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On time derivatives for $\langle\hat{x}\rangle$ and $\langle\hat{p}\rangle$: formal 1D calculations

(Sobre as derivadas com respeito ao tempo para $\langle\hat{x}\rangle$ e $\langle\hat{p}\rangle$: cálculos formais em 1D)

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We present formal 1D calculations of the time derivatives of the mean values of the position ($\hat{x}$) and momentum ($\hat{p}$) operators in the coordinate representation. We call these calculations formal because we do not care for the appropriate class of functions on which the involved (self-adjoint) operators and some of its products must act. Throughout the paper, we examine and discuss in detail the conditions under which two pairs of relations involving these derivatives (which have been previously published) can be formally equivalent. We show that the boundary terms present in $d\langle\hat{x}\rangle/dt$ and $d\langle\hat{p}\rangle/dt$ can be written so that they only depend on the values taken there by the probability density, its spatial derivative, the probability current density and the external potential $V = V(x)$. We also show that $d\langle\hat{p}\rangle/dt$ is equal to $-\langle dV/dx\rangle + \langle f_Q\rangle$ plus a boundary term ($f_Q = -\partial Q/\partial x$ is the quantum force and Q is the Bohm's quantum potential). We verify that $\langle f_Q\rangle$ is simply obtained by evaluating a certain quantity on each end of the interval containing the particle and by subtracting the two results. That quantity is precisely proportional to the integrand of the so-called Fisher information in some particular cases. We have noted that f_Q has a significant role in situations in which the particle is confined to a region, even if V is zero inside that region.
Keywords: quantum mechanics, Schrödinger equation, probability density, probability density current, Bohm's quantum potential, quantum force.

Apresentamos cálculos formais em 1D das derivadas com respeito ao tempo dos valores médios dos operadores da posição ($\hat{x}$) e do momento linear ($\hat{p}$) na representação de coordenadas. Chamamos esses cálculos formais porque não nos preocupamos com o tipo apropriado de funções sobre as quais devem atuar os operadores (auto-adjuntos) envolvidos e alguns de seus produtos. Ao longo do artigo, examinamos e discutimos em detalhe as condições em que dois pares de relações que envolvem essas derivadas (que foram previamente publicadas) podem ser formalmente equivalentes. Mostramos que os termos de fronteira presentes em $d\langle\hat{x}\rangle/dt$ e $d\langle\hat{p}\rangle/dt$ podem ser escritos de modo que eles só dependem dos valores aí tomados pela densidade de probabilidade, sua derivada espacial, a densidade de corrente de probabilidade e do potencial externo $V = V(x)$. Também mostramos que $d\langle\hat{p}\rangle/dt$ é igual a $-\langle dV/dx\rangle + \langle f_Q\rangle$ mais um termo de fronteira ($f_Q = -\partial Q/\partial x$ é a força quântica e Q é o potencial quântico de Bohm). Verificamos que $\langle f_Q\rangle$ é obtido simplesmente através do cálculo de uma certa quantidade em cada extremidade do intervalo contendo a partícula e subtraindo os dois resultados. Em alguns casos particulares essa quantidade é justamente proporcional ao integrando da assim chamada informação de Fisher. Notamos que f_Q tem um papel significativo em situações em que a partícula é confinada a uma região, mesmo se V é zero dentro dessa região.
Palavras-chave: mecânica quântica, equação de Schrödinger, densidade de probabilidade, densidade de corrente de probabilidade, potencial quântico de Bohm, força quântica.

1. Introduction

Almost any book on quantum mechanics states that the mean values of the position and momentum operators ($\langle\hat{x}\rangle_t$ and $\langle\hat{p}\rangle_t$) satisfy, in a certain sense, the same equations of motion that the classical position and momentum ($x = x(t)$ and $p = p(t)$) satisfy. This result, which establishes a clear correspondence between the classical and quantum dynamics is the Ehrenfest theorem [1, 2]:

$$\frac{d}{dt}\langle\hat{x}\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{x}]\rangle = \frac{1}{m}\langle\hat{p}\rangle, \tag{1}$$

$$\frac{d}{dt}\langle\hat{p}\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{p}]\rangle = \langle\hat{f}\rangle. \tag{2}$$

Note that Eq. (2) contains the average value of the external classical force operator $\hat{f} = f(x) = -dV/dx$,

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rather than the own force evaluated at $x = \langle \hat{x} \rangle$. As a result, we are clarifying the statement preceding Eq. (1).

When trying to prove Ehrenfest's theorem in a rigorous way, the difficulty arises that each of the operators involved ($\hat{x}$, $\hat{p}$ and $\hat{H}$, which must be preferably self-adjoint) has its own domain, and some plausible common domain must be found in which Eq. (1) and/or Eq. (2) are/is valid, which is a non-trivial and complicated matter. To review some of the difficulties that may arise, as well as certain aspects of these domains, Refs. [3–6] can be consulted (Ref. [4], which was recently discovered by the present author, is especially important). For a rigorous mathematical derivation of the Ehrenfest equations (which does not use overly stringent assumptions), see Ref. [7]. For a more general (and rigorous) derivation, see Ref. [8]. For a nice treatment of this theorem (specifically, for the problem of a particle-in-a-box) that is based on the use of the classical force operator for a particle in a finite square well potential, which then becomes infinitely deep (effectively confining the particle to a box), see Ref. [9]. For a study of the force exerted by the walls of an infinite square well potential, and the Ehrenfest relations between expectation values as related to wave packet revivals and fractional revivals, see Ref. [10].

The usual formal (or heuristic) demonstration in textbooks of Eqs. (1) and (2) in the coordinate representation with $x \in (-\infty, +\infty)$ appears to have no problem; however, it is known that the quantities $\langle \hat{x} \rangle$ and $\langle \hat{p} \rangle$ with $x \in \Omega = [a, b]$ (where Ω is a finite interval) do not always obey the Ehrenfest theorem [3, 6]. This problem occurs because boundary terms that are not necessarily zero arise in the formal calculation of the time derivatives of $\langle \hat{x} \rangle$ and $\langle \hat{p} \rangle$. To verify this result in this article, we carefully reexamine the formal traditional approach to the Ehrenfest theorem in the coordinate representation from the beginning. Hence, we do not consider the domains of the involved (self-adjoint) operators. Specifically, in this article, we do not care for the appropriate class of functions on which these operators and some of its products must act. In our study, the notion of self-adjointness of an operator (or strict self-adjointness) is essentially replaced by the hermiticity (or formal self-adjointness), which is known to be less restrictive. We believe that a formal study of this problem alone is worthy and pertinent; in fact, the strict considerations related to the domains of the involved operators and their compositions seem to be too demanding. In our paper, we also examine and discuss in detail the conditions under which two pairs of relations involving $d\langle \hat{x} \rangle/dt$ and $d\langle \hat{p} \rangle/dt$ (which were published in Refs. [5, 6]) can be formally equivalent.

We start with the position and momentum operators, $\hat{x} = x$ and $\hat{p} = -i\hbar\partial/\partial x$, for a non-relativistic quantum particle moving in the region $x \in \Omega$ (which may be finite or infinite). The inner product for the functions $\Psi = \Psi(x, t)$ and $\Phi = \Phi(x, t)$ (belonging at least to the Hilbert space $\mathcal{L}^2(\Omega)$, and on which $\hat{x}$ and $\hat{p}$ act) is $\langle \Psi, \Phi \rangle = \int_\Omega \bar{\Psi}\Phi$, where the bar represents complex conjugation. The corresponding mean values of these operators in the (complex) normalized state $\Psi = \Psi(x, t)$ ($\|\Psi\|^2 \equiv \langle \Psi, \Psi \rangle = 1$) are as follows

$$\langle \hat{x} \rangle \equiv \langle \Psi, \hat{x}\Psi \rangle = \int_\Omega dx\, x\, \bar{\Psi}\Psi, \tag{3}$$

$$\langle \hat{p} \rangle \equiv \langle \Psi, \hat{p}\Psi \rangle = -i\hbar \int_\Omega dx\, \bar{\Psi} \frac{\partial \Psi}{\partial x}. \tag{4}$$

The operator $\hat{x}$ is hermitian because it automatically satisfies the following relation

$$\langle \Psi, \hat{x}\Phi \rangle - \langle \hat{x}\Psi, \Phi \rangle = 0, \tag{5}$$

where Ψ and Φ are functions belonging to $\mathcal{L}^2(\Omega)$. The time derivative of expressions (3) and (4) leads us to the following relations

$$\frac{d}{dt} \langle \hat{x} \rangle = \int_\Omega dx\, x \frac{\partial}{\partial t} \left(\bar{\Psi}\Psi\right) = \int_\Omega dx\, x \left(\frac{\partial \bar{\Psi}}{\partial t}\Psi + \bar{\Psi}\frac{\partial \Psi}{\partial t} \right) \tag{6}$$

and

$$\frac{d}{dt} \langle \hat{p} \rangle = -i\hbar \int_\Omega dx \frac{\partial}{\partial t} \left(\bar{\Psi} \frac{\partial \Psi}{\partial x} \right)$$
$$= -i\hbar \int_\Omega dx \left[\frac{\partial \bar{\Psi}}{\partial t}\frac{\partial \Psi}{\partial x} + \bar{\Psi}\frac{\partial}{\partial x}\left(\frac{\partial \Psi}{\partial t}\right) \right]. \tag{7}$$

In the last expression, we have used the commutativity of the operators $\partial/\partial x$ and $\partial/\partial t$.

In non-relativistic quantum mechanics, the wave function Ψ evolves in time according to the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\Psi = \hat{H}\Psi = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V \right)\Psi, \tag{8}$$

where $\hat{H}$ is the Hamiltonian operator of the system and $V = V(x)$ is the (real) external classical potential. By substituting in Eqs. (6) and (7) the time derivatives of Ψ and $\bar{\Psi}$ (which are obtained from Eq. (8) and its complex conjugate), we obtain $d\langle \hat{x} \rangle/dt$ and $d\langle \hat{p} \rangle/dt$. As will be discussed in the next two sections, these derivatives always have terms that are evaluated at the ends of the interval Ω. However, if these derivatives must be real-valued, certain mathematical conditions (which are, of course, physically justified) should be imposed on the boundary terms. We will show that these boundary terms can be written so that they can only depend on the values taken by the probability density, its spatial derivative, the probability current density and the external potential V at the boundary.

2. Time derivatives for $\langle \hat{x} \rangle$

For example, the time derivative of the average value of $\hat{x}$ specifically depends on the values taken by the probability density and the probability current density in these extremes. In fact, the following result can be formally proven (see formula (A.1) in Ref. [5])

$$\frac{d}{dt}\langle \hat{x} \rangle = \left(-xj + i\frac{\hbar}{2m}\rho \right)\Big|_a^b + \frac{i}{\hbar}\langle [\hat{H}, \hat{x}] \rangle \tag{9}$$

where we use the notation $f|_a^b = f(b,t) - f(a,t)$ here and in further discussion. The function $j = j(x,t)$ is the probability current density

$$j = \frac{\hbar}{m}\,\mathrm{Im}\left(\bar{\Psi}\frac{\partial \Psi}{\partial x} \right) = \frac{i\hbar}{2m}\left(\frac{\partial \bar{\Psi}}{\partial x}\Psi - \bar{\Psi}\frac{\partial \Psi}{\partial x} \right), \tag{10}$$

and $\rho = \rho(x,t)$ is the probability density

$$\rho = \bar{\Psi}\Psi. \tag{11}$$

These two real quantities (which are sometimes called "local observables") can be integrated on the region of interest, and each of these integrals is essentially the average value of some operator. Indeed, the integral of j is

$$\begin{aligned}\int_a^b dx\, j &= \frac{i\hbar}{2m}\int_\Omega dx \left(\frac{\partial \bar{\Psi}}{\partial x}\Psi - \bar{\Psi}\frac{\partial \Psi}{\partial x} \right) \\ &= \frac{i\hbar}{2m}\int_\Omega dx \left[\frac{\partial}{\partial x}\left(\bar{\Psi}\Psi \right) - 2\bar{\Psi}\frac{\partial \Psi}{\partial x} \right] \\ &= \frac{i\hbar}{2m}\,\rho|_a^b + \frac{1}{m}\int_\Omega dx\, \bar{\Psi}(-i\hbar)\frac{\partial}{\partial x}\Psi.\end{aligned}$$

The integral on the right-hand side in this last expression is precisely the average value of the operator $\hat{p} = -i\hbar\partial/\partial x$ (see formula (4)). Finally, we can write

$$\int_\Omega dx\, j = \frac{i\hbar}{2m}\,\rho|_a^b + \frac{1}{m}\langle \hat{p} \rangle. \tag{12}$$

The integral of ρ (which is a finite number only if the probability density is calculated for a state $\Psi \in \mathcal{L}^2(\Omega)$) is precisely the mean value of the identity operator $\hat{1} = \int_\Omega dx \mid x \rangle\langle x \mid$.

It is important to note that the operator $\hat{p}$ satisfies the relation

$$\langle \Psi, \hat{p}\Phi \rangle - \langle \hat{p}\Psi, \Phi \rangle = -i\hbar\, \bar{\Psi}\Phi\big|_a^b, \tag{13}$$

for the functions Ψ and Φ belonging to $\mathcal{L}^2(\Omega)$. If the boundary conditions imposed on Ψ and Φ lead to the cancellation of the term evaluated at the endpoints of the interval Ω, we can write the relation as $\langle \Psi, \hat{p}\Phi \rangle = \langle \hat{p}\Psi, \Phi \rangle$. In this case, $\hat{p}$ is a hermitian operator. If we make $\Psi = \Phi$ in this last expression and Eq. (13), we obtain the following condition (see formula (11))

$$\rho|_a^b = 0. \tag{14}$$

Moreover, $\langle \Psi, \hat{p}\Psi \rangle = \langle \hat{p}\Psi, \Psi \rangle = \overline{\langle \Psi, \hat{p}\Psi \rangle} \Rightarrow \mathrm{Im}\,\langle \Psi, \hat{p}\Psi \rangle = 0$, *i.e.*, $\langle \hat{p} \rangle \in \mathbb{R}$. These last two results are consistent with Eq. (12).

Formula (9) was obtained from the following formal relation (formula (11) in Ref. [5] with $\hat{A} = \hat{x}$):

$$\begin{aligned}\frac{d}{dt}\langle \hat{x} \rangle &= \frac{i}{\hbar}\left(\langle \hat{H}\Psi, \hat{x}\Psi \rangle - \langle \Psi, \hat{x}\hat{H}\Psi \rangle \right) \\ &= \frac{i}{\hbar}\left(\langle \hat{H}\Psi, \hat{x}\Psi \rangle - \langle \Psi, \hat{H}\hat{x}\Psi \rangle \right) + \frac{i}{\hbar}\langle [\hat{H}, \hat{x}] \rangle.\end{aligned} \tag{15}$$

In the case where $\hat{x} = x$ and $\hat{H} = i\hbar\partial/\partial t$, this equation is precisely Eq. (6) (compare the first equality in Eq. (15) with Eq. (6)). To check Eq. (9), formula (15) can be developed by first calculating the following two scalar products:

$$\langle \hat{H}\Psi, \hat{x}\Psi \rangle = -\frac{\hbar^2}{2m}\int_\Omega dx\, x\, \frac{\partial^2 \bar{\Psi}}{\partial x^2}\Psi + \int_\Omega dx\, x\, V\, \bar{\Psi}\Psi,$$

$$\langle \Psi, \hat{H}\hat{x}\Psi \rangle = \langle \hat{H}\hat{x} \rangle = -\frac{\hbar^2}{2m}\int_\Omega dx\, \bar{\Psi}\frac{\partial^2}{\partial x^2}(x\Psi) + \int_\Omega dx\, x\, V\, \bar{\Psi}\Psi.$$

Before subtracting these two expressions, we develop the first integral in $\langle \Psi, \hat{H}\hat{x}\Psi \rangle$. Then, we use the relation

$$\frac{\partial^2 \bar{\Psi}}{\partial x^2}\Psi - \bar{\Psi}\frac{\partial^2 \Psi}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial \bar{\Psi}}{\partial x}\Psi - \bar{\Psi}\frac{\partial \Psi}{\partial x} \right),$$

and the definitions of the probability current density (Eq. (10)) and the probability density (Eq. (11)). After identifying the terms that depend on $\partial(xj)/\partial x$ and $\partial\rho/\partial x$, we obtain the following result

$$\langle \hat{H}\Psi, \hat{x}\Psi \rangle - \langle \Psi, \hat{H}\hat{x}\Psi \rangle = \left(i\hbar\, xj + \frac{\hbar^2}{2m}\rho \right)\Big|_a^b, \tag{16}$$

which is substituted into Eq. (15), leading to formula (9). The average value of the commutator $[\hat{H}, \hat{x}]$ in formula (9) is calculated as follows:

$$\begin{aligned}\langle [\hat{H}, \hat{x}] \rangle = \langle \hat{H}\hat{x} \rangle - \langle \hat{x}\hat{H} \rangle &= -\frac{\hbar^2}{2m}\int_\Omega dx\, \bar{\Psi}\frac{\partial^2}{\partial x^2}(x\Psi) \\ &\quad + \int_\Omega dx\, x\, V\bar{\Psi}\Psi \\ &\quad + \frac{\hbar^2}{2m}\int_\Omega dx\, x\, \bar{\Psi}\frac{\partial^2 \Psi}{\partial x^2} - \int_\Omega dx\, x\, V\bar{\Psi}\Psi.\end{aligned}$$

By developing this expression, we obtain

$$\langle [\hat{H}, \hat{x}] \rangle = -\frac{i\hbar}{m}\int_\Omega dx\, \bar{\Psi}(-i\hbar)\frac{\partial}{\partial x}\Psi = -\frac{i\hbar}{m}\langle \hat{p} \rangle. \tag{17}$$

Finally, substituting results (14) and (17) into formula (9), we obtain the following

$$\frac{d}{dt}\langle \hat{x} \rangle = (-xj)|_a^b + \frac{1}{m}\langle \hat{p} \rangle. \tag{18}$$

In the writing of this formula, we used the condition $\langle \Psi, \hat{p}\Phi \rangle = \langle \hat{p}\Psi, \Phi \rangle$ (*i.e.*, $\hat{p}$ is a hermitian operator), but Eq. (18) is also consistent with the hermiticity of $\hat{x}$ ($\Rightarrow \langle \hat{x} \rangle \in \mathbb{R}$).

It is convenient to mention here a result that pertains to the Hamiltonian of the system, $\hat{H}$. Indeed, this operator satisfies the following relation

$$\langle \Psi, \hat{H}\Phi \rangle - \langle \hat{H}\Psi, \Phi \rangle = -\frac{\hbar^2}{2m} \left(\bar{\Psi} \frac{\partial \Phi}{\partial x} - \frac{\partial \bar{\Psi}}{\partial x} \Phi \right) \Big|_a^b , \quad (19)$$

for the functions Ψ and Φ belonging to $\mathcal{L}^2(\Omega)$. If the boundary conditions imposed on Ψ and Φ lead to the cancellation of the term evaluated at the endpoints of the interval Ω, we can write the relation $\langle \Psi, \hat{H}\Phi \rangle = \langle \hat{H}\Psi, \Phi \rangle$. In this case $\hat{H}$ is a hermitian operator. If we make $\Psi = \Phi$ in this last expression, as well as in Eq. (19), we obtain the following condition (see formula (10))

$$j|_a^b = 0. \quad (20)$$

Moreover, $\langle \Psi, \hat{H}\Psi \rangle = \langle \hat{H}\Psi, \Psi \rangle = \overline{\langle \Psi, \hat{H}\Psi \rangle} \Rightarrow \mathrm{Im}\langle \Psi, \hat{H}\Psi \rangle = 0$, *i.e.*, $\langle \hat{H} \rangle \in \mathbb{R}$. In formula (18), condition (20) is not sufficient to eliminate the term evaluated at the boundaries of the interval Ω.

We can now compare result (18) with the result obtained in Ref. [6] (see formula (17) in Ref. [6])

$$\frac{d}{dt} \langle \hat{x} \rangle = \left(-x\, R^2\, v \right) \Big|_a^b + \langle v \rangle \, . \quad (21)$$

From the beginning, Ref. [6] uses real-valued expressions for the temporal evolution of $\hat{x}$ and $\hat{p}$. For example, Eq. (21) is obtained from the following

$$\frac{d}{dt} \langle \hat{x} \rangle = -\frac{2}{\hbar} \, \mathrm{Im}\langle \hat{H}\Psi, \hat{x}\Psi \rangle. \quad (22)$$

That is, Eq. (21) is consistent with the hermiticity of $\hat{x}$. In fact (as we observed after Eq. (15)), because $\hat{H} = i\hbar\partial/\partial t$, formula (6) can be written as follows:

$$\frac{d}{dt} \langle \hat{x} \rangle = \frac{i}{\hbar} \left(\langle \hat{H}\Psi, \hat{x}\Psi \rangle - \langle \Psi, \hat{x}\hat{H}\Psi \rangle \right).$$

Furthermore, because $\langle \Psi, \hat{x}\hat{H}\Psi \rangle = \langle \hat{x}\Psi, \hat{H}\Psi \rangle$, Eq. (22) is obtained. As observed from the discussion that follows formula (12) in Ref. [6], $R^2 = \bar{\Psi}\Psi = |\Psi|^2 = \rho$ is the probability density and $v = v(x,t)$ is the velocity field, which is related to the probability current density as follows: $j = \rho\, v$. From this last formula we can write

$$\int_\Omega dx\, j = \int_\Omega dx\, v\, \bar{\Psi}\Psi = \langle v \rangle \, . \quad (23)$$

Comparing Eq. (23) with formula (12) (after applying condition (14)), the relation $\langle v \rangle = \langle \hat{p} \rangle / m$ is obtained. Returning to formula (21), it is clear that it is equal to formula (18), and the latter is equal to formula (9), provided that formula (14) is verified. We can then say that the time derivative of the mean value of the operator $\hat{x}$ is not always equal to $\langle \hat{p} \rangle / m$. For example, Ref. [3] shows a specific example that confirms the validity of Eq. (18).

In summary, the temporal evolution of the mean value of $\hat{x}$ is given by Eq. (18) and also by Eq. (21). Assuming that (in addition to $\hat{x}$ and $\hat{p}$) the operator $\hat{H}$ is hermitian, we can write the following expression:

$$\frac{d}{dt} \langle \hat{x} \rangle = -(b-a)\, j(a,t) + \frac{1}{m} \langle \hat{p} \rangle \quad (24)$$

(in which we used relation (20)). Only one boundary condition involving the vanishing of the boundary term in Eq. (13), but also leading to the vanishing of the probability current density at the ends of the interval Ω, gives the equation $d\langle \hat{x} \rangle / dt = \langle \hat{p} \rangle / m$. This scenario is clearly possible, for example, for the Dirichlet boundary condition $\Psi(a,t) = \Psi(b,t) = 0$. However, the same is not necessarily true for the periodic boundary conditions $\Psi(a,t) = \Psi(b,t)$ and $(\partial\Psi/\partial x)(a,t) = (\partial\Psi/\partial x)(b,t)$ [3].

3. Time derivatives for $\langle \hat{p} \rangle$

Next, we consider the momentum operator $\hat{p}$. The following result was formally proved in Ref. [5] (see formula (A.2) in Ref. [5])

$$\frac{d}{dt} \langle \hat{p} \rangle = -\frac{\hbar^2}{2m} \left(\frac{\partial \bar{\Psi}}{\partial x} \frac{\partial \Psi}{\partial x} - \bar{\Psi} \frac{\partial^2 \Psi}{\partial x^2} \right) \Big|_a^b + \frac{i}{\hbar} \langle [\hat{H}, \hat{p}] \rangle. \quad (25)$$

This formula was obtained from the following formal relation (formula (11) in Ref. [5] with $\hat{A} = \hat{p}$)

$$\frac{d}{dt} \langle \hat{p} \rangle = \frac{i}{\hbar} \left(\langle \hat{H}\Psi, \hat{p}\Psi \rangle - \langle \Psi, \hat{H}\hat{p}\Psi \rangle \right) + \frac{i}{\hbar} \langle [\hat{H}, \hat{p}] \rangle. \quad (26)$$

In the case where $\hat{p} = -i\hbar\partial/\partial x$ y $\hat{H} = i\hbar\partial/\partial t$, this equation simplifies to Eq. (7) (*i.e.*, in writing Eq. (26), no special condition has been imposed). If we want to verify the validity of Eq. (25), we can begin to develop formula (26). Thus, we first compute the following scalar products present there:

$$\langle \hat{H}\Psi, \hat{p}\Psi \rangle = i\hbar \frac{\hbar^2}{2m} \int_\Omega dx\, \frac{\partial^2 \bar{\Psi}}{\partial x^2} \frac{\partial \Psi}{\partial x} - i\hbar \int_\Omega dx\, V\, \bar{\Psi} \frac{\partial \Psi}{\partial x},$$

$$\langle \Psi, \hat{H}\hat{p}\Psi \rangle = \langle \hat{H}\hat{p} \rangle = i\hbar \frac{\hbar^2}{2m} \int_\Omega dx\, \bar{\Psi} \frac{\partial^2}{\partial x^2} \left(\frac{\partial \Psi}{\partial x} \right) - i\hbar \int_\Omega dx\, V\, \bar{\Psi} \frac{\partial \Psi}{\partial x}.$$

By integrating by parts the first integral in $\langle \Psi, \hat{H}\hat{p}\Psi \rangle$ and then subtracting these two expressions, we obtain the following result:

$$\langle \hat{H}\Psi, \hat{p}\Psi \rangle - \langle \Psi, \hat{H}\hat{p}\Psi \rangle = i\hbar \frac{\hbar^2}{2m} \left(\frac{\partial \bar{\Psi}}{\partial x} \frac{\partial \Psi}{\partial x} - \bar{\Psi} \frac{\partial^2 \Psi}{\partial x^2} \right) \Big|_a^b , \quad (27)$$

which can be substituted into (26) to produce formula (25). Likewise, the mean value of the commutator $[\hat{H}, \hat{p}]$

in formula (26) can be explicitly computed using $\langle\hat{H}\hat{p}\rangle$ and calculating $\langle\hat{p}\hat{H}\rangle$; in fact,

$$\langle[\hat{H},\hat{p}]\rangle = \langle\hat{H}\hat{p}\rangle - \langle\hat{p}\hat{H}\rangle = \langle\hat{H}\hat{p}\rangle$$

$$-i\hbar\frac{\hbar^2}{2m}\int_\Omega dx\,\bar{\Psi}\frac{\partial}{\partial x}\left(\frac{\partial^2\Psi}{\partial x^2}\right) + i\hbar\int_\Omega dx\,\bar{\Psi}\frac{\partial}{\partial x}(V\Psi).$$

By developing the derivative in the last integral above and simplifying, we obtain an expected result (see Refs. [1,2], for example)

$$\langle[\hat{H},\hat{p}]\rangle = i\hbar\int_\Omega dx\,\frac{dV}{dx}\,\bar{\Psi}\Psi = i\hbar\left\langle\frac{dV}{dx}\right\rangle \equiv -i\hbar\langle\hat{f}\rangle, \tag{28}$$

where we have also identified the external classical force operator $\hat{f} = f(x) = -dV/dx$. Finally, formula (25) can be written as follows

$$\frac{d}{dt}\langle\hat{p}\rangle = -\frac{\hbar^2}{2m}\left(\frac{\partial\bar{\Psi}}{\partial x}\frac{\partial\Psi}{\partial x} - \bar{\Psi}\frac{\partial^2\Psi}{\partial x^2}\right)\Bigg|_a^b + \langle\hat{f}\rangle. \tag{29}$$

Note that formula (27) is obtained by making $\Phi = \hat{p}\Psi$ in relation (19). Thus, if the boundary term in Eq. (19) is zero because of the boundary conditions (and consequently, $\hat{H}$ is hermitian), the boundary term in Eq. (29) does not necessarily vanish. An example of this scenario is provided by the Dirichlet boundary condition, $\Psi(a,t) = \Psi(b,t) = 0$. Indeed, with this boundary condition $\hat{H}$, is hermitian, but the boundary term in Eq. (29) is not zero. Within the case of the periodic boundary condition, $\Psi(a,t) = \Psi(b,t)$ and $(\partial\Psi/\partial x)(a,t) = (\partial\Psi/\partial x)(b,t)$, the operator $\hat{H}$ is also hermitian, but the boundary term in Eq. (29) does vanish (from the Schrödinger equation in (8) we also know that $(\partial^2\Psi/\partial x^2)(a,t) = (\partial^2\Psi/\partial x^2)(b,t)$ if the potential satisfies $V|_a^b = 0$). Similarly, in an open interval ($\Omega = (a,b) = (-\infty,+\infty)$) the boundary term in Eq. (29) is zero if $\Psi(x,t)$ and its derivative, $\partial\Psi(x,t)/\partial x$, tend to zero at the ends of that interval. Specifically, if a wave function tends to zero for $x \to \pm\infty$, at least as $|\,x\,|^{-\frac{1}{2}-\epsilon}$ (where $\epsilon > 0$), then its derivative also tends to zero there, and the boundary term in both in Eqs. (19) and (29) vanishes (as a result, we also have $\Psi(x,t) \in \mathcal{L}^2(\Omega)$). This result provides the formal argument for the cancellation of these two boundary terms. Clearly, if Ψ satisfies a homogeneous boundary condition for which $\hat{H}$ is hermitian and $\partial\Psi/\partial x$ satisfies the same boundary condition, the boundary term in Eq. (29) vanishes (this result seems to be very restrictive).

Consequently, result (25) was obtained from formula (26). Likewise, the following expression for $d\langle\hat{p}\rangle/dt$ was also obtained from formula (26) (see formula (19) in Ref. [6])

$$\frac{d}{dt}\langle\hat{p}\rangle = -R^2\left(\frac{m}{2}v^2 - V - Q\right)\Bigg|_a^b + \langle\hat{f}\rangle - \left\langle\frac{\partial Q}{\partial x}\right\rangle, \tag{30}$$

where (as we said before) $R^2 = \rho$, $v = j/\rho$ and $\hat{f} = f(x) = -dV/dx$; moreover, $Q = Q(x,t)$ is Bohm's quantum potential,

$$Q \equiv -\frac{\hbar^2}{2m}\frac{1}{|\Psi|}\frac{\partial^2|\Psi|}{\partial x^2} = -\frac{\hbar^2}{2m}\frac{1}{\sqrt{\rho}}\frac{\partial^2\sqrt{\rho}}{\partial x^2}$$

$$= \frac{\hbar^2}{4m}\left[\frac{1}{2}\left(\frac{1}{\rho}\frac{\partial\rho}{\partial x}\right)^2 - \frac{1}{\rho}\frac{\partial^2\rho}{\partial x^2}\right]. \tag{31}$$

Now let us verify and reexamine the validity of Eq. (30). Returning to result (26), it is clear that it can also be written as follows:

$$\frac{d}{dt}\langle\hat{p}\rangle = \frac{i}{\hbar}\left(\langle\hat{H}\Psi,\hat{p}\Psi\rangle - \langle\hat{H}\hat{p}\rangle\right) + \frac{i}{\hbar}\left(\langle\hat{H}\hat{p}\rangle - \langle\Psi,\hat{p}\hat{H}\Psi\rangle\right),$$

and, if the condition

$$\langle\Psi,\hat{p}\hat{H}\Psi\rangle = \langle\hat{p}\Psi,\hat{H}\Psi\rangle, \tag{32}$$

is used, we can write

$$\frac{d}{dt}\langle\hat{p}\rangle = \frac{i}{\hbar}\left(\langle\hat{H}\Psi,\hat{p}\Psi\rangle - \langle\hat{p}\Psi,\hat{H}\Psi\rangle\right)$$

$$= \frac{i}{\hbar}\left(\langle\hat{H}\Psi,\hat{p}\Psi\rangle - \overline{\langle\hat{H}\Psi,\hat{p}\Psi\rangle}\right).$$

Therefore, the time derivative of $\langle\hat{p}\rangle$ is given by the following

$$\frac{d}{dt}\langle\hat{p}\rangle = -\frac{2}{\hbar}\,\mathrm{Im}\langle\hat{H}\Psi,\hat{p}\Psi\rangle, \tag{33}$$

which is automatically real-valued. It is important to note that the formula

$$\langle\Psi,\hat{p}\hat{H}\Psi\rangle - \langle\hat{p}\Psi,\hat{H}\Psi\rangle = \hbar^2\,\bar{\Psi}\frac{\partial\Psi}{\partial t}\Bigg|_a^b \tag{34}$$

is obtained by setting $\Phi = \hat{H}\Psi$ in relation (13). If the boundary conditions imposed on Ψ lead to the cancellation of the boundary term in Eq. (34), then formula (32) is verified; however, that same boundary condition can also cancel the boundary term in Eq. (13), with $\Psi = \Phi$ (the latter would imply that $\hat{p}$ is hermitian). The spatial part of the boundary term in Eq. (34) is unaffected by the presence of the time derivative.

As is known, by substituting the polar form of the wave function in the Schrödinger Eq. (8) (*i.e.*, $\Psi = \sqrt{\rho}\exp(iS/\hbar)$), where $S = S(x,t) \in \mathbb{R}$ is essentially the phase of the wave function) and then separating the real and imaginary parts, we obtain (i) the quantum Hamilton-Jacobi equation

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 + Q + V = 0, \tag{35}$$

and (ii) the continuity equation

$$\frac{\partial\rho}{\partial t} + \frac{\partial j}{\partial x} = 0. \tag{36}$$

The probability current density j can also be written in terms of ρ and S after replacing the polar form of Ψ in formula (10)

$$j = \frac{1}{m}\rho\frac{\partial S}{\partial x}. \tag{37}$$

Formula (33) can be written as follows

$$\frac{d}{dt}\langle \hat{p}\rangle = +2\hbar\int_{\Omega} dx\, \mathrm{Im}\left(\frac{\partial \bar{\Psi}}{\partial t}\frac{\partial \Psi}{\partial x}\right), \tag{38}$$

and by substituting the relation $\Psi = \sqrt{\rho}\exp(iS/\hbar)$ in Eq. (38), we obtain the following result

$$\frac{d}{dt}\langle \hat{p}\rangle = \int_{\Omega} dx\left(\frac{\partial \rho}{\partial t}\frac{\partial S}{\partial x} - \frac{\partial \rho}{\partial x}\frac{\partial S}{\partial t}\right). \tag{39}$$

By solving for $\partial S/\partial t$ and $\partial \rho/\partial t$ in Eqs. (35) and (36), respectively, and substituting them into Eq. (39), formula (30) is obtained (after some simple calculations).

The boundary term in formula (29) is real-valued if Eq. (14) is verified. To obtain this result, we first write that boundary term separately but in terms of ρ and j (or $v = j/\rho$):

$$-\frac{\hbar^2}{2m}\frac{\partial \bar{\Psi}}{\partial x}\frac{\partial \Psi}{\partial x}\bigg|_a^b + \frac{\hbar^2}{2m}\bar{\Psi}\frac{\partial^2 \Psi}{\partial x^2}\bigg|_a^b$$
$$= \left[-\frac{\hbar^2}{8m}\frac{1}{\rho}\left(\frac{\partial \rho}{\partial x}\right)^2 - \rho\frac{m}{2}v^2\right]\bigg|_a^b$$
$$+ \left(-\rho Q - \rho\frac{m}{2}v^2 + i\frac{\hbar}{2}\frac{\partial j}{\partial x}\right)\bigg|_a^b \tag{40}$$

(Eq. (40) is, in fact, also valid without vertical bars, $|_a^b$). As we have observed before, the hermiticity of $\hat{p}$ ($\Rightarrow \langle \hat{p}\rangle \in \mathbb{R}$) requires that the probability density (for the state Ψ) satisfies formula (14). Differentiating that formula with respect to time, we obtain the following:

$$\left(\frac{\partial \rho}{\partial t}\right)(b,t) - \left(\frac{\partial \rho}{\partial t}\right)(a,t) = \frac{\partial \rho}{\partial t}\bigg|_a^b = 0.$$

Now, using the continuity equation (Eq. (36)), we obtain the condition

$$\frac{\partial j}{\partial x}\bigg|_a^b = 0. \tag{41}$$

With this last result, the entire boundary term in Eq. (40) (and therefore in Eq. (29)) is real-valued (the first term in (40) is always real). Consistently, $d\langle \hat{p}\rangle/dt$ and $\langle \hat{f}\rangle$ are both real-valued quantities in Eq. (29).

In the proof of the formula (30), the condition given in Eq. (32) was used; thus, the results in Eq. (29) (or Eq. (25)) and Eq. (30) are not equivalent. However, from the expression for $d\langle \hat{p}\rangle/dt$ that is written after Eq. (31), we can write the following:

$$\frac{d}{dt}\langle \hat{p}\rangle = \frac{i}{\hbar}\left(\langle \hat{H}\Psi, \hat{p}\Psi\rangle - \langle \Psi, \hat{p}\hat{H}\Psi\rangle\right).$$

Now, instead of using Eq. (32), we use relation (34) (from which we solve for $\langle \Psi, \hat{p}\hat{H}\Psi\rangle$). This process leads to the following expression

$$\frac{d}{dt}\langle \hat{p}\rangle = -\frac{2}{\hbar}\,\mathrm{Im}\langle \hat{H}\Psi, \hat{p}\Psi\rangle - \bar{\Psi}\hat{H}\Psi\Big|_a^b \tag{42}$$

(in which we have used $\hat{H} = i\hbar\partial/\partial t$ to write the boundary term in Eq. (42)). Indeed, formulas (29) and (42) are equivalent. The first term on the right-hand side of Eq. (42) is precisely the entire right-hand side of Eq. (30). Additionally, the boundary term in Eq. (42) can be rewritten using Eq. (8). In this way, we obtain the following result:

$$\frac{d}{dt}\langle \hat{p}\rangle = -\rho\frac{m}{2}v^2\Big|_a^b + \frac{\hbar^2}{2m}\bar{\Psi}\frac{\partial^2 \Psi}{\partial x^2}\bigg|_a^b + \rho Q|_a^b - \left\langle \frac{\partial Q}{\partial x}\right\rangle + \langle \hat{f}\rangle.$$

Now, we use the following (remarkable) relation:

$$\frac{\partial}{\partial x}\left[-\frac{\hbar^2}{8m}\frac{1}{\rho}\left(\frac{\partial \rho}{\partial x}\right)^2\right] = \frac{\partial \rho}{\partial x}Q$$

(where we have made use of the definition of the Bohm's quantum potential given by Eq. (31)), to write

$$\rho Q|_a^b - \left\langle \frac{\partial Q}{\partial x}\right\rangle = \int_a^b dx\,\frac{\partial \rho}{\partial x}Q = -\frac{\hbar^2}{8m}\frac{1}{\rho}\left(\frac{\partial \rho}{\partial x}\right)^2\bigg|_a^b, \tag{43}$$

which leads us to the following result:

$$\frac{d}{dt}\langle \hat{p}\rangle = \left[-\frac{\hbar^2}{8m}\frac{1}{\rho}\left(\frac{\partial \rho}{\partial x}\right)^2 - \rho\frac{m}{2}v^2\right]\bigg|_a^b$$
$$+\frac{\hbar^2}{2m}\bar{\Psi}\frac{\partial^2 \Psi}{\partial x^2}\bigg|_a^b + \langle \hat{f}\rangle. \tag{44}$$

Finally, because the following relation is verified:

$$\left[-\frac{\hbar^2}{8m}\frac{1}{\rho}\left(\frac{\partial \rho}{\partial x}\right)^2 - \rho\frac{m}{2}v^2\right]\bigg|_a^b = -\frac{\hbar^2}{2m}\frac{\partial \bar{\Psi}}{\partial x}\frac{\partial \Psi}{\partial x}\bigg|_a^b$$

(see Eq. (40)), formula (44) is precisely result (29) (*i.e.*, Eqs. (42) and (29) are equivalent).

Recapitulating, the temporal evolution of the mean value of $\hat{p}$ is given by Eq. (29), but the boundary term must be real-valued if the mean value of $\hat{p}$ is real. As we have demonstrated (see Eq. (40)), to accomplish this, it is enough that the boundary conditions satisfy Eq. (14), which implies that Eq. (41) is also satisfied because the continuity equation is verified. After substituting Eqs. (40) and (41) in Eq. (29), this formula (Eq. (29)) can be written as follows:

$$\frac{d}{dt}\langle \hat{p}\rangle = \left[-\frac{\hbar^2}{8m}\frac{1}{\rho}\left(\frac{\partial \rho}{\partial x}\right)^2 - \rho\frac{m}{2}v^2\right]\bigg|_a^b$$

$$+\left(-\rho Q-\rho\frac{m}{2}v^2\right)\Big|_a^b+\langle\hat{f}\rangle. \tag{45}$$

Formula (30) also gives us the average value of $\hat{p}$, but this equation must also be consistent with Eq. (14) (because $\hat{p}$ is hermitian) and the boundary conditions should cancel the boundary term that appears in Eq. (34). This term is precisely

$$\hbar^2\,\bar{\Psi}\frac{\partial\Psi}{\partial t}\Big|_a^b=\frac{\hbar^2}{2}\frac{\partial\rho}{\partial t}\Big|_a^b+i\hbar\,\rho\frac{\partial S}{\partial t}\Big|_a^b, \tag{46}$$

and because $(\partial\rho/\partial t)|_a^b=0$ (as a result of the validity of Eq. (14)), we have that the vanishing of the left-hand side in Eq. (46) implies the following

$$\rho\frac{\partial S}{\partial t}\Big|_a^b=0. \tag{47}$$

Now, multiplying the quantum Hamilton-Jacobi equation (Eq. (35)) by ρ and substituting the expression $\partial S/\partial x=mv$ (Eq. (37) with $j=\rho v$) and Eq. (47), the following relation is obtained (in this way, this result is also a consequence of the elimination of the left-hand side in Eq. (46))

$$\rho V|_a^b=\left(-\rho Q-\rho\frac{m}{2}v^2\right)\Big|_a^b. \tag{48}$$

Now, returning to formula (30) and substituting relation (43), we obtain the following result

$$\frac{d}{dt}\langle\hat{p}\rangle=\left[-\frac{\hbar^2}{8m}\frac{1}{\rho}\left(\frac{\partial\rho}{\partial x}\right)^2-\rho\frac{m}{2}v^2\right]\Big|_a^b+\rho V|_a^b+\langle\hat{f}\rangle. \tag{49}$$

Formula (49) becomes formula (45), as long as relation (48) is obeyed (this is an expected result!). Thus, Eqs. (29) and (30), together with the condition given by Eq. (14) (which is consistent with the hermiticity of $\hat{p}$), give us identical results if the boundary term in Eq. (34) vanishes (which occurs if $\hat{p}$ is hermitian); *i.e.*, if Eq. (48) is verified (see the comment after Eq. (34)). In conclusion, Eqs. (49) and (29) show that the time derivative of the mean value of $\hat{p}$ is always equal to a term evaluated at the ends of the interval containing the particle plus the mean value of the external classical force operator. However, as is shown in Eq. (49), the boundary term may depend only on the values taken at $x=a$ and $x=b$ by the probability density, its first spatial derivative, the probability current density and the external potential.

In agreement with the previous results (see the discussion that follows Eq. (29)), all of the boundary terms in Eq. (49) do not vanish for the solutions to the Schrödinger equation $\Psi=\Psi(x,t)$ satisfying the Dirichlet boundary condition. In this case, both the density of probability and the probability current density vanish at the ends of the interval, *i.e.*, $j|_a^b=0-0=0$ and $\rho|_a^b=0-0=0$. Therefore, we have $\rho V|_a^b=0$ and $(\rho m v^2/2)|_a^b=(0/0)-(0/0)=0$. The latter result because $j=\rho v$, $\rho(a)=\rho(b)$ (Eq. (14)) and $j(a)=j(b)$ (Eq. (20)). Moreover, we also know that $\rho Q|_a^b=0$, which is consistent with Eq. (48). Thus, we can write the following result

$$\frac{d}{dt}\langle\hat{p}\rangle=-\frac{\hbar^2}{8m}\frac{1}{\rho}\left(\frac{\partial\rho}{\partial x}\right)^2\Big|_a^b+\langle\hat{f}\rangle. \tag{50}$$

The boundary term in Eq. (50) can be written as follows:

$$-\frac{\hbar^2}{2m}\left(\frac{\partial\sqrt{\rho}}{\partial x}\right)^2\Big|_a^b,$$

and (in this case) it coincides with $\langle-\partial Q/\partial x\rangle$ (this result comes from Eq. (43)). Also (in this case), the boundary term coincides with the following expression:

$$-\frac{\hbar^2}{2m}\frac{\partial\bar{\Psi}}{\partial x}\frac{\partial\Psi}{\partial x}\Big|_a^b=-\frac{\hbar^2}{2m}\left|\frac{\partial\Psi}{\partial x}\right|^2\Big|_a^b$$

(see the relation that follows Eq. (44)). Consequently, the mean value of the quantum force $f_Q=f_Q(x,t)\equiv-\partial Q/\partial x$ can be calculated by simply evaluating a quantity (which, in this case, only depends on ρ and $\partial\rho/\partial x$) at $x=b$ and at $x=a$ and then subtracting these two results. Similarly, if we assign the following expressions to f_Q:

$$f_Q\rightarrow-\frac{\hbar^2}{2m}\frac{1}{|\Psi|^2}\frac{\partial}{\partial x}\left|\frac{\partial\Psi}{\partial x}\right|^2$$

or

$$f_Q\rightarrow-\frac{\hbar^2}{2m}\frac{1}{\rho}\frac{\partial}{\partial x}\left(\frac{\partial\sqrt{\rho}}{\partial x}\right)^2,$$

which are clearly distinct from each another and also from $-\partial Q/\partial x$, the correct value for $\langle f_Q\rangle$ is obtained. However, an exact expression for f_Q can be obtained using the relation that precedes Eq. (43), in which $Q\,\partial\rho/\partial x=\partial(\rho Q)/\partial x-\rho\,\partial Q/\partial x$. The result is the following

$$f_Q=\frac{1}{\rho}\frac{\partial}{\partial x}\left[-\rho Q-\frac{\hbar^2}{8m}\frac{1}{\rho}\left(\frac{\partial\rho}{\partial x}\right)^2\right]. \tag{51}$$

Clearly, $\langle f_Q\rangle$ is always equal to a boundary term. Formula (51) can be written without the explicit presence of Bohm's quantum potential. Indeed, by substituting the expression for Q (the expression to the right in Eq. (31)) in Eq. (51), we obtain the following

$$f_Q=\frac{1}{\rho}\frac{\partial}{\partial x}\left[\frac{\hbar^2}{4m}\rho\frac{d^2}{dx^2}\ln(\rho)\right]. \tag{52}$$

This last result has been known in hydrodynamic formulations of Schrödinger's theory; see, for example, the following recent [11] (and further references therein).

Now, if we return to Eq. (50) and assume that the external potential is zero ($\Rightarrow \langle \hat{f} \rangle = 0$), we can write the following

$$\frac{d}{dt}\langle \hat{p} \rangle = -\frac{\hbar^2}{2m}\left(\frac{\partial\sqrt{\rho}}{\partial x}\right)^2\Bigg|_a^b = -\frac{\hbar^2}{2m}\left|\frac{\partial\Psi}{\partial x}\right|^2\Bigg|_a^b = \langle f_Q \rangle. \tag{53}$$

Consequently, the mean value of the force encountered by a free particle confined to a region and colliding with the two walls is precisely $\langle f_Q \rangle$. Then, from Eq. (53), and because the formula that follows Eq. (44) (which is also valid without vertical bars, $|_a^b$) with $(\rho m v^2/2)\big|_{(x=b)} = (\rho m v^2/2)\big|_{(x=a)} = 0$ is verified, we can say that the average force on the particle when it hits the wall at $x = b$ is given by the following

$$-\frac{\hbar^2}{2m}\left(\frac{\partial\sqrt{\rho}}{\partial x}\right)^2\Bigg|_{(x=b)} = -\frac{\hbar^2}{2m}\left|\frac{\partial\Psi}{\partial x}\right|^2\Bigg|_{(x=b)}, \tag{54}$$

At $x = a$, the expression for this force is obtained from Eq. (54) by making the following replacements: $b \to a$ and $- \to +$. Let us now consider the example of the confined (free) particle moving between $x = 0\,(= a)$ and $x = L\,(= b)$, and in some of its possible stationary states

$$\Psi = \Psi_n(x,t) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)\exp\left(-i\frac{E_n}{\hbar}t\right), \tag{55}$$

where $E_n = \hbar^2\pi^2 n^2/2mL^2$, with $n = 1, 2, \ldots$ (naturally, the corresponding probability density $\rho = \rho_n(x) = |\Psi_n(x,t)|^2$ is independent of time). Using these results in Eq. (54) (in either of the two expressions), we can determine that the average force on the particle at $x = L$ is given by $-2E_n/L$, and at $x = 0$ it is given by $+2E_n/L$; therefore, $\langle f_Q \rangle = 0$ (this same result was obtained in Ref. [12] following a procedure different from that shown here). However, if the state Ψ is a linear combination of the solutions (55) (and hence, the corresponding probability density is also a function of time), $\langle f_Q \rangle$ does not necessarily vanish (in this specific case, the average force on the particle at $x = L$ is not always minus the value ($(-1)\times$) at $x = 0$) [13]. In Ref. [13] the issue of the average forces for a particle ultimately restricted to a finite one-dimensional interval, either because there exists an infinite potential or because we put the particle in the interval and neglect the rest of the line, has been recently treated.

Consistently with previous results (see the discussion following Eq. (29)), the entire boundary term in Eq. (49) vanishes for the solutions $\Psi = \Psi(x,t)$ satisfying the periodic boundary condition. Indeed, we know that $\rho|_a^b = j|_a^b = 0$; therefore, $\rho V|_a^b = 0$ (provided that $V|_a^b = 0$) and $\rho Q|_a^b = 0$ (see Eq. (48)). Finally, because

$$\frac{\partial\rho}{\partial x}\Bigg|_a^b = 2\,\mathrm{Re}\left(\bar{\Psi}\frac{\partial\Psi}{\partial x}\right)\Bigg|_a^b,$$

all of the boundary terms in Eq. (49) vanish, and the result $d\langle \hat{p} \rangle/dt = \langle \hat{f} \rangle$ is reached. However, in this case, we also know that $d^2\langle \hat{x} \rangle/dt^2 \neq \langle \hat{f} \rangle/m$. This result occurs because the boundary term in Eq. (24) is not zero (because the probability current density does not vanish at the ends of Ω), and its derivative with respect to t does not vanish either. Clearly, this situation does not occur when the relation $j(a) = j(b) = 0$ is obeyed (as in the case of the Dirichlet boundary condition).

Finally, as was explained before (see the discussion following Eq. (29)), the boundary term in Eq. (29) is zero in an open interval ($\Omega = (-\infty, +\infty)$), provided that appropriate conditions can be satisfied as $x \to \pm\infty$ (*i.e.*, Ψ and its derivative should vanish at infinity). Equivalently, the boundary term in Eq (45) is also zero, as well as that in Eq. (49) (because Eq. (48) is satisfied). We can then conclude (from Eq. (43)) that $\langle f_Q \rangle = 0$; therefore, $d\langle \hat{p} \rangle/dt = \langle \hat{f} \rangle$. From Eq. (24), relation $d\langle \hat{x} \rangle/dt = \langle \hat{p} \rangle/m$ is also verified; consequently, $d^2\langle \hat{x} \rangle/dt^2 = \langle \hat{f} \rangle/m$.

4. Conclusions

We have formally calculated time derivatives of $\langle \hat{x} \rangle$ and $\langle \hat{p} \rangle$ in one dimension. Simultaneously, we have identified the conditions under which two pairs of these derivatives, which have been previously published, can be equivalent. When the particle is in a finite interval, we have observed that the Ehrenfest theorem is generally not verified. In fact, because of the large variety of boundary conditions that can be imposed in this case (and for which $\hat{p}$ and $\hat{H}$ are hermitian operators), the boundary terms that appear in $d\langle \hat{x} \rangle/dt$ and $d\langle \hat{p} \rangle/dt$ (which may depend only on the values taken there by the probability density, its spatial derivative, the probability current density and the external potential) do not always vanish. Particularly, if the boundary term in $d\langle \hat{x} \rangle/dt$ does not vanish, we generally know that $d^2\langle \hat{x} \rangle/dt^2 \neq \langle \hat{f} \rangle/m$. If the particle is at any part of the real line, but there is a very small chance for it to exist at infinity, the time derivatives of $\langle \hat{x} \rangle$ and $\langle \hat{p} \rangle$ obey the usual Ehrenfest relations, as expected. As we have demonstrated, $d\langle \hat{x} \rangle/dt$ is equal to $\langle \hat{p} \rangle/m$, plus a boundary term, but we can also say that $d\langle \hat{p} \rangle/dt$ is equal to $\langle \hat{f} \rangle + \langle f_Q \rangle$ plus a boundary term. In the first formula, the respective boundary term is zero whenever the probability current density vanishes at the ends of the interval (see Eq. (24)). As a case in point, the same result is observed in the second formula when the probability density and current are zero there (see, for example, Eq. (45) conjointly with Eq. (43)).

If a free particle ($V = \text{const} \Rightarrow \hat{f} = 0 \Rightarrow \langle \hat{f} \rangle = 0$) is confined to a box, the quantum force f_Q (or rather, its mean value $\langle f_Q \rangle$) is the quantity that reports the existence of the box's impenetrable walls (at least for the Dirichlet boundary condition). In all cases, the average value of $f_Q = -\partial Q/\partial x$ is simply obtained by evaluating a certain quantity at each end of the interval occupied by the particle and subtracting the two results (see Eq. (51)). That quantity is precisely proportional to the integrand of the so-called probability density's Fisher information, $\mathcal{F}(\rho)$, in particular cases; for example, when $\rho = 0$ at the ends of the interval. In effect, for a particle in an interval $\Omega = [a, b]$, we obtain the following (see, for instance, Refs. [11, 14]):

$$\mathcal{F}(\rho) = \int_a^b dx \, \frac{1}{\rho} \left(\frac{\partial \rho}{\partial x} \right)^2 .$$

Clearly, in this case, we obtain $\langle f_Q \rangle$ by evaluating the integrand in $\mathcal{F}(\rho)$ (times $-\hbar^2/8m$) at $x = a$ and $x = b$ (see Eq. (51)).

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