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On average forces and the Ehrenfest theorem for a particle in a semi-infinite interval

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We study the issues of average forces and the Ehrenfest theorem for a particle restricted to a semi-infinite interval by an impenetrable wall. We consider and discuss two specific cases: (i) a free particle in an infinite step potential, and (ii) a free particle on a half-line. In each situation, we show that the mean values of the position, momentum and force, as functions of time, verify the Ehrenfest theorem (the state of the particle being a general wave packet that is a continuous superposition of the energy eigenstates for the Hamiltonian). However, the involved force is not the same in each case. In fact, we have the usual external classical force in the first case and a type of nonlocal boundary quantum force in the second case. In spite of these different forces, the corresponding mean values of these quantities give the same results. Accordingly, the Ehrenfest equations in the two situations are equivalent. We believe that a careful and clear consideration of how the two cases differ but, in the end, agree, is pertinent, and has not been included in the literature.

Keywords: Quantum mechanics; Schrödinger equation; Ehrenfest theorem; average forces.

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1. Introduction

The problem of a Schrödinger particle of mass M moving in a one-dimensional step potential of finite height (or a potential barrier) is one of the simplest problems in quantum mechanics. In fact, this problem can be found in almost any quantum mechanics textbook [1-3]. Let us assume that the barrier is located at $x = 0$ and that the potential is defined by $V(x < 0) = 0$ and $V(x > 0) = V_0$. If the energy of the particle is such that $\varepsilon < V_0$, the particle penetrates some distance into the barrier. If we want to restrict the movement of the particle precisely to the semi-space $x \leq 0$ (the half-line), we have two specific methods to achieve that restriction. The first method is to take the limit of $V_0 \to \infty$ in the finite step potential. In this case, the (free) particle lives on the entire real line, which is then forever restricted to the half-line. We call this case "a particle-in-an-infinite-step-potential". The second method is to consider from the beginning that the (free) particle has always lived on the half-line. In this case, an external potential is not necessary to restrict the particle; only boundary conditions are necessary. We call this case "a particle-on-a-half-line", and we only use the Dirichlet boundary condition ($u(x = 0) = 0$) in this paper.

The problem of a particle restricted to move on a semi-infinite interval (either because there exists an infinite potential or because we put the particle on the half-line and neglect the rest of the line) has been variously studied [4-16]. The purpose of this paper is to examine and relate the two specific methods (mentioned above) to achieve the restriction of the movement of a particle to a semi-infinite region (*i.e.*, to a half-line). We include in the discussion the issues of average forces, and the time evolution of the mean values of the position and momentum operators (*i.e.*, the Ehrenfest theorem). Recently, we did a study similar to that in the present article but for the system of a particle confined to a closed interval (*i.e.*, to a box) [17]. Because, in the present case, the relevant spatial integration range for some matrix elements goes from $-\infty$ to 0, one could expect some complications in the evaluation of these quantities. We also address this issue herein.

The outline of the paper is as follows. In Sec. 2, we present some basic results for the problem of a particle in a finite step potential. In Sec. 3, we examine the limiting procedure that permits us to obtain the mean value of the external classical force ($\hat{F} = -dV(x)/dx$) for the problem of the particle-in-an-infinite-step-potential from the problem of the particle in a finite step potential (the state of the particle being a stationary state). Then, we obtain an expression for the mean value of $\hat{F}$ for the particle-in-an-infinite-step-potential (the state of the particle being a complex general state). In this section, we also calculate explicit general expressions for the mean values of the position ($\hat{X}$) and momentum ($\hat{P}$) operators. We conveniently avoid the problems associated with the integration range over the interval $(-\infty, 0]$ by considering certain generalized limits. Then, we confirm the Ehrenfest theorem for a particle-in-an-infinite-step-potential (*i.e.*, $d\langle\hat{X}\rangle/dt = \langle\hat{P}\rangle/M$ and $d\langle\hat{P}\rangle/dt = \langle\hat{F}\rangle$). In Sec. 4, we present the formal time derivatives of the mean values of the position ($\hat{x}$) and momentum operators ($\hat{p}$) for a particle-on-a-half-line. By using the Dirichlet boundary condition at $x = 0$ while also supposing that the wave function tends to zero at $x = -\infty$, we find the following results: $d\langle\hat{x}\rangle/dt = \langle\hat{p}\rangle/M$ and $d\langle\hat{p}\rangle/dt = \mathrm{b.t.} + \langle\hat{f}\rangle$, where $\mathrm{b.t.}$ denotes a boundary term and $\hat{f} = -d\varphi(x)/dx$ is the external classical force upon the particle-on-a-half-line. Moreover, that boundary term can be written as the mean value of a (nonlocal) quantity that we call the boundary quantum force, f_B. Incidentally, by supposing that the first spatial derivative of the wave function tends to zero at $x = -\infty$, the $\mathrm{b.t.}$ is simply equal to a certain quantity evaluated at $x = 0$. By using the latter condition and considering a wave packet that is a continuous superposition of the energy eigenfunctions of the Hamiltonian describing a particle-on-a-half-line, with $\varphi(x) = 0$ ($\Rightarrow \hat{f} = 0$), we obtain the meaningful result that the $\mathrm{b.t.}$ is equal to the mean value of the external classical force operator for a particle-in-an-infinite-step-potential; *i.e.*, we find that $d\langle\hat{p}\rangle/dt$ is equal to $\langle\hat{F}\rangle$. Hence, the Ehrenfest theorem for a particle-on-a-half-line is completed with the formula $d\langle\hat{p}\rangle/dt = \langle f_B\rangle$. Note that, throughout this paper, we use capital letters to denote the operators in the particle-in-an-infinite-step-potential problem and lowercase letters in the particle-on-a-half-line-problem. Finally, some concluding remarks are given in Sec. 5.

2. Particle in a finite step potential

Let us first consider the following (external) finite step potential of height V_0:

$$V(x) = V_0\Theta(x) \quad (-\infty < x < +\infty), \tag{1}$$

where $\Theta(y)$ is the Heaviside step function ($\Theta(y < 0) = 0$ and $\Theta(y > 0) = 1$). Because the derivative of $\Theta(y)$ is the Dirac delta function ($\delta(y)$), the external classical force upon the particle ($\hat{F} = F(x) = -dV(x)/dx$) can be written as follows:

$$F(x) = -V_0\delta(x) \quad (-\infty < x < +\infty). \tag{2}$$

The eigensolutions of the (eigenvalue) Schrödinger equation $\hat{H}\phi_k(x) = \varepsilon_k\phi_k(x)$ for positive energies $0 < \varepsilon_k < V_0$ can be written as follows:

$$\phi_k(x) = \Theta(-x)\left[\exp(ikx) + \frac{ik+\alpha_k}{ik-\alpha_k}\exp(-ikx)\right] + \Theta(x)\frac{2ik}{ik-\alpha_k}\exp(-\alpha_k x) \quad (-\infty < x < +\infty), \tag{3}$$

where $k \equiv \sqrt{2M\varepsilon_k}/\hbar$ and $\alpha_k \equiv \sqrt{2M(V_0-\varepsilon_k)}/\hbar$ are real-valued and positive quantities. The Hamiltonian operator

$$\hat{H} = \hat{T} + V(x) = \frac{1}{2M}\hat{P}^2 + V(x) = -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} + V(x) \tag{4}$$

(where $\hat{T}$ is the kinetic energy operator and $\hat{P} = -i\hbar\partial/\partial x$ is the momentum operator) describes a particle living on the whole real line, $\mathbb{R}$. As usual, one assumes that this (self-adjoint) operator (for a finite V_0) acts on continuously differentiable functions belonging (as do their second derivatives) to the well-known space $\mathcal{L}^2(\mathbb{R})$ [18]. Thus, any eigenfunction of $\hat{H}$, $\phi_k(x)$, and its derivative, $\phi'_k(x)$, must be continuous at $x = 0$. Therefore, at $x = 0$, we write $\phi_k(0-)=\phi_k(0+)\equiv\phi_k(0)$ and $\phi'_k(0-)=\phi'_k(0+) \equiv \phi'_k(0)$ (where $\phi_k(x\pm) \equiv \lim_{\epsilon\to 0}\phi_k(x\pm\epsilon)$, with $\epsilon > 0$). Likewise, the probability current density

$$j_k(x) = \frac{\hbar}{M}\mathrm{Im}\left[\bar{\phi}_k(x)\frac{d}{dx}\phi_k(x)\right] \tag{5}$$

(where the horizontal bar represents complex conjugation) verifies $j_k(0-) = j_k(0+) \equiv j_k(0)$. In addition, the probability density, $\varrho_k(x) = |\phi_k(x)|^2$, verifies $\varrho_k(0-)=\varrho_k(0+)\equiv\varrho_k(0)$. Note that, $j_k(x > 0) = 0$; therefore, $j_k(0) = 0$. However, the probability density does not vanish at $x = 0$ (although the probability density in the region $x > 0$ decreases rapidly as x increases). Thus, the potential barrier of a finite height (at $x = 0$) is not strictly an impenetrable barrier [19,20]. In fact, the finite barrier at $x = 0$ represents a very simple type of point interaction. This type of interaction can be modelled through boundary conditions only (without any singular potential at $x = 0$); *i.e.*, the corresponding (self-adjoint) Hamiltonian operator has the form given in (4) (with $x \in \mathbb{R} - \{0\}$), where V in this case is just the (bounded) finite step potential. This operator has in its domain a general boundary condition that depends on four (real) parameters [21]. Moreover, for each function belonging to this domain, we obtain that the probability current density is continuous at $x = 0$.

As is well known, the standard formula to calculate the mean value of an operator $\hat{A}$ in the normalized state χ is given by $\langle\hat{A}\rangle_\chi = \langle\chi, \hat{A}\chi\rangle$. By using the latter formula to calculate the mean value of the force operator $\hat{F}$ (Eq. (2)) in the stationary state $\phi_k(x)$, the result is the following:

$$\langle\hat{F}\rangle_{\phi_k} = \langle\phi_k, \hat{F}\phi_k\rangle = \int_{-\infty}^{+\infty} dx\, F(x)\,|\phi_k(x)|^2 = -V_0\varrho_k(0). \tag{6}$$

Obviously, $\phi_k(x)$ is not a normalized state (because of its behaviour at $x = -\infty$); *i.e.*, $\phi_k(x)$ is not a square-integrable function. In addition, $\phi_k(x)$ is not even normalizable; thus, it makes no sense to divide the right hand side of (6) by $\langle\phi_k, \phi_k\rangle \propto \delta(0)$. Thus, we write the formula $\langle\hat{F}\rangle_{\phi_k} = \langle\phi_k, \hat{F}\phi_k\rangle$ (which gives us a finite result) as a matter of convenience only. Nevertheless, as we will see in the next section, this choice has no impact on the results that we obtain.

3. Particle-in-an-infinite-step-potential

The eigensolutions of the Hamiltonian operator (Eq. (4)) in the potential

$$V(x) = \lim_{V_0\to\infty} V_0\Theta(x) \quad (-\infty < x < +\infty), \tag{7}$$

are obtained from Eq. (3). Clearly, if $V_0 \to \infty$, all of the eigenfunctions verify the result $\phi_k(x) \to 0 \equiv \psi_k(x)$ for $x \geq 0$ because

$$\alpha_k \approx \frac{\sqrt{2MV_0}}{\hbar} \to \infty,$$

and also

$$\frac{2ik}{ik-\alpha_k} \approx \frac{2i\sqrt{\varepsilon_k}}{i\sqrt{\varepsilon_k}-\sqrt{V_0}} \approx -2i\sqrt{\frac{\varepsilon_k}{V_0}} \to 0.$$

The latter result leads us to write the following:

$$\phi_k(0+)\,(\equiv \phi_k(0)) \approx -2i\sqrt{\frac{\varepsilon_k}{V_0}} \;\Rightarrow$$

$$\rho_k(0+)(\equiv \rho_k(0)) = |\phi_k(0)|^2 \approx \frac{4\varepsilon_k}{V_0}. \tag{8}$$

Likewise, to obtain $\phi_k(x)$ in the region $x<0$ (*i.e.*, $\psi_k(x)$), we need to use the following result:

$$\frac{ik+\alpha_k}{ik-\alpha_k} \approx \frac{i\sqrt{\varepsilon_k}+\sqrt{V_0}}{i\sqrt{\varepsilon_k}-\sqrt{V_0}} \to -1.$$

(Throughout this article, we use the approximation sign "≈" in any expression in which $V_0 \gg \varepsilon_k$). Thus, the eigensolutions of the Hamiltonian $\hat{H}$ with the potential given in Eq. (7) have the form

$$\psi_k(x) = \Theta(-x)\,[\exp(ikx) - \exp(-ikx)]$$
$$= \Theta(-x)2i\,\sin(kx) \quad (-\infty < x < +\infty), \tag{9}$$

for the energies $\varepsilon_k \to E_k = \hbar^2k^2/2M \in (0,\infty)$ (Note: we prefer to use the symbol E_k in the case of the infinite step potential). We have chosen $k \in (0,\infty)$ so that $\exp(ikx)$ in (9) represents a plane wave moving to the right and $-\exp(-ikx)$ represents a plane wave moving to the left (*i.e.*, the incident wave is all reflected, but the reflected wave at $x=0$ is shifted in phase from the incident at $x=0$ by a factor of -1). Note also that $\psi_k(x)$ satisfies the "extended" Dirichlet boundary condition $\psi_k(x\geq 0)=0$.

The corresponding mean value $\langle\hat{F}\rangle_{\psi_k} = \langle\psi_k, \hat{F}\psi_k\rangle$ is truly independent of V_0 (which is valid when V_0 tends to infinity). In effect, one obtains

$$\langle\hat{F}\rangle_{\psi_k} = \lim_{V_0\to\infty}\langle\hat{F}\rangle_{\phi_k} = \lim_{V_0\to\infty} -V_0\rho_k(0) = -4E_k \tag{10}$$

(in which we used the results given in Eqs. (6) and (8), with $\varepsilon_k \to E_k$). More precisely, we should write $\langle\hat{F}\rangle_{\psi_k} = -4E_k\,|A(k)|^2$, where $A(k)$ is a complex-valued function of the "momenta" k, which multiplies the right-hand side of the solutions $\phi_k(x)$ (Eq. (3)) and also $\psi_k(x)$ (Eq. (9)). So, we may say that the average force upon the particle (in a stationary state) when the particle hits the infinite wall at $x=0$ is proportional to $-4E_k\,|A(k)|^2$. Incidentally, the specific result that $\langle\hat{F}\rangle$ in a stationary state is independent of the height V_0 of one of the walls of a finite square well (when $V_0\to\infty$), was obtained in Ref. 22.

Let us write an (assumed normalized) complex general wave packet $\Psi=\Psi(x,t)$ of the following form:

$$\Psi(x,t) = \int_0^\infty \frac{dk}{\sqrt{2\pi}}\,A(k)\,\psi_k(x)$$
$$\times \exp\left(-i\frac{E_k}{\hbar}t\right)\;(-\infty < x < +\infty), \tag{11}$$

where $\psi_k(x)$ is given by Eq. (9). By substituting Eq. (9) into (11), we can also write the following:

$$\Psi(x,t){=}\Theta(-x)\int_0^\infty \frac{dk}{\sqrt{2\pi}}\,A(k)\,u_k(x)\exp\left(-i\frac{E_k}{\hbar}t\right), \tag{12}$$

where the functions $u_k(x)$ are given by

$$u_k(x) = 2i\,\sin(kx). \tag{13}$$

In the region $x\in(-\infty,0]$, $u_k(x)$ obviously coincides with $\psi_k(x)$ (Eq. (9)). The Hamiltonian for a free particle living on the half-line is simply $\hat{h}\equiv\hat{T}$ (see Eq. (4)) and acts (essentially) on the functions $u(x)\in\mathcal{L}^2((-\infty,0])$ such that $(\hat{h}u)(x)$ is also in $\mathcal{L}^2((-\infty,0])$ while obeying the Dirichlet boundary condition, $u(0)=0$. The eigenfunctions to $\hat{h}$ are precisely the functions $u_k(x)$, and its eigenvalues are the same as those of $\hat{H}$.

The mean value of the force operator at time t in the state given by Eq. (11), $\langle\hat{F}\rangle_\Psi = \langle\Psi,\hat{F}\Psi\rangle$, takes the form:

$$\langle\hat{F}\rangle_\Psi = \int_0^\infty\int_0^\infty \frac{dk\,dk'}{2\pi}\,\bar{A}(k)A(k')\,(\hat{F})(k,k')$$
$$\times \exp\left[i\frac{(E_k-E_{k'})}{\hbar}t\right], \tag{14}$$

where the matrix elements of $\hat{F}$, $(\hat{F})(k,k') = \langle\psi_k,\hat{F}\psi_{k'}\rangle = \lim_{V_0\to\infty}\langle\phi_k,\hat{F}\phi_{k'}\rangle$, are given by the following (see Eq. (2)):

$$(\hat{F})(k,k') = \lim_{V_0\to\infty} -V_0\bar{\phi}_k(0)\phi_{k'}(0). \tag{15}$$

Substituting the result of the left-hand side in (8) into Eq. (15) (with $\varepsilon_{k;k'}\to E_{k;k'}$), we obtain the following noteworthy result:

$$(\hat{F})(k,k') = \lim_{V_0\to\infty} -V_0\,2i\sqrt{\frac{E_k}{V_0}}$$
$$\times(-2i)\sqrt{\frac{E_{k'}}{V_0}} = -4\sqrt{E_kE_{k'}}. \tag{16}$$

Thus, by substituting Eq. (16) into (14), we can write a general expression for the average value of the operator $\hat{F}$ when $V_0\to\infty$:

$$\langle\hat{F}\rangle_\Psi = -4\int_0^\infty\int_0^\infty \frac{dk\,dk'}{2\pi}\,\bar{A}(k)A(k')$$
$$\times\sqrt{E_kE_{k'}}\,\exp\left[i\frac{(E_k-E_{k'})}{\hbar}t\right]. \tag{17}$$

Now let us check that the mean values of the position ($\hat{X}=x$) and momentum ($\hat{P}=-i\hbar\partial/\partial x$) operators at time

t for the general state Ψ verify the Ehrenfest theorem. The expectation value of the position operator is the expression

$$\langle \hat{X} \rangle_\Psi = \int_0^\infty \int_0^\infty \frac{dk\, dk'}{2\pi}\, \bar{A}(k) A(k')\, (\hat{X})(k,k') \times \exp\left[i \frac{(E_k - E_{k'})}{\hbar} t \right], \tag{18}$$

where the matrix elements of $\hat{X}$,

$$(\hat{X})(k,k') = \langle \psi_k, \hat{X} \psi_{k'} \rangle = \int_{-\infty}^{+\infty} dx\, \bar{\psi}_k(x)\, x\, \psi_{k'}(x),$$

i.e.,

$$(\hat{X})(k,k') = \int_{-\infty}^{0} dx\, \bar{u}_k(x)\, x\, u_{k'}(x),$$

are given by the following improper integral (in the ordinary sense):

$$(\hat{X})(k,k') = -4 \int_0^\infty dx\, x\, \sin(kx)\, \sin(k'x). \tag{19}$$

This (nonconvergent) integral can also be written in terms of the Fourier cosine transform

$$F_c(k) \equiv \mathcal{F}_c[f(x)] = \int_0^\infty dx\, f(x)\, \cos(kx)$$

($k > 0$) [23]:

$$(\hat{X})(k,k') = -2 \left[F_c(k - k') - F_c(k + k') \right], \tag{20}$$

where $f(x) = x$. (The latter function is not absolutely integrable over $[0, \infty)$; thus, it follows that $(\hat{X})(k,k')$ is a divergent quantity). However, if $(\hat{X})(k,k')$ is considered to be a distribution, we obtain

$$(\hat{X})(k,k') = \lim_{N\to\infty} -4 \int_0^N dx\, x\, \sin(kx)\, \sin(k'x) = \frac{8kk'}{(k^2 - k'^2)^2}, \tag{21}$$

where we have used the following generalized limits:

$$\lim_{N\to\infty} \cos\left[(k \pm k')N\right] = 0,$$

and also

$$\lim_{N\to\infty} \sin\left[(k \pm k')N\right] = 0.$$

These two results are a consequence of the so-called Riemann-Lebesgue Lemma, *i.e.*,

$$\int_a^b dx\, f(x) \left\{ \begin{array}{c} \cos(Nx) \\ \sin(Nx) \end{array} \right\} = 0,$$

for $N \to \infty$ (where $f(x)$ should be an absolutely integrable function over the interval (a, b)) [24]. Clearly, because N is very large, $f(x)$ does not change significantly while $\cos(Nx)$ or $\sin(Nx)$ are producing cancelling areas [25]. Thus, the result (21) must be interpreted as

$$\int_0^\infty \int_0^\infty dk\, dk' \left(\right) (\hat{X})(k,k') = \int_0^\infty \int_0^\infty dk\, dk' \left(\right) \frac{8kk'}{(k^2 - k'^2)^2}, \tag{22}$$

where we might have a function of k and/or k' inside the parentheses. From Eqs. (18) and (22), we can write a general expression for the average value of the operator $\hat{X}$:

$$\langle \hat{X} \rangle_\Psi = \frac{4\hbar^2}{M} \int_0^\infty \int_0^\infty \frac{dk\, dk'}{2\pi} \bar{A}(k) A(k') \times \frac{\sqrt{E_k E_{k'}}}{(E_k - E_{k'})^2} \exp\left[i \frac{(E_k - E_{k'})}{\hbar} t \right], \tag{23}$$

where we also used $k = \sqrt{2ME_k}/\hbar$, and $k' = \sqrt{2ME_{k'}}/\hbar$. Likewise, the mean value of the momentum operator is as follows:

$$\langle \hat{P} \rangle_\Psi = \int_0^\infty \int_0^\infty \frac{dk\, dk'}{2\pi}\, \bar{A}(k) A(k')\, (\hat{P})(k,k') \times \exp\left[i \frac{(E_k - E_{k'})}{\hbar} t \right], \tag{24}$$

where the matrix elements of $\hat{P}$,

$$(\hat{P})(k,k') = \langle \psi_k, \hat{P} \psi_{k'} \rangle = -i\hbar \int_{-\infty}^{+\infty} dx\, \bar{\psi}_k(x)\, \psi'_{k'}(x),$$

i.e.,

$$(\hat{P})(k,k') = \int_{-\infty}^{0} dx\, \bar{u}_k(x)\, u'_{k'}(x),$$

are given by the following improper integral (in the ordinary sense):

$$(\hat{P})(k,k') = i\hbar\, 4k' \int_0^\infty dx\, \sin(kx)\, \cos(k'x). \tag{25}$$

By also considering $(\hat{P})(k,k')$ as a distribution, we obtain

$$(\hat{P})(k,k') = \lim_{N\to\infty} i\hbar\, 4k' \int_0^N dx\, \sin(kx)\, \cos(k'x) = i\hbar \frac{4kk'}{k^2 - k'^2}. \quad (26)$$

This result must be interpreted as

$$\int_0^\infty \int_0^\infty dk\, dk' \left(\,\right) (\hat{P})(k,k') = i\hbar \int_0^\infty \int_0^\infty dk\, dk' \left(\,\right) \frac{4kk'}{k^2 - k'^2}. \quad (27)$$

Now, from Eqs. (24) and (26), we can write a general expression for the average value of the operator $\hat{P}$:

$$\langle \hat{P} \rangle_\Psi = i\hbar\, 4 \int_0^\infty \int_0^\infty \frac{dk\, dk'}{2\pi} \bar{A}(k) A(k') \times \frac{\sqrt{E_k E_{k'}}}{E_k - E_{k'}} \exp\left[i \frac{(E_k - E_{k'})}{\hbar} t \right]. \quad (28)$$

Note that the operators $\hat{X}$ and $\hat{P}$ act on functions that are square-integrable on $\mathbb{R}$ and (generally) different from zero only in the semi-space $x < 0$.

Clearly, expressions (23) and (28) verify the expected result:

$$\frac{d}{dt} \langle \hat{X} \rangle_\Psi = \frac{1}{M} \langle \hat{P} \rangle_\Psi. \quad (29)$$

Likewise, from Eqs. (17) and (28), another desired result is obtained:

$$\frac{d}{dt} \langle \hat{P} \rangle_\Psi = \langle \hat{F} \rangle_\Psi. \quad (30)$$

In this manner, the Ehrenfest theorem for a particle-in-an-infinite-step-potential has been explicitly confirmed for the general state Ψ given by Eq. (11).

4. Particle-on-a-half-line

In this section, we begin by presenting the formal time derivatives of the mean values of the position ($\hat{x} = x$) and momentum ($\hat{p} = -i\hbar\partial/\partial x$) operators for a particle-on-a-half-line ($x \in (-\infty, 0] \equiv \Omega$). The formal computation of these derivatives for a particle living in the entire real line lead us to the standard Ehrenfest theorem (provided that the state and its derivative tend to zero at infinity) [26]. For a particle moving in a closed interval (*i.e.*, in a box), a strictly formal study of the quantities $d\langle \hat{x} \rangle/dt$ and $d\langle \hat{p} \rangle/dt$ as well their corresponding boundary terms has been recently made [27].

Let $\hat{o}$ be a time-independent operator (such as $\hat{x}$ or $\hat{p}$). The time derivative of this operator's mean value $\langle \hat{o} \rangle_u = \langle u, \hat{o}u \rangle$ in the normalized state $u = u(x,t) \in \mathcal{L}^2(\Omega)$, which evolves in time according to the Schrödinger equation $\partial u/\partial t = -i\hat{h}u/\hbar$ (the Hamiltonian operator is

$$\hat{h} = -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial x^2} + \varphi(x), \quad (31)$$

and $\varphi(x)$ is the external potential inside Ω), can be calculated as follows:

$$\frac{d}{dt} \langle \hat{o} \rangle_u = \left\langle \frac{\partial u}{\partial t}, \hat{o}u \right\rangle + \left\langle u, \hat{o}\frac{\partial u}{\partial t} \right\rangle = \frac{i}{\hbar} \langle \hat{h}u, \hat{o}u \rangle - \frac{i}{\hbar} \langle u, \hat{o}\hat{h}u \rangle = \frac{i}{\hbar} \Big(\langle \hat{h}u, \hat{o}u \rangle - \langle u, \hat{h}\hat{o}u \rangle \Big) + \frac{i}{\hbar} \langle u, [\hat{h}, \hat{o}]u \rangle, \quad (32)$$

where $[\hat{h}, \hat{o}] = \hat{h}\hat{o} - \hat{o}\hat{h}$, as usual. In the case where $\hat{o} = \hat{x}$, the following results are obtained

$$\langle \hat{h}u, \hat{x}u \rangle - \langle u, \hat{h}\hat{x}u \rangle = -\frac{\hbar^2}{2M} \left[x \left(u \frac{\partial \bar{u}}{\partial x} - \bar{u} \frac{\partial u}{\partial x} \right) - \bar{u}u \right] \Bigg|_{-\infty}^{0}, \quad (33)$$

and

$$\langle u, [\hat{h}, \hat{x}]u \rangle = -\frac{i\hbar}{M} \langle \hat{p} \rangle_u. \quad (34)$$

For the (free) particle-on-a-half-line, we take $\varphi(x) = 0$. Moreover, we impose the Dirichlet boundary condition, $u(0,t) = 0$; however, we also expect that $u(-\infty, t)$ tends strongly to zero. These boundary conditions imply that the boundary term in (33) is zero. Note that, with the Dirichlet boundary condition at $x = 0$ (and, as usual, ignoring the exact behaviour of the functions in question at $x = -\infty$, *i.e.*, by assuming that these are essentially normalized functions in Ω), the operators $\hat{p}$ and $\hat{h}$ (in addition to $\hat{x}$) are Hermitian. Moreover, $\hat{h}$ is also self-adjoint; in fact, there exists a one-parameter family of self-adjoint Hamiltonians (see, for example, the pedagogical Refs. 7 and 28). However, the momentum operator is not self-adjoint and has no self-adjoint extension [7]. After substituting Eqs. (33) and (34) into Eq. (32) (with $\hat{o} = \hat{x}$), we obtain the expected result:

$$\frac{d}{dt} \langle \hat{x} \rangle_u = \frac{1}{M} \langle \hat{p} \rangle_u. \quad (35)$$

Likewise, in the case where $\hat{o} = \hat{p}$, the following results are obtained:

$$\langle \hat{h}u, \hat{p}u \rangle - \langle u, \hat{h}\hat{p}u \rangle = i\hbar \frac{\hbar^2}{2m} \left(\frac{\partial u}{\partial x} \frac{\partial \bar{u}}{\partial x} - \bar{u} \frac{\partial^2 u}{\partial x^2} \right) \Bigg|_{-\infty}^{0}, \quad (36)$$

and

$$\langle u, [\hat{h}, \hat{p}]u \rangle = i\hbar \left\langle \frac{d\varphi}{dx} \right\rangle_u = -i\hbar \langle \hat{f} \rangle_u. \quad (37)$$

where $\hat{f} = -d\varphi(x)/dx$ is the external classical force upon the particle on the half-line. By substituting Eqs. (36)

and (37) into Eq. (32) (with $\hat{o} = \hat{p}$) and after imposing $\varphi(x) = 0$ ($\Rightarrow \hat{f} = 0$) and the boundary conditions $u(0,t) = 0$ and $u(-\infty,t) = 0$, we obtain the following result:

$$\frac{d}{dt}\langle\hat{p}\rangle_u = -\frac{\hbar^2}{2M}\left|\frac{\partial u}{\partial x}\right|^2\Bigg|_{-\infty}^{0}. \qquad (38)$$

If the wave function $u = u(x,t)$ tends to zero for $x \to -\infty$, at least as $|\, x \,|^{-\frac{1}{2}-\epsilon}$ with $\epsilon > 0$ (and therefore $u \in \mathcal{L}^2(\Omega)$), then its derivative $\partial u(x,t)/\partial x$ also tends to zero there. Hence, relation (38) reduces to

$$\frac{d}{dt}\langle\hat{p}\rangle_u = -\frac{\hbar^2}{2M}\left|\frac{\partial u}{\partial x}\right|^2\Bigg|_{(x=0)} \qquad (39)$$

This specific result has been previously noted [15, 29]. Notice that the right-hand side of Eq. (38) can be written as the mean value of the (nonlocal) quantum force

$$f_B = f_B(x,t) \equiv -\frac{\hbar^2}{2M}\frac{1}{|u|^2}\frac{\partial}{\partial x}\left|\frac{\partial u}{\partial x}\right|^2. \qquad (40)$$

Because

$$\langle f_B\rangle_u = \int_{\Omega} dx\, f_B(x,t)\,|u(x,t)|^2$$

is always equal to a certain quantity evaluated at one end (say, $x = 0$) minus the same quantity evaluated at the other end ($x = -\infty$), f_B can be considered a boundary quantum force. Thus, in this case, the Ehrenfest theorem consists of Eq. (35) and the following expression:

$$\frac{d}{dt}\langle\hat{p}\rangle_u = \langle f_B\rangle_u. \qquad (41)$$

Note that, for a particle-in-an-infinite-step-potential (*i.e.*, $u \to \Psi$, $(x = 0) \to (x = +\infty)$), the boundary term in (36) is zero (*i.e.*, $\langle f_B\rangle_\Psi = 0$). In fact, in the open interval $\Omega = (-\infty, +\infty)$, Ψ and its derivative $\partial\Psi/\partial x$ tend to zero for $x \to \pm\infty$.

Let us write the wave packet $u = u(x,t)$ in the following form:

$$u(x,t) = \int_0^\infty \frac{dk}{\sqrt{2\pi}}\,A(k)\,u_k(x)\,\exp\left(-i\frac{E_k}{\hbar}t\right)$$
$$(-\infty < x \le 0), \qquad (42)$$

where the eigenfunctions $u_k(x)$ are given in Eq. (13). Clearly, the general state $\Psi(x,t)$ given in Eq. (11) can be written as follows (see Eq. (12)): $\Psi(x,t) = u(x,t)\Theta(-x)$. Hence, the mean values, $\langle\hat{X}\rangle_\Psi$ and $\langle\hat{P}\rangle_\Psi$, are equal to $\langle\hat{x}\rangle_u$ and $\langle\hat{p}\rangle_u$, respectively. Thus, Eqs. (29) and (35) are equivalent. Now, by substituting the wave packet $u(x,t)$ into the right-hand-side of Eq. (39), we obtain:

$$\langle f_B\rangle_u = -4\int_0^\infty\int_0^\infty \frac{dk\,dk'}{2\pi}\,\bar{A}(k)A(k')$$
$$\times\sqrt{E_k E_{k'}}\,\exp\left[i\frac{(E_k - E_{k'})}{\hbar}t\right]. \qquad (43)$$

This result is precisely the mean value $\langle\hat{F}\rangle_\Psi$ for a particle-in-an-infinite-step-potential (see Eq. (17)). This is an important result of our paper. Consequently, Eqs. (30) and (41) are also equivalent. Final note: we very recently learned of Ref. 30 in which it was proved that the right-hand side of formula (39) is equal to the mean value of the external classical force for a particle-in-an-infinite-step-potential ($\hat{F} = -dV(x)/dx$). However, in that reference, this specific result was directly obtained by multiplying the Schrödinger equation for Ψ by $\partial\bar{\Psi}/\partial x$, adding the respective complex conjugate relation, and integrating each term of the resulting expression over a small interval $(-\epsilon, +\epsilon)$, $\epsilon \to 0$ [30].

5. Conclusions

We have studied the Ehrenfest theorem and the issue of average forces for a particle ultimately restricted to a semi-infinite interval by an impenetrable wall in one dimension (inside the latter region, our particle is a free particle after all). We have noticed two ways to achieve that restriction. One of these leads us to the particle-in-an-infinite-step-potential, and we inevitably have the Dirichlet boundary condition (in our paper, at $x = 0$). The other method leads us to the particle-on-a-half-line, and the Dirichlet boundary condition is just one more condition. In fact, there exists a one-parameter family of boundary conditions for the (self-adjoint) Hamiltonian for a particle-on-a-half-line. In each situation, we have shown that the mean values of the position, momentum and force, as functions of time, verify an Ehrenfest theorem that makes sense (the state of the particle being in each case a general wave packet that is a continuous superposition of energy eigenstates for the respective Hamiltonian). However, the involved force is not the same in each case. In fact, we have the usual external classical force in the first case and a type of nonlocal boundary quantum force in the second case. In spite of these differences, the corresponding mean values of these quantities give the same results. Accordingly, the Ehrenfest equations in the two situations are equivalent, and the internal consistency of the formalism of quantum mechanics is assured. We hope that our article will be of genuine interest to all those who are interested in the fundamental aspects of quantum mechanics.

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