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ON A LAGRANGE-HAMILTON FORMALISM DESCRIBING POSITION AND MOMENTUM UNCERTAINTIES

Dieter Schuch
Institut für Theoretische Physik
J.W. Goethe-Universität
Robert-Mayer-Str. 8-10, W-6000 Frankfurt am Main, FRG

Abstract

According to Heisenberg's uncertainty relation, in quantum mechanics it is not possible to determine simultaneously exact values for position and momentum of a material system. Calculating the mean value of the Hamiltonian operator with the aid of exact analytic Gaussian wave packet solutions, these uncertainties cause an energy contribution additional to the classical energy of the system. For the harmonic oscillator, e.g., this nonclassical energy represents the ground state energy. It will be shown that this additional energy contribution can be considered as a Hamiltonian function, if it is written in appropriate variables. With the help of the usual Lagrange-Hamilton formalism known from classical particle mechanics, but now considering this new Hamiltonian function, it is possible to obtain the equations of motion for position and momentum uncertainties.

1 Introduction

According to quantum mechanics it is in principle impossible to simultaneously determine the exact values of two canonically conjugate variables like position and momentum. These values can be given only with a finite uncertainty, a mean square deviation or fluctuation $\langle \tilde{x}^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$ and $\langle \tilde{p}^2 \rangle = \langle p^2 \rangle - \langle p \rangle^2$, where the brackets $\langle ... \rangle$ denote quantum mechanical mean values. The lower bound of these uncertainties, the minimum uncertainty product is defined by Heisenberg's uncertainty relation

$$U = \langle \tilde{x}^2 \rangle \langle \tilde{p}^2 \rangle \geqq \frac{\hbar^2}{4} . \tag{1}$$

In this paper the most simple but also most important one-dimensional problems, the free motion and the harmonic oscillator (HO) will be discussed in detail (the results for the free motion can be obtained in the limit $\omega \to 0$, where ω is the frequency of oscillation). The corresponding time-dependent Schrödinger equation (SE) (in position space),

$$i\hbar \frac{\partial}{\partial t} \Psi(x,t) = H_{op} \Psi(x,t) = \{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\} \Psi(x,t) , \tag{2}$$

has exact analytic Gaussian-shaped wave packet-type (WP) solutions Ψ(x,t). The uncertainty of position, reflecting the wave aspect, causes the finite width of this function, which can be time-dependent as it is known from the spreading of the "free-particle" WP. The particle aspect is expressed by the fact that the maximum of the WP follows the trajectory of the corresponding classical problem.

Calculating the mean value of the Hamiltonian operator H_op with the help of the Gaussian WPs to obtain the energy of the system,

$$\begin{aligned} \langle E \rangle &= \langle H_{op} \rangle = \frac{1}{2m} \langle p^2 \rangle + \frac{m}{2} \omega^2 \langle x^2 \rangle \\ &= (\frac{1}{2m} \langle p \rangle^2 + \frac{m}{2} \omega^2 \langle x \rangle^2) + (\frac{1}{2m} \langle \tilde{p^2} \rangle + \frac{m}{2} \omega^2 \langle \tilde{x}^2 \rangle) \qquad (3) \\ &= E_{cl} + \tilde{E} \; . \end{aligned}$$

the uncertainty of position and momentum causes, that in addition to the classical energy E_{cl}, a contribution $\tilde{E}$ occurs.

In classical mechanics, the (conserved) energy E_{cl} of the system is equivalent to the Hamiltonian function, $E_{cl} = H$, which also determines the dynamics of the system via the Hamiltonian equations of motion.

In this work, it will be shown that in analogy to classical particle mechanics, the additional contribution $\tilde{E}$ in (3) can be considered as Hamiltonian function for the position and momentum uncertainties. Therefore, the dynamics of these properties reflecting the (nonclassical), wave aspect, i.e. the equations of motion, can be obtained from this Hamiltonian function in exactly the same way as it is known from the formalism for classical particles.

For this purpose, $\tilde{E}$ has to be expressed in terms of appropriate variables and corresponding canonically conjugate momenta to provide the Hamiltonian $\tilde{\mathcal{H}}_L$.

2 Appropriate Variables for the Uncertainties

Using the Gaussian WP-solutions of the SE, exact analytic expressions for E_{cl} and $\tilde{E}$ can be obtained. In the case of the HO $\tilde{E}$ just represents the groundstate energy, usually given in the form $E_{GS} = \frac{1}{2}\hbar\omega$. However, there is much more information contained in $\tilde{E}$, especially connected with the dynamics of position and momentum uncertainties. In order to extract this information, the Gaussian WP used to calculate the mean values shall be given in the form

$$\Psi_L(x,t) = N(t) exp \left\{ i[y(t)\tilde{x}^2 + \frac{1}{\hbar}\langle p \rangle \tilde{x} + K(t)] \right\} , \qquad (4)$$

where $\tilde{x} = x - \langle x \rangle = x - \eta(t)$ (the explicit form of N(t) and K(t) is not relevant for the following discussion). The maximum of the WP at position x = $\langle x \rangle$ follows the classical trajectory $\eta(t)$. The WP width $\sqrt{\langle \tilde{x}^2 \rangle}$ is connected with the imaginary part y_I of the complex coefficient of $\tilde{x}^2$ in the exponent, y(t), via

$$\frac{2\hbar}{m}\, y_I = \frac{\hbar}{2m\langle\tilde{x}^2\rangle} = \frac{1}{\alpha^2(t)} . \tag{5}$$

Inserting the WP into the SE proves that $\langle x\rangle = \eta(t)$ obeys the classical Newtonian equation for a corresponding point particle,

$$\ddot{\eta} + \omega^2\, \eta = 0 . \tag{6}$$

To determine the time dependence of the WP width, the complex (quadratically) nonlinear equation of Ricatti-type,

$$\frac{2\hbar}{m}\,\dot{y} + \left(\frac{2\hbar}{m}\, y\right)^2 + \omega^2 = 0 , \tag{7}$$

has to be solved. With the help of the new variable $\alpha(t)$ introduced in Eq.(5), the complex Ricatti equation can finally be transformed into the real (nonlinear) Newton-type equation

$$\ddot{\alpha} + \omega^2\alpha = \frac{1}{\alpha^3} . \tag{8}$$

In contrast to the equation for the WP maximum, Eq.(6), the equation for the QP width, Eq.(8), contains an inverse cubic term on the rhs.

Additional insight into the dynamics of the investigated systems can be obtained by linearizing the Ricatti equation (7) with the help of

$$\frac{2\hbar}{m}\, y = \frac{\dot{\lambda}}{\lambda} , \tag{9}$$

introducing a new *complex* variable $\lambda = \hat{u} + i\hat{z} = \alpha e^{i\varphi}$, to provide the complex linear equation of motion

$$\ddot{\lambda} + \omega^2\lambda = 0 , \tag{10}$$

which has exactly the same form as Eq. (6), but now for a complex variable.

It can be shown [1-3] that in cartesian coordinates, $\hat{z}$ is directly proportional to the classical trajectory,

$$\frac{\hat{z}\alpha_0 p_0}{m} = \langle x \rangle = \eta(t) , \tag{11}$$

and in polar coordinates, the absolute value α is identical with $\alpha(\mathrm{t}) = (2\mathrm{m}\langle\tilde{x}^2\rangle/\hbar)^{\frac{1}{2}}$ from Eq. (8), and thus directly proportional to the WP width.

Furthermore, $\hat{u}$ and $\hat{z}$ (in cartesian coordinates), or α and φ (in polar coordinates), respectively, are not independent of each other, but coupled via the relation

$$\dot{\hat{z}}\hat{u} - \dot{\hat{u}}\hat{z} = \alpha^2\dot{\varphi} = 1 . \tag{12}$$

The physical meaning of this relation is that $\lambda(\mathrm{t})$ moves in the *complex* plane like a particle in a real two-dimensional plane with *conserved angular momentum.* Therefore, the $1/\alpha^3$-term in Eq. (8) represents the "centrifugal force" for this motion in the *complex* plane.

3 Lagrange and Hamilton Functions for Uncertainties

In Eq. (5) it is shown how the mean square deviation of position, $\langle\tilde{x}^2\rangle$, is connected with y_I or α (and thus λ), respectively. In a similar way the momentum uncertainty $\langle\tilde{p}^2\rangle$ is connected with y_R and y_I or $\dot{\alpha}$ and $\dot{\varphi}$ (and thus $\dot{\lambda}$, respectively, via

$$\langle\tilde{p}^2\rangle = \hbar^2\,\frac{y_R^2 + y_I^2}{2\,y_I} = \frac{\hbar m}{2}\,(\dot{\lambda}\dot{\lambda}^*) = \frac{\hbar m}{2}\,(\dot{\alpha}^2 + \alpha^2\dot{\varphi}^2) . \tag{13}$$

Therefore, the energy contribution $\tilde{E}$ can be written as

$$\tilde{E} = \frac{\hbar}{4}(\dot{\lambda}\dot{\lambda}^* + \omega^2\,\lambda\lambda^*) = \frac{\hbar}{4}\,(\dot{\alpha}^2 + \alpha^2\dot{\varphi}^2 + \omega^2\alpha^2) . \tag{14}$$

Assuming that α and φ are the required appropriate generalized coordinates, still the canonically conjugate momenta have to be determined in order to express $\tilde{E}$ in a proper Hamiltonian form. In analogy to classical mechanics, a Lagrangian function for the position and momentum uncertainties can be obtained by simply changing the sign of the potential energy contribution into minus, leading to

$$\tilde{\mathcal{L}}_L(\alpha,\varphi,\dot{\alpha},\dot{\varphi}) = \frac{\hbar}{4}\,(\dot{\alpha}^2 + \alpha^2\dot{\varphi}^2 - \omega^2\alpha^2) . \tag{15}$$

Thus, the generalized momenta are given by

$$\frac{\partial \tilde{\mathcal{L}}_L}{\partial \dot{\alpha}} = \frac{\hbar}{2}\,\dot{\alpha} \;=\; p_\alpha \tag{16}$$

$$\frac{\partial \tilde{\mathcal{L}}_L}{\partial \dot{\varphi}} = \frac{\hbar}{2}\,\alpha^2\dot{\varphi} \;=\; p_\varphi\;. \tag{17}$$

With the help of these definitions, the energy fluctuation $\tilde{E}$ can be written in the correct Hamiltonian form

$$\tilde{\mathcal{H}}_L = \frac{p_\alpha^2}{\hbar} + \frac{p_\varphi^2}{\hbar\alpha^2} + \frac{\hbar}{4}\,\omega^2\alpha^2\;. \tag{18}$$

This Hamiltonian function $\tilde{\mathcal{H}}_L$ provides the equations of motion for the variables describing the *wave* aspect in exactly the same way as the classical Hamiltonian function of particle mechanics yields the equations of motion for the variables describing the *particle* aspect.

In addition, an interesting consequence follows from Eq. (17), defining the angular momentum p_φ. As mentioned in the previous section, this is an angular momentum property connected with the motion of λ in the *complex* plane under the additional condition, that the "conservation law" $\dot{\varphi} = \frac{1}{\alpha^2}$ is fulfilled.

However, inserting this into (17) shows that the conserved angular momentum-type quantity p_φ has the constant value

$$p_\varphi = \frac{\hbar}{2}\;, \tag{19}$$

a value that usually does not describe an orbital angular momentum but the nonclassical angular momentum-type property spin!

Furthermore, it should be mentioned that the uncertainty product (1), if it is written in terms of the new coordinates and momenta, takes the form

$$U(t) = p_\varphi^2 + (\alpha p_\alpha)^2\;. \tag{20}$$

From Eq. (19) follows that $p_\varphi^2 = \hbar^2/4$, i.e. it is just the (constant) minimum uncertainty. The second term, however, represents the square at the position-momentum correlations, as

$$\langle[\tilde{x},\tilde{p}]_+\rangle \;=\; \langle\tilde{x}\tilde{p}+\tilde{p}\tilde{x}\rangle \;=\; \frac{\hbar}{2}\,\frac{\partial}{\partial t}\,(\lambda\lambda^*) = \hbar\dot{\alpha}\alpha \;=\; 2\,(\alpha p_\alpha) \tag{21}$$

is valid.
For $p_\alpha = 0$ and thus $\dot{\alpha} = 0$, i.e. the WP width is constant and no correlations between position and momentum exist.

4 Conclusions

The information on the dynamics of the considered systems contained in the time-dependent SE can also be obtained from a corresponding Newtonian equation for these systems, if a complex variable is used, where the imaginary part of this variable is proportional to the classical trajectory and the real part is uniquely connected with the imaginary part. The connecting relation expresses a kind of conservation of angular momentum for the two-dimensional motion in the complex plane.

In polar coordinates, the absolute value of the complex variable, $\alpha(t)$, is directly proportional to the WP width $\sqrt{\langle \tilde{x}^2 \rangle}$, and thus to the uncertainty $\langle \tilde{x}^2 \rangle$.

It is possible to express the difference between the mean value of the Hamiltonian operator, $\langle H_{op} \rangle$, and the classical energy, E_{cl}, in terms of the coordinates α and φ and the corresponding canonically conjugate momenta. Thus, it is possible to write $\tilde{E}$ in the form of the Hamiltonian function $\mathcal{H}_L$, where from the correct equations of motion for the "wave properties" (uncertainties) can be obtained in exactly the same way as the equations of motion for the particle properties can be obtained from the classical energy, respectively Hamiltonian function.

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