

ALTERNATIVE DESCRIPTIONS OF WAVE AND PARTICLE ASPECTS OF THE HARMONIC OSCILLATOR

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Abstract

The dynamical properties of the wave and particle aspects of the harmonic oscillator can be studied with the help of the time-dependent Schrödinger equation (SE). Especially the time-dependence of maximum and width of Gaussian wave packet solutions allow to show the evolution and connections of those two complementary aspects. The investigation of the relations between the equations describing wave and particle aspects leads to an alternative description of the considered systems. This can be achieved by means of a Newtonian equation for a complex variable in connection with a conservation law for a nonclassical angular momentum-type quantity. With the help of this complex variable it is also possible to develop a Hamiltonian formalism for the wave aspect contained in the SE, which allows to describe the dynamics of the position and momentum uncertainties. In this case the Hamiltonian function is equivalent to the difference between the mean value of the Hamiltonian operator and the classical Hamiltonian function.

1 Introduction

In wave mechanics a complex equation, the Schrödinger equation (SE), is used to describe the dynamics and energetics of the particle and wave aspects of a material system under the influence of conservative forces, e.g., the harmonic force of an undamped oscillator. In classical mechanics Newton's equation of motion is a *real* equation which is only capable of describing the particle aspect. It will be shown that it is possible to also take into account the wave aspect by changing to a *complex* Newtonian equation. However, real and imaginary parts of the new complex variable are not independent of each other, but are coupled by a well-defined relation which is connected with a conservation law for a nonclassical angular momentum-type quantity. With the help of this new complex variable it is also possible to express the groundstate energy \tilde{E} in a way that it can serve as a Hamiltonian function for the position and momentum uncertainties.

2 Dynamics of Particle and Wave Aspects

The wave mechanical equation (SE) for the harmonic oscillator (HO)

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = \left\{ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{m}{2} \omega^2 x^2 \right\} \Psi(x, t), \quad (1)$$

possesses exact analytic solutions of the form of Gaussian wave packets (WP). The dynamics of the particle aspect is reflected by the fact that the maximum of the WP follows the classical trajectory of the corresponding particle. The wave aspect is expressed by the finite width of the WP. This width can also be time-dependent. This time-dependence is closely connected with a contribution to the convective current density in the continuity equation for the (real) density function corresponding to the (complex) WP. Inserting the Gaussian WP given in the form

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

(where $\tilde{x} = x - \langle x \rangle = x - \eta(t)$ and $\langle p \rangle = m \frac{d}{dt} \langle x \rangle$ denotes the mean value of momentum p , the explicit form of $N(t)$ and $K(t)$ is not relevant for the following discussion), into the SE(1) shows that the maximum at position $\langle x \rangle = \eta(t)$ fulfills the classical Newtonian equation of motion

$$\ddot{\eta} + \omega^2 \eta = 0. \quad (3)$$

The WP width, $\sqrt{\langle \tilde{x}^2 \rangle}$ (where $\langle \tilde{x}^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$), is connected with the imaginary part of the complex coefficient of \tilde{x}^2 in the exponent, $y(t)$, via

$$\frac{2\hbar}{m} y_I = \frac{\hbar}{2m \langle \tilde{x}^2 \rangle} = \frac{1}{\alpha^2(t)}. \quad (4)$$

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

$$\frac{2\hbar}{m} \dot{y} + \left(\frac{2\hbar}{m} y \right)^2 + \omega^2 = 0 \quad (5)$$

has to be solved.

With the aid of the variable $\alpha(t)$ as defined in Eq. (4) (which is apart from a constant factor identical with the WP width), the corresponding real part turns into

$$\frac{2\hbar}{m} y_R = \frac{\dot{\alpha}}{\alpha} \quad (6)$$

and Eq. (5) yields the (real) nonlinear Newtonian equation

$$\ddot{\alpha} + \omega^2 \alpha = \frac{1}{\alpha^3} . \quad (7)$$

The only difference between this equation, determining the dynamics of the WP width, and Eq. (3) for the dynamics of the WP maximum is the inverse cubic term on the rhs of Eq. (7). In order to elucidate the meaning of this additional term, the Ricatti Eq. (5) has to be reconsidered. Using the substitution

$$\frac{2\hbar}{m} y = \frac{\dot{\lambda}}{\lambda} \quad (8)$$

with the new complex variable $\lambda = \hat{u} + i\hat{z}$, Eq. (5) can be linearized to yield the *complex* linear Newtonian equation

$$\ddot{\lambda} + \omega^2 \lambda = 0 . \quad (9)$$

This equation is formally identical with the Newtonian Eq. (3) for the WP maximum. It can be shown (e.g. by expressing the WP(2) in terms of λ or with the help of a Green-function, see [1-3]) that the imaginary part of λ is directly proportional to the classical trajectory, i.e.

$$\frac{\dot{z}\alpha_0 p_0}{m} = \langle x \rangle = \eta(t) , \quad (10)$$

(where α_0 and p_0 are the initial values of $\alpha(t)$ and $\langle p \rangle(t)$, respectively). Furthermore, in the same way it can be shown (see e.g. [1-3]) that real and imaginary parts of λ are uniquely connected via the relation

$$\dot{z}\hat{u} - \dot{u}\hat{z} = 1 . \quad (11)$$

Equation (8) for the time evolution of λ was obtained from the Ricatti Equation (5), which describes the evolution of the WP width, as shown in Eq. (7) for $\alpha(t)$. In order to show how the wave aspect is contained in λ , it shall be written in polar coordinates,

$$\lambda = \alpha e^{i\varphi} = \alpha \cos \varphi + i \alpha \sin \varphi . \quad (12)$$

Inserting this form into Eq. (8), comparison with the definitions given in Eqs. (4) and (6) shows that the quantity α in Eq. (12) denoting the absolute value of λ is identical with the quantity α denoting the WP width in Eq. (7), if the relation

$$\dot{\varphi} = \frac{1}{\alpha^2} \quad (13)$$

is fulfilled. However, the validity of Eq. (13) can easily be proven by inserting (12) into Eq. (11).

The physical meaning of Eq. (13) becomes more transparent, when the motion of $\lambda(t)$ in the *complex* plane is compared with the motion of a two-dimensional harmonic oscillator in the *real* physical space, written in polar coordinates (see e.g. [1-3]). This comparison shows that relation (13) (and thus the equivalent relation (11) in cartesian coordinates) corresponds to the *conservation of angular momentum* in real space.

Furthermore, it shows that the inverse cubic term on the rhs of Eq. (7) corresponds to a *centrifugal force* in real space.

So, it can be stated that the complex quantity $\lambda(t)$ fulfilling the Newtonian Eq. (9) contains the information about the dynamics of both particle and wave aspects of the system. Written in cartesian coordinates, the imaginary part of λ directly provides the information about the dynamics of the particle aspect, the WP maximum, written in polar coordinates, the absolute value of λ directly provides the information about the dynamics of the wave aspect, the WP width.

3 Energetics of Particle and Wave Aspects

It shall be mentioned only briefly here (for further details see e.g. [2,3]) that this new complex variable λ can also provide new information contained in the groundstate energy of the harmonic oscillator, usually only given in the form $\tilde{E} = \frac{1}{2}\hbar\omega$. The notation \tilde{E} is used to already indicate that this energy contribution is just the difference between the mean value of the Hamiltonian operator (calculated with the WP-solution (2)) and the classical energy E_{class} , respectively

$$\begin{aligned} \langle E \rangle &= \langle H \rangle = \frac{1}{2m} \langle p^2 \rangle + \frac{m}{2} \omega^2 \langle x^2 \rangle \\ &= \left(\frac{1}{2m} \langle p \rangle^2 + \frac{m}{2} \omega^2 \langle x \rangle^2 \right) + \left(\frac{1}{2m} \langle \bar{p}^2 \rangle + \frac{m}{2} \omega^2 \langle \bar{x}^2 \rangle \right) \\ &= E_{class} + \tilde{E} . \end{aligned} \quad (14)$$

In classical mechanics the energy E_{class} of the HO is identical with the classical Hamiltonian function, H_{class} , which also provides the equations of motion for the particle aspect.

Writing the difference of kinetic and potential energy uncertainties in terms of the polar coordinates of λ , i.e.

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

this quantity can be used as Lagrangian function for the position and momentum uncertainties. From $\tilde{\mathcal{L}}$ the canonically conjugate momenta to the coordinates α and φ can be obtained in the usual way and the groundstate energy can be written in the form of a Hamiltonian function that provides the equations of motion for the position and momentum uncertainties.

In this context it is interesting that the canonical angular momentum p_φ , obtained from the Lagrangian (15), is not only constant, as already mentioned in connection with Eqs. (11) and (13), but has the value

$$p_\varphi = \frac{\hbar}{2} . \quad (16)$$

Thus, the complex variable $\lambda(t)$, obeying the simple Newtonian Eq. (9), follows a path in the *complex* plane similar to the path of a particle in a two-dimensional HO-field. However, the quantity corresponding to the conserved classical angular momentum in *real* space is the quantity $p_\varphi = \hbar/2$ in *complex* space. This is rather surprising, because even in wave mechanics orbital angular momenta are integer multiples of \hbar . Half-integer multiples of \hbar are usually connected with the purely quantum mechanical property spin. Whether there are any relations between p_φ and spin shall not be further discussed in this work.

4 Conclusions

The information on the dynamics of the considered system contained in the time-dependent SE can also be obtained from a corresponding Newtonian equation for this system, 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 addition, the value of this conserved nonclassical angular momentum property is $\hbar/2$, usually only known from the quantum mechanical property spin.

With the help of this complex quantity $\lambda = \hat{u} + i\hat{z} = \alpha \exp(i\varphi)$, it is possible to obtain equations of motion for the particle aspect, $\langle x \rangle = \eta = (\alpha_0 p_0 / m) \hat{z}$, as well as for the wave aspect, $\langle x^2 \rangle = \hbar/2m \alpha^2$.

Furthermore, it is possible to express the difference between the mean value of the Hamiltonian operator and the classical energy E_{class} 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 a Hamiltonian function, wherefrom 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.

5 Acknowledgments

The author gratefully acknowledges financial support and a fellowship from the *Deutsche Forschungsgemeinschaft*.

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