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Ehrenfest's theorem and Bohm's quantum potential in a "one-dimensional box"

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Abstract

The time evolution of the mean values of the position and momentum operators for a Schrödinger particle in a one-dimensional box is reviewed. The connection of both $(d/dt)\langle X\rangle$ and $(d/dt)\langle P\rangle$ with local densities and Bohm's quantum potential is pointed out. New boundary non-local terms are obtained. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

In this Letter we are interested in the time evolution of the mean values of the position and momentum operators (Ehrenfest theorem [1]) applied to a particle in a one-dimensional box. Different approaches have been introduced [2]; however, some important aspects were not properly considered. The point is that for any quantum mechanical expression like, for example, $(d/dt)\langle A\rangle = (i/\hbar)\langle[H, A]\rangle$, in the Schrödinger picture, we are giving for granted that the involved operators have well defined domains. For a particle in a box X is a bounded operator, but H and P are unbounded, thus, we must pay attention to the domains of the involved operators.

Recently, the Ehrenfest theorem was considered showing that its usual form is not always valid [3], in particular for the X and P operators we generally have $(d/dt)\langle X\rangle \neq (i/\hbar)\langle[H, X]\rangle$ and $(d/dt)\langle P\rangle \neq (i/\hbar) \times \langle[H, P]\rangle$. Now, our aim is the connection between these results and the probability and current densities, as well as with Bohm's quantum potential [4]. In the last years, Bohm's quantum potential Q has been considered by many authors with various purposes, some of them are mentioned in Refs. [5,6], however, as far as we know, the relation between the Ehrenfest theorem and Q for a Schrödinger particle in a one-dimensional box was not considered in the literature.

2. Time evolution of the mean value of an operator

In this section some general features of the time evolution of the mean value of an operator are summarized. In the Schrödinger picture, the time derivative of the mean value of a given explicitly time independent self-adjoint operator A in the normalized state

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$\Psi = \Psi(x,t)$ is

$$\frac{d}{dt}\langle A\rangle = -\frac{2}{\hbar}\,\mathrm{Im}(H\Psi, A\Psi), \tag{1}$$

where $\Psi \in \mathrm{Dom}(A) \cap \mathrm{Dom}(H) \cap \mathrm{Ran}(H) \equiv D$, for all t ($H\Psi \equiv \mathrm{Ran}(H)$ is the range of H) [3]. In particular, when $\Psi \in D \cap \mathrm{Ran}(A)$, we obtain

$$\frac{d}{dt}\langle A\rangle = \frac{i}{\hbar}\big\langle [H, A]\big\rangle. \tag{2}$$

So, for the position and momentum operators we can write

$$\frac{d}{dt}\langle X\rangle = \frac{i}{\hbar}\big\langle [H, X]\big\rangle = \frac{1}{m}\langle P\rangle,$$
$$\frac{d}{dt}\langle P\rangle = \frac{i}{\hbar}\big\langle [H, P]\big\rangle, \tag{3}$$

where both $X\Psi$ and $P\Psi$ belong to $\mathrm{Dom}(H)$. These two equations constitute the usual Ehrenfest theorem. It is important to note that Eq. (2) cannot be obtained just by taking the mean value of the analogous evolution equation in the Heisenberg picture, unless the domain problems be considered. On the other hand, if both $X\Psi$ and $P\Psi$ do not belong to $\mathrm{Dom}(H)$, the time derivative of the mean value of the position and momentum operators must be written as

$$\frac{d}{dt}\langle X\rangle = -\frac{2}{\hbar}\,\mathrm{Im}(H\Psi, X\Psi),$$
$$\frac{d}{dt}\langle P\rangle = -\frac{2}{\hbar}\,\mathrm{Im}(H\Psi, P\Psi), \tag{4}$$

which do not require the existence of the commutators [3].

3. Operators for a particle in a box

In this section we present the position, momentum and Hamiltonian operators for a particle in a one-dimensional box in the interval $\Omega = [0, L]$. The Hilbert space of the system, on which all these operators are defined, is $\mathsf{H} = \mathsf{L}^2(\Omega)$, with scalar product denoted by $(\Psi_1, \Psi_2) = \int_0^L \overline{\Psi_1}\Psi_2\,dx$, where $\overline{\Psi}$ is the complex conjugate of Ψ. The position is a bounded and multiplicative operator and its domain is the whole space. The momentum is an unbounded derivative operator and its domain is [3,7]

$$\mathrm{Dom}(P) = \big\{\Psi \mid \Psi \in \mathsf{H},\ \text{a.c. in } \Omega,\ P\Psi \in \mathsf{H},\ \Psi \text{ fulfills } \Psi(L) = \Psi(0),\ \forall t\big\}, \tag{5}$$

where hereafter a.c. means absolutely continuous functions. As is well known, there exists a one-parameter family of boundary conditions for which P is self-adjoint [8], nevertheless, we select only the periodic boundary condition: $\Psi(L,t) = \Psi(0,t)$, since for this, the operator P transforms as a vector and the parity symmetry operation of the Hamiltonian operator $(P\cdot P)/2m$ is not spontaneously broken [7].

The Hamiltonian operator is defined by

$$H\Psi(x,t) = \left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi(x,t). \tag{6}$$

H is also unbounded and the most general domain, for which it is self-adjoint, can be written in terms of only one family of boundary conditions [3]

$$\mathrm{Dom}(H) = \Bigg\{\Psi \mid \Psi \in \mathsf{H},\ \Psi \text{ and } \Psi' \text{ a.c. in } \Omega,\ H\Psi \in \mathsf{H},\ \Psi \text{ fulfills} \begin{pmatrix} \Psi(L) - i\lambda\Psi'(L) \\ \Psi(0) + i\lambda\Psi'(0) \end{pmatrix} = U \begin{pmatrix} \Psi(L) + i\lambda\Psi'(L) \\ \Psi(0) - i\lambda\Psi'(0) \end{pmatrix},\ U^{-1} = U^{+},\ \forall t\Bigg\}. \tag{7}$$

The primes hereafter mean differentiation with respect to x, the parameter λ is inserted for dimensional reasons and the symbol $+$ denotes the adjoint of a vector or a matrix. The unitary matrix U may be written as

$$U = \begin{pmatrix} e^{i\mu}e^{i\tau}\cos\theta & e^{i\mu}e^{i\gamma}\sin\theta \\ e^{i\mu}e^{-i\gamma}\sin\theta & -e^{i\mu}e^{-i\tau}\cos\theta \end{pmatrix}$$

with $0 \leqslant \theta < \pi$, $0 \leqslant \mu, \tau, \gamma < 2\pi$. The potential $V(x)$ inside the box is bounded from below. We see that there is a four-parameter family of boundary conditions, each of which leads, for a fixed set of parameters $\theta, \mu, \tau, \gamma$, to a unitary time evolution. It can be shown that for every wavefunction $\Psi \in \mathrm{Dom}(H)$, the current density

$$j = j(x,t) \equiv \frac{-\hbar}{2im}\left(\frac{\partial\overline{\Psi}}{\partial x}\Psi - \frac{\partial\Psi}{\partial x}\overline{\Psi}\right)$$

satisfies at the walls of the box: $j(0,t) = j(L,t)$. In order to classify physically the boundary conditions it is convenient to split (7) into three subfamilies:

Family 1.

$$\begin{pmatrix} \Psi(L) \\ \lambda\Psi'(L) \end{pmatrix} = e^{i\gamma} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \Psi(0) \\ \lambda\Psi'(0) \end{pmatrix}. \tag{8}$$

Family 2.

$$\begin{pmatrix} \Psi(0) \\ \lambda\Psi'(0) \end{pmatrix} = e^{-i\gamma} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} \begin{pmatrix} \Psi(L) \\ \lambda\Psi'(L) \end{pmatrix}, \tag{9}$$

where

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \frac{1}{\sin\theta} \times \begin{pmatrix} \cos\mu + \cos\tau\cos\theta & \sin\mu - \sin\tau\cos\theta \\ -\sin\mu - \sin\tau\cos\theta & \cos\mu - \cos\tau\cos\theta \end{pmatrix}. \tag{10}$$

These two families can be considered as a single subfamily of boundary conditions, for all t. In fact, for each one of them we have $\sin\theta \neq 0$. Note that the 2×2 matrices in (8) and (9) are real and their parameters take only finite values. Moreover, $ad - bc = 1$.

Family 3.

$$\Psi(L) = -\operatorname{ctn}\left(\frac{\mu+\tau}{2}\right)\lambda\Psi'(L),$$
$$\Psi(0) = -\tan\left(\frac{\mu-\tau}{2}\right)\lambda\Psi'(0). \tag{11}$$

Note that in these cases $\sin\theta = 0 \Rightarrow \theta = 0$. Moreover, since $0 \leqslant \mu, \tau < 2\pi$, then $\operatorname{ctn}((\mu+\tau)/2)$ and $\tan((\mu-\tau)/2)$ belong to $\Re$ with $\pm\infty$. These families of boundary conditions (family $1+2$ and family 3) are similar to those studied by Kurasov, Albeverio et al. [9] for a free particle on a line with a hole (a point interaction). For this system, which is characterized in terms of boundary conditions for a Schrödinger Hamiltonian perturbed at one point, we have a similar story. In fact, we can imagine bringing the extremities of the interval $\Omega = [0, L]$ close to each other, making it looks like a circle with a hole, so our results are also applied to this system (in this case it is enough to replace $0 \to 0-$ and $L \to 0+$). There exist very localized interactions, for example, between a particle and an impurity or a local defect in a solid. For those cases, two half-lines connected by a transition point ($x = 0$) can be regarded as a simple model of point interactions. The case consisting of three half-lines whose ends are connected also has been considered in the literature (see Exner and Šeba [10]). Actually, quantum mechanics on networks (or graphs) of one-dimensional wires connected at nodes has been extensively studied [10]. In all these cases the Hilbert space for the whole system is taken to be the direct sum $\mathsf{H} = \bigoplus_{i=1}^{n} \mathsf{H}_i = \bigoplus_{i=1}^{n} \mathsf{L}^2([0,\infty))$. For a positive half-line ($[0,\infty)$) the respective Hamiltonian extensions are obtained using only one of Eqs. (11) making $L \to 0+ \equiv 0$. In this case, as is well known, $x = 0$ is always an impenetrable barrier. It is worth pointing out that the wires between two nodes may be described using some of the boundary conditions of a “particle in a box”.

Finally, we can say that the three families of boundary conditions described above represent, for all t, as well as the general boundary condition included in (7), the whole family of boundary conditions for which the Schrödinger Hamiltonian operator for a particle in a box is self-adjoint. It is worth pointing out that for the boundary conditions included in the first and second family, $\sin\theta \neq 0$, so, the current density $j = j(x,t)$ satisfies $j(0,t) = j(L,t) \neq 0$. This is a necessary condition in order to have a “free” particle in a box, i.e., in a box, but not confined to the box, which permits us to say that the walls are transparent to the current. For the boundary conditions of the third family, $\sin\theta = 0$, so, the current density satisfies $j(0,t) = j(L,t) = 0$. This is a necessary condition in order to have a confined particle in a box [3]. Thus, there exist several boundary conditions for the momentum and Hamiltonian operator in a box, however, the problem of choosing the appropriate boundary condition is certainly related to the physics of the problem under discussion.

4. Time evolution of mean values and Bohm’s quantum potential

In this section we study the time evolution of the mean value of the operators X and P in the box. Let us first consider the polar form of the wavefunction Ψ

(Madelung–de Broglie's substitution) [4,11]:

$$\Psi(x,t) = Re^{iS/\hbar}, \tag{12}$$

where $R = R(x,t)$ and $S = S(x,t)$ are real functions. Inserting (12) in the Schrödinger equation, the following equations are obtained:

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 + Q + V = 0, \tag{13}$$

$$\frac{\partial}{\partial t}\left(R^2\right) + \frac{1}{m}\frac{\partial}{\partial x}\left(R^2\frac{\partial S}{\partial x}\right) = 0, \tag{14}$$

where Q is Bohm's quantum potential

$$Q \equiv -\frac{\hbar^2}{2m}\frac{1}{R}\frac{\partial^2 R}{\partial x^2}. \tag{15}$$

Eqs. (13) and (14) are equivalent to the Schrödinger equation. As is well known, Eq. (14) is just the continuity equation. Indeed, the probability and current densities are respectively given by

$$\left|\Psi(x,t)\right|^2 = R^2$$

and

$$j(x,t) = \frac{1}{m}R^2\frac{\partial S}{\partial x} \equiv R^2 v,$$

where v is the Bohmian velocity or "velocity field". In the classical limit ($\hbar \to 0$), the function $S(x,t)$ becomes the action of the classical Hamilton–Jacobi equation. Because of its close resemblance with this equation, Eq. (13) is called the quantum Hamilton–Jacobi equation.

For a particle in a box, let us insert into $(d/dt)\langle X\rangle$ in (4) the polar form of the wavefunction, then,

$$\frac{d}{dt}\langle X\rangle = -\frac{2}{\hbar}\,\mathrm{Im}(H\Psi, X\Psi) = \int_0^L \frac{\partial}{\partial t}\left(R^2\right)x\,dx. \tag{16}$$

Using Eq. (14), one obtains

$$\frac{d}{dt}\langle X\rangle = \left(-R^2 x v\right)\Big|_0^L + \langle v\rangle. \tag{17}$$

The boundary term can also be written as

$$\left(-R^2 x v\right)\Big|_0^L = -Lj(0,t).$$

For all boundary conditions included in family $1+2$, this term does not vanish because $j(0,t) = j(L,t) \neq 0$. In particular, for a "free" particle, i.e., with periodic boundary condition, one has

$$\frac{d}{dt}\langle X\rangle = -Lj(0,t) + \langle v\rangle.$$

For a confined particle, that is, for all boundary conditions included in family 3,

$$\frac{d}{dt}\langle X\rangle = \langle v\rangle$$

because $j(0,t) = j(L,t) = 0$.

Analogously,

$$\frac{d}{dt}\langle P\rangle = -\frac{2}{\hbar}\,\mathrm{Im}(H\Psi, P\Psi) = \int_0^L \left[\frac{\partial}{\partial t}\left(R^2\right)\frac{\partial S}{\partial x} - \frac{\partial}{\partial x}\left(R^2\right)\frac{\partial S}{\partial t}\right]dx. \tag{18}$$

Using again Eqs. (13) and (14), we have

$$\frac{d}{dt}\langle P\rangle = \left[-R^2\left(\frac{m}{2}v^2 - V - Q\right)\right]\Bigg|_0^L - \left\langle\frac{dV}{dx}\right\rangle - \left\langle\frac{\partial Q}{\partial x}\right\rangle. \tag{19}$$

When a bounded potential is present inside the box, which satisfies $V(0) = V(L)$, it can be shown that the boundary term in (19) vanishes. In fact, since $\Psi(x,t) \in \mathrm{Dom}(P)$, then $R(0,t) = R(L,t)$, $S(0,t) = S(L,t) + 2\pi n$, $n = 0, \pm1, \pm2, \ldots.$ Moreover, if $V(0) = V(L)$ and $H\Psi(x,t) \in \mathrm{Dom}(P)$, then

$$\left(\frac{\partial^2\Psi}{\partial x^2}\right)(0,t) = \left(\frac{\partial^2\Psi}{\partial x^2}\right)(L,t). \tag{20}$$

Likewise, $\Psi(x,t) \in \mathrm{Dom}(H) \Rightarrow j(0,t) = j(L,t)$, then $(\partial S/\partial x)(0,t) = (\partial S/\partial x)(L,t)$, because $R^2(0,t) = R^2(L,t)$. Finally, substituting $\Psi(x,t) = Re^{iS/\hbar}$ in (20) and using all these conditions, we obtain

$$\left[-R^2\left(\frac{m}{2}v^2 - V - Q\right)\right]\Bigg|_0^L = 0 \tag{21}$$

with

$$v^2 = \frac{1}{m^2}\left(\frac{\partial S}{\partial x}\right)^2$$

and

$$R^2 Q = -\frac{\hbar^2}{2m}R\frac{\partial^2 R}{\partial x^2}.$$

So, Eq. (19) can always be written as

$$\frac{d}{dt}\langle P\rangle = -\left\langle\frac{dV}{dx}\right\rangle - \left\langle\frac{\partial Q}{\partial x}\right\rangle. \tag{22}$$

It is worth pointing out that the one-dimensional Schrödinger particle does not have spin, however, there is still content for the Bohm's quantum potential, in contrast with what is claimed in [6] where the existence of Q was strictly related to the spin of the particle.

Then, for a free particle in a box (i.e., $V(x) = 0$) the time evolutions of the mean values of the operators X and P can be obtained from the equations

$$\frac{d}{dt}\langle X\rangle = -Lj(0,t) + \langle v\rangle,$$
$$\frac{d}{dt}\langle P\rangle = -\left\langle\frac{\partial Q}{\partial x}\right\rangle. \tag{23}$$

In summary, the right-hand sides of the time evolutions of $\langle X\rangle$ and $\langle P\rangle$ can be physically understood as mean values of velocities or forces. In this way, we have recovered the true sense of the original Ehrenfest theorem.

As follows, by considering two examples of wavefunctions $\Psi(x,t)$ which are simple linear combinations of stationary states for their respective simple boundary conditions (with the restrictions obtained in Section 2), relations (24) are verified.

5. Two examples

Among the boundary conditions satisfying $j(0,t) = j(L,t) \neq 0$, we have the periodic condition (this boundary condition is obtained making $\theta = \pi/2$, $\mu = \gamma = 0, \pi$ in the matrix U in domain (7))

$$\Psi(0) = \Psi(L) \neq 0, \qquad \Psi'(0) = \Psi'(L) \neq 0.$$

In this case the particle in a box is "free" (i.e., at the box, but not confined to the box) if the domain of the Hamiltonian operator consists of functions satisfying these boundary conditions. The Hamiltonian $(P\cdot P)/2m$ is the kinetic energy, being this operator a function of the momentum operator in a box [3].

Since the wavefunctions $\Psi(x,t)$ may be expanded in terms of the Hamiltonian eigenfunctions $\psi_j(x)$,

$$\Psi(x,t) = \sum_j c_j\psi_j(x)e^{-i(E_j/\hbar)t},$$

we write here the corresponding eigenfunctions and eigenvalues:

$$\psi_n(x) = \frac{1}{\sqrt{L}}e^{i(2n\pi/L)x},$$
$$E_n = \frac{\hbar^2}{2m}\left(\frac{2n\pi}{L}\right)^2, \quad n = 0, \pm1, \pm2, \ldots,$$

where

$$\psi_n(x) \in \mathrm{Dom}(X)\cap\mathrm{Dom}(H),$$
$$(H\psi_n)(x) \in \mathrm{Dom}(X), \quad \forall n,$$
$$\psi_n(x) \in \mathrm{Dom}(P)\cap\mathrm{Dom}(H),$$
$$(H\psi_n)(x) \in \mathrm{Dom}(P), \quad \forall n,$$

and

$$(P\psi_n)(x) \in \mathrm{Dom}(H), \quad \forall n \neq 0,$$

but

$$(X\psi_n)(x) \notin \mathrm{Dom}(H), \quad \forall n.$$

(Note that the ground-state eigenfunction $\psi_0(x) = 1/\sqrt{L}$ does not verify the periodic condition imposed upon the derivative, in fact, $(\psi_0)'(0) = (\psi_0)'(L) = 0$. In this case the probability current is null at the box.)

Without loss of generality, let us choose a linear combination of the eigenfunctions ψ_1 and ψ_2,

$$\Psi(x,t) = \frac{1}{\sqrt{2}}\left[\psi_1(x)e^{-i(E_1/\hbar)t} + \psi_2(x)e^{-i(E_2/\hbar)t}\right].$$

Now it is important to note that

$$\Psi(0,t) = \Psi(L,t) \neq 0,$$
$$\left(\frac{\partial\Psi}{\partial x}\right)(0,t) = \left(\frac{\partial\Psi}{\partial x}\right)(L,t) \neq 0$$
$$\Rightarrow \quad \Psi(x,t) \in \mathrm{Dom}(P)\cap\mathrm{Dom}(H),$$
$$\left(\frac{\partial^2\Psi}{\partial x^2}\right)(0,t) = \left(\frac{\partial^2\Psi}{\partial x^2}\right)(L,t) \neq 0$$
$$\Rightarrow \quad (H\Psi)(x,t) \in \mathrm{Dom}(P),$$
$$0 = (x\Psi)(0,t) \neq (x\Psi)(L,t) \neq 0$$
$$\Rightarrow \quad (X\Psi)(x,t) \notin \mathrm{Dom}(H),$$
$$\left(\frac{\partial\Psi}{\partial x}\right)(0,t) = \left(\frac{\partial\Psi}{\partial x}\right)(L,t) \neq 0$$
$$\Rightarrow \quad (P\Psi)(x,t) \in \mathrm{Dom}(H),$$

then, for the position operator,

$$\frac{d}{dt}\langle X\rangle = -\frac{2}{\hbar}\,\mathrm{Im}(H\Psi, X\Psi) = -Lj(0,t) + \langle v\rangle = -\frac{3\pi\hbar}{mL}\cos(\omega_{21}t) \neq \frac{1}{m}\langle P\rangle,$$

where

$$\omega_{21} \equiv \frac{E_2 - E_1}{\hbar} = \frac{6\hbar\pi^2}{mL^2},$$

$$-Lj(0,t) = -\frac{3\pi\hbar}{mL} - \frac{3\pi\hbar}{mL}\cos(\omega_{21}t)$$

and

$$\langle v\rangle = \frac{1}{m}\langle P\rangle = \frac{3\pi\hbar}{mL}.$$

Similarly, for the momentum operator,

$$\frac{d}{dt}\langle P\rangle = -\frac{2}{\hbar}\,\mathrm{Im}(H\Psi, P\Psi) = \frac{i}{\hbar}\big\langle [H,P]\big\rangle = -\left\langle \frac{\partial Q}{\partial x}\right\rangle = 0,$$

so, the quantum force vanishes. It is worth mentioning that this result is independent of the particular linear combination chose for $\Psi(x,t)$, provided it verifies the periodic boundary condition.

Among the boundary conditions satisfying $j(0,t) = j(L,t) = 0$, we choose the Dirichlet boundary condition (this boundary condition is obtained making $\theta = 0$, $\{\mu = \tau\} = \pi/2, 3\pi/2$ in the matrix U in domain (7))

$$\Psi(0) = \Psi(L) = 0.$$

In this case the particle is confined to the box. The Hamiltonian operator with this boundary condition is $(1/2m)P^2$, but P^2 is not defined as $P \cdot P$ [3,12]. We write here the corresponding eigenfunctions and eigenvalues:

$$\psi_N(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{N\pi}{L}x\right),$$

$$E_N = \frac{\hbar^2}{2m}\left(\frac{N\pi}{L}\right)^2, \quad N = 1,2,3,\ldots,$$

where

$$\psi_N(x) \in \mathrm{Dom}(X) \cap \mathrm{Dom}(H),$$
$$(H\psi_N)(x) \in \mathrm{Dom}(X), \quad \forall N,$$
$$\psi_N(x) \in \mathrm{Dom}(P) \cap \mathrm{Dom}(H),$$
$$(H\psi_N)(x) \in \mathrm{Dom}(P), \quad \forall N,$$

and

$$(X\psi_N)(x) \in \mathrm{Dom}(H), \quad \forall N,$$

but

$$(P\psi_N)(x) \notin \mathrm{Dom}(H), \quad \forall N.$$

Let us also choose a linear combination of the eigenfunctions ψ_1 and ψ_2 corresponding to this boundary condition,

$$\Psi(x,t) = \frac{1}{\sqrt{2}}\left[\psi_1(x)e^{-i(E_1/\hbar)t} + \psi_2(x)e^{-i(E_2/\hbar)t}\right].$$

Now we see that

$$\Psi(0,t) = \Psi(L,t) = 0 \quad \Rightarrow \quad \Psi(x,t) \in \mathrm{Dom}(P) \cap \mathrm{Dom}(H),$$

$$\left(\frac{\partial^2\Psi}{\partial x^2}\right)(0,t) = \left(\frac{\partial^2\Psi}{\partial x^2}\right)(L,t) = 0 \quad \Rightarrow \quad (H\Psi)(x,t) \in \mathrm{Dom}(P),$$

$$(x\Psi)(0,t) = (x\Psi)(L,t) = 0 \quad \Rightarrow \quad (X\Psi)(x,t) \in \mathrm{Dom}(H),$$

$$0 \neq \left(\frac{\partial\Psi}{\partial x}\right)(0,t) \neq \left(\frac{\partial\Psi}{\partial x}\right)(L,t) \neq 0 \quad \Rightarrow \quad (P\Psi)(x,t) \notin \mathrm{Dom}(H),$$

then,

$$\frac{d}{dt}\langle X\rangle = -\frac{2}{\hbar}\,\mathrm{Im}(H\Psi, X\Psi) = \frac{i}{\hbar}\big\langle [H,X]\big\rangle = \langle v\rangle = \frac{1}{m}\langle P\rangle = \frac{8\hbar}{3mL}\sin(\omega_{21}t),$$

where

$$\omega_{21} \equiv \frac{E_2 - E_1}{\hbar} = \frac{3\hbar\pi^2}{2mL^2}.$$

Analogously,

$$\frac{d}{dt}\langle P\rangle = -\frac{2}{\hbar}\,\mathrm{Im}(H\Psi, P\Psi) = -\left\langle \frac{\partial Q}{\partial x}\right\rangle = \frac{8E_1}{L}\cos(\omega_{21}t),$$

so, for this boundary condition the quantum force does not vanish, in spite of $V = 0$!

6. Conclusions

The time evolution of the mean values of the position and momentum operators for a Schrödinger particle in a one-dimensional box has been reviewed. Some restrictions on the circumstances in which these time evolutions hold as they are usually written in the literature have been found. In general, for any observable A (being both H and A self-adjoint operators) the relation $(d/dt)\langle A\rangle = (i/\hbar)\langle [H, A]\rangle$ is only verified when $A\Psi \in \mathrm{Dom}(H)$. Otherwise, if $A\Psi \notin \mathrm{Dom}(H)$ we must write $(d/dt)\langle A\rangle = -(2/\hbar)\,\mathrm{Im}(H\Psi, A\Psi)$.

We have studied the connection between the time derivatives $(d/dt)\langle X\rangle$ and $(d/dt)\langle P\rangle$ with the probability and current densities and Bohm's quantum potential for a particle in a one-dimensional box. A new boundary non-local term for $(d/dt)\langle X\rangle$ was obtained:

$$\frac{d}{dt}\langle X\rangle = -\frac{2}{\hbar}\,\mathrm{Im}(H\Psi, X\Psi) = -Lj(0,t) + \langle v\rangle, \quad (24)$$

where $\Psi \in \mathrm{Dom}(X) \cap \mathrm{Dom}(H)$ and $H\Psi \in \mathrm{Dom}(X)$.

By calculating $(d/dt)\langle P\rangle$, a term which depends on the gradient of Q, was identified:

$$\frac{d}{dt}\langle P\rangle = -\frac{2}{\hbar}\,\mathrm{Im}(H\Psi, P\Psi) = -\left\langle \frac{dV}{dx}\right\rangle - \left\langle \frac{\partial Q}{\partial x}\right\rangle, \quad (25)$$

where $\Psi \in \mathrm{Dom}(P) \cap \mathrm{Dom}(H)$ and $H\Psi \in \mathrm{Dom}(P)$.

If $X\Psi \in \mathrm{Dom}(H)$ then (24) may be written as

$$\frac{d}{dt}\langle X\rangle = \frac{i}{\hbar}\big\langle [H, X]\big\rangle, \quad (26)$$

where the term $(i/\hbar)\langle [H, X]\rangle$ is not necessarily equal to $(1/m)\langle P\rangle$ because the function Ψ in (26) does not necessarily belongs to $\mathrm{Dom}(P)$.

If, in addition, $P\Psi \in \mathrm{Dom}(H)$ then (25) can also be written as

$$\frac{d}{dt}\langle P\rangle = \frac{i}{\hbar}\big\langle [H, P]\big\rangle = -\left\langle \frac{dV}{dx}\right\rangle, \quad (27)$$

which implies that $\langle \partial Q/\partial x\rangle = 0$ (in this last case we can write $(i/\hbar)\langle [H, X]\rangle = (1/m)\langle P\rangle$, since the validity of (26) is supposed).

In the case of a confined particle in a box with $V(x) = 0$, with Dirichlet boundary condition, by having recourse to Bohm's quantum potential the familiar quasiclassical interpretation of the Ehrenfest theorem was recovered:

$$\frac{d}{dt}\langle P\rangle = -\left\langle \frac{\partial Q}{\partial x}\right\rangle.$$

We have examined this problem without having recourse to the heuristic procedure of taking limits of a finite potential at the walls of the box, which yields only the Dirichlet boundary condition. Actually, our procedure can be applied to any of the infinite boundary conditions.

Obviously, we may conclude that a bounded classically free motion (with $V(x) = 0$) is not in general quantum mechanically free [13]. In fact, even distant features of the boundary can profoundly affect the particle movement in a non-local way through the gradients of the wavefunction at the boundary.

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