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Quantized Discrete Space Oscillators

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A quasi-canonical sequence of finite dimensional quantizations has been found which has canonical quantization as its limit. In order to demonstrate its practical utility and its numerical convergence, this formalism is applied to the eigenvalue and "eigenfunction" problem of several harmonic and anharmonic oscillators.

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I. Introduction

Harmonic and anharmonic oscillators have long been used to illustrate new approximation techniques. Here they are used to demonstrate the application of an approximation procedure based upon the approach of a sequence of discrete non-canonical quantizations to the standard canonical quantization limit .

Consider a discrete one dimensional space in which the coordinates of allowed positions are interger multiples of a fundamental scale parameter a having dimensions of length. Although it is well known that the canonical commutation relation

$$[Q, P] = i\hbar I \tag{1}$$

does not admit finite dimensional matrix representations,[1] one can ask whether a limit procedure exists such that sequences of matrices $\{Q_N, P_N\}$ satisfy in some way

$$\lim_{N\to\infty} [Q_N, P_N] = i\hbar I \tag{2}$$

in the weak sense. We have found the answer to be in the affirmative[2] and therefore briefly sketch the theoretical analysis and apply the formalism to the numerical eigenvalue and eigenstate problems of harmonic and anharmonic oscillators.

II. Brief Analysis

The quantum mechanical scalar product of two wave functions in the Schroedinger representation can be written in the form

$$(\Psi, \Phi) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Psi(q)\delta(q - q')\Phi(q')dqdq', \tag{3}$$

a form equivalent to the traditional one. With respect to this scalar product the Schroedinger coordinate and momentum representatives have the form

$$Q(q, q') = q\delta(q - q'), \tag{4}$$

$$P(q, q') = -i\hbar \frac{\partial}{\partial q} \delta(q - q'). \tag{5}$$

On the other hand in a finite discrete space representation of the canonical coordinates and momenta one defines the Schroedinger representative of the coordinate operator by the diagonal matrix

$$Q_N = a\begin{pmatrix} (N-1)/2 & 0 & . & . & . & . & . & 0 \\ 0 & . & & & & & . & . \\ . & & . & & & . & & . \\ . & & & 1/2 & 0 & & & . \\ . & & 0 & . & -1/2 & & & . \\ . & & . & & & . & & . \\ . & . & & & & & . & 0 \\ 0 & . & . & . & . & . & 0 & -(N-1)/2 \end{pmatrix}, \tag{6}$$

or equivalently in component notation by

$$Q^r_{Ns} = ra\delta^r_s. \tag{7}$$

Here a defines the distance between neighboring points in space and N is a power of 2.

The components of the momentum operator are taken from the discrete Fourier transform of the diagonal part of Q_N,

$$P^r_{Ns} = \frac{\hbar^2}{N}\sum_{k=-(N-1)/2}^{(N-1)/2}\frac{2\pi k}{Na}\exp\left\{-\frac{2\pi ik}{N}(r-s)\right\}. \tag{8}$$

Thus P_N is a Toeplitz matrix. The expressions (4) and (5) follow from a proper definition of the state space scalar product and limiting procedure.

The state space scalar product is defined by

$$(\Phi,\Psi) = \frac{1}{a}\sum_{k=-(N-1)/2}^{(N-1)/2}\overline{\Phi^k}\Psi^k \tag{9}$$

where the bar denotes complex conjugation. With respect to this scalar product it is convenient for the sake of the weak limiting procedure to write the rth eigenvector of Q_N as either

$$\underset{r}{q}^s = \underset{r}{\delta}^s, \tag{10}$$

or equivenently expressed in terms of the finite discrete Fourier transform as

$$\underset{r}{q}^{s} = \frac{1}{N} \sum_{k=-(N-1)/2}^{(N-1)/2} \exp\left\{-\frac{2\pi i k}{N}(r-s)\right\}. \tag{11}$$

Using the latter one can verify that

$$(\underset{r}{q}, \underset{s}{q}) = \frac{1}{a} \underset{rs}{\delta} = \frac{1}{Na} \sum_{k=-(N-1)/2}^{(N-1)/2} \exp\left\{-\frac{2\pi i k}{N}(r-s)\right\} \tag{12}$$

One can now define the refinement or weak limit as that in which

$$Na \to \infty, a \to 0, ra \to q, sa \to q', \tag{13}$$

so that the matrix product summations carry over into integrals (in the same way that a Fourier series can be carried over into a Fourier integral). Note that this approach differs from those of others in which the domain of the right hand side of (2) is restricted to a subspace of the Hilbert space.[3]

For a small enough and N, r, s large enough one can get as close as desired to any real valued q or q'. In this case using the right hand side of (12) one can see that in the refinement or weak limit

$$(\underset{r}{q}, \underset{s}{q}) \to \delta(q - q'). \tag{14}$$

Similarly one can see that (2)and (7) and (8) have the weak limits

$$(\underset{r}{q}, [Q, P]\, \underset{s}{q}) \to i\hbar q \frac{\partial}{\partial q} \delta(q - q'), \tag{15}$$

$$(\underset{r}{q}, Q\, \underset{s}{q}) \to \delta(q - q'), \tag{16}$$

$$(\underset{r}{q}, P\, \underset{s}{q}) \to i\hbar \frac{\partial}{\partial q} \delta(q - q'). \tag{17}$$

Note that with all of these weak limits the factor $\frac{1}{a}$ associated with the implied metric tensor in the scalar product (9) is essential.

The existence of these limits is considered sufficient justification for investigating the practical utility of this finite dimensional quasi-canonical quantization. Hence we investigate the eigenvalue problem of several of the oscillators described by the Hamiltonian

$$H = \frac{P^2}{2m} + FQ + m\omega^2 \frac{Q^2}{2} + \lambda m \frac{Q^4}{4}. \tag{18}$$

III. Oscillator Eigenstates and Eigenvalues

Given (8) and (7) the Hamiltonian (18) can be written in the form

$$H^r_{Ns} = \frac{1}{N} \sum_{k=-(N-1)/2}^{(N-1)/2} \left(\frac{(2\pi\hbar k)^2}{2m(Na)^2} + Fra + \frac{m\omega^2}{2}(ra)^2 + \frac{m\lambda}{4}(ra)^4 \right) \exp\left\{ -2\pi k \frac{(r-s)}{N} \right\}. \tag{19}$$

It now remains to make proper choices of N and a and to carry out the numerical calculations in a manner compatible with a refinement process.

Define exponents n and l such that

$$N = 2^n, a = a_0 2^{-\alpha}, L = a_0 2^{n-\alpha}, n - \alpha > 0, \tag{20}$$

where a_0 is a length scale appropriate to the problem and where L gives the physical size of our one dimensional space. Clearly n sets the dimensionality of the matrix and α the refinement. The size of the space is L,while the rth eigenvector $\underset{r}{q}$ corresponds to the physical coordinate $ra_0 2^{n-\alpha}$.

A. The Harmonic Oscillator

For the case of the harmonic oscillator ($F = \lambda = 0$) it is convenient to choose

$$a_0 = \left(\frac{\hbar}{m\omega} \right)^{1/2}. \tag{21}$$

With the choices (19),(20), and (21) the discretized dimensionless form for the Hamiltonian is

$$\frac{H}{\hbar\omega} = \sum_{k=-(N-1)/2}^{(N-1)/2} \left(\frac{(2\pi k)}{2^{2\alpha-3n+1}}^2 + \frac{2^{2\alpha-n}}{2} r^2 \right) \exp\left\{ -2\pi k \left(\frac{r-s}{N} \right) \right\}., \tag{22}$$

One has different approximations for different choices of n and α. Figure I. illustrates the first 4 normalized "wave" eigenvectors for the discrete Harmonic Oscillator ($F = \lambda = 0$) with $n = 8, \alpha = 1$. Amazingly, for the first two eigenvectors of $\frac{H}{\hbar\omega}$ the absolute value of the error between a component of the eigenvector and the exact corresponding eigenfunction solution to the Schroedinger equation is less that 10^{-3} for the ground state and 10^{-2} for the first excited state at any of the allowed positions in the discrete space.

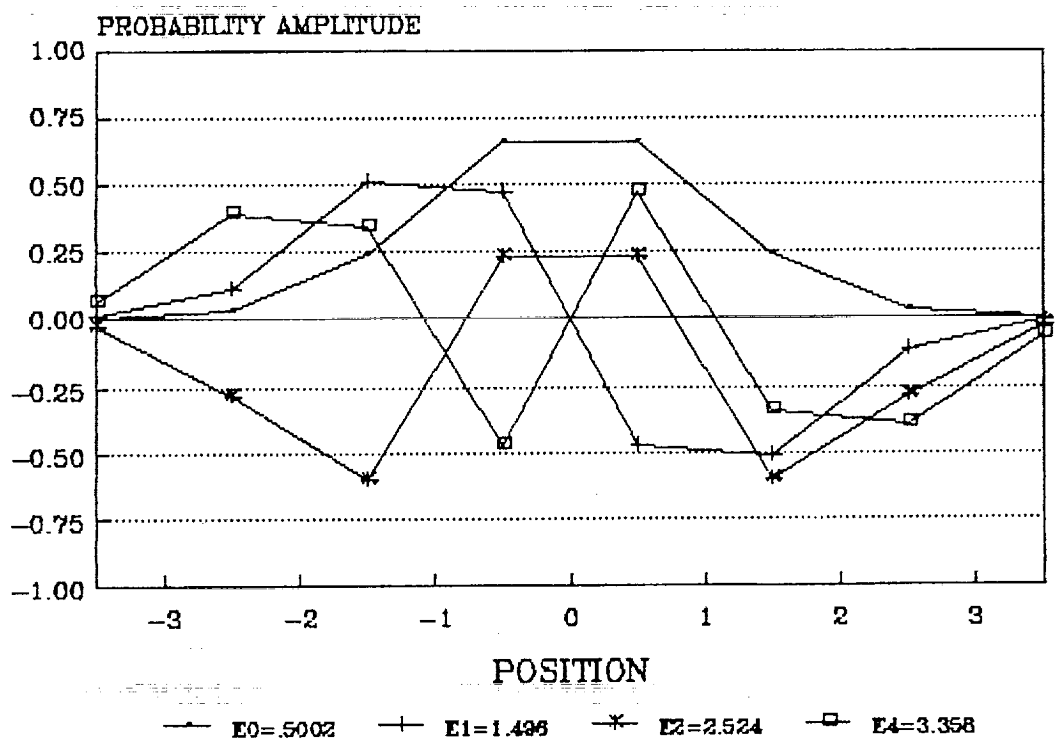

FIGURE I. HARMONIC OSC WAVEVECTORS (8,0)

Table I illustrates the numerical convergence of the 1st four harmonic oscillator eigenvalues as a function of matrix dimensionality N and α.

Table I H.O.

	$N=2, \alpha=0$	$N=4, \alpha=0$	$N=8, \alpha=0$	$N=16, \alpha=1$
E_0	1.3587	.5410	.50018	.5000001
E_1	1.3587	1.2186	1.4961	1.499984
E_2	–	3.1156	2.5241	2.500205
E_3	–	3.7933	3.3582	3.497943

B. The Asymmetric Oscillator

For the case of the asymmetric oscillator we take the choice

$$a_0 = \left(\frac{2\hbar^2}{Fm}\right)^{\frac{1}{3}}, \omega^2 = -\frac{8F}{ma_0}, \lambda = \frac{F}{ma_0^3}. \tag{23}$$

The components of the dimensionless Hamiltonian now have the form

$$\frac{H^{\tau}_{N_s}}{Fa_0} = \sum_{k=-(N-1)/2}^{(N-1)/2} \left(\frac{(2\pi k)^2}{2^{2\alpha-3n+1}} + 2^{\alpha-n}r - 8\cdot 2^{2\alpha-n}r^2 + \frac{2^{4\alpha-n}r^4}{4}\right) \exp\left\{-2\pi k\frac{(r-s)}{N}\right\}$$

Figure II illustrates the asymmetric potential while Figure III illustrates the solutions to the eigenvector problem for this asymmetric oscillator. Of interest is the "trapping" in the virtual potential well occuring with the 4th energy level, an effect not easily accounted for with other approximation techniques.

Table II illustrates the numerical convergence of the first four eigenvalues using several choices of N and α.

Table II ASYM OSC.

	$N=2, \alpha=0$	$N=4, \alpha=0$	$N=8, \alpha=0$	$N=16, \alpha=1$	$N=64, \alpha=2$
E_0	−.7507	−9.3999	−19.1162	−19.6787	−19.6803
E_1	−1.2493	−3.2519	−16.5510	−15.6227	−15.6025
E_2	–	−0.6331	−9.1040	−11.7496	−11.7147
E_3	–	2.0159	−8.9120	−8.6628	−8.65986

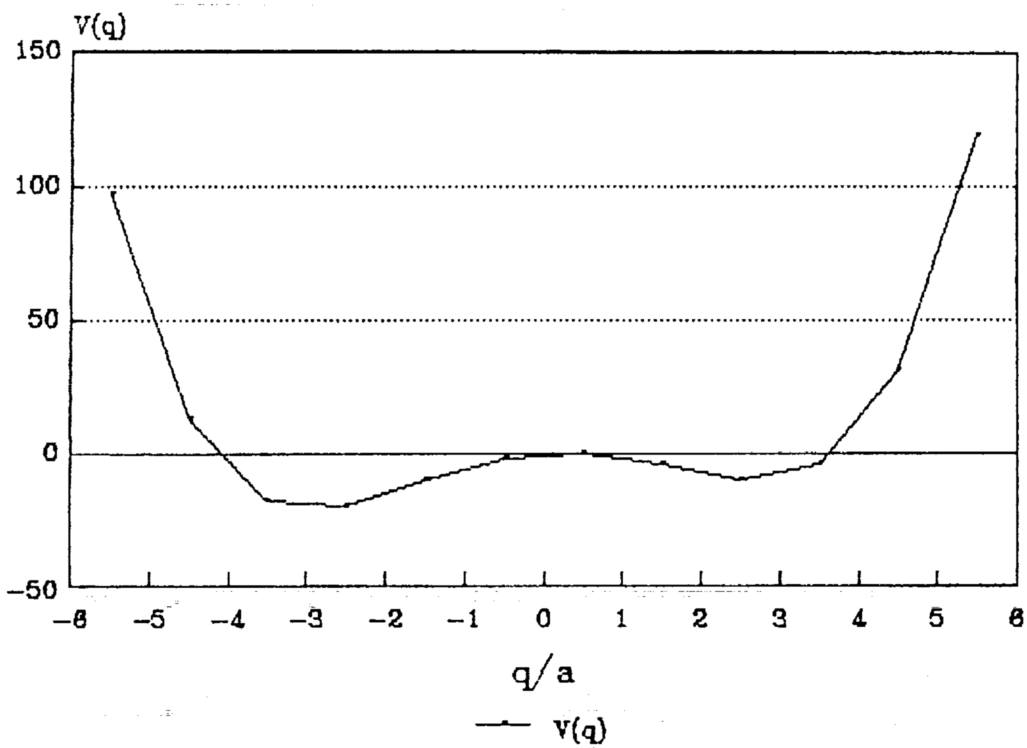

FIGURE II. ASYMMETRIC OSC POTENTIAL

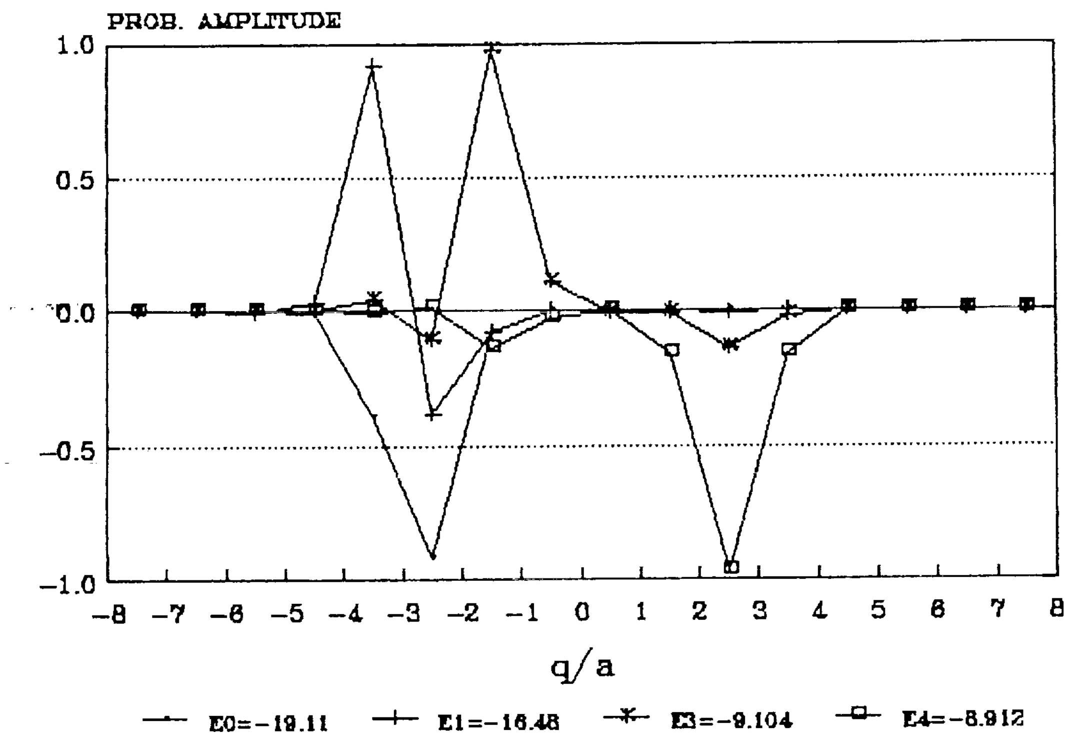

FIGURE III. ASYM OSC WAVEVECTORS (8,0)

C. The Quartic Oscillator

In the case of the quartic oscillator (F=$\omega = 0$) the choice

$$a_0 = \left(\frac{2\pi\hbar}{m\lambda^{1/2}} \right)^{\frac{1}{3}} \tag{24}$$

suffices. In this case the components of the dimensionless Hamiltonian have the form

$$\frac{H'_{Ns}}{\lambda a_0^4} = \sum_{k=-(N-1)/2}^{(N-1)/2} \left(\frac{(2\pi k)^2}{2^{2\alpha-3n+1}} + \frac{2^{4\alpha-n} r^4}{4} \right) \exp\left\{ -2\pi k \frac{(r-s)}{N} \right\}$$

The quartic oscillator is included here because it has been a frequent subject of study and its eigenvalues are numerically established. Table III illustrates the numerical convergence for the first four eigenvalues and gives the "exact" eigenvalues as numerically established by others[456] using distinct techniques.

Table III QUARTIC OSC

	$N=2, \alpha=0$	$N=4, \alpha=0$	$N=8, \alpha=0$	$N=16, \alpha=1$	"*exact*"
E_0	1.2493	.4498	.4217	.420805	.420804
E_1	1.2493	1.2760	1.5587	1.50790	1.50790
E_2	–	3.0895	2.9422	2.95880	2.95880
E_3	–	3.9157	3.8709	4.62128	4.62122

IV. Summary.

The purpose here has been to demonstrate the numerical application of the quasi-canonical quantization procedure to 1 dimensional oscillatory systems. With this application it is clear that numerical convergence occurs for each of the potentials.

The calculation procedure is computationally straightforward since the momentum matrix (8) can be conveniently calculated using well established signal processing techniques.[7] In particular, fast Fourier transform (FFT)[8] techniques allow for rapid determination of "state" vectors and quantum numbers.

The approximation procedure utilized here is based not upon the truncation of the wave functions but rather on how well the canonical commutation relation is approximated. In contrast to usual perturbation theories the number of allowed states in each order is thesame as the number of allowed positions. The convergence of this discrete quantization to a canonical one and detailed derivations of results quoted in the Section II will be discussed elsewhere. However it is useful to note two important facts about the procedure. First, the use of the discrete fourier transform (and numerical use of FFT's[8]) does not implies the periodicity of space, rather the quantization is carried out over a finite region of space. Secondly, the matrix Q_N as a $N=2^n$dimensional matrix insures not only the faster speed of the FFT's utilized but also that on the discrete scale that Q_N is an invertible matrix for which the eigenvalue zero exists only as a refinement or weak limit. Thus one should not expect numerical problems in dealing with coulomb like potentials.

Finally, with the refinement limit we note that one can get as close as one wishes to canonical quantization with discrete space, suggesting that quantum theory cannot readily distinguish between discrete and continuous space time. In addition, please note that the combination (9) and (11) allows a sequence of matrices to serve as the definition of required generalized functions, as in (14,15,16,17), somewhat in analogy to the good functions of Lighthill[9].[10]

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