$$\theta_{n+1}(z) = \frac{z^n}{n!\sqrt{(n+1)!}}, \quad n = 0,1,2,\ldots, \qquad (26)$$

form an orthonormal basis of $\mathcal{F}$ so that $g(z)$ may be written

$$g(z) = \sum_{n=0}^{\infty} c_{n+1}\theta_{n+1}(z). \qquad (27)$$

Notice that the function $\delta(z,z') = {}_0F_2(1,2;z\bar{z}')$ plays the role of the delta function in $\mathcal{F}$.

Finally, we want to know what is the abstract realization of the operators acting on $\mathcal{F}$ as a multiplication by z and as a derivation $\partial/\partial z$. Let us consider the function

$$zg(z) = \sum_{n=0}^{\infty} c_{n+1}\frac{z^{n+1}}{n!\sqrt{(n+1)!}} = \sum_{m=1}^{\infty} m\sqrt{m+1}\, c_m\theta_{m+1}(z). \qquad (28)$$

On the other hand, the action of the operator $A^\dagger$ on $|g\rangle$ is

$$A^\dagger|g\rangle\bigg| = b^\dagger a^\dagger b \sum_{m=0}^{\infty} c_{m+1}|\theta_{m+1}\rangle = \sum_{n=1}^{\infty} c_n n\sqrt{n+1}\,|\theta_{n+1}\rangle. \tag{29}$$

Then, $A^\dagger$ is the operator whose realization in $\mathcal{F}$ is a multiplication by z. Let us consider now the function

$$\frac{\partial g(z)}{\partial z} = \sum_{m=1}^{\infty} c_{m+1}\frac{z^{m-1}}{(m-1)!\sqrt{(m+1)!}} = \sum_{m=1}^{\infty} \frac{c_{m+1}}{\sqrt{m+1}}\,\theta_m(z). \tag{30}$$

As $[A, A^\dagger] \neq I$, the abstract operator corresponding to the derivative is not A. Therefore, we have to find an operator B such that

$$B|g\rangle = \sum_{m=0}^{\infty} c_{m+1}B|\theta_{m+1}\rangle = \sum_{m=1}^{\infty} \frac{c_{m+1}}{\sqrt{m+1}}\,|\theta_m\rangle. \tag{31}$$

We suppose it has the form

$$B = b^\dagger a f(N)b, \quad N = a^\dagger a, \tag{32}$$

and the function f becomes

$$f(N) = \frac{1}{N(1+N)}. \tag{33}$$

It is easy to see that

$$[B, A^\dagger] = I, \qquad [A, B^\dagger] = I, \tag{34}$$

and therefore, up to normalization,

$$|z\rangle = \exp(zB^\dagger)|\theta_1\rangle. \tag{35}$$

However, it is not possible to obtain $|z\rangle$ as the action of a unitary representation of the algebras in (34).

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FINITE-ELEMENT TIME EVOLUTION OPERATOR
FOR THE ANHARMONIC OSCILLATOR

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Abstract

The finite-element approach to lattice field theory is both highly accurate (relative errors $\sim 1/N^2$, where N is the number of lattice points) and exactly unitary (in the sense that canonical commutation relations are exactly preserved at the lattice sites). In this talk I construct matrix elements for dynamical variables and for the time evolution operator for the anharmonic oscillator, for which the continuum Hamiltonian is $H = p^2/2 + \lambda q^4/4$. Construction of such matrix elements does not require solving the implicit equations of motion. Low order approximations turn out to be extremely accurate. For example, the matrix element of the time evolution operator in the harmonic oscillator ground state gives a result for the anharmonic oscillator ground state energy accurate to better than 1%, while a two-state approximation reduces the error to less than 0.1%.

1   Introduction

For over a decade now, the finite-element method has been developed for application to quantum systems. (For a review of the program see [1].) The essence of the approach is to put the Heisenberg equations of motion for the quantum system on a Minkowski space-time lattice in such a way as to preserve exactly the canonical commutation relations at each lattice site. Doing so corresponds precisely to the classical finite-element prescription of requiring continuity at the lattice sites while imposing the equations of motion at the Gaussian knots, a prescription chosen to minimize numerical error. We have applied this technique to examples in quantum mechanics and to quantum field theories in two and four space-time dimensions. In particular, recent work has concentrated on Abelian and non-Abelian gauge theories [2, 3, 4].

Because it is the equations of motion that are discretized, a lattice Lagrangian does not exist in Minkowski space. This is because the equations of motion are in general nonlocal, involving fields at all previous (but not later) times. Similarly, a lattice Hamiltonian does not exist, in the sense of an operator from which the equations of motion can be derived.

However, because the formulation is unitary, a unitary time-evolution operator must exist which carries fields from one lattice time to the next. For linear finite elements this operator in quantum mechanics has been explicitly constructed [5]. Construction of this operator requires solving the equations of motion, which are implicit. Therefore, it is most useful, and perhaps surprising, that when matrix elements of the time evolution operator are constructed in a harmonic oscillator basis, they do not require the solution of the equations of motion [6]. Although these

general formulas were derived some years ago, it seems they have not been exploited. My purpose here is to study, in a simple context, the matrix elements of the evolution operator, and see how accurately spectral information may be extracted. My goal, of course, is to apply similar techniques in gauge theories, for example, to study chiral symmetry breaking in QCD.

2 Review of the Finite-Element Method

Let us consider a quantum mechanical system with one degree of freedom governed by the continuum Hamiltonian

$$H = \frac{p^2}{2} + V(q), \tag{1}$$

from which follow the Heisenberg equations

$$\dot{p} = -V'(q), \quad \dot{q} = p. \tag{2}$$

These equations are to be solved subject to the initial condition

$$[q(0), p(0)] = i. \tag{3}$$

It immediately follows from (2) that the same relation holds at any later time

$$[q(t), p(t)] = i. \tag{4}$$

Now suppose we introduce a time lattice by subdividing the interval $(0, T)$ into N subintervals each of length h. On each subinterval ("finite element") we express the dynamical variables as rth degree polynomials

$$p(t) = \sum_{k=0}^{r} a_k (t/h)^k, \quad q(t) = \sum_{k=0}^{r} b_k (t/h)^k, \tag{5}$$

where t is a local variable ranging from 0 to h. We determine the $2(r + 1)$ operator coefficients a_k, b_k, as follows:

1. On the first finite element let

$$a_0 = p_0 = p(0), \quad b_0 = q_0 = q(0). \tag{6}$$

2. Impose the equations of motion (2) at r points within the finite element, at $\alpha_i h$, $i = 1, 2, \ldots, r$, where $0 < \alpha_1 < \alpha_2 < \cdots < \alpha_r < 1$. This then gives

$$p(h) \approx p_1 = \sum_{k=0}^{r} a_k, \quad q(k) \approx q_1 = \sum_{k=0}^{r} b_k. \tag{7}$$

3. Proceed to the next finite element by requiring continuity (but not continuity of derivatives) at the lattice sites, that is, on the second finite element, set

$$a_0 = p_1, \quad b_0 = q_1, \tag{8}$$

and again impose the equations of motion at $\alpha_i h$, and so on.

How are the α_i's determined? By requiring preservation of the canonical commutation relations at each lattice site,

$$[q_1, p_1] = [q_0, p_0] = i, \tag{9}$$

one finds

$$r = 1 \quad \text{(linear finite elements)} \quad \alpha = \frac{1}{2} \tag{10}$$

$$r = 2 \quad \text{(quadratic finite elements)} \quad \alpha_{\pm} = \frac{1}{2} \pm \frac{1}{2\sqrt{3}} \tag{11}$$

$$r = 3 \quad \text{(cubic finite elements)} \quad \alpha_{1,3} = \frac{1}{2} \mp \frac{\sqrt{3}}{2\sqrt{5}}, \quad \alpha_2 = \frac{1}{2} \tag{12}$$

These points are exactly the Gaussian knots, that is, the roots of the rth Legendre polynomial,

$$P_r(2\alpha - 1) = 0. \tag{13}$$

Amazingly, these are precisely the points at which the numerical error is minimized. It is known for classical equations that if one uses N rth degree finite elements the relative error goes like N^{-2r}, while imposing the equations at any other points would give errors like N^{-r}.

Let us consider a simple example. The quartic anharmonic oscillator has continuum Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{4}\lambda q^4, \tag{14}$$

for which the equations of motion are

$$\dot{q} = p \quad \dot{p} = -\lambda q^3. \tag{15}$$

If we use the linear ($r = 1$) finite-element prescription given above, the corresponding discrete lattice equations are

$$\frac{q_1 - q_0}{h} = \frac{p_1 + p_0}{2}, \quad \frac{p_1 - p_0}{h} = -\frac{\lambda}{8}(q_1 + q_0)^3. \tag{16}$$

(Notice the easily remembered mnemonic for linear finite elements: Derivatives are replaced by forward differences, while undifferentiated operators are replaced by forward averages.) By commuting the first of these equations with $p_1 + p_0$ and the second with $q_1 + q_0$ the unitarity condition (9) follows immediately. These equations are implicit, in the sense that we must solve a nonlinear equation to find q_1 and p_1 in terms of q_0 and p_0. Although such a solution can be given, let use make a simple approximation, by expanding the dynamical operators at time 1 in powers of h, with operator coefficients at time 0. Those coefficients are determined by (16), and a very simple calculation yields

$$q_1 = q_0 + hp_0 - \frac{\lambda}{2}h^2 q_0^3 + \ldots,$$

$$p_1 = p_0 - \lambda h q_0^3 - \frac{3}{2}\lambda h^2 q_0 p_0 q_0 + \ldots. \tag{17}$$

We can define Fock space creation and annihilation operators in terms of the initial-time operators

$$q_0 = \gamma\frac{(a + a^\dagger)}{\sqrt{2}}, \quad p_0 = \frac{(a - a^\dagger)}{i\sqrt{2}\gamma}, \tag{18}$$

which satisfy

$$[a, a^\dagger] = 1. \tag{19}$$

Here we have introduced an arbitrary variational parameter γ. The Fock-space states (harmonic oscillator states) are created and destroyed by these operators:

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle, \tag{20}$$

which states are not energy eigenstates of the anharmonic oscillator. We can now take matrix elements in these states of the dynamical operators at lattice site 1, using (17):

$$\langle 1|p_1|0\rangle \approx \langle 1|p_0|0\rangle(1 + i\frac{3}{2}h\lambda\gamma^4 - \frac{3}{4}h^2\lambda\gamma^2 + \ldots)$$
$$\approx \langle 1|p_0|0\rangle(1 + i\omega h - \frac{1}{2}\omega^2 h^2 + \ldots), \tag{21}$$

and

$$\langle 1|q_1|0\rangle \approx \langle 1|q_0|0\rangle(1 + i\frac{h}{\gamma^2} - \frac{3}{4}h^2\lambda\gamma^2 + \ldots)$$
$$\approx \langle 1|q_0|0\rangle(1 + i\omega h - \frac{1}{2}\omega^2 h^2 + \ldots), \tag{22}$$

where we have assumed approximately exponential dependence on the energy difference ω. Equating the coefficients of the terms through order h^2 constitutes four equations in two unknowns. These equations are consistent and yield

$$\omega = \frac{3}{2}\lambda\gamma^4 = \frac{1}{\gamma^2}, \tag{23}$$

so the energy difference between the ground state and the first excited state is approximately

$$\omega = \left(\frac{3}{2}\lambda\right)^{1/3} \approx 1.145\lambda^{1/3} \tag{24}$$

which is only 5% higher than the exact result $E_{01} = 1.08845\lambda^{1/3}$. A similar calculation using quadratic finite elements ($r = 2$) reduces the error to 0.5%.

3 The Time-Evolution Operator

Because the canonical commutation relations are preserved at each lattice site, we know that there is a unitary time evolution operator that carries dynamical variable forward in time:

$$q_{n+1} = Uq_nU^\dagger, \quad p_{n+1} = Up_nU^\dagger, \tag{25}$$

For the system described by the continuum Hamiltonian (1) in the linear finite-element scheme, we have found [5] the following formula for U:

$$U = e^{ihp_n^2/4}e^{ihA(q_n)}e^{ihp_n^2/4}, \tag{26}$$

where

$$A(x) = \frac{2}{h^2}[x - g^{-1}(4x/h^2)]^2 + V(g^{-1}(4x/h^2)), \tag{27}$$

$$g(x) = \frac{4}{h^2}x + V'(x). \tag{28}$$

The implicit nature of the finite-element prescription is evident in the appearance of the inverse of the function g.

Given the time evolution operator, a lattice Hamiltonian may be defined by $U = \exp(ih\mathcal{H})$. For linear finite elements $\mathcal{H}$ differs from the continuum Hamiltonian by terms of order h^2. For example,

$$V = \frac{1}{2}m^2q^2 : \quad \mathcal{H} = \frac{2}{mh}\tan^{-1}\left(\frac{mh}{2}\right)\left[\frac{1}{2}p^2 + \frac{1}{2}m^2q^2\right], \tag{29}$$

$$V = \frac{\lambda}{3}q^3 : \quad \mathcal{H} = \frac{1}{2}p^2 + \frac{1}{3}\lambda q^3 + h^2\left[\frac{\lambda}{12}pqp + p^3\right] + \ldots, \tag{30}$$

$$V = \frac{\lambda}{4}q^4 : \quad \mathcal{H} = \frac{1}{2}p^2 + \frac{1}{4}\lambda q^4 + h^2\left[-\frac{\lambda^2}{24}q^6 - \frac{\lambda}{8}qp^2q\right] + \ldots. \tag{31}$$

If one uses quadratic finite elements $\mathcal{H}$ differs from the continuum Hamiltonian by terms of order h^4, etc.

4   Matrix Elements of Dynamical Variables

Remarkably, it is not necessary to solve the equations of motion to compute matrix elements of the dynamical variable. Introduce creation and annihilation operators as in (18). Then, in terms of harmonic oscillator states (20) the following formula is easily derived [6] for a general matrix element of q_1:

$$\langle m|q_1|n\rangle = -\frac{\gamma}{\sqrt{2}}(\sqrt{m}\delta_{n,m-1} + \sqrt{n}\delta_{m,n-1})$$

$$+\frac{e^{-i\theta(m-n)}}{R\sqrt{\pi 2^{n+m}n!m!}} \int_{-\infty}^{\infty} dz\, ze^{-g^2(z)/4R^2}g'(z)H_n(g(z)/2R)H_m(g(z)/2R), \tag{32}$$

where g is given by (28), $H_n(x)$ is the nth Hermite polynomial, and we have introduced the abbreviations

$$R^2 = \frac{4\gamma^2}{h^4} + \frac{1}{h^2\gamma^2}, \quad e^{-i\theta} = \frac{2\gamma}{Rh^2} + \frac{i}{Rh\gamma}. \tag{33}$$

For the example of the harmonic oscillator, this formula gives for the ground state–first excited state energy difference $\omega = (2/h)\tan^{-1}(h/2)$, consistent with (29), while for the anharmonic oscillator if we expand in h we obtain precisely the expansion (22).

5 Matrix Elements of the Time Evolution Operator

A similar formula can be derived for the harmonic oscillator matrix elements of the time evolution operator. (There is an error in the formula printed in [6].)

$$\langle m|U|n\rangle = \frac{1}{2R}\frac{1}{\sqrt{\pi 2^{n+m}n!m!}}e^{-i(n+m+1)\theta}$$
$$\times \int_{-\infty}^{\infty}dz\,g'(z)H_n(g(z)/2R)H_m(g(z)/2R)e^{[ihV(z)+ih^3V'(z)^2/8-h^2g(z)^2e^{-i\theta}/8\gamma R]}, \quad (34)$$

which again is expressed in terms of g not g^{-1}.

For the harmonic oscillator, where $V = q^2/2$, (34) gives for the ground-state energy

$$\langle 0|U|0\rangle = e^{i\omega_0 h}, \quad \omega_0 = \frac{1}{h}\tan^{-1}\frac{h}{2}, \quad (35)$$

which follows from (29). For the anharmonic oscillator, $V = \lambda q^4/4$, again, for a first look, we expand in powers of h, with the result, for the harmonic oscillator ground state,

$$\langle 0|U|0\rangle = 1 + h\left(\frac{i}{4\gamma^2} + \frac{3i}{16}\lambda\gamma^4\right) + h^2\left(-\frac{3}{32\gamma^4} + \frac{9}{64}\lambda\gamma^2 - \frac{105}{512}\lambda^2\gamma^8\right) + \cdots$$

$$\approx 1 + i\omega_0 h - \frac{1}{2}\omega_0^2 h^2 + \cdots, \quad (36)$$

which is also derivable from (31). Equating powers of h gives us two equations, which are to be solved first for the dimensionless number $\lambda\gamma^6 = \alpha$. Once the number α is determined, the value of ω_0 is expressed as

$$\omega_0 = \lambda^{1/3}f(\alpha), \quad f(\alpha) = \frac{1}{4\alpha^{1/3}}\left(1 + \frac{3}{4}\alpha\right). \quad (37)$$

For a first estimate, we use the "principle of minimum sensitivity", that is, use the stationary value of α,

$$f'(\alpha) = 0 \Rightarrow \alpha = \frac{2}{3} \Rightarrow f(\alpha) = 0.4293, \quad (38)$$

which is about 2% higher than the exact value of 0.42081 [7]. In fact, when we solve (36) for α we find a complex value

$$\alpha = \frac{1}{2} \pm \frac{i}{2\sqrt{3}} \Rightarrow f(\alpha) = 0.4178 \mp 0.0077i. \quad (39)$$

The imaginary part is small, and the real part is only 0.7% low. The failure of (39) to be real does not indicate any breakdown of unitarity, but only that the one state approximation is not exact. We do much better by making a two-state approximation, where we must diagonalize the 2×2 matrix

$$\begin{pmatrix} U_{00} & U_{02} \\ U_{20} & U_{22} \end{pmatrix}. \quad (40)$$

We then find the following relation between $\omega_{0,2}$ and $\alpha = \lambda\gamma^6$:

$$\omega_{0,2} = \frac{\lambda^{1/3}}{16}\alpha^{-1/3}[12 + 21\alpha \mp 2\sqrt{3}(8 + 16\alpha + 33\alpha^2)^{1/2}], \quad (41)$$

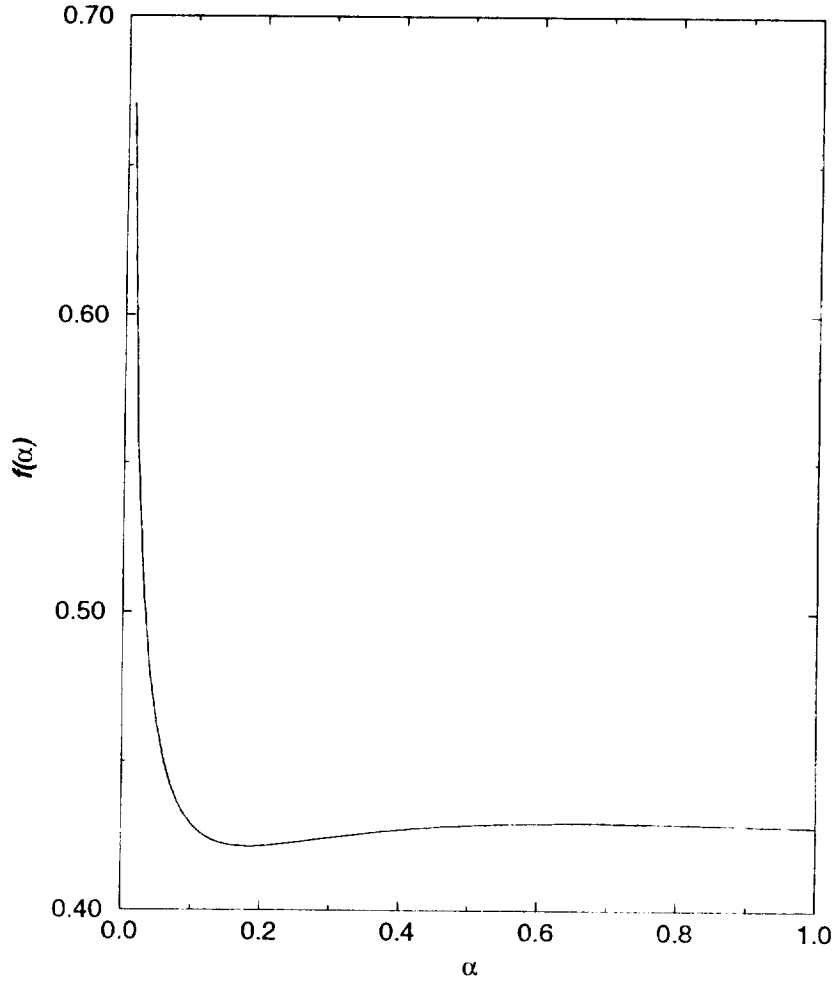which, for the − sign, is plotted in Fig. 1:

FIG. 1. Ground-state energy for the anharmonic oscillator as a function of $\alpha = \lambda\gamma^6$, in the second approximation. Here $\omega_0 = \lambda^{1/3}f(\alpha)$, $f(\alpha)$ given by (41).

This graph shows that the ground-state energy is very insensitive to the value of α. The principle of minimum sensitivity give spectacular agreement with the exact result,

$$\omega_0 = 0.421235\lambda^{1/3}, \tag{42}$$

being only 0.1% high, while it gives a good value for the third state, $\omega_2 = 2.992\lambda^{1/3}$. Solving for α from the eigenvalues of (40) gives even better results:

$$\omega_0 = \lambda^{1/3}(0.42054 + 2 \times 10^{-6}i), \quad \omega_2 = \lambda^{1/3}(2.94328 - .022029i), \tag{43}$$

where the ground state energy is now low by 0.06%, the imaginary part being negligible.

6 Conclusions

The simple calculations given here for the quantum-mechanical anharmonic oscillator are the beginning of a program to develop use of lattice Hamiltonian techniques to explore gauge theories in the finite-element context. The astute reader will note that the numerical results presented in Sec. 5 also hold in the continuum, by virtue of (31). It is in two or more space-time dimensions that the essential nature of the lattice in such calculations comes into play [3, 4, 8]. The high accuracy contrasted with the simplicity of the approach leads us to expect that we can extract spectral information, anomalies, and symmetry breaking from an examination of the time-evolution operator.

Acknowledgments

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q-BOSONS

and the

q-ANALOGUE QUANTIZED FIELD

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Abstract

The q-analogue coherent states $|z>_q$ are used to identify physical signatures for the presence of a q-analogue quantized radiation field in the $|z>_q$ classical limit where $|z|$ is large. In this quantum-optics-like limit, the fractional uncertainties of most physical quantities (momentum, position, amplitude, phase) which characterize the quantum field are $O(1)$. They only vanish as $O(1/|z|)$ when $q = 1$. However, for the number operator, N, and the N-Hamiltonian for a free q-boson gas, $H_N = \hbar\omega(N + 1/2)$, the fractional uncertainties do still approach zero . A signature for q-boson counting statistics is that $(\Delta N)^2/ < N > \to 0$ as $|z| \to \infty$. Except for its $O(1)$ fractional uncertainty, the q-generalization of the Hermitian phase operator of Pegg and Barnett, $\hat{\phi}_q$, still exhibits normal classical behavior. The standard number-phase uncertainty-relation, $\Delta N \Delta\hat{\phi}_q = 1/2$, and the approximate commutation relation, $[N, \hat{\phi}_q] = i$, still hold for the single-mode q-analogue quantized field. So, N and $\hat{\phi}_q$ are almost canonically conjugate operators in the $|z>_q$ classical limit. The $|z>_q$ CS's minimize this uncertainty relation for moderate $|z|^2$.

1 Motivation and Introduction

In considering the potential importance of quantum algebras to quantum field theory and to physics[1], I am reminded of the twenty year development of Yang-Mills theory and the strong interactions (now called QCD or quantum chromodynamics):

- 1954: YM theory was proposed to generalize U(1) QED to an $SU(2)_{Isospin}$ theory for the strong interactions with the ρ meson as the analogue of the photon.

- 1966: Nambu suggested that YM theory may be relevant to the color degree of freedom of constituent quarks.

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- 1968: Experiments at SLAC discovered scaling of the strong interactions at short-distances.

- 1972-3: Asymptotic freedom was discovered for $SU(3)_{Color}$ YM theory (i.e. the weak coupling of the strong interactions at short distances).

In 1954, both the ultra-violet and infra-red(if the ρ were taken massless) properties of YM theory were regarded as *complicated*. But inspite of the theory's mathematical beauty, it took 20 years for theorists to discover its important physical property of asymptotic freedom; and, in fact, this occurred only after the hint provided by a Nobel prize winning experiment!

For comparison, the recent history of quantum algebras is

- 1979-87: q-algebra symmetries investigated in quantum and statistical mechanical models [1].

- 1989: q-oscillators introduced to realize the new symmetries of q-algebras [2].

- ????: ???

If this historical parallel is of significance, we need to know the physical implications of these novel symmetry structures. If there are q-oscillators in nature which realize these new algebras, it seems reasonable to expect that there will also exist a q-analogue quantum field which has such q-oscillators as its normal modes[4]. We need to know its canonical physical properties—what are its number and phase signatures? Since the usual quasi-classical coherent states (CS) approximately characterize many types of cooperative behavior in the q=1 case, it is natural to use the q-CS's to investigate and identify empirical signatures[4,6] of a generic q-field for cooperative phenomena, whether in quantum optics, many body physics, particle physics ....

The q-analogue coherent states $|z>_q$ satisfy $a|z>_q = z|z>_q$ where the q-oscillator algebra is ($q \to 1$, usual bosons)

$$aa^\dagger - q^{\pm 1/2}a^\dagger a = q^{\mp N/2} \tag{1}$$

with $[N, a^\dagger] = a^\dagger$, $[N, a] = -a$, and the physically important bosonic $[a, a] = 0$. We take q real, and $0 < q < 1$.

In the $|n>_q$ basis, $<m|n> = \delta_{mn}$ and[2]

$$a^\dagger|n> = \sqrt{[n+1]}|n+1> \qquad a|n> = \sqrt{[n]}|n-1> \qquad a|0> = 0 \tag{2}$$

where $[x]_q = [x] \equiv (q^{x/2} - q^{-x/2})/(q^{1/2} - q^{-1/2})$ is the "q-deformation" of x. More simply $[x] = \sinh(sx/2)/\sinh(s/2)$ where $q = \exp s$. Note that

$$a^\dagger a|n> = [N]|n> = [n]|n> \qquad N|n> = n|n> \qquad a|0> = 0 \tag{3}$$

It follows that with $< z|z> = 1$ the q-CS's are

$$|z>_q = N(z) \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{[n]!}}|n>, \qquad N(z) = e_q(|z|^2)^{-1/2} \tag{4}$$

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[2]From now on the sub-q's are usually implicit!

in terms of the "q-exponential function"

$$e_q(z) \equiv \sum_{n=0}^{\infty} \frac{z^n}{[n]!}, \qquad [n]! \equiv [n][n-1]\cdots[1], \qquad [0]! = 1 \tag{5}$$

which is an order zero entire function [5], and $|e_q(z)| \leq e_q(|z|) \leq exp(|z|)$. For $x > 0$, it's positive, but for $x < 0$ and $q < (q_1^* \sim 0.14)$ there are an infinite number of increasing amplitude oscillations of decreasing frequency as $x \to (-\infty)$. The infinite number of real zeros are approximately at $\tilde{\mu}_n = -q^{(1-n)/2}/(1-q)$; $n = 1, 2, \ldots$. As q increases, these zeros collide in pairs and move off the real axis as a complex conjugate pair. In this manner, $e_q(z) \to exp(z)$ as $q \to 1$.

In analyzing the q-boson field in the $|z>_q$ classical limit, we use the Heisenberg representation, consider a specific mode, and suppress the $\vec{k}$ mode and $\hat{\epsilon}$ polarization indices for the generic electric and magnetic fields, etc. . Notice that the q-analogue coherent states $|z>_q$ are good candidates for studying the classical limit of the q-analogue quantized radiation field because they are minimum uncertainty states. They minimize the fundamental commutation relation

$$U_{Q,P} \equiv \frac{2\Delta Q \Delta P - |<[Q,P]>|}{|<[Q,P]>|} \geq 0 \tag{6}$$

with $U|_{|z>} = 0$, but $U|_{|n>\neq|0>} = \frac{(3[n]+[n+1])}{([n+1]-[n])}$. Also, the n^{th} order correlation function factorizes, i.e.

$$Tr(\rho E^-(x)E^+(y)) = \mathcal{E}^-(x)\mathcal{E}^+(y), \ldots \tag{7}$$

In addition, there exists a resolution of unity[3-5] for the q-CS's

$$\int |z><z| \, d\mu(z) + \int |\tilde{z}><\tilde{z}| \, d\tilde{\mu} = I \tag{8}$$

with, respectively, a continuous (q-integration) measure

$$d\mu(z) = \frac{1}{2\pi} e_q(|z|^2)e_q(-|z|^2)d_q|z|^2 \, d\theta \tag{9}$$

and a discrete measure

$$d\tilde{\mu}_k = \frac{1}{2\pi} e_q(q^{1/2}|\tilde{z}_k|^2)e_q(-|\tilde{z}_k|^2)d\theta. \tag{10}$$

Note that $|\tilde{z}_k|^2 = q^{k/2}\zeta_i$ with $k = 0, 1, \ldots$ and $\zeta_i = $ minus the i^{th} zero of $e_q(z)$. The q-discrete auxiliary states,[4], $|\tilde{z}_k>_q$ satisfy

$$\tilde{a}_k|\tilde{z}_k>_q = (q^{1/4}\tilde{z}_k)|\tilde{z}_k>_q \tag{11}$$

The $\tilde{a}_k$ obey the q-commutation relations, (1).

Consequently the q-CS's are non-orthogogonal and overcomplete. There are q-analogue generalizations[4,6] of the P-, Q-, and W-phase space representations of quantum optics. However, as we next discuss, there also are important differences in the $|z>_q$ basis for other coherence and uncertainty properties of the q-analogue quantized field[3] .

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[3]For more details see [6].

2 Fractional Uncertainties in the $|z>_q$ Classical Limit

With the usual definitions $\hat{P} = -i(\hbar\omega/2)^{1/2}(a - a^\dagger)$, $\hat{Q} = (\hbar/2\omega)^{1/2}(a + a^\dagger)$, the fractional uncertainties $\frac{\Delta\hat{Q}}{|<\hat{Q}>|}$ and $\frac{\Delta\hat{P}}{|<\hat{P}>|}$ are of $O(1)$ for $|z| \to \infty$ and

$$< z|[Q, P]|z > = i\hbar < z|[a, a^\dagger]|z > = i\hbar < z|\hat{\Lambda}|z > = i\hbar\lambda(z) \geq i\hbar \tag{12}$$

This defines the resolution operator $\hat{\Lambda} \equiv [a, a^\dagger]$. The q-boson "resolution function" ($q = \exp s$, and $N(z)$ is the CS norm.)

$$\lambda(z) \equiv N(z)^2 \sum_{n=0}^{\infty} \frac{|z|^{2n} \cosh(s(2n + 1)/4)}{[n]!\, \cosh(s/4)} \tag{13}$$

goes as $(q^{-1/2} - 1)|z|^2 + 1$ as $|z| \to \infty$. This follows because

$$\lambda(z) \equiv < z|[N + 1]|z > - < z|[N]|z > = ((q^{-1/2} - 1)|z|^2 + (e_q(q^{1/2}|z|^2)/e_q(|z|^2))) \tag{14}$$

Note that $\lambda(z)$ is bounded from above and below.

For the generic q-electromagnetic field, the fractional uncertainties in amp $\hat{E}$, in amp $\hat{B}$, and in the "Hermitian" Pegg-Barnett phase operator, $\hat{\phi}_q$, are also of $O(1)$ [7,4,6].

Note[4] that the quadratic $\hat{P}, \hat{Q}$ single-mode hamiltonian, which has an $O(1)$ fractional uncertainty,

$$H_{\hat{P},\hat{Q}} = (1/2)\hbar\omega(a^\dagger a + aa^\dagger) = (1/2)(\hat{P}^2 + \omega^2\hat{Q}^2). \tag{15}$$

is proportional to the anti-commutator. Hence for $q \neq 1$, $H_{\hat{P},\hat{Q}}$ is not mathematically independent of the basic commutator $\hat{\Lambda} \equiv [a, a^\dagger]$ because of the fundamental operator identity

$$(-(i/\hbar)[Q, P]\cosh(s/4))^2 - ((2/\hbar\omega)H_{\hat{P},\hat{Q}}\sinh(s/4))^2 = 1. \tag{16}$$

In striking contrast to these $O(1)$ fractional uncertainties, both the usual N operator and the elementary N-Hamiltonian operator

$$H_N = \hbar\omega(N + 1/2) \tag{17}$$

possess zero fractional uncertainties as $|z| \to \infty$. Also, H_N does indeed possess the conventional field-theoretic properties of the classic $q = 1$ Hamiltonian operator.

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[4]For $H_{\hat{P},\hat{Q}}$, the energy is not additive for two widely separated systems, violating the usual cluster decomposition "axiom" in quantum field theory. For q-quanta this is not so surprising since the fractional uncertainty in the energy based on $H_{\hat{P},\hat{Q}}$ is $O(1)$ in the $|z>$ basis and the quanta by (1) are compelled to be always interacting,i.e. by exclusion-principle-like q-forces! So it is doubtful that $H_{\hat{P},\hat{Q}}$ permits the usual physical interpretation based on a smooth limit to a conventional, free quantized field.

3   q-Boson Counting Statistics

The physically important $[a, a] = 0$ implies that the usual Bose-Einstein energy distribution still follows for a free q-boson gas . Note that (9) above does imply a non-degenerate equally-spaced spectrum. On the other hand, the q-CS's do not give a Poisson number distribution for $q \neq 1$ since [2,8]

$$P_n{}^q(z) = |< n|z >|^2 = \frac{|z|^{2n}}{[n]! e_q(|z|^2)}. \tag{18}$$

Note that for $q \neq 1$, $|z|^2$ is the eigenvalue of the deformed number operator, [N], in the $|z >_q$ basis. The mean value of usual number operator N goes as $< N >= 2\alpha_q log|z| + \beta_q$ for $1 < |z|^2 < few 100$, where α_q and β_q are q-dependent constants. For fixed $|z|^2$, as q decreases the peak of $P_n{}^q(z)$ narrows and shifts to smaller n. Therefore, the behavior of the fractional uncertainty $(\Delta N)/ < N >$ is not very q-dependent.

However, since $\Delta N \to \eta_q$ as $|z| \to \infty$, where η_q is a q-dependent constant for $q \neq 1$, there is the very important signature for q-boson counting statistics that

$$(\Delta N)^2 / < N > \to 0 \tag{19}$$

as $|z| \to \infty$. This is in contrast to a thermal source where the "rhs" of (19) equals $< N + 1 >$ for all $|z|$, and for laser light (and q=1 CS's) where the "rhs" equals "one" as $|z| \to \infty$. So in principle it is possible by q-boson counting experiments to very simply identify a q-boson gas in this limit in spite of the ordinary Bose-Einstein frequency distribution.

4   The q-Analogue of the Pegg-Barnett Phase Operator, $\hat{\phi}_q$

Recall $z = |z| \exp(i\theta)$. While mathematically a hermitian phase operator conjugate to N, or to $[N] \equiv a^\dagger a$ does not exist [9], q-generalizations of the phase operators of Susskind-Glogower [9,10] and of Pegg-Barnett [7] have been constructed [4,6]. The q-generalization of the Pegg and Barnett operator[5] is obtained by introducing a complete, orthonormal basis of $(s + 1)$ phase states $|\theta_m >_q = (s + 1)^{-1/2} \sum_{m=0}^s \exp(in\theta_m)|n >_q$, $\theta_m = \theta_0 + 2m\pi/(s + 1)$, with $m = 0, 1, \ldots, s,$. These are eigenstates of the respectively hermitian and unitary

$$\hat{\phi}_q \equiv \sum_{m=0}^s \theta_m |\theta_m >< \theta_m| \tag{20}$$

$$\exp(i\hat{\phi}_q) \equiv |0 >< 1| + \cdots + |s - 1 >< s| + \exp(i(s + 1)\theta_0)|s >< 0| \tag{21}$$

which is manifestly q-independent and unitary. In the analysis of $SU(2)_q$ Chaichian and Ellinas[11] introduce a polar decomposition operator that is the same as $\exp(i\hat{\phi})_q$ when the reference phase is chosen to be $\phi_R = (s + 1)\theta_0$.

For arbitrary q, it still follows that

$$[cos\hat{\phi}_q, sin\hat{\phi}_q] = 0 \qquad cos^2 \hat{\phi}_q + sin^2 \hat{\phi}_q = 1 \tag{22}$$

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[5] The number-phase properties of the q-generalized SG operators are treated in [6]. For research prior to PB on phase operators in spaces of finite dimension see T.S. Santhanam (*this conference*) and see the two recent general reviews of phase operators [12].

and that $< n|\cos^2 \hat{\phi}_q|n >=< n|\sin^2 \hat{\phi}_q|n >= 1/2$ for $n = 1, 2, \ldots$. In particular, the q-boson vacuum state $|0 >_q$ has a random phase.

The mean-value of $\hat{\phi}_q$ in the $|z >_q$ basis is

$$< \hat{\phi}_q >= \frac{1}{2\pi} \int_0^{2\pi} \theta_m \bar{P}_q(\theta_m)\, d\theta_m \ = \ \theta \ = \ Arg(z) \qquad (23)$$

in terms of the q-boson phase distribution(the conjugate distribution to $P_n{}^q(z)$)

$$\bar{P}_q(\theta_m) \ = \ \lim_{s \to \infty}(s+1)| < \theta_m|z >_q |^2 \qquad (24)$$

with the normalization $\frac{1}{2\pi} \int_0^{2\pi} \bar{P}_q(\theta_m)\, d\theta_m = 1$. The variance of the phase operator

$$(\Delta \hat{\phi}_q)^2 \to 1/(2\eta_q)^2 \qquad (25)$$

as $|z| \to \infty$, where η_q is the same q-dependent constant found for ΔN as $|z| \to \infty$.

5 Approximate $[N, \hat{\phi}_q] = i$ in $|z >_q$ Classical Limit

Thus, from the reciprocal-dependencies on η_q of ΔN and $\Delta \hat{\phi}_q$, it follows that there are the ususal (though approximate) number-phase and energy-phase uncertainty relations

$$\Delta N\, \Delta \hat{\phi}_q \ \geq \ 1/2 \qquad \Delta H_N\, \Delta \hat{\phi}_q \ \geq \ \hbar\omega/2 \qquad (26)$$

In the $|z >_q$ basis, the q-boson phase distribution $\bar{P}_q(\theta_m)$ function also appears in Dirac's approximate number-phase commutation relation

$$< z|[N, \hat{\phi}_q]|z > = \ i \ - \ i\, \bar{P}_q(\theta_0) \qquad (27)$$

where θ_0 is the Pegg-Barnett indicial angle used above in (20). So for large $|z|$, for $q \neq 1$,

$$\lim_{s \to \infty} < z|[N, \hat{\phi}_q]|z > \ = \ i \ - \ i\, 2\pi\, \delta_q(\theta - \theta_0) \qquad (28)$$

for $\hat{\phi}_q$ eigenvalues from the indicial θ_0 to $(\theta_0 + 2\pi)$. This extra δ_q term is a "bell-shaped" function. This term serves a physical role analogous to that of a smeared "magnetic monopole" string in that it appears in the classical limit to uniquely specify the classical phyase angle. For $q = 1$, the smearing is absent and δ_q is replace by a Dirac-delta-function distribution. This smearing is in agreement with the greater fractional uncertainty of $\hat{\phi}_q$ for $q \neq 1$.

So, neglecting the indicial-referencing term, we conclude that the $|z >_q$ coherent states both give and minimize Dirac's commutation relation, i.e. in $|z >_q$ basis for $|z|$ large

$$[N, \hat{\phi}_q] = i \qquad (29)$$

Hence, for the q-boson quantum field the operators N and $\hat{\phi}_q$ are almost canonically conjugate in the $|z >_q$ classical limit. This is in contrast to the extra $\lambda(z)$ "resolution factor" in the commutation relation for the position and momentum operators. Given the physical importance

of Dirac's commutation relation to cooperative phenomena in many different fields of physics, it is very encouraging that for arbitrary q values Eq.(29) still holds for the q-boson quantum field [13].

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AN ALGORITHM FOR THE BASIS
OF THE FINITE FOURIER TRANSFORM

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Abstract

The Finite Fourier Transformation matrix (F.F.T.) plays a central role in the formulation of quantum mechanics in a finite dimensional space studied by the author over the past couple of decades. An outstanding problem which still remains open is to find a complete basis for F.F.T. In this paper we suggest a simple algorithm to find the eigenvectors of F.F.T.

I. INTRODUCTION

The finite Fourier transform matrix (F.F.T.) plays a fundamental role in many contexts and has been studied extensively [1-3]. It is central in the discussions on finite dimensional quantum mechanics based on Weyl's commutation relations [4] studied by the author in a series of publications [5]. The eigenvalues of this matrix were determined by Schur [1] and a simple argument to recover this result has been given earlier [6]. The calculation of the eigenvectors is not straight-forward and many methods have been given in particular, by Mehta [7]. In Section IV, we present a new algorithm to find the eigenvectors.

II. EIGENVALUES OF S

The F.F.T. matrix S, which is unitary, is defined by

$$S_{\alpha\beta} = \frac{1}{\sqrt{n}} \exp \left[\frac{2\pi i}{n} \alpha \beta \right] ,$$

$$\alpha, \beta = 0,1,2,\ldots n-1 \qquad (2.1)$$

$$i = \sqrt{-1}$$

and has many interesting properties

$$1) \quad (S^2)_{\alpha\beta} \equiv I'_{\alpha\beta} = \delta_{\alpha + \beta, o} \qquad (2.2)$$
$$(\text{mod } n)$$

Since $S^2 f_\alpha = f_{-\alpha \bmod n,}$ for a vector f_α with n components, S^2 is called the parity operator

$$2) \quad (S^4)_{\alpha\beta} = \delta_{\alpha\beta} \qquad (2.3)$$

like the usual Fourier transform.

3) The matrix S, which is by definition a symmetric matrix will diagonalize any circulant matrix.

From Equation (2-3), it is clear that the eigenvalues of S are simply ±1 and $\pm i$. There is then a degeneracy of the eigenvalues. The first problem will be to determine this. Luckily, Equations (2.1)-(2.3) can be repeatedly used to fix this [6]. If k_1, k_2, k_3 and k_4 denote the multiplicity of the eigenvalues taken in the order (1, -1, i, -i), Equation (2.1) implies that

$$\text{Tr } S = \frac{1}{\sqrt{n}} \sum_{\ell=0}^{n-1} [\exp \frac{2\pi i}{n}]^{\ell^2}$$

$$= \frac{1}{2} (1 + i) [1 + \exp(\frac{-i\pi n}{2})], \tag{2.4}$$

and hence

$$\text{Tr } S = (k_1 - k_2) + i(k_3 - k_4)$$

$$= 1 \text{ for } n = 4k + 1,$$

$$= 0 \text{ for } n = 4k + 2,$$

$$= i \text{ for } n = 4k + 3,$$

$$= (1 + i) \text{ for } n = 4k,$$

$$k = 0,1,2,\ldots \tag{2.5}$$

From Equation (2) we infer that

$$\text{Tr } S^2 = (k_1 + k_2) - (k_3 + k_4)$$

$$= 1 \text{ for } n \text{ odd},$$

$$= 2 \text{ for } n \text{ even}.$$

We also have

$$\text{Tr } S^4 = n = k_1 + k_2 + k_3 + k_4.$$

Equations (2.5), (2.6) and (2.7) can be used to solve for k_1, k_2, k_3 and k_4 and one finds that

	$n = 4k + 1$	$n = 4k + 2$	$n = 4k + 3$	$n = 4k$
k_1	$k + 1$	$k + 1$	$k + 1$	$k + 1$
k_2	k	$k + 1$	$k + 1$	k
k_3	k	k	$k + 1$	k
k_4	k	k	k	$k - 1$

III. EIGENVECTORS OF S

Let us decompose S into its primitive idempotents as

$$S = \sum_{j=1}^{4} i^j B(j),$$

where

$$B(1) = \frac{1}{2}s + \frac{1}{4}(I - I')$$

$$B(2) = -\frac{1}{2}c + \frac{1}{4}(I + I'),$$

$$B(3) = -\frac{1}{2}s + \frac{1}{4}(I - I'),$$

$$B(4) = \frac{1}{2}c + \frac{1}{4}(I + I'), \tag{3.2}$$

$$C_{\alpha\beta} = \frac{1}{\sqrt{n}} \cos\left(\frac{2\pi}{n}\alpha\beta\right)$$

$$s_{\alpha\beta} = \frac{1}{\sqrt{n}} \sin\left(\frac{2\pi}{n}\alpha\beta\right),$$

$$\alpha, \beta = 0,1,2,\ldots n-1 \tag{3.3}$$

It is easily verified that

$$S B(j) = i^j B(j), \tag{3.4}$$

thus the nonzero columnus of $B(j)$ yield the eigenvectors of S with eigen-value i^j. Also, in analogy with the standard case, Mehta [7] has been able to express these eigenvectors in terms of Hermite functions with

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discrete arguments.

IV. EIGENVECTORS OF S; AN ALTERNATE METHOD

Since the F.F.T. matrix S satisfies Equation (2.1) we construct the matrix [10]

$$T = S^3 + S^2 S_d + S S_d^2 + S_d^3$$

$$= I'(S + S_d) + (S + S_d) S_d^2 , \qquad (4.1)$$

where

$$S_d = \text{diagonal } S . \qquad (4.2)$$

We find that

$$S T = S(S^3 + S^2 S_d + S S_d^2 + S_d^3)$$

$$= (I + S^3 S_d + S^2 S_d^2 + S S_d^3)$$

$$= (S_d^3 + S^3 + S^2 S_d + S S_d^2) S_d$$

$$= T S_d . \qquad (4.3)$$

If T is nonsingular,

$$T^+ S T = S_d \qquad (4.4)$$

Therefore, the columns of T automatically provide the eigenvectors of S. The degenerate eigenvectors of S corresponding to the repeated eigenvalues can be made orthonormal by using Gram-Schmidt process. This will render T unitary. While the process is quite general, we shall illustrate this for some special cases

case of $n = 2$

$$S = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} , \qquad (4.5)$$

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and

$$S_d = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} , \qquad (4.6)$$

Since $S^2 = S_d^2 = I$, $\qquad (4.7)$

We get from Equation (4.1)

$$T = 2 \ (S + S_d),$$

$$= 2 \begin{pmatrix} 1 + \dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{2}} \\[2mm] \dfrac{1}{\sqrt{2}} & -1 - \dfrac{1}{\sqrt{2}} \end{pmatrix} \qquad (4.8)$$

We unitarized matrix of the eigenvectors of S is therefore

$$U_2 = \frac{1}{\sqrt{2\sqrt{2} \ (\sqrt{2} + 1)}} \begin{pmatrix} \sqrt{2} + 1 & 1 \\[2mm] 1 & -(\sqrt{2} + 1) \end{pmatrix} \qquad (4.9)$$

case of n = 3

$$S = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1 \\ 1 & \varepsilon & \varepsilon^2 \\ 1 & \varepsilon^2 & \varepsilon \end{pmatrix} ,$$

$$\varepsilon = \exp \frac{2\pi i}{3} . \qquad (4.10)$$

From Equation (2.8) we see that

$$S_d = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & i \end{pmatrix} \qquad (4.11)$$

one finds from Equation (4.1) that the unitarized matrix of the eigen-

vectors of S is

$$U_3 = \frac{1}{\sqrt{2}\ \sqrt{3}\ (\sqrt{3}+1)} \begin{pmatrix} \sqrt{3}+1 & \sqrt{2} & 0 \\ 1 & \dfrac{1+\sqrt{3}}{\sqrt{2}} & i\sqrt{3+\sqrt{3}} \\ 1 & \dfrac{1+\sqrt{3}}{\sqrt{2}} & -i\sqrt{3+\sqrt{3}} \end{pmatrix} \cdot \tag{4.12}$$

case of n = 4

In this case we have

$$S = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -i \\ 1 & -i & -1 & i \end{pmatrix} \tag{4.13}$$

and

$$S_d = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & i \end{pmatrix} \tag{4.14}$$

It is easily calculated that

$$T = \begin{pmatrix} 3 & 1 & 1 & 0 \\ 1 & 1 & -1 & 2i \\ 1 & -1 & -1 & 0 \\ 1 & 1 & -1 & -2i \end{pmatrix} \tag{4.15}$$

The first two column vectors correspond to the eigenvalue = +1, the third one to -1 and the last to -i.

By a simple use of Gram-Schmidt orthogonalization procedure one can find the unitarized matrix corresponding to the eigenvectors of S as

$$U_4 = \frac{1}{\sqrt{2\sqrt{4}\ (\sqrt{4} + 1)}} \begin{pmatrix} 3 & 0 & \sqrt{3} & 0 \\ 1 & \sqrt{2} & -\sqrt{3} & i\sqrt{6} \\ 1 & -2\sqrt{2} & -\sqrt{3} & 0 \\ 1 & \sqrt{2} & -\sqrt{3} & -i\sqrt{6} \end{pmatrix} \qquad (4.16)$$

ACKNOWLEDGMENTS

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[10] This can be easily generalized to $A^{n-1} + A^{n-2} A_d + A^{n-3} A_d^2 + \ldots$ $+ A A_d^{n-2} + A_d^{n-1}$ for the case of a general involution matrix satisfying the relation $A^n = I$.

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A NOTE ON THE ANGULAR
FOURIER TRANSFORMATION

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ABSTRACT

It is demonstrated that an angular Fourier transformation is obtained by making a rotation around the non-compact axis of So(2,1), the Lorentz group in three dimensions.

I. INTRODUCTION

The conventional fourier transformation has been at the root of quantum mechanics. If $\hat{q}$, $\hat{p}$ represent the position and momentum self adjoint operators of quantum mechancis, they satisfy the commutation relation *[1]

$$[\hat{q}, \hat{p}] = \hat{q}\hat{p} - \hat{p}\hat{q} = i \ . \tag{1}$$

It is also well known that this relation implies that

$$(\Delta p)^2 \ (\Delta q)^2 \geq \frac{1}{4} \ , \tag{2}$$

where

$$(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2 \ . \tag{3}$$

Equation (1) is known to imply that

$$|p\rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp(ipq)|q\rangle dq \ .$$

i.e. the basis $|q\rangle$ in which the operator $\hat{q}$ is diagonal is related to the basis in which the operator $\hat{p}$ is diagonal through the Fourier Transform operator $\hat{S}$

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*We use the unit where units $\dfrac{h}{2\pi} = 1$, where he is the plank constant

It is also known [2] that the classical fourier transform operator S can be represented as,

$$\hat{S} = \exp\{i\Pi\{(\hat{p}^2 + \hat{q}^2)/4 - \frac{1}{4}\}\} , \qquad (5)$$

where $\hat{S}$ is defined as

$$\langle q|\hat{S}\Psi\rangle = \frac{1}{\sqrt{2\Pi}} \int_{-\infty}^{\infty} \exp(iqq')\langle q'|\Psi\rangle dq' , \qquad (6)$$

where Ψ is the wave function which satisfies the Schröedinger wave euqation [1].

In this paper we show that the conventional fourier transform operator $\hat{S}$ when rotated by an angle θ through the non compact generator Γ_4 of the Lorentz group SO(2,1) yields the Angular Fourier Transformation (AFT). We also analyze the properties of the AFT from this perspective and relate it to the recent work of L. B. Almeida [23] who has derived the AFT from a different point of view.

In Section 2 we summarize the properties of the group SO(2,1). In section 3, we study some properties of the AFT from this perspective and relate this to the work of Almeida. In the last section we offer some conclusions on the discretization of the transform.

II. THE LORENTZ GROUP SO(2,1)

We define the three operators by Γ_4, Γ_0, T as

$$\begin{aligned}
\Gamma_0 &= (1/4) \times \{\hat{p}^2 + \hat{q}^2\} , \\
\Gamma_4 &= (-1/4) \times \{\hat{p}^2 - \hat{q}^2\} , \\
T &= (-1/4) \times \{\hat{q}\,\hat{p} + \hat{p}\,\hat{q}\} = (-1/2) \times \{\hat{p}\,\hat{q} + \frac{i}{2}\} . \quad (7)
\end{aligned}$$

It is easily verified that Γ_4, Γ_0, T satisfy the following commutation relations.

$$[\Gamma_0, \Gamma_4] = iT \quad , \tag{8}$$

$$[T, \Gamma_0] = i\Gamma_4 \quad , \tag{9}$$

$$[T, \Gamma_4] = i\Gamma_0 \quad , \tag{10}$$

and the Lie algebra so obtained is that of the Lorentz group SO(2,1) in (2+1) dimensions [4]. It is recognized that the classical Fourier Transform operator in Equation (5) can be rewritten as

$$\hat{S} = \exp\{i\Pi(\Gamma_0 - \tfrac{1}{4})\} \quad . \tag{11}$$

The generator Γ_4 is called the non compact generator of the Lorentz group SO(2,1), reflecting the fact that it is not bounded in support. From the commutation relations we can verify using Equations (8, 9, 10) that

$$\hat{K}_\theta(\hat{p}, \hat{q}) = \exp(i\theta\Gamma_4)\cdot(\hat{S})\cdot\exp(i\theta\Gamma_4) \quad , \tag{12}$$

$$\hat{K}_\theta(\hat{p}, \hat{q}) = \exp(-i\tfrac{\pi}{4})\cdot\exp(\tfrac{\pi}{4}\sinh\theta)\cdot\exp(i\pi\{\{\tfrac{\hat{p}^2+\hat{q}^2}{4}\cosh\theta-\{\hat{p}\,\hat{q}\}\sinh\theta\}). \tag{13}$$

It may also be verified that

$$\langle q|\hat{K}_\theta\Psi\rangle = N_\theta\int_{-\infty}^{\infty}\exp(i\{\{\tfrac{q^2+q'^2}{2}\}\sinh\theta-\{qq'\}\cosh\theta\})\langle q'|\Psi\rangle dq', \tag{14}$$

Where N_θ is a normalization constant that is dependent on θ.

If we now set $\sinh\theta = \cot\alpha$ and $\cosh\theta = \csc\alpha$ then we obtain the kernel of L. B. Almeida where the variables are (t,u) instead of (q,q'). Thus the kernel of the AFT gets a meaning as a rotation in the (t,w) plane. The variables (q,q') are the canonical variables and can be substituted with any pair of variables that satisfy equation (1).

III. PROPERTIES OF THE ANGULAR FOURIER TRANSFORM

It becomes clear after substituting $\sinh\theta = \cot\alpha$ and $\cosh\theta = \csc\alpha$ that

$$\theta = \ln(\cot(\frac{\alpha}{2})) \ , \tag{15}$$

which implies that as $\theta \to \infty$, $\alpha \to 2n\Pi$ and $\theta \to -\infty$, $\alpha \to (2n + 1)\Pi$. With the above identifications our kernel in Equation (13) is identical to that of Almeida who has shown that the kernel exhibits the following properties

$$(1) \quad K\alpha(t,u) = K\alpha(u,t) \ , \tag{16}$$

$$(2) \quad \int_{-\infty}^{\infty} K\alpha(t,u)K*\alpha(t,u')dt = \delta(u-u') \ , \tag{17}$$

$$(3) \quad Ko(t,\omega) = \frac{1}{\sqrt{2\pi}} \exp\{-it\omega\} \ . \tag{18}$$

For further properties use reference [3]. As envisaged in reference [3] the AFT can be applied to the study of frequency swept filters.

IV. CONCLUSIONS

In this paper we have used the properties of the group SO(2,1) to define the AFT as a rotation of the fourier transform operator $\hat{S}$ by an angle θ through the non compact generator Γ_4 of the group, which will reduce to the conventional Fourier Transform as $\theta \to \infty$.

The study of a discrete version of this transform and fast algorithms for it's computation is of great interest and has been carried out [5].

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C-4.

NEURODYNAMIC OSCILLATORS

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Abstract

Oscillation of electrical activity has been found in many nervous systems, from invertebrates to vertebrates including man. There exists experimental evidence of very simple circuits with the capability of oscillation. Neurons with intrinsic oscillation have been found and also neural circuits where oscillation is a property of the network. These two types of oscillations coexist in many instances. It is nowadays hypothesized that behind synchronization and oscillation there is a system of coupled oscillators responsible for activities that range from locomotion and feature binding in vision to control of sleep and circadian rhythms.

The huge knowledge that has been acquired on oscillators from the times of Lord Rayleigh has made the simulation of neural oscillators a very active endeavor. This has been enhanced with more recent physiological findings about small neural circuits by means of intracellular and extracellular recordings as well as imaging methods. The future of this interdisciplinary field looks very promising; some researchers are going into quantum mechanics with the idea of trying to provide a quantum description of the brain.

In this work we describe some simulations using neuron models by means of which we form simple neural networks that have the capability of oscillation. We analyze the oscillatory activity with root locus method, cross- correlation histograms, and phase planes. In the more complicated neural network models there is the possibility of chaotic oscillatory activity and we study that by means of Lyapunov exponents. The companion paper shows an example of that kind.

1   Introduction

Recent advances in nonlinear dynamics, chaos and fractals have been of great benefit not only in Physics and Mathematics but as well as in the study of the dynamic activity of the brain. These tools allow to characterize neural phenomena that are usually described by means of graphical methods as it is the case of electroencephalography (EEG) and some other similar recordings.

A topic that has pervaded neurophysiology along decades of this century has been the observation of oscillations in external (scalp) EEG. Likewise, oscillations of neuronal activity have

been found in extracellular and intracellular electrical recordings in cortical and subcortical areas of the brain of man and animals. These observations of oscillating electrical activity have been described since the works of Mayer, Carlson, and Sherrington in 1906, as well as in the studies of Gray and Lissman in 1950 and in the work of Wilson in 1961 [1]. From then to the eighties there exist many other descriptions in the literature about oscillatory behavior. The common feature of these observations is the lack of a theoretical framework where to place them and the ignorance about the mechanisms and function of oscillatory activity.

In recent years the study of neural oscillation has been renewed applying analytical and computational tools. Among them the more notorious are nonlinear dynamics, spectral analysis, signal processing methods, chaos, and artificial neural networks. On the one hand, these tools allow to characterize neural oscillation in a manner not possible before and, on the other hand, they also allow to model and simulate oscillating phenomena in such a way that it is possible to make inferences about the mechanisms that at the level of neuronal circuits could be responsible of producing, modulating and using the oscillatory capabilities of neurons, neural networks, and neural systems.

It has been said that we do not know what could be the use of oscillations and chaos in the brain [2], but we have the tools to detect and quantify them in such a way that could lead us towards new knowledge and new tools.

2 Biological Oscillation

It is well known that oscillatory activity can be detected in the EEG. According to the brain state different oscillatory bands can be defined, namely: delta(1-4 Hz), theta(5-8 Hz), alpha(10 Hz), beta(20-30 Hz) and gamma(30-50 Hz). Beta and gamma bands are related to very active states. If at the same time the activity of neurons is recorded, it is possible to find rhythmic firing that is coherent with the beta or gamma oscillations. The most prominent example of this fact is the discovery by Singer, Gray and others [3] of oscillations of 40 Hz in the cat visual cortex. They recorded the EEG in two different places and found strong coherence between them. At the same time, the firing of neurons recorded in the same locations is rhythmically synchronized with the EEG. Since there is evidence that the features of an object are processed in parallel channels along the visual pathway they think that response synchronization of cortical neurons is a possible mechanism for feature binding in the visual system. This is probably the most important role that has been given to neural oscillation. However, it has to be realized that feature binding is not equivalent to perception.

The hippocampus is another example of oscillation where three different components can be discriminated in the hippocampal EEG: A rhythmic slow activity (RSA) or theta rhythm (with harmonics), an irregular slow activity (ISA) that may be high-amplitude (large irregular activity, LIA) or small-amplitude (small irregular activity, SIA), and fast waves or beta rhythms. It is not known what role, if any, these components play in the hippocampal functioning.

One important question is what neuronal circuits underlie both the generation of rhythmic firing and the oscillations in the EEG. There are single neurons that have the machinery for rhythmic firing and others fire rhythmically due to the properties of the network which they belong to. According to Getting [4] some simple biological circuits employ one of the following arrangements: mutual excitation, recurrent inhibition, reciprocal inhibition, and feedback inhibition. It has been

shown that in biological neural systems both ways of producing rhythmic firing are used, even in combination.

3 Models of Oscillation

Modeling is an important tool for understanding biological phenomena. There are several approaches to simulate oscillatory activity. Here we show several examples. In one of them oscillation is produced by the intrinsic properties of a dynamic linear system and in the other two examples the firing pattern depends on the connectivity properties of a simple neural network where single neurons have increasing complexity in their mathematical modeling.
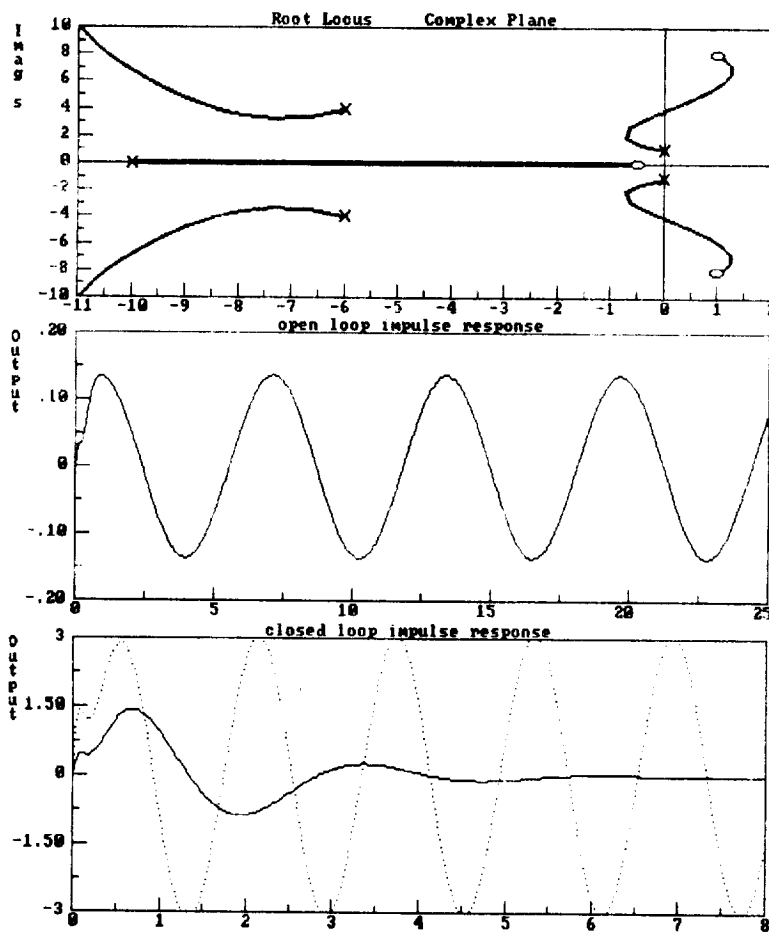
FIG. 1. Model of linear oscillator with complex dynamics. The behavior is dependent on the gain.

For the model in FIG. 1, the upper plot shows the root locus for a fifth order linear model of a dynamic system which in open loop practically behaves as a linear harmonic oscillator due to the dominance of the imaginary poles. Due to its intrinsic characteristics, the open loop response of the model produces a periodic oscillation as shown in the middle plot in FIG. 1. When negative feedback is added to the model, new properties appear, for one, the possibility of two different

types of oscillation. One transient oscillation (continuous curve in lower plot of FIG. 1) when a given gain produces complex poles in the left-hand side of the complex plane, and periodic oscillation (dotted curve in lower plot of FIG. 1) when another gain produces imaginary poles. Notice that the frequency of periodic oscillation is different between the open loop and the closed loop responses. The complexity of responses of a simple model like this can be enriched by adding a nonlinear element in the forward path and a delay in the feedback path. A system like this has been proposed to model the fast rhythm generation in the hippocampus [5].

For the first case of the second example, Net 1, Net 2, and Net 3 shown in FIG. 2 are simple neural networks in which we study the conditions to achieve periodic firing patterns. The neuron models (circles) are not endogenous units: to initiate their activity it is necessary one activating element (fiber).
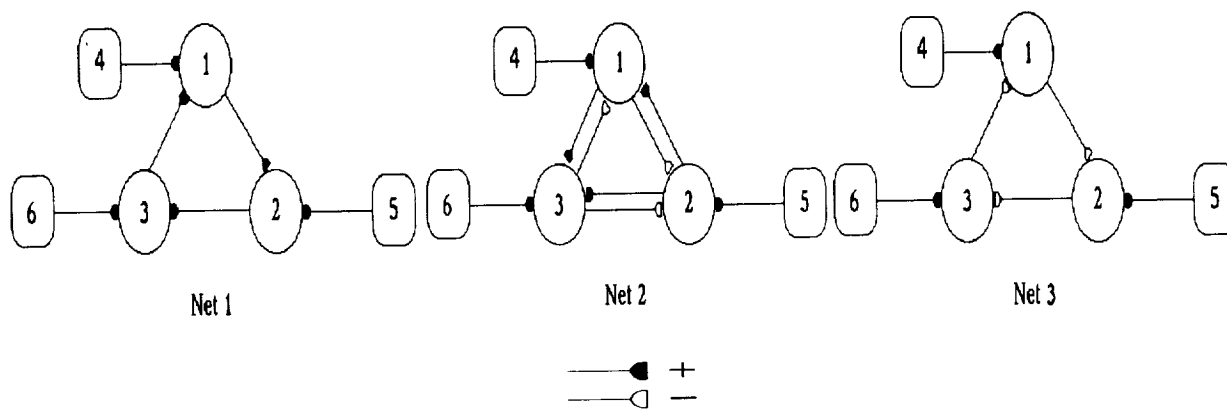

FIG. 2. Neural networks with periodic firing patterns.

The firing patterns shown in FIG. 3 were obtained by varying the synaptic intensity (weight) in each connection of the network and keeping unaltered other biological parameters. The cross-correlation histograms are useful for inferring functional connectivity and for assessing temporal relations between the firing patterns. In the histograms shown we see an increasing degree of synchronous activity in the firing patterns from Net 1 to Net 3. Actually, in Net 3 we observe a rhythmic oscillation.

For the second case of the second example, the electrical properties of individual neurons are described with Hodgkin- Huxley type voltage and time-dependent ionic currents. Neurotransmitter fluxes are additional state variables in such networks and the action of chemical synapses is modeled by additional kinetic equations. In FIG. 4 and FIG. 5 we show in the left column the firing activity of the neurons and in the right column the phase planes. A single neuron model can fire rhythmically, as exhibited by type 1 neuron in the upper part of FIG. 4, or it can display the apparently chaotic activity seen at the bottom of the figure. The difference between the two models is simply the value of a time-dependent sodium current variable.

We formed a network with recurrent inhibition like the one in Net 3 (see FIG. 2). In FIG. 5 we show the activity of the neurons in the ring-network. When type 1 neurons are used, the individual activities remain rhythmic. By contrast, when type 2 neurons are used in the network the activity becomes rhythmic in all three neurons, which is made more evident in the corresponding phase plane plots. The overall behavior of the second network is different from the behavior of the single components.
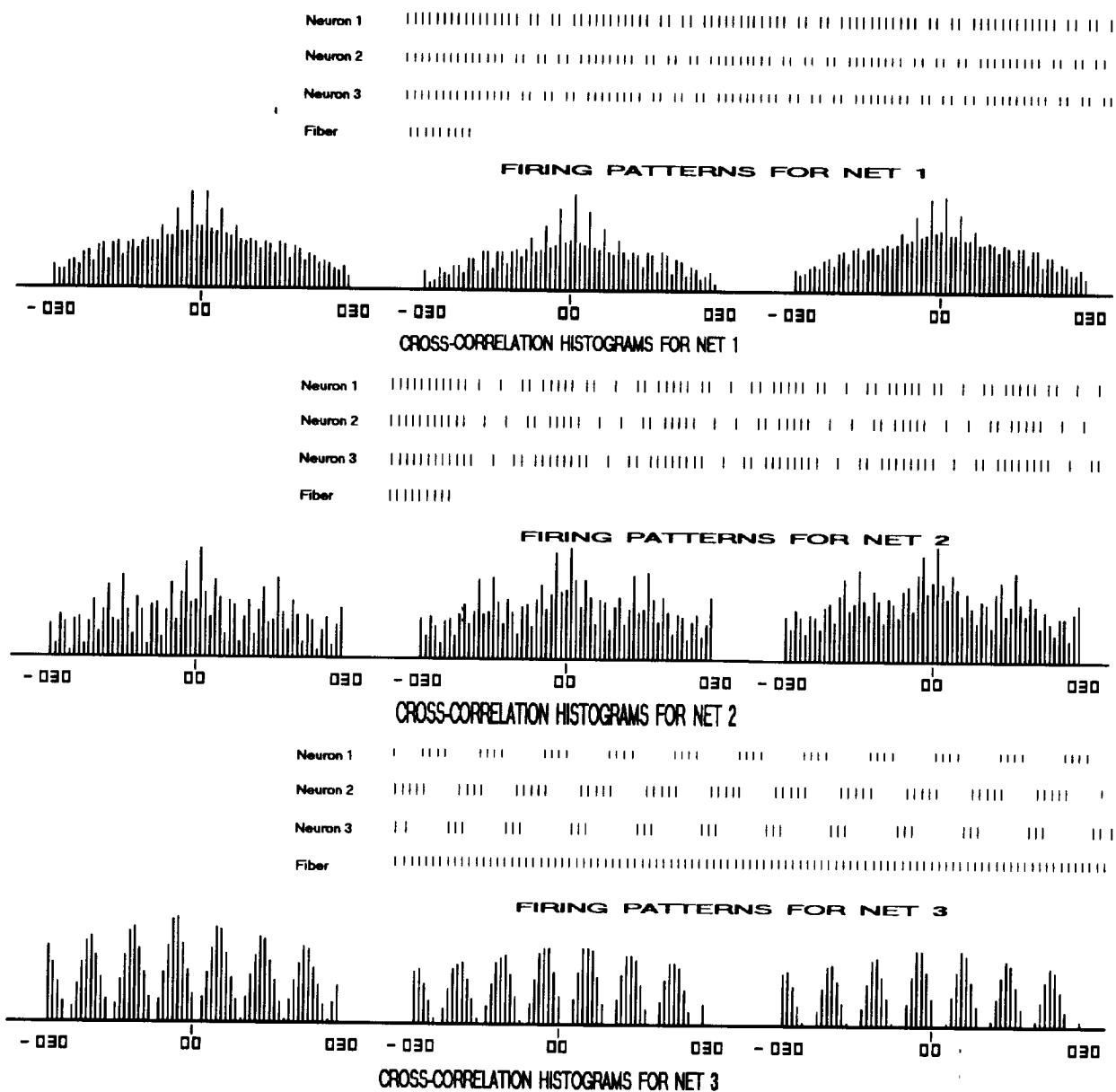
FIG. 3. Firing patterns and cross-correlation histograms for nets of Fig.2. From left to right, the histograms show the cross-correlation between neurons 1-2, 2-3, and 3-1, respectively. The weights between neurons 1-2, 2-3, and 3-1 are: 10, 4, 5 for Net 1; 5/-6, 12/-6, 5/-6 for Net 2; and -12, -16, -24 for Net 3. Negative weights indicate inhibitory connections.

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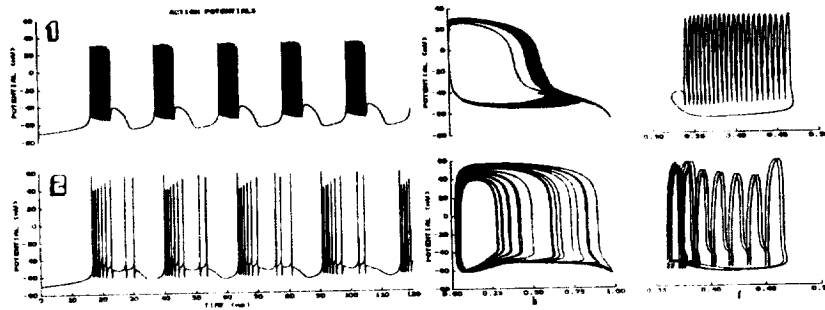
FIG 4. Examples of activity in single neurons. Type 1 neuron shows a periodic attractor while type 2 neuron exhibits an apparently chaotic attractor.
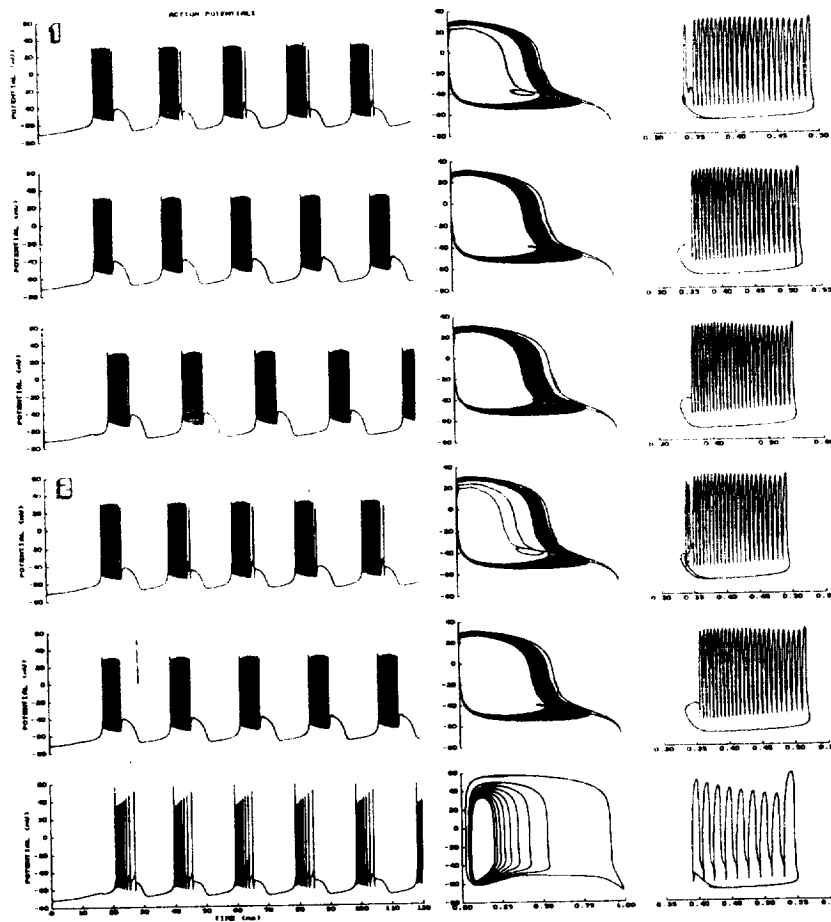
FIG. 5. Neuron activity in a ring-net similar to Net 3 of FIG. 2. Type 1 neurons were used for the first net and type 2 for the second one. Type of neuron notwithstanding all neurons display a rhythmic activity in the net.

4   Concluding Remarks

As it happens in High-Energy Physics where powerful colliders allow to look for new elementary particles, in Neuroscience, instruments like Magnetic Resonance Imaging (MRI) and Positron-Emitted Tomography (PET), allow to look for unknown mechanisms involved in normal brain functioning. However, unlike Physics, Neuroscience does not possess theoretical frameworks with the power of Quantum Theory and Classical Mechanics, that is, there is not a brain theory which could embrace the evidence provided by experiments at the molecular level as well as at the system level.

Many neuroscientists think that understanding of the mechanisms underlying perception, memory, learning and consciousness will require a quantum theory framework which would include nonlinear dynamics and chaos [6].

For example, brain waves and neuromuscular systems have attracted the use of harmonic analysis and feedback control theory since the times of Wiener [7] and Ashby [8]. In the same line but in a different field was Hebb with his reberveratory circuits [9]. They were using these tools as a mathematical characterization of macro-events in physiological systems. More recently, in trying to understand special mechanisms in the organization of biological neural networks, the theory of feedback has been brought to light again, namely by Humphrey [10] and by Edelman [11] with his idea of reentrant loops. In including negative or positive feedback in a system the conditions for oscillation are highly likely.

On the other hand, Penrose [12] has argumented that consciousness will not be understood on a computational basis, but it will require a fuller understanding of quantum mechanics, specifically the application of micro quantum mechanics to macro events [13]. However, Crick remarks that Penrose considers physics incomplete because there is as yet no theory of quantum gravity and hopes that an adequate theory of it might explain consciousness but he is very vague as to how it might do so [14]. On the side of perception, Pribram describes works which propose a quantum neurodynamics based on the Schröedinger equation and also a neural wave equation akin to Schröedinger's. He also mentions that Heisenberg matrices have been identified as instruments for the evolution of group structures, a process shown capable of accounting for the neural processes entailed in the perception of objects [6]. It is agreed at this time that all the hypotheses on consciousness are very vague as to exactly what is crucial for it and the same can be said about perception.

It is important to notice that a single neuron has a great molecular complexity [15]. However, it is in neural nets and systems of nets where higher brain functions are supposed to take place [14]. Moreover, advances in molecular neurobiology point to the place where two neurons communicate -called the synapse- as very important for higher brain functions, mainly the events that occur at the dendritic tree and the dendritic spines which are the sites that have the molecular machinery (receptors and channels) for receiving the molecules of neurotransmitter coming from the sending neuron. These phenomena could be studied by means of coupled harmonic oscillators as it has been done for finding soluble models in molecular physics [16]. After all, it was the great quantum theorist Schröedinger whose lectures in Dublin, when published in 1944 with the title "What Is Life?", had a major influence on the development of molecular biology [13]. In that book Schröedinger had one question and one answer: "How can the events in space and time which take place within the spatial boundary of a living organism be accounted for by physics and

chemistry? The obvious inability of present-day physics and chemistry to account for such events is no reason at all for doubting that they can be accounted for by those sciences." [17].

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LYAPUNOV EXPONENTS FROM CHUA'S CIRCUIT TIME SERIES USING ARTIFICIAL NEURAL NETWORKS

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Abstract

In this paper we present the general problem of identifying if a nonlinear dynamic system has a chaotic behavior. If the answer is positive the system will be sensitive to small perturbations in the initial conditions which will imply that there is a chaotic attractor in its state space. A particular problem would be that of identifying a chaotic oscillator. We present an example of three well known different chaotic oscillators where we have knowledge of the equations that govern the dynamical systems and from there we can obtain the corresponding time series. In a similar example we assume that we only know the time series and, finally, in another example we have to take measurements in the Chua's circuit to obtain sample points of the time series. With the knowledge about the time series the phase plane portraits are plotted and from them, by visual inspection, it is concluded whether or not the system is chaotic. This method has the problem of uncertainty and subjectivity and for that reason a different approach is needed. A quantitative approach is the computation of the Lyapunov exponents. We describe several methods for obtaining them and apply a little known method of artificial neural networks to the different examples mentioned above. We end the paper discussing the importance of the Lyapunov exponents in the interpretation of the dynamic behavior of biological neurons and biological neural networks.

1 Introduction

In the companion paper [1] we described some findings about biological oscillators that have been presented in the recent literature. We also showed some examples of oscillator models. Here we want to review some models of chaotic oscillators with the goal of extending the analysis to time series (trains of action potentials) coming from biological oscillators where there are some hints that they are chaotic.

There are many experimental situations where there is no idea of what the mathematical model of a system could be or where the form of the equations is known but the parameters are unknown. There is an extensive literature about methods for systems identification but they are

usually limited to linear models. Since the conditions for chaotic behavior arise from the presence of nonlinear elements, the use of linear methods is limited.

In recent years there have been many advances in the understanding of nonlinear dynamic systems and that has produced many methods for identifying whether or not a given system is chaotic. For testing these methods various simple chaotic systems have been discovered or invented. In some of them the equations that govern the system are well known but in others only some sort of approximation is known. In the former case, it is possible to generate the corresponding time series with very high approximation, in the latter case, the measurements yield a sampled version of the corresponding time series. Having at hand the equations and the time series, or at least the time series, it is possible, in very different ways, to compute the asymptotic properties of the system. Two measures are used for this: the Lyapunov exponents in which a positive one indicates chaotic dynamics, and the attractor's topological dimension which indicates topological characteristics and is directly related to the number of non-negative Lyapunov exponents [2].

It is usual to ascertain the existence of chaotic dynamic by means of visual inspection of the phase plane portrait. However, such method presents a considerable amount of uncertainty and subjectiveness. Taking that into account, it is important to have a quantitative method like the one provided by the computation of the Lyapunov exponents.

2 Lyapunov Exponents

To determine if a system possess chaotic dynamics it is necessary to know if it is sensitive to small perturbations on the initial conditions. When this occurs it is then impossible to predict the final state of the system after a finite time. To be able of characterizing a chaotic attractor it is necessary to establish quantitative measures concerning the sensitivity to initial conditions. The spectrum of Lyapunov exponents gives a method of quantifying the dynamics. The Lyapunov exponents describe the average rate of growing or shrinking of small perturbations in different directions in the state space. When the attractor has at least one positive exponent then it has the property of being sensitive to the initial conditions and it is called a chaotic attractor.

There are several methods for computing the Lyapunov exponents. Wolf *et al.* [3] were the first in suggesting a method to compute them directly from the time series, without knowing the equations that govern the system's dynamics. Kurths and Herzel [4] proposed another algorithm. However, in these algorithms the estimations are sensitive to the number of observations, to the sampling frequency and to the noise in the observations [3]. Trying to avoid these problems, Gencay and Dechert [5] designed an algorithm that computes the m Lyapunov exponents from an unknown m-dimensional dynamic system directly from a few observations on the attractor, in such a way that the estimation is robust even for certain amount of noise. This algorithm is based on a result by Hornik *et al.* [6] in which they show that the m Lyapunov exponents of a diffeomorphism that is topologically conjugate to the process that generates the data, are also the m Lyapunov exponents of that process. To obtain a robust estimation considering both few observations on the attractor and the presence of noise, Gencay and Dechert [5] applied artificial neural networks with a cascade architecture. Such procedure is a non-parametric estimation that Hornik *et al.* [6] [7] have shown to be universal approximators, that is, they can asymptotically approximate a function and its derivatives.

3 Computation of the Lyapunov Exponents

The Lyapunov exponents are constants, except for a zero-measure set, and describe the direction of nearby paths that converge or diverge in the state space of a dynamic system. The Lyapunov exponents λ_i are defined as the logarithm of the eigenvalues μ_i $\forall$ $i = 1, 2, \cdots, m$ of the symmetric positive matrix

$$\Lambda_x = \lim_{t \to \infty} \left[Y(\mathbf{x}; t)^{tr} Y(\mathbf{x}; t) \right]^{1/2t}, \tag{1}$$

where the matrix Y is dependent on the differential equation that characterizes the dynamical system. A direct application of the above definition is not practical since the Y matrix grows exponentially due to the fast convergence of the columns in the direction of greater expansion. Using topological properties and an appropriate QR decomposition, the Lyapunov exponents are found by computing

$$\lambda_i = \frac{1}{\Delta t} \lim_{t \to \infty} \frac{1}{n} \sum_{j=0}^{n-1} \ln \left(R_{ii}^j \right), \tag{2}$$

where R_{ii} are the diagonal elements of the triangular matrix R.

An alternative to the aforementioned algorithm is the use of neural networks which are capable of recovering a nonlinear map from a time series of iterates [8]. Here an unknown function is estimated and then it is possible to compute the Lyapunov exponents using the properties of the dynamic system [5].
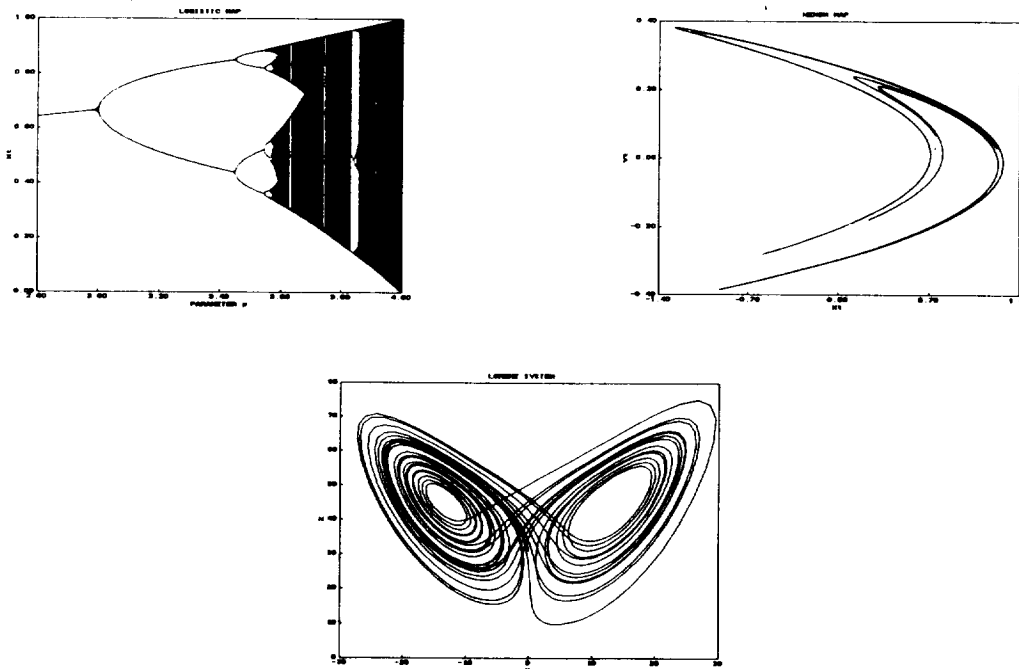

FIG. 1. Phase Plane Portraits for the Logistic Map, the Hénon Map, and the Lorenz System.

4 Examples of chaotic oscillators

To be able of testing the effectiveness of the Lyapunov exponents one has to have at hand dynamical systems with proved chaotic behavior. Many mathematical model systems are known, for instance: Hénon, Rossler-chaos, Lorenz, Rossler- hyperchaos, Mackey-Glass, and others [3]. Physical model systems are more difficult to produce, however we have the Belousov-Zhabotinsky chemical reaction [9] and Chua's nonlinear circuit family [10]. Obviously, there are real physical chaotic systems but they are extremely complex as it is the case of atmospheric turbulence.

TABLE I. True Lyapunov Exponents, equations representing the chaotic systems, initial conditions and parameters.

True Lyapunov Exponents		
Logistic map	Hénon map	Lorenz system
0.673	**0.440** **-1.620**	**1.51** **0.00** **-22.5**
$x_{t+1} = \mu x_t(1 - x_t)$	$x_t = 1 - ax_t^2 + y_t$ $y_t = bx_t$	$\dot{x} = a(x - y)$ $\dot{y} = x(b - z) - y$ $\dot{z} = xy - cz$
$x_0 = 0.3, \mu = 4.0$	$x_0 = 0.1, y_0 = 0.0$ $a = 1.4, b = 0.3$	$x_0 = 0.0, y_0 = 1.1, z_0 = 0.0$ $a = 16.0, b = 45.92, c = 4.0$

TABLE II. Estimated Lyapunov Exponents. Logistic Map ($q = 5$, $T = 100$). Hénon Map ($q = 10$, $T = 200$). Lorenz System ($q = 15$, $T = 1000$). The error is less than 1×10^{-3}. The non-spurious Lyapunov exponents are shown in boldface.

Estimated Lyapunov Exponents			
p	Logistic map	Hénon map	Lorenz system
1	**0.6794**		
2	**0.6401** -6.7823	**0.3670** **-1.5673**	
3	**0.6350** -2.4378 -2.4930	**0.4502** **-1.7331** -2.8164	**1.7285** **0.0411** **-23.72**
4	**0.6434** -1.61106 -1.7342 -5.0200	**0.4119** **-1.4803** -3.3658 -5.2263	**1.5910** **-0.0710** **-20.973** -80.325
5	**0.6790** -0.9073 -1.3544 -1.8468 -3.2313	**0.4385** **-1.5473** -1.4859 -1.7651 -2.5605	**1.4799** **0.0067** **-20.977** -60.702 -92.584

We divided this section of examples in three parts. In the first part the ordinary differential equations for the Lorenz model were integrated using the SDRIV2 subroutines form Kahaner *et al.* [12]. For the QR decomposition use used the subroutines in [13]. In the second and third parts we computed the Lyapunov exponents by means of the neural networks approach [5].

For the first part of the section we show the results of computing the Lyapunov exponents for mathematical model systems with well known chaotic dynamics [3] [5] [8]. We computed the Lyapunov exponents for the Logistic Map, for the Hénon map and for the Lorenz system [3] [5]. The corresponding phase plane portraits are shown in FIG. 1, and the equations, parameters and computed true values of the Lyapunov exponents are shown in TABLE I above.

For the second part of the section we show the results when we assume that for the same chaotic systems than above, the equations are not known, only the time series. In TABLE II we show the computed Lyapunov exponents where the presence of one positive exponent indicates that the system is chaotic.

According to the established notation for neural network architectures [11], p represents the number of nodes in the input layer and q represents the number of nodes in the hidden layer. The output layer has one node. The error is the quadratic average summation of the differences between the real and the estimated values for the time series, being T the total number of sample points in the sequence.

For the third part of the section we show the results obtained when we used a nonlinear circuit of the Chua's family with the parameters, components and initial conditions shown in FIG. 2. The temporal series was acquired by means of a digital storage scope, the x-coordinate is the voltage in the linear capacitor C1 and the y-coordinate is the voltage in the linear capacitor C2. A part of the phase plane portrait is also shown in FIG. 2, from it the temporal series was obtained using a sampling frequency of 500 Hz.
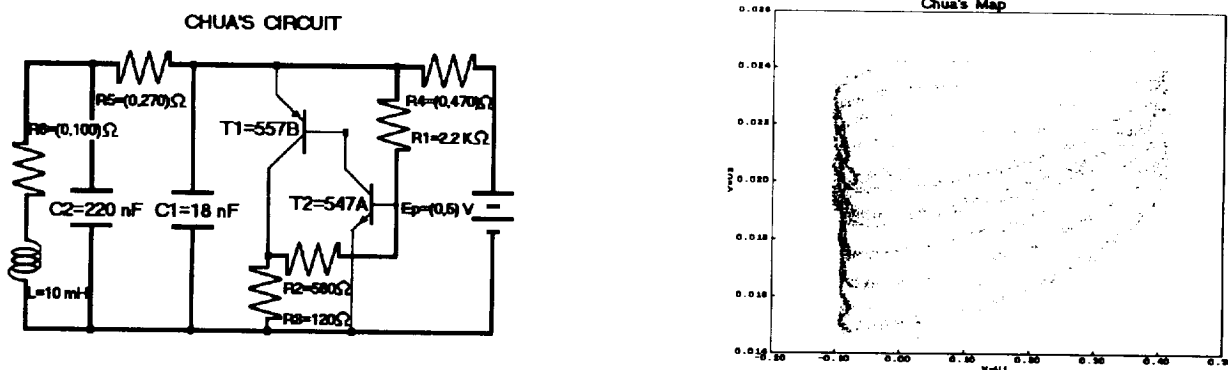
FIG. 2. Nonlinear Circuit of the Chua's Family and a part of its phase plane portrait that was plotted using as state variables the voltages in the capacitors C1 and C2. The phase plane portrait changes when the parameters in the circuit are varied between the limits denoted in the diagram.

The estimated Lyapunov exponents for the Chua's circuit are shown in TABLE III, when using the estimation for $q = 15$ and $T = 2500$. The error was less than 5×10^{-2}. Notice that λ_1 is a positive exponent which means that the dynamic behavior of the circuit is chaotic, as expected.

TABLE III. Estimated Lyapunov Exponents for the Chua's Circuit.

Estimated Lyapunov Exponents	
p	Chua's Circuit
3	$\lambda_1 = +4.07216$
	$\lambda_2 = -0.32160$
	$\lambda_3 = -3.58462$

5 Concluding Remarks

We have shown well known examples of mathematical models of chaotic attractors: Logistic, Hénon, and Lorenz. We also showed an electronic model of a chaotic attractor: a circuit of the Chua's family. In all these examples we computed the Lyapunov exponents as a measure of the system's sensitivity to small perturbations in the initial conditions. For the example where we know the equations we used the standard method; for the other two examples, we used the method of Gencay and Dechert [5] that applies a neuronal network algorithm. We went from the easier examples to the difficult one, that is, the Chua's circuit where the time series is obtained from direct measurements in the circuit. In the former examples the true values of the Lyapunov exponents are known whereas in the Chua's circuit the Lyapunov exponents are estimated and to this has to be added the differences or variations, for any reason, in the parameters for the circuit's components. The justification for such trouble is that in a real chaotic system there is a complexity even worse that in the electronic model. Therefore, the circuit provides a very valuable experience that afterwards can benefit the understanding of the real chaotic attractor.

Recent experimental evidence points to biological neurons and biological neural networks as very likely sources of chaotic attractors. As in the case of chaotic chemical reactions the biological significance given to such behavior is speculative [9] [14]. Nevertheless, the application of the techniques described in this paper might be very useful for interpreting data from neurophysiological experiments where the electrical activity from many neurons is recorded simultaneously.

Similar to Chua's circuit situation, due to the usual difficult conditions of neurophysiological experimentation, in a biological neural network we can only obtain a short duration record of the compound time series (train of action potentials). The individual time series have to be separated and that procedure produces and additional source of uncertainty and every tool available for interpreting the results is welcomed [15].

As a very simple example (for details see companion paper [1]) let us consider the rhythmic firing single neuron (1) shown in the upper plot in FIG. 3. This time series was obtained from the simulation of a mathematical model for a single neuron and two of its phase plane portraits for two different physiological parameters $(V - f, V - h)$ chosen as state variables show very clearly the possibility of chaotic behavior. In the lower plot in FIG. 3 we show another simulation of the rhythmic firing of a neuron (2) that belongs to a recurrent-ring network composed of single neurons like the ones given in (1). From the two phase plane portraits we cannot conclude that the neuron (2) in the network is chaotic and the conclusion about neuron (1) required of an expert. This ambiguity can be surmounted if the Lyapunov exponents are computed for these

time series and from there the importance of making such calculations and having experimental testing circuits for improving the confidence in the results.
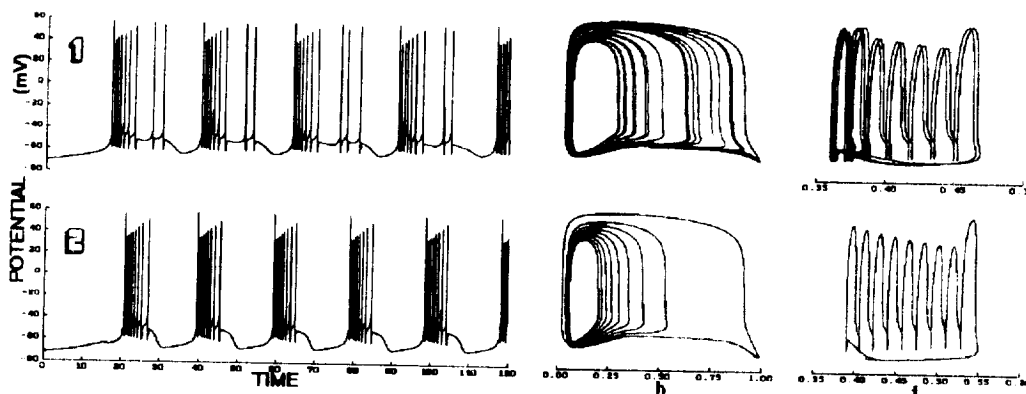
FIG. 3. *(1)* Rhytmically firing single neuron. *(2)* Rhytmically firing neuron belonging to a network formed with type *(1)* neurons.

On the other hand, in biological experiments there are problems similar to the ones present when making measurements in the Chua's circuit. When doing an extracellular recording, the duration of it is limited to a few minutes and afterwards a considerable amount of preprocessing is required to get to the individual contribution of each neuron recorded [16] [17]. The calculation of the Lyapunov exponents for these individual contributions could be added to help understanding the functional role of oscillatory neurons and oscillatory networks. That is the work that we are about to pursue.

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A METHOD OF SOLVING
SIMPLE HARMONIC OSCILLATOR SCHRÖDINGER
EQUATION.

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Abstract

A usual step in solving totally Schrödinger equation is to try first the case when dimensionless position independent variable w is large. In this case the Harmonic Oscillator equation takes the form $(d^2/dw^2 - w^2)F = 0$, and following $W.K.B.$ method, it gives the intermediate corresponding solution $F = \exp(-w^2/2)$, which actually satisfies exactly another equation, $(d^2/dw^2 + 1 - w^2)F = 0$.

We apply a different method, useful in anharmonic oscillator equations, similar to that of Rampal and Datta [1], and although it is slightly more complicated however it is also more general and systematic.

After some arrangements Schrödinger equation for a simple harmonic oscillator is set as in (1):

$$(d^2/du^2 + c_0 - c_2 u^2)N(u) = 0 \tag{1}$$

$$\hbar^2 c_0 = 2mE \qquad \hbar^2 c_2 = (m\omega_0)^2 \tag{2}$$

where c_0 and c_2 are the parameters of the differential equation, $u = x - a$ is the distance from the particle to the point where potential energy is a minimum, ω_0 is the classical angular frequency of the movement, E is the total energy and N is the probability amplitude for the particle to be found at u . In a very common procedure, (1) is first transformed to equation (3), in which w is a dimensionless independent variable, obtained by the mathematical manipulation (4):

$$(d^2/dw^2 + b - w^2)f(w) = o \tag{3}$$

$$w^2\hbar = m\omega_0 u^2 \qquad \hbar\omega_0 b = 2E \tag{4}$$

Some authors [2] get the solution of (3) for large w as a decaying exponential function of $w/2$, by means of the $W.K.B.$ method, which is a factor in the total wave function.

But others [3] simply propose the change of dependent variable (5) without mentioning the $W.K.B.$ method:

$$f = \exp(-w^2/2)P(w) \qquad (5)$$

And a few ones [4] consider that the dominant term, when w is large, is w^2 and they write (6) with $b = 0$ as an approximation of (3); and assert that (7) are its solutions:

$$(d^2/dw^2 - w^2)F = 0 \qquad (6)$$

$$F = \exp(\pm w^2/2) \qquad (7)$$

But after choosing the negative sign in (7), for the good behaviour of F, it is easy to demonstrate that (7) does not satisfy (6), and rather satisfies (3) when $b = 1$. We will use a method whose intermediate steps at all stages are correct.

Starting with (1), the Ansatz (8) is composed of two factors: P that gives information of the zeros of N, and G:

$$N = \exp(-G)P \qquad (8)$$

Non linear equation (9) is obtained from (8) and (1), with unknowns P and G:

$$[P'' - 2P'G'] + [(G')^2 - G'']P = [-c_0 + c_2 u^2]P \qquad (9)$$

$$[(G')^2 - G''] = -c_0(0) + c_2 u^2 \qquad (10)$$

(' means derivative with respect to u).

If P is an n degree polynomial P_n, then for $n = 0$, P_0 is a constant, and (10) is a non-linear equation with only one unknown. By watching (10) it is noticed that (11) is the solution of (10) if constraints (12) hold:

$$G = \beta u^2 \qquad (11)$$

$$4\beta^2 = c_2 \qquad 2\beta = c_0(0) \qquad (12)$$

The first eigenvalue $E(0)$ can be obtained from (2) and (12). Consequently, (13) is the solution of the Schrödinger equation for $n = 0$; βu^2 as the argument of the exponential function must be dimensionless:

$$N = f_0 = P_0 \exp(-\beta u^2) \qquad (13)$$

Therefore w becomes a dimensionless variable and (1) is transformed into (7), and taking into account (12):

$$w^2 = \alpha\beta u^2 \qquad (14)$$

$$[d^2/dw^2 + c_0(n)/\alpha\beta - 4w^2/\alpha^2]f_n(w) = 0 \qquad (15)$$

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(15) is precisely (3), with $b(n) = c_0(n)/\alpha\beta$, and $b(0) = c_0(o)/\alpha\beta = 2/\alpha$.(16) is the correct solution of (15) and (17) is the differential equation of the polynomial P_n:

$$N_n = P_n \exp(-w^2/2) \tag{16}$$

$$[d^2/dw^2 - (4w/\alpha)d/dw + 2(b-1)/\alpha]P_n = 0 \tag{17}$$

For $\alpha = 2$ and $b(n) = 2n + 1$, (17) is the equation of Hermite, and $P_n = H_n$ are Hermite's polynomials. The energy eigenvalues can easily be obtained.

The Simple Harmonic Oscillator Schrödinger equation is perhaps the known differential equation with the most accurate solution. It would not be worthy to obtain that solution again, if methodological aspects are not taken into account. If a physicist plans to work in problems related to differential equations, it is useful to give her (him) general and powerful methods. As the Simple Harmonic Oscillator is the first approximation to many physical models, and one of the first problems with which the students are put into contact, it is good to take advantage of methods that can be used in better approximations to more complex physical models, and more exact formulations, as relativistic ones for instance. The author has made a review of the relativistic and non- relativistic isotropic harmonic oscillators, and uniform magnetic fields [5], using this method. With polar coordinates and centrifugal potentials, other polynomials depending on two quantum numbers, and one extra factor are the solutions of the radial equations. First the author had used the method in solving anharmonic rectilinear oscillators, and anharmonic isotropic oscillator equations [6], and continues working further these topics.In all those cases mentioned, and here, we consider that writing equations (9) and (10), is the most important step that permits to find the solution for large w, and the independent dimensionless variable.

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WIGNER DISTRIBUTION FUNCTION AND ENTROPY
OF THE DAMPED HARMONIC OSCILLATOR
WITHIN THE THEORY OF OPEN QUANTUM SYSTEMS

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(Presented by G. Nemes)

Abstract

The harmonic oscillator with dissipation is studied within the framework of the Lindblad theory for open quantum systems. By using the Wang-Uhlenbeck method, the Fokker-Planck equation, obtained from the master equation for the density operator, is solved for the Wigner distribution function, subject to either the Gaussian type or the δ-function type of initial conditions. The obtained Wigner functions are two-dimensional Gaussians with different widths. Then a closed expression for the density operator is extracted. The entropy of the system is subsequently calculated and its temporal behaviour shows that this quantity relaxes to its equilibrium value.

1 Introduction

In the last two decades, the problem of dissipation in quantum mechanics, i.e. the consistent description of open quantum systems, was investigated by various authors [1, 2, 3, 4, 5]. Because dissipative processes imply irreversibility and, therefore, a preferred direction in time, it is generally thought that quantum dynamical semigroups are the basic tools to introduce dissipation in quantum mechanics. In the Markov approximation the most general form of the generators of such semigroups was given by Lindblad [6]. This formalism has been studied for the case of damped harmonic oscillators [7, 8, 9] and applied to various physical phenomena, for instance, the damping of collective modes in deep inelastic collisions in nuclear physics [10] and the interaction of a two-level atom with the electromagnetic field [11].

In the present work, also dealing with the damping of the harmonic oscillator within the Lindblad theory for open quantum systems, we will explore the physical aspects of the Fokker-Planck equation which is the c-number equivalent equation to the master equation for the density operator. Generally the master equation gains considerably in clarity if it is represented in terms of the Wigner distribution function which satisfies the Fokker-Planck equation. It is worth mentioning that these master and Fokker-Planck equations agree in form with the corresponding equations formulated in quantum optics [12, 13, 14, 15, 16].

The content of the paper is arranged as follows. In Sec. 2 we review the derivation of the master equation of the harmonic oscillator. In Sec. 3 we transform the master equation into the Fokker-Planck equation by means of the well-known methods [17, 18, 19]. Then the Fokker-Planck equation for the Wigner distribution, subject to either the Gaussian type or the δ-function type of initial conditions, is solved by the Wang-Uhlenbeck method. Sec. 4 derives an explicit form of the density operator involved in the Lindblad master equation, formulates the entropy using the explicit form of the density operator and discusses its temporal behaviour. Finally, concluding remarks are given in Sec. 5.

2 Master equation for the damped harmonic oscillator

The rigorous formulation for introducing the dissipation into a quantum mechanical system is that of quantum dynamical semigroups [2, 3, 6]. According to the axiomatic theory of Lindblad [6], the usual von Neumann-Liouville equation ruling the time evolution of closed quantum systems is replaced in the case of open systems by the following equation for the density operator ρ:

$$\frac{d\Phi_t(\rho)}{dt} = L(\Phi_t(\rho)). \tag{1}$$

Here, Φ_t denotes the dynamical semigroup describing the irreversible time evolution of the open system in the Schrödinger representation and L the infinitesimal generator of the dynamical semi-group Φ_t. Using the structural theorem of Lindblad [6] which gives the most general form of the bounded, completely dissipative Liouville operator L, we obtain the explicit form of the most general time-homogeneous quantum mechanical Markovian master equation:

$$\frac{d\rho(t)}{dt} = L(\rho(t)) = -\frac{i}{\hbar}[H, \rho(t)] + \frac{1}{2\hbar}\sum_j([V_j\rho(t), V_j^+] + [V_j, \rho(t)V_j^+]). \tag{2}$$

Here H is the Hamiltonian of the system and the operators V_j and V_j^+ are bounded operators on the Hilbert space of the Hamiltonian.

We should like to mention that the Markovian master equations found in the literature are of this form after some rearrangement of terms, even for unbounded Liouville operators. In this connection we assume that the general form of the master equation given by (2) is also valid for unbounded Liouville operators.

In this paper we impose a simple condition to the operators H, V_j, V_j^+ that they are functions of the basic observables $\hat{q}$ and $\hat{p}$ of the one-dimensional quantum mechanical system (with $[\hat{q}, \hat{p}] = i\hbar$) of such kind that the obtained model is exactly solvable. A precise version for this last condition is that linear spaces spanned by first degree (respectively second degree) noncommutative polynomials in $\hat{q}$ and $\hat{p}$ are invariant to the action of the completely dissipative mapping L. This condition implies [7] that V_j are at most first degree polynomials in $\hat{q}$ and $\hat{p}$ and H is at most a second degree polynomial in $\hat{q}$ and $\hat{p}$. Then the harmonic oscillator Hamiltonian H is chosen of the form

$$H = H_0 + \frac{\mu}{2}(\hat{q}\hat{p} + \hat{p}\hat{q}), \quad H_0 = \frac{1}{2m}\hat{p}^2 + \frac{m\omega^2}{2}\hat{q}^2. \tag{3}$$

With these choices the Markovian master equation can be written [8]:

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H_0, \rho] - \frac{i}{2\hbar}(\lambda + \mu)[\hat{q}, \rho\hat{p} + \hat{p}\rho] + \frac{i}{2\hbar}(\lambda - \mu)[\hat{p}, \rho\hat{q} + \hat{q}\rho]$$
$$-\frac{D_{pp}}{\hbar^2}[\hat{q}, [\hat{q}, \rho]] - \frac{D_{qq}}{\hbar^2}[\hat{p}, [\hat{p}, \rho]] + \frac{D_{pq}}{\hbar^2}([\hat{q}, [\hat{p}, \rho]] + [\hat{p}, [\hat{q}, \rho]]), \tag{4}$$

where D_{pp}, D_{qq} and D_{pq} are the diffusion coefficients and λ the friction constant. They satisfy the following fundamental constraints [8]:

$$\text{i) } D_{pp} > 0, \quad \text{ii) } D_{qq} > 0, \quad \text{iii) } D_{pp}D_{qq} - D_{pq}^2 \geq \frac{\lambda^2\hbar^2}{4}. \tag{5}$$

In the particular case when the asymptotic state is a Gibbs state

$$\rho_G(\infty) = e^{-\frac{H_0}{kT}}/\text{Tr}e^{-\frac{H_0}{kT}}, \tag{6}$$

these coefficients reduce to

$$D_{pp} = \frac{\lambda + \mu}{2}\hbar m\omega \coth\frac{\hbar\omega}{2kT}, \quad D_{qq} = \frac{\lambda - \mu}{2}\frac{\hbar}{m\omega}\coth\frac{\hbar\omega}{2kT}, \quad D_{pq} = 0, \tag{7}$$

where T is the temperature of the thermal bath.

3 Wigner distribution function

One useful way to study the consequences of the master equation (4) for the density operator of the one-dimensional damped harmonic oscillator is to transform it into more familiar forms, such as the equations for the c-number quasiprobability distributions Glauber P, antinormal ordering Q and Wigner W associated with the density operator [20]. In this case the resulting differential equations of the Fokker-Planck type for the distribution functions can be solved by standard methods [17, 19, 21] employed in quantum optics and observables directly calculated as correlations of these distribution functions.

The Fokker-Planck equation, obtained from the master equation and satisfied by the Wigner distribution function $W(x_1, x_2, t)$ of real variables x_1, x_2 corresponding to the operators $\hat{q}, \hat{p}$

$$x_1 = \sqrt{\frac{m\omega}{2\hbar}}q, \quad x_2 = \frac{1}{\sqrt{2\hbar m\omega}}p, \tag{8}$$

has the form [20]:

$$\frac{\partial W}{\partial t} = \sum_{i,j=1,2} A_{ij}\frac{\partial}{\partial x_i}(x_j W) + \frac{1}{2}\sum_{i,j=1,2} Q_{ij}^W\frac{\partial^2}{\partial x_i\partial x_j}W, \tag{9}$$

where

$$A = \begin{pmatrix} \lambda - \mu & -\omega \\ \omega & \lambda + \mu \end{pmatrix}, \quad Q^W = \frac{1}{\hbar}\begin{pmatrix} m\omega D_{qq} & D_{pq} \\ D_{pq} & D_{pp}/m\omega \end{pmatrix}. \tag{10}$$

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Since the drift coefficients are linear in the variables x_1 and x_2 and the diffusion coefficients are constant with respect to x_1 and x_2, Eq. (9) describes an Ornstein-Uhlenbeck process [22, 23]. Following the method developed by Wang and Uhlenbeck [23], we shall solve this Fokker-Planck equation, subject to either the wave-packet type or the δ-function type of initial conditions.

1) When the Fokker-Planck equation is subject to a Gaussian (wave-packet) type of the initial condition (x_{10} and x_{20} are the initial values of x_1 and x_2 at $t = 0$, respectively)

$$W_w(x_1, x_2, 0) = \frac{1}{\pi\hbar} \exp\{-2[(x_1 - x_{10})^2 + (x_2 - x_{20})^2]\}, \tag{11}$$

the solution is found to be

$$W_w(x_1, x_2, t) = \frac{\Omega}{\pi\hbar\omega\sqrt{|B_w|}} \exp\{-\frac{1}{B_w}[\phi_w(x_1 - \bar{x}_1)^2 + \psi_w(x_2 - \bar{x}_2)^2 + \chi_w(x_1 - \bar{x}_1)(x_2 - \bar{x}_2)]\}, \tag{12}$$

where

$$B_w = g_1 g_2 - \frac{1}{4}g_3^2, \quad g_1 = g_2^* = \frac{\mu a}{\omega}e^{2\Lambda t} + \frac{d_1}{\Lambda}(e^{2\Lambda t} - 1), \quad g_3 = 2[e^{-2\lambda t} + \frac{d_2}{\lambda}(1 - e^{-2\lambda t})], \tag{13}$$

$$\phi_w = g_1 a^{*2} + g_2 a^2 - g_3, \quad \psi_w = g_1 + g_2 - g_3, \quad \chi_w = 2(g_1 a^* + g_2 a) - g_3(a + a^*). \tag{14}$$

We have put $a = (\mu - i\Omega)/\omega$, $\Lambda = -\lambda - i\Omega$ and $d_1 = (a^2 m\omega D_{qq} + 2aD_{pq} + D_{pp}/m\omega)/\hbar$, $d_2 = (m\omega D_{qq} + 2\mu D_{pq}/\omega + D_{pp}/m\omega)/\hbar$ and $\Omega^2 = \omega^2 - \mu^2$. The functions $\bar{x}_1$ and $\bar{x}_2$, which are also oscillating functions, are given by

$$\bar{x}_1 = e^{-\lambda t}[x_{10}(\cos\Omega t + \frac{\mu}{\Omega}\sin\Omega t) + x_{20}\frac{\omega}{\Omega}\sin\Omega t], \tag{15}$$

$$\bar{x}_2 = e^{-\lambda t}[x_{20}(\cos\Omega t - \frac{\mu}{\Omega}\sin\Omega t) - x_{10}\frac{\omega}{\Omega}\sin\Omega t]. \tag{16}$$

2) If the Fokker-Planck equation (9) is subject to the δ-function type of initial condition, the Wigner distribution function is given by

$$W(x_1, x_2, t) = \frac{\Omega}{\pi\hbar\omega\sqrt{|B|}} \exp\{-\frac{1}{B}[\phi_d(x_1 - \bar{x}_1)^2 + \psi_d(x_2 - \bar{x}_2)^2 + \chi_d(x_1 - \bar{x}_1)(x_2 - \bar{x}_2)]\}, \tag{17}$$

where

$$B = f_1 f_2 - f_3^2, \quad f_1 = f_2^* = \frac{d_1}{\Lambda}(e^{2\Lambda t} - 1), \quad f_3 = \frac{d_2}{\lambda}(1 - e^{-2\lambda t}), \tag{18}$$

$$\phi_d = f_1 a^{*2} + f_2 a^2 - 2f_3, \quad \psi_d = f_1 + f_2 - 2f_3, \quad \chi_d = 2[f_1 a^* + f_2 a - f_3(a + a^*)]. \tag{19}$$

So, the Wigner functions are 2-dimensional Gaussian distributions with the average values $\bar{x}_1$ and $\bar{x}_2$ and different widths.

When time $t \to \infty$, $\bar{x}_1$ and $\bar{x}_2$ vanish and we obtain the steady state solution:

$$W(x_1, x_2) = \frac{1}{2\pi\sqrt{\det\sigma^W(\infty)}} \exp[-\frac{1}{2}\sum_{i,j=1,2}(\sigma^W)_{ij}^{-1}(\infty)x_i x_j]. \tag{20}$$

The stationary covariance matrix $\sigma^W(\infty)$ can be determined from the algebraic equation

$$A\sigma^W(\infty) + \sigma^W(\infty)A^T = Q^W. \tag{21}$$

4 Entropy and effective temperature

Entropy is a quantity which may be visualized physically as a measure of the lack of knowledge of the system. When we denote by $\rho(t)$ the density operator in the Schrödinger picture for the harmonic oscillator, the entropy $S(t)$ is given by

$$S(t) = -k\mathrm{Tr}(\rho \ln \rho). \tag{22}$$

For calculating the entropy we shall compute straightway the expectation value of the logarithmic operator $< \ln \rho > = \mathrm{Tr}(\rho \ln \rho)$. Accordingly, the problem amounts to derive the explicit form of the density operator for the damped harmonic oscillator.

To get the explicit expression for the density operator, we use the relation $\rho = 2\pi\hbar\mathbf{N}\{W_s(q,p)\}$, where W_s is the Wigner distribution function in the form of standard rule of association and $\mathbf{N}$ is the normal ordering operator [17, 24] which acting on the function $W_s(q,p)$ moves all p to the right of the q. By the standard rule of association is meant the correspondence $p^m q^n \to \hat{q}^n \hat{p}^m$ between functions of two classical variables (q,p) and functions of two quantum mechanical canonical operators $(\hat{q}, \hat{p})$. The calculation of the density operator is then reduced to a problem of transformation of the Wigner distribution function by the $\mathbf{N}$ operator, provided that W_s is known. A special care is necessary for the $\mathbf{N}$ operation when the Wigner function is in the exponential form of a second order polynomial of q and p. The Wigner distribution function previously obtained corresponds however to the form of the Weyl rule of association [25]. The solution (12) of the Fokker-Planck equation (9), subject to the wave-packet type of initial condition (11) can be written in terms of the coordinate and momentum as:

$$W(q,p,t) = \frac{1}{2\pi\sqrt{\delta}}\exp\{-\frac{1}{2\delta}[\phi(q- < \hat{q} >)^2 + \psi(p- < \hat{p} >)^2 - 2\chi(q- < \hat{q} >)(p- < \hat{p} >)]\}, \tag{23}$$

where

$$< \hat{q} > = \sqrt{\frac{2\hbar}{m\omega}}x_1, \quad < \hat{p} > = \sqrt{2\hbar m\omega}x_2, \tag{24}$$

$$\varphi \equiv \sigma_{pp} = < \hat{q}^2 > - < \hat{q} >^2 = -\frac{\hbar\omega^2}{4\Omega^2}\frac{1}{m\omega}\psi_w, \tag{25}$$

$$\psi \equiv \sigma_{qq} = < \hat{p}^2 > - < \hat{p} >^2 = -\frac{\hbar\omega^2}{4\Omega^2}m\omega\phi_w. \tag{26}$$

$$\chi \equiv \sigma_{pq}(t) = \frac{1}{2} < \hat{q}\hat{p} + \hat{p}\hat{q} > - < \hat{q} >< \hat{p} > = \frac{\hbar\omega^2}{8\Omega^2}\chi_w, \quad \delta = \phi\psi - \chi^2 \tag{27}$$

and $< \hat{A} > = \mathrm{Tr}(\rho\hat{A})$ denotes the expectation value of an operator $\hat{A}$. The Wigner distribution function (23) can be transformed into the form of standard rule of association [26] by

$$W_s(q,p) = \exp(\frac{1}{2}i\hbar\frac{\partial^2}{\partial p\partial q})W(q,p). \tag{28}$$

Upon performing the operation on the right-hand side, we get the Wigner distribution function W_s, which has the same form as the original W multiplied by $\hbar$ but with $\chi - i\hbar/2$ in place of χ. The normal ordering operation of the Wigner function W_s in Gaussian form can be carried out by applying McCoy theorem [24, 27, 28]. The explicit form of the density operator is the following:

$$\rho = \frac{\hbar}{\sqrt{\xi}} \exp\left[\frac{1}{2} \ln \frac{\xi}{\xi - i\hbar\chi'} - \frac{1}{2\hbar\sqrt{\xi - i\hbar\chi' + \frac{1}{4}\hbar^2}} \cosh^{-1}(1 + \frac{\hbar^2}{2(\xi - i\hbar\chi')}) \right.$$

$$\times \left\{\phi(\hat{q} - <\hat{q}>)^2 + \psi(\hat{p} - <\hat{p}>)^2 - (\chi' + i\frac{\hbar}{2})[2(\hat{q} - <\hat{q}>)(\hat{p} - <\hat{p}>) - i\hbar]\right\}], \qquad (29)$$

where

$$\xi = \phi\psi - \chi'^2, \quad \chi' = \chi - i\frac{\hbar}{2}. \qquad (30)$$

The density operator (29) is in a Gaussian form, as was expected from the initial form of the Wigner distribution function. While the density operator is expressed in terms of operators $\hat{q}$ and $\hat{p}$, the Wigner distribution is a function of real variables q and p. When time t goes to infinity, the density operator approaches to

$$\rho(\infty) = \frac{\hbar}{\sqrt{\sigma - \frac{\hbar^2}{4}}} \exp\left[-\frac{1}{2\hbar\sqrt{\sigma}} \ln \frac{2\sqrt{\sigma} + \hbar}{2\sqrt{\sigma} - \hbar} [\sigma_{pp}(\infty)\hat{q}^2 + \sigma_{qq}(\infty)\hat{p}^2 - \sigma_{pq}(\infty)(\hat{q}\hat{p} + \hat{p}\hat{q})], \qquad (31)$$

where $\sigma = \sigma_{pp}(\infty)\sigma_{qq}(\infty) - \sigma_{pq}^2(\infty)$ and [8]:

$$\sigma_{pp}(\infty) = \frac{1}{2\lambda(\lambda^2 + \omega^2 - \mu^2)}((m\omega)^2\omega^2 D_{qq} + (2\lambda(\lambda - \mu) + \omega^2)D_{pp} - 2m\omega^2(\lambda - \mu)D_{pq}), \qquad (32)$$

$$\sigma_{qq}(\infty) = \frac{1}{2(m\omega)^2\lambda(\lambda^2 + \omega^2 - \mu^2)}((m\omega)^2(2\lambda(\lambda + \mu) + \omega^2)D_{qq} + \omega^2 D_{pp} + 2m\omega^2(\lambda + \mu)D_{pq}), \qquad (33)$$

$$\sigma_{pq}(\infty) = \frac{1}{2m\lambda(\lambda^2 + \omega^2 - \mu^2)}(-(\lambda + \mu)(m\omega)^2 D_{qq} + (\lambda - \mu)D_{pp} + 2m(\lambda^2 - \mu^2)D_{pq}). \qquad (34)$$

In the particular case (7)

$$\sigma_{qq}(\infty) = \frac{\hbar}{2m\omega} \coth \frac{\hbar\omega}{2kT}, \quad \sigma_{pp}(\infty) = \frac{\hbar m\omega}{2} \coth \frac{\hbar\omega}{2kT}, \quad \sigma_{pq}(\infty) = 0 \qquad (35)$$

and the asymptotic state is a Gibbs state (6):

$$\rho_G(\infty) = 2\sinh \frac{\hbar\omega}{2kT} \exp\left[-\frac{1}{kT}(\frac{1}{2m}\hat{p}^2 + \frac{m\omega^2}{2}\hat{q}^2)\right]. \qquad (36)$$

Because of the presence of the exponential form in the density operator, the construction of the logarithmic density is straightforward. In view of the relations (25-27), the expectation value of the logarithmic density becomes

$$< \ln \rho > = \ln \hbar - \frac{1}{2} \ln(\delta - \frac{\hbar^2}{4}) - \frac{\sqrt{\delta}}{\hbar} \ln \frac{2\sqrt{\sigma} + \hbar}{2\sqrt{\sigma} - \hbar}. \tag{37}$$

By putting $\hbar\nu = \sqrt{\delta} - \hbar/2$, we finally get the entropy in a closed form:

$$S(t) = k[(\nu + 1)\ln(\nu + 1) - \nu \ln \nu]. \tag{38}$$

It is worth noting that the entropy depends only upon the variance of the Wigner distribution. When time $t \to \infty$, the function ν goes to $s = \omega(d_2^2/\lambda^2 - |d_1|^2/(\lambda^2 + \Omega^2))^{1/2}/2\Omega - 1/2$ and the entropy relaxes to its equilibrium value $S(\infty) = k[(s + 1)\ln(s + 1) - s \ln s]$. It should also be noted that the expression (38) has the same form as the entropy of a system of harmonic oscillators in thermal equilibrium. In the later case ν represents, of course, the average of the number operator [29]. While the formal expression (38) for the entropy has a well-known appearance, the form of the function ν displays clearly a specific feature of the present entropy. We see that the time dependence of the entropy is represented by the damping factor $\exp(-2\lambda t)$ and also by the oscillating function $\sin^2(\Omega t)$. The entropy relaxes to its equilibrium value $S(\infty)$.

5   Concluding remarks

Recently we assist to a revival of interest in quantum Brownian motion as a paradigm of quantum open systems. There are many motivations. The possibility of preparing systems in macroscopic quantum states led to the problems of dissipation in tunneling and of loss of quantum coherence (decoherence). These problems are intimately related to the issue of quantum-to-classical transition. All of them point the necessity of a better understanding of open quantum systems and all requires the extension of the model of quantum Brownian motion. The Lindblad theory provides a selfconsistent treatment of damping as a possible extension of quantum mechanics to open systems. In the present paper we have studied the one-dimensional harmonic oscillator with dissipation within the framework of this theory. From the master equation of the damped quantum oscillator we have derived the corresponding Fokker-Planck equation in the Wigner W representation. The obtained equation describes an Ornstein-Uhlenbeck process. By using the Wang-Uhlenbeck method we have solved this equation for the Wigner function, subject to either the Gaussian type or the δ-function type of initial conditions and showed that the Wigner functions are two-dimensional Gaussians with different widths. Then we have obtained the density operator. The density operator in a Gaussian form is a function of $\hat{q}, \hat{p}$ in addition to several time dependent factors. The explicit form of the density operator has been subsequently used to calculate the entropy. It relaxes to its equilibrium value.

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The relativistic many body problem with an oscillator interaction

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Abstract

We start with the total energy E for a system of three scalar relativistic particles that, because of Einstein's relation, will have square roots of functions of the momenta. By taking powers of this relation, we finally get a fourth degree polynomial in E^2, where the square roots have disappeared, and which we can convert into a type of Schroedinger equation. To be in the center of mass frame we pass to Jacobi momenta and then replace them by creation and annihilation operators. We thus get an equation in terms of the generators of a U(2) group, which, in principle, we can solve in an elementary way. Finally we rewrite our equation in a Poincaré invariant form.

1 Introduction

In the II Harmonic Oscillator Conference I presented a paper dealing with systems of relativistic particles interacting through Dirac oscillators. The results were later applied to the mass spectra of baryons and mesons [1,2,3].

As all the results presented had already been published I prefer to deal in this paper with a new approach, restricted here to scalar particles, that seems to me a systematic way to attack many body problems with oscillator interactions.

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I will start by considering a non relativistic problem of n free particles and indicate the steps by which later it can be reduced to a system with oscillator interactions, which will serve as a model for the relativistic problem we wish to analyze.

2   The non-relativistic problem

Let us first start with a system of n free non-relativistic particles of the same mass m, and take units

$$\hbar = m = c = 1, \tag{2.1},$$

where the velocity of light will appear only in the next section, but we want to start from the beginning with units in which everything is dimensionless.

The classical total energy is then

$$E = (1/2) \sum_{s=1}^{n} \mathbf{p}_s \cdot \mathbf{p}_s \tag{2.2}$$

where $\mathbf{p}_s$ are the three dimensional classical momentum vectors of particle s.

From the beginning we would like to work in the center of mass frame, because our interest will be the internal energy of the system and not the contribution from its center of mass motion. The best way to achieve this is to pass to Jacobi coordinates [4] defined by the orthogonal transformation

$$\mathbf{p}'_s = [s(s+1)]^{-\frac{1}{2}} \left[\sum_{t=1}^{s} \mathbf{p}_t - s\mathbf{p}_{s+1} \right], s = 1, 2, \ldots n - 1, \tag{2.3a}$$

$$\mathbf{p}'_n = n^{-\frac{1}{2}} \sum_{t=1}^{s} \mathbf{p}_s, \tag{2.3b}$$

Clearly $\mathbf{p}'_n$ is proportional to the total momentum and in the center of mass system it will vanish, so Eq. (2.2) reduces to

$$E = \tfrac{1}{2} \sum_{s=1}^{n-1} \mathbf{p}'_s \cdot \mathbf{p}'_s \tag{2.4}$$

The Schroedinger equations corresponding to (2.4) is obtained when we replace $\mathbf{p}'_s$ by the operator

$$\mathbf{p}'_s = \frac{1}{i} \frac{\partial}{\partial \mathbf{x}'_s}, \tag{2.5}$$

with $\mathbf{x}'_s$ being the corresponding Jacobi coordinate vector. As the $\mathbf{p}'_s$ are hermitian operators we can also write Schroedinger equation as

$$\frac{1}{2} \sum_{s=1}^{n-1} \left(\mathbf{p}'^{\dagger}_s \cdot \mathbf{p}'_s \right) \psi = E\psi \tag{2.6}$$

We can easily transform this into an hermitian oscillator operator equation if we make the replacement

$$\mathbf{p}'_s \to \mathbf{p}'_s - i\omega\mathbf{x}'_s, \tag{2.7a}$$

$$\mathbf{p}'^{\dagger}_s \to \mathbf{p}'_s + i\omega\mathbf{x}'_s, \tag{2.7b}$$

where the second equation follows from the first as *both* $\mathbf{p}'_s, \mathbf{x}'_s$ are hermitian operators.

Thus we now get a Schroedinger equation of the form

$$\frac{1}{2} \sum_{s=1}^{n-1} \left[p'^2_s + \omega^2 x'^2_s - (3/2)\omega(n-1) \right] \psi = E\psi, \tag{2.8}$$

whose eigenvalue for the energy E will be

$$E = \omega N, \tag{2.9}$$

with N being the total number of quanta *i.e.*

$$N = \sum_{s=1}^{n-1} \nu_s. \tag{2.10}$$

The previous analysis is standard except for the fact that we start from a system of n free particles. Furthermore our notation in terms of three vectors and Jacobi coordinates, avoids the worry about the Galilean invariance of the whole procedure. We will now consider a similar set of steps for a relativistic problem.

3   The system of three relativistic particles

Rather than discuss the system of n relativistic particles, we shall restrict ourselves to $n = 3$, as we will see that the case is general enough, with only the algebraic steps becoming more complicated as n increases.

In our units the total energy for a system of three free relativistic particles can be written as

$$E = \pm\Pi_1 \pm \Pi_2 \pm \Pi_3, \tag{3.1}$$

where $\Pi_s, s = 1, 2, 3$ is defined as

$$\Pi_s = (p_s^2 + 1)^{\frac{1}{2}}. \tag{3.2}$$

It is very important to note that, in our units, Einstein relation is $E^2 = p^2 + 1$, and when reduced to the E itself gives both the square root in (3.2) and the $\pm$ signs in (3.1).

Obviously we can not get a Schroedinger equation from the relation (3.1), but we can take $\pm\Pi_3$ to the right hand side and square both sides. Then we can square again and again appropriately, and we easily arrive at the fact that (3.1) becomes an eight degree equation in E (actually of fourth degree in E^2) of the form

$$\Phi(E^2, \Pi_s^2) \equiv$$

$$E^8 - 4AE^6 + (4A^2 + 2B)E^4 - (4C^2 + 4AB)E^2 + B^2 = 0 \tag{3.3}$$

where A, B, C are functions of $\Pi_s^2, s = 1, 2, 3$ given by

$$A \equiv \Pi_1^2 + \Pi_2^2 + \Pi_3^2, \tag{3.4a}$$

$$B \equiv \Pi_1^4 + \Pi_2^4 + \Pi_3^4 - 2\Pi_1^2\Pi_2^2 - 2\Pi_2^2\Pi_3^2 - 2\Pi_1^2\Pi_3^2, \tag{3.4b}$$

$$C^2 \equiv 16\Pi_1^2\Pi_2^2\Pi_3^2. \tag{3.4c}$$

Now we can write an equation that does not have E as an eigenvalue, but in which it appears as a parameter, if we replace $\mathbf{p}_s$ by $-i\partial/\partial \mathbf{x}_s$ as in (2.5), so that Π_s^2 become the operators

$$\hat{\Pi}_s^2 = (-\nabla_s^2 + 1), \tag{3.5}$$

and we get

$$\Phi(E^2, \hat{\Pi}_s^2)\psi = 0 \tag{3.6}$$

Thus far we have obtained nothing useful because $\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3$ considered as operators of the form (2.5), commute with the operator Φ and so are integrals of motion, so that ψ can be written as

$$\psi = \exp[i(\mathbf{p}_i \cdot \mathbf{x}_1 + \mathbf{p}_2 \cdot \mathbf{x}_2 + \mathbf{p}_3 \cdot \mathbf{x}_3)], \tag{3.7}$$

where now $\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3$ are ordinary numbers and we are returned to equation (3.3) whose eight roots for the energy E are obviously given by (3.1) with all the possible combination of the signs $\pm$.

Before proceeding further, along the lines of the previous section, we again remark that we would like to work in the center of mass frame, as our interest is restricted to the internal energy of the system. Thus we go, as in section 2, to the Jacobi momenta $\mathbf{p}'_s, s = 1, 2, 3$ which from (2.3) are given now by the matrix relation

$$
\begin{pmatrix} \mathbf{p}'_1 \\ \mathbf{p}'_2 \\ \mathbf{p}'_3 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & -\sqrt{\frac{2}{3}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{pmatrix} \begin{pmatrix} \mathbf{p}_1 \\ \mathbf{p}_2 \\ \mathbf{p}_3 \end{pmatrix} .
\tag{3.8}
$$

As the matrix is orthogonal, transposing it we get $\mathbf{p}_s$ in terms of $\mathbf{p}'_s$, and as we want to be in the center of mass frame $\mathbf{p}'_3 = 0$, so we get finally

$$
\mathbf{p}_1 = \frac{1}{\sqrt{2}}\mathbf{p}'_1 + \frac{1}{\sqrt{6}}\mathbf{p}'_2, \mathbf{p}'_2 = \frac{1}{\sqrt{2}}\mathbf{p}'_1 - \frac{1}{\sqrt{6}}\mathbf{p}'_2, \mathbf{p}_3 = -\sqrt{\frac{2}{3}}\mathbf{p}'_2,
\tag{3.9}
$$

As Eq. (3.6) contains only powers of $\hat{\Pi}^2_s, s = 1, 2, 3$, we can write the latter using the hermitian property of $\mathbf{p}'_s$, now considered as operators of the type (2.6), as

$$
\hat{\Pi}^2_1 = \frac{1}{2}\mathbf{p}'^\dagger_1 \cdot \mathbf{p}'_1 + \frac{1}{6}\mathbf{p}'^\dagger_2 \cdot \mathbf{p}'_2 + \frac{1}{2\sqrt{3}}(\mathbf{p}'^\dagger_1 \cdot \mathbf{p}'_2 + \mathbf{p}'^\dagger_2 \cdot \mathbf{p}'_1) + 1,
\tag{3.10a}
$$

$$
\hat{\Pi}^2_2 = \frac{1}{2}\mathbf{p}'^\dagger_1 \cdot \mathbf{p}'_1 + \frac{1}{6}\mathbf{p}'^\dagger_2 \cdot \mathbf{p}'_2 - \frac{1}{2\sqrt{3}}(\mathbf{p}'^\dagger_1 \cdot \mathbf{p}'_2 + \mathbf{p}'^\dagger_2 \cdot \mathbf{p}'_1) + 1,
\tag{3.10b}
$$

$$
\hat{\Pi}^2_3 = \frac{2}{3}\mathbf{p}'^\dagger_2 \cdot \mathbf{p}'_2 + 1
\tag{3.10c}
$$

The interesting point is to introduce the oscillator interaction, exactly as in the replacement we made in (2.7) in the non-relativistic problem. For notational purposes we introduce the creation and annihilation operators

$$
\boldsymbol{\eta}_s \equiv \frac{1}{\sqrt{2}}(\omega^{\frac{1}{2}}\mathbf{x}'_s - i\omega^{-\frac{1}{2}}\mathbf{p}'_s), s = 1, 2,
\tag{3.11a}
$$

$$
\boldsymbol{\xi}_s \equiv \frac{1}{\sqrt{2}}(\omega^{\frac{1}{2}}\mathbf{x}'_s + i\omega^{-\frac{1}{2}}\mathbf{p}'_s), s = 1, 2,
\tag{3.11b}
$$

so that the relations (2.7) can be written as

$$
\mathbf{p}'_s \rightarrow -i\omega^{\frac{1}{2}}\sqrt{2}\boldsymbol{\xi}_s,
\tag{3.12a}
$$

$$
\mathbf{p}'^\dagger_s \rightarrow i\omega^{\frac{1}{2}}\sqrt{2}\boldsymbol{\eta}_s,
\tag{3.12b}
$$

Under this replacement the $\hat{\Pi}^2_s$ operators become then

$$
\hat{\Pi}^2_1 = \omega[C_{11} + \frac{1}{3}C_{22} + \frac{1}{\sqrt{3}}(C_{12} + C_{21})] + 1
\tag{3.13a}
$$

$$\hat{\Pi}_2^2 = \omega[C_{11} + \frac{1}{3}C_{22} - \frac{1}{\sqrt{3}}(C_{12} + C_{21})] + 1 \tag{3.13b}$$

$$\hat{\Pi}_3^2 = \frac{4}{3}\omega C_{22} + 1, \tag{3.13c}$$

where the operator $C_{st}, s, t = 1, 2$ are defined by

$$C_{st} = \boldsymbol{\eta}_s \cdot \boldsymbol{\xi}_t \tag{3.14}$$

From the fact that

$$[\xi_{it}, \eta_{js}] = \delta_{ij}\delta_{st} \ ; \ i, j = 1, 2, 3 \ ; \ s = 1, 2, \tag{3.15}$$

we have the commutation relations

$$[C_{st}, C_{s't'}] = C_{st'}\delta_{s't} - C_{s't}\delta_{st'}, \tag{3.16}$$

and thus they are generators [5] of a U(2) group. Therefore the operators $\hat{\Pi}_1^2, \hat{\Pi}_2^2, \hat{\Pi}_3^2$, appearing in the equation (3.6), are linear functions of the generators of this group.

To obtain from Eq.(3.6) the eigenvalues of the energy for this relativistic oscillator problem we can proceed as follows: First we note that the first order Casimir operator of U(2) group is

$$\hat{N} = C_{11} + C_{22}, \tag{3.17}$$

and that it has an SU(2) subgroup whose generators are

$$\hat{F}_+ \equiv C_{12}, \tag{3.18a}$$

$$\hat{F}_o \equiv (\tfrac{1}{2})(C_{11} - C_{22}), \tag{3.18b}$$

$$\hat{F}_- \equiv C_{21}, \tag{3.18c}$$

with a corresponding Casimir operator of the form

$$\hat{F}^2 \equiv \hat{F}_-\hat{F}_+ + \hat{F}_o(\hat{F}_o + 1). \tag{3.19}$$

The $\hat{N}, \hat{F}^2$ by definition commute with all C_{st} and among themselves, so from (3.13), they will be integrals of motion of the operator $\Phi(E^2, \Pi_s^2)$. Thus the eigenstates of the Eq. (3.6) can be characterized by the eigenvalues of $\hat{N}, \hat{F}^2$ which we denote respectively by

$$N, f(f + 1) \tag{3.20}$$

with f taking the values $(N/2, (N/2) - 1$, down to $1/2$ or 0 depending on whether N is odd or even.

Another operator that commutes with $\hat{N}, \hat{F}^2$ is obviously $\hat{F}_o$ and we shall designate its eigenvalue by

$$\nu = f, f - 1, \ldots, -f, \qquad (3.21)$$

so the eigenstates associated with $\hat{N}, \hat{F}^2, \hat{F}_o$ could be represented by the ket

$$|Nf\nu>, \qquad (3.22)$$

and the solution ψ of Eq. (3.6) is necessarily a linear combination of these kets $i.e.$

$$\psi = \sum_{\nu=-f}^{f} a_\nu |Nf\nu>, \qquad (3.23)$$

as $\hat{N}, \hat{F}^2$ are integrals of motion.

To obtain the eigenvalues of the internal energy E as function of N, f we need first to consider the matrix elements of the operator Φ of (3.6) in the basis (3.22) $i.e.$

$$< Nf\nu'|\Phi(E^2, \hat{\Pi}_s^2)|Nf\nu >, \qquad (3.24)$$

which from (3.13), (3.17), (3.18) is a straightforward, but laborious, calculation of the type familiar in angular momentum theory, as the group there is also SU(2).

To get the internal energy

$$E(N, f, \alpha), \qquad (3.25)$$

with α indicating the rest of the indices, we need to evaluate the determinant of the $(2f + 1) \times (2f + 1)$ matrix whose elements are (3.24) and equate it to zero. This gives us a numerical equation of degree $4(2f + 1)$ in the variable E^2 and its solution provides us with values indicated symbolically in (3.25).

As our purpose is to provide the *method* of solution for the internal energy of relativistic three body oscillator problem, we will only carry the calculation of (3.24) for the single case when

$$N = f = \nu = 0 \qquad (3.26)$$

which implies that

$$< 000|\hat{\Pi}_s^2|000 >= 1, \quad s = 1, 2, 3 \qquad (3.27)$$

and so A, B, C^2 in (3.4) become respectively

$$A = 3, \qquad B = -3, \qquad C^2 = 16, \qquad (3.28)$$

and the equation for the energy is given by

$$E^8 - 12E^6 + 30E^4 - 28E^2 + 9 = 0, \qquad (3.29)$$

whose four roots for E^2 are $E^2 = 1$, repeated three times, and $E^2 = 9$, with $E = \pm 3$ and ± 1 as we expect from (3.1).

So far we have discussed, and given a method for solving, the equation related with a three body relativistic problem with an oscillator interaction. In the next section we proceed to show that we can formulate it in a Poincaré invariant form.

4 Poincaré invariance of the three body relativistic equation with oscillator interactions

To express Eq. (3.6) in a Poincaré invariant form we start with definition of the total four momentum for the three particle problem *i.e.*

$$P_\mu = p_{\mu 1} + p_{\mu 2} + p_{\mu 3}, \qquad (4.1)$$

where $\mu = 0, 1, 2, 3$ with $p_{os}, s = 1, 2, 3$, being the time like component while $p_{is}, i = 1, 2, 3$, are the space like components of the vector $\mathbf{p}_s$ of the previous section.

We shall require also a unit time like four vector u_μ which we shall define as

$$u_\mu = P_\mu (-g^{\sigma\tau} P_\sigma P_\tau)^{-\frac{1}{2}}, \qquad (4.2)$$

where repeated indices σ, τ are summed over 0,1,2,3 and our metric tensor is taken as

$$g^{\sigma\tau} = 0 \quad \text{if} \quad \sigma \neq \tau, \ g_{11} = g_{22} = g_{33} = -g_{oo} = 1 \qquad (4.3)$$

Clearly in the center of mass frame where $P_i = 0, i = 1, 2, 3, u_\mu$ takes the value

$$(u_\mu) = (1, 0, 0, 0) \qquad (4.4)$$

The operators $\boldsymbol{\eta}_s, \boldsymbol{\xi}_s, s = 1, 2$, defined in (3.11) are space like three component vectors which could be denoted by $\eta_{is}, \xi_{is}, i = 1, 2, 3$. A time like component could be added through the definition (3.11) just by putting p'_{os}, x'_{os} instead of p'_{is}, x'_{is} and thus we would get η_{os}, ξ_{os} which, together with η_{is}, ξ_{is}, form the four vectors

$$\eta_{\mu s}, \xi_{\mu s}; \ \mu = 0, 1, 2, 3; \ s = 1, 2. \qquad (4.5)$$

We do not want to use these operators directly in the definition of the C_{st} of (3.14), but rather utilize their transversal parts defined by

$$\eta_{\mu s}^{\perp} \equiv \eta_{\mu s} + (g^{\sigma\tau}\eta_{\sigma s}u_\tau)u_\mu, \tag{4.6a}$$

$$\xi_{\mu s}^{\perp} \equiv \xi_{\mu s} + (g^{\sigma\tau}\xi_{\sigma s}u_\tau)u_\mu. \tag{4.6b}$$

These transverse operators have the property that in the center of mass frame where $(u_\mu) = (1000)$ we have, because of the matrix (4.3), that

$$\eta_{os}^{\perp} = 0, \quad \xi_{os}^{\perp} = 0, \quad \eta_{is}^{\perp} = \eta_{is}, \quad \xi_{is}^{\perp} = \xi_{is}. \tag{4.7}$$

Thus now the generator $C_{st}, s,t = 1,2$, appearing in the definitions (3.13) of $\hat{\Pi}_1^2, \hat{\Pi}_2^2, \hat{\Pi}_3^2$ can be expressed in a Lorentz invariant way by

$$C_{st} = g^{\sigma\tau}\eta_{\sigma s}^{\perp}\xi_{\tau t}^{\perp}, \tag{4.8}$$

as in the center of mass frame it takes the form (3.14) *i.e.* $C_{st} = \boldsymbol{\eta}_s \cdot \boldsymbol{\xi}_t$.

As for the energy E^2 appearing in Eq. (3.6) it can be substituted by the operator

$$E^2 \to (-g^{\sigma\tau}P_\sigma P_\tau), \tag{4.9}$$

because in the center of mass frame $P_i = 0, i = 1,2,3$, and from the metric tensor (4.3), we see that the parenthesis in (4.9) reduces to P_o^2, which is the time like component of the four momentum vector squared and thus corresponds to the square of the total energy of the system.

With the definitions (4.8) of C_{st} and (4.9) of E^2 substituted in Eq.(3.6) we get a Poincaré invariant equation for our problem, as C_{st}, given in terms of Jacobi coordinates and momenta, is also invariant under translation in space time, and thus commutes with P_μ.

We have then arrived at a procedure for deriving a Poincaré invariant equation for a three particle system with oscillator interactions which, in the center of mass reference frame, can be solved by a simple group theoretical procedure, which leads eventually to algebraic equations of degree $4(2f + 1)$ for E^2, that can be solved numerically to give the spectrum of the problem.

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COVARIANT HARMONIC OSCILLATORS AND COUPLED HARMONIC OSCILLATORS

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Abstract

It is shown that the system of two coupled harmonic oscillators shares the basic symmetry properties with the covariant harmonic oscillator formalism which provides a concise description of the basic features of relativistic hadronic features observed in high-energy laboratories. It is shown also that the coupled oscillator system has the SL(4,r) symmetry in classical mechanics, while the present formulation of quantum mechanics can accommodate only the Sp(4,r) portion of the SL(4,r) symmetry. The possible role of the SL(4,r) symmetry in quantum mechanics is discussed.

1 Introduction

The covariant harmonic oscillator formalism developed by the present authors has been shown to be effective in explaining the basic phenomenological features of relativistic extended hadrons observed in high-energy laboratories. In particular, the formalism shows that the quark model and Feynman's parton picture are two different manifestations of one relativistic entity. In addition, the formalism constitutes a representation of Wigner's little group for a massive particle with internal space-time structure [1].

Since the classical mechanics of two coupled harmonic oscillators is discussed in Goldstein's text book [2], there is a tendency to believe that this oscillator problem is completely understood and that nothing new can be learned from it. We disagree. In this paper, we show that this coupled oscillator system can serve as an analog computer for the above-mentioned covariant oscillator formalism.

From the mathematical point of view, the standard approach is to construct a suitable representation of the symmetry group after writing down its generators. The first symmetry group in the present case is $Sp(4,r)$ with ten generators [3, 4, 5]. The second symmetry group is $SL(4,r)$ which contains a number of $Sp(4)$-like subgroups. In constructing these groups, we shall note that each oscillator has its own $Sp(2)$ symmetry, and that the coupling of the two oscillator also has a

$Sp(2)$-like symmetry. It was pointed out that these three $Sp(2)$ groups can be combined into one $Sp(4)$ group.

Since $Sp(4)$ is locally isomorphic to the deSitter group $O(3,2)$, it can explain the Lorentz transformation properties, particularly that of the covariant harmonic oscillator formalism. In this paper, we concentrate on the issue of a lack of information on one oscillator affecting the uncertainty and the entropy of the other oscillator.

2   Covariant Harmonic Oscillators

The covariant harmonic oscillator formalism has been discussed exhaustively in the literature, and it is not necessary to give another full-fledged treatment in the present paper. Instead, we shall concentrate on the issue of entropy in this paper. The entropy is a measure of our ignorance and is computed from the density matrix [6, 7]. The density matrix is needed when the experimental procedure does not analyze all relevant variables to the maximum extent consistent with quantum mechanics. The purpose of the present note is to discuss a concrete example of the entropy arising from our ignorance in relativistic quantum mechanics.

Let us consider a bound state of two particles. For convenience, we shall call the bound state the hadron, and call its constituents quarks. Then there is a Bohr-like radius measuring the space-like separation between the quarks. There is also a time-like separation between the quarks, and this variable becomes mixed with the longitudinal spatial separation as the hadron moves with a relativistic speed.

However, there are at present no quantum measurement theories to deal with the above-mentioned time-like separation. We shall study in the present paper how this ignorance is translated into the entropy. Within the framework of the covariant harmonic oscillator formalism [1], it will be shown that the entropy increases as the hadron gains its speed. The entropy defined in this way is a more fundamental quantity than the hadronic temperature [4]. It is independent of the question of whether the temperature can be defined [8].

Let us consider a hadron consisting of two quarks. If the space-time positions of two quarks are specified by x_a and x_b respectively, the system can be described by the variables [9]

$$X = (x_a + x_b)/2, \qquad x = (x_a - x_b)/2\sqrt{2}. \tag{1}$$

The four-vector X specifies where the hadron is located in space and time, while the variable x measures the space-time separation between the quarks. In the convention of Feynman *et al* [9], the internal motion of the quarks bound by a harmonic oscillator potential of unit strength can be described by the Lorentz-invariant equation

$$\frac{1}{2}\left\{x_\mu^2 - \frac{\partial^2}{\partial x_\mu^2}\right\}\psi(x) = \lambda\psi(x). \tag{2}$$

We use here the space-favored metric: $x^\mu = (x, y, z, t)$.

It is possible to construct a representation of the Poincaré group from the solutions of the above differential equation [1]. If the hadron is at rest, the solution should take the form

$$\psi(x, y, z, t) = \psi(x, y, z)\left(\frac{1}{\pi}\right)^{1/4}\exp\left(-t^2/2\right), \tag{3}$$

where $\psi(x, y, z)$ is the wave function for the three-dimensional oscillator with appropriate angular momentum quantum numbers. There are no excitations along the t direction. Indeed, the above wave function constitutes a representation of Wigner's $O(3)$-like little group for a massive particle [1].

Since the three-dimensional oscillator differential equation is separable in both spherical and Cartesian coordinate systems, $\psi(x, y, z)$ consists of Hermite polynomials of x, y, and z. If the Lorentz boost is made along the z direction, the x and y coordinates are not affected, and can be dropped from the wave function. The wave function of interest can be written as

$$\psi^n(z, t) = (\tfrac{1}{\pi})^{1/4} \exp(-t^2/2) \, \psi_n(z), \tag{4}$$

with

$$\psi^n(z) = \left(\frac{1}{\pi n! 2^n} \right)^{1/2} H_n(z) \exp(-z^2/2), \tag{5}$$

where $\psi^n(z)$ is for the n-th excited oscillator state. The full wave function $\psi^n(z, t)$ is

$$\psi_0^n(z, t) = \left(\frac{1}{\pi n! 2^n} \right)^{1/2} H_n(z) \exp\left\{ -\frac{1}{2} \left(z^2 + t^2 \right) \right\}. \tag{6}$$

The subscript 0 means that the wave function is for the hadron at rest. The above expression is not Lorentz-invariant, and its localization undergoes a Lorentz squeeze as the hadron moves along the z direction [1].

It is convenient to use the light-cone variables to describe Lorentz boosts. The light-cone coordinate variables are

$$u = (z + t)/\sqrt{2}, \qquad v = (z - t)/\sqrt{2}. \tag{7}$$

In terms of these variables, the Lorentz boost along the z direction,

$$\begin{pmatrix} z' \\ t' \end{pmatrix} = \begin{pmatrix} \cosh\eta & \sinh\eta \\ \sinh\eta & \cosh\eta \end{pmatrix} \begin{pmatrix} z \\ t \end{pmatrix}, \tag{8}$$

takes the simple form

$$u' = e^\eta u, \qquad v' = e^{-\eta} v, \tag{9}$$

where η is the boost parameter and is $\tanh^{-1}(v/c)$. The wave function of Eq.(6) can be written as

$$\psi_0^n(z, t) = \left(\frac{1}{\pi n! 2^n} \right)^{1/2} H_n\left((u + v)/\sqrt{2} \right) \exp\left\{ -\frac{1}{2}(u^2 + v^2) \right\}. \tag{10}$$

If the system is boosted, the wave function becomes

$$\psi_\eta^n(z, t) = \left(\frac{1}{\pi n! 2^n} \right)^{1/2} H_n\left((e^{-\eta}u + e^\eta v)/\sqrt{2} \right) \exp\left\{ -\frac{1}{2} \left(e^{-2\eta}u^2 + e^{2\eta}v^2 \right) \right\}. \tag{11}$$

As was discussed in the literature for several different purposes, this wave function can be expanded as [1]

$$\psi_\eta^n(z, t) = (1/\cosh\eta)^{n+1} \sum_k \left(\frac{(n+k)!}{n! k!} \right)^{1/2} (\tanh\eta)^k \psi_{n+k}(z) \psi_n(t). \tag{12}$$

In both Eqs. (10) and (11), the localization property of the wave function in the uv plane is determined by the Gaussian factor, and it is sufficient to study the ground state only for the essential feature of the boundary condition. Eq.(10) and Eq.(11) then respectively become

$$\psi_0^n(z,t) = \left(\frac{1}{\pi}\right)^{1/2} \exp\left\{-\frac{1}{2}(u^2 + v^2)\right\}.$$ (13)

If the system is boosted, the wave function becomes

$$\psi_\eta(z,t) = \left(\frac{1}{\pi}\right)^{1/2} \exp\left\{-\frac{1}{2}\left(e^{-2\eta}u^2 + e^{2\eta}v^2\right)\right\}.$$ (14)

We note here that the transition from Eq.(13) to Eq.(14) is a squeeze trasnformation. The wave function of Eq.(13) is distributed within a circular region in the uv plane, and thus in the zt plane. On the other hand, the wave function of Eq.(14) is distributed in an elliptic region. This ellipse is a "squeezed" circle with the same area as the circle. This Lorentz-squeezed wave function can be expaned as

$$\psi_\eta(z,t) = \frac{1}{\cosh\eta} \sum_k (\tanh\eta)^k \psi_k(z)\psi_k(t).$$ (15)

From this wave function, we can construct the pure-state density matrix

$$\rho_\eta(z,t;z',t') = \psi_\eta(z,t)\psi_\eta(z',t'),$$ (16)

which satisfies the condition $\rho^2 = \rho$:

$$\rho_\eta(z,t;z',t') = \int \rho_\eta(z,t;z'',t'')\rho_\eta(z'',t'';z',t')dz''dt''.$$ (17)

However, there are at present no measurement theories which accommodate the time-separation variable t. Thus, we can take the trace of the ρ matrix with respect to the t variable. Then the resulting density matrix is

$$\begin{aligned}
\rho_\eta(z,z') &= \int \psi_\eta(z,t)\left\{\psi_\eta(z',t)\right\}^* dt \\
&= \left(\frac{1}{\cosh\eta}\right)^2 \sum_k (\tanh\eta)^{2k}\psi_k(z)\psi_k^*(z').
\end{aligned}$$ (18)

The trace of this density matrix is one, but the trace of ρ^2 is less than one, as

$$\begin{aligned}
Tr\left(\rho^2\right) &= \int \rho_\eta(z,z')\rho_\eta(z',z)dz'dz \\
&= \left(\frac{1}{\cosh\eta}\right)^4 \sum_k (\tanh\eta)^{4k},
\end{aligned}$$ (19)

which is less than one. This is due to the fact that we do not know how to deal with the time-like separation in the present formulation of quantum mechanics. Our knowledge is less than complete. The standard way to measure this ignorance is to calculate the entropy defined as [6, 7]

$$S = -Tr\left(\rho\ln(\rho)\right).$$

If we pretend to know the distribution along the time-like direction and use the pure-state density matrix given in Eq.(16), then the entropy is zero. However, if we do not know how to deal with the distribution along t, then we should use the density matrix of Eq.(18) to calculate the entropy, and the result is

$$S \doteq 2\left\{(\cosh\eta)^2 \ln(\cosh\eta) - (\sinh\eta)^2 \ln(\sinh\eta)\right\}. \tag{20}$$

In terms of the velocity v of the hadron,

$$S = -\ln[1 - (v/c)^2] - \frac{(v/c)^2 \ln(v/c)^2}{1 - (v/c)^2}. \tag{21}$$

We can also calculate the density matrix using the Gaussian form of the wave function given in Eq.(17), and the result is

$$\rho(z, z') = \left(\frac{1}{\pi \cosh 2\eta}\right)^{1/2} \exp\left\{-\frac{1}{4}[(z + z')^2 / \cosh 2\eta + (z - z')^2 \cosh 2\eta]\right\}, \tag{22}$$

This expression also leads to the entropy given in Eq.(20)

The diagonal elements of the above density matrix is

$$\rho(z, z) = \left(\frac{1}{\pi \cosh 2\eta}\right)^{1/2} \exp\left(-z^2 / \cosh 2\eta\right). \tag{23}$$

The width of the distribution becomes $(\cosh\eta)^{1/2}$, and becomes wide-spread as the hadronic speed increases. Likewise, the momentum distribution becomes wide-spread. This simultaneous increase in the momentum and position distribution widths is called the parton phenomenon in high-energy physics. The position-momentum uncertainty becomes $\cosh\eta$. This increase in uncertainty is due to our ignorance about the physical but unmeasurable time-separation variable.

The use of an unmeasurable variable as a "shadow" coordinate is not new in physics and is of current interest [10, 11, 12, 13]. Feynman's book on statistical mechanics contains the following paragraph [14].

When we solve a quantum-mechanical problem, what we really do is divide the universe into two parts - the system in which we are interested and the rest of the universe. We then usually act as if the system in which we are interested comprised the entire universe. To motivate the use of density matrices, let us see what happens when we include the part of the universe outside the system.

In the present paper, we have identified Feynman's rest of the universe as the time-separation coordinate in a relativistic two-body problem. Our ignorance about this coordinate leads to a density matrix for a non-pure state, and consequently to an increase of entropy. It is interesting to note that the density matrix of Eq.(22) becomes that of the harmonic oscillator in a thermal equilibrium state if $(\tanh\eta)^2$ is identified as the Boltzmann factor [15].

We have thus far studied the properties of covariant harmonic oscillators where the longitudinal and time-like coordinates undergo squeeze transformations. The word "squeeze" is relatively new in physics. However, squeeze transformations are almost everywhere in physics. In the rest of this paper, we shall discuss the role of squeeze transformations in the system of two coupled harmonic oscillators. We shall see that the problem of covariant harmonic oscillators with two variables is the same as that of two coupled harmonic oscillators.

3 Linear Canonical and Non-Canonical Transformations in Classical Mechanics

For a dynamical system consisting of two pairs of canonical variables x_1, p_1 and x_2, p_2, we can introduce the four-dimensional coordinate system:

$$(\eta_1, \eta_2, \eta_3, \eta_4) = (x_1, x_2, p_1, p_2).$$ (24)

Then the transformation of the variables from η_i to ξ_i is canonical if

$$MJ\tilde{M} = J,$$ (25)

where

$$M_{ij} = \frac{\partial}{\partial \eta_j} \xi_i,$$

and

$$J = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}.$$

For linear canonical transformations, we can work with the group of four-by-four real matrices satisfying the condition of Eq.(25). This group is called the four-dimensional symplectic group or $Sp(4)$. While there are many physical applications of this group, we are interested here in constructing the representations relevant to the study of two coupled harmonic oscillators.

It is more convenient to discuss this group in terms of its generators G, defined as

$$M = \exp(-i\alpha G),$$ (26)

where G represents a set of purely imaginary four-by-four matrices. The symplectic condition of Eq.(25) dictates that G be symmetric and anticommute with J or be antisymmetric and commute with J.

In terms of the Pauli spin matrices and the two-by-two identity matrix, we can construct the following four antisymmetric matrices which commute with J of Eq.(25).

$$J_1 = \frac{i}{2} \begin{pmatrix} 0 & \sigma_1 \\ -\sigma_1 & 0 \end{pmatrix}, \qquad J_2 = \frac{1}{2} \begin{pmatrix} \sigma_2 & 0 \\ 0 & \sigma_2 \end{pmatrix},$$

$$J_3 = \frac{i}{2} \begin{pmatrix} 0 & \sigma_3 \\ -\sigma_3 & 0 \end{pmatrix}, \qquad J_0 = \frac{i}{2} \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}.$$ (27)

The following six symmetric generators anticommute with J.

$$K_1 = \frac{i}{2} \begin{pmatrix} 0 & \sigma_3 \\ \sigma_3 & 0 \end{pmatrix}, \qquad K_2 = \frac{i}{2} \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \qquad K_3 = -\frac{i}{2} \begin{pmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{pmatrix},$$

and

$$Q_1 = \frac{i}{2} \begin{pmatrix} -\sigma_3 & 0 \\ 0 & \sigma_3 \end{pmatrix}, \qquad Q_2 = \frac{i}{2} \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \qquad Q_3 = \frac{i}{2} \begin{pmatrix} \sigma_1 & 0 \\ 0 & -\sigma_1 \end{pmatrix}.$$ (28)

These generators satisfy the commutation relations:

$$[J_i, J_j] = i\epsilon_{ijk}J_k, \qquad [J_i, K_j] = i\epsilon_{ijk}K_k, \qquad [K_i, K_j] = [Q_i, Q_j] = -i\epsilon_{ijk}J_k,$$

$$[J_i, J_0] = 0, \qquad [K_i, Q_j] = i\delta_{ij}J_o,$$

$$[J_i, Q_j] = i\epsilon_{ijk}Q_k, \qquad [K_i, J_o] = iQ_i, \qquad [Q_i, J_o] = -iK_i. \tag{29}$$

The group of homogeneous linear transformations with this closed set of generators is called the symplectic group $Sp(4)$. The J matrices are known to generate rotations while the K and Q matrices generate squeezes [4].

It is often more convenient to study the physics of four-dimensional phase space using the coordinate system

$$(\xi_1, \xi_2, \xi_3, \xi_4) = (x_1, p_1, x_2, p_2). \tag{30}$$

The transformation from $(\eta_1, \eta_2, \eta_3, \eta_4)$ is

$$\begin{pmatrix} \xi_1 \\ \xi_2 \\ \xi_3, \\ \xi_4 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \\ \eta_4 \end{pmatrix}, \tag{31}$$

and the J matrix becomes

$$J = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}. \tag{32}$$

In this new coordinate system, the rotation generators take the form

$$J_1 = \frac{-1}{2}\begin{pmatrix} 0 & \sigma_2 \\ \sigma_2 & 0 \end{pmatrix}, \qquad J_2 = \frac{i}{2}\begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix},$$

$$J_3 = \frac{-1}{2}\begin{pmatrix} \sigma_2 & 0 \\ 0 & -\sigma_2 \end{pmatrix}, \qquad J_0 = \frac{-1}{2}\begin{pmatrix} \sigma_2 & 0 \\ 0 & \sigma_2 \end{pmatrix}. \tag{33}$$

The squeeze generators become

$$K_1 = \frac{i}{2}\begin{pmatrix} \sigma_1 & 0 \\ 0 & -\sigma_1 \end{pmatrix}, \qquad K_2 = \frac{i}{2}\begin{pmatrix} \sigma_3 & 0 \\ 0 & \sigma_3 \end{pmatrix}, \qquad K_3 = -\frac{i}{2}\begin{pmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{pmatrix},$$

$$Q_1 = \frac{i}{2}\begin{pmatrix} -\sigma_3 & 0 \\ 0 & \sigma_3 \end{pmatrix}, \qquad Q_2 = \frac{i}{2}\begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_1 \end{pmatrix}, \qquad Q_3 = \frac{i}{2}\begin{pmatrix} 0 & \sigma_3 \\ \sigma_3 & 0 \end{pmatrix}. \tag{34}$$

In addition to the ten generators given in Eq.(33) and also in Eq.(34), we can consider the scale transformation in which both the position and momentum of the first coordinate are expanded and those of the second coordinate contracted. The Hamiltonian given in Eq.(46) suggests such a transformation, and the transformation can be generated by

$$S_0 = \frac{i}{2}\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}. \tag{35}$$

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This matrix generates scale transformations in phase space. The transformation leads to a radial expansion of the phase space of the first coordinate [16] and contracts the phase space of the second coordinate. What is the physical significance of this operation? As we discussed in Sec. 7, the expansion of phase space leads to an increase in uncertainty and entropy. Mathematically speaking, the contraction of the second coordinate should cause a decrease in uncertainty and entropy. Can this happen? The answer is clearly No, because it will violate the uncertainty principle. This question will be addressed in future publications.

In the meantime, let us study what happens when the matrix S_0 is introduced into the set of matrices given in Eq.(33) and Eq.(34). It commutes with J_0, J_3, K_1, K_2, Q_1, and Q_2. However, its commutators with the rest of the matrices produce four more generators:

$$[S_0, J_1] = \frac{i}{2} \begin{pmatrix} 0 & -\sigma_2 \\ \sigma_2 & 0 \end{pmatrix}, \qquad [S_0, J_2] = \frac{1}{2} \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix},$$

$$[S_0, K_3] = \frac{1}{2} \begin{pmatrix} 0 & \sigma_1 \\ -\sigma_1 & 0 \end{pmatrix}, \qquad [S_0, Q_3] = \frac{1}{2} \begin{pmatrix} 0 & -\sigma_3 \\ \sigma_3 & 0 \end{pmatrix}. \tag{36}$$

If we take into account the above five generators in addition to the ten generators of $Sp(4)$, there are fifteen generators. They form the closed set of commutation relations for the the group $SL(4,r)$. This $SL(4,r)$ symmetry of the coupled oscillator system may have interesting physical implications.

4 SL(4,r) Formulation of Two Coupled Oscillators

Let us consider a system of two coupled harmonic oscillators. The Hamiltonian for this system is

$$H = \frac{1}{2} \left\{ \frac{1}{m_1} p_1^2 + \frac{1}{m_2} p_2^2 + A' x_1^2 + B' x_2^2 + C' x_1 x_2 \right\}. \tag{37}$$

where

$$A' > 0, \qquad B' > 0, \qquad 4A'B' - C'^2 > 0. \tag{38}$$

By making scale changes of x_1 and x_2 to $(m_1/m_2)^{1/4} x_1$ and $(m_2/m_1)^{1/4} x_2$ respectively, it is possible to make a canonical transformation of the above Hamiltonian to the form [17, 18]

$$H = \frac{1}{2m} \left\{ p_1^2 + p_2^2 \right\} + \frac{1}{2} \left\{ A x_1^2 + B x_2^2 + C x_1 x_2 \right\}, \tag{39}$$

with $m = (m_1 m_2)^{1/2}$. We can decouple this Hamiltonian by making the coordinate transformation:

$$\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} \cos(\alpha/2) & -\sin(\alpha/2) \\ \sin(\alpha/2) & \cos(\alpha/2) \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}. \tag{40}$$

Under this rotation, the kinetic energy portion of the Hamiltonian in Eq.(39) remains invariant. Thus we can achieve the decoupling by diagonalizing the potential energy. Indeed, the system becomes diagonal if the angle α becomes

$$\tan \alpha = \frac{C}{B - A}. \tag{41}$$

This diagonalization procedure is well known.

We now introduce the new parameters K and η defined as

$$K = \sqrt{AB - C^2/4}, \qquad \exp(-2\eta) = \frac{A + B + \sqrt{(A - B)^2 + C^2}}{\sqrt{4AB - C^2}}, \tag{42}$$

in addition to the rotation angle α. In terms of this new set of variables, A, B and C take the form

$$A = K \left(e^{2\eta} \cos^2 \frac{\alpha}{2} + e^{-2\eta} \sin^2 \frac{\alpha}{2} \right),$$

$$B = K \left(e^{2\eta} \sin^2 \frac{\alpha}{2} + e^{-2\eta} \cos^2 \frac{\alpha}{2} \right),$$

$$A = K \left(e^{-2\eta} - e^{2\eta} \right) \sin \alpha. \tag{43}$$

the Hamiltonian can be written as

$$H = \frac{1}{2m} \left\{ q_1^2 + q_2^2 \right\} + \frac{K}{2} \left\{ e^{2\eta} y_1^2 + e^{-2\eta} y_2^2 \right\}, \tag{44}$$

where y_1 and y_2 are defined in Eq.(40), and

$$\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = \begin{pmatrix} \cos(\alpha/2) & -\sin(\alpha/2) \\ \sin(\alpha/2) & \cos(\alpha/2) \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \end{pmatrix}. \tag{45}$$

This form will be our starting point. The above rotation together with that of Eq.(40) is generated by J_0.

If we measure the coordinate variable in units of $(mK)^{1/4}$, and use $(mK)^{-1/4}$ for the momentum variables, the Hamiltonian takes the form

$$H = \frac{\omega}{2} e^{\eta} \left(e^{-\eta} q_1^2 + e^{\eta} y_1^2 \right) + \frac{\omega}{2} e^{-\eta} \left(e^{\eta} q_2^2 + e^{-\eta} y_2^2 \right), \tag{46}$$

where $\omega = \sqrt{K/m}$. If $\eta = 0$, the system becomes decoupled, and the Hamiltonian becomes

$$H = \frac{\omega}{2} \left(p_1^2 + x_1^2 \right) + \frac{\omega}{2} \left(p_2^2 + x_2^2 \right). \tag{47}$$

In Sec. 8, we will be dealing with the problem of what happens when no observations are made on the second coordinate. If the system is decoupled, as the above Hamiltonian indicates, the physics in the first coordinate is solely dictated by the Hamiltonian

$$H_1 = \frac{\omega}{2} \left(p_1^2 + x_1^2 \right). \tag{48}$$

It is important to note that the Hamiltonian of Eq.(47) cannot be obtained from Eq.(46) by canonical transformation. For this reason, the Hamiltonian of the form

$$H' = \frac{\omega}{2} \left(e^{-\eta} q_1^2 + e^{\eta} y_1^2 \right) + \frac{\omega}{2} \left(e^{\eta} q_2^2 + e^{-\eta} y_2^2 \right) \tag{49}$$

may play a useful role in our discussion. This Hamiltonian can be transformed into the decoupled form of Eq.(47) through a canonical transformation.

5 Quantum Mechanics of Coupled Oscillators

It is remarkable that both the Hamiltonian H of Eq.(46) and H' of Eq.(49) lead to the same Schrödinger wave function. If y_1 and y_2 are measured in units of $(mK)^{1/4}$, the ground-state wave function for this oscillator system is

$$\psi_0(x_1, x_2) = \frac{1}{\sqrt{\pi}} \exp\left\{-\frac{1}{2}(e^\eta y_1^2 + e^{-\eta} y_2^2)\right\}. \tag{50}$$

The wave function is separable in the y_1 and y_2 variables. However, for the variables x_1 and x_2, the story is quite different. If we write this wave function in terms of x_1 and x_2, then

$$\psi(x_1, x_2) = \frac{1}{\sqrt{\pi}} \exp\left\{-\frac{1}{2}\left[e^\eta (x_1 \cos\frac{\alpha}{2} - x_2 \sin\frac{\alpha}{2})^2 \right.\right.$$
$$\left.\left. + e^{-\eta}(x_1 \sin\frac{\alpha}{2} + x_2 \cos\frac{\alpha}{2})^2\right]\right\}. \tag{51}$$

If $\eta = 0$, this wave function becomes

$$\psi_0(x_1, x_2) = \frac{1}{\sqrt{\pi}} \exp\left\{-\frac{1}{2}(x_1^2 + x_2^2)\right\}. \tag{52}$$

For other values of η, the wave function of Eq.(51) can be obtained from the above expression by a unitary transformation.

$$\sum_{m_1 m_2} A_{m_1 m_2}(\alpha, \eta)\psi_{m_1}(x_1)\psi_{m_2}(x_2), \tag{53}$$

where $\psi_m(x)$ is the m[th] excited state wave function. The coefficients $A_{m_1 m_2}(\eta)$ satisfy the unitarity condition

$$\sum_{m_1 m_2} |A_{m_1 m_2}(\alpha, \eta)|^2 = 1. \tag{54}$$

It is possible to carry out a similar expansion in the case of excited states [1].

As for unitary transformations applicable to wave functions, let us go back the generators of canonical transformations in classical mechanics. As was stated before, they are also applicable to the Wigner phase-space distribution function. The canonical transformation of the Wigner function is translated into a unitary transformation of the Schrödinger wave function. There are therefore ten generators of unitary transformations applicable to Schrödinger wave functions [4, 3].

The Wigner phase-space picture is often more convenient for studying the problems of coupled harmonic oscillators. Unitary transformations in the Schrödinger picture can be achieved through canonical transformations in phase space. It has been known that canonical transformations are uncertainty-preserving transformations. They are also entropy-preserving transformations [5]. Are there then non-canonical transformations in quantum mechanics?

In the present case of coupled harmonic oscillators, we assume that we are not able to measure the x_2 coordinate. It is often more convenient to use the Wigner phase-space distribution function to study the density matrix, especially when we want to study the uncertainty products in detail [18, 14].

For two coordinate variables, the Wigner function is defined as [18]

$$W(x_1, x_2; p_1, p_2) = \left(\frac{1}{\pi}\right)^2 \int \exp\left\{-2i(p_1 y_1 + p_2 y_2)\right\}$$

$$\times \psi^*(x_1 + y_1, x_2 + y_2)\psi(x_1 - y_1, x_2 - y_2)dy_1 dy_2. \tag{55}$$

The Wigner function corresponding to the oscillator wave function of Eq.(51) is

$$W(x_1, x_2; p_1, p_2) = \left(\frac{1}{\pi}\right)^2 \exp\left\{-e^{\eta}(x_1 \cos\frac{\alpha}{2} - x_2 \sin\frac{\alpha}{2})^2\right.$$

$$-e^{-\eta}(x_1 \sin\frac{\alpha}{2} + x_2 \cos\frac{\alpha}{2})^2 - e^{-\eta}(p_1 \cos\frac{\alpha}{2} - p_2 \sin\frac{\alpha}{2})^2$$

$$\left. -e^{\eta}(p_1 \sin\frac{\alpha}{2} + p_2 \cos\frac{\alpha}{2})^2\right\}. \tag{56}$$

If we do not make observations in the $x_2 p_2$ coordinates, the Wigner function becomes

$$W(x_1, p_1) = \int W(x_1, x_2; p_1, p_2)dx_2 dp_2. \tag{57}$$

The evaluation of the integral leads to

$$W(x_1, p_1) = \left\{\frac{1}{\pi^2(1 + \sinh^2\eta \sin^2\alpha)}\right\}^{1/2}$$

$$\times \exp\left\{-\left(\frac{x_1^2}{\cosh\eta - \sin\eta\cos\alpha} + \frac{p_1^2}{\cosh\eta + \sin\eta\cos\alpha}\right)\right\}. \tag{58}$$

This Wigner function gives an elliptic distribution in the phase space of x_1 and p_1. This distribution gives the uncertainty product of

$$(\Delta x)^2(\Delta p)^2 = \frac{1}{4}(1 + \sinh^2\eta \sin^2\alpha). \tag{59}$$

This expression becomes $1/4$ if the oscillator system becomes uncoupled with $\alpha = 0$. Because x_1 is coupled with x_2, our ignorance about the x_2 coordinate, which in this case acts as Feynman's rest of the universe, increases the uncertainty in the x_1 world which, in Feynman's words, is the system in which we are interested.

In the Wigner phase-space picture, the uncertainty is measured in terms of the area in phase space where the Wigner function is sufficiently different from zero. According to the Wigner function for a thermally excited oscillator state, the temperature and entropy are also determined by the degree of the spread of the Wigner function phase space.

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COHERENT STATES FOR THE RELATIVISTIC HARMONIC OSCILLATOR

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Abstract

Recently we have obtained, on the basis of a group approach to quantization, a Bargmann-Fock-like realization of the Relativistic Harmonic Oscillator as well as a generalized Bargmann transform relating Fock wave functions $< z|n >$ and a set of relativistic Hermite polynomials $H_n^N(x)$, $(N = mc^2/\hbar\omega)$. Nevertheless, the relativistic creation and annihilation operators satisfy typical relativistic commutation relations $[\hat{z}, \hat{z}^\dagger] \approx$ Energy (an $SL(2,R)$ algebra). Here we find higher-order polarization operators on the $SL(2,R)$ group, providing canonical creation and annihilation operators satisfying $[\hat{a}, \hat{a}^\dagger] = \hat{1}$, the eigenstates of which are "true" coherent states.

1 Group Quantization and the Relativistic Harmonic Oscillator (RHO) in the Bargmann-Fock-like realization.

The quantization of relativistic systems in a manifestly covariant way requires the use of commutation relation of the form $[\hat{x}, \hat{p}] \approx$ Energy, which means a deviation from the canonical rules. If the Hamiltonian, $\hat{x}$ and $\hat{p}$ close a Lie algebra, it is possible to resort to some kind of group quantization method, i.e. some technique of obtaining unitary irreducible representations of a group the Lie algebra of which coincides with the Poisson algebra of the physical system. In the present case there is a Lie algebra, a central extension of $SL(2,R)$ ($SO(3,2)$ in 3+1 dimensions):

$$[\hat{E}, \hat{x}] = -i\frac{\hbar}{m}\hat{p}, \quad [\hat{E}, \hat{p}] = im\omega^2\hbar\hat{x}, \quad [\hat{x}, \hat{p}] = i\hbar(\hat{1} + \frac{1}{mc^2}\hat{E}), \quad (1)$$

which reproduces the Poincaré algebra under the $\omega \to 0$ limit and the Newton (non-relativistic harmonic oscillator) algebra when $c \to \infty$ and that, therefore, earns to be considered as the algebra of a relativistic harmonic oscillator.

Then, our starting point will be a central pseudo-extension of the group $SL(2, R)$, denoted by $SL(2, R)\tilde{\otimes}U(1)$ [1], whose coboundary is generated by a function which is an integer power of the parameter of the Cartan subgroup. The precise techniques of the group-quantization procedure [2] will be explained on the way.

The $\tilde{G} \equiv SL(2, R)\tilde{\otimes}U(1)$ group law is:

$$z'' = z'\eta^{-2} + z\kappa' + \frac{z}{N(1+\kappa)}(z^*z'\eta^{-2} + z'^*z\eta^2)$$

$$z^{*''} = z'^*\eta^2 + z^*\kappa' + \frac{z^*}{N(1+\kappa)}(zz'^*\eta^2 + z'z^*\eta^{-2})$$

$$\eta'' = \sqrt{\frac{2}{1+\kappa''}}\left[\sqrt{\frac{1+\kappa'}{2}}\sqrt{\frac{1+\kappa}{2}}\eta'\eta + \sqrt{\frac{2}{1+\kappa'}}\sqrt{\frac{2}{1+\kappa}}\left(\frac{z'z^*}{2N}\eta'\eta^* + \frac{z'^*z}{2N}\eta'^*\eta\right)\right] \quad (2)$$

$$\zeta'' = \zeta'\zeta(\eta''\eta'^{-1}\eta^{-1})^{-2N},$$

where

$$\kappa \equiv \sqrt{1 + \frac{2zz^*}{N}}$$

$$\kappa'' = \kappa'\kappa + \frac{1}{N}\left(z^*z'\eta^{-2} + z'^*z\eta^2\right),$$

and $z \in C$, $\eta \in U(1) \subset SL(2, R)$, $\zeta \in U(1)$ and $N \equiv \frac{mc^2}{\hbar\omega}$. It must be noted that N is quantized ($N = 1, 3/2, 2, 5/2, ...$) on $SL(2, R)$ but a positive number on the Universal covering group.

The coboundary

$$\Delta \equiv \left(\eta''\eta'^{-1}\eta^{-1}\right)^{-2N} : SL(2, R) \times SL(2, R) \to U(1), \quad (3)$$

which is generated by

$$\eta^{-2N} : SL(2, R) \to U(1), \quad (4)$$

realizes a pseudo-extension. We say that Δ is a pseudo-cocycle and realizes a pseudo-extension rather than a trivial cocycle (coboundary) realizing a trivial extension because in the $c \to \infty$ limit, $(\eta''\eta'^{-1}\eta^{-1})^{-2N}$ goes to a true cocycle on the non-relativistic harmonic oscillator (Newton) group (see [3] for a general study of the contraction process under which a true cocycle is generated by a coboundary).

Group quantization uses the (exponential of the) right-invariant vector fields, which act on $U(1)$-equivariant complex functions on $\tilde{G}$ as ordinary derivatives, to define a group representation (Bohr-Sommerfeld quantization). This representation is reducible, as can be stated by the existence of non-trivial operators (all the left-invariant vector fields) commuting with the representation.

The full quantization is achieved by reducing this representation in a way compatible with the action of right vector fields. The reduced Hilbert space is made of complex functions Ψ on $\tilde{G}$ such that

$$\Psi(\zeta * g) = \zeta \cdot \Psi(g) , \quad \zeta \in U(1), g \in G$$

$$\tilde{X}^L\Psi = 0 , \quad \forall \tilde{X}^L \in \mathcal{P}$$

where a Polarizarion $\mathcal{P}$ is a maximal left subalgebra containing the generators in the kernel of Δ and excluding the central generator $\Xi \equiv \tilde{X}^L_\zeta$ of $U(1)$.

The left- and right-invariant vector fields are:

$$\tilde{X}^L_z = \kappa \frac{\partial}{\partial z} + \frac{iz^*}{2N(1+\kappa)}\left(i\eta \frac{\partial}{\partial \eta}\right) - \frac{iz^*}{1+\kappa}\Xi$$

$$\tilde{X}^L_{z^*} = \kappa \frac{\partial}{\partial z^*} - \frac{iz}{2N(1+\kappa)}\left(i\eta \frac{\partial}{\partial \eta}\right) + \frac{iz}{1+\kappa}\Xi$$

$$\tilde{X}^L_\eta = i\eta \frac{\partial}{\partial \eta} - 2iz \frac{\partial}{\partial z} + 2iz^* \frac{\partial}{\partial z^*} \tag{5}$$

$$\tilde{X}^L_\zeta = i\zeta \frac{\partial}{\partial \zeta} \equiv \Xi,$$

$$\tilde{X}^R_z = \frac{\eta^{-2}}{(1+\kappa)}\left[\frac{(1+\kappa)^2}{2}\frac{\partial}{\partial z} + \frac{z^{*2}}{N}\frac{\partial}{\partial z^*} - i\frac{z^*}{N}\left(i\eta \frac{\partial}{\partial \eta}\right) + iz^*\Xi\right]$$

$$\tilde{X}^R_{z^*} = \frac{\eta^2}{(1+\kappa)}\left[\frac{(1+\kappa)^2}{2}\frac{\partial}{\partial z^*} + \frac{z^2}{N}\frac{\partial}{\partial z} + i\frac{z}{N}\left(i\eta \frac{\partial}{\partial \eta}\right) - iz\Xi\right] \tag{6}$$

$$\tilde{X}^R_\eta = i\eta \frac{\partial}{\partial \eta}$$

$$\tilde{X}^R_\zeta = i\zeta \frac{\partial}{\partial \zeta} \equiv \Xi.$$

The operators are

$$\hat{z} \equiv \tilde{X}^R_{z^*}, \qquad \hat{z}^\dagger \equiv -\tilde{X}^R_z, \qquad \hat{H} \equiv \frac{i}{2}\tilde{X}^R_\eta = \frac{i}{\omega}\tilde{X}^R_t = \frac{1}{\hbar\omega}\hat{E}, \tag{7}$$

where $\eta = e^{i\theta}$ and $\theta = \frac{\omega t}{2}$, with the commutation relations

$$\left[\hat{H}, \hat{z}\right] = -\hat{z}, \qquad \left[\hat{H}, \hat{z}^\dagger\right] = \hat{z}^\dagger, \qquad \left[\hat{z}, \hat{z}^\dagger\right] = \hat{1} + \frac{1}{N}\hat{H} \tag{8}$$

A polarization is given by $\mathcal{P} =< \tilde{X}^L_\eta, \tilde{X}^L_z >$, with solutions

$$\Psi = \zeta \sum_n e^{-2in\theta} c_n \Phi^N_n(z, z^*)$$

$$\Phi^N_n(z, z^*) \equiv \frac{1}{\pi\sqrt{n!}}\sqrt{\frac{(2N+n-1)!}{(2N-1)!(2N)^n}}\sqrt{\frac{2N-1}{2N}}\left(\frac{1+\kappa}{2}\right)^{-N-n} z^{*n} \tag{9}$$

which constitute the Fock-Bargmann-like space with the group invariant measure $\frac{dz\,dz^*}{\kappa}$[1].
The relativistic Fock space is given by:

$$< 0|0 >= 1, \qquad |n> = \frac{(\hat{z}^\dagger)^n|0>}{\sqrt{n! \prod_{s=1}^{n-1}(1 + \frac{s}{2N})}}, \tag{10}$$

---

[1]In reality the measure on the whole group is $\frac{dz\,dz^*\,d\theta}{\kappa}$ but the time variable (or θ) can be factorized out.

$$\hat{z}|n> = \sqrt{n(1+\frac{n-1}{2N})}|n-1>$$

$$\hat{z}^\dagger|n> = \sqrt{(n+1)(1+\frac{n}{2N})}|n+1> \qquad (11)$$

$$\hat{H}|n> = n|n>$$

2 Relativistic coherent states (RCS).

In the group-quantization scheme, the coherent states (generalizing the standard non-relativistic coherent states [4]), as well as the wave functions given above, are defined by mean of infinitesimal relations (differential polarization equations), rather than a finite group action on the vacuum associated with a previously given representation of the group [5,6] (see [7,8,9] for a more general study of overcomplete families of satates non-necessarily associated with groups). They are defined simply as:

$$|z> \equiv \sum_n \Phi_n^{N^*}(z,z^*)|n> \quad \leftrightarrow \quad \Phi_n^N(z,z^*) = <z|n> \qquad (12)$$

The associated (time-independent) wave functions $< z'|z >\equiv \Phi_z(z')$ correspond to the choice $c_n \equiv c_n(z) = \Phi_n^N(z,z^*)$ in $\Psi(z')$.

The RCS are identified with the generalized coherent states on the unit complex disk [5] once the change of variables $z_D = \sqrt{\frac{2}{N}}\frac{z}{1+\kappa} \in D$ ($z \in C$), has been made, where D is the unit complex disk.

The expectation values of $\hat{z}$ and $\hat{z}^\dagger$ in the coherent states are $< \hat{z} >\equiv \frac{<z|\hat{z}|z>}{<z|z>} = z$ and $< \hat{z}^\dagger >= z^*$, making the variables $z,z^* \in C$ specially suitable to describe the Bargmann-Fock-like representation. Defining the operators $\hat{x}$ and $\hat{p}$ in the usual way, i.e.

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{z}+\hat{z}^\dagger\right), \qquad \hat{p} = \sqrt{\frac{m\omega\hbar}{2}}\left(\hat{z}^\dagger - \hat{z}\right) \qquad (13)$$

we get $< \hat{x} >= x$, $< \hat{p} >= p$, where x and p are defined in the same way, constituting the phase-space coordinates for Anti-deSitter space-time.

Repeating the group quantization in the new variables we obtain the x-representation in terms of the relativistic Hermite Polynomials [10]. Both representations are related through the Relativistic Bargmann transform [11], the kernel of which is nothing other than the configuration-space wave function of the coherent states $|z>$ defined above:

$$< x|z >= \hat{C}^N\left(\frac{1+\kappa}{2}\right)^{-N}\alpha^N\left[1+\frac{s_0^2}{N}\right]^{-N}, \qquad (14)$$

where

$$s_0 \equiv \sqrt{\frac{m\omega}{\hbar}}x - \frac{\sqrt{2}z\alpha}{1+\kappa}, \qquad \alpha \equiv \sqrt{1+\frac{\omega^2 x^2}{c^2}}$$

$$\hat{C}^N \equiv \frac{1}{\sqrt{\pi}}\left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}}\sqrt{\frac{2N-1}{2N}}\sqrt{\frac{\Gamma(N)}{\sqrt{N}\Gamma(N-\frac{1}{2})}} \qquad (15)$$

In the non-relativistic limit we regain the usual coherent states in configuration space:

$$< x|z >^{N.R.} = \frac{1}{\sqrt{\pi}} \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} e^{-z^2/2+\sqrt{2m\omega/\hbar}xz} e^{-\frac{1}{2}(\frac{m\omega}{\hbar}x^2+|z|^2)} \tag{16}$$

The uncertainty relations for the operators $\hat{x}$ and $\hat{p}$ are:

$$\Delta\hat{x}\Delta\hat{p} = \frac{\hbar}{2}\sqrt{\kappa^2 + \frac{1}{4N^2}[4|z|^4 - (z^2 + z^{*2})]} \geq \frac{1}{2}\hbar\kappa = \frac{1}{2}| < [\hat{x}, \hat{p}] > | \tag{17}$$

The equality holds for $z = |z|e^{in\pi}$, i.e. $z \in R$, defining the so-called "intelligent states", but only for $z = 0$ (the vacuum) we reach the absolute minimum (see [12] for the calculations in the unit Disk).

3 Canonical (higher-order) creation and annihilation operators: canonical, relativistic coherent states.

The definition of polarization in group quantization can be generalized so as to admit operators in the left enveloping algebra. This generalization has been already exploited in finding a position operator for the free relativistic particle [13] (as well as in solving anomalous problems [2]). In the present case it also makes sense to look for basic operators satisfying canonical (versus manifestly covariant) commutation relations. Let us then seek a power series in $\tilde{X}_z^L$ and $\tilde{X}_{z^*}^L$,

$$\tilde{X}_{z^*}^{L\,HO} = \tilde{X}_{z^*}^L + \frac{\alpha}{N}\tilde{X}_z^L \tilde{X}_z^L \tilde{X}_{z^*}^L + ...$$

$$\tilde{X}_\eta^{L\,HO} = \tilde{X}_\eta^L - \mu\tilde{X}_z^L \tilde{X}_{z^*}^L - \frac{\nu}{N}\tilde{X}_z^L \tilde{X}_z^L \tilde{X}_{z^*}^L \tilde{X}_{z^*}^L + ..., \tag{18}$$

such that $\mathcal{P}^{HO} =< \tilde{X}_\eta^{L\,HO}, \tilde{X}_{z^*}^{L\,HO} >$ contains $\tilde{X}_\eta^L$ and excludes $\tilde{X}_\zeta^L$. The coefficients of the power series are determined by the requirement that $\mathcal{P}^{HO}$ is a polarization and the corresponding right operators define a unitary action on the wave functions Ψ which fortunately are the same as before. More concretely,

$$\left[\tilde{X}_\eta^{L\,HO}, \tilde{X}_{z^*}^{L\,HO}\right] = -2\tilde{X}_{z^*}^{L\,HO}$$

$$\left[\tilde{X}_z^{R\,HO}, \tilde{X}_{z^*}^{R\,HO}\right] = \hat{1} \tag{19}$$

The resulting higher-order (canonical) creation and annihilation operator are:

$$\hat{z}^{HO} \equiv \hat{a} = \hat{z} - \left(\frac{1}{4N} - \frac{3}{32N^2}\right)\hat{z}^\dagger\hat{z}\hat{z} + \frac{7}{32N^2}\hat{z}^\dagger\hat{z}^\dagger\hat{z}\hat{z}\hat{z} + ... \equiv \sqrt{\frac{2}{1+\hat{\kappa}}}\hat{z} \tag{20}$$

$$\hat{z}^{\dagger\,HO} \equiv \hat{a}^\dagger = \hat{z}^\dagger\sqrt{\frac{2}{1+\hat{\kappa}}}$$

and the energy operator is:

$$\hat{H}^{HO} = N(\hat{\kappa} - 1) = \hat{a}^\dagger\hat{a} \tag{21}$$

where $\hat{\kappa} \equiv \sqrt{1 + \frac{2}{N}\left(\hat{z}^{\dagger}\hat{z}\right)}$ and the operator $\sqrt{\frac{2}{1+\hat{\kappa}}}$ must be considered as functions of the single operator $\left(\hat{z}^{\dagger}\hat{z}\right)$.

The commutation relations,

$$
\begin{aligned}
\left[\hat{a}, \hat{a}^{\dagger}\right] &= \hat{1} \\
\left[\hat{H}^{HO}, \hat{a}\right] &= -\hat{a} \\
\left[\hat{H}^{HO}, \hat{a}^{\dagger}\right] &= \hat{a}^{\dagger},
\end{aligned}
\tag{22}
$$

have the non-relativistic (canonical) form. Their action on the Fock space is:

$$
\begin{aligned}
\hat{a}|n> &= \sqrt{n}|n-1> \\
\hat{a}^{\dagger}|n> &= \sqrt{(n+1)}|n+1> \\
\hat{H}^{HO}|n> &= n|n>,
\end{aligned}
\tag{23}
$$

which reproduces the non-relativistic harmonic oscillator representation, although it must be stressed that the estates $|n>$ are the same relativistic energy eigenstates as before.

3.1 Canonical coherent states.

It seems quite natural to define canonical coherent states $|a>$ as the eigenstates of the canonical annihilation operator, $\hat{a}|a>= a|a>$, with solutions:

$$
|a> = e^{-|a|^2/2} \sum_{n} \frac{a^n}{\sqrt{n!}}|n>,
\tag{24}
$$

and define a non-relativistic Bargmann-Fock space in the usual way:

$$
<a|n> = <n|a>^* = e^{-|a|^2/2}\frac{a^{*n}}{\sqrt{n!}} \equiv \Psi_n^{N.R.}(a)
\tag{25}
$$

The connection to the relativistic Bargmann-Fock space is given by

$$
\begin{aligned}
\Psi_a(z) \equiv <z|a> &= \sum_{n} <z|n><n|a> = \sum_{n} \Psi_n(z)\Psi_n^{N.R.}(a)^* \\
&= \frac{1}{\pi}\sqrt{\frac{2N-1}{2N}}e^{-|a|^2/2}\left(\frac{1+\kappa}{2}\right)^{-N}\sum_{n}\frac{1}{n!}\sqrt{\frac{(2N)_n}{(2N)^n}}\left(\frac{2az^*}{1+\kappa}\right)^n \\
&\approx \frac{1}{\pi}e^{-|a|^2/2}e^{-|z|^2/2}e^{az^*}\left\{1 - \frac{1}{4N}\left[1 - \frac{1}{2}\left(|z|^2 - az^*\right)\left(3|z|^2 - az^*\right)\right] + ...\right\}
\end{aligned}
\tag{26}
$$

The expectation value $<a|\hat{z}|a>$ defines a classical function $z = z(a)$ relating the variables a, a^* and z, z^* as follows:

$$
<a|\hat{z}|a> = a\sum_{n} c_n <a|\left(\hat{a}^{\dagger}\hat{a}\right)^n|a>
\tag{27}
$$

where c_n are the coefficients of the power series of $f(u) = \sqrt{1 + \frac{u}{2N}}$. Then we define:

$$z(a) = \sqrt{1 + \frac{|a|^2}{2N}}\, a \tag{28}$$

Note that although $< a| \left(\hat{a}^\dagger \hat{a}\right)^n |a > \neq < a|\hat{a}^{\dagger\,n}\hat{a}^n|a > = |a|^{2n}$, any operator of the form $\hat{F} = \hat{O}\hat{a}^m$ (or $\hat{G} = \hat{a}^{\dagger\,p}\hat{O}$), where $\left[\hat{H}^{HO}, \hat{O}\right] = 0$, defines a classical function $F(a)$ (or $G(a)$) by the formula:

$$F(a) = a^m \sum_n o_n |a|^{2n} , \quad G(a) = a^{*p} \sum_n o_n |a|^{2n} , \tag{29}$$

where $< a|\hat{O}|a > = \sum_n o_n < a| \left(\hat{H}^{HO}\right)^n |a > $.

The functions

$$a(z) = \sqrt{\frac{2}{1+\kappa}}\, z , \quad a^*(z) = \sqrt{\frac{2}{1+\kappa}}\, z^* \tag{30}$$

turn out to be the Darboux coordinates taking the symplectic form $\Omega \equiv \frac{1}{\kappa} dz \wedge dz^*$ to canonical form $\Omega = da \wedge da^*$.

Finally, we define

$$\hat{q} \equiv \sqrt{\frac{\hbar}{2m\omega}} \left(\hat{a} + \hat{a}^\dagger\right)$$

$$\hat{\pi} \equiv \sqrt{\frac{m\omega\hbar}{2}} \left(\hat{a}^\dagger - \hat{a}\right) \tag{31}$$

satisfying

$$[\hat{q}, \hat{\pi}] = i\hbar \hat{1} , \tag{32}$$

and their corresponding classical functions. For these operators we obviously obtain

$$\Delta\hat{q}\Delta\hat{\pi} = \frac{\hbar}{2} \tag{33}$$

on the $|a>$ states.

4 Final Remarks

The construction of the canonical (higher-order) creation and annihilation operators $\hat{a}^\dagger$ and $\hat{a}$ in the 1+1-D relativistic harmonic oscillator is a matter of convenience rather than a necessity since a first-order polarization, the manifestly covariant one, $\mathcal{P} = < \check{X}_\eta^L, \check{X}_z^L > $ exists. However, the situation become quite different for the relativistic harmonic oscillator with spin, at least from a geometrical point of view. The reason is that the doubly pseudo-extended $SO(3,2)$ (anti-de Sitter) Lie algebra, containing the commutators

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}(\hat{1} + \frac{1}{mc^2}\hat{E}) \tag{34}$$

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accounting for the mass, and the commutator

$$[\hat{J}_+, \hat{J}_-] = 2\left(\hat{J}_3 + j\hat{1}\right) \tag{35}$$

accounting for the spin, does not admit a consistent way (i.e. compatible with the rest of the symmetry) of defining two sets of first-order conjugated creation-annihilation (hor co-ordinate-momentum) operators. In other words, the system does not admit a (first-order) polarization and therefore the Hilbert space of $U(1)$-equivariant complex functions on the group can be only partially reduced [14]. The full reduction then requires the introduction of higher-order operators in the polarization, generalizing those introduced here and accounting for proper *intrinsic spin* operators.

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ON PSEUDOSUPERSYMMETRIC OSCILLATORS AND REALITY OF RELATIVISTIC ENERGIES FOR VECTOR MESONS

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Abstract

Specific oscillators - hereafter called pseudosupersymmetric oscillators - appear as interesting nonrelativistic concepts in connection with the study of relativistic vector mesons interacting with an external constant magnetic field when the real character of the energy eigenvalues is required as expected. A new pseudosupersymmetric quantum mechanics can then be developed and the corresponding pseudosupersymmetries can be pointed out.

1. Introduction

There are two old problems which appear when we study the interaction of relativistic vector mesons (spin one particles with nonzero rest mass) with external constant magnetic fields chosen, in particular, as directed along the z-axis, i.e. $\vec{B}$ = (0,0,B). The first one which will be of special interest here is mainly connected to the energy eigenvalue problem subtended by the inclusion of an anomalous moment coupling inside the relativistic equation of motion ensuring that the spin 1-boson has a gyromagnetic ratio value of g = 2. A survey of such a question has recently been presented in the Daicic-Frankel study[1] where further references can also be found. We will refer to that paper in order to save place here. The second problem is concerned with the fulfilment of the causality principle through the corresponding wave equation

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describing such an interaction. Its discussion can be referred to another contribution[2] where the so-called method of characteristics[3] plays the prominent role. Let us only comment on the fact that our final equation will satisfy all the requirements needed by the causality principle but it will not be discussed here, so that we can polarize our attention mainly on the first problem.

After a short remark pointing out the first difficulty (§2), we want to insist on our understanding of the so-called parasupersymmetric quantum mechanics (PSSQM)[4,5] for motivating our way of eliminating the above problem (§3) and for studying the new (nonrelativistic) formulation and Hamiltonian that we get in that way (§4). Besides the usual bosons, we are led to the introduction of a new kind of fermions that we call "pseudofermions" (§5) and to new symmetries that we call "pseudosupersymmetries" as it will be clear in the following by comparison with well known supersymmetries[6] and parasupersymmetries[4,5].

2. On the reality of (relativistic) energy eigenvalues

By exploiting the remarkable Johnson-Lippmann contribution[7] developed for spin $\frac{1}{2}$-particles, it is easy[1] to decompose the spin 1-formalism in a z-part associated with the so-called $H_{//}$ and, in a (x,y)-part, associated with the so-called $H_\perp$, the latter being readily studied through 1-dimensional harmonic oscillator characteristics. Then, the energy eigenvalue problem for vector mesons leads to information such that

$$E^2 = 1 + e B (n + \frac{1}{2}) - 2 e B s \qquad (2.1)$$

where e is the charge of the vector meson, n the Landau-level quantum number ($n = 0,1,2,\cdots$) and s the eigenvalues of the third component of the spin operator ($s = 0,\pm 1$), when we have chosen $\hbar = 1$, $m = 1$, $c = 1$ and defined the angular frequency $\omega = e B$ of the resulting harmonic oscillator. In eq.(2.1), the first term in the righthand side corresponds to the relativistic rest mass term, the second one to the original discussion of $H_\perp$ and the third one to the presence of an anomalous magnetic moment coupling[1]. Such an equation evidently permits

$$E^2 < 0 \qquad (2.2)$$

when $eB > 1$, $n = 0$, $s = 1$, so that we are dealing with the problem of possible complex energy eigenvalues for intense magnetic fields of critical magnitudes.

3. Some observations from PSSQM

PSSQM has been proposed by Rubakov and Spiridonov[4] and slightly modified by us[5]. Both approaches consider the superposition of bosons and parafermions[8] of order 2 and lead to 3-fold degeneracies in the energy spectrum. But, if, in the Rubakov-Spiridonov context[4], the groundstate is characterized by a negative energy eigenvalue, our groundstate has a null energy eigenvalue[9]. We have thus pointed out that the relativistic result (2.2) could have a direct connection with the nonrelativistic Rubakov-Spiridonov approach and that, consequently, we could handle the problem by exploiting our approach and its relativistic counterpart excluding results such as those given by eqs.(2.1) and (2.2).

In fact, such a method has recently been developed by one of us[10] by following strictly our PSSQM-context[5]. Here, we want, in a certain complementary way, to center our attention on new harmonic oscillatorlike characteristics ensuring the reality ot the energy eigenvalues.

4. To a new nonrelativistic Hamiltonian

We have modified the relativistic formulation of vector mesons interacting with our B-magnetic field in such a way that we get a six-component Klein-Gordon type equation of the form

$$p_0^2 \chi(x) = (1 + \pi_1^2 + \pi_2^2 + p_3^2 + eB - 2eB\Sigma_3) \chi(x) \tag{4.1}$$

where

$$\pi_i = p_i - eA_i, \quad i = 1,2, \tag{4.2}$$

$$A_1 = -\frac{1}{2}By, \quad A_2 = \frac{1}{2}Bx, \tag{4.3}$$

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$$\Sigma_3 = \begin{pmatrix} s_3 & 0 \\ 0 & s_3 \end{pmatrix}, \quad s_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{4.4}$$

This 6 by 6 formulation leads to a bounded energy spectrum ($E_0 \geq 0$) with 3-fold degeneracies and admits a nonrelativistic (NR) limit characterized by the Hamiltonian

$$H_{NR} = \frac{1}{2}(\pi_1^2 + \pi_2^2) + \frac{e\,B}{2}(1 - 2\,s_3). \tag{4.5}$$

Such developments solve our (relativistic) problem connected with eqs.(2.1) and (2.2). They also point out a new Hamiltonien (4.5) which, now, has to be visited.

5. From this new relativistic Hamiltonian : the appearance of "pseudofermions"

From supersymmetric[6] as well as parasupersymmetric[4,5] considerations, we immediately observe that the Hamiltonian (4.5) is made of two contributions : the first term is a purely bosonic part constructed in terms of even bosonic operators π_1 and π_2 while the second term looks like a purely "fermionic" part constructed in terms of odd "fermionic" operators called hereafter A and B. In fact, we propose to construct new charges

$$Q_1 = A\,\pi_1 + B\,\pi_2, \quad Q_2 = -B\,\pi_1 + A\,\pi_2, \tag{5.1}$$

where

$$A = \frac{1}{2\sqrt{2}}\begin{pmatrix} 0 & 0 & 1+i \\ 0 & 0 & -1+i \\ 1-i & -1-i & 0 \end{pmatrix}, \quad B = \frac{1}{2\sqrt{2}}\begin{pmatrix} 0 & 0 & 1-i \\ 0 & 0 & 1+i \\ 1+i & 1-i & 0 \end{pmatrix}. \tag{5.2}$$

The matrices A and B are Hermitean (so that the charges also are) and have a manifestly odd character. It is straightforward to show that, with $i, j = 1, 2$, we have

$$Q_i^3 = Q_i\,H_{NR}, \quad [Q_i, H_{NR}] = 0, \tag{5.3a}$$

$$Q_i^2 Q_j = Q_j Q_i^2 = -Q_i Q_j Q_i = Q_j H_{NR}, \quad i \neq j. \qquad (5.3b)$$

Such a structure is neither a Lie superalgebra[11], nor a Lie parasuperalgebra[12]. It is more clearly characterized when we refer to the two charges

$$Q = c(Q_1 - i Q_2), \quad Q^\dagger = c(Q_1 + i Q_2), \quad c \in \mathbb{R}. \qquad (5.4)$$

Indeed they lead to the structure relations

$$Q^2 = 0, \quad Q^{\dagger 2} = 0, \quad [H_{NR}, Q] = [H_{NR}, Q^\dagger] = 0,$$

$$Q Q^\dagger Q = 4 c^2 Q H_{NR}, \quad Q^\dagger Q Q^\dagger = 4 c^2 Q^\dagger H_{NR}, \qquad (5.5)$$

already obtained by Semenov and Chumakov[13] as possible ones associated with the discussion of 3-level systems. By searching for the charges (5.4) in terms of annihilation and creation (oscillatorlike) operators, we define

$$Q = \frac{1}{2}(A + i B)(\pi_1 - i \pi_2) = \sqrt{\omega}\, b\, a^\dagger, \quad Q^\dagger = \sqrt{\omega}\, b^\dagger a, \qquad (5.6)$$

with

$$a = \frac{1}{\sqrt{2\omega}}(\pi_1 + i \pi_2) \qquad (5.7)$$

as usual. We then get information on our "fermionic" operators b and $b^\dagger$ such that

$$b^2 = b^{\dagger 2} = 0, \quad b b^\dagger b = b, \quad b^\dagger b b^\dagger = b^\dagger. \qquad (5.8)$$

These relations mean that the corresponding particles are bosons (see eq.(5.7)) and "a new kind of fermions" (see eq.(5.8)) that we call "pseudofermions". The first equalities in eqs.(5.8) corresponding to nilpotencies show that they are not far to satisfy the Pauli principle but the last equalities say that they are not at all usual fermions. Moreover, we can prove that they are neither parafermions[8], nor quons[14], nor orthofermions[15].

For $c = 1$ or $\frac{1}{2}$, eqs.(5.4) and (5.5) appear to be compatible with those of PSSQM developed by Rubakov-Spiridonov[4] or by us[5], respectively. Moreover, the corresponding structure relations of supersymmetric developments[6] imply the eqs.(5.5).

These properties suggest that our symmetries (evidently called "pseudosuper-symmetries") are, in a certain sense, "between" super- and parasupersymmetries. We have thus the basic ingredients of a new tool that we call "pseudosupersymmetric quantum mechanics" which could be developed in terms of two "pseudopotentials" W_1 and W_2.

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ON PARASUPERSYMMETRIC OSCILLATORS
AND RELATIVISTIC VECTOR MESONS
IN CONSTANT MAGNETIC FIELDS

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Abstract

Johnson-Lippmann considerations on oscillators and their connection with the minimal coupling schemes are visited in order to introduce a new Sakata-Taketani equation describing vector mesons in interaction with a constant magnetic field. This new proposal, based on a specific parasupersymmetric oscillatorlike system, is characterized by real energies as opposed to previously pointed out relativistic equations corresponding to this interacting context.

1.   Relativistic descriptions of free vector mesons

Free vector mesons can be described through many (well known) equations, f.i.

- the KEMMER equation[1]

$$\left(\beta^{\mu} p_{\mu} - 1 \right) \psi = 0$$

where the (10×10) matrices β_{μ} generate the Kemmer algebra

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$$\beta_\mu \beta_\nu \beta_\lambda + \beta_\lambda \beta_\nu \beta_\mu = g_{\mu\nu} \beta_\lambda + g_{\lambda\nu} \beta_\mu .$$

- the SAKATA-TAKETANI equation[2]

$$i \frac{\partial}{\partial t} \varphi = \left[(I \otimes \sigma_2) + \frac{\vec{p}^2}{2} I \otimes (\sigma_2 + i\sigma_1) - i S_j S_i p_j p_i \otimes \sigma_1 \right] \varphi$$

$$\equiv H_{ST} \varphi$$

where the (6×6) matrices are direct products of $D^{(1)}$ and Pauli matrices. Notice that, in the two above equations, we take as units the rest mass, the velocity of light and the Dirac constant. Our choice is also to use the metric tensor

$$G = \{ g^{\mu\nu} \,|\, g^{00} = -g^{ii} = 1 \} .$$

The Kemmer equation reduces to the Sakata-Taketani one when one considers the (six) physical components, only. Namely, the Hamiltonian form of the equation (1.1) together with the initial condition write

$$i \frac{\partial}{\partial t} \psi = \left([\beta_0, \beta_j] p_j + \beta_0 \right) \psi \equiv H_\kappa \psi , \tag{1.3a}$$

$$\left(H_\kappa \beta_0 - 1 \right) \psi = 0 . \tag{1.3b}$$

One can then shows that, through the action of the transformation $S = 1 + \beta_j \beta_0^2 p_j$, the above system becomes

$$\left(\beta_0^2 - 1 \right) \psi' = 0 , \tag{1.4a}$$

$$i \frac{\partial}{\partial t} \psi' = H_{ST} \psi' \tag{1.4b}$$

if
$$\psi' = S \psi = \begin{pmatrix} \varphi \\ 0 \end{pmatrix} . \tag{1.5}$$

2. Relativistic descriptions for vector mesons interacting with constant magnetic fields

The corresponding equations hold for vector mesons <u>interacting with constant magnetic fields directed along the x_3-axis</u>, i.e.

- in the KEMMER case [3]

$$\left(\beta^\mu \pi_\mu - 1 + (1 - \beta_5^2) e B S_3\right) \psi = 0 \qquad (2.1)$$

where
$$\pi_\mu = p_\mu - e A_\mu, \qquad (2.2)$$

$$A_0 = 0, \quad A_1 = -\frac{B}{2} x_2, \quad A_2 = \frac{B}{2} x_1, \quad A_3 = 0, \qquad (2.3)$$

$$\beta_5 = \frac{i}{4} \varepsilon_{\mu\nu\rho\sigma} \beta^\mu \beta^\nu \beta^\rho \beta^\sigma, \quad \varepsilon_{0123} = 1, \qquad (2.4)$$

$$S_3 = i\left[\beta_1, \beta_2\right]; \qquad (2.5)$$

- in the SAKATA-TAKETANI case [4]

$$i \frac{\partial}{\partial t} \varphi = \left[(I \otimes \sigma_2) + \frac{\vec{\pi}^2}{2} I \otimes (\sigma_2 + i \sigma_1) - i S_j S_l \pi_j \pi_l \otimes \sigma_1 + e B S_3 \otimes \sigma_2\right] \varphi. \quad (2.6)$$

The eigenvalues E corresponding to the physical components write [3,4] in both cases

$$E^2 = 1 + e B (n + \frac{1}{2}) + 2 e B S, \quad S = 0, \pm 1, \quad n = 0, 1, 2, \cdots, \qquad (2.7)$$

if we limit ourselves to the so-called perpendicular part (i.e. in the plane (x_1, x_2)). So, for the particular values $n = 0$ and $S = -1$, we obtain

$$E^2 = 1 - e B \qquad (2.8)$$

which could, for sufficiently large magnetic fields, lead to complex energies. This is an old problem [5] and we propose to solve it by investigating a very recent tool : the so-called "parasupersymmetric oscillators"

3. Parasupersymmetry and the corresponding new Sakata-Taketani equation

The nonrelativistic limit corresponding to the interacting Sakata-Taketani or Kemmer Hamiltonians (2.1) and (2.6) is

$$H_{NR} = \frac{1}{2}(\pi_1^2 + \pi_2^2) + e\,B\,S_3.\tag{3.1}$$

Taking

$$\omega = e\,B,\tag{3.2a}$$

$$a = \frac{1}{\sqrt{2\,e\,B}}(\pi_1 + i\,\pi_2)\tag{3.2b}$$

$$a^\dagger = \frac{1}{\sqrt{2\,e\,B}}(\pi_1 - i\,\pi_2),\tag{3.2c}$$

we get

$$H_{NR} = \frac{\omega}{2}\{a, a^\dagger\} + \omega\,S_3 = \frac{\omega}{2}\{a, a^\dagger\} + \omega\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix},\tag{3.3}$$

and

$$E_{NR} = \omega\left(n + \frac{1}{2}\right) + \omega\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.\tag{3.4}$$

These are the RUBAKOV-SPIRIDONOV parasupersymmetric Hamiltonian and spectrum for an oscillatorlike interaction[6]. A specific feature of this parasupersymmetric model is the existence of negative eigenvalues. This evidently leads to complex relativistic energies for sufficiently large magnetic fields and confirms the Tsai results[5].

We propose here to eliminate this defect by using another parasupersymmetric model : the BECKERS-DEBERGH parasupersymmetric oscillator [7] characterized by positive energies, only. More precisely, the BECKERS-DEBERGH spectrum corresponds to

$$E_{NR} = \omega \left(n + \frac{1}{2} \right) + \frac{\omega}{2} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

(3.5)

Thus, the remaining point is to construct a Sakata-Taketani Hamiltonian whose nonrelativistic limit would lead to such a spectrum. We take [8]

$$H_{ST} = (I \otimes \sigma_2) + \frac{\pi_1^2 + \pi_2^2}{2} I \otimes (\sigma_2 - i \sigma_1) + \frac{i}{2} (\pi_1^2 + \pi_2^2) S_3^2 \otimes \sigma_1$$

$$- (\pi_1^2 + \pi_2^2) \lambda + (\Pi_1^2 + \Pi_2^2) \lambda - \frac{i}{2} (\pi_1 \Pi_1 - \pi_2 \Pi_2) (S_1^2 - S_2^2) \otimes \sigma_1$$

$$- \frac{i}{2} (\pi_1 \Pi_2 - \pi_2 \Pi_1) \{ S_1 , S_2 \} \otimes \sigma_1 + e B \eta,$$

(3.6)

where λ, η are undetermined and

$$\Pi_a = p_a + e A_a, \quad a = 1, 2,$$

(3.7)

In order to solve our problem, we have to impose different conditions like

$$\left\{ \lambda , (S_1^2 - S_2^2) \otimes \sigma_1 \right\} = \left\{ \lambda , \{ S_1 , S_2 \} \otimes \sigma_1 \right\} = 0,$$

(3.8a)

$$- \frac{i}{2} \left\{ (S_1^2 - S_2^2) \otimes \sigma_1 , \eta \right\} + 2 \left(\{ S_1 , S_2 \} \otimes \sigma_1 \right) \lambda - \frac{i}{2} \{ S_1 , S_2 \} \otimes \sigma_3 = 0,$$

(3.8b)

$$- \frac{i}{2} \left\{ \{ S_1 , S_2 \} \otimes \sigma_1 , \eta \right\} - 2 \left((S_1^2 - S_2^2) \otimes \sigma_1 \right) \lambda + \frac{i}{2} (S_1^2 - S_2^2) \otimes \sigma_3 = 0,$$

(3.8c)

in order to the eliminate terms like $(\pi_1^2 + \pi_2^2)^2, \cdots$.

We then obtain

$$\lambda = \begin{pmatrix} a_1 & 0 & 0 & -\dfrac{i}{4} & a_3 & 0 \\[6pt] 0 & a_1 & 0 & -a_3 & -\dfrac{i}{4} & 0 \\[6pt] 0 & 0 & 0 & 0 & 0 & a_2 \\[6pt] \dfrac{i}{4} & a_3 & 0 & -a_1 & 0 & 0 \\[6pt] -a_3 & \dfrac{i}{4} & 0 & 0 & -a_1 & 0 \\[6pt] 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\eta = \begin{pmatrix} \alpha_1 & -2i\,a_1 & 0 & \alpha_4 & \alpha_3 & 0 \\[6pt] 2i\,a_1 & \alpha_1 & 0 & -\alpha_3 & \alpha_4 & 0 \\[6pt] 0 & 0 & \alpha_5 & 0 & 0 & \alpha_2 \\[6pt] 4i\,a_3 - \alpha_4 & \alpha_3 & 0 & -\alpha_1 & 2i\,a_1 & 0 \\[6pt] -\alpha_3 & 4i\,a_3 - \alpha_4 & 0 & -2i\,a_1 & -\alpha_1 & 0 \\[6pt] 0 & 0 & \alpha_6 & 0 & 0 & -\alpha_5 \end{pmatrix},$$

together with constraints like

$$a_1^2 - a_3^2 = -\frac{1}{16}, \quad a_3\,\alpha_3 = a_1\,\alpha_1, \quad \cdots .$$

Taking now

$$a_1 = 0, \quad a_2 = -\frac{i}{2}, \quad a_3 = \frac{1}{4},$$

$$\alpha_1 = \frac{i}{\omega}\sqrt{3}, \quad \alpha_2 = i, \quad \alpha_3 = 0, \quad \alpha_4 = -\frac{i}{\omega} + \frac{i}{2}, \quad \alpha_5 = \frac{i}{\omega}, \quad \alpha_6 = \frac{i}{\omega},$$

we finally have

$$E_{NR} = \omega\left(n' + \frac{1}{2}\right) + \frac{\omega}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \equiv E_{NR}^{B.D.} \tag{3.9a}$$

with

$$n' \equiv n_1 + n_2 . \tag{3.9b}$$

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Of course, in these developments, we have exploited Johnson-Lippmann considerations[9] relating the motion in a constant magnetic field with oscillatorlike interactions and implying in particular that the eigenvalues of the operators $\frac{1}{2}(\pi_1^2 + \pi_2^2)$ and $\frac{1}{2}(\Pi_1^2 + \Pi_2^2)$ are $\omega(n_1 + \frac{1}{2})$ and $\omega(n_2 + \frac{1}{2})$, respectively. As a result, a Sakata-Taketani type Hamiltonian avoiding the complexity of the energies is

$$H_{ST} = (I \otimes \sigma_2) + i(I \otimes \sigma_3) + i(\sqrt{3} - 1)S_3^2 \otimes \sigma_3$$

$$+ \frac{i}{2}I \otimes (\sigma_1 - i\sigma_2) + \frac{i}{2}S_3^2 \otimes (\sigma_1 + i\sigma_2)$$

$$+ \frac{1}{4}(\pi_1^2 + \pi_2^2)\left(-iS_3 \otimes \sigma_1 + iS_3^2 \otimes \sigma_1 + I \otimes (\sigma_2 - i\sigma_1)\right)$$

$$+ \frac{1}{4}(\Pi_1^2 + \Pi_2^2)\left(iS_3 \otimes \sigma_1 + iS_3^2 \otimes \sigma_1 + I \otimes (\sigma_2 - i\sigma_1)\right)$$

$$- \frac{i}{2}(\pi_1\Pi_1 - \pi_2\Pi_2)(S_1^2 - S_2^2) \otimes \sigma_1 - \frac{i}{2}(\pi_1\Pi_2 + \pi_2\Pi_1)\{S_1, S_2\} \otimes \sigma_1$$

$$+ eB\left(\frac{i}{2}I \otimes (\sigma_1 + i\sigma_2) + \frac{1}{2}S_3^2 \otimes \sigma_2\right). \tag{3.10}$$

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Pseudoclassical description of the Dirac Oscillator.

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Abstract

In this paper we discuss the Dirac Oscillator wave equation in terms of a pseudoclassical language, using Grassmann variables to describe the internal degrees of freedom of the oscillator. Regarding the original wave equation as a classical constraint, we use the theory of constrained systems, to develop a reparametrization invariant lagrangian, which is the pseudoclassical equivalent of the quantum case. The consistency of the Hamiltonian formalism and the quantization procedure are also analized.

1. Introduction

As is well known, in the second decade of this century Dirac developed the square root method, to analyze the internal spin degrees of freedom in quantum mechanics. Dirac accomplished his task by means of a Clifford algebra for these degrees. Altought at that time the Grassmann algebras were already known, there existed no classical counterpart available for his approach. In present day point of view, however, we know that this old problem can be formulated using anticommuting, fermionic variables, to reproduce the behavior of the spin degrees of freedom at the classical level. Since the Grassmann variables have no direct physical meaning, the theories formulated with them are usually

called pseudoclassical.

One important point of the approach formulated above is that, associated with the anticommuting variables and involving also the rest of the non-Grassmann dynamical variables of the theory, (called bosonic variables), there exist a supersymmetric gauge invariance in the formulation. One of the reasons for this supersymmetry is the fact that any quantum wave equation present in the theory is translated at the classical level as a first class constraint. According to Dirac conjecture, all first class constraints generate gauge transformations, but since in this case the Grassmann and the bosonic variables are mixed up by the gauge transformation they become, in fact, supersymmetric.

This way of reasoning has been analyzed by several authors [1,2,3,4] as a pevious step to quantization. The idea is in some sense based in Dirac's point of view that we should first try to fully understand a problem at a classical level, and only then try to quantize it [5]. One consequence of this procedure is that we can apply it to systems which we don't fully understand, for instance in the case of two body, or more, relativistic wave equations [1]. The interesting point here is that the time evolution of the dynamical variables are just the Euler Lagrange equations, which in principle are known, thus solving the dynamics of the problem, at least at the classical level.

2. The Dirac Oscillator

Let us begin with a simple introduction to the Dirac Oscillator. Some years ago, Moshinsky and Szczepaniak introduced a relativistic wave equation linear in momentum and in position which has an harmonic oscillator spectrum plus a strong spin-orbit coupling term [6]. This equation is obtained by the replacement of the momentum of the particle in the Dirac equatiom by

$$\mathbf{p} \rightarrow \mathbf{p} - im\omega\mathbf{r}\beta, \qquad\qquad 1)$$

where $\mathbf{p}$ is the momentum, m the mass of the particle and r is its position, ω is the frequency of the oscillator, and β the Dirac γ^0 matrix. Taking advantage of the frame dependence vector u^μ, it is easy to show that the Dirac oscillator equation can be put in

the manifestly covariant form

$$(\theta \cdot P + m\theta_5)\psi = 0, \qquad\qquad 2)$$

where

$$P^\mu \equiv p^\mu - 2im\omega x_\perp^\mu (\hat{u} \cdot \theta)\theta_5, \qquad\qquad 3.a)$$

and

$$x_\perp^\mu \equiv x^\mu + (\hat{u} \cdot x)\hat{u}^\mu \qquad\qquad 3.b)$$

The operators θ^μ and θ_5, are expressed in terms of the Dirac matrices in the following way

$$\theta^\mu \equiv \frac{i}{\sqrt{2}}\gamma_5\gamma^\mu, \quad \mu = 0,1,2,3$$
$$\theta_5 = \frac{i}{\sqrt{2}}\gamma_5, \qquad\qquad\qquad 3.c)$$

where $\gamma_5 = i\gamma^0\gamma^1\gamma^2\gamma^3$. We use natural units in which $\hbar = c = 1$ and our metric is given by $(\eta_{\mu\nu}) = \text{diag.}(-1,1,1,1)$. We recover the original Dirac Oscillator in the frame in which $\hat{u}^\mu = (1,0,0,0)$. The solution, spectrum degeneracy, hidden supersymetry and other important properties are discussed in [8,9], (and references therein).

3. Pseudoclassical description

Now, the idea is to reformulate the problem in a pseudoclassical language. This is done in a natural way by translating Eq. 2) into a first class constraint

$$\mathcal{J} \equiv \theta \cdot P + m\theta_5 \approx 0, \qquad\qquad 4)$$

where $\approx$ means weak equality and the dynamical variables become pseudoclassical ones

$$\{\theta^\mu, \theta^\nu\} = i\eta^{\mu\nu},$$
$$\{\theta_5, \theta_5\} = i. \qquad\qquad 5.a)$$

Of course we know that

$$\{x^\mu, p^\nu\} = \eta^{\mu\nu}. \qquad\qquad 5.b)$$

The Poisson braket of the first class constraint $\mathcal{J}$ with itself, is the classical equivalent of the square of the Dirac Oscillator. In this way, thus, we generate another constraint

which could be called the pseudoclassical analogue of the Klein Gordon equation. This new constraint is constructed in such a way to be again a first class, altought secondary, constraint. Of course, if there is any second class constraint we should replace the Poisson braket for the Dirac one, in order to get rid of them.

In our case the superalgebra obeyed by the constraints is given by

$$\{\mathcal{J}, \mathcal{J}\} = i\mathcal{H} = i(P^2 + m^2 - 4im\omega\lambda) \approx 0,$$

$$\{\mathcal{J}, \mathcal{H}\} = 0, \qquad\qquad 6)$$

$$\{\mathcal{H}, \mathcal{H}\} = 0.$$

In this equation, λ is given by

$$\lambda \equiv (\theta \cdot x_\perp)\hat{u} \cdot (m\theta - \theta_5 P). \qquad\qquad 7)$$

Notice that the first of this constraints is precisely the pseudoclassical Klein Gordon equation. Is in this sense that we say that we translate the square root method into a classical language. We also note from Eq. 7) that $\mathcal{J}$ and $\mathcal{H}$ are first class.

Following the procedure described in Ref. [7], we can construct the Lagrangian of the problem. Since the whole dynamics of the theory is contained in the constraints, the Hamiltonian of the system is a linear combination of them

$$H = N\mathcal{H} + iM\mathcal{J} \equiv 0, \qquad\qquad 8)$$

where N and M are gauge fixing parameters. This in turn means that the Hamiltonian is weakly zero, implying a reparametrization invariant Lagrangian as a consequence. According to Ref. [7] the whole action is given by

$$S = \int_{\tau_2}^{\tau_1} d\tau \{-m\sqrt{-z^2}[1 - 2i\omega(\theta \cdot x_\perp)(\hat{u} \cdot \theta)] + i/2[\dot{\theta}^\mu \theta_\mu + \dot{\theta}_5 \theta_5]$$
$$- 2im\omega(\theta \cdot x_\perp)\theta_5(\hat{u} \cdot z) + 2im\omega(z \cdot x_\perp)(\hat{u}\theta)\theta_5 \qquad\qquad 9)$$
$$- 2m\omega M(\theta \cdot x_\perp)(\hat{u} \cdot \theta)\theta_5 - imM\theta_5.$$

Where $z^\mu \equiv \dot{x}^\mu - iM\theta^\mu$.

It is not hard to prove that this action is the correct answer to our problem. From the Hamiltonian formalism, we know that the time evolution of any dynamical variable F is given by

$$\dot{F} = \{F, H\}. \qquad\qquad 10)$$

Hence, for the dynamical variables in our case we obtain that

$$\dot{x}^\mu = iM\theta^\mu + 2NP^\mu + 4im\omega N(\theta \cdot x_\perp)\theta_5 u^\mu$$

$$\dot{\theta}^\mu = 4m^2\omega N[x_\perp^\mu(\hat{u} \cdot \theta) - (\theta \cdot x_\perp)\hat{u}^\mu] + MP^\mu \qquad 11)$$

$$\dot{\theta}_5 = mM - 2imM\omega(\theta \cdot x_\perp)(\hat{u} \cdot \theta) - 4m\omega N(x_\perp \cdot P)(\hat{u} \cdot \theta) + 4m\omega N(\theta \cdot x_\perp)(\hat{u} \cdot P),$$

which are precisely the Euler-Lagrange equations of the action 9) provided

$$N(\tau) = \frac{\sqrt{-z^2}}{2m}[1 + 2i\omega(\theta \cdot x_\perp)(\hat{u} \cdot \theta)]. \qquad 12)$$

This result proves the complete agreement between the Hamiltonian and Lagrangian formalisms, and as a result we are confident that action 9) is the corect answer. What Eq. 12) tells us is that we can specify the gauge by giving a value to $\sqrt{-z^2}$, usually $\sqrt{-z^2} = -1$. In the same way we can construct the supergauge transformations for each dynamical variable F by means of the equations

$$\delta F = \{F, \epsilon^a(\tau)\phi_a\}, \quad a = 1,2 \qquad 13)$$

where ϕ_a represent our two constraints, and $\epsilon^a(\tau)$ are two time dependent infinitesimal parameters. The result is too long to be given here, (see reference [7]), the only point we want to remark here is that, as we already mentioned, they express the full dynamics of the theory, as is suggested by the comparisson of Eqs. 10) and 13).

4. Conclusions

We note form Eq. 3.a) that the Dirac Oscillator interaction term is θ-dependent. In cases like this, the quantization procedure should be done carefully, since some properties of the Grassmann variables changes radically when quantized. For example, the θ_5 variable has the property that $\theta_5{}^2 = 0$ at the classical level, but at the quantum level (Eq. 3.c) $\theta_5{}^2 = -1/2$. Thus if we consider for instance, the Taylor expansion of a θ_5 dependent function, we obtain different results depending wether the quantization is done before or after the series expansion.

In the case of the system studied here, if we put in Eq. 6) the square of P^μ given by 3.a) and proceed to quantize by means of definitions (3.c), we obtain a wrong result. The

central point here, is that we should regard P^μ as a basic quantity to quantize. If instead of developing the square of P^μ, we first quantize Eq. 6) and regard 3.a) as a quantum operator identity, we obtain a complete compatibilty with the Klein Gordon wave equation associated with the Dirac Oscillator. Finally, we would like to remark that our approach could be useful to problems that are not fully understood at the quantum level, but that have θ-dependent interaction terms, such as the afforementioned two body relativistic wave equations and some supergravity theories [7].

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NOTES ON OSCILLATOR-LIKE INTERACTIONS OF VARIOUS SPIN RELATIVISTIC PARTICLES*

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Abstract

The equations for various spin particles with oscillator-like interactions are discussed in this talk. Contents: 1. Comment on "The Klein-Gordon Oscillator"; 2. The Dirac oscillator in quaternion form; 3. The Dirac-Dowker oscillator; 4. The Weinberg oscillator; 5. Note on the two-body Dirac oscillator.

1   Comment on "The Klein-Gordon Oscillator"

In connection with the publications of Moshinsky *et al.*, e. g. [1], the interest in the model with the $j = 1/2$ Hamiltonian that is linear in both momenta and coordinates has grown recently [2]. Analogous type of interaction has been considered for the case of $j = 0$ and $j = 1$ Duffin-Kemmer field [3] and for the case of $j = 0$ Klein-Gordon field [4].

In the paper [4] the operators $\vec{Q}$, coordinate, and $\vec{P}$, momentum, have been represented in $n \otimes n$ matrix form

$$\vec{Q} = \hat{\eta}\vec{q}, \qquad \vec{P} = \hat{\eta}\vec{p}, \tag{1.1}$$

with $\hat{\eta}^2 = 1$. The interaction in the Klein-Gordon equation has been introduced in the following way:

$$\vec{P} \to \vec{P} - im\hat{\gamma}\hat{\Omega} \cdot \vec{Q}, \tag{1.2}$$

where for the sake of completeness $\hat{\Omega}$ is chosen by $3 \otimes 3$ matrix with coefficients $\hat{\Omega}_{ij} = \omega_i \delta_{ij}$. The $\hat{\gamma}$ matrix obeys the following anticommutation relations $\{\hat{\gamma}, \hat{\eta}\} = 0$, $\hat{\gamma}^2 = 1$.

The Klein-Gordon equation for $\Psi(\vec{q}, t)$, the wave function which could be expanded in two-component form, is then

$$-\frac{\partial^2}{\partial t^2}\Psi(\vec{q}, t) = \left(\vec{p}^2 + m^2\vec{q} \cdot \hat{\Omega}^2 \cdot \vec{q} + m\hat{\gamma}\, tr\Omega + m^2\right)\Psi(\vec{q}, t), \tag{1.3}$$

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what gives the energy spectrum [4]

$$E^2_{(a)N_i} - m^2 = 2m\left(\omega_1 N_1 + \omega_2 N_2 + \omega_3 N_3\right), \qquad N_1, N_2, N_3 = 0, 1, 2 \ldots$$

$$E^2_{(b)N_i} - m^2 = 2m\left(\omega_1(N_1 + 1) + \omega_2(N_2 + 1) + \omega_3(N_3 + 1)\right). \tag{1.4}$$

However, the physical sense of implementing the matrices $\hat{\eta}$ and $\hat{\gamma}$ in [4] is obscure. In this Section we try to attach some physical foundations to this procedure. It is well-known some ways to recast the Klein-Gordon equation in the Hamiltonian form e. g. [5, 6]. First of all, the Klein-Gordon equation could be re-written to the system of two coupled equations [6,p.98]

$$\frac{\partial \Psi}{\partial x^\alpha} = \kappa \Xi_\alpha, \qquad \frac{\partial \Xi^\alpha}{\partial x^\alpha} = -\kappa \Psi, \tag{1.5}$$

where $\kappa = mc/\hbar$ (in the following we use the system where $c = \hbar = 1$). By means of redefining the components they are easy to present in the matrix Hamiltonian form (cf. with [7])

$$i\frac{\partial}{\partial t}\begin{pmatrix} \phi \\ \chi_1 \\ \chi_2 \\ \chi_3 \end{pmatrix} = \left[\begin{pmatrix} 0 & p_1 & p_2 & p_3 \\ p_1 & 0 & 0 & 0 \\ p_2 & 0 & 0 & 0 \\ p_3 & 0 & 0 & 0 \end{pmatrix} + m\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}\right]\begin{pmatrix} \phi \\ \chi_1 \\ \chi_2 \\ \chi_3 \end{pmatrix} \tag{1.6}$$

provided that $\phi = i\partial_t \Psi + m\Psi$, $\chi_i = -i\nabla_i \Psi = \vec{p}_i \Psi$. Using matrices $\vec{\alpha}$ and β, corresponding to this case, and introducing interaction analogously [1a] we come to the equation for upper component

$$(E^2 - m^2)\phi = \left[\vec{p}^2 + m^2\omega^2\vec{r}^2 - 3m\omega\right]\phi \tag{1.7}$$

what coincides with Eq. (10a) of ref. [4] in the case $\omega_1 = \omega_2 = \omega_3$.

The similar formulation also originated from the Duffin-Kemmer approach. In this case the wave function $\Phi = column(\phi_1, \phi_2, \chi_i)$ is five-dimensional and its components are $\phi_1 = (i\partial_t \Psi + m\Psi)/\sqrt{2}$, $\phi_2 = (i\partial_t \Psi - m\Psi)/\sqrt{2}$, $\chi_i = -i\nabla_i \Psi = \vec{p}_i \Psi$. It satisfies the equation

$$i\frac{\partial \Phi}{\partial t} = \left(\vec{B}\vec{p} + m\beta_0\right)\Phi, \qquad B_\mu = [\beta_0, \beta_\mu]_- \tag{1.8}$$

(our choice of $5 \otimes 5$ dimension β-matrices corresponds to ref. [3]). As shown there, the substitution $\vec{p} \to \vec{p} - im\omega\eta_0\vec{r}$ leads to the equation (1.7) for both ϕ_1 and ϕ_2. Let us remark, in both the approach based on Eq. (1.6) and the Duffin-Kemmer approach, Eq. (1.8), we have the equation

$$(E^2 - m^2)\chi_i = (p_i - im\omega x^i)(p_j + im\omega x^j)\chi_j \tag{1.9}$$

for down component, which seems to not be reduced to oscillator-like equation.

Then, Sakata-Taketani approach, e. g. [5], is characterized by the equation which we write in the form:

$$i\frac{\partial}{\partial t}\Phi = \left\{\frac{\vec{p}(\tau_3 + i\tau_2)\vec{p}}{2m} + m\tau_3\right\}\Phi, \tag{1.10}$$

with τ_i being the Pauli matrices. $\Phi = column(\phi, \chi)$ is the two-component wave function with components which could be written as following: $\phi = (\Psi + \frac{i}{m}\partial_t \Psi)/\sqrt{2}$, $\chi = (\Psi - \frac{i}{m}\partial_t \Psi)/\sqrt{2}$.

From the previous experience we learned that in order to get the oscillator-like equation we need to do substitution with matrix which anticommutes with matrix structure of the momentum part of the equation. In our case the matrix which has this property is τ_1 matrix. Therefore, we do the substitution $\vec{p} \to \vec{p} - im\omega\tau_1\vec{r}$ and come to

$$E^2\xi = \left[\vec{p}^2 + m^2\omega^2\vec{r}^2 - 3m\omega + m^2\right]\xi, \tag{1.11}$$

where $\xi = \phi + \chi$, and to the analogous equation for $\eta = \phi - \chi = \frac{E}{m}(\phi + \chi)$. In the process of calculations we convinced ourselves that the interaction Hamiltonian

$$\mathcal{H} = \frac{1}{2m}\left(\vec{p}^2 + m^2\omega^2\vec{x}^2 - 3m\omega\right)(\tau_3 + i\tau_2) + m\tau_3 \tag{1.12}$$

is the same as in [3, formula (3.9)] since $\tau_1(\tau_3 + i\tau_2)\tau_1 = -(\tau_3 + i\tau_2)$ and $(\tau_3 + i\tau_2)\tau_1 = \tau_3 + i\tau_2$.

2 The Dirac oscillator in quaternion form

The quaternion (and conjugated to it) with real coefficient is defined as $q = q_0 + iq_1 + jq_2 + kq_3$, $\bar{q} = q_0 - iq_1 - jq_2 - kq_3$. The basis vectors satisfy the equations $i^2 = j^2 = k^2 = -1$ and $ij = -ji = k$ with cyclic permutations. Considering a two-component quaternionic spinor (or $SL(2, H)$ spinor) one could write the free Dirac equation as following, ref. [8c,d],

$$\tilde{\Gamma} \cdot \partial\Psi - m\tau_3\Psi k = 0. \tag{2.1}$$

Anticommutation relations for $\tilde{\Gamma}$ are given in [8d,p.222]. In Pauli representation ($i \to -\sqrt{-1}\tau_1$, $j \to -\sqrt{-1}\tau_2$ and $k \to -\sqrt{-1}\tau_3$) it goes through to usual Dirac equation and its complex conjugate. As mentioned in [8] it is convenient to diagonalize the matrices entering in Eq. (2.1) using matrix

$$T = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -\sqrt{-1} \\ 1 & \sqrt{-1} \end{pmatrix}. \tag{2.2}$$

In such a way we come to biquaternionic formulation ($q_i \in \mathbb{C}$):

$$\begin{cases} \bar{\partial}\psi_L + im\bar{\psi}_R^\dagger = 0 \\ \partial\bar{\psi}_R^\dagger + im\psi_L = 0, \end{cases} \tag{2.3}$$

where $\psi_L \equiv \psi p_+$, $\psi_R \equiv \psi p_-$. This decomposition of Ψ into left ideals is carried out by means of the projection operators $p_\pm = (b_0 \pm b_3)/2$. New basis is $b_0 \equiv 1, b_1 \equiv \sqrt{-1}i, b_2 \equiv \sqrt{-1}j, b_3 \equiv \sqrt{-1}k$ and $\bar{b}_0 = b_0, \bar{b}_\alpha = -b_\alpha$. Introducing interaction in the form $\partial_i \to \partial_i + \tau_3 V_i(\vec{x})$, V is the compensating field for this type of $Sp(1, Q)$ transformations, and taking into account that the vectors of biquaternionic basis anticommute $b_\alpha\bar{b}_\beta + b_\beta\bar{b}_\alpha = -2\eta_{\alpha\beta}$, $\eta_{\alpha\beta} = diag(-1, 1, 1, 1)$, we come to the equations for the left and right spinor-quaternions in the following form:

$$(E^2 - m^2)\psi_L = \left[(\vec{p}^2 + k^2\vec{x}^2) - 3k - 2\epsilon_{ijk}b_k x_i p_j\right]\psi_L \tag{2.4}$$

$$(E^2 - m^2)\bar{\psi}_R^\dagger = \left[(\vec{p}^2 + k^2\vec{x}^2) + 3k + 2\epsilon_{ijk}b_k x_i p_j\right]\bar{\psi}_R^\dagger \tag{2.5}$$

if we choose $V_i(\vec{x}) = kx_i$. Eqs. (2.4) and (2.5) are the Dirac oscillator equations in the Pauli rep, $b_k \to \tau_k$. Analogous equations for ψ_R and $\bar{\psi}_L^\dagger$ could be obtained from (2.3) if one choose the opposite signs at the mass terms.

3 The Dirac-Dowker oscillator

In this Section we start from the equation for any spin given by Dirac [9] in the form written down by Corson, ref. [6,p.154], (here we use Corson's notation)

$$\begin{cases} \partial^{\dot{A}B} v_B(k+\tfrac{1}{2})\psi(k+\tfrac{1}{2}, l-\tfrac{1}{2}) - m\left(\tfrac{2k+1}{2l}\right)^{1/2} v^{\dot{A}}(l)\psi(k,l) = 0 \\[2mm] \partial_{\dot{A}B} v^{\dot{A}}(l)\psi(k,l) + m\left(\tfrac{2l}{2k+1}\right)^{1/2} v_B(k+\tfrac{1}{2})\psi(k+\tfrac{1}{2}, l-\tfrac{1}{2}) = 0, \end{cases} \tag{3.1}$$

where v_A and $v_{\dot{A}}$ are the rectangular spinor-matrices of $2k$ rows and $2k+1$ columns (see, e. g., section 17b of ref. [6] for the details). The wave function $\psi(k,l)$ belongs to the (k,l) representation of the homogeneous Lorentz group. The choice $l = 1/2$ and $k = j - 1/2$, j is the spin of a particle, permits one to reduce a number of subsidiary conditions. Moreover, the equations (3.1) are shown by Dowker [10] to recast to the matrix form which is similar to the well-known Dirac equation for $j = 1/2$ particle

$$\begin{cases} \alpha^\mu \partial_\mu \Phi = m\Upsilon \\[2mm] \bar{\alpha}^\mu \partial_\mu \Upsilon = -m\Phi. \end{cases} \tag{3.2}$$

The $4j$- component function Φ could be identified with the wave function in $(j,0) \oplus (j-1,0)$ representation. Then, Υ, which also has $4j$ components, is written down

$$\Upsilon = (-1)^{2j}(2j)^{-\frac{1}{2}} \begin{pmatrix} v_{\dot{A}}(j-\tfrac{1}{2}) \otimes v^{\dot{A}}(\tfrac{1}{2}) \\ u_{\dot{A}}(j) \otimes v^{\dot{A}}(\tfrac{1}{2}) \end{pmatrix} \psi(j - \tfrac{1}{2}, \tfrac{1}{2}). \tag{3.3}$$

and it belongs to $(j - 1/2, 1/2)$ representation. The matrices α^μ and $\bar{\alpha}^\mu = \alpha_\mu$ obeys all the algebraic relations of the Pauli matrices $\bar{\alpha}^{(\mu}\alpha^{\nu)} = g^{\mu\nu}$, except for completeness.

Defining $p_\mu = -i\partial_\mu$ and the analogs of γ- matrices as following:

$$\gamma^\mu = \begin{pmatrix} 0 & -i\bar{\alpha}^\mu \\ i\alpha^\mu & 0 \end{pmatrix} \tag{3.4}$$

the set of equations (3.2) is written down to the form of the Dirac equation

$$(p_\mu \gamma^\mu - m)\begin{pmatrix} \Phi \\ \Upsilon \end{pmatrix} = 0. \tag{3.5}$$

However, let us not forget that Φ and Υ are 2-spinors only in the case of $j = 1/2$.

In the case of spin $j = 1/2$ it is well-known the set of γ- matrices is defined up to the unitary transformation and Eq. (3.5) could be recast to the Hamiltonian form given by Dirac (with α_k and β matrices) by means of the unitary matrix. It is easy to carry out the same procedure $(\alpha^k = S\gamma^0\gamma^k S^{-1}$ and $\beta = S\gamma^0 S^{-1})$ for γ- matrices, Eq. (3.4), and functions of arbitrary spin $(\Psi = S^{-1}\Phi)$. For our aims it is convenient to chose the unitary matrix as following:

$$S = \frac{1}{\sqrt{2}}\begin{pmatrix} \mathbb{1}_{4j\otimes 4j} & i\mathbb{1}_{4j\otimes 4j} \\ i\mathbb{1}_{4j\otimes 4j} & \mathbb{1}_{4j\otimes 4j} \end{pmatrix}. \tag{3.6}$$

After standard substitution $\vec{p} \rightarrow \vec{p} - im\omega\gamma^0\vec{r}$ we obtain

$$E\phi = -i\left[\alpha_0(\vec{\alpha}\vec{p}) + im\omega(\vec{\alpha}\vec{r})\right]v + m\alpha_0\phi, \tag{3.7}$$

$$Ev = i\left[\alpha_0(\vec{\alpha}\vec{p}) - im\omega(\vec{\alpha}\vec{r})\right]\phi - m\alpha_0v. \tag{3.8}$$

Since it follows from the anticommutation relations that $\alpha_i\alpha_0 = \alpha_0\alpha_i$ we have the equations which coincide with Eq. (8) of ref. [1a] or Eqs. (3.6) and (3.12) of ref. [1d] except for $\tau_\mu \rightarrow \alpha_\mu$, i. e. their explicit forms,

$$(E^2 - m^2)\phi = \left[\vec{p}^2 + m\omega\vec{r}^2 - 3\alpha_0 m\omega - m\omega\alpha_0\alpha^{[i}\bar{\alpha}^{j]}r^i\nabla_j\right]\phi \tag{3.9}$$

$$(E^2 + m^2)v = \left[\vec{p}^2 + m\omega\vec{r}^2 + 3\alpha_0 m\omega + m\omega\alpha_0\alpha^{[i}\bar{\alpha}^{j]}r^i\nabla_j\right]v. \tag{3.10}$$

Thus, we convinced ourselves that we got the same oscillator-like interaction and the similar spectrum as for the case of $j = 1/2$ particles in [1a].

4 The Weinberg oscillator

The principal equation of $2(2j + 1)$- component approach [11] in the case of spin $j = 1$ is

$$(\gamma_{\mu\nu}p_\mu p_\nu + M^2)\Psi^{(j=1)}(x) = 0, \tag{4.1}$$

with $\gamma_{\alpha\beta}$ being $6 \otimes 6$ covariantly defined matrices. The $j = 1$ Hamiltonian has been given in refs. [11b,c]:

$$\mathcal{H} = \frac{2E^2}{2E^2 - M^2}(\vec{\alpha}\vec{p}) + \beta\left[E - \frac{2E}{2E^2 - M^2}(\vec{\alpha}\vec{p})^2\right], \tag{4.2}$$

where

$$\vec{\alpha} \equiv \begin{pmatrix} \vec{S} & 0 \\ 0 & -\vec{S} \end{pmatrix}, \qquad \beta \equiv \begin{pmatrix} 0 & \mathbb{1}_{3\otimes3} \\ \mathbb{1}_{3\otimes3} & 0 \end{pmatrix}.$$

(S_i are the spin matrices for a vector particle).

In general, the upper and down components of 6- component wave function do not uncouple neither under the interaction $\vec{p} \rightarrow \vec{p} - im\omega\beta\vec{r}$ nor under $\gamma_{5,\mu\nu}u_\mu r_\nu$. However, if we introduce the Dirac oscillator interaction so that the conditions of the longitudity of $\Psi = column(\phi_i, \chi_i)$ respective to $\vec{r}$, i. e. $\vec{r}\times\vec{\phi} = 0$, $\vec{r}\times\vec{\chi} = 0$ are fulfilled, we come to the equations more simple

$$(2E^2 - M^2)\xi = E(\vec{S}\vec{p})\eta + \left[(\vec{S}\vec{p}) - k(\vec{S}\vec{r})\right](\vec{S}\vec{p})\xi, \tag{4.3}$$

$$E(\vec{S}\vec{p})\xi = \left[(\vec{S}\vec{p}) + k(\vec{S}\vec{r})\right](\vec{S}\vec{p})\eta \tag{4.4}$$

($\xi = \phi - \chi$, $\eta = \phi + \chi$), which could be uncoupled to the following form ($k = im\omega$)

$$(\vec{S}\vec{p})(E^2 - M^2)(\vec{S}\vec{p})\xi = (\vec{S}\vec{p})\left[\vec{p}^2 + m\omega^2\vec{r}^2 + 3m\omega + 4m\omega\vec{S}[\vec{r}\times\vec{p}]\right](\vec{S}\vec{p})\xi \tag{4.5}$$

$$(\vec{S}\vec{p})(E^2 - M^2)(\vec{S}\vec{p})\eta = (\vec{S}\vec{p})\left[\vec{p}^2 + m\omega^2\vec{r}^2 - 3m\omega - 4m\omega\vec{S}[\vec{r}\times\vec{p}]\right](\vec{S}\vec{p})\eta -$$
$$-im\omega(2E^2 - M^2)(\vec{S}\vec{r})(\vec{S}\vec{p})\eta \tag{4.6}$$

These equations can be considered as the extension of the equations with Dirac oscillator interaction to the $j = 1$ case, for the components $(\vec{S}\vec{p})\xi$ and $(\vec{S}\vec{p})\eta$. However, remark that one has the additional spin-orbit term acting as earlier at η.

5 Note on the two-body Dirac oscillator

The two-body Dirac Hamiltonian with oscillator-like interaction is given by (see, e. g., ref. [1c])

$$\mathcal{H}\psi == \left[\frac{1}{\sqrt{2}}(\vec{\alpha}_1 + \vec{\alpha}_2) \cdot \vec{P} + \frac{1}{\sqrt{2}}(\vec{\alpha}_1 - \vec{\alpha}_2) \cdot \vec{p} - \frac{i}{\sqrt{2}}(\vec{\alpha}_1 - \vec{\alpha}_2) \cdot \vec{r}B + m(\beta_1 + \beta_2) \right] \psi. \tag{5.1}$$

In the c.m.s. it is possible to equate $\vec{P} = 0$. The matrices are given by the direct products

$$\vec{\alpha}_1 = \begin{pmatrix} 0 & \vec{\sigma}_1 \\ \vec{\sigma}_1 & 0 \end{pmatrix} \otimes \begin{pmatrix} \mathbb{1}_{2\otimes2} & 0 \\ 0 & \mathbb{1}_{2\otimes2} \end{pmatrix}, \quad \vec{\alpha}_2 = \begin{pmatrix} \mathbb{1}_{2\otimes2} & 0 \\ 0 & \mathbb{1}_{2\otimes2} \end{pmatrix} \otimes \begin{pmatrix} 0 & \vec{\sigma}_2 \\ \vec{\sigma}_2 & 0 \end{pmatrix}, \tag{5.2}$$

$$B = \beta_1 \otimes \beta_2 = \begin{pmatrix} \mathbb{1}_{2\otimes2} & 0 \\ 0 & -\mathbb{1}_{2\otimes2} \end{pmatrix} \otimes \begin{pmatrix} \mathbb{1}_{2\otimes2} & 0 \\ 0 & -\mathbb{1}_{2\otimes2} \end{pmatrix}, \tag{5.3}$$

$$\Gamma_5 = \gamma_1^5 \otimes \gamma_2^5 = \begin{pmatrix} 0 & \mathbb{1}_{2\otimes2} \\ \mathbb{1}_{2\otimes2} & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & \mathbb{1}_{2\otimes2} \\ \mathbb{1}_{2\otimes2} & 0 \end{pmatrix}. \tag{5.4}$$

Now we apply the same procedure like that was used for transformation the Bargmann-Wigner equation to the Proca equations. The 16- component wave function of the two-body Dirac equation could be expanded on the complete set of matrices: $(\gamma^\mu C)$, $(\sigma^{\mu\nu} C)$ and C, $(\gamma^5 C)$, and $(\gamma^5 \gamma^\mu C)$. We consider the system multiplied by C, the matrix of charge conjugation, in order to trace for the symmetric properties under oscillator-like potentials. The wave function is decomposed in symmetric and antisymmetric parts using the above-mentioned complete system of matrices:

$$\psi_{\{\alpha\beta\}} = \gamma_{\alpha\eta}^\mu C_{\eta\beta} A_\mu + \sigma_{\alpha\eta}^{\mu\nu} C_{\eta\beta} F_{\mu\nu} \tag{5.5}$$

$$\psi_{[\alpha\beta]} = C_{\alpha\beta}\phi + \gamma_{\alpha\eta}^5 C_{\eta\beta}\tilde{\phi} + \gamma_{\alpha\epsilon}^5 \gamma_{\epsilon\eta}^\mu C_{\eta\beta}\tilde{A}_\mu. \tag{5.6}$$

In such a way we obtain the set of equations:

$$EA_0 = 0, \quad E\tilde{A}_0 = -2m\tilde{\phi}, \quad E\phi = 2i\sqrt{2}(\vec{p}_i - i\vec{r}^i)F^{i0} \tag{5.7}$$

$$E\tilde{\phi} = -2m\tilde{A}_0 + \sqrt{2}\epsilon_{ijk}(\vec{p}_i + i\vec{r}^i)F^{jk} \tag{5.8}$$

$$E\tilde{A}^i = -i\sqrt{2}\epsilon_{ijk}(\vec{p}_j \mp i\vec{r}^j)A^k \tag{5.9}$$

$$EA^i = 4imF^{0i} + i\sqrt{2}\epsilon_{ijk}(\vec{p}_j \pm i\vec{r}^j)\tilde{A}^k \tag{5.10}$$

$$EF^{0i} = -2imA^i + i\sqrt{2}(\vec{p}_i + i\vec{r}^i)\phi \tag{5.11}$$

$$EF_{jk} = \frac{1}{\sqrt{2}}\epsilon_{ijk}(\vec{p}_i - i\vec{r}^i)\tilde{\phi} \tag{5.12}$$

Let us mention that for another type of Dirac oscillator-like interaction $\sim (\vec{\alpha}_1 - \vec{\alpha}_2)B\Gamma_5$ the only changes are the sign changes at the term $i\vec{r}$ in Eqs. (5.9) and (5.10) of the above system. The two-body Dirac oscillator equations in the form (5.7)-(5.12) could be uncoupled on the set containing only functions ϕ, $\tilde{\phi}$ and $\tilde{A}_\mu$ and the another one containing only A_μ and $F_{\mu\nu}$:

$$1) \qquad (E^2 - 8m^2)\phi = 4(\vec{p}_i - i\vec{r}^i)(\vec{p}_i + i\vec{r}^i)\phi - \frac{1}{E}\left\{ \begin{pmatrix} 16m\epsilon_{ijk}\vec{r}^i\vec{p}_j \\ 0 \end{pmatrix} \right\}\tilde{A}^k \tag{5.13}$$

$$(E^2 - 4m^2)\tilde{\phi} = 2(\vec{p}_i + \vec{r}^i)(\vec{p}_i - i\vec{r}^i)\tilde{\phi} \tag{5.14}$$

$$E\tilde{A}_0 = -2m\tilde{\phi} \tag{5.15}$$

$$(E^2 - 8m^2)\tilde{A}^i = 2(\vec{p}_j \mp i\vec{r}^j)(\vec{p}_i \pm i\vec{r}^i)\tilde{A}^j - 2(\vec{p}_j \mp i\vec{r}^j)(\vec{p}_j \pm i\vec{r}^i)\tilde{A}^i +$$

$$+ \frac{1}{E}\left\{ \begin{pmatrix} 16m\epsilon_{ijk}\vec{r}^j\vec{p}_k \\ 0 \end{pmatrix} \right\} \phi \tag{5.16}$$

2) $\qquad EA_0 = 0 \tag{5.17}$

$$(E^2 - 8m^2)F^{0i} = 4(\vec{p}_i + i\vec{r}^i)(\vec{p}_j - i\vec{r}^j)F^{0j} -$$

$$- 4i\frac{m}{E}(\vec{p}_j \pm i\vec{r}^j)(\vec{p}_i \mp i\vec{r}^i)A^j + 4i\frac{m}{E}(\vec{p}_j \pm i\vec{r}^j)(\vec{p}_j \mp i\vec{r}^j)A^i \tag{5.18}$$

$$E^2 A^i = 2(\vec{p}_j \pm i\vec{r}^j)(\vec{p}_i \mp i\vec{r}^i)A^j - 2(\vec{p}_j \pm i\vec{r}^j)(\vec{p}_j \mp i\vec{r}^j)A^i + 4imEF^{0i}$$

$$(E^2 - 4m^2)F^{jk} = \epsilon_{ijk}\epsilon_{lmn}(\vec{p}_i - i\vec{r}^i)(\vec{p}_l + i\vec{r}^l)F^{mn}. \tag{5.19}$$

This fact proves the Dirac oscillator interaction, like the case of introduction of electrodynamic interaction in the Proca or the Bargmann-Wigner equations, does not mix $S = 1$ and $S = 0$ states. Next, the interaction term of the following form:

$$\mathcal{V}^{int} = \frac{1}{r}\frac{dV(r)/dr}{1 - [V(r)]^2}(\vec{\alpha}_1 - \vec{\alpha}_2)B\Gamma_5\vec{r} \tag{5.20}$$

has been deduced [12] from the equation of Relativistic Quantum Constraint Dynamics (RQCR) or N- particle Barut equation. In [12] it proved to lead to the Dirac oscillator-like interactions provided that the definite choice of the function $V(r)$. In connection with that let us remark the curious behavior of the another potential $V(r)$ which has been proposed in ref. [13b,c]:

$$V(r) = -g^2\frac{coth\,(rm\pi)}{4\pi r} = -g^2\frac{coth\,(\kappa r)}{4\pi r}. \tag{5.21}$$

It could be deduced from the one-boson exchange quasipotential $V(\vec{p}, \vec{k}; E) = -g^2(p - k)^{-2}$ by means of the transformation into the relativistic configurational representation (RCR) using the complete set of Shapiro plane-wave functions: $\xi(\vec{\Delta}, \vec{r}) = (\Delta_0 - \vec{\Delta}\vec{n}/m)^{-1-irm}$, $\Delta_0 = \sqrt{\vec{\Delta}^2 + m^2}$, $\vec{n} = \vec{r}/|\vec{r}|$.

In the case of the quasipotential (5.21) the interaction term $\mathcal{V}$, Eq. (5.20), has the different asymptotic behavior in three regions $(g^2/(4\pi) = 1)$. Namely,

$$\mathcal{V}^{int} \simeq \frac{1}{r(r^2 - 1)}(\vec{\alpha}_1 - \vec{\alpha}_2)B\Gamma_5\vec{r} \simeq$$

$$\simeq \begin{cases} (1/r^3)(\vec{\alpha}_1 - \vec{\alpha}_2)B\Gamma_5\vec{r}, & \text{if} \quad r \gg \frac{1}{\kappa} \quad \text{and} \quad r > 1 \\ -(1/r)(\vec{\alpha}_1 - \vec{\alpha}_2)B\Gamma_5\vec{r}, & \text{if} \quad \frac{1}{\kappa} \ll r < 1, \end{cases} \tag{5.22}$$

in the infrared region ($r \gg \frac{1}{\kappa}$, large distances); and

$$\mathcal{V}^{int} \simeq -2\kappa(\vec{\alpha}_1 - \vec{\alpha}_2)B\Gamma_5\vec{r}, \qquad \text{if} \quad r \ll \frac{1}{\kappa}, \tag{5.23}$$

in the ultraviolet region (small distances). In one of the regions one has the Dirac oscillator-like behavior.

Acknowledgments

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THE DUFFIN-KEMMER-PETIAU OSCILLATOR

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Abstract

In view of current interest in relativistic spin-one systems and the recent work on the Dirac Oscillator, we introduce the Duffin-Kemmer-Petiau (DKP) equation obtained by using an external potential linear in r. Since, in the non-relativistic limit, the spin 1 representation leads to a harmonic oscillator with a spin-orbit coupling of the Thomas form, we call the equation the DKP oscillator. This oscillator is a relativistic generalisation of the quantum harmonic oscillator for scalar and vector bosons. We show that it conserves total angular momentum and that it is *exactly* solvable. We calculate and discuss the eigenspectrum of the DKP oscillator in the spin 1 representation.

1   The DKP Oscillator

The focus of attention in this paper is to generalise the concept of the quantum harmonic oscillator to relativistic vector bosons.

For a free scalar or vector boson of mass m, the relativistic DKP equation [1] is

$$(c\beta \cdot \mathbf{p} + mc^2)\psi = i\hbar\beta^0\frac{\partial\psi}{\partial t} \tag{1.1}$$

where the internal variables β^μ ($\mu = 0,1,2,3$) satisfy the commutation relation

$$\beta^\mu\beta^\nu\beta^\lambda + \beta^\lambda\beta^\nu\beta^\mu = g^{\mu\nu}\beta^\lambda + g^{\nu\lambda}\beta^\mu. \tag{1.2}$$

In the spin 1 representation, the β^μ are 10×10 matrices while the dynamical state ψ is a ten-component spinor.

For the external potential which we introduce with the non-minimal substitution

$$\mathbf{p} \longrightarrow \mathbf{p} - im\omega\eta^0\mathbf{r}, \tag{1.3}$$

where ω is the oscillator frequency and $\eta^0 = 2\beta^{0^2} - 1$, the DKP equation for the system is

$$[c\beta \cdot (\mathbf{p} - im\omega\eta^0\mathbf{r}) + mc^2]\psi = i\hbar\beta^0\frac{\partial\psi}{\partial t}. \tag{1.4}$$

This external potential, which is of Lorentz tensor type, does not conserve the orbital and spin angular momenta, since

$$[\beta\eta^0 \cdot \mathbf{r}, \mathbf{L}] = -i(\beta\eta^0 \wedge \mathbf{r}) \quad \text{and} \quad [\beta\eta^0 \cdot \mathbf{r}, \mathbf{S}] = i(\beta\eta^0 \wedge \mathbf{r}), \tag{1.5}$$

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but it does conserve the total angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$.

In the spin 1 representation of eq.(4), the dynamical state ψ is chosen as the 10-component spinor

$$\psi(\mathbf{r}) = \begin{pmatrix} i\varphi \\ \mathbf{A}(\mathbf{r}) \\ \mathbf{B}(\mathbf{r}) \\ \mathbf{C}(\mathbf{r}) \end{pmatrix} \quad \text{with} \quad \mathbf{A} \equiv \begin{pmatrix} A_1 \\ A_2 \\ A_3 \end{pmatrix}, \quad \mathbf{B} \equiv \begin{pmatrix} B_1 \\ B_2 \\ B_3 \end{pmatrix}, \quad \text{and} \quad \mathbf{C} \equiv \begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix} \quad (1.6)$$

so that, for stationary states, the equation of motion eq.(4) decomposes into

$$\begin{cases} mc^2\varphi = ic\mathbf{p}^- \cdot \mathbf{B} \\ mc^2\mathbf{A} = E\mathbf{B} - c\mathbf{p}^+ \wedge \mathbf{C} \\ mc^2\mathbf{B} = E\mathbf{A} + ic\mathbf{p}^+\varphi \\ mc^2\mathbf{C} = -c\mathbf{p}^- \wedge \mathbf{A} \end{cases} \quad (1.7)$$

where $\mathbf{p}^\pm = \mathbf{p} \pm im\omega\mathbf{r}$. Since $\mathbf{A}$ is the 3-component spinor analogous to the Dirac upper component, we seek the wave equation for $\mathbf{A}$. It is straightforward to eliminate φ, $\mathbf{B}$ and $\mathbf{C}$ in favor of $\mathbf{A}$ so that one gets

$$(E^2 - m^2c^4)\mathbf{A} = [c^2(\mathbf{p}^2 + m^2\omega^2\mathbf{r}^2) - 3\hbar\omega mc^2 - 2\hbar\omega mc^2\mathbf{L}\cdot\mathbf{s}]\mathbf{A} - \frac{1}{m^2}\mathbf{p}^+\{\mathbf{p}^- \cdot [\mathbf{p}^+ \wedge (\mathbf{p}^- \wedge \mathbf{A})]\} \quad (1.8)$$

where $\mathbf{L}$ is the orbital angular momentum and $\mathbf{s}$ the 3×3 spin one operator. In the non-relativistic limit $\varepsilon \ll mc^2$, the fourth term in eq.(1.8) becomes negligible, since it is of order $1/m^3$, so that the wave equation for $\mathbf{A}$ can be written

$$\varepsilon\mathbf{A} \simeq [\frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\omega^2\mathbf{r}^2 - \frac{3}{2}\hbar\omega - \hbar\omega\mathbf{L}\cdot\mathbf{s}]\mathbf{A} \quad (1.9)$$

which characterises the usual harmonic oscillator in addition to a spin-orbit coupling, absent for scalar DKP bosons, of strength $-\hbar\omega$. Note that the strength of this coupling is half the one obtained from the Dirac oscillator [2].

Since the spin 1 representation of eq.(1.4) leads to the usual three-dimensional (3D) oscillator, in the non-relativistic limit, we refer to the system it describes as the Duffin-Kemmer-Petiau oscillator.

2   Solution to the vector DKP oscillator problem

For the S = 1 central field problem, the general eigenfunction we use takes the form [3]

$$\psi_{JM}(\mathbf{r}) = \frac{1}{r} \begin{pmatrix} i\phi_{nJ}(r)Y_{JM}(\Omega) \\ \sum_L F_{nJL}(r)\mathbf{Y}_{JL1}^M(\Omega) \\ \sum_L G_{nJL}(r)\mathbf{Y}_{JL1}^M(\Omega) \\ \sum_L H_{nJL}(r)\mathbf{Y}_{JL1}^M(\Omega) \end{pmatrix}. \quad (2.1)$$

Putting ψ_{JM} into eq.(1.4) results in ten coupled radial differential equations which can be decoupled into two sets associated with $(-1)^J$ and $(-1)^{J+1}$ parities. We call the $(-1)^J$ solutions

natural-parity (or magnetic-like) states while we refer to the $(-1)^{J+1}$ solutions as unnatural-parity (or electric-like) states. With the notation

$$R_{nJJ}(r) = R_o \quad , \quad R_{nJJ\pm1}(r) = R_{\pm1}, \qquad R \equiv F, G, H \tag{2.2}$$

the set associated with $(-1)^J$ parity is

$$E F_o = mc^2 G_o \tag{2.3}$$

$$\hbar c \left(\frac{d}{dr} - \frac{J+1}{r} + \frac{m\omega r}{\hbar} \right) F_o = -\frac{1}{\zeta_J} mc^2 H_1 \tag{2.4}$$

$$\hbar c \left(\frac{d}{dr} + \frac{J}{r} + \frac{m\omega r}{\hbar} \right) F_o = -\frac{1}{\alpha_J} mc^2 H_{-1} \tag{2.5}$$

$$-\zeta_J \left(\frac{d}{dr} + \frac{J+1}{r} - \frac{m\omega r}{\hbar} \right) H_1 - \alpha_J \left(\frac{d}{dr} - \frac{J}{r} - \frac{m\omega r}{\hbar} \right) H_{-1} = \frac{1}{\hbar c} \left(mc^2 F_o - E G_o \right) . \tag{2.6}$$

For unnatural parity states, the radial differential equations are coupled in the following way :

$$\hbar c \left(\frac{d}{dr} - \frac{J+1}{r} - \frac{m\omega r}{\hbar} \right) H_o = -\frac{1}{\zeta_J} \left(mc^2 F_1 - E G_1 \right) \tag{2.7}$$

$$\hbar c \left(\frac{d}{dr} + \frac{J}{r} - \frac{m\omega r}{\hbar} \right) H_o = -\frac{1}{\alpha_J} \left(mc^2 F_{-1} - E G_{-1} \right) \tag{2.8}$$

$$-\zeta_J \left(\frac{d}{dr} + \frac{J+1}{r} + \frac{m\omega r}{\hbar} \right) F_1 - \alpha_J \left(\frac{d}{dr} - \frac{J}{r} + \frac{m\omega r}{\hbar} \right) F_{-1} = \frac{1}{\hbar c} mc^2 H_o \tag{2.9}$$

$$\hbar c \left(\frac{d}{dr} - \frac{J+1}{r} - \frac{m\omega r}{\hbar} \right) \phi = -\frac{1}{\alpha_J} \left(mc^2 G_1 - E F_1 \right) \tag{2.10}$$

$$\hbar c \left(\frac{d}{dr} + \frac{J}{r} - \frac{m\omega r}{\hbar} \right) \phi = \frac{1}{\zeta_J} \left(mc^2 G_{-1} - E F_{-1} \right) \tag{2.11}$$

$$-\alpha_J \left(\frac{d}{dr} + \frac{J+1}{r} + \frac{m\omega r}{\hbar} \right) G_1 + \zeta_J \left(\frac{d}{dr} - \frac{J}{r} + \frac{m\omega r}{\hbar} \right) G_{-1} = \frac{1}{\hbar c} mc^2 \phi. \tag{2.12}$$

To obtain the exact solution for the magnetic-like states, we eliminate G_o, $H_\pm$ in favor of F_o in eq.(2.6). This yields the eigenvalues [4]

$$\frac{1}{2mc^2} (E_{N,J}^2 - m^2 c^4) = (N+1)\hbar\omega \tag{2.13}$$

with the principal quantum number $N = 2n + J$ (n is the radial quantum number). Note that the oscillator levels are equidistant and degenerate; the zero-point energy differs here from the one we found for the scalar DKP bosons.

The exact eigenvalues of the radial equations associated with unnatural-parity states can be shown [4] to be

$$\frac{1}{2mc^2}(E_\pm^2 - m^2c^4) = (N + \frac{3}{2})\hbar\omega + J(J+1)\frac{(\hbar\omega)^2}{mc^2} \mp \Delta \qquad (2.14)$$

where

$$\Delta = \hbar\omega \left(J + \frac{1}{2} \right) \left(1 + \frac{a_1}{a_0}\frac{\hbar\omega}{mc^2} + \frac{a_2}{a_0}\left(\frac{\hbar\omega}{mc^2}\right)^2 \right)^{\frac{1}{2}} \qquad (2.15)$$

with $a_0 = (2J+1)^2$, $a_1 = 4J(J+1)(2N+3)$ and $a_2 = 4J^2(J+1)^2$ where N, a positive integer, is the principal quantum number.

As shown in eq.(23), the energy of the DKP oscillator in unnatural parity states involves the usual 3-dimensional harmonic oscillator energy, a second term proportional to $J(J+1)$ which appears as some kind of rotational energy and a third energy contribution Δ which is a complicated function of the oscillator frequency, J and N with no obvious physical interpretation.

In the limit where the oscillator frequencies are such that $\hbar\omega \ll mc^2$, keeping only the first-order term in ω in eqs.(2.14-15) leads to

$$\frac{1}{2mc^2}(E_+^2 - m^2c^4) \equiv \epsilon_{n.r.}^+ \simeq (N - J + 1)\hbar\omega \qquad (2.16)$$

$$\frac{1}{2mc^2}(E_-^2 - m^2c^4) \equiv \epsilon_{n.r.}^- \simeq (N + J + 2)\hbar\omega \qquad (2.17)$$

This is best illustrated in fig.1 which shows, for fixed values of N and J, the variations of the relativistic and non-relativistic eigen-energies with $\hbar\omega/mc^2$.
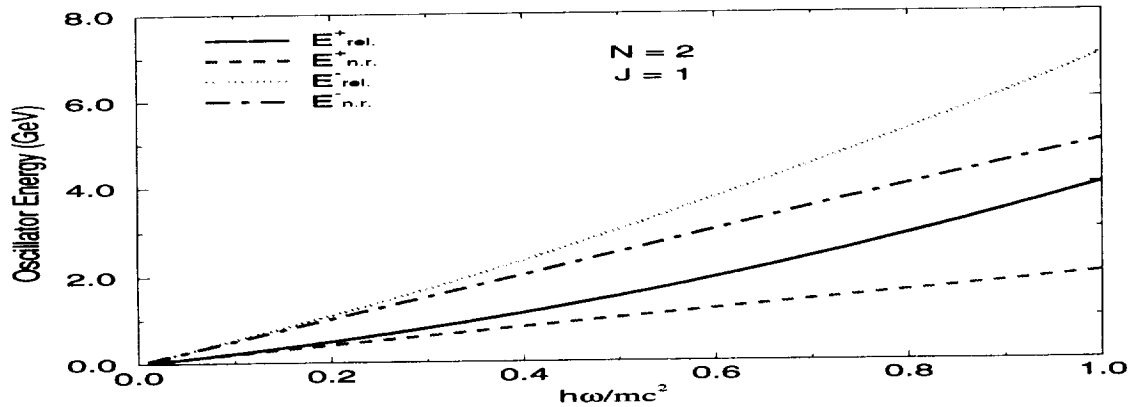
Figure 1: *Variation of the DKP and non-relativistic oscillator energies with ω.*

This shows that our solutions have the correct non-relativistic limits since the levels in eqs.(2.16-17) are those of a usual 3D non-relativistic oscillator with a spin-orbit coupling of strength $-\hbar\omega$. In this limit, they could have also been obtained directly from eq.(1.9). Furthermore, taking this limit suggests the interpretation of the E_+ and E_- energies as "spin-orbit partners", E_+ being associated with $J = L + 1$ and E_- with $J = L - 1$.

The unnatural parity E_+ levels for $N \leq 9$ are presented in fig.2 alongside the $\epsilon^+_{n.r.}$ and the $(N + \frac{3}{2})\hbar\omega$ levels for reference. For a given value of $N - J$, all the non-relativistic energy levels (N, J^π) (with $N - J$ odd and $J < N$) are infinitely degenerate. This accidental degeneracy is not present in the exact DKP oscillator E_+ eigenspectrum whose levels are found to cluster in several groups of states belonging to the same $N - J$ oscillator shell.
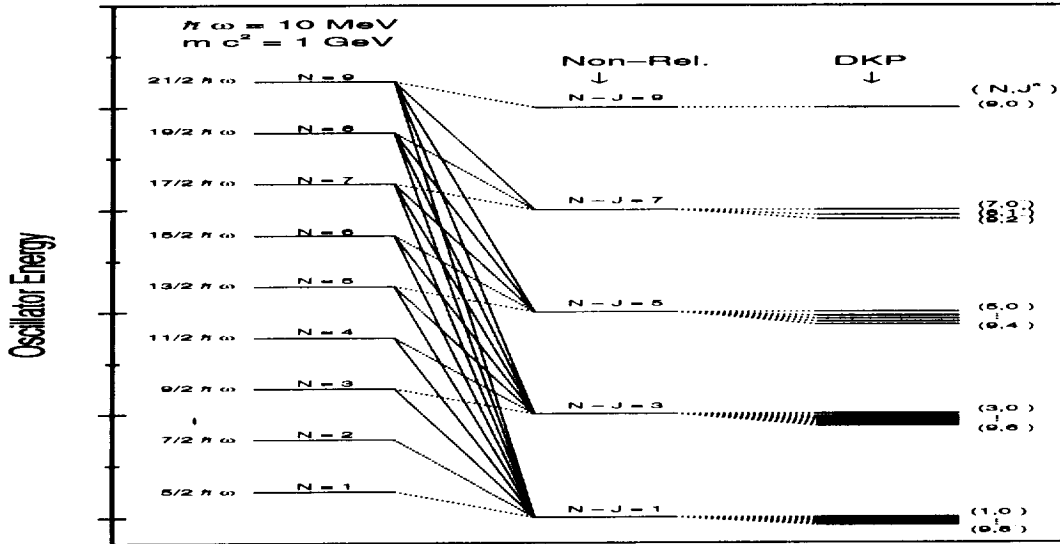
Figure 2: DKP and non-relativistic spectra associated with $J = L + 1$ for $N \leq 9$. The dotted lines between the DKP and non-relativistic oscillator levels link states with the same quantum numbers (N, J^π).

The E_- eigenspectrum is now presented in fig.3 together with the non-relativistic $\epsilon^-_{n.r.}$ energy levels for $N \leq 9$.
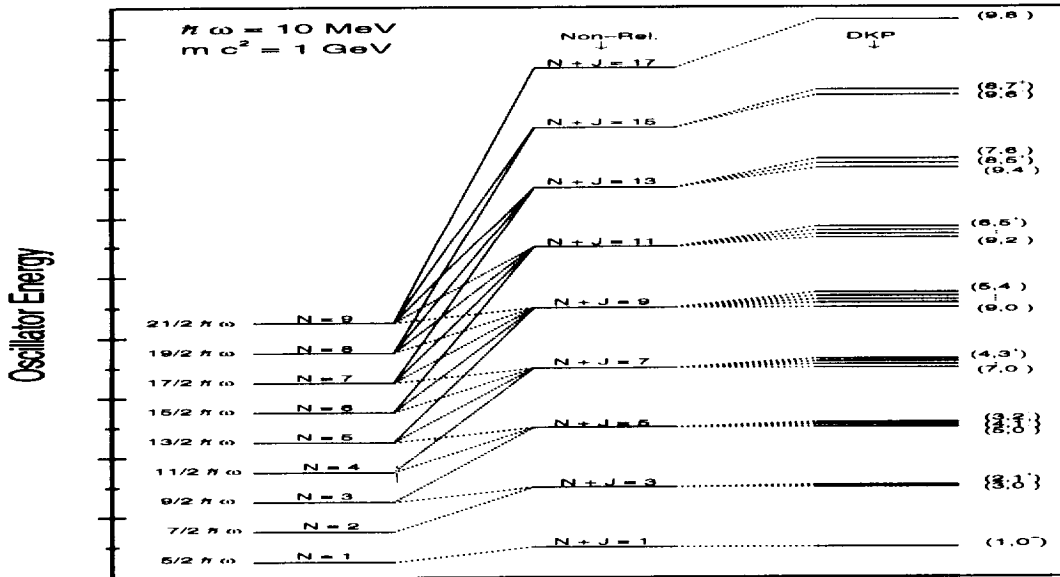

Figure 3: DKP and non-relativistic spectra associated with $J = L - 1$ for $N \leq 9$.

While all the non-relativisitic (N, J^π) levels associated with the same $N + J$ oscillator shell are degenerate, with a finite degeneracy in this case, their relativistic analogues are not. The

exact DKP oscillator states are found to cluster into bands of states belonging to specific values of $N + J$.

For a more quantitative analysis of the E_- bands of the DKP oscillator spectrum, we plotted in fig.4 the E_- energy levels, belonging to the $N + J = 49$ band for instance, against $J(J + 1)$ for different oscillator frequencies.
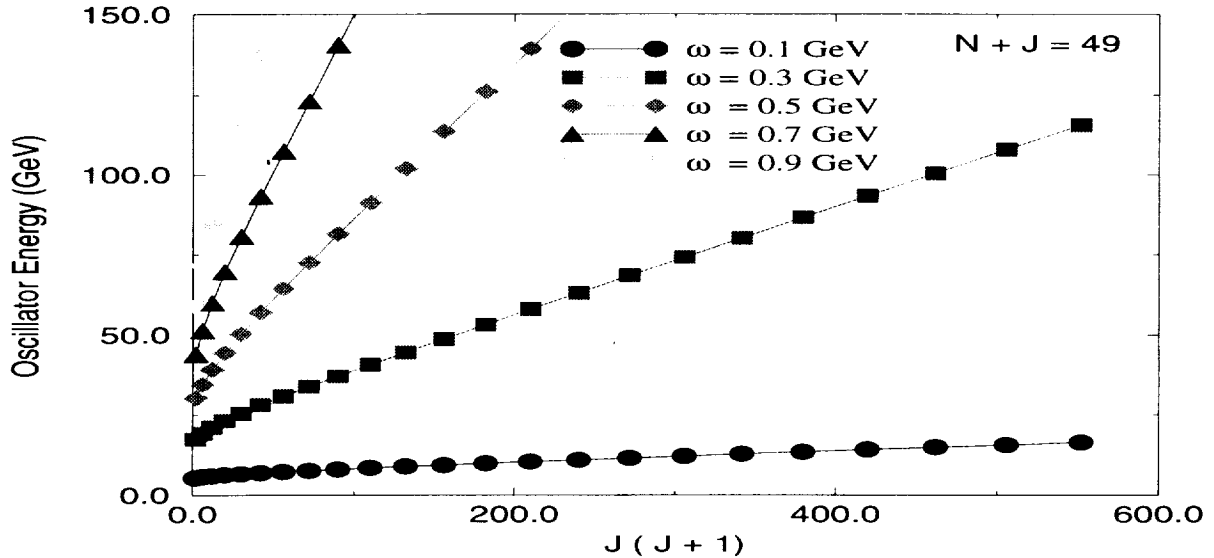
Figure 4: *Energy levels of the* $N + J = 49$ *band as a function of* $J(J + 1)$ *for different oscillator frequencies.*

It is indeed remarkable that the DKP oscillator energies constitute nearly perfect rotational bands. There are deviations from the rotational patterns at low angular momenta. These single particle rotational bands are of the finite type since for $N + J$ fixed they terminate at some J_{max}. The effective rotational moments of inertia are sensitive to the oscillator frequencies since the slopes of the bands are found to vary substantially with increasing ω.

Figure 5: *Energy levels of the* $N + J = 23, 29, 35, 41, 49$ *band as a function of* $J(J + 1)$ *for* $\hbar\omega = 0.2 GeV$.

Fig.5 alternately represents the energies of five different $N + J$ bands for a specific oscillator frequency as a function of $J(J + 1)$. The DKP oscillator energies now lie on rotational bands whose slopes hardly change with $N + J$ which implies that the effective rotational moments of inertia are rigid and insensitive to such variations.
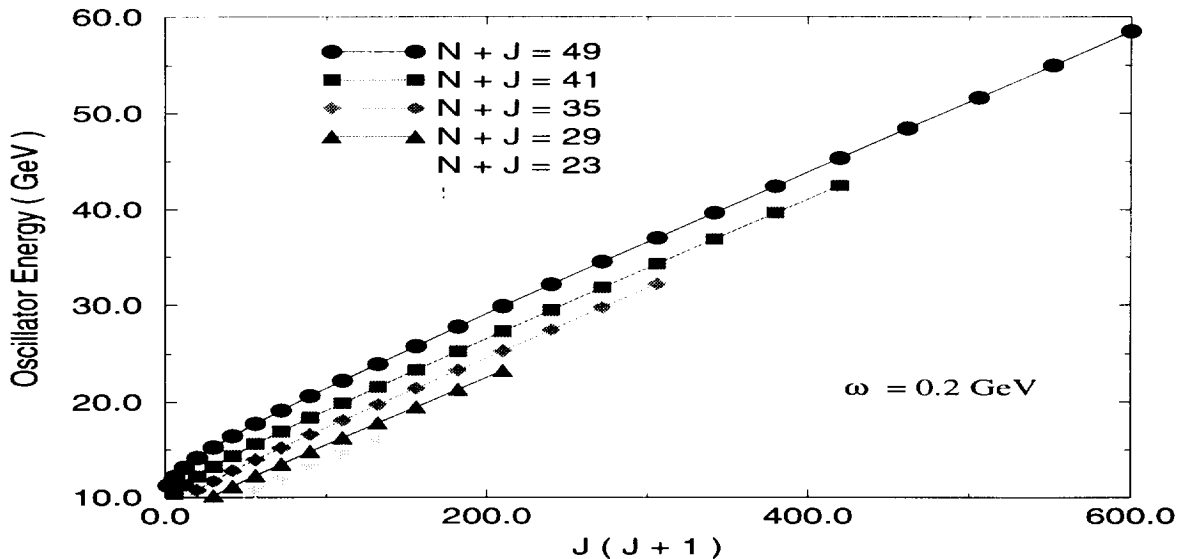
Of course, it should be pointed out that these rotational bands are unlike the usual ones where the levels are associated with the same intrinsic motion but different angular momenta. Here the single particle states involve different radial as well as rotational motions. Note that this behaviour is not particularly tied to this DKP oscillator. Buck [5] also found that, when solving the Schrödinger equation for deep, bell-shaped potentials, the levels with a fixed value of $N = 2n + \ell$ (these states are degenerate for a harmonic oscillator) lie on a straight line when plotted against $\ell(\ell+1)$. Geometric arguments in terms of the shapes of the potentials which can give rise to these rotational-like bands have been put forward to explain this behaviour [5][6].

3   Conclusion

We have introduced a new potential in the DKP equation. Since, in the non-relativistic limit, the DKP equation of motion leads to the usual harmonic oscillator with a spin-orbit coupling of the Thomas form, we call the system a DKP oscillator. This oscillator is a relativistic generalisation of the quantum harmonic oscillator for vector bosons. We have shown that it conserves the total angular momentum, that it is exactly soluble and we have computed and discussed its eigen-solutions.

The renewed interest in the Dirac oscillator has generated studies of its group theoretical properties [7] and hidden supersymmetry [8][9] among others. Such investigations of the DKP oscillator would be most useful to gain further insight into the physical meaning of this oscillator.

This study is on the other hand relevant to the work on relativistic equations for two fermions and particularly to those of Krolikowski's type [10]. Since they tend to the DKP equation in the point-like limit of tightly bound-states, exact solutions of the latter may provide useful information about this class of relativistic two-body equations.

Acknowledgments

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HARMONIC OSCILLATORS AND RESONANCE SERIES GENERATED BY A PERIODIC UNSTABLE CLASSICAL ORBIT

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Abstract

The presence of an unstable periodic classical orbit allows one to introduce the decay time as a purely classical magnitude: inverse of the Lyapunov index which characterizes the orbit instability. The Uncertainty Relation gives the corresponding resonance width which is proportional to the Planck constant. The more elaborate analysis is based on the parabolic equation method where the problem is effectively reduced to the multidimensional harmonic oscillator with the time-dependent frequency. The resonances form series in the complex energy plane which is equidistant in the direction perpendicular to the real axis. The applications of the general approach to various problems in atomic physics are briefly exposed.

1   Introduction

The quantum quasistationary states may be subdivided into three types (although these types are not absolutely independent): (*i*) the shape resonances which decay by penetration through some potential barrier; (*ii*) the Feshbach resonances, i.e. the quasibound states of the particle in the field of the excited core, for instance, the doubly excited states of the helium atom; (*iii*) the resonances related with the unstable periodic classical orbits. The latter type of resonances is probably the less known one. The peculiarities of the density of states, corresponding to the periodic orbit (or cycle), were analyzed by Gutzwiller [1] and by Balian and Bloch [2]. The role of such orbits is a subject of intensive discussion in the current literature.

The connection between the stable periodic classical orbit and the quantum mechanical eigenvalues is obvious from the physical point of view: such trajectories are similar to the effective channels in space along which the wavefunction is concentrated. The pioneer study of the problem by Gutzwiller [1] suffers a number of deficiencies. For instance, the Gutzwiller theory does not give true value for the total amount of quantum numbers labeling the state (in this case it should be equal to the dimensionality of the configurational space). This deficiencies were discussed by Miller [3]. However it seems that the most appropriate method to treat the problem is the parabolic equation approach developed initially in the theory of radio wave propagation (see e.g. the monograph by Babich and Buldyrev [4] and the discussion below in Sec.2). This method provides adequate basis for the description of the eigenfunctions which are localized at the vicinity of the periodic stable orbit.

The case of the unstable periodic classical orbit was not the subject of such a detailed study. In particular Voros [5] showed that the expansion of the density of states over the closed orbits due

to Gutzwiller [1] is not convergent and thus has not rigorous mathematical meaning. We do not discuss the problem on such a rigorous level and do not analyze the density of states expansion. Instead of it we consider only the relatively narrow resonances which can be well manifested in the physical observables. The resonances of this type are shown below to be related with the short-period long-living unstable orbits.

The natural characteristics of the classical orbit lifetime is the inverse of the Lyapunov index which is commonly used to describe the orbit instability. Thus in this case the concept of lifetime is introduced exclusively within the framework of classical mechanics without an appeal to the quantum tunneling and the channels interaction as in the case of the resonance types (i) and (ii). Namely this circumstance allows us to single out the third type of resonances in the classification introduced above.

The unstable orbits were discussed by Heller [6] who demonstrated that in the vicinity of the orbits the wavefunctions are enhanced and the 'scars' are formed on them. The explanation is obvious: the classical system stays long in this region. We show that the individual unstable orbit is naturally related with the whole series of resonances and give the simplified description of the wavefunctions. The complex eigenenergies representing the series form an equidistant pattern in the direction of the imaginary energy axis. The basic ideas of the present approach were outlined by the authors some times ago [7]. Here they are developed further and elucidated. Some recent applications to the problems of atomic physics are discussed.

2 Parabolic Equation Method

We start our analysis with the trivial comment. In the classical mechanics the particle with the energy close to the top of the potential barrier stays near the top for a long time. In quantum mechanics one can associate with the barrier top the series of 'eigenstates' with the imaginary energies (see also [8]). Indeed, consider the one- or two-dimensional *parabolic barrier*. In the first case the particle coordinate is x, in the second case the cylindrical radial coordinate is denoted as ρ. The stationary Schrödinger equation (for the particle with unit mass) is written respectively as

$$\left(-\frac{\hbar}{2}\frac{d^2}{dx^2} - \frac{1}{2}\alpha^2 x^2 \right)\psi = E^{(1)}\psi \tag{1}$$

and

$$\left(-\frac{\hbar}{2}\Delta_2^2 + \mu L_3 - \frac{1}{2}\alpha^2\rho^2 \right)\psi = E^{(2)}\psi, \tag{2}$$

where Δ_2 is the two-dimensional Laplace operator, L_3 is the corresponding angular momentum operator, α and μ are the potential parameters. The substitution of new variables $(x', \rho') = (x', \rho')\exp(-i\pi/4)$ transforms the equations (1), (2) into these for the harmonic oscillators. Respectively, the wave functions containing only the outgoing waves in the asymptotes are transformed into the oscillator eigenstates. Thus if the equations (1), (2) are considered with the outgoing wave boundary condition, then the imaginary 'eigenvalues' are obtained:

$$E^{(1)} = -i\alpha\hbar\left(n + \frac{1}{2}\right), \qquad E^{(2)} = \mu\hbar m - i\hbar\alpha\left(2n + \mid m \mid +1\right). \tag{3}$$

It should be stressed that the corresponding 'eigenstates' form the natural basis set for the description of the time-evolution of the wave packet which is localized initially near the barrier top (e.g., for $\psi(x)\mid_{t=0}= \exp(-\beta x^2)/(1+\gamma x^2$) with some positive parameters β and γ). The imaginary part of the energy generally describes the short-time evolution of the wave packet and is not necessarily related with the true ionization process, i.e. escape to infinitely large distances (this situation is described by the notion *Diabatic Quasistaionary State* (DQS) introduced by the authors, see Ref.[7]).

The method of parabolic equation allows one to apply these simple formulae to the more general problem. Its essence is summarized below.

Consider the vicinity of the unstable orbit. One can introduce the natural local reference system at this region related with the trajectory. Let the system origin move with the particle along the unstable periodic orbit. The transversal coordinate axes q_i ($i = 1, 2, 3, \ldots N - 1$; N is the dimensionality of the system configurational space) are directed normally to the orbit. The longitudinal coordinate s is the distance along the orbit. Let q_i be chosen so that $q_i = 0$ on the orbit. Since our subsequent consideration is confined to the orbit vicinity this definition is quite sufficient to our purposes. In these variables the system Hamiltonian can be written as

$$H = -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial s^2} + H_{tr}(p_i, q_i, s), \tag{4}$$

where M is the effective mass (we treat here the transition to the new curvilinear coordinates in somewhat simplified manner what is unimportant for the subsequent discussion). The transversal motion Hamiltonian H_{tr} contains momenta p_i conjugate to the transversal coordinates q_i. It includes also the periodic parametric dependence on the coordinate s.

In the framework of the parabolic equation method the motion along the longitudinal coordinate s is treated semiclassically. This implies the following representation of the wave function:

$$\psi(q_1, q_2, \cdots q_{n-1}, s) = v_{E_0}^{-1/2}\exp\left(iS_{E_0}(t)/\hbar\right)\varphi\left(q_1, q_2, \cdots q_{n-1}, t\right). \tag{5}$$

Here S_{E_0} and v_{E_0} are respectively the action $(\int pdq)$ and the velocity for the classical motion along the trajectory for the energy E_0 ($v_{E_0} = M^{-1}dS_{E_0}/ds$). The new 'time' variable t is directly related with the longitudinal coordinate s: $v_{E_0}dt = ds$. Substituting the wave function (5) into the Schrodinger equation $(H - E)\psi = 0$ one obtains (in the lowest order in the Planck constant $\hbar$) the following equation for the function φ:

$$i\hbar\frac{\partial\varphi}{\partial t} = \left(H_{tr}(p_i, q_i, t) - H_{tr}(0, 0, t) - E + E_0\right)\varphi. \tag{6}$$

The latter equation has the mathematical form of the *non-stationary* (*parabolic*) Schrodinger equation with the *mock* 'time' variable t directly related to the coordinate s. Note that our treatment starts with the *stationary* Schrodinger equation. Therefore the *true* time does not appear here.

The rigorous formulation of the method based on the asymptotic (semiclassical type) techniques implies that the Hamiltonian of the non-stationary problem should be replaced by its approximation quadratic in the coordinates q_i. These statements present the essence of the parabolic equation method introduced originally by Leontovich and Fock [9] (see also Ref.[10]).

3 Quantization Conditions

The important point for the further development is that the Hamiltonian H_{tr} is periodic in 'time' t since the orbit is periodic. The natural way to treat such a problem is to consider the *quasienergetic or Floquet states* (see e.g. the review Ref. [11]). The latter is introduced so that after the period T the corresponding wave function acquires the phase factor which contains the quasi energy ϵ:

$$\psi(t + T) = \exp(i\epsilon T)\psi(t). \qquad (7)$$

Let now choose the function φ to be the quasi energy state. After the passage over the periodic orbit the total wave function ψ (5) should remain unchanged. This gives the following quantization condition:

$$E - E_0 - \epsilon + S_{E_0}(T)/T = 2\pi n\hbar/T, \qquad (8)$$

where T is the period of the orbit, n is an integer. Note that the parabolic equation method assumes naturally the semiclassical condition for the motion over s-coordinate: $S_{E_0}/\hbar \geq 1$.

Since we assume here the quadratic approximation for the Hamiltonian H_{tr}, then the non-stationary Schrodinger equation (6) describes the $(N - 1)$-dimensional oscillator with the parameters depending on the 'time' t.

The quasi energy spectrum for the time-periodic quadratic (in the coordinates and the conjugated momenta) system was discussed in the monograph by Malkin and Man'ko [12]. Their study is based on the mathematically rigorous analysis by Sugiura [13] and Williamson [14]. Here we give only the list of the statements which seems to be quite appealing.

(i) In the case of quadratic time-dependent Hamiltonian the classical Hamilton equations are linear and coincide with the quantum Heizenberg equations for the momentum and coordinate operators $\hat{p}$ and $\hat{q}$.

(ii) Let the general solution of the classical equations to be known:

$$(p(t),\ q(t)) = \Lambda(t)(p(0),\ q(0)), \qquad (9)$$

where $\Lambda(t)$ is the evolution matrix acting on the array of the system coordinates q and canonically conjugated momenta p. Then the solution of the Heizenberg equations takes the form

$$(\hat{p}(t),\ \hat{q}(t)) = \Lambda(t)(\hat{p}(0),\ \hat{q}(0)) \qquad (10)$$

with the same evolution matrix.

(iii) For an arbitrary fixed t_0 one can find the *time-independent* quadratic (in the coordinates and momenta) Hamiltonian $H_{eff}^{(t_0)}$ which generates the same result for the system evolution at the time t as the initial *time-dependent* Hamiltonian. This implies that the exact time-evolution operator can be presented as $\exp(iH_{eff}^{(t_0)}t_0)$.

(iv) The matrix $\Lambda(t)$ which describes the system evolution over its period is called the *monodromy* matrix. The spectrum of the corresponding operator $H_{eff}^{(T)}$ coincides with the quasi energy spectrum. We should emphasize here that this operator must be considered as a continuous limit $(t \to T)$ of the operator $H_{eff}^{(t)}$. For instance, in the one-dimensional case the phase point in principle can perform several 2π-rotations around the origin which do not influence the monodromy

matrix. However this rotations should be taken into account in the construction of the operator $H_{eff}^{(T)}$.

Thus the problem of finding the quasi energies is reduced to the analysis of the spectrum of the monodromy matrix (we assume further that its eigenvalues are non-degenerate). Moreover, the eigenvalues of the monodromy matrix are essentially the exponents of the eigenvalues of some quadratic Hamiltonian. The latter does not necessarily correspond to the real *oscillator* since the case of the *quadratic potential barrier* also can be realized. The spectrum of such a barrier was discussed above at the beginning of the Section 2. Taking all these possibilities into account one finds that the following basic types of the eigenvalues sets are feasible (the most general description is given by Williamson [14]):

$$\exp(i\omega T), \tag{11}$$

$$\exp(\pm\alpha T), \tag{12}$$

$$\exp(\pm i\mu T \pm \alpha T). \tag{13}$$

The first one corresponds to the real oscillator with the frequency ω in the normal mode of the Hamiltonian $H_{eff}^{(T)}$ whereas the second and the third cases are related respectively with the parabolic barriers (1) and (2). Note that in (13) four various eigenvalues are contained according to various choice of the signs.

The parameter α in (12) and (13) coincides with the Lyapunov index which characterizes the instability of the classical periodic orbit in the linear approximation for the equations of motion. Indeed, the Lyapunov index is defined by the relation $q_i(T)/q_i(0) = \exp(\alpha T)$. According to the statement (ii) it is related with the description of the quantum system.

The eigenstates of the time-evolution operator coincide with those of the operator $H_{eff}^{(T)}$. One has to bear in mind that in the multidimensional system the eigenstates of each type can appear several times. In order to distinguish them we introduce below the lower indexes. The diagonalization of $H_{eff}^{(T)}$ generates the subdivision of the transversal coordinate subspace into the direct sum of the subspaces each of which corresponds to some set of the eigenvalues discussed above. The natural coordinate basis in each subspace is given by the normal coordinates. Depending on the type of the eigenvalue (see above) the quadratic Hamiltonian $H_{eff}^{(T)}$ in each subspace is of the oscillatory type (with some frequency ω_{j_1}, $j_1 = 1, 2, ...N_1$) or corresponds to the quadratic barrier described by Eq. (1) or (2) with the related parameters α_{j_2} ($j_2 = 1, 2, ...N_2$) in the case (1) or the parameters α_{j_3} and μ_{j_3} ($j_3 = 1, 2, ...N_3$) in the case (2). The lower indexes enumerate the eigenvalues. The total amount of the eigenvalues is $N_1 + N_2 + N_3 = N - 1$.

Taking into account the relation (7) we obtain the quasi energy spectrum of the system:

$$\epsilon(\{n\}, \{m\}) = \sum_{j_1} \hbar\omega_{j_1}\left(n_{j_2} + \frac{1}{2}\right) - i\sum_{j_2}\hbar\alpha_{j_2}\left(n_{j_2} + \frac{1}{2}\right) + \tag{14}$$
$$+ \sum_{j_3}\hbar\left(\omega_{j_3}m_{j_3} - i\alpha_{j_3}\left(2n_{j_3} + \mid m_{j_3} \mid + 1\right)\right)$$

with some integer n_j ($n_j > 0$), m_j. The summation is performed over all eigenvalues described above. The eigenfunctions φ are expressed readily as the products of the Hermit functions of the normal coordinates.

Let us summarize the meaning of the quantum numbers. The quantum number n quantizes the motion along the periodic orbit. The quantum numbers n_{j_1} quantize the stable vibrational modes of the transversal motion whereas n_{j_2} and n_{j_3} are theirs analogs in the case of unstable transversal modes. The quantum number m_{j_3} are the azimuthal quantum number for the rotations in the plane locally perpendicular to the cycle.

We should emphasize that the total amount of the quantum numbers (including n, see (8)) coincides with the dimensionality of the configuration space. However, since the resonance series lie along the imaginary axis in the complex energy plane, this series is manifested in the experimental observations as one peak. Thus some of the quantum numbers prove to be 'hidden' and the amount of the 'observable' quantum numbers is effectively reduced.

4 Discussion

The formulae (8) and (14) contain the essence of the present paper. They are quite transparent from the physical point of view. Let the orbit energy E_0 be chosen to satisfy the semiclassical quantization condition for the motion along the periodic orbit:

$$S_{E_0} = 2\pi n\hbar. \tag{15}$$

Then from (8) we obtain

$$E = E_0 + \epsilon. \tag{16}$$

Thus the quantization problem is separated: first, the motion over the unstable cycle should be quantized according to Eq.(15) and, second, the motion over the transversal coordinates is quantized giving the quasi energy spectrum (14). The analogous equations were discussed by Miller [3] in the case of stable orbit. They reflects effective separation of variables in the vicinity of the cycle: the quantum number n is large but the other quantum numbers are small being incorporated into the quasi energy spectrum.

These formulae are also in close relation to the Gutzwiller formula for the density of levels in the two-dimensional case:

$$\rho(E) = \frac{T}{2\pi} \text{Im} \sum_{n=1}^{\infty} \frac{1}{\sinh(n\alpha T/2)} \exp(inS/\hbar). \tag{17}$$

This sum can be rearranged similarly to the Miller [3] paper:

$$\rho(E) = \frac{T}{2\pi} \text{Im} \sum_{n=1}^{\infty} [1 - \exp(-n\alpha T)]^{-1} \exp[n(iS/\hbar - \alpha T/2)] = \tag{18}$$

$$= \frac{T}{2\pi} \text{Im} \sum_{m=0}^{\infty} [1 - \exp(iS/\hbar - m\alpha)]^{-1} \exp[n(iS/\hbar - 3\alpha T/2)].$$

Thus the density of states has the poles at the complex energies given by the equations (8) and (14) (since $S_E = S_{E_0} + (\partial S/\partial E)(E - E_0)$, $\partial S/\partial E = T$). However the expression (17) is not applicable in the complex energy plane. Moreover the expansion of the states density over the

periodic trajectories does not converge [5]. Therefore the proper description of the individual resonance states given in the present paper is essential.

Our principle qualitative conclusion is as follows. Since the unstable closed classical orbit can be characterized by some 'decay time' (namely, the inverse of Lyapunov index), the Uncertainty Relation gives the related resonance width which is linear in the Planck constant $\hbar$ (in contradistinction to the shape resonances where the width is exponentially small). Moreover whole resonance series correspond to the individual orbit with the resonances lying in the complex energy plane equidistantly on the line parallel to the imaginary axis (see formula (14)).

The first point to be stressed is that the quadratic approximation demands localization of the wave function in the vicinity of the orbit whereas the resonance functions constructed above do not satisfy this requirement since they rise exponentially in the case of the quadratic potential barrier. This contradiction is removed if one notices that the complex transformation of the transversal coordinates $q = q' \exp(i\pi/8)$ makes the eigenfunctions decreasing. The close analogy is traced here with the method of the complex rotation of the coordinates. This method of the resonance states calculation proves to be very efficient in the analysis of quite complex atomic systems [15]. The physical meaning of this states follows from theirs role in the description of the initially prepared wave packet (see discussion in the Sec.2).

The formula (14) implies that the quantum numbers n_j are not too large in order to confine the major part of the probability to the applicability domain of the quadratic approximation for the Hamiltonian H_{tr}. Nevertheless it is worth to stress that the resonances of this type generate series in the complex energy plane (in the quadratic approximation the series are equidistant in the direction of the imaginary energy axis). This constitutes the principle difference between the resonances discussed in the present paper and the shape or Feshbach resonances. In particular, this difference is manifested in the shape of the resonance profiles in the physical observables such as the cross sections, transition probabilities etc.

In principle the situation is feasible when the quadratic approximation is not applicable even for the lowest values of n_i ($n_i = 0$). This problem is not important for the general construction of the present theory since in fact its small parameter is the Planck constant (or inverse particle mass). However it can limit applicability of the theory to the concrete systems. If the quadratic approximation is dropped, then the theory is reduced to the description of the quasi energy states of the periodic Hamiltonian with the more general (non-quadratic) dependence on the coordinates. The practical realozation of this approach (see the next Section) gives good results.

5   Some Applications to Atomic Physics

In this Section some recent applications to the atomic physics are briefly discussed. We emphasize some modifications of the general scheme which are necessary in the concrete applications. The states of the atom in the uniform electric field serve in the text books as a typical example of the shape resonances. These resonances have negative energy and decay by the penetration of the potential barrier. The resonances exist also for positive energies where they have different origin being related with the unstable periodic classical trajectory. The electron moves between the atomic nucleus and the turning point against the force exerted on it by the uniform field. The calculations [16], [17] within the present approach demonstrate an excellent agreement with the accurate numerical data both for the resonance positions and widths.

For the motion of the electron in the field of two Coulomb centers the unstable classical trajectory also represents an interval of line. The calculations of the resonances were carried in this case by Du *et al* [18].

In the cited examples the resonance width corresponds to the true ionization (transitions to the continuum). An alternative situation appears for the helium atom where Klar [19] have found classical unstable equilibrium configurations (in which the electron-electron and electron-nucleus separations do not vary with time but the system rotates as a whole). Within the present approach these configurations are related [20] with the Rydberg series of broad resonances (doubly excited states) which are interpreted as DQS. Their widths describe not the transitions to the continuum (autoionization) but the interaction of the diabatic configurations.

The equilibrium electron configurations in the helium atom give an example of the correlated motion of the electrons which is not described by the effective central field approximation conventional in the theory of atoms. The description of the electron correlations is one of the fundamental problems in atomic physics.

The other example of the correlated electron motion appears in the study to the two-electron continuum states which are the final states in the electron impact ionization ((e, 2e) process) or double photoionization ((γ, 2e) process) of the atom. In the near-threshold domain the theory of the process was developed by Wannier [21] (see also the review by Read [22]). The physical idea is that the electrons fly apart from the core (with the charge Z) being at equal distances from it, i.e. at the so called Wannier ridge $r_1 = r_2$ ($\vec{r}_1$, $\vec{r}_2$ are the electron vectors relative to the atomic nucleus). Otherwise one of the electrons is decelerated and is captured into the high lying Rydberg state. Hence sliding off the Wannier ridge leads to the population of the one-electron continuum. For the double escape process this part of the flux is lost. In the framework of the present approach this is described in terms of the effective width and the whole double escape process is presented [23] as the system survival on the Wannier ridge.

Due to the Coulomb electron-electron repulsion the emission of the electrons in the opposite direction has the highest probability, i.e. $\theta_{12} \approx \pi$, where θ_{12} is the angle between $\vec{r}_1, \vec{r}_2$).

It is convenient to use collective hyperspherical coordinates: hyperradius $R = (r_1^2 + r_2^2)^{1/2}$ and hyperangle $\alpha_h = \tan(r_1/r_2)$. The Wannier treatment presumes two basic assumptions:

(i) The vicinity of the Wannier saddle configuration $\vec{r}_1 = -\vec{r}_2$ (i.e. $\alpha_h = \frac{1}{4}\pi$), $\theta_{12} = \pi$ is considered with the quadratic approximation in the variables $(\alpha_h - \frac{1}{2}\pi)$ and $(\pi - \theta_{12})$.

(ii) The motion over the hyperradius R is treated semiclassically.

The hyperradius R plays the role of the longitudinal coordinate s of the Sections 2, and $(\alpha_h - \frac{1}{4}\pi)$ and $(\pi - \theta_{12})$ are the transversal coordinates q_i. In the original Wannier theory [21], [22] the processes in the small-R region (inner zone, $R < R_0$) are not considered. They are replaced by some boundary condition on the border R_0 and the system evolution in the outer zone to the free electron motion regime ($R \to \infty$) is considered. Thus in contradistinction to the previous examples we do not have the *periodic* classical trajectory in this case. The basic trajectory corresponds to the double electron escape and terminates at $R \to \infty$.

The analysis of the *total* double escape cross sections within the present approach was carried out in Ref. [23]. Some special treatment is required to account for the electrons deceleration (as R increases) due to the Coulomb attraction to the residual core. This effect becomes crucial when the energy excess E above the double ionization threshold is small. The postadiabatic scheme was developed which allowed us to reproduce not only the Wannier power threshold law but also the

deviations from it for small but finite E.

In addition to the total double escape cross section the final electron distributions over the angles and energies is of great interest as a direct manifestation of the electron correlations. In a good approximation the angular coordinate θ_{12} is separated from the hyperangle α_h. Then the general scheme of the Sections 2 and 3 shows that the angular dependent wave function obeys [24], [25] the non-stationary Schrodinger equation for the harmonic oscillator with the time-dependent frequency (it is worth reiterating that the mock time is simply related with the longitudinal coordinate R). The final ($R \to \infty$) angular distributions depend crucially on the boundary (or initial) condition imposed on the border of the reaction zone. Although this point is completely obvious in the present formulation via the non-stationary harmonic oscillator (see also Ref. [26]), it was missed by the previous authors [27] who claimed that the Gaussian angular correlation pattern universally appear.

In the present approach the problem of the angular correlations is formulated in terms of the wave packet propagation from R_0 to $R \to \infty$. Some general features of the propagation can be established in the harmonic approximation for the problem under consideration [24], [25]. The more accurate scheme of the calculations drops the harmonic approximation. It incorporates the exact Coulomb interaction between the electrons and also the effective centrifugal potential which appears for the double continuum states with the non-zero orbital momentum L. The quantitative agreement with the experimental data is achieved along this way and a number of new qualitative features of the double escape process are revealed [28] - [30].

Acknowledgments

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Shannon-Wehrl entropy
for cosmological and black-hole squeezing

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Abstract

We discuss the Shannon-Wehrl entropy within the squeezing vocabulary for the cosmological and black hole particle production.

Models and concepts of quantum optics have been applied to quantum cosmology (cosmological particle production) already in the seventies [1]. More recently Grishchuk and Sidorov [GS] [2] used the formalism of squeezed states to discuss the spectrum of relic gravitons from inflation, the spectrum of primordial density perturbations, and even the Hawking radiation of Schwarzschild black holes. Apparently there is no new physics entailed [3]. However, the squeezing language may well be more effective in characterizing those physical processes which are of basic theoretical interest. Therefore many authors started to use this language in the cosmological context.

Here we apply the Shannon-Wehrl entropy (S_{sw}) [4] to the squeezing approach of [GS] [5].

In quantum optics S_{sw} is known as an important parameter which is employed to distinguish among various types of coherent states, measuring the relative degree of squeezing with respect to pure coherent states for which $S_{sw} = 1$ is minimum [6]. It is defined as follows

$$S_{sw} = -\frac{1}{\pi} \int d^2\alpha Q(\alpha) \ln Q(\alpha) \qquad (1)$$

where $Q(\alpha)$ is the Q representation of the density operator satisfying the normalization condition $\frac{1}{\pi} \int d^2\alpha Q(\alpha) = 1$.

The calculation of S_{sw} for various types of states is not difficult [7]. Here we quote two results of which we shall make use in the following. For the one-mode squeezed states

$$S_{sw} = 1 + \frac{1}{2} \ln(\sinh^2 r - |\epsilon|^2) \qquad (2)$$

where ϵ is the coherent percent component of the squeezed state. $\epsilon = 0$ means the squeezed vacuum state. For the thermal states the S_{sw} parameter may be written

$$S_{sw} = 1 - \ln(1 - \xi) \qquad (3)$$

where ξ is the inverse of the Boltzmann modal factor $\xi = \exp(-\beta\hbar\omega)$.

Let us pass now to the squeezing approach of [GS]. The main idea is that gravitons created from zero point fluctuations of an initial vacuum cosmological state are at present in an one-mode squeezed quantum state as the result of the parametric amplification due to the interaction with the variable gravitational background. The squeezing coefficient r is a function of the cosmological evolution. Most authors [8] use an expansion in three stages: inflationary (i), radiation-dominated (r), and matter-dominated (m), with the transitions between stages considered in the 'sudden' approximation in which the kinematic effects of the transitions are neglected. Thus the Universe remains in the same quantum state as before transitions [9], and only a redistribution (squeezing) of the quasiparticles takes place. The parametric amplification occurs mainly at the inflationary stage, where the variation of the background is most rapid. The squeezing coefficient can be obtained from the ratios of the dimensionless scale factors at the returning (either at r-stage or m-stage) and exit of a given mode out of the Hubble sphere at the i-stage, as follows

$$\exp r = a(\eta_{ret})/a(\eta_{ex}) \tag{3}$$

According to [GS] r increased from $r \sim 1$ up to $r \sim 100$ for waves with present-day frequencies ranging from $\nu \approx 10^{-8} - 10^{-16}$Hz, which were amplified at the inflationary stage only. For waves in the range $\nu \approx 10^{-16} - 10^{-18}$Hz, the squeezing parameter may reach a value of 120 due to the additional amplification at the matter-dominated transition. We see that cosmological squeezing is about two orders of magnitude bigger than ordinary laboratory squeezing. This is indicative of the huge mean number of quasiparticles in every mode. Making use of the numerical values of the cosmological squeezing coefficient we can plot the S_{sw} entropic parameter for the one-mode squeezed graviton states according to Eq.(2).
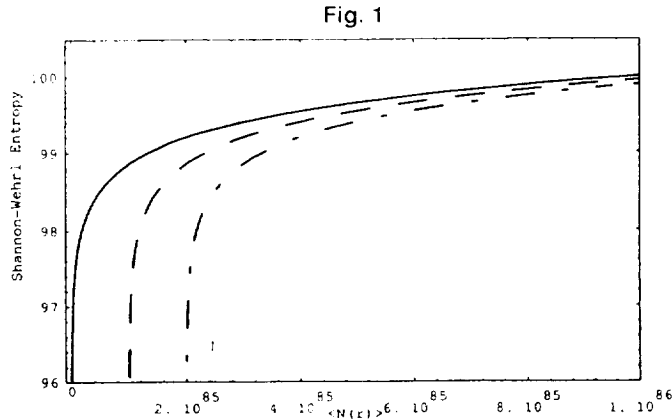
Fig. 1

Fig. 1: Shannon-Wehrl entropy for graviton squeezed states with different coherent components ϵ (full line $\epsilon = 0\%$, slash line $\epsilon = 10\%$, slash-dot line $\epsilon = 20\%$).

The non-zero coherent component we allowed for would correspond to possible deviations of the initial quantum state of gravitons from the vacuum state [10].

In the case of Schwarzschild black holes a two-mode squeezing comes into play for any type of radiation detected at asymptotic infinity. However due to the special causal structure of the black hole spacetime, the asymptotic observations are limited to one mode only. Under

such conditions the detected states turn into thermal ones. Actually, Hawking radiation is a distorted blackbody radiation, but we can consider it as an effective thermal one [11]. Therefore we plotted S_{sw} according to Eq.(3), with γ in the effective Boltzmann factor defined by

$$\frac{1}{\exp(\gamma) - 1} = \frac{\Gamma(\omega)}{\exp(\beta_h \hbar \omega) - 1} \tag{4}$$

where β_h is the horizon inverse temperature parameter, and $\Gamma(\omega)$ is the penetration factor of the curvature and angular momentum barrier around the black hole.
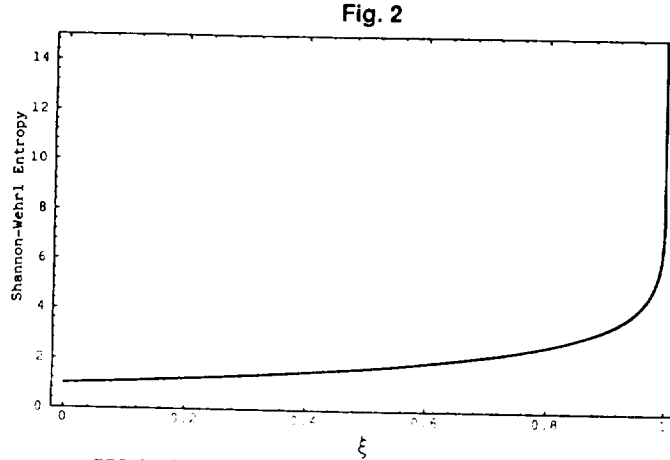
Fig. 2

Fig. 2: Shannon-Wehrl entropy for the 'thermal' radiation of a $M = 10^{17}$ g Schwarzschild black hole as a function of the inverse of the effective Bolzmann factor.

We chose the mass of the black hole so that no massive particles are emitted. This would better correspond to the analogy with quantum optics.

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REAL LASERS AND OTHER DEFORMED OBJECTS[1]

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. *Heard at the Second Harmonic Oscillator Conference:*
"There are no harmonic oscillators in Nature." K.B. Wolf
"Tell that to the quantum opticians!" M.M. Nieto

Abstract

In this talk we re-examine three important properties of quantum laser systems:
(i) Photon counting statistics (ii) Squeezing (iii) Signal-to-Quantum Noise Ratio.
None of these phenomena depends on the choice of hamiltonian; indeed, we analyze them initially without restriction to any specific form of the commutation relations.

1   Introduction

Although most of the recent motivation for deforming the bosonic canonical commutation relations has been derived from considerations of theory, in this note we should like to take a different tack. To what extent does the assumption of modified (*deformed*) commutation relations lead to new, even non-intuitive, physical predictions? Ideally, such predictions should not be based on the choice of a specific hamiltonian, due to the additional ambiguity involved in such a choice; unfortunately, this rules out delicate tests involving frequency measurements, some of the most refined of physics. And, initially at any rate, it would be of interest to embark on the analysis without resorting to a specific form of deformed commutation relations, although ultimately any quantitative result will depend on a specific set.

With this *minimalist* philosophy in mind, let us consider the ingredients necessary for a theory of quantum photons. First of all, we need an operator a which annihilates photons one at a time; and its hermitian conjugate $a^\dagger$ which creates them. We also postulate a number operator N which counts photons; $N|n\rangle = n|n\rangle$. The set $\{|n\rangle; n = 0,\ldots,\}$ provides a denumerable basis for the Hilbert space (Fock space). Thus the number operator N satisfies $[N, a] = -a$, just as for the usual (non-deformed) boson operators. Necessarily, since the vacuum state $|0\rangle$ is defined to have no photons, $N|0\rangle = 0$ and $a|0\rangle = 0$. Clearly the combination $a^\dagger a$ does not change the number of photons, so it commutes with N and must be a function of N. We write this function conventionally as $[N]$ (read "box N"). Thus we have

$$a^\dagger a = [N].$$

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Clearly $aa^\dagger$ is also a function of N; from evaluation of

$$a(a^\dagger a)|n> = (aa^\dagger)a|n> \tag{1}$$

this function may easily be seen to be

$$aa^\dagger = [N+1].$$

The generalized commutation relations may therefore be written

$$aa^\dagger - a^\dagger a = [N+1] - [N] \tag{2}$$

where [ ] is some (analytic) function.

For example, the two most commonly used deformations of the canonical commutation relations which have been considered are:

(a) "Maths" Boson:

$$aa^\dagger - qa^\dagger a = I. \tag{3}$$

This was introduced by Arik and Coon [1], who also described the corresponding q-coherent states. In the commutator form, this may be written as

$$aa^\dagger - a^\dagger a = q^N \tag{4}$$

where q is some real parameter. We refer to this deformed boson as a "Maths" (or M-) boson as the "basic" numbers (cf. Equation (15)) and special functions, q-functions, associated with this operator have been investigated in the mathematical literature for over 150 years; see, for example, [2].

(b) "Physics" Boson:

$$aa^\dagger - qa^\dagger a = q^{-N}. \tag{5}$$

In the commutator form, this may be written as

$$aa^\dagger - a^\dagger a = \cosh(2N+1)s/\cosh s \tag{6}$$

where $q = \exp(2s)$.

This deformation was introduced [3, 4] in order to provide a realization of the "quantum groups" [5] (non-cocommutative Hopf algebras) which arise naturally in the solution of certain lattice models [6].

An alternate formulation of Equation 2 is [7]

$$aa^\dagger - f(N)a^\dagger a = 1 \tag{7}$$

with the correspondence [8]

$$
\begin{aligned}
[n] &= 1 + f(n-1) + f(n-1)f(n-2) + f(n-1)f(n-2)f(n-3) \\
&\quad + \cdots + f(n-1)f(n-2)\cdots f(2)f(1) \tag{8}
\end{aligned}
$$

$$= \sum_{k=0}^{n-1} \frac{f(n-1)!}{f(k)!}. \tag{9}$$

Following the pioneering work of Jackson, we may introduce a generalized calculus related to our general deformation characterized by the analytic function [ ]. We define an operator D_x such that

$$D_x = \frac{1}{x}\left[x\frac{d}{dx}\right].$$ (10)

This acts as a generalized derivative operator, e.g.

$$D_x\, x^n = [n]x^{n-1}.$$ (11)

The eigenfunction $E(x)$ of D_x given by

$$E(x) = \sum_{n=0}^{\infty} \frac{x^n}{[n]!}.$$ (12)

is well–defined provided the function [ ] satisfies appropriate convergence criteria. This plays the role of a generalized exponential function.

A related generalized quantum optics may be described [8], starting with the generalized coherent states $|\lambda\rangle$ defined to satisfy

$$a|\lambda\rangle = \lambda|\lambda\rangle.$$ (13)

Since $a\, E(\lambda a^\dagger)|0\rangle = \lambda E(\lambda a^\dagger)|0\rangle$, we can use $E(x)$ to define analogues of coherent states as normalized eigenstates of the generalized annihilation operator.

$$|\lambda\rangle = \{E(|\lambda|^2)\}^{-\frac{1}{2}} E(\lambda a^\dagger)|0\rangle.$$ (14)

The q-coherent states associated with the special cases of the bosons described by Equation 3 and Equation 5 have been investigated by several authors e.g. [4, 9]. For these two special cases, $[n]$ is given by

$$[n] = \begin{cases} \dfrac{1-q^n}{1-q} & \text{M-case} \\[2ex] \dfrac{q^n - q^{-n}}{q - q^{-1}} & \text{P-case} \end{cases}$$ (15)

We now consider in turn each of three phenomena in quantum optics from our new generalized viewpoint:

- Photon counting statistics

- Squeezing

- Signal-to-Quantum Noise Ratio.

2 Photon Counting Statistics

The states of an ideal laser are conventionally described by Glauber coherent states [10]. However, real lasers do not strictly adhere to this description; in particular, the photon number statistics of real lasers are not exactly Poissonian [11]. Furthermore, various non-linear interactions give rise to well-defined deviations from the Poissonian distribution [12]. Recently, deformations of the commutation rules of boson operators have been considered as models for physical systems which deviate from the ideal cases [13]. We approach the problem of the "real" laser in this latter phenomenological spirit, and show that indeed a coherent state of the deformed boson (q-coherent state) provides a more accurate model of a non-ideal laser, at least as far as the photon number statistics is concerned.

An *ideal* laser may be described as a normalized eigenstate of the photon annihilation operator a, where a and its hermitian conjugate $a^\dagger$ (photon creation operator) satisfy

$$[a, a^\dagger] \equiv aa^\dagger - a^\dagger a = I. \tag{16}$$

The normalized eigenstate satisfying $a|\alpha> = \alpha|\alpha>$ is easily seen to be

$$|\alpha> = \exp(-\frac{|\alpha|^2}{2}) \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n> . \tag{17}$$

The number eigenstates are $|n>$, and this coherent state gives rise to the Poisson distribution

$$P_n = | <n|\alpha> |^2 = \exp(-|\alpha|^2) \frac{|\alpha|^{2n}}{n!}. \tag{18}$$

The factorial moments of this distribution are

$$<n> = |\alpha|^2$$

$$<n(n-1)> = |\alpha|^4$$

$$<n(n-1)(n-2)> = |\alpha|^6$$

etc., from which the variance is found to be

$$\sigma^2 = <n^2> - <n>^2 = |\alpha|^2$$

A convenient measure of the deviation of a distribution from the Poisson distribution is the Mandel parameter

$$Q = \frac{\sigma^2}{<n>} - 1 = \frac{<n(n-1)>}{<n>} - <n>$$

which vanishes for the Poisson distribution, is positive for a super-Poissonian distribution, and negative for a sub-Poissonian distribution.

In order to enter into the phenomenological spirit of our approach, and to compare with the experimental data, we need to specify the form of the commutation relations Equation 2; that is, specify a choice of the function [ ]. It is sufficient for our purposes here to compare the distributions arising from the M and P forms Equation 3 and Equation 5 respectively. One can

easily check that the P-type q-Poisson distribution is sub-Poissonian ($Q \leq 0$) for all values of q, reducing to the conventional Poisson distribution for $q = 1$. On the other hand, the M-type q-Poisson distribution is super-Poissonian for $q < 1$ and sub-Poissonian for $q > 1$.

The q-Poissonian q-factorial moments are $< [n] > = |\alpha|^2$, $< [n][n-1] > = |\alpha|^4$, etc.

To evaluate the average number of photons and the Mandel parameter for the q-Poisson distribution we note that the corresponding factorial moments satisfy

$$< n > = \left. \frac{x}{E_q(x)} \cdot \frac{\partial E_q(x)}{\partial x} \right|_{x=|\alpha|^2}$$

$$< n(n-1) > = \left. \frac{x^2}{E_q(x)} \cdot \frac{\partial^2 E_q(x)}{\partial^2 x} \right|_{x=|\alpha|^2}$$

These expressions may be used to provide estimates of the q-Poissonian parameters q and $|\alpha|^2$ corresponding to a distribution which is specified in terms of given values of $< n >$ and Q . The values of q corresponding to given pairs of values of $< n >$ and Q , and the corresponding values of $|\alpha|^2$ were tabulated in reference [14].

For small deviations from a Poissonian distribution we define $q = e^{-s}$ and obtain in the M-case

$$s = \frac{2Q}{< n >}$$

which is positive (*i.e.*, $q < 1$) for a super-Poissonian distribution and negative ($q > 1$) for a sub-Poissonian distribution. In the P-case we obtain

$$s^2 = -\frac{3Q}{< n > (< n > + \frac{3}{2})}$$

so that only the sub-Poissonian distribution ($Q < 0$) corresponds to a real value of s (and q).

Another useful result is

$$\rho \equiv \lim_{<n> \to 0} \frac{Q}{< n >} = \begin{cases} \dfrac{1-q}{1+q} & \text{M-case} \\[2mm] \dfrac{2}{q+q^{-1}} - 1 & \text{P-case} \end{cases} \tag{19}$$

In the M-case the range of ρ is $-1 < \rho < 1$, corresponding to a sub-Poissonian distribution for $\rho < 0$ and to a super-Poissonian distribution for $\rho > 0$. In the P-case the range of ρ is $-1 < \rho \leq 0$, exhibiting only a sub-Poissonian distribution.

From Equation (19) we obtain

$$q = \begin{cases} \dfrac{1-\rho}{1+\rho} & \text{M-case} \\[2mm] \dfrac{1}{1+\rho} \pm \sqrt{\dfrac{1}{(1+\rho)^2} - 1} & \text{P-case} \end{cases} \tag{20}$$

Using the three highest peaks in the experimental data pertaining to the photon statistics of a He-Ne laser just above threshold [15] we obtain $\frac{P_2^2}{P_1 P_3} = \frac{[3]}{[2]} = 1.319$, which in the M-case is a

quadratic equation in q, yielding $q = 0.747$. Note that the corresponding equation for the P-case can be shown to rule out the P-boson as a model of this system since for all real and positive q the inequality $\frac{[3]}{[2]} \geq \frac{3}{2}$ holds.

If one compares the best fit for the M-boson q-coherent state against the experimental data [15] and the ideal (Glauber) coherent state, one finds that the value of q corresponding to the best fit is 0.749, in very close agreement with the value estimated above using the highest three peaks. It is not surprising that a better fit is obtained with the q-coherent state, due to the extra parameter q. However, certain constraints are satisfied (for example, the convergence criterion for the M-type q-exponential function demands that $(1 - q)|\alpha|^2 \leq 1$ and is satisfied here) and, as we have already remarked, the P-boson model is ruled out.

Experimental studies of the photon statistics of a laser at different intensities above the threshold were reported in refs. [16] and [17]. Since super-Poissonian statistics is exhibited, only M-type analysis is warranted. In both cases it is found that for counting times short relative to the intensity correlation time the distributions agree with q-Poissonian statistics, the value of q increasing from a value which could be close to zero at threshold to a value close to unity (Poissonian distribution) for intensities about an order of magnitude higher than the threshold intensity. At twice the threshold intensity values of q ranging between roughly 0.3 and 0.8 were obtained from the different sets of experimental data.

Another set of experimental data, exhibiting a sub-Poissonian distribution, involves the photons emitted by single-atom resonance fluorescence [18]. Using the data for P_0, P_1, P_2 we obtained in Reference [14] $q_M = 2.44$ or $q_P = 3.12$. This is in agreement with the estimate for q_M obtained using Equation (20) and the data reported in [18], $< n > = 6.23 \cdot 10^{-3}$ and $Q = -2.52 \cdot 10^{-3}$, from which $q_M = 2.36$.

The examples of this section illustrate cases from quantum optics where a more accurate model of a physical system may be obtained by use of quantum group ideas.

3   Squeezing

The electromagnetic field components x and p are given by

$$x = \frac{1}{\sqrt{2}}(a + a^\dagger) \quad \text{and} \quad p = \frac{1}{i\sqrt{2}}(a - a^\dagger). \tag{21}$$

As usual, we define the variances (Δx) and (Δp) by

$$(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2 \quad \text{and} \quad (\Delta p)^2 = \langle p^2 \rangle - \langle p \rangle^2. \tag{22}$$

In the vacuum state

$$(\Delta x)_0 = \frac{1}{\sqrt{2}} \quad \text{and} \quad (\Delta p)_0 = \frac{1}{\sqrt{2}}. \tag{23}$$

and so

$$(\Delta x)_0 (\Delta p)_0 = \frac{1}{2}. \tag{24}$$

The commutation relation Equation (16) for a and $a^\dagger$ leads to the following uncertainty principle

$$(\Delta x)(\Delta p) \geq \frac{1}{2}|\langle [x, p] \rangle| = \frac{1}{2}. \tag{25}$$

Thus the vacuum state attains the lower bound for the uncertainty, as do the coherent states.

While it impossible to lower the product $(\Delta x)(\Delta p)$ below the vacuum uncertainty value, it is nevertheless possible to define *squeezed* states [19] for which (at most) one quadrature lies below the vacuum value, i.e.

$$(\Delta x) < (\Delta x)_0 = \frac{1}{\sqrt{2}} \quad \text{or} \quad (\Delta p) < (\Delta p)_0 = \frac{1}{\sqrt{2}}. \tag{26}$$

If we now consider the generalized bosonic operators given by (2), using the same definitions for the the field quadratures, x and p, as in (21) we find that, just as in the conventional case, the vacuum uncertainty product $(\Delta x)_0(\Delta p)_0 = \frac{1}{2}$ is a lower bound for all *number* states.

However, unlike the conventional case, it is not a global lower bound.

Consider the quadrature values in eigenstates of the generalized annihilation operator.

Then

$$\langle x \rangle_\lambda = \langle \lambda | \frac{1}{\sqrt{2}}(a^\dagger + a) | \lambda \rangle = \frac{1}{\sqrt{2}}(\lambda + \bar{\lambda}) \tag{27}$$

and

$$\langle x^2 \rangle_\lambda = \langle \lambda | \frac{1}{2}((a^\dagger)^2 + a^2 + a^\dagger a + aa^\dagger) | \lambda \rangle \tag{28}$$

$$= \frac{1}{2}\{(\bar{\lambda} + \lambda)^2 + 1 - \varepsilon_{f,\lambda}|\lambda|^2\} \tag{29}$$

where

$$\varepsilon_{f,\lambda} = 1 - \langle f(N+1) \rangle_\lambda. \tag{30}$$

If we choose $0 < f(n) < 1$, then it can be shown that $\varepsilon_{f,\lambda}|\lambda|^2 \in (0,1)$ for λ within the radius of convergence of the generalized exponential (12).

Hence

$$(\Delta x)_\lambda^2 = \frac{1}{2}\{1 - \varepsilon_{f,\lambda}|\lambda|^2\}. \tag{31}$$

Evaluating the variance for the other component, we find that $(\Delta p)_\lambda^2 = (\Delta x)_\lambda^2$ so

$$(\Delta x)_\lambda(\Delta p)_\lambda = \frac{1}{2}\{1 - \varepsilon_{f,\lambda}|\lambda|^2\} < \frac{1}{2}. \tag{32}$$

However, it can also be shown that

$$\frac{1}{2}\{1 - \varepsilon_{f,\lambda}|\lambda|^2\} = \frac{1}{2}|\langle [x,p] \rangle_\lambda| \tag{33}$$

so

$$(\Delta x)_\lambda(\Delta p)_\lambda = \frac{1}{2}|\langle [x,p] \rangle_\lambda| \tag{34}$$

Thus we see that these generalized q–coherent states satisfy a restricted form of the Minimum Uncertainty Property (M.U.P.) of the conventional coherent states. Additionally we see that there is a general noise reduction in both quadratures compared to their vacuum value. In conventional coherent states there is no noise reduction relative to the vacuum value. In conventional squeezed states, there is noise reduction in only one component.

We can apply the preceding analysis to the two usual forms of q-deformed bosons:

(a) 'Physics' q–bosons
First consider the q-bosons of Equation 5. The deformed commutation relation

$$aa^\dagger - q\,a^\dagger a = q^{-N}. \tag{35}$$

can be rewritten [20] as

$$aa^\dagger - f(N)\,a^\dagger a = 1 \tag{36}$$

where $f(N) = \frac{q^{N+2}+1}{q(q^N+1)}$.

In this case, for normalizable eigenstates, the function $\varepsilon_{f,\lambda}$ is negative and so simultaneous two–component noise reduction does not take place. This is in agreement with the findings of Katriel and Solomon [21] and Chiu et al [22]. However, it can be shown that ordinary *squeezing* i.e. noise reduction in one component compared to the vacuum (with a corresponding noise amplification in the other component) does take place [23, 24].

(b) 'Maths' q–bosons
We now consider the q-boson described by Arik and Coon [1]. which is characterised by the deformed commutation relation

$$aa^\dagger - q\,a^\dagger a = 1 \tag{37}$$

For $q \in (0,1)$, the Jackson q-exponential $E_q(|\lambda|^2)$ converges, provided

$$\varepsilon_q|\lambda|^2 = (1-q)|\lambda|^2 < 1.$$

Given this condition on λ, we have normalizable q-analogue coherent states satisfying (13) in which

$$(\Delta x)_\lambda^2 = (\Delta p)_\lambda^2 = (\Delta x)_\lambda(\Delta p)_\lambda = \frac{1}{2}\{1 - \varepsilon_q|\lambda|^2\} < \frac{1}{2}. \tag{38}$$

Hence, for this type of q–boson, we do obtain noise reduction in both quadratures with respect to the vacuum value.

4 Signal-to-Quantum Noise Ratio

In a classic paper, Yuen [19] showed that for a radiation field of photons the maximum signal-to-quantum noise ratio ρ for fixed energy has the value $4n_s(n_s+1)$, where n_s gives the upper limit on the number of photons in the signal (effectively a maximum power per unit frequency constraint).

The only mathematical input to this result consisted of the canonical commutation relations for the photon annihilation operato r a, namely;

$$[a, a^\dagger] = 1 \qquad (39)$$

with the photon number operator given by $N = a^\dagger a$.

The hermitian components x, p of the electromagnetic field corresponding to our *generalized* photons of Equation 2 (which we now write as $a_q^\dagger, a_q$ to distinguish from the conventional ones) satisfy

$$[x_q, p_q] = i([N + 1] - [N]) \qquad (40)$$

which reduces to the canonical commutation relation $[x, p] = i$ when $[N] = N$.

We now consider a state, which we write as $<, >$, although everything which follows applies equally to a general state described by a density function. Introducing the hermitian operators

$$X \equiv x_q - < x_q >, \quad P \equiv p_q - < p_q >,$$

the quantum dispersion (quantum noise) in each of the components is measured by the quantities $(\Delta x_q)^2 \equiv < X^2 >$ and $(\Delta p_q)^2 \equiv < P^2 >$. The positivity of the number $< A(t)A^\dagger(t) >$ for all t, where $A(t) \equiv tX + iP$, leads immediately to the modified uncertainty principle

$$(\Delta x_q)^2 (\Delta p_q)^2 \geq \frac{1}{4} < [N + 1] - [N] >^2 . \qquad (41)$$

This uncertainty product exceeds the conventional value of $\frac{1}{4}$ in the "Physics" case (5), and in the "Maths" case (3) for $q \geq 1$.

The signal-to-quantum noise ratio

$$\rho_q \equiv < x_q >^2 / (\Delta x_q)^2$$

must be maximized subject to the constraint

$$< a_q^\dagger a_q > \leq [n_s] \qquad (42)$$

where n_s is the maximum number of q-photons for the frequency under consideration, and inequality (41) above. We may rewrite constraint (42) as

$$< x_q >^2 + < p_q >^2 + (\Delta x_q)^2 + (\Delta p_q)^2 - < [N + 1] - [N] > \leq 2[n_s] \qquad (43)$$

where we have substituted

$$< x_q^2 > = < x_q >^2 + (\Delta x_q)^2, \quad < p_q^2 > = < p_q >^2 + (\Delta p_q)^2.$$

Consideration of (43) leads us to infer that it is favourable to use all the available energy; that is, $< N > = n_s$: and to use it in the x-component alone, so that $< p_q > = 0$. The inequality thus becomes the equation

$$< x_q >^2 + (\Delta x_q)^2 + (\Delta p_q)^2 = [n_s] + [n_s + 1]. \qquad (44)$$

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It is a straightforward exercise in the calculus to show that the ratio ρ_q is maximized, subject to the constraints (41) and (44), at a value

$$\rho_q = 4[n_s][n_s + 1]/([n_s + 1] - [n_s])^2. \tag{45}$$

Given two types of "photon" described by $[\ ]_1$ and $[\ ']_2$, it is a straightforward exercise in inequalities to show that the corresponding signal-to-quantum noise ratios ρ_1, ρ_2 satisfy

$$\rho_1 \quad \le \rho_2 \quad \text{if} \quad \frac{[n+1]_1}{[n]_1} \ge \frac{[n+1]_2}{[n]_2}.$$

Taking $[n]_2 = n$ ("ordinary" photons) and $[n]_1$ as the q-photons defined by Equations (3) and (5) in turn, we obtain:

$$\rho_{q\le 1}^M \ge \rho \ge \rho^P \ge \rho_{q\ge 1}^M$$

on comparing with Yuen's result for the conventional case

$$\rho = 4n_s(n_s + 1). \tag{46}$$

Therefore states based on the usual q-photons Equation (5), and Equation (3) for $q \ge 1$, (which are the more physical cases satisfying the conventional uncertainty principle) will not lead to an enhanced signal-to-quantum noise ratio over the conventional photon case.

5 Conclusions

In this talk we have given three examples where we are able to model physically observable properties of real photons by means of deformed photons satisfying very general deformations of the canonical commutation relations. The viewpoint we have adopted is the phenomenological one; we do not assume that "real" photons satisfy other than the conventional commutation relations. Rather, we have shown that simple models involving "dressed" photons, satisfying very general constraints, may be invoked to describe observed, and sometimes non-intuitive, phenomena.

This by no means addresses the still open question as to whether deformed commutation relations describe real particles, whatever that means.

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SUPERSYMMETRIC OSCILLATOR IN OPTICS

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Abstract

We show that the supersymmetric structure (in the sense of supersymmetric quantum mechanics) appears in Helmholtz optics describing light propagation in waveguides. For the case of elliptical waveguides, with the accuracy of paraxial approximation it admits a simple physical interpretation. The supersymmetry connects light beams of different colors. The difference in light frequencies for the supersymmetric beams is determined by the transverse gradient of the refractive index. These beams have the same wavelength in the propagation direction and can form a stable interference pattern.

1 Introduction

There is a correspondence between quantum mechanics and optics in the paraxial regime [1] and in the global one [2]. Consequently, many notions can be transported from one to the other, such as coherent and squeezed states (see, *e.g.*, Ref. [3, 4]). Here we describe an optical system that exhibits supersymmetry in the sense of supersymmetric quantum mechanics (SUSY QM).

Supersymmetry in quantum mechanics connects two Hamiltonians with the same spectrum except for the ground state (unbroken supersymmetry [5], see [6] and references therein.) SUSY has been successfully applied in atomic [7] and nuclear physics [8]. The supersymmetric form of the Dirac equation in an external field [9, 10, 11] presents the Dirac equation as the square root of the Klein-Gordon equation; the kind of supersymmetry we have here is analogous and finds the square root of the Helmholtz equation. The supersymmetric structure of Helmholtz optics describes light propagation in a waveguide and admits a very clear physical interpretation.

We consider optical waveguides along the z-axis, *i.e.*, media that are inhomogeneous only in the x direction. From the wave equation in $2 + 1$ dimensions for solutions of time frequency ν we have the Helmholtz equation

$$\left[\partial_z^2 + \partial_x^2 + \nu^2 n^2(x)/c^2\right] f(x, z) = 0. \tag{1}$$

In Section 2 we present the supersymmetric structure of Eq. (1), in Section 3 a physical reinterpretation, and some concluding remarks in Section 4. Note that until Section 3 we do not use the paraxial approximation.

2 Supersymmetric structure

We start with a system of two first-order equations for a two-component wave function of the x and z-coordinates,

$$\partial_z \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} = \begin{pmatrix} ik & v_+ \\ v_- & -ik \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix}, \qquad (2)$$

where k is a constant and

$$v_\pm \equiv \pm\partial_x + W(x),$$

with an arbitrary function $W(x)$. The second z-derivative involves the square of this 2×2 matrix,

$$\partial_z^2 \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} = \begin{pmatrix} -k^2 + v_+v_- & 0 \\ 0 & -k^2 + v_-v_+ \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix}.$$

Therefore we have two different Helmholtz equations for the components:

$$\left[\partial_z^2 + \partial_x^2 + k^2 - W_x - W^2\right] \Psi_1 = 0,$$
$$\left[\partial_z^2 + \partial_x^2 + k^2 + W_x - W^2\right] \Psi_2 = 0. \qquad (3)$$

where $W_x \equiv dW/dx$. Now, for a given wavenumber κ in z direction that is common to both wavefunctions, we write

$$\Psi_{1,2}(x, z) = \Phi_{1,2}(x)e^{-i\kappa z}. \qquad (4)$$

Equations (3) then become the eigenvalue equations for the components,

$$\left[-\partial_x^2 - W_x + W^2\right] \Phi_1 = \left[k^2 - \kappa^2\right] \Phi_1,$$
$$\left[-\partial_x^2 + W_x + W^2\right] \Phi_2 = \left[k^2 - \kappa^2\right] \Phi_2. \qquad (5)$$

Now we introduce the supersymmetric structure by considering the component Φ_1 as representing the 'boson' and Φ_2 the 'fermion' sectors of the supersymmetric Hamiltonian eigenfunctions. The supercharge operators are

$$Q_- = \begin{pmatrix} 0 & 0 \\ v_+ & 0 \end{pmatrix}, \qquad Q_+ = \begin{pmatrix} 0 & v_- \\ 0 & 0 \end{pmatrix}.$$

The supersymmetric Hamiltonian, defined as the anticommutator of the two supercharges, is

$$H_s = \{Q_-, Q_+\} = \begin{pmatrix} v_-v_+ & 0 \\ 0 & v_+v_- \end{pmatrix}, \qquad [H_s, Q_\pm] = 0.$$

The eigenvalue equations for H_s are then

$$v_-v_+\Phi_1 = \left(k^2 - \kappa^2\right) \Phi_1,$$
$$v_+v_-\Phi_2 = \left(k^2 - \kappa^2\right) \Phi_2.$$

These equations coincide with Eqs. (5). Operators v_-v_+ and v_+v_- have the same spectrum except for the ground state, which has to be a normalizable solution of one of the two equations $v_+\phi_1 = 0$ or $v_-\phi_2 = 0$. Therefore, SUSY connects solutions of Helmholtz equations of two different waveguides with index profiles

$$\nu^2 n^2(x)/c^2 = k^2 \mp W_x - W^2. \qquad (6)$$

3 Physical Reinterpretation

We now reinterpret these formulas in another way to describe two *different* beams in the *same* waveguide. We choose

$$W(x) = w\,x. \tag{7}$$

The eigenvalue equations (5) are then two Schrödinger equations for harmonic oscillators with displaced energy levels,

$$\left[-\partial_x^2 + w^2 x^2\right]\Phi_{1,2} = \left(k^2 \mp w - \kappa^2\right)\Phi_{1,2}. \tag{8}$$

Meanwhile, seen as Helmholtz equations, Eqs. (8) correspond to

$$\nu^2 n^2(x)/c^2 = k^2 \mp w - w^2 x^2, \tag{9}$$

with the same refractive index $n(x)$. In the absence of material dispersion, n is independent of ν. This is an *elliptic* index-profile waveguide; it approximates the usual parabolic index-profile waveguide in the paraxial regime [12]. The eigenvalues of the operator on the left of (8) are well known to be

$$E_m = w(2m+1), \qquad m = 0,1,2,\ldots. \tag{10}$$

We now find conditions for a supersymmetric pair of Helmholtz solutions propagating in the same waveguide. Into this waveguide $n^2(x) = n_0^2 - n_1^2 x^2$ we inject two light beams with slightly different time frequencies

$$\nu_{1,2}^2 = \nu_0^2(1 \mp \epsilon).$$

To fulfill Eqs. (9), we substitute $k = n_0\nu_0/c$, $w = n_1\nu_0/c$ and find the conditions

$$\epsilon = \frac{n_1}{n_0 k} = \frac{w}{k^2}, \qquad \frac{\nu_2^2 - \nu_1^2}{\nu_0^2} = 2\epsilon. \tag{11}$$

This determines the frequency shift in terms of the transverse index profile of the waveguide.

From the standard quantum harmonic oscillator solution we know that the Gaussian beam width in x-direction is $\Delta x = (2w)^{-1/2}$. Therefore, the parameter

$$\epsilon = [2k^2(\Delta x)^2]^{-1} \sim (\text{wavelength/beam width})^2$$

should be small. The two light beams with the frequencies $\nu_{1,2}$ obey the Helmholtz equations with

$$\nu_{1,2}^2 n^2(x)/c^2 = k^2 \mp w - w^2 x^2(1 \mp \epsilon). \tag{12}$$

When $\epsilon \to 0$, these two Helmholtz equations become a supersymmetric pair that is slightly broken by the term $\epsilon w^2 x^2$.

It is easy to see that SUSY has the same accuracy as the paraxial approximation. Solution of the Helmholtz equation (1) with the term (12) (compare with Eqs. (8)) shows that the z-propagation wavenumbers of the two beams are

$$\kappa_{1,2}^2(m) = k^2 - w[(1 \pm \epsilon)(2m+1) \pm 1], \qquad m = 0,1,\ldots$$

or

$$\frac{\kappa_{1,2}(m)}{k} \simeq 1 - \epsilon\left(m + \frac{1}{2} \pm \frac{1}{2}\right) - \frac{\epsilon^2}{2}\left(m + \frac{1}{2} \pm \frac{1}{2}\right)^2 \mp \epsilon^2\left(m + \frac{1}{2}\right) + \cdots.$$

The term of order $\epsilon = w/k^2$ exhibits exact SUSY; except for the ground state $\kappa_2(0) = k$, the z-wavenumbers of the two beams coincide

$$\kappa_1(m-1) = \kappa_2(m) + O(\epsilon^2), \qquad m = 1, 2, \cdots, \tag{13}$$

The two terms of order ϵ^2 respectively give a nonlinear correction to the paraxial approximation and break supersymmetry. Therefore, SUSY is exact in the paraxial approximation and is broken beyond this regime.

Thus, supersymmetry (13) connects light beams of different frequencies $\nu_{1,2}^2$ in the same waveguide [cf. Eq. (11)], but having the same wavelength $2\pi/\kappa$ in the propagation direction z [Eq. (4)]. These two beams form a stable interference pattern along the waveguide axis.

4 Conclusions

We have considered the propagation of light in a planar waveguide ruled by the two-dimensional Helmholtz equation. Two Helmholtz equations with different refractive indices (3) form a supersymmetric pair in the sense of SUSY QM.

Supersymmetry *also* describes the propagation of light beams of *different* colors in the *same* waveguide when the transversal index profile is elliptic. This profile determines the difference of light frequencies. SUSY is exact in the paraxial approximation, and broken beyond. In the paraxial regime, supersymmetric light beams of different colors have the same wavelength along the axis of the waveguide, giving rise to a stable interference pattern.

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OSCILLATOR-LIKE COHERENT STATES
FOR THE JAYNES-CUMMINGS MODEL

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Abstract

A new way of diagonalizing the Jaynes-Cummings Hamiltonian is proposed, which allows the definition of annihilation operators and coherent states for this model. Mean values and dispersions over these states are computed and interpreted.

1   Introduction

The Jaynes-Cummings (J.C.) model [1], which is extensively used in Quantum Optics, describes, in its simplest version, the interaction of a cavity mode with a two-level system. In the rotating-wave approximation, it may be described by the Hamiltonian [1, 2]

$$H_{\mathrm{JC}} = \omega \left(a^\dagger a + \frac{1}{2} \right) \sigma_0 + \frac{\omega_0}{2}\sigma_3 + \kappa(a^\dagger \sigma_- + a\sigma_+) , \tag{1}$$

where $\{\sigma_1, \sigma_2, \sigma_3\}$ are Pauli matrices, σ_0 is the identity, $\sigma_\pm = \sigma_1 \pm i\sigma_2$, and $a^\dagger$ and a are the photon creation and annihilation operators. Moreover, κ is the coupling constant, ω is the field mode frequency, and ω_0 is the atomic frequency. Let us also introduce the detuning $\Delta = \omega - \omega_0$. The exact solvability of this model is well-known. Working in the Fock space

$$\mathcal{F} = \mathcal{F}_b \otimes \mathcal{F}_f = \left\{ |n,-\rangle = \begin{pmatrix} 0 \\ |n\rangle \end{pmatrix} , \ |n,+\rangle = \begin{pmatrix} |n\rangle \\ 0 \end{pmatrix} , \ n = 0, 1, 2, \ldots \right\} , \tag{2}$$

the energy eigenstates take the form (for $n = 0, 1, 2, \ldots$)

$$|E_0^-\rangle = |0,-\rangle , \tag{3}$$

$$|E_{n+1}^-\rangle = \frac{1}{R(n+1)} \left(\kappa\sqrt{n+1}|n,+\rangle + \left(\frac{\Delta}{2} + \kappa\, r(n+1) \right)|n+1,-\rangle \right) , \tag{4}$$

$$|E_n^+\rangle = \frac{1}{R(n+1)} \left(\left(\frac{\Delta}{2} + \kappa\, r(n+1) \right)|n,+\rangle - \kappa\sqrt{n+1}|n+1,-\rangle \right) , \tag{5}$$

where

$$r(n) = (\delta + n)^{1/2}, \quad \delta = \left(\frac{\Delta}{2\kappa} \right)^2 , \quad R(n) = \left[\left(\frac{\Delta}{2} + \kappa\, r(n) \right)^2 + \kappa^2 n \right]^{1/2} . \tag{6}$$

In the expression of $r(n)$ we have introduced the parameter δ which will be important in the following. The corresponding energy eigenvalues are

$$E_n^- = \omega n + \kappa r(n), \quad E_n^+ = \omega(n+1) - \kappa r(n+1). \tag{7}$$

The interest of this model, its solvability and its applications have long been discussed. More precisely, dynamical properties have been obtained through the use of states which are initially harmonic oscillator coherent states [3], but that evolve according to the J.C. Hamiltonian [2, 4]. Here, we construct new coherent states which correspond to eigenstates of an annihilation operator for H_{JC}. To do that, we have to find first such an annihilation operator through the diagonalization of the Jaynes-Cummings Hamiltonian (1). Second, we use the theoretical approach, based on the direct product of the Weyl-Heisenberg group with SU(2), to evaluate those coherent states. Finally, we exhibit some of their properties. More details can be found in [5].

2 Annihilation operators and coherent states for H_{JC}

The diagonalization of H_{JC} is performed by the unitary operator $\mathcal{O}$, so that

$$H_d \equiv \mathcal{O}^\dagger H_{JC} \mathcal{O} = \begin{pmatrix} \omega(N+1) - \kappa r(N+1) & 0 \\ 0 & \omega N + \kappa r(N) \end{pmatrix}, \tag{8}$$

where $N = a^\dagger a$, and the definition of $r(N)$ is given in Eq. (6). This operator $\mathcal{O}$ has the form

$$\mathcal{O} = \begin{pmatrix} \dfrac{1}{R(N+1)}\left[\dfrac{\Delta}{2} + \kappa r(N+1)\right] & \dfrac{\kappa}{R(N+1)}\, a \\ -a^\dagger \dfrac{\kappa}{R(N+1)} & \dfrac{1}{R(N)}\left[\dfrac{\Delta}{2} + \kappa r(N)\right] \end{pmatrix}. \tag{9}$$

Clearly, an annihilation operator for H_d is given by $A_d = a\,\sigma_0$. Since the states depend also on the spin index $\pm$, we introduce the spinorial annihilation and creation operators:

$$\Sigma_{-d} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad \Sigma_{+d} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}. \tag{10}$$

We then obtain candidates to be annihilation and creation operators for H_{JC} as:

$$A = \mathcal{O} A_d \mathcal{O}^\dagger, \quad A^\dagger = \mathcal{O} A_d^\dagger \mathcal{O}^\dagger, \quad \Sigma_\pm = \mathcal{O} \Sigma_{\pm d} \mathcal{O}^\dagger. \tag{11}$$

For the determination of coherent states, the situation is particularly simple when we work with H_d in (8), since the energy eigenstates are the Fock-space basis vectors (2). The group theoretical approach to coherent states leads us to define

$$|z, \beta\rangle_d = T(z, \beta)_d |0, -\rangle, \quad z, \beta \in \mathbf{C}, \tag{12}$$

in terms of the unitary representation of the direct product of the Weyl-Heisenberg group with $SU(2)$

$$T(z, \beta)_d = \exp[z A_d^\dagger - \bar{z} A_d + \beta \Sigma_{+d} - \bar{\beta} \Sigma_{-d}]. \tag{13}$$

The coherent states for $H_{\rm JC}$ are then given by

$$|z,\beta\rangle = \mathcal{O}|z,\beta\rangle_d = T(z,\beta)|E_0^-\rangle = \mathcal{O}T(z,\beta)_d\mathcal{O}^\dagger|E_0^-\rangle\,. \tag{14}$$

From the harmonic oscillator coherent states we easily get

$$|z,\beta\rangle_d = \cos(\theta/2)\begin{pmatrix} 0 \\ |z\rangle \end{pmatrix} + e^{i\phi}\sin(\theta/2)\begin{pmatrix} |z\rangle \\ 0 \end{pmatrix} = \cos(\theta/2)\,|z-\rangle_d + e^{i\phi}\sin(\theta/2)\,|z+\rangle_d\,, \tag{15}$$

with $\beta = (\theta/2)e^{i\phi}$, and $|z\rangle$ the normalized state $|z\rangle = e^{-|z|^2/2}\sum_{n=0}^\infty (z^n/\sqrt{n!})|n\rangle$. The state $|z,\beta\rangle_d$ is a linear combination of the "fundamental coherent states" $|z+\rangle_d$ and $|z-\rangle_d$, which are both eigenstates of A_d (but not of Σ_{-d}). Similar fundamental coherent states are defined by using such a decomposition of $|z,\beta\rangle$ in (14).

To be complete, we give the time evolution of such states; the one of the general state (15) will be obtained easily by linear combination. We start with the diagonal case, for which the evolution operator is

$$U_d(t) = e^{-itH_d} = \begin{pmatrix} \bar{e}^{it[\omega(N+1)-\kappa r(N+1)]} & 0 \\ 0 & \bar{e}^{it[\omega N+\kappa r(N)]} \end{pmatrix}\,, \tag{16}$$

and we compute $|z,\pm,t\rangle = \mathcal{O}U_d(t)|z,\pm\rangle_d = U_{\rm JC}(t)\mathcal{O}|z,\pm\rangle_d$. More precisely, we get

$$\begin{aligned}
|z,+,t\rangle &= e^{-|z|^2/2}e^{-i\omega t}\sum_{n=0}^\infty \frac{(ze^{-i\omega t})^n}{\sqrt{n!}}e^{it\kappa r(n+1)}|E_n^+\rangle\,, \\
|z,-,t\rangle &= e^{-|z|^2/2}\sum_{n=0}^\infty \frac{(ze^{-i\omega t})^n}{\sqrt{n!}}e^{-it\kappa r(n)}|E_n^-\rangle\,.
\end{aligned} \tag{17}$$

These are similar to the states obtained by the evolution of the harmonic oscillator coherent states, except for the supplementary oscillation for each n in the sum. This implies that the coherent state does not evolve in time to another coherent state, unlike to the case of the harmonic oscillator. Moreover, our states (17) are different from those considered in other approaches [2, 4]. Indeed, all these authors deal with the states $|z,\pm\rangle_d$ (or a mixture of them) and their evolution is

$$U_{\rm JC}(t)|z,\pm\rangle_d = e^{-itH_{\rm JC}}|z,\pm\rangle_d\,. \tag{18}$$

3   Relevant physical quantities

Let us recall the introduction of the parameter δ in the expression of $r(n)$ in (6). It will be used as a variable in the following. It contains both the detuning Δ and the coupling parameter κ and leads to the exact resonance case when $\delta = 0$ or to the weak coupling limit when $\delta \to \infty$. The parameter $x = |z|^2$ is also introduced, and will be proved to be a good approximation of the number of photons. We will deal with the function

$$G(\delta,x) = e^{-x}\sum_{n=0}^\infty \frac{x^n}{n!}r(n+1) = e^{-x}\sum_{n=0}^\infty \frac{x^n}{n!}\sqrt{\delta+n+1}\,. \tag{19}$$

Its asymptotic behaviour is $G(\delta,x) \sim \sqrt{x}$, which is independent of δ. The calculations will be done explicitly over the states (17), and for a general state $|z,\beta,t\rangle$. We can use (15) to write

the mean value and dispersion of an operator X. Indeed, defining $\langle X \rangle_{\pm} = \langle z, t, \pm | X | z, t, \pm \rangle$ and $\langle X \rangle_{\pm \mp} = \langle z, t, \pm | X | z, t, \mp \rangle$, the mean value of X over a general coherent state is

$$\langle X \rangle = \frac{1 - \cos\theta}{2} \langle X \rangle_{+} + \frac{1 + \cos\theta}{2} \langle X \rangle_{-} + \frac{\sin\theta}{2} \left(e^{i\phi} \langle X \rangle_{+-} + e^{-i\phi} \langle X \rangle_{-+} \right). \tag{20}$$

In the case of having $\langle X \rangle_{+-} = \langle X \rangle_{-+} = 0$, the square of the dispersion is simply

$$(\Delta X)^2 \equiv \langle X^2 \rangle - \langle X \rangle^2 = \frac{1 - \cos\theta}{2} (\Delta X)^2_{+} + \frac{1 + \cos\theta}{2} (\Delta X)^2_{-} + \frac{\sin^2\theta}{4} [\langle X \rangle_{+} - \langle X \rangle_{-}]^2. \tag{21}$$

Let us now compute the relevant physical magnitudes. The operator $\mathcal{N} = (a^\dagger a + 1/2)\sigma_0 + \sigma_3/2$ corresponds to the total number of particles. It is a constant of motion and is invariant under the transformation by $\mathcal{O}$. We then get

$$\langle \mathcal{N} \rangle_{+} = x + 1, \quad \langle \mathcal{N} \rangle_{-} = x, \quad (\Delta\mathcal{N})^2_{+} = (\Delta\mathcal{N})^2_{-} = x. \tag{22}$$

(Those are known results in connection with the susy harmonic oscillator.)

The evaluation of the mean values of the number of photons $N = a^\dagger a$ is less trivial, and gives

$$\langle N \rangle_{+} = x + \frac{1}{2} - \frac{\Delta}{4\kappa} e^{-x} \sum_{n=0}^{\infty} \frac{x^n}{n!} \frac{1}{r(n+1)}, \quad \langle N \rangle_{-} = x - \frac{1}{2} + \frac{\Delta}{4\kappa} e^{-x} \sum_{n=0}^{\infty} \frac{x^n}{n!} \frac{1}{r(n)}. \tag{23}$$

Comparing with the harmonic oscillator, where $\langle N \rangle = x$, we have a correction due to the interaction. Since κ is usually small, a good approximation to the average number of photons is x. Indeed, the contribution of the terms containing the series is, in this case, approximately $1/2$.

We can compute the mean values and dispersions of the energy in the fundamental states and study their behaviour with respect to both x and δ. Since $\langle H_{\rm JC} \rangle_{+-} = \langle H_{\rm JC} \rangle_{-+} = 0$, the calculations over the general coherent states through Eqs. (20)–(21) do not give anything new with respect to the results for the fundamental states. Indeed, we can see from (21) that the dispersion attains his minimum over the pure states. The mean values are easily computed and take the simple form

$$\langle H_{\rm JC} \rangle_{+} = \omega \left[(x + 1) - \lambda G(\delta, x) \right], \quad \langle H_{\rm JC} \rangle_{-} = \omega \left[x + \lambda G(\delta - 1, x) \right], \tag{24}$$

while the values of the dispersion are more complicated and present interesting features

$$(\Delta H_{\rm JC})^2_{+} = \omega^2 \left[\lambda^2(1 + \delta) + (1 + \lambda^2)x + 2\lambda x (G(\delta, x) - G(\delta + 1, x)) - \lambda^2 (G(\delta, x))^2 \right], \tag{25}$$

$$(\Delta H_{\rm JC})^2_{-} = \omega^2 \left[\lambda^2 \delta + (1 + \lambda^2)x - 2\lambda x (G(\delta - 1, x) - G(\delta, x)) - \lambda^2 (G(\delta - 1, x))^2 \right]. \tag{26}$$

We have introduced $\lambda = \kappa/\omega$. When a large number of photons is considered, we can use the asymptotic behaviour of $G(\delta, x)$ to see that

$$\frac{(\Delta H_{\rm JC})_{\pm}}{\langle H_{\rm JC} \rangle_{\pm}} \sim \frac{1}{\sqrt{x}}, \tag{27}$$
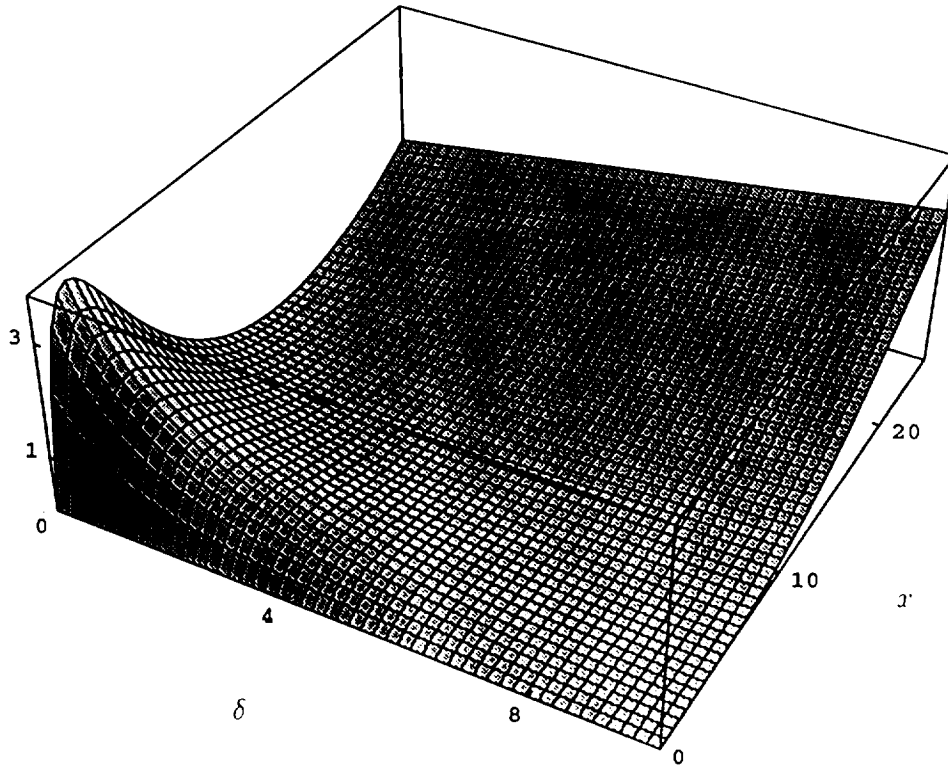
as in the harmonic oscillator case.

Fig. 1. Behaviour of $(\Delta H_{\rm JC})^2_+/\omega^2$ as a function of δ and x for $\lambda = 8$.

If we want to see how the dispersion evolves with respect to a variation of the characteristics of the system δ and λ, we analyse the form of $(\Delta H_{\rm JC})^2_+$, since $(\Delta H_{\rm JC})^2_-$ shows a similar qualitative behaviour. If we fix λ, the typical behaviour of $(\Delta H_{\rm JC})^2_+$ is as in Fig. 1. It can be proved that for fixed values of δ smaller than a certain δ_0, $(\Delta H_{\rm JC})^2_+$ has a minimum for $x \neq 0$.

The atomic inversion is the last quantity we will consider. Over a general coherent state, we have

$$\langle \sigma_3 \rangle = \frac{1}{2} e^{-x} \sum_{n=0}^{\infty} \frac{x^n}{n!} \left[\frac{\Delta}{2\kappa} \left(\frac{1 - \cos\theta}{r(n+1)} - \frac{1 + \cos\theta}{r(n)} \right) + 2\sin\theta \frac{\cos\varphi_n(t)}{r(n+1)} \right], \tag{28}$$

where $\varphi_n(t) = \phi + 2t\kappa r(n+1)$. If we take $\Delta = 0$ and $\theta = -\phi = \pi/2$, we have a temporal behaviour which is similar to the one obtained by Narozhny et $al.$ [2] (let us recall that their states are different from ours). It consists of Rabi oscillations, as shown in Fig. 2:

$$\langle \sigma_3 \rangle = \frac{1}{2} e^{-x} \left[-1 + 2 \sum_{n=0}^{\infty} \frac{x^n}{n!} \frac{\sin(2t\kappa\sqrt{n+1})}{\sqrt{n+1}} \right]. \tag{29}$$

The derivative of this function with respect to t is essentially the value obtained in Ref. [2]. In Fig. 2, we show the graph of our $\langle \sigma_3 \rangle$ for $x = 20$. It is similar to those obtained in many other papers, and that although the expression of $\langle \sigma_3 \rangle$ is not exactly the same in all the cases.

These results indicate that it is reasonable to analyze the coherent states associated to the J.C. Hamiltonian in the way we are doing, but we do not know for the present if they could be interesting for the experiments.

$$x = 20$$
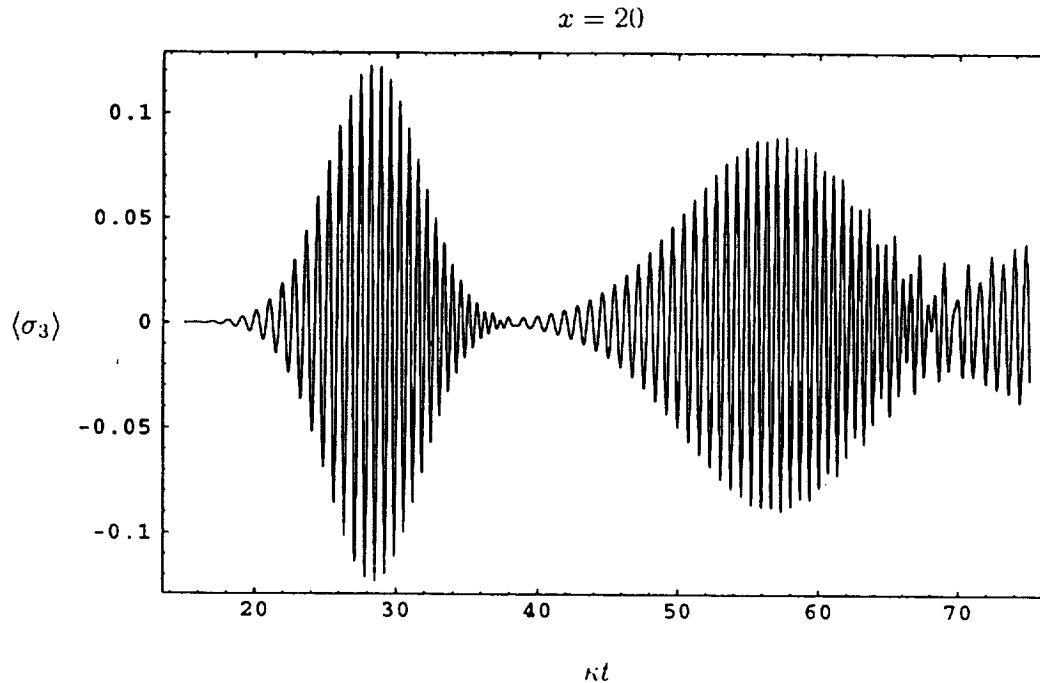
Fig. 2. Collapses and revivals of the atomic inversion in a general coherent state for $x = 20$ and $\delta = 0$.

4 Acknowledgments

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SLIGHTLY ANHARMONIC SYSTEMS IN QUANTUM OPTICS

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Abstract

We consider an arbitrary atomic system (n-level atom or many such atoms) interacting with a strong resonant quantum field. The approximate evolution operator for a quantum field case can be produced from the atomic evolution operator in an external classical field by a 'quantization prescription', passing the operator arguments to Wigner D-functions. Many important phenomena arising from the quantum nature of the field can be described by such a way.

1 Introduction

The behaviour of atomic systems interacting with a quantized electromagnetic field in a cavity has been studied for a long time. Even the simplest model of a single two-level system interacting with a single field mode in a lossless cavity, the Jaynes-Cummings model (JCM) [1], reveals interesting properties like collapses and revivals of atomic inversion oscillations, trapping states, Schrödinger Cats, etc. [1-3]. They stem from the nonlinear nature of the JCM.

For a linear system, the Hamiltonian is usually a linear function of generators of some representation of a finite-dimensional Lie algebra, and the Evolution operator (EO) belongs to the corresponding Lie group representation. This property is referred as a *Dynamical Symmetry*. The most familiar examples are the Harmonic oscillator and the spin rotation in an external magnetic field. Their dynamical groups are, correspondingly, $SU(1,1)$ and $SU(2)$. Dynamical symmetry results in an equidistant spectrum (or a spectrum consisted of several equidistant parts), coherent states (i.e., nonspreading wave packets) and many other attributes of 'harmonic behaviour' [4, 5].

Real systems are oftenly nonlinear. Interesting phenomena appear, if the nonlinearity is 'weak', i.e., the dynamics is 'almost harmonic' one. For instance, the JCM in the classic field limit is equivalent to the spin-1/2 rotation in the external field, that gives the simplest example of the dynamical symmetry (two-dimensional representation of $SU(2)$). JCM collapses and revivals appear in the case of a strong quantum field, when the system is slightly nonlinear.

JCM dynamics is very instructive and we may say more about it. The JCM possesses an exact solution and its EO can be found explicitly. It is 2×2-matrix with coefficients depending

on photon operators, see, e.g. [3]. On the other hand, the number of excitation N is a constant of motion in this model, and its EO can be written as a direct sum of infinitely many 2×2-matrices corresponding to different values of N. Every matrix is similar to the spin-1/2 rotation around x-axis, but different blocks rotate with different frequencies, Ω_N, called quantum Rabi frequencies. The spectrum consists from infinitely many pairs of levels separated by $2\Omega_N$, and anharmonicity results in a nonlinear dependence of quantum Rabi frequency on the excitation number, $\Omega_N = g\sqrt{N}$ (g is a coupling constant). Therefore, the JCM can be considered as an interesting example of a nonlinear system, however possessing the exact dynamical symmetry.

Treating the field classically, we put $\Omega_N \rightarrow \overline{\Omega} \sim g\sqrt{\overline{n}}$, using the classical Rabi frequency rather than quantum ones. (Here $\overline{n}$ is the field intensity in units of photon number.) For a strong quantum field with Poisson photon distribution, different Ω_N contribute to dynamics, $\overline{n} - \sqrt{\overline{n}} < N < \overline{n} + \sqrt{\overline{n}}$. The difference in frequencies $g\sqrt{\overline{n}+\Delta n} - g\sqrt{\overline{n}-\Delta n} g \sim \sqrt{\Delta n/\overline{n}} \sim g$ becomes important for times $\sim g^{-1}$. This is just the JCM collapse time. It is in the range of modern experimental possibilities, both for Rydberg atom micromasers and for optical microcavities (see the references in the review [1]). The frequency of revivals is proportional to $g/\sqrt{\overline{n}}$. Thus, it is not surprising, that JCM collapses and revivals can be described in the frame of expansion over the inverse field intensity [3].

Natural generalizations of JCM involve more resonant levels and more atoms. Already a system of many two-level atoms (the Dicke model [6]) does not allow an exact solution. However, for very general class of atomic systems interacting with the quantum field under the Rotating Wave Approximation, the excitation number remains a constant of motion. If one of the field modes contains a lot of photons, we can neglect the other modes and develop a perturbation theory with the inverse excitation number as a small parameter. Precisely, the initial number of photons must be much larger then the maximum possible number of atomic excitations $\mathcal{A}$. This program has been realized at the level of wave functions for the Dicke model in Refs. [7] and for more general systems in Ref. [8].

Here, we shall find an explicit form of the EO for an arbitrary atomic system interacting with a strong resonant quantum field. The atomic operators for such a system form a finite-dimensional representation of some compact Lie algebra (see, e.g., [9]). For the case of identical atoms, the algebra depends on the number of levels while the representation depends on the number of atoms and symmetry properties of initial atomic state under the atomic permutations. For instance, the case of A identical two-level atoms excited from a symmetric state leads to the $(A+1)$-dimensional representation of $SU(2)$. The exact EO can be written as a direct sum of finite dimensional-blocks with different excitation numbers. The dimension of blocks for the case $N > \mathcal{A}$ is determined by the atomic algebra representation, but the exact Hamiltonian in every block is a nonlinear function of the representation generators (see Eq. (9) below). However, we shall show that the dynamical symmetry can be restored in the zeroth- and the first-order approximations. It means that the evolution operator in every block can be well approximated by the operator from the corresponding Lie group representation. In the Dicke model case this approximate motion is a rotation of the collective atomic pseudospin (of the length $A/2$) around x-axis. Once again, the rotation frequencies in different blocks depend nonlinearly on the excitation number (see Eq. (10) below). Therefore, our zeroth-order approximation possesses a dynamical symmetry in the same sense as the exact JCM solution. The difference is that the motion in every block is described by the appropriate representation of atomic algebra instead of spinor $SU(2)$ representations for

JCM. Being restricted to JCM case our theory just reproduces its exact solution.

The work is organized as follows. In the next section we shall describe the model. In Sec. 3 the asymptotic evolution operator for an arbitrary atomic system interacting with a strong quantum field is found. It has a matrix form in the atomic basis with coefficients depending on the photon operators. Let us remind, that the evolution operator for the atomic system in an external classical field (*semiclassical EO*) is a matrix of a finite rotation from the atomic group representation. The corresponding matrix elements are calculated by the group representation theory (see, e.g., [10]).

Remarkably, the approximate 'quantum' EO can be obtained from the semiclassical one by a simple 'quantization prescription' (see the text before Eq. (23)), which introduces the operator arguments into the Wigner D-functions. Therefore, our results enable to write (without calculations) approximate matrix elements of the quantum evolution operator as far as the ones of the semiclassical EO are known.

We demonstrate the convenience of the form (23) for the EO in Sec. 4, where it is used to reproduce the wave functions found in Ref. [8] and to prove the approximate factorization of the system wave function for special initial conditions. Making use of Eq. (23) drastically simplifies the original proof of factorization [8]. The wave functions of Ref. [8] contain the information about collapses and revivals, trapping states and Schrödinger cats and provide the correct structure of the field quasiprobability distribution for the systems under study. Therefore, the proposed asymptotic form for the EO describes all these phenomena connected with the quantum nature of the field.

2 Description of the model

We shall work with the following Hamiltonian

$$\hat{H} = \omega(\hat{n} + \hat{h}) + \hat{V}, \quad \hat{V} = g(a\hat{X}_+ + a^\dagger \hat{X}_-). \tag{1}$$

Here, $a, a^\dagger, \hat{n} = a^\dagger a$ are the photon annihilation, creation and number operators, describing a cavity quantized field mode with the frequency ω. g is the coupling constant with resonant atoms placed into the cavity, (we consider the exact resonance case for simplicity). $\hat{h}$ is the bare atomic system Hamiltonian determining the configuration of atomic levels, $\hat{X}_\pm$ are atomic operators describing transitions between resonant levels and obeying commutation relations

$$[\hat{h}, \hat{X}_-] = -\hat{X}_-, \quad [\hat{h}, \hat{X}_+] = \hat{X}_+. \tag{2}$$

Hamiltonian (1) with conditions (2) describes quite general atomic system interacting with a resonant mode of quantized field under the Rotating Wave Approximation. The Dicke model corresponds to the particular case when an atomic system consists of A two-level atoms [6]. Then the operators $\hat{h}, \hat{X}_\pm$ belong to the $(A+1)$-dimensional representation of $su(2)$ algebra and obey the additional commutation relation

$$[\hat{X}_+, \hat{X}_-] = 2\hat{h} \tag{3}$$

The simplest case of the JCM corresponds to the two-dimensional representation of $su(2)$.

We define the basis of the atomic algebra representation as

$$|k, \gamma\rangle_{at}, \quad 0 \le k \le A, \quad \hat{h}|k, \gamma\rangle_{at} = (k - C)|k, \gamma\rangle_{at}, \tag{4}$$

where k is a number of excitations in the atomic system, $\mathcal{A}$ is its maximal value, C is a constant corresponding to the bottom energy level of the atomic system ($k = 0$). γ denotes all the other atomic indexes (atomic level populations), which are given by eigenvalues of the operators from the Cartan subalgebra. For example, in the case of $su(2)$ algebra we have the only Cartan operator $\hat{h}$ and there are no additional indexes. Then the maximum possible number of atomic excitations $\mathcal{A}$ is equal to the number of atoms A, and the bottom level of atomic energy is $C = A/2$. In the presence of additional indexes (say, for three-level atoms) the bare atomic levels may be degenerate and the dimension of the representation is then larger than $\mathcal{A}+1$.

It follows from Eqs. (2) that the excitation number operator commutes with the Hamiltonian

$$\hat{N} = a^+ a + \hat{h}, \quad [\hat{N}, \hat{H}] = 0. \tag{5}$$

It is useful to introduce the basis

$$|N, k\rangle = |N-k\rangle_f \otimes |k\rangle_{at}, \quad 0 \le k \le \mathcal{A}, \quad \hat{N}|N, k\rangle = (N-C)|N, k\rangle, \tag{6}$$

where $|n\rangle_f$ is a Fock field states, $|k\rangle_{at}$ is a bare atomic state (4). For a fixed value of N, the Hamiltonian (1) in the basis (6) is a finite dimensional matrix. It's rows and columns are numerated by the indexes k and γ. (In Eq. (6) and below, we omit the index γ.)

We shall explore the field phase operators defined as [11]

$$a^\dagger = \exp(-i\hat{\phi})\sqrt{\hat{n}+1}, \quad a = \sqrt{\hat{n}+1}\exp(i\hat{\phi}),$$
$$\exp(-i\hat{\phi})|n\rangle_f = |n+1\rangle_f \quad \exp(i\hat{\phi})|n\rangle_f = |n-1\rangle_f, \quad n > 0. \tag{7}$$

These phase operators are unitary and provide the correct physical results for large n's. The following commutation relations are valid:

$$f(\hat{n})\exp(-i\hat{\phi}) = \exp(-i\hat{\phi})f(\hat{n}+1), \quad \exp(i\hat{\phi})f(\hat{n}) = f(\hat{n}+1)\exp(i\hat{\phi}), \tag{8}$$

where $f(\hat{n})$ is an arbitrary function of the photon number operator (determined by its Taylor expansion). Eqs. (8) follow from similar relations for the operators $a, a^\dagger$.

3 The Evolution Operator for the strong field case

We consider here the case of initially strong field. Then, the total number of excitations is larger than the maximum possible atomic excitation number, i.e. "$\hat{N} \sim \hat{n} \gg \hat{h}$", and we can build a perturbation theory with $\hat{N}^{-1}$ as a small parameter. It is convenient to divide the derivation into subsequent steps.

1. We eliminate $a, a^\dagger$ and $\hat{n}$ from the Hamiltonian (1) using Eqs. (7) and the excitation number conservation, $\hat{n} = \hat{N} - \hat{h}$,

$$\hat{V} = g\left(\sqrt{\hat{N}-\hat{h}+1}\,\exp(i\hat{\phi})\hat{X}_+ + \hat{X}_-\exp(-i\hat{\phi})\sqrt{\hat{N}-\hat{h}+1.}\right) \tag{9}$$

2. The square roots in the last equation can be written as series of powers of the operator

$$(\hat{N} + 1/2)^{-1} \equiv g^2/\hat{\Omega}^2, \quad \hat{\Omega}(\hat{N}) \equiv g\sqrt{\hat{N} + 1/2}. \tag{10}$$

We get

$$\hat{V} = \hat{\Omega}\left[\hat{H}_0 + \frac{g^2}{\hat{\Omega}^2}\hat{H}_1 + \ldots\right], \tag{11}$$

$$\hat{H}_0 = \exp\left(i\hat{\phi}\right)\hat{X}_+ + \exp\left(-i\hat{\phi}\right)\hat{X}_-, \tag{12}$$

$$\hat{H}_1 = -1/2\{\hat{h},\hat{H}_0\}_+,\ldots. \tag{13}$$

Here $\{,\}_+$ stands for anticommutator.

Our choice of a small parameter (Eq. (10) rather than $\hat{N}^{-1}$) is important, since it provides vanishing first order corrections to eigenfrequencies, as it has been shown in Ref. [7]. In fact, the first-order corrections are in such a way included into the zeroth-order ones, that improves the quality of the zeroth-order approximation. According to Eq. (11), the whole time scale is determined by the factor $\hat{\Omega}(\hat{N})$, which plays the role of the Rabi frequency for the problem under study.

3. It is convenient to use the following transformation

$$\hat{Q} = \exp\left[i\hat{\phi}(\hat{h} + C)\right]. \tag{14}$$

This operator is unitary on the states $n > \mathcal{A} \geq k$. Acting on the basis vectors it gives

$$\hat{Q}|k\rangle_{at} \otimes |n\rangle_f = \exp(i\hat{\phi}k)|k\rangle_{at} \otimes |n\rangle_f = |k\rangle_{at} \otimes |n-k\rangle_f = |N=n,k\rangle. \tag{15}$$

Since the operator $\hat{h}+C$ has an integer spectrum, the operator $\hat{Q}$ is a direct sum of different powers of the phase operator.

Directly from the definitions (14),(7) and from the commutators (2),(8) we find

$$f(\hat{n})\hat{Q}^{-1} = \hat{Q}^{-1}f(\hat{n} + \hat{h} + C), \quad \hat{Q}f(\hat{n}) = f(\hat{n} + \hat{h} + C)\hat{Q}, \tag{16}$$

$$\hat{Q}\hat{X}_+\hat{Q}^{-1} = \exp(i\hat{\phi})\hat{X}_+, \qquad \hat{Q}\hat{X}_-\hat{Q}^{-1} = \exp(-i\hat{\phi})\hat{X}_+. \tag{17}$$

4. Here we shall find the zeroth-order EO. (Wave functions in the second order for the Dicke model have been calculated in Ref. [7].) Applying the Q-transformation to the zeroth-order Hamiltonian and using Eqs. (16),(17) we have

$$\hat{V} \approx \hat{\Omega}(\hat{n}+\hat{h}) = \hat{Q}\,\hat{\Omega}(\hat{n}-C)\,\hat{H}_{cl}\hat{Q}^{-1}, \qquad \hat{H}_{cl} \equiv \hat{X}_+ + \hat{X}_-. \tag{18}$$

Therefore, Q-transformation removes the nondiagonal photon operators from the zeroth-order Hamiltonian. It transforms the operator $\hat{H}_0$ into the purely atomic operator $\hat{H}_{cl}$, which has a sense of the atomic system Hamiltonian in an external constant classical field. Moreover, the Q-transformation removes the field operators from the coefficients $\hat{H}_0,\hat{H}_1,\ldots$ in all the orders. Simultaneously, the Q-transformation changes the expansion parameter, $\hat{\Omega}(\hat{N}) \to \hat{\Omega}(\hat{n}-C)$, transforming it into the function of the photon number operator. Therefore, the Q-transformation separates field and atomic variables in the expansion (11) in such a way, that atomic operators appear in the coefficients and the photon number operator is included into the expansion parameter. Thus, the calculation of high order corrections involve only the atomic operators.

5. Now we can calculate the matrix elements of the EO with the Hamiltonian (18)

$$\exp(-it\hat{V}) \approx \exp\left[-it\hat{\Omega}(\hat{N})\hat{H}_0\right] = \hat{Q}\exp\left[-\hat{\Omega}(\hat{n} - C)\hat{H}_{cl}\right]\hat{Q}^{-1} \tag{19}$$

between the atomic states (they are still operators in the field space). Taking into account the action of the Q-operator on the atomic states, we find

$$_{at}\langle k| \exp(-it\hat{V})|m\rangle_{at} \approx e^{i\hat{\phi}k} \, _{at}\langle k| \exp\left[-it\hat{\Omega}(\hat{n}-C)\hat{H}_{cl}\right]|m\rangle_{at} \, e^{-i\hat{\phi}m}$$

$$= \, _{at}\langle k| \exp\left[-it\hat{\Omega}_k\hat{H}_{cl}\right]|m\rangle_{at} \, \exp(i\hat{\phi}(k-m)), \qquad (20)$$

where we have denoted

$$\hat{\Omega}_k \equiv \hat{\Omega}(\hat{n}+k-C) = g\sqrt{\hat{n}+k-C+1/2}. \qquad (21)$$

Shifting $e^{i\hat{\phi}k}$ to the right in the last line of Eq. (20), we have used the commutator (7).

What profit have we got with Eq. (20)? We have separated the field phase operators, writing them on the right. The operator $\hat{\Omega}_k\hat{H}_{cl}$ contains the only field operator $\hat{n}$ which commutes with all the other ingredients and may be treated as a Q-number in the calculation of the exponent. Thus, we can reconstruct the quantum field EO if we know the atomic EO in the external classical field

$$\hat{U}_{cl}(\omega) = \exp(-it\omega\hat{H}_{cl}). \qquad (22)$$

The matrix $\hat{U}_{cl}(\omega)$ is the rotation operator from the atomic group representation. It's matrix elements are known from the standard group representation theory. For the Dicke model case, the operator $\hat{H}_{cl} = \hat{X}_+ + \hat{X}_- = 2\hat{S}_x$ is just a generator of rotations around x-axis, and the matrix elements of $\exp(-it\omega 2\hat{S}_x)$ are the usual Wigner D-functions.

The quantum EO matrix elements can be produced from the matrix $\hat{U}_{cl}(\omega)$ by the following 'quantization prescription':

(i) to substitute the group parameter ω in the (k,γ)-th row of the matrix $\hat{U}_{cl}(\omega)$ by the operator $\omega \to \hat{\Omega}_k = \sqrt{\hat{n}+k-C+1/2}$, (here k is the atomic excitation number in the row (k,γ));

(ii) to multiply every matrix element $_{at}\langle k,\gamma|\hat{U}|m,\gamma'\rangle_{at}$ from the right by the power of the phase operator $\exp(i\hat{\phi}(k-m))$.

Writing explicitly in Eq. (20) the additional atomic indexes γ, we have

$$_{at}\langle k,\gamma|\hat{U}|m,\gamma'\rangle_{at} = \, _{at}\langle k,\gamma|\hat{U}_{cl}(\hat{\Omega}_k)|m,\gamma'\rangle_{at} \, \exp(i\hat{\phi}(k-m)). \qquad (23)$$

This equation is our principal result. It corresponds to the wave functions found in Ref. [8]. Being restricted to the case of a single two-level atom, it gives the exact JCM EO (see, e.g., [3]). The quantization prescription formulated above can be easily generalized to include detuning [12].

4 The wave function factorization

The most remarkable feature of dynamics with the EO (23) is an approximate wave function factorization for special initial states. Let the field initially be in a coherent state, $|in\rangle_f = |\alpha\rangle$, $\alpha \equiv \sqrt{\bar{n}}e^{i\phi}$, where $\bar{n}$ and ϕ are the initial photon number and the phase of the field. (The number $e^{i\phi}$ may not be confused with the phase operator $\exp(i\hat{\phi})$). The initial atomic state is taken as an eigenstate of the operator

$$\hat{H}_{cl}(\phi) = e^{i\phi}\hat{X}_+ + e^{-i\phi}\hat{X}_- = e^{i\phi\hat{h}}\hat{H}_{cl}e^{-i\phi\hat{h}}, \quad \hat{H}_{cl}(\phi)|\underline{p(\phi)}\rangle_{at} = \lambda_p|\underline{p(\phi)}\rangle_{at}, \quad |\underline{p(\phi)}\rangle_{at} = e^{i\phi\hat{h}}|\underline{p}\rangle_{at}.$$

Here, $\hat{H}_{cl}$ is determined by Eq. (18). We shall call λ_p and $|p(\phi)\rangle_{at}$ as semiclassical eigenvalues and eigenvectors. The vector $|\underline{p}\rangle_{at}$ is also an eigenvector of the semiclassical evolution operator (22)

$$\hat{U}_{cl}(\omega)|\underline{p}\rangle_{at} = \exp\left(-i\omega\lambda_p t\right)|\underline{p}\rangle_{at}. \tag{24}$$

It is known [13], that coherent states with large photon numbers are approximately eigenstates of the phase operators. More precisely,

$$\exp(ik\hat{\phi})|\alpha\rangle = \exp(ik\phi)|\alpha\rangle + O(k/\sqrt{\bar{n}}). \tag{25}$$

Now we act by the EO (23) to the initial state $|in\rangle = |\alpha\rangle \otimes |p\rangle_{at}$. Multiplying the equation from the left by an arbitrary atomic vector $\langle k|_{at}$ and substituting the EO matrix element, Eq. (23) we have

$$\begin{aligned}
{}_{at}\langle k|\, \hat{U}\, |\alpha\rangle_f \otimes |\underline{p(\phi)}\rangle_{at} &\approx \sum_m e^{i\phi(k-C)} {}_{at}\langle k|\hat{U}_{cl}(\hat{\Omega}_k)|m\rangle_{at\ at}\langle m|\underline{p}\rangle_{at} \otimes |\alpha\rangle_f \\
&= {}_{at}\langle k|e^{i\phi(k-C)}e^{-it\lambda_p\hat{\Omega}_k}|\underline{p}\rangle_{at} \otimes |\alpha\rangle_f \\
&= {}_{at}\langle k|\exp\left(-it\lambda_p g\sqrt{\hat{n}+\hat{h}+1/2}\right)|\underline{p(\phi)}\rangle_{at} \otimes |\alpha\rangle_f. \tag{26}
\end{aligned}$$

Here, in the first line, the phase factor coming from the action of the field phase operator $e^{i\hat{\phi}(k-m)}$ on the coherent state, Eq. (25) cancels the atomic phase factor ${}_{at}\langle m|\underline{p(\phi)}\rangle = e^{i\phi(m-C)} {}_{at}\langle m|\underline{p}\rangle_{at}$ to give $e^{i\phi(k-C)}$. In the second line we use the property (24), that is $\hat{U}_{cl}(\hat{\Omega}_k)|\underline{p}\rangle_{at} = e^{-it\lambda_p\hat{\Omega}_k}|\underline{p}\rangle_{at}$. We stress, that the operator-valued group parameter $\hat{\Omega}_k$ depends on the number of the row, so for rows with different k's we must use different semiclassical EO's with different values of the group parameter. Finally, in the last line of Eq. (26) we substitute $e^{i\phi(k-C)} {}_{at}\langle k|\underline{p}\rangle_{at} = {}_{at}\langle k|\underline{p(\phi)}\rangle_{at}$ and ${}_{at}\langle k|e^{-it\lambda_p\hat{\Omega}_k} = {}_{at}\langle k|\exp(-it\lambda_p g\sqrt{\hat{n}+\hat{h}+1/2})$. Since ${}_{at}\langle k|$ is an arbitrary atomic state, we can write the wave function in the form

$$\hat{U}(t)|in\rangle \approx \exp\left[-it\lambda_p g\sqrt{\hat{n}+\hat{h}+1/2}\right]|in\rangle.$$

Introducing the notation $\overline{\Omega} \equiv g\sqrt{\bar{n}+1/2}$ we can approximate the square root as

$$\sqrt{\hat{n}+\hat{h}+1/2} \approx \sqrt{\hat{n}+1/2} + \frac{\hat{h}}{2\sqrt{\bar{n}+1/2}} + O\left(\hat{n}^{-3/2}\right), \qquad \frac{1}{\sqrt{\hat{n}+1/2}} \approx \frac{g}{\overline{\Omega}} + O\left(\frac{1}{\bar{n}}\right)$$

and we find the factorized wave function

$$\begin{aligned}
|\Psi(t)\rangle &\cong |\Phi_p(t)\rangle \otimes |A_p(t)\rangle, \\
|\Phi_p(t)\rangle &= \exp\left(-itg\lambda_p\sqrt{\hat{n}+1/2}\right)|\alpha\rangle_f, \\
|A_p(t)\rangle &= \exp\left[-itg^2\lambda_p\hat{h}/(2\overline{\Omega})\right]|\underline{p}\rangle_{at}, \tag{27}
\end{aligned}$$

This wave function has been found by a different way in Ref. [8] and used for the discussion of the trapping states, collapses, revivals and Schrödinger Cat states for the systems under study.

If different semiclassical eigenstates contribute to the initial state, the wave function is a superposition of corresponding factorized states (27). The evolution operator Eq. (23) describes the dynamics from any initial state, such that the initial photon number is much larger then the maximum number of atomic excitations.

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COHERENT CONTROL IN SIMPLE QUANTUM SYSTEMS

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Abstract

Coherent dynamics of two-, three-, and four-level quantum systems, simultaneously driven by concurrent laser pulses of arbitrary and different forms, is treated by using a nonperturbative group-theoretical approach. The respective evolution matrices are calculated in an explicit form. General aspects of controllability of few-level atoms by using laser fields are treated analytically.

1. INTRODUCTION

We analyze the general aspects of the problem of dynamical coherent control of atomic populations in the framework of semiclassical approach when an external (laser) field is considered as an inexaustible energy reservoir and only the atomic behaviour is considered to be controllable. The natural controllers are strengths, frequencies and phases of the components of a polychromatic laser field driving simultaneously different atomic transitions. An initial atomic state may be also considered as a controller.

The dynamics of any nonstationary quantum system is described by the time evolution equation

$$i \frac{\partial}{\partial t} U(t,0) = H(t) \; U(t,0) \; , \quad U(0,0) = I \; , \quad \hbar = 1 \qquad (1)$$

with the Hamiltonian

$$H(t) = \sum_{k=1}^{m} h_k(t) \; H_k \; . \qquad (2)$$

which depends on time explicitely. It is not an easy task to solve the eq.1 analitically even for a two-level system exposed to an

arbitrary varying external field. Usualy used adiabatic and weak-field approximations as well as the approximation with slowly varying amplitudes breaks down if we deal with short and/or intense laser pulses. The well-known Floke method is useful only in the case of periodic excitations. The high level of control of atomic populations by using designed laser fields calls for a new nonperturbative technique that should be, on the one hand, rather general to enable one to treat uniformely the atomic dynamics under various excitation conditions, and on the other hand, it should be able to result in explicit solutions of the evolution equation (1).

The group-theoretical technique will be applied to solve this task for two-, three-, and four-level atoms exposed to an arbitrary time-varying polychromatic laser field. It is based on the concept of dynamical symmetry of nonstationary quantum processes [1-3].

After solving the eq.1 for a given model system, the problem of finite control [4] is to find such values of controllers $\{h_j(t)$, $j=1,\ldots,m\}$ that enables us to transform the system from an initial state to the desired final state at the target time $T > 0$. Such a transition is governed by the equation

$$| s(T) > = U(T,0) | s(0) >.$$ (3)

Generally speaking, the solution of this task is not unique. In addition one can put the task of optimal control which is to find such values of controllers that minimizes a given loss functional or maximizes a desired quality criterion [5].

2. GENERAL BACKGROUND

A single atom with N nondegenerate and nonequidistant levels

$$H_0 |s_m> = w_m |s_m>, \quad m = 1,2,\ldots,N,$$ (4)

interacts with amplitude- modulated components of a polychromatic field

$$E = (1/2) \sum_{l>} \sum_{k} E_{kl} (t) \exp (i \ w_{kl} \ t) + c.c.$$ (5)

by such a way that only one $(k,1)$-component of the field E_{k1} is in resonance with the $(k,1)$- atomic transition. If one deals with the electric dipole transitions

$$H_{int} = -E(t) \, d(t) \, ,$$

then by the parity reasons the energetic matrix $H_0 + H_{int}$ turns out to be tridiagonal. However, we will treat the general case (when all the $N(N-1)/2$ atomic transitions are driven independently on each other) to be able to include into consideration, if necessary, other interactions that may couple nonadjacent levels. The complex variable $E_{k1}(t)$ measures amplitude, phase, and polarization of the respective component.

Writing the state vector of a N-level atom in the form

$$|s(t)\rangle = \sum_{m=1}^{N} c_m(t) \, |s_m\rangle \exp \, (-i \, w_m \, t), \qquad (6)$$

one can obtain from the nonstationary Scrodinger equation the following set of equations for the probability amplitudes in the rotating wave approximation

$$i\dot{s}_k(t) = \sum_{k<1} h_{k1}(t) \, s_1(t) + c.c., \qquad (7)$$

where

$$h_{k1}(t) = - \, (1/2) \, E_{k1}(t) \, d_{k1}(t). \qquad (8)$$

The resonant Hamiltonian has the following structure

$$H_{nn}(t) = 0, \qquad H_{k1}(t) = h_{k1}(t) = H_{1k}^{*}(t) \, , \quad k \neq 1. \qquad (9)$$

Finally, the probability of finding our N-level system on level n at time t is expressed in terms of the evolution-matrix elements and the initial populations P_m as follows

$$P_n(t) = \sum_{m=1}^{N} |U_{nm}(t)|^2 \, P_m(0). \qquad (10)$$

3. COHERENT CONTROL ON THE SU(2) DYNAMICAL GROUP

A quantum system with the SU(2) dynamical symmetry is a fundamental model in the semiclassical theory of field-matter interactions. The hermitean Hamiltonian of such an arbitrarily driven system can be cast in the form

$$H(t) = h_0(t) R_0 + h^*(t) R_- + h(t) R_+ \qquad (11)$$

with the generators satisfying the commutation relations

$$[R_+, R_-] = 2R_0, \quad [R_0, R_{+,-}] = \pm R_{+,-}, \qquad (12)$$

where c-number parameters h_0 and h are assumed to be arbitrary analytic functions. Writing the evolution operator in the factorized Wei-Norman form [6]

$$U = \exp \left(g_0 - i\int_0^t h_0(\tau) \, d\tau \right) R_0 \, \exp g_- R_- \, \exp g_+ R_+, \qquad (13)$$

one can obtain the governing equation for $g = \exp(g_0/2)$

$$\ddot{g} - \left(\frac{\dot{h}}{h} + i \, h_0 \right) \dot{g} + |h|^2 \, g = 0, \quad g(0) = 1, \quad \dot{g}(0) = 0. \qquad (14)$$

Once the eq.14 is solved all the other SU(2) group parameters are found in quadratures [6,2,3] It follows from the unitariry of (13) the simple conservation laws

$$|g|^2 - g_- g_+ = 1, \quad |g|^2 (1 + |g_+|^2) = 1. \qquad (15)$$

In the two-dimensional representation we get the expression

$$U^{(1/2)} = \begin{bmatrix} g & [2i(\dot{g})^* + h_0 g^*]/2h^* \\ (2i \, \dot{g} - h_0 g)/2h & g^* \end{bmatrix} \qquad (16)$$

which is the time-evolution matrix for a two-level system driven by an external field with arbitrary amplitude and frequency modulation. In terms of populations the complete formal solution of the problem of two-level control is given by the formula

$$|g(T)|^2 = [2P_1(0) - 1]^{-1} [P_1(T) + P_1(0) - 1], \qquad (17)$$

where $P_1(0)$ and $P_1(T)$ are the input and the output values of the first level population, respectively. Since the evolution is unitary one has $P_1(t) + P_2(t) = 1$.

4. POPULATION CONTROL OF A RESONANTLY DRIVEN THREE-LEVEL SYSTEM

Let us consider the coherent dynamics of a three-state system with an arbitrary level configuration simultaneously driven in resonance by three lasers with arbitrary and different time dependences of their amplitudes. Choosing the phases in an appropriate way we can write the system Hamiltonian in the matrix form with the following nonvanishing elements

$H_{12} = H_{21} = h_{12}(t)$, $H_{23} = H_{32} = h_{23}(t)$, $H_{13} = -H_{31} = -ih_{13}(t)$.

If we write this matrix in terms of the generators of the standard representation of the SU(2) group, then the time-evolution matrix is simply the three-dimensional representation of this group [7]

$$U^{(1)} = \begin{pmatrix} u^2 & \sqrt{2}uv & v^2 \\ -\sqrt{2}uv^* & |u|^2-|v|^2 & \sqrt{2}u^*v \\ (v^*)^2 & -\sqrt{2}u^*v^* & (u^*)^2 \end{pmatrix}, \tag{18}$$

where $u \equiv g$ and $v^* \equiv -(2i\dot{g} - h_0 g)/2h$. The governing equation for the driven three-level system is given by

$$\ddot{g} - [(\dot{h}_{12}-i\dot{h}_{23})(h_{12}-ih_{23})^{-1} + ih_{13}]\dot{g} + (1/4)(h_{12}^2 + h_{23}^2)\, g = 0.$$

The complete formal solution of the problem of three-level population control is given by the formula

$$|g(T)|^2 = \frac{(P_1(0)-P_2(0))(P_1(T)-P_2(0)) - (P_3(0)-P_2(0))(P_3(T)-P_2(0))}{(P_1(0)-P_3(0))(P_1(0)+P_3(0)-2P_2(0))}.$$

The useful relation exists between two variables u and v

$$|u(t)|^4 - |v(t)|^4 = [P_1(0) - P_3(0)]^{-1} [P_1(t) - P_3(t)].$$

Using the eqs. 10 and (18) we can now easily find simple exact conditions for complete transfer of population from one level to another and for complete return of population to an initial level. Let at t=0 level 1 is fully populated, i.e. $P_1(0)= 1$, $P_2(0)= P_3(0)= 0$, then the population is transfered completely to the level 3 at time t, i.e. $P_3(t)= 1$, $P_1(t) = P_2(t)= 0$, if g(t) = 0. For the same initial conditions the population returns to the first level at time t, i.e. $P_1(t) = 1$, $P_2(t)= P_3(t)= 0$, when $|g(t)| = 1$.

5. POPULATION DYNAMICS OF A RESONANTLY DRIVEN FOUR-LEVEL SYSTEM

The resonant Hamiltonian of a four-level system simultaneously driven by six lasers with arbitrary and different time dependences of amplitudes is given by the eq.9 with N=4. If the phases are choosen in such a way that all the Rabi frequencies (8) are purely imagine ones then the four-level Hamiltonian generates the following 4x4-matrix realization of the SO(4) algebra

$$R_1^{32} = R_2^{13} = R_3^{21} = -R_1^{23} = -R_2^{31} = -R_3^{12} = J_1^{14} = J_2^{24} = J_3^{34} = -J_1^{41} = -J_2^{42} = -J_3^{43} = 1,$$

with zero remaining matrix elements and with the following commutation relations

$$[R_j, R_k] = e_{jkl} R_l, \quad [J_j, J_k] = e_{jkl} R_l, \quad [R_j, J_k] = e_{jkl} J_l.$$

One can rearrange this basis by such a way to obtain from the matrices R_j and J_k two mutually commuting sets of matrices $A_{0,+,-}$ and $B_{0,+,-}$ with the commutation relations (12). Now we can rewrite our Hamiltonian in the form

$$H(t) = \sum_{m=0,+,-} a_m(t) A_m + b_m(t) B_m, \quad (19)$$

where the following short-hand notations are introduced

$$a_0 \equiv i(h_{12} - h_{34}), \quad 2a_- \equiv ih_{23} + h_{13} - ih_{14} + h_{24},$$

$$2a_+ \equiv ih_{23} - h_{13} - ih_{14} - h_{24}, \quad b_0 \equiv i(h_{12} + h_{34}), \quad (20)$$

$$2b_- \equiv ih_{23} + h_{13} + ih_{14} - h_{24}, \quad b_+ \equiv ih_{23} - h_{13} + ih_{14} + h_{24}.$$

Since H(t) exactly equals to the sum of the two SU(2) Hamiltonians, commuting with each other, we may use all the results obtained for the SU(2) dynamical symmetry. Thus the system posesses SU(2) ⊕ SU(2) dynamical symmetry [8] and the evolution operator can be written in the factorized form $U = U_g U_f$, where

$$U_g = \exp (g_0 A_0) \exp (g_- A_-) \exp (g_+ A_+),$$

$$U_f = \exp (f_0 B_0) \exp (f_- B_-) \exp (f_+ B_+) \quad (21)$$

The governing equations for our four-level system take the form

$$\ddot{g} - \dot{a}_{+}a_{+}^{-1}\dot{g} + (1/2)(i\dot{a}_0 - ia_0\dot{a}_{+}a_{+}^{-1} + 2a_-a_+ + (1/2)a_0^2)g = 0,$$

$$\ddot{f} - \dot{b}_{+}b_{+}^{-1}\dot{f} + (1/2)(i\dot{b}_0 - ib_0\dot{b}_{+}b_{+}^{-1} + 2b_-b_+ + (1/2)b_0^2)f = 0,$$

with the variables $g \equiv \exp(g_0/2)$ and $f \equiv \exp(f_0/2)$ respectively. In an explicit form the evolution matrices are the following

$$
U_g = g^{-1}
\begin{vmatrix}
g\ \text{Reg} & g\ \text{Img} & \text{Reg}_- & -\text{Img}_- \\
-g\ \text{Img} & g\ \text{Reg} & \text{Img}_- & \text{Reg}_- \\
-\text{Reg}_- & -\text{Img}_- & g\text{Reg} & -g\ \text{Img} \\
\text{Img}_- & -\text{Reg}_- & g\ \text{Img} & g\ \text{Reg}
\end{vmatrix},
$$

$$
U_f = f^{-1}
\begin{vmatrix}
f\ \text{Ref} & f\ \text{Imf} & \text{Ref}_- & \text{Imf}_- \\
-f\ \text{Im}\,f & f\ \text{Ref} & \text{Imf}_- & -\text{Ref}_- \\
-\text{Ref}_- & -\text{Imf}_- & f\ \text{Ref} & f\ \text{Imf} \\
-\text{Imf}_- & \text{Ref}_- & -f\ \text{Imf} & f\ \text{Ref}
\end{vmatrix},
$$

where $g_- = g\ (2i\dot{g} - a_0\ g)/2a_+$ and $f_- = f\ (2i\dot{f} - b_0\ f)/2b_+$.

Let at $t = 0$ the first level is occupied with probability one, i.e. $P_1(0) = 1$, $P_2(0) = P_3(0) = P_4(0) = 0$. Then the exact condition for complete transfer of population to the upper level is given by

$$|g^{-1}(\text{Ref Img}_- + \text{Reg}_-\ \text{Imf}) - f^{-1}(\text{Reg Imf} + \text{Ref}_-\ \text{Img}_-)|^2 = 1 \quad (22)$$

and the condition for the first level to be completely depleted of population is

$$\text{Reg Imf} - \text{Img Imf} - (gf)^{-1}\ (\text{Reg}_-\ \text{Ref}_- - \text{Img}_-\ \text{Imf}_-) = 0. \quad (23)$$

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KRAVCHUK FUNCTIONS
FOR THE FINITE OSCILLATOR APPROXIMATION[1]

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Abstract

Kravchuk orthogonal functions — Kravchuk polynomials multiplied by the square root of the weight function — simplify the inversion algorithm for the analysis of discrete, finite signals in harmonic oscillator components. They can be regarded as the best approximation set. As the number of sampling points increases, the Kravchuk expansion becomes the standard oscillator expansion.

1   Introduction

In a harmonic oscillator environment, such as Fourier optics in a multimodal parabolic index-profile fiber, **sampling on a finite set of discrete observation points** reconstructs the wavefunction through partial wave synthesis. For the harmonic oscillator eigenfunctions, one must invert a nondiagonal matrix with the dimension of the number of data.

We show that Kravchuk orthogonal functions optimize the algorithm for the expansion coeffients, because the matrix **is already** diagonal.

- Kravchuk functions [1, 2] are solutions of the difference analogue of the Schrödinger equation describing a discrete harmonic oscillator system.

- Kravchuk functions have a well-defined analytical structure *inside* the measurement interval.

- Kravchuk functions become the standard oscillator wavefunctions, as the number of sampling points increases.

This contribution is a résumé of Ref. [3].

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2 Harmonic oscillator expansions over a lattice of sampling points

The standard harmonic oscillator eigenfuctions are

$$\psi_n(\xi) = \frac{1}{\sqrt{\sqrt{\pi}2^n n!}} H_n(\xi)\, e^{-\xi^2/2}, \qquad n = 0, 1, 2, \ldots,$$

where $H_n(\xi)$ are the Hermite polynomials, $\xi = \sqrt{m\omega/\hbar}\, x$, m is oscillator mass, ω is oscillation frequency, and the position coordinate is x. This function set is orthonormal under the $\mathcal{L}^2(\Re)$ inner product:

$$(\psi_m, \psi_n)_\Re = \int_{-\infty}^{\infty} d\xi\, \psi_m(\xi)\, \psi_n(\xi) = \delta_{m,n} = \left\{ \begin{array}{ll} 1, & \text{when } m = n, \\ 0, & \text{when } m \neq n. \end{array} \right.$$

Thus, an arbitrary function $f(\xi) \in \mathcal{L}^2(\Re)$ can be approximated in the norm as

$$f(\xi) = \sum_{n=0}^{\infty} c_n\, \psi_n(\xi),$$

where the expansion coefficients $\{c_n\}_{n=0}^{\infty}$ are determined by

$$c_n = (\psi_n, f)_\Re = \int_{-\infty}^{\infty} d\xi\, \psi_n(\xi)\, f(\xi).$$

When the $N + 1$ values $\{f(\xi_j)\}_{j=0}^{N}$ of function $f(\xi)$ are sampled on the points

$$\xi_0 = -\tfrac{1}{2}Nh, \ldots\ \xi_j = \left(-\tfrac{1}{2}N + j\right)h, \ldots\ \xi_N = \tfrac{1}{2}Nh,$$

then

$$f(\xi_j) = \sum_{n=0}^{N} c_n^{(N)}\, \psi_n(\xi_j), \quad j = 0, 1, \ldots N. \tag{2.1}$$

The task to determine the $N + 1$ coefficients $\{c^{(N)}\}_{n=0}^{N}$ is formulated in matrix form as

$$\mathbf{f} = \mathbf{\Psi}^{(N)}\, \mathbf{c}^{(N)},$$

where

$$\mathbf{f} = \begin{pmatrix} f(\xi_0) \\ f(\xi_1) \\ \vdots \\ f(\xi_N) \end{pmatrix}, \qquad \mathbf{c}^{(N)} = \begin{pmatrix} c_0^{(N)} \\ c_1^{(N)} \\ \vdots \\ c_N^{(N)} \end{pmatrix},$$

and

$$\mathbf{\Psi}^{(N)} = \begin{pmatrix} \psi_0(\xi_0) & \psi_0(\xi_1) & \cdots & \psi_0(\xi_N) \\ \psi_1(\xi_0) & \psi_1(\xi_1) & \cdots & \psi_1(\xi_N) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_N(\xi_0) & \psi_N(\xi_1) & \cdots & \psi_N(\xi_N) \end{pmatrix}$$

This is the $N \times N$ matrix that **has to be inverted** to find the coefficients in (2.1).

3 Kravchuk functions are difference analogs of the oscillator eigenfunctions

Kravchuk **polynomials** $k_n^{(p)}(x, N)$ are:

- polynomials of degree $0 \le n \le N$,

- in the variable $x \in [0, N]$,

- of the parameter $0 < p < 1$.

These polynomials are related to the binomial distribution of probability theory [4, 5]. They form an orthogonal set

$$\sum_{j=0}^{N} \varrho(j) \, k_m^{(p)}(j, N) \, k_n^{(p)}(j, N) = d_n^2 \delta_{m,n}$$

with respect to a discrete binomial weight function

$$\varrho(x) = C_N^x \, p^x (1 - p)^{N-x}.$$

Kravchuk functions are defined as

$$\phi_n^{(p)}(x, N) = d_n^{-1} \, k_n^{(p)}(Np + x, N) \, \varrho^{1/2}(x + Np),$$

$$0 \le n \le N, \qquad -Np \le x \le (1 - p)N$$

(*cf.* definition of the Hermite functions in Ref. [6]). They obey the three-term recurrence relation

$$[x - n - p(N - 2n)]k_n^{(p)}(x, N) = (n + 1)k_{n+1}^{(p)}(x, N) + p(1 - p)(N - n + 1)k_{n-1}^{(p)}(x, N),$$

and satisfy the equation

$$\mathbf{H}^{(N)}(x) \, \phi_n^{(p)}(x, N) = (n + \tfrac{1}{2})\phi_n^{(p)}(x, N),$$

with the difference **Hamiltonian**

$$\mathbf{H}^{(N)}(x) = (1 - 2p)x + 2p(1 - p)N + \tfrac{1}{2} - \sqrt{p(1 - p)}[\alpha(x) \, e^{-\partial_x} + \alpha(x + 1) \, e^{\partial_x}],$$

namely

$$[(1 - 2p)x - n + 2p(1 - p)N]\phi_n^{(p)}(x, N) = \sqrt{p(1 - p)} \, [\alpha(x)\phi_n^{(p)}(x - 1, N) + \alpha(x + 1)\phi_n^{(p)}(x + 1, N)].$$

The oscillator equation of motion in the Schrödinger representation [7] is $[H, [H, x]] = (\hbar\omega)^2 x$. The difference analogue of this relation satisfied by this Hamiltonian is [1]

$$[\mathbf{H}^{(N)}(x), [\mathbf{H}^{(N)}(x), x]] = x.$$

Finally, the limit $N \to \infty$ of Kravchuk functions is

$$\lim_{N \to \infty} h^{-1/2}\phi_n^{(p)}(h^{-1}\xi, N) = \psi_n(\xi).$$

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The set of Kravchuk functions $\phi_n^{(p)}(x, N)$, $n = 0, 1, \ldots, N$ forms a basis for irreducible representations of the rotation group $SO(3)$ [8], corresponding to the eigenvalues $\ell = \frac{1}{2}N$ of the invariant Casimir operator; the eigenvalues of generator J_z are the integer $m = n - \frac{1}{2}N = n - \ell$. The representations corresponding to different values of the parameter p turn out to be unitarily equivalent [1], so it is sufficient to consider a set of functions $\phi_n^{(p)}(x, N)$ with some fixed value of this parameter. It is convenient to choose the value $p = \frac{1}{2}$, since these Kravchuk functions have definite parity with respect to reflections of x,

$$\phi_n^{(1/2)}(-x, N) = (-1)^n \phi_n^{(1/2)}(x, N).$$

We thus use henceforth the **symmetric Kravchuk functions**

$$\phi_n(x, N) = 2^{n-N/2} k_n(x + \frac{1}{2}N, N) \sqrt{\frac{n! \, (N - n)!}{\Gamma(\frac{1}{2}(N + x + 1)) \Gamma(\frac{1}{2}(N - x + 1))}}.$$

4 Finite approximation by Kravchuk functions

A function $f(\xi)$ that 'lives in a harmonic oscillator environment', of which the values on $N + 1$ equidistant points ξ_j are known, is meaningfully expanded in symmetric Kravchuk functions as

$$f(\xi_j) = \frac{1}{\sqrt{h}} \sum_{n=0}^{N} \kappa_n^{(N)} \phi_n(\xi_j/h, N), \quad j = 0, 1, \ldots N.$$

To find the expansion coefficients $\{\kappa_n^{(N)}\}_{n=0}^{N}$, we multiply the above equation by $\phi_m(\xi_j/h, N)$ and sum over the sample points ξ_j:

$$\kappa_n^{(N)} = \sqrt{h} \sum_{j=0}^{N} \phi_n(\xi_j/h, N) \, f(\xi_j).$$

We thus have only to multiply the sampled values $f(\xi_j)$ by the (numerically calculated) values of the Kravchuk functions at the points $x_j = \xi_j/h$, for $n = 0, 1, \ldots, N$, to find the expansion coefficients. **No matrix inversion is necessary.**

The sum

$$f(\xi, N) = \frac{1}{\sqrt{h}} \sum_{n=0}^{N} \kappa_n^{(N)} \phi_n(\xi/h, N), \quad j = 0, 1, \ldots, N,$$

interpolates the original function defined on discrete points to the interval $[\xi_0, \xi_N]$ and is a **finite approximation** to the square-integrable function $f(\xi)$. This approximant is *finite* because for any fixed N it has a *finite support* $(-h - h^{-1}, h + h^{-1})$ with $h = \sqrt{2/N}$. When N grows, the approximation to $f(\xi)$ becomes better. The time evolution of the approximating function multiplies each $\phi_n(\xi_j, N)$ by the usual time dependence $\exp(-iE_n t/\hbar)$, with the equally spaced energy eigenvalues $E_n = \hbar\omega(n + \frac{1}{2})$.

5 Position and momentum functions

The canonical vector basis of **position** functions

$$\Lambda_0 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad \Lambda_1 = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}, \quad \cdots \quad \Lambda_N = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}$$

is interpolated to

$$f(\xi_j) = \sum_{k=0}^{N} f_k^{(N)} \Lambda_k(\xi_j, N) = f_j^{(N)}, \quad j = 0, 1, \ldots N.$$

These basis functions can be expanded in terms of Kravchuk functions as

$$\Lambda_k(\xi_j, N) = \frac{1}{\sqrt{h}} \sum_{n=0}^{N} \lambda_{k,n}^{(N)} \phi_n(\xi_j/h, N), \quad j = 0, 1, \ldots N,$$

where the coefficients are

$$\lambda_{k,n}^{(N)} = \sqrt{h}\, \phi_n(\xi_k/h, N)$$

for $k = 0, 1, \ldots [N/2]$ and continuous ξ. These functions are the localized states of the discrete oscillator.

Momentum basis functions are defined in the same way, because Kravchuk functions are self-reproducing under the discrete Fourier transformation [2], *i.e.*

$$\tilde{\Lambda}_k(\xi, N) = \sum_{n=0}^{N} i^n \phi_n(\xi_k/h, N)\, \phi_n(\xi/h, N).$$

Acknowledgments

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PHASE SPACE ANALYSIS IN
ANISOTROPIC OPTICAL SYSTEMS

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Abstract

From the minimal action principle follow the Hamilton equations of evolution for geometric optical rays in anisotropic media. As in classical mechanics of velocity-dependent potentials, the velocity and the canonical momentum are not parallel, but differ by an anisotropy vector potential, similar to that of linear electromagnetism. Descartes' well known diagram for refraction is generalized and a factorization theorem holds for interfaces between two anisotropic media.

1 Fermat's principle

Fermat's principle states that the light ray joining two points in an optical medium takes the path where it employs an extremal time [1]:

$$\delta \int_A^B dt = \delta \int_A^B ds\, n(\vec{q}(s), \dot{\vec{q}}(s)) = 0.$$

Here we denote by ds the *length* element along the ray $\vec{q}$, the ray direction by $\dot{\vec{q}} = \dfrac{d\vec{q}}{ds}$ and by n the *refractive index* of the medium. The refractive index characterizes the optical medium. Constant n indicates that the medium is *homogeneous* (invariant under translations) and *isotropic* (invariant under rotations). In *anisotropic media*, the refractive index depends also on the *direction* of the ray [2].

We use one of the Cartesian coordinates of $\mathcal{R}^3$ as the evolution parameter to describe the evolution of the ray $\vec{q} = \begin{pmatrix} \mathbf{q} \\ z \end{pmatrix}$. Defining $\mathbf{v} = \dfrac{d\mathbf{q}}{dz}$ with $ds = \dfrac{dz}{\sqrt{1 - \dot{\mathbf{q}}^2}} = dz\,\sqrt{1 + \mathbf{v}^2}$ we write Fermat's principle as [3]

$$\delta \int_{z_A}^{z_B} dz\, L(\mathbf{q}(z), z; \mathbf{v}(z)) = 0,$$

with the Lagrangian function $L(\mathbf{q}, z; \mathbf{v}) = \sqrt{1 + \mathbf{v}^2}\, n(\mathbf{q}, z; \mathbf{v})$.

2 Evolution equations

The Euler-Lagrange equations that follow from the Fermat principle are [4]

$$\frac{d}{dz}\mathbf{p} = \frac{\partial L}{\partial \mathbf{q}},$$

where the canonical *momentum* is

$$\mathbf{p} = \frac{\partial L}{\partial \mathbf{v}} = \frac{n\mathbf{v}}{\sqrt{1+\mathbf{v}^2}} + \sqrt{1+\mathbf{v}^2}\,\frac{\partial n}{\partial \mathbf{v}} = n\dot{\mathbf{q}} + \mathbf{A}(\mathbf{q}, z, \dot{\mathbf{q}}),$$

and we define the *anisotropy vector*

$$\mathbf{A} = \sqrt{1+\mathbf{v}^2}\,\frac{\partial n}{\partial \mathbf{v}} = (1 - \dot{\mathbf{q}}\,\dot{\mathbf{q}}^T)\,\frac{\partial n(\mathbf{q}, z, \dot{\mathbf{q}})}{\partial \dot{\mathbf{q}}}.$$

We obtain the Hamilton evolution equations through the Legendre transformation

$$\frac{d\mathbf{q}}{dz} = \frac{\partial H}{\partial \mathbf{p}}, \qquad \frac{d\mathbf{p}}{dz} = -\frac{\partial H}{\partial \mathbf{q}},$$

with the Hamiltonian function

$$H(\mathbf{q}, z; \mathbf{p}) = \mathbf{p}\cdot\mathbf{v} - L(\mathbf{q}, z; \mathbf{v}) = -\sqrt{n^2 - |\mathbf{p} - \mathbf{A}|^2} + \frac{(\mathbf{p} - \mathbf{A})\cdot\mathbf{A}}{\sqrt{n^2 - |\mathbf{p} - \mathbf{A}|^2}}.$$

In anisotropic media, the three-vectors of ray direction $\dot{\vec{q}}$, momentum $\vec{p}$, and anisotropy $\vec{A}$, are thus characterized by:

$$\vec{p} = n\dot{\vec{q}} + \vec{A}(\vec{q}, \dot{\vec{q}}), \qquad p_z = -H, \qquad |\dot{\vec{q}}| = 1, \qquad |\vec{p} - \vec{A}| = n(\vec{q}, \dot{\vec{q}}),$$

i.e., we have the orthogonal decomposition of momentum $\vec{p}$ into ray direction $\dot{\vec{q}}$ and the anisotropy three-vector

$$\vec{A} = \nabla_{\dot{\vec{q}}} n \big|_{|\dot{\vec{q}}|=1} = (1 - \dot{\vec{q}}\dot{\vec{q}}^T)\,\frac{\partial n}{\partial \dot{\vec{q}}}\bigg|_{|\dot{\vec{q}}|=1} = \hat{\mathbf{e}}_\theta\,\frac{\partial n}{\partial \theta} + \frac{\hat{\mathbf{e}}_\phi}{\sin\theta}\,\frac{\partial n}{\partial \phi}.$$

The anisotropy vector is orthogonal to the direction of ray propagation $\dot{\vec{q}}$.

While $|\dot{\vec{q}}|$ sweeps over the ray direction sphere $\mathcal{S}_2$, the vector $\vec{p} - \vec{A}$ draws out a closed surface $n(\vec{q}, \dot{\vec{q}})$—the *ray surface* at the space point $\vec{q}$, and the three-vector $\vec{p}$ ranges correspondingly over another closed surface that we call the *Descartes ovoid* of the anisotropic medium at $\vec{q}$.

The Hamilton equations are thus written in manifestly euclidean-covariant form as

$$\frac{d\vec{q}}{dz} = \frac{\partial H}{\partial \vec{p}} = \frac{\vec{p} - \vec{A}}{p_z - A_z}, \qquad \frac{d\vec{p}}{dz} = -\frac{\partial H}{\partial \vec{q}} = \frac{n}{p_z - A_z}\,\frac{\partial n}{\partial \vec{q}}.$$

From the second equation it follows that $d\vec{p} \times \dfrac{\partial n}{\partial \vec{q}} = \vec{0}$. As in the isotropic case, we get the Ibn Sahl [5] Snell law of refraction between two anisotropic media [6].

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FIGURE 1. Dipole medium: the momentum $\vec{p}$ of a ray is obtained by adding the direction vector $\vec{q}$ times n^0 to the dipole vector of the medium $\vec{D}$. The anisotropy vector $\vec{A}$ ranges over a cardioid-type surface.
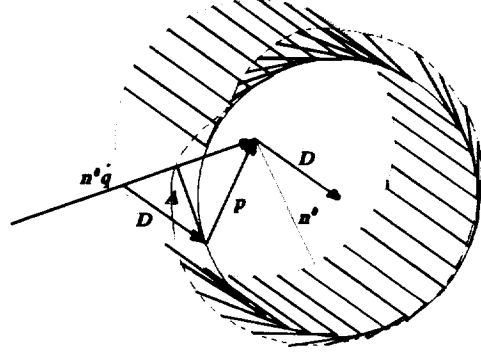
3   Dipole anisotropic media

Consider the refractive index with linear dependence on ray direction

$$n(\vec{q},\dot{\vec{q}}) = n^0(\vec{q}) + D(\vec{q},\dot{\vec{q}}),$$
$$D(\vec{q},\dot{\vec{q}}) = \sum_{j=x,y,z} D_j(\vec{q})\dot{q_j} = \vec{D}(\vec{q})^T\dot{\vec{q}}.$$

We call n^0 the *monopole* part of the medium and $\vec{D}$ its *dipole* vector. The anisotropy vector is

$$\vec{A}^{(1)} = (1 - \dot{\vec{q}}\dot{\vec{q}}^T)\vec{D} = \vec{D} - \vec{D}^T(\dot{\vec{q}})\dot{\vec{q}} = (\dot{\vec{q}} \times \vec{D}) \times \dot{\vec{q}}.$$

This vector lies in the plane of $\dot{\vec{q}}$ and $\vec{D}$, and is orthogonal to the ray direction $\dot{\vec{q}}$. The relation between ray direction and optical momentum is $\vec{p} = n^0\dot{\vec{q}} + \vec{D}$. While $\dot{\vec{q}} \in \mathcal{S}_2$, the Descartes ovoid is a sphere of radius $n^0(\vec{q})$ and center at $\vec{D}$. (See Figure 1).

4   Quadrupole media

Consider now a refractive index with quadratic dependence on ray direction $\dot{\vec{q}}$

$$n(\vec{q},\dot{\vec{q}}) = n^0(\vec{q}) + Q(\vec{q},\dot{\vec{q}}),$$
$$Q(\vec{q},\dot{\vec{q}}) = \sum_{j,k=x,y,z} Q_{j,k}\,\dot{q_j}\dot{q_k} = \dot{\vec{q}}^T\hat{Q}\dot{\vec{q}}.$$

We have a $\dot{\vec{q}}$-quadratic summand with coefficients $Q_{j,k}$ in a 3×3 *optical quadrupole matrix* $\hat{Q}$ that must be symmetric and traceless. It is common to restrict consideration to *principal axes*; in that frame of reference, $\hat{Q} = \mathrm{diag}\,(Q_x,Q_y,Q_z)$ and $Q_x + Q_y + Q_z = 0$. Then, the anisotropy and momentum vectors are

$$\vec{A}^{(2)} = 2(1 - \dot{\vec{q}}\dot{\vec{q}}^T)\hat{Q}\dot{\vec{q}} = 2[\hat{Q}\dot{\vec{q}} - Q(\vec{q},\dot{\vec{q}})\,\dot{\vec{q}}],$$

$$\vec{p} = [n(\vec{q},\dot{\vec{q}}) + 2(1 - \dot{\vec{q}}\dot{\vec{q}}^T)\hat{Q}]\dot{\vec{q}} = (n^0 + 2\hat{Q} - \dot{\vec{q}}^T\hat{Q}\dot{\vec{q}})\dot{\vec{q}}.$$

In two-dimensional optics, 2×2 symmetric traceless matrices have two independent coefficients that describe the ellipticity and orientation of the figure. When $\dot{\vec{q}}$ ranges over the sphere of directions $\mathcal{S}_2$, $\vec{p}$ will range over the Descartes ovoid of the quadrupole medium. (See Figure 2).

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FIGURE 2. $n^0\dot{\vec{q}}$ ranges over the sphere (circle in the two dimensions of the figure) of radius n^0, $n\dot{\vec{q}}$ over the peanut-shaped surface, and the momentum $\vec{p}$ draws a Descartes oval. The thin lines joining points on the circle and on the oval relate the direction of the ray with the corresponding direction of the momentum vector.
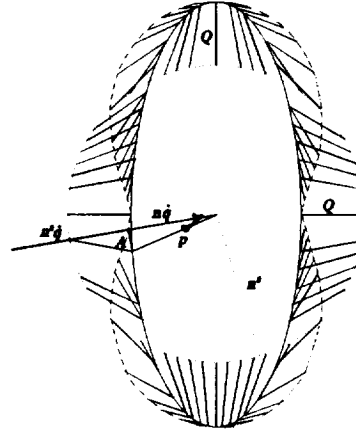
5 Free propagation in homogeneous uniaxial media

For the uniaxial quadrupole media we can write the refractive index as

$$n(\dot{\vec{q}}) = n^0 + (\dot{x}, \dot{y}, \dot{z}) \begin{pmatrix} \nu & 0 & 0 \\ 0 & \nu & 0 \\ 0 & 0 & -2\nu \end{pmatrix} \begin{pmatrix} \dot{x} \\ \dot{y} \\ \dot{z} \end{pmatrix}$$

where n^0 is the monopole part and ν is a quadrupole anisotropy coefficient.

Putting $\dot{\mathbf{q}}$ in terms of $\mathbf{v}$, we can write out the components of momentum as

$$\mathbf{p} = (n^0 + 4\nu)\dot{\mathbf{q}} - 3\nu\dot{\mathbf{q}}^2\,\dot{\mathbf{q}} = (1 + \mathbf{v}^2)^{-3/2}[(n^0 + 4\nu) + (n^0 + \nu)\mathbf{v}^2]\mathbf{v}$$

For free propagation, the Hamilton equations and their solutions are:

$$\frac{d\mathbf{q}}{dz} = \mathbf{v} \Rightarrow \mathbf{q}(z) = \mathbf{q}(0) + z\mathbf{v}, \qquad \frac{d\mathbf{p}}{dz} = 0 \Rightarrow \mathbf{p}(z) = \mathbf{p}(0).$$

Although the solutions are apparently independent of the anisotropy of the medium (they are straight lines in space), the anisotropy is expressed through the relation between the ray momentum $\mathbf{p}$ and the ray direction $\mathbf{v}$. In isotropic media, the momentum vector is n times the direction vector and we can easily invert this particular case to [7]

$$\mathbf{v} = \frac{\mathbf{p}}{\sqrt{(n^0)^2 - \mathbf{p}^2}} = \frac{\mathbf{p}}{p_z}, \qquad |\mathbf{v}| = n^0\tan\theta \qquad (\nu = 0).$$

In the more general uniaxial anisotropic case, to find a simple closed inversion, we expand this equation with a Taylor series in $(\mathbf{v}^2)^k\mathbf{v}$ for $k = 0, 1, 2, \ldots$ and propose a similar expansion of $\mathbf{v}$ in powers of $(\mathbf{p}^2)^k\mathbf{p}$. Equating the series we find the expansion coefficients

$$\mathbf{v}(\mathbf{p}) = \frac{1}{n^0 + 4\nu}\mathbf{p} + \frac{\frac{1}{2}n^0 + 5\nu}{(n^0 + 4\nu)^4}\mathbf{p}^2\mathbf{p} + \frac{\frac{3}{8}(n^0)^2 + \frac{15}{2}n^0\nu + 51\nu^2}{(n^0 + 4\nu)^7}(\mathbf{p}^2)^2\mathbf{p}$$
$$+ \frac{\frac{5}{16}(n^0)^3 + \frac{75}{8}(n^0)^2\nu + 114n^0\nu^2 + 650\nu^3}{(n^0 + 4\nu)^{10}}(\mathbf{p}^2)^3\mathbf{p} + \cdots .$$

FIGURE 3. Descartes diagram to construct refraction angles between two anisotropic media.
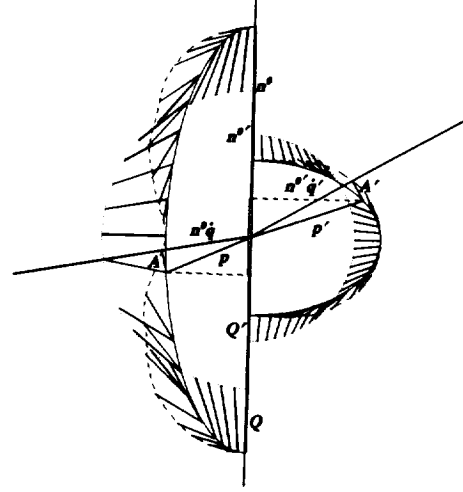
The evolution Hamiltonian is then

$$
\begin{aligned}
H(\mathbf{p}) &= \mathbf{p} \cdot \mathbf{v} - (n^0 - 2\nu)\sqrt{1 + \mathbf{v}^2} - 3\nu\,\frac{\mathbf{v}^2}{\sqrt{1 + \mathbf{v}^2}} \\
&= -(n^0 - 2\nu) + \frac{1}{2n^e}\,\mathbf{p}^2 + \frac{n^0 + 10\nu}{8(n^e)^4}\,(\mathbf{p}^2)^2 + \frac{3(n^0)^2 + 60n^0\nu + 408\nu^2}{16(n^e)^7}\,(\mathbf{p}^2)^3 \\
&\quad + \frac{5(n^0)^3 + 150(n^0)^2\nu + 1824n^0\nu^2 + 10\,400\,\nu^3}{128(n^e)^{10}}\,(\mathbf{p}^2)^4 + \cdots \,,
\end{aligned}
$$

where $n^e = n^0 + 4\nu$ plays the role of an effective paraxial refractive index. In the isotropic case (when $\nu = 0$), this is the expansion of $-\sqrt{n^2 - \mathbf{p}^2}$, the well-known optical Hamiltonian for such a media [8].

6   Finite refraction

Let us consider the case when rays cross the flat interface $z = 0$ between two different aligned uniaxial quadrupole anisotropic media. Let their refractive indices in two half-spaces be $n(\vec{q})$ and $n'(\vec{q})$ with monopole parameters n^0 and $n^{0\prime}$, and quadrupole anisotropy coefficients ν and ν', respectively. The refraction law claims that the projection of the momentum vector on the refracting surface is *conserved*, which for our refracting surface gives $\mathbf{p} = \mathbf{p}'$. Generally, the incident and refracted rays are not coplanar with the surface normal. However, in the aligned uniaxial case both refractive indexes are axially symmetric (under rotations around z-axis) and the two anisotropic vectors are coplanar with the suface normal (z-axis). Refraction in our case is thus coplanar.

Using 'ruler, compass and plotter' on the plane Figure 3, we construct the Descartes diagram for the point at the interface joining two 'half Descartes diagrams' and matching the length of the momentum vectors $\mathbf{p}$ and $\mathbf{p}'$ on the interface. To find the angle of refraction θ' in terms of the angle of incidence θ, we construct $\dot{\mathbf{q}}'(\dot{\mathbf{q}}; n^0, \nu; n^{0\prime}, \nu')$ expanded in series of sines, and find

$$
\sin\theta' = \frac{n^e}{n^{e\prime}}\sin\theta + \frac{3}{n^{e\prime}}\left[\left(\frac{n^e}{n^{e\prime}}\right)\nu' - \nu\right]\sin^3\theta + \frac{27}{(n^{e\prime})^2}\left(\frac{n^e}{n^{e\prime}}\right)^2\nu'\left[\left(\frac{n^e}{n^{e\prime}}\right)^3\nu' - \nu\right]\sin^5\theta
$$

$$-\frac{81}{(n^{e'})^3}\left(\frac{n^e}{n^{e'}}\right)\nu'\left[\left(\frac{n^e}{n^{e'}}\right)^3\nu'-\nu\right]\left[\left(4\frac{n^e}{n^{e'}}\right)^3\nu'-\nu\right]\sin^7\theta+\cdots.$$

The first summand is the very well know law of sines (Ibn Sahl–Snell law [5]); it is here also the *paraxial approximation* with the ratio of effective refractive coefficients. The succeding terms are corrections of orders ν^k and $\sin^{2k+1}\theta$ due to anisotropy.

7   The roots of refraction

We consider now the ray transformation due to refraction at a smooth surface $S(\vec{q}) = \zeta(\mathbf{q}) - z = 0$ between two general anisotropic, homogeneous media $n(\vec{q})$ and $n'(\vec{q})$. The rays in the first and in the second media are given correspondingly by the equations

$$\mathbf{q}(z) = \mathbf{q} + z\mathbf{v}, \quad \mathbf{p}(z) = \mathbf{p}, \quad z < \bar{z},$$
$$\mathbf{q}'(z) = \mathbf{q}' + z\mathbf{v}', \quad \mathbf{p}'(z) = \mathbf{p}', \quad z > \bar{z},$$

where we have indicated the point of impact at the refracting surface by bars $\vec{\bar{q}} = (\bar{\mathbf{q}}, \bar{z} = \zeta(\bar{\mathbf{q}}))$. We can formally consider the second pair of equations also on the left of the refracting surface, $z < \bar{z}$. It allows to parametrize the rays behind the surface by the coordinate $\mathbf{q}'$ and momentum $\mathbf{p}'$ on the same screen $z = 0$; $\mathbf{v}$ and $\mathbf{v}'$ are the two ray directions on the screen. Thus, the point of impact coordinates can be written in two ways:

$$\mathbf{q}(\bar{z}) = \mathbf{q} + \zeta(\bar{\mathbf{q}})\mathbf{v} = \bar{\mathbf{q}} = \mathbf{q}' + \zeta(\bar{\mathbf{q}})\mathbf{v}' = \mathbf{q}'(\bar{z}).$$

This is the *first root equation* of refraction [9]; it is an implicit equation for $\bar{\mathbf{q}}$.

The *second root equation* follows from the conservation of the tangential component of momentum and implies the refraction law. If the normal to the surface S is denoted by $\vec{\nabla}S(\vec{q}) = (\zeta_x, \zeta_y, -1) \equiv (\boldsymbol{\Sigma}(\mathbf{q}), -1)$ then we have $(\vec{p} - \vec{p}') \times \vec{\nabla}S(\vec{q}) = 0$. As we know, the momentum vector has components $\vec{p} = (p_x, p_y, p_z) = (\mathbf{p}, -H)$. Denoting the Hamiltonians before and after the refracting suface as H and H' we can rewrite the last equation containing the vector product as

$$\mathbf{p} - H(\mathbf{p})\boldsymbol{\Sigma}(\bar{q}) = \bar{\mathbf{p}} = \mathbf{p}' - H'(\mathbf{p}')\boldsymbol{\Sigma}(\bar{q}).$$

This is the second root equation determaning explicitly $\bar{p}$ once $\bar{q}$ has been found.

We have thus determined the root transformation for generic surfaces $S = \zeta(\mathbf{q}) - z = 0$ between homogeneous, anisotropic media. On optical phase space the root transformation is

$$\mathcal{R}_{n;\zeta} : \mathbf{q} \mapsto \bar{\mathbf{q}} = \mathbf{q} + \mathbf{v}(\mathbf{p})\,\zeta(\bar{\mathbf{q}}),$$
$$\mathcal{R}_{n;\zeta} : \mathbf{p} \mapsto \bar{\mathbf{p}} = \mathbf{p} - H(\mathbf{p})\,\boldsymbol{\Sigma}(\bar{\mathbf{q}}),$$

where $\mathbf{v}(\mathbf{p})$ and $H(\mathbf{p})$ contain the refractive index function $n(\vec{q})$. From our construction follows that the refracting surface transformation

$$\mathcal{S}_{n,n';\zeta} : (\mathbf{q}, \mathbf{p}) \mapsto (\mathbf{q}', \mathbf{p}')$$

thus factorizes into the product of the root transformation in the first medium and the inverse root transformation in the second medium, $\mathcal{S}_{n,n';\zeta} = \mathcal{R}_{n;\zeta}\,(\mathcal{R}_{n';\zeta})^{-1}$. When the surface S is a

FIGURE 4. Refraction at a surface is a map between phase space points $(\mathbf{q}, \mathbf{p})$ and $(\mathbf{q}', \mathbf{p}')$. This transformation visibly factors into transformations back and forth from the point of impact $\mathbf{q}$ on the surface $z = \zeta(\mathbf{q})$.

$z = $ constant plane, the second root transformation is simple free flight by generic z. The root transformation is illustrated in figure 4.

Let us consider explicitly the example of the symmetrical surface under rotations around z-axis

$$\zeta(\mathbf{q}) = \zeta_2 \mathbf{q}^2 + \zeta_4 \mathbf{q}^4 + \cdots .$$

The refraction by such a surface is determined to third aberration order as [9]

$$\mathbf{q}' = \mathbf{q} - \zeta_2 \left(\frac{1}{n^{0\prime} + 4\nu'} - \frac{1}{n^0 + 4\nu} \right) \mathbf{q}^2 \mathbf{p} + 2\zeta_2^2 \frac{[n^{0\prime} - 2\nu'] - [n^0 - 2\nu]}{n^{0\prime} + 4\nu} \mathbf{q}^2 \mathbf{q},$$

$$\mathbf{p}' = \mathbf{p} + 2\zeta_2([n^{0\prime} - 2\nu'] - [n^0 - 2\nu])\mathbf{q} + \zeta_2 \left(\frac{1}{n^{0\prime} + 4\nu'} - \frac{1}{n^0 + 4\nu} \right) \mathbf{p}^2 \mathbf{q}$$

$$-4\zeta_2^2 \frac{[n^{0\prime} - 2\nu'] - [n^0 - 2\nu]}{n^{0\prime} + 4\nu} \mathbf{p} \cdot \mathbf{q}\mathbf{q} - 2\zeta_2^2 \frac{[n^{0\prime} - 2\nu'] - [n^0 - 2\nu]}{n^{0\prime} + 4\nu} \mathbf{q}^2 \mathbf{p}$$

$$+4 \left(\zeta_2^3 \frac{([n^{0\prime} - 2\nu'] - [n^0 - 2\nu])^2}{n^{0\prime} + 4\nu} - \zeta_4 ([n^{0\prime} - 2\nu'] - [n^0 - 2\nu]) \right) \mathbf{q}^2 \mathbf{q}.$$

The paraxial part of the transformation is recognizably that of a quadratic surface.

Acknowledgments

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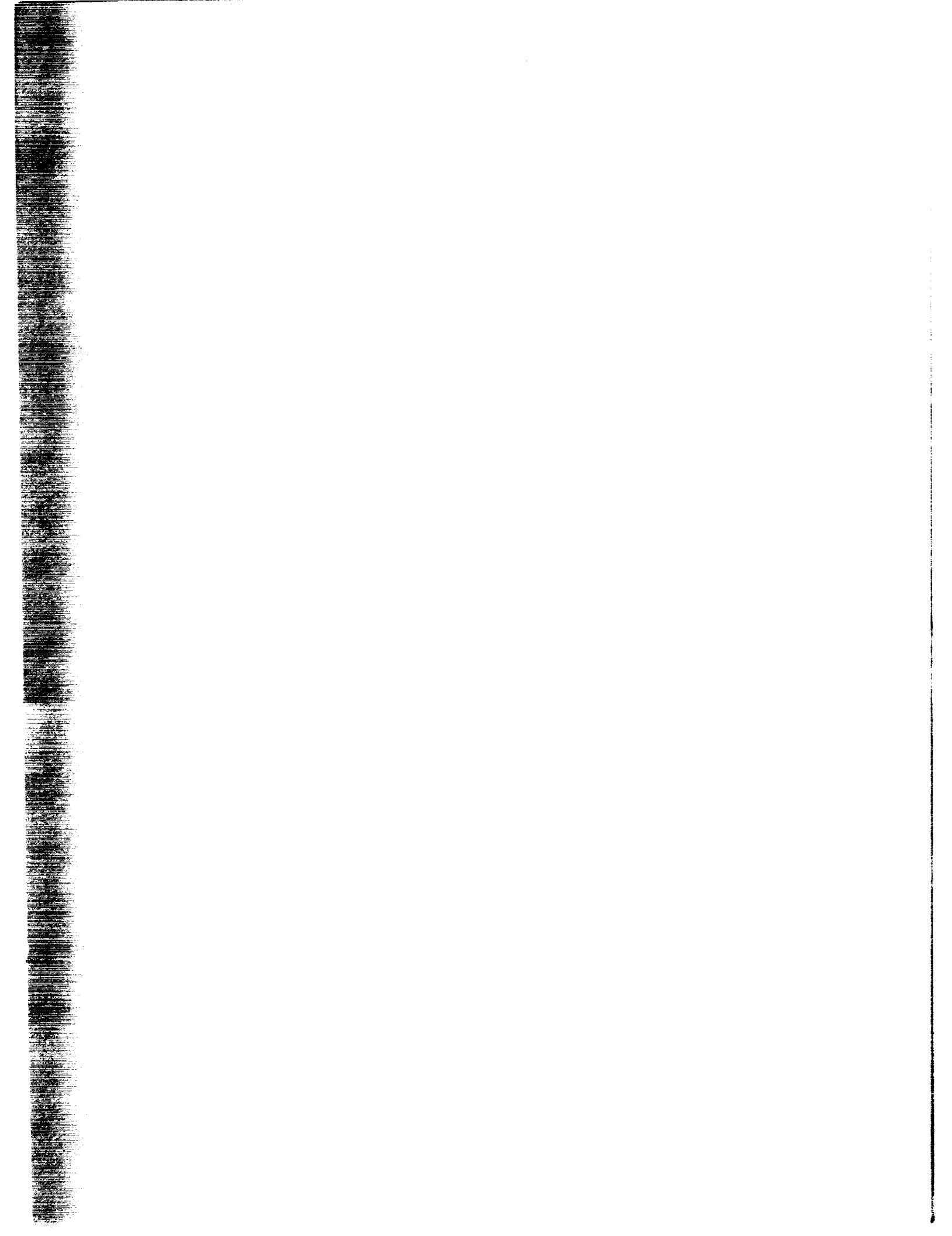
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13. ABSTRACT *(Maximum 200 words)*

The second International Workshop on Harmonic Oscillators was held at the Hotel Hacienda Cocoyoc March 23-25, 1994. The Workshop was attended by 67 participants; there were 10 invited lectures, 30 plenary oral presentations, 15 posters, and plenty of discussion divided into the five sessions of this volume. The organizing committee was asked by the chairmen of several Mexican funding agencies exactly what was meant by harmonic oscillators, and for what purpose the new research could be useful. Harmonic oscillator, in group theory, is a name for a family of mathematical models based on the theory of Lie algebras and groups, with applications in a growing range of physical theories and technologies: molecular, atomic, nuclear, and particle physics; quantum optics; and communication theory. The Harmonic Oscillators II Workshop was funded and organized through the Centro Internacional de Fisica y Matematicas Aplicadas (CIFMA). The Cuernavaca Center adds to the existing networks initiated by the Centro Latino Americano de Fisica, in Brazil, and the Centro Internacional de Fisica, in Colombia. The First Harmonic Oscillators meeting was held at the College Park campus of the University of Maryland (March 25-28, 1992).

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