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# Confinement, average forces, and the Ehrenfest theorem for a one-dimensional particle

SALVATORE DE VINCENZO
Escuela de Física, Facultad de Ciencias, Universidad Central de Venezuela,
A.P. 47145, Caracas 1041-A, Venezuela
E-mail: salvatore.devincenzo@ucv.ve

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**Abstract.** The topics of confinement, average forces, and the Ehrenfest theorem are examined for a particle in one spatial dimension. Two specific cases are considered: (i) A free particle moving on the entire real line, which is then permanently confined to a line segment or 'a box' (this situation is achieved by taking the limit $V_0 \to \infty$ in a finite well potential). This case is called 'a particle-in-an-infinite-square-well-potential'. (ii) A free particle that has always been moving inside a box (in this case, an external potential is not necessary to confine the particle, only boundary conditions). This case is called 'a particle-in-a-box'. After developing some basic results for the problem of a particle in a finite square well potential, the limiting procedure that allows us to obtain the average force of the infinite square well potential from the finite well potential problem is re-examined in detail. A general expression is derived for the mean value of the external classical force operator for a particle-in-an-infinite-square-well-potential, $\hat{F}$. After calculating similar general expressions for the mean value of the position ($\hat{X}$) and momentum ($\hat{P}$) operators, the Ehrenfest theorem for a particle-in-an-infinite-square-well-potential (i.e., $\mathrm{d}\langle\hat{X}\rangle/\mathrm{d}t = \langle\hat{P}\rangle/M$ and $\mathrm{d}\langle\hat{P}\rangle/\mathrm{d}t = \langle\hat{F}\rangle$) is proven. The formal time derivatives of the mean value of the position ($\hat{x}$) and momentum ($\hat{p}$) operators for a particle-in-a-box are re-introduced. It is verified that these derivatives present terms that are evaluated at the ends of the box. Specifically, for the wave functions satisfying the Dirichlet boundary condition, the results, $\mathrm{d}\langle\hat{x}\rangle/\mathrm{d}t = \langle\hat{p}\rangle/M$ and $\mathrm{d}\langle\hat{p}\rangle/\mathrm{d}t = \text{b.t.}+\langle\hat{f}\rangle$, are obtained where b.t. denotes a boundary term and $\hat{f}$ is the external classical force operator for the particle-in-a-box. Thus, it appears that the expected Ehrenfest theorem is not entirely verified. However, by considering a normalized complex general state that is a combination of energy eigenstates to the Hamiltonian describing a particle-in-a-box with $v(x) = 0$ ($\Rightarrow \hat{f} = 0$), the result that the b.t. is equal to the mean value of the external classical force operator for the particle-in-an-infinite-square-well-potential is obtained, i.e., $\mathrm{d}\langle\hat{p}\rangle/\mathrm{d}t$ is equal to $\langle\hat{F}\rangle$. Moreover, the b.t. is written as the mean value of a quantity that is called boundary quantum force, $f_\mathrm{B}$. Thus, the Ehrenfest theorem for a particle-in-a-box can be completed with the formula $\mathrm{d}\langle\hat{p}\rangle/\mathrm{d}t = \langle f_\mathrm{B}\rangle$.

**Keywords.** Quantum mechanics; Schrödinger equation; confinement in one dimension; average forces; Ehrenfest theorem.

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## 1. Introduction

The problem of a non-relativistic quantum particle with a mass of $M$ moving in a square well potential of finite (arbitrary) depth $V_0$ and width $a$ is one of the basic problems in one-dimensional (1D) quantum mechanics [1,2]. Some time ago, Rokhsar considered this problem as a starting model to verify Newton's second law in mean values (or in Ehrenfest's version), $\mathrm{d}\langle\hat{P}\rangle/\mathrm{d}t = \langle\hat{F}\rangle$, in the case in which the well is infinitely deep [3]. In fact, the (external) classical force for a particle-in-a-finite-square-well-potential was explicitly used in that reference. It was noted by Rokhsar that, in the approximation $V_0 \gg E$ (where $E$ is the energy of the particle), i.e., when the well depth becomes very large, the matrix elements of the force do not always vanish, and these do not depend on $V_0$. Hence (through a pedagogical example), the equation $\mathrm{d}\langle\hat{P}\rangle/\mathrm{d}t = \langle\hat{F}\rangle$ could be verified for a particle constrained to move in the real line but walled in by two impenetrable barriers or infinite potential walls. We have seen a similar treatment to that used in ref. [3] in a somewhat old book of solved problems in quantum mechanics [4]. In fact, problem 25(1) of that reference proposed an estimate of the average force applied by the particle upon a wall of the infinite square well, i.e., an infinitely high wall (the state of the particle being a stationary state). Very recently, we realized that the specific topic 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, has also been treated [5].

The purpose of this paper is to examine and relate the topics of confinement, average forces, and the Ehrenfest theorem for a particle in one spatial dimension. We consider two specific cases or modes of confinement that we have identified: (i) A free particle moving on the entire real line, which is then permanently confined to a line segment or 'a box' (this result is achieved by taking the limit $V_0 \to \infty$ in a finite well potential). We shall call this case 'a particle-in-an-infinite-square-well-potential' (and its respective wave function satisfies the 'extended' Dirichlet boundary condition $\psi(x \le 0) = \psi(x \ge a) = 0$). (ii) A free particle that has always been moving inside a box (in this case, an external potential is not necessary to confine the particle; rather, it is confined by boundary conditions). We shall call this case 'a particle-in-a-box', and one of the boundary conditions that the wave function can satisfy is the Dirichlet boundary condition, $u(x = 0) = u(x = a) = 0$ (in relation to this case, we only consider this boundary condition in this paper). After developing some basic results for the problem of a particle in a finite square well potential (§2), we re-examine in detail the somewhat little known limiting procedure that allows us to obtain the average force for the problem of the infinite square well potential from the finite well potential problem (§3). We have certainly seen in some articles that the eigenfunctions and eigenvalues of the infinite square well potential are obtained from the eigenfunctions and eigenvalues of the finite well potential [3,6,7] (i.e., by explicitly taking the limit $V_0 \to \infty$ in the latter $V_0$-dependent quantities). Also, in §3, we derive a general expression for the mean value of the external classical force operator for the particle-in-an-infinite-square-well-potential, $\hat{F} = -\mathrm{d}V(x)/\mathrm{d}x$. This formula was written in terms of the energy eigenvalues of the infinite square well potential (which are equal to those for the particle-in-a-box). In this calculation, the state of the particle is zero everywhere, but it is a combination of energy eigenstates of the Hamiltonian describing a particle-in-a-box just inside the infinite square well potential. In §4, after calculating similar general expressions of the mean value of the position ($\hat{X}$) and momentum ($\hat{P}$) operators, the Ehrenfest theorem for a particle-in-an-infinite-square-well-potential (i.e., $\mathrm{d}\langle\hat{X}\rangle/\mathrm{d}t = \langle\hat{P}\rangle/M$ and $\mathrm{d}\langle\hat{P}\rangle/\mathrm{d}t = \langle\hat{F}\rangle$) is proven. In §5, we start out by presenting the formal time derivatives of the mean values of the position ($\hat{x}$) and momentum ($\hat{p}$) operators for a particle-in-a-box. These derivatives present terms that are evaluated at the ends of the box. Specifically, for the Dirichlet boundary condition we find that $\mathrm{d}\langle\hat{x}\rangle/\mathrm{d}t = \langle\hat{p}\rangle/M$; nevertheless, $\mathrm{d}\langle\hat{p}\rangle/\mathrm{d}t$ is equal to a boundary term plus $\langle\hat{f}\rangle$ (where $\hat{f} = -\mathrm{d}v(x)/\mathrm{d}x$ is the external classical force upon the particle inside the box). Hence, it appears that the expected (or usual) Ehrenfest theorem is not entirely verified. However, by considering a normalized complex general state that is a combination of energy eigenstates of the Hamiltonian describing a particle-in-a-box, with $v(x) = 0$ ($\Rightarrow \hat{f} = 0$), we obtain the significant result that the boundary term for a particle-in-a-box is just equal to the mean value of the external classical force operator for the particle-in-an-infinite-square-well-potential, i.e., $\mathrm{d}\langle\hat{p}\rangle/\mathrm{d}t = \langle\hat{F}\rangle$. Moreover, that boundary term can be written as the average value of a quantity, which we call a boundary quantum force, $f_{\mathrm{B}}$. Thus, the Ehrenfest theorem for a particle-in-a-box is completed with the formula $\mathrm{d}\langle\hat{p}\rangle/\mathrm{d}t = \langle f_{\mathrm{B}}\rangle$. Note that, throughout the article, we use capital letters to denote the operators in the particle-in-an-infinite-square-well-potential problem, and lower-case letters in the particle-in-a-box problem. Finally, we draw some conclusions in §6. We believe that the content and results that follow should be enlightening to all those who are interested in the fundamental aspects of quantum mechanics.

## 2. The finite square-well

Let us consider the following finite square-well (external) potential of depth $V_0$:

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

where $\Theta(y)$ is the Heaviside step function. Note that $V(x) = 0$ for $0 < x < a$ and $V(x) = +V_0$ elsewhere (in the limit $V_0 \to \infty$, we obtain the infinite square well potential). Because the derivative of $\Theta(y)$ is the Dirac delta function ($\delta(y)$), the external classical force (or force operator) upon the particle ($\hat{F} = F(x) = -\mathrm{d}V(x)/\mathrm{d}x$) can be written as follows:

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

The most general solution of the (eigenvalue) Schrödinger equation $\hat{H}\phi(x) = \varepsilon\phi(x)$ for energies $V_0 > \varepsilon > 0$ can be written as follows:

$$\phi(x) = \begin{cases} A\exp(+\kappa x), & x \le 0, \\ B\exp(+ikx) + C\exp(-ikx), & 0 \le x \le a, \\ D\exp(-\kappa x), & x \ge a, \end{cases} \tag{3}$$

where $A$, $B$, $C$ and $D$ are constants to be determined from the boundary conditions imposed on $\phi(x)$ and its normalization. Moreover, $\kappa = \sqrt{2M(V_0-\varepsilon)}/\hbar$ and $k = \sqrt{2M\varepsilon}/\hbar$ 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 permanently living on the whole real line, $\mathbb{R}$. This (self-adjoint) operator (for a finite $V_0$) is assumed to act on continuously differentiable functions belonging (and their second derivatives) to the well-known space $\mathcal{L}^2(\mathbb{R})$ [6]. Thus, any eigenfunction of $\hat{H}$, $\phi(x)$, and its derivative, $\phi'(x)$, must be continuous at $x = 0$ and $x = a$. Therefore, at $x = 0$ we have $\phi(0-) = \phi(0+)$ and $\phi'(0-) = \phi'(0+)$ (where $\phi(x\pm) \equiv \lim_{\epsilon\to 0}\phi(x \pm \epsilon)$, with $\epsilon > 0$). By using these boundary conditions, we obtain the following:

$$\begin{aligned} B &= \frac{(\kappa + ik)}{2ik}A, \\ C &= \frac{(-\kappa + ik)}{2ik}A, \end{aligned} \quad \Rightarrow \ -\frac{B}{C} = \frac{\kappa + ik}{\kappa - ik}. \tag{5}$$

Also, at $x = a$ we have $\phi(a-) = \phi(a+)$ and $\phi'(a-) = \phi'(a+)$. By using these boundary conditions, we obtain the following:

$$\begin{aligned} B &= \frac{(-\kappa + ik)}{2ik}\exp(-\kappa a)\exp(-ika)D, \\ C &= \frac{(\kappa + ik)}{2ik}\exp(-\kappa a)\exp(ika)D, \end{aligned} \quad \Rightarrow \ -\frac{B}{C}\exp(2ika) = \frac{\kappa - ik}{\kappa + ik}. \tag{6}$$

Substituting eq. (5) into eq. (6), we obtain the formula that gives us the possible (discrete) eigenvalues of $\hat{H}$ (i.e., the spectral equation for the bound states):

$$\left(\frac{\kappa - ik}{\kappa + ik}\right)^2 = \exp(2ika). \tag{7}$$

Let us first consider the case in which the solution of eq. (7) is given by the following equation:

$$\frac{\kappa - ik}{\kappa + ik} = -\exp(ika) \ \Rightarrow \ \tan\left(\frac{ka}{2}\right) = \frac{\kappa}{k}. \tag{8}$$

From the definitions given in the beginning for $\kappa$ and $k$, we can write the following formula:

$$\kappa^2 + k^2 = k_0^2, \tag{9}$$

where $k_0 = \sqrt{2MV_0}/\hbar$. Now, by substituting eq. (8) into eq. (9), we obtain the following:

$$\cos^2\left(\frac{ka}{2}\right) = \left(\frac{k}{k_0}\right)^2 \ \Rightarrow \ \left|\cos\left(\frac{ka}{2}\right)\right| = \frac{k}{k_0}. \tag{10}$$

The first set of numerical values for the allowed energies is obtained from the transcendental equation (10). For example, this equation can be solved graphically by intersecting a straight line with a slope of $1/(k_0 a)$ with the absolute value of the cosine of the half-angle (by considering $ka$ as the independent variable). Note that these values depend on the depth of the well. The respective eigenfunctions are obtained, for example, by expressing the constants $B$, $C$, and $D$ in $\phi(x)$ (eq. (3)) in terms of $A$. In fact, the constant $B$ as a function of $A$ ($B(A)$) is one of the equations in (5). Likewise, by using the second result in eq. (5) ($B(C)$) and the first result in eq. (8), we first obtain the relation $C = \exp(ika)B$; then, by using $B(A)$, we can write $C = (\kappa + ik)\exp(ika)A/2ik$. To express $D$ in terms of $A$, we first substitute $\exp(ika)$ (obtained from the first result in eq. (8)) into '$B$ vs. $D$' given in eq. (6). Then, by eliminating the constant $B$ with $B(A)$ we finally obtain $D = \exp(\kappa a)A$. Now, we can write $\phi(x)$ as follows:

$$\phi(x) = \begin{cases} A\exp(+\kappa x), & x \le 0, \\ A\left(\dfrac{\kappa + ik}{2ik}\right)\{\exp(+ikx) + \exp[-ik(x-a)]\}, & 0 \le x \le a, \\ A\exp[-\kappa(x-a)], & x \ge a, \end{cases} \tag{11}$$

where the remaining constant $A$ is determined by normalization. Note that these eigenfunctions satisfy the relation $\phi(0) = \phi(a)$. Therefore, the respective probability density, $\rho(x) = |\phi(x)|^2$, verifies $\rho(0) = \rho(a)$. In fact, we can define space-shifted eigenfunctions, $\tilde{\phi}(x) \equiv \phi(u)$, where $u \equiv x + (a/2)$, which verify $\tilde{\phi}(x) = \tilde{\phi}(-x)$, i.e., they are positive-parity states.

Let us now consider the case in which the solution of eq. (7) is given by the following equation:

$$\frac{\kappa - ik}{\kappa + ik} = \exp(ika) \Rightarrow \tan\left(\frac{ka}{2}\right) = -\frac{k}{\kappa}. \tag{12}$$

By substituting eq. (12) into eq. (9), we obtain the following:

$$\sin^2\left(\frac{ka}{2}\right) = \left(\frac{k}{k_0}\right)^2 \Rightarrow \left|\sin\left(\frac{ka}{2}\right)\right| = \frac{k}{k_0}. \tag{13}$$

This transcendental equation gives us the second set of eigenvalues of the Hamiltonian in eq. (4). The respective eigenfunctions are obtained analogously to the previous case, but now eq. (12) is used instead of eq. (8). The result is the following:

$$\phi(x) = \begin{cases} A\exp(+\kappa x), & x \le 0, \\ A\left(\dfrac{\kappa + ik}{2ik}\right)\{\exp(+ikx) - \exp[-ik(x-a)]\}, & 0 \le x \le a, \\ -A\exp[-\kappa(x-a)], & x \ge a. \end{cases} \tag{14}$$

Note that these eigenfunctions satisfy the relation $\phi(0) = -\phi(a)$. Hence, the probability density verifies $\rho(0) = \rho(a)$ again. Moreover, the space-shifted eigenfunctions ($\tilde{\phi}(x)$) verify $\tilde{\phi}(x) = -\tilde{\phi}(-x)$, i.e., they are negative-parity states. If one calculates the mean value of the operator $\hat{F}$ (eq. (2)) in any stationary state $\phi(x)$, the result is always zero. In effect, the following equation can be written:

$$\langle\hat{F}\rangle_\phi = \langle\phi, \hat{F}\phi\rangle = \int_{-\infty}^{+\infty} \mathrm{d}x\, F(x)\,|\phi(x)|^2 = -V_0\,[\rho(a) - \rho(0)] = 0. \tag{15}$$

## 3. The infinite well depth limit

In the limit $V_0 \to \infty$, the finite square well becomes an infinite square well. The eigenvalues of the Hamiltonian operator (eq. (4)) in the potential

$$V(x) = \lim_{V_0\to\infty} V_0 \left[\Theta(-x) + \Theta(x-a)\right], \quad -\infty < x < +\infty, \tag{16}$$

are obtained from eqs (10) and (13). By using the definitions for $k$ and $k_0$, we obtain the following results, respectively:

$$\left|\cos\left(\frac{ka}{2}\right)\right| = \frac{k}{k_0} = \sqrt{\frac{\varepsilon}{V_0}} \to 0 \Rightarrow k \to \frac{\pi}{a}, \frac{3\pi}{a}, \frac{5\pi}{a}, \ldots,$$

$$\left|\sin\left(\frac{ka}{2}\right)\right| = \frac{k}{k_0} = \sqrt{\frac{\varepsilon}{V_0}} \to 0 \Rightarrow k \to \frac{2\pi}{a}, \frac{4\pi}{a}, \frac{6\pi}{a}, \ldots.$$

Therefore,

$$k \to \frac{n\pi}{a} \equiv K_n \Rightarrow \varepsilon \to \frac{\hbar^2}{2M}\left(\frac{n\pi}{a}\right)^2 \equiv E_n, \quad n = 1, 2, 3, \ldots. \tag{17}$$

Note that the corresponding eigenfunctions for odd (even) $n$ are obtained from the solution given in eq. (11) (eq. (14)). Clearly, in the limit $V_0 \to \infty$, all the eigenfunctions verify the result $\phi(x) \to 0 \equiv \psi_n(x)$ for $x \leq 0$ and $x \geq a$ (this is true because $1/\kappa \approx \hbar/\sqrt{2MV_0} \to 0$). In order to obtain $\phi(x)$ inside the (infinite) well (i.e., $\psi_n(x)$), we need to use the following two results:

$$\exp(ika) = \mp\left(\frac{\kappa - ik}{\kappa + ik}\right) \approx \mp\left(\frac{\sqrt{V_0} - i\sqrt{\varepsilon}}{\sqrt{V_0} + i\sqrt{\varepsilon}}\right) \to \mp 1,$$

where the minus (plus) sign applies to the solution given in eq. (11) (eq. (14)), and

$$\frac{\kappa + ik}{2ik} \approx \frac{1}{2i}\sqrt{\frac{V_0}{\varepsilon}}.$$

Throughout this paper, we use the approximation sign '$\approx$' in any expression in which $V_0 \gg \varepsilon$. By substituting these results into $\phi(x)$ for the interval $0 \leq x \leq a$ (see eqs (11) and (14)), with $k \to n\pi/a$ and $\varepsilon \to E_n$, we obtain the following equation:

$$\phi(x) \equiv \phi_n(x) \approx A\sqrt{\frac{V_0}{E_n}} \sin\left(\frac{n\pi x}{a}\right), \quad n = 1, 2, 3, \ldots, \quad 0 \leq x \leq a. \tag{18}$$

Because $V_0 \gg \varepsilon$, there is practically no contribution from the regions outside the well to the normalization. Thus, we can write the following (with $A \in \mathbb{R}$):

$$1 = \lim_{V_0\to\infty} \int_{-\infty}^{+\infty} \mathrm{d}x \; |\phi_n(x)|^2 = \lim_{V_0\to\infty} \int_0^a \mathrm{d}x \; |\phi_n(x)|^2$$
$$\approx A^2 \frac{V_0}{E_n} \int_0^a \mathrm{d}x \; \sin^2\left(\frac{n\pi x}{a}\right).$$

By integrating, we obtain the following equation:

$$A \approx \sqrt{\frac{2}{a}}\sqrt{\frac{E_n}{V_0}}. \tag{19}$$

If we substitute this result into eq. (18), we arrive at the usual result:

$$\phi_n(x) \approx \sqrt{\frac{2}{a}}\sqrt{\frac{E_n}{V_0}}\sqrt{\frac{V_0}{E_n}}\sin\left(\frac{n\pi x}{a}\right),$$

$$\Rightarrow \psi_n(x) = \lim_{V_0\to\infty}\phi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right), \quad n = 1, 2, 3, \ldots . \tag{20}$$

Note that this result is independent of $V_0$ at the end, i.e., even before explicitly taking the limit of $V_0 \to \infty$. Summing up, the eigenfunctions of the Hamiltonian $\hat{H}$ (eq. (4)) with the infinite square well potential (eq. (16)) can be written as follows:

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)[\Theta(x) - \Theta(x-a)], \quad n = 1, 2, 3, \ldots, \tag{21}$$

where $x \in (-\infty, +\infty)$. Moreover, they satisfy the 'extended' Dirichlet boundary condition $\psi_n(x \le 0) = \psi_n(x \ge a) = 0$. We would like to stress that, precisely because of this boundary condition, the operator $\hat{H}$ can be considered equivalent to a non-self-adjoint kinetic energy operator $\hat{T}$ (see eq. (4)) acting on functions $\psi(x) \in \mathcal{L}^2(\mathbb{R})$ with $(\hat{T}\psi)(x) \in \mathcal{L}^2(\mathbb{R})$ and verifying the somewhat strong boundary condition $\psi(x \le 0) = \psi(x \ge a) = 0$ [8].

The procedure we have used to obtain $\psi_n(x)$, although correct, does not give us directly the approximate value that the eigenfunctions assume for $x = 0-$ and $x = a+$ as functions of $V_0$ (when $V_0 \gg \varepsilon$). We can solve this issue by introducing a new constant $A'$, which is related to $A$ as follows (observe the solutions in eqs (11) and (14)):

$$A = \frac{k}{\kappa + ik}A'. \tag{22}$$

By substituting eq. (22) into eqs (11) and (14) and using the result $A \approx \sqrt{E_n/V_0}\,A'$, we obtain the following result:

$$\phi(x) \equiv \phi_n(x) \approx \begin{cases} A'\sqrt{\dfrac{E_n}{V_0}}\exp(+\kappa x), & x \le 0, \\ A'\dfrac{1}{2i}\{\exp(+iK_n x) \pm \exp[-iK_n(x-a)]\}, & 0 \le x \le a, \\ \pm A'\sqrt{\dfrac{E_n}{V_0}}\exp[-\kappa(x-a)], & x \ge a, \end{cases} \tag{23}$$

where the upper (lower) sign applies to the solution given in eq. (11) (eq. (14)). Moreover, $\kappa \approx \sqrt{2MV_0}/\hbar$ and $\exp(iK_n a) = \mp 1$. Clearly, from (23), we have that $\phi_n(x) \to 0 \equiv \psi_n(x)$ for $x \notin (0, a)$ and $\psi_n(x) = A' \sin(n\pi x/a)$ for $x \in [0, a]$, where $A' = \sqrt{2/a}$. This result is consistent with the result given in eq. (21). Nevertheless (from (23)), we can also write the results as follows:

$$\phi_n(0) \approx \sqrt{\frac{2}{a}}\sqrt{\frac{E_n}{V_0}}\,, \quad \phi_n(a) \approx (-1)^{n+1}\sqrt{\frac{2}{a}}\sqrt{\frac{E_n}{V_0}}\,, \quad n = 1, 2, 3, \ldots . \tag{24}$$

Therefore, the respective stationary-state probability density, $\rho_n(x) = |\phi_n(x)|^2$, satisfies the periodic boundary condition:

$$\rho_n(0) = \rho_n(a) \approx \frac{2}{a}\frac{E_n}{V_0}\,, \quad n = 1, 2, 3, \ldots . \tag{25}$$

As a consequence, the mean value of the force operator is zero (see expression (15)). However, it is also important to note that $\langle \hat{F} \rangle_{\psi_n} = \langle \psi_n, \hat{F}\psi_n \rangle$ is really independent of $V_0$ (which is valid when $V_0$ tends to infinity). In effect, if we substitute the relations given in eq. (25) into eq. (15), we obtain the following:

$$\langle \hat{F} \rangle_{\psi_n} = \lim_{V_0 \to \infty} -V_0\,[\rho_n(a) - \rho_n(0)] = \lim_{V_0 \to \infty} -V_0 \left( \frac{2}{a}\frac{E_n}{V_0} - \frac{2}{a}\frac{E_n}{V_0} \right)$$
$$= -\left( \frac{2}{a}E_n - \frac{2}{a}E_n \right) = 0\,, \quad n = 1, 2, 3, \ldots . \tag{26}$$

This result also tells us that the average force encountered by the particle when it hits the (infinite) wall at $x = 0$ is $+2E_n/a$, and at $x = a$ it is $-2E_n/a$ (which is precisely the result obtained in ref. [4]).

In order to procure a non-trivial mean value of the force operator, let us consider a normalized complex general state $\Psi = \Psi(x, t)$ of the following form:

$$\Psi(x, t) = \sum_{n=1} A_n\, \psi_n(x) \exp\left( -i\frac{E_n}{\hbar}t \right), \quad -\infty < x < +\infty, \tag{27}$$

where $\psi_n(x)$ is given by eq. (21). Moreover, we have $\sum_{n=1} |A_n|^2 = 1$ because $\|\Psi\|^2 \equiv \langle \Psi, \Psi \rangle = 1$ (for all $t$). By substituting eq. (21) into eq. (27), we can also write the following result:

$$\Psi(x, t) = \sum_{n=1} A_n u_n(x) \exp\left( -i\frac{E_n}{\hbar}t \right) [\Theta(x) - \Theta(x - a)]\,, \tag{28}$$

where $x \in (-\infty, +\infty)$ and the functions $u_n(x)$ are given by the following expression:

$$u_n(x) = \sqrt{\frac{2}{a}} \sin\left( \frac{n\pi x}{a} \right), \quad n = 1, 2, 3, \ldots . \tag{29}$$

Clearly, in the region $0 \le x \le a$, i.e., just inside the infinite well (the box), $u_n(x)$ coincides with $\psi_n(x)$. The Hamiltonian for a (free) particle permanently confined to a box is simply $\hat{h} \equiv \hat{T}$ (see eq. (4)), and it acts (essentially) on functions $u(x) \in \mathcal{L}^2([0, a])$ such that $(\hat{h}u)(x)$ is also in $\mathcal{L}^2([0, a])$ but obeying the Dirichlet boundary condition, $u(0) = u(a) = 0$. The normalized eigenfunctions to $\hat{h}$ are precisely the functions $u_n(x)$, and its eigenvalues are the same as those of $\hat{H}$ (see eq. (17)).

The mean value of the force operator at time $t$ in the general state given in eq. (27), $\langle \hat{F} \rangle_\Psi = \langle \Psi, \hat{F}\Psi \rangle$, can be written as follows:

$$\langle \hat{F} \rangle_\Psi = \sum_{n,m=1} A_n^* A_m \, (\hat{F})_{n,m} \, \exp\left[ i \frac{(E_n - E_m)}{\hbar} t \right], \tag{30}$$

where the matrix elements of $\hat{F}$, $(\hat{F})_{n,m} = \langle \psi_n, \hat{F}\psi_m \rangle = \int_{-\infty}^{+\infty} \mathrm{d}x \; \psi_n^*(x) F(x) \psi_m(x)$, are given by the following equation (see eq. (2)):

$$(\hat{F})_{n,m} = \lim_{V_0 \to \infty} -V_0 \left[ \phi_n^*(a)\phi_m(a) - \phi_n^*(0)\phi_m(0) \right]. \tag{31}$$

Substituting the results given in eq. (24) into eq. (31), we obtain the following formula:

$$\begin{aligned}(\hat{F})_{n,m} &= \lim_{V_0 \to \infty} -V_0 \left[ (-1)^{n+m} \frac{2}{a} \frac{\sqrt{E_n E_m}}{V_0} - \frac{2}{a} \frac{\sqrt{E_n E_m}}{V_0} \right] \\ &= -\frac{2}{a} \sqrt{E_n E_m} \left[ (-1)^{n+m} - 1 \right].\end{aligned} \tag{32}$$

This result confirms that these matrix elements are really independent of $V_0$ (in the limit $V_0 \to \infty$) [3]. Moreover, they do not vanish when $n$ is even (odd) and $m$ is odd (even). Substituting the formula for $(\hat{F})_{n,m}$ given in eq. (32) into eq. (30), we can write a general expression for the average value of the operator $\hat{F}$:

$$\langle \hat{F} \rangle_\Psi = -\frac{2}{a} \sum_{n,m=1} A_n^* A_m \sqrt{E_n E_m} \left[ (-1)^{n+m} - 1 \right] \exp\left[ i \frac{(E_n - E_m)}{\hbar} t \right]. \tag{33}$$

Importantly, $\langle \hat{F} \rangle_{\Psi \in \mathcal{L}^2(\mathbb{R})}$ is valid in the limit as $V_0$ approaches infinity. Thus, this result should also be formally equal to the mean value of a boundary quantum force (for example, $f_\mathrm{B}$) but employing functions $u \in \mathcal{L}^2([0, a])$ that obey the Dirichlet boundary condition, $u(0) = u(a) = 0$. It is clear that $f_\mathrm{B}$ cannot be simply written as the derivative of the external potential inside the box ($0 \leq x \leq a$) because this potential may be zero. However, the mean value of $f_\mathrm{B}$ (in a state $u \in \mathcal{L}^2([0, a])$) does not vanish. We return to this point in §5.

## 4. Ehrenfest's theorem for a particle-in-an-infinite-square-well-potential

Now we show 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 state $\Psi$ that we used before to calculate the average force have the expected relationship. First, the expectation value of the position operator is the following:

$$\langle \hat{X} \rangle_\Psi = \sum_{n,m=1} A_n^* A_m (\hat{X})_{n,m} \, \exp\left[ i \frac{(E_n - E_m)}{\hbar} t \right], \tag{34}$$

where the matrix elements of $\hat{X}$, $(\hat{X})_{n,m} = \langle \psi_n, \hat{X}\psi_m \rangle = \int_{-\infty}^{+\infty} \mathrm{d}x \; \psi_n^*(x) x \psi_m(x)$, i.e., $(\hat{X})_{n,m} = \int_0^a \mathrm{d}x \; u_n^*(x) x u_m(x)$, are given by the following expression:

$$(\hat{X})_{n,m} = \begin{cases} \dfrac{a}{2}, & n = m, \\ \dfrac{2\hbar^2}{Ma} \dfrac{\sqrt{E_n E_m}}{(E_n - E_m)^2} \left[ (-1)^{n+m} - 1 \right], & n \neq m. \end{cases} \tag{35}$$

Then, we can write a general expression for the average value of the operator $\hat{X}$:

$$\langle\hat{X}\rangle_\Psi = \frac{a}{2} + \frac{2\hbar^2}{Ma}\sum_{n\neq m=1} A_n^* A_m \frac{\sqrt{E_n E_m}}{(E_n - E_m)^2}\left[(-1)^{n+m} - 1\right] \times \exp\left[i\frac{(E_n - E_m)}{\hbar}t\right], \tag{36}$$

where the latter summation sign means $\sum_{n=1}\sum_{m=1}$ with $n \neq m$. Likewise, the expectation value of the momentum operator is as follows:

$$\langle\hat{P}\rangle_\Psi = \sum_{n,m=1} A_n^* A_m (\hat{P})_{n,m} \exp\left[i\frac{(E_n - E_m)}{\hbar}t\right], \tag{37}$$

where the matrix elements of $\hat{P}$, $(\hat{P})_{n,m} = \langle\psi_n, \hat{P}\psi_m\rangle = -i\hbar\int_{-\infty}^{+\infty} \mathrm{d}x\ \psi_n^*(x)\ \psi_m'(x)$, i.e., $(\hat{P})_{n,m} = -i\hbar\int_0^a \mathrm{d}x\ u_n^*(x)u_m'(x)$, are given by the following expression:

$$(\hat{P})_{n,m} = \begin{cases} 0, & n = m, \\ i\dfrac{2\hbar}{a}\dfrac{\sqrt{E_n E_m}}{E_n - E_m}\left[(-1)^{n+m} - 1\right], & n \neq m. \end{cases} \tag{38}$$

Thus, we obtain a general expression for the average value of the operator $\hat{P}$:

$$\langle\hat{P}\rangle_\Psi = i\frac{2\hbar}{a}\sum_{n\neq m=1} A_n^* A_m \frac{\sqrt{E_n E_m}}{E_n - E_m}\left[(-1)^{n+m} - 1\right]\exp\left[i\frac{(E_n - E_m)}{\hbar}t\right]. \tag{39}$$

Note that these two (Hermitian) operators act on functions in $\mathcal{L}^2(\mathbb{R})$ that are different from zero in the (open) interval $(0, a)$ (although, of course, these functions may have nodes there).

It readily follows from eqs (36) and (39) that

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{X}\rangle_\Psi = \frac{1}{M}\langle\hat{P}\rangle_\Psi, \tag{40}$$

and, considering eq. (33), we arrive at the desired result:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{P}\rangle_\Psi = \langle\hat{F}\rangle_\Psi. \tag{41}$$

Thus, the Ehrenfest theorem for a particle-in-an-infinite-square-well potential has been explicitly confirmed for the general state given in eq. (27), which belongs to $\mathcal{L}^2(\mathbb{R})$.

## 5. Ehrenfest's theorem for a particle-in-a-box

In this section, we begin by presenting the formal time derivatives of the mean value of the position ($\hat{x} = x$) and momentum ($\hat{p} = -i\hbar\partial/\partial x$) operators for a particle-in-a-box. Actually, the formal calculation of these derivatives for a particle moving in the entire real line leads us to the Ehrenfest theorem [9,10] (provided that the state and its derivative vanish at infinity). However, for a particle-in-a-box ($x \in [0, a] \equiv \Omega$), the quantities $\mathrm{d}\langle\hat{x}\rangle/\mathrm{d}t$ and $\mathrm{d}\langle\hat{p}\rangle/\mathrm{d}t$ do not always satisfy this theorem. In fact, certain boundary terms (that are not necessarily zero) arise in the formal calculation of these derivatives. Naturally, there is a large variety of boundary conditions that can be imposed in this case, one of them is the Dirichlet boundary condition.

In the (standard) textbooks demonstration of the Ehrenfest theorem, one commonly notes the presence of the commutators $[\hat{h}, \hat{x}]$ and $[\hat{h}, \hat{p}]$, where $\hat{h}$ is the Hamiltonian. Indeed, the formal evaluation of the mean values of these quantities always leads to the Ehrenfest theorem. However, to be strict, the writing of these commutators may be meaningless (especially for the particle-in-a-box problem) unless a proper analysis related to the domains of the involved operators (and their compositions) is made. To examine some of the difficulties that may arise, as well as the weak points of the formal argument, refs [11–14] can be consulted (ref. [12], which was recently discovered by the present author, is particularly important). For a rigorous mathematical derivation of the Ehrenfest theorem (under some not-too-stringent assumptions), see ref. [15]. For a more general (and rigorous) derivation, see ref. [16]. Recently, we have presented a new, pertinent, strictly formal study of this problem in which the boundary terms present in the derivatives of $\langle\hat{x}\rangle$ and $\langle\hat{p}\rangle$ are also written only in terms of the probability density, its spatial derivative, the probability current density, and the external potential [17].

Let $\hat{o}$ be a time-independent operator (such as $\hat{x}$ or $\hat{p}$). The time derivative of its mean value $\langle\hat{o}\rangle_u = \langle u, \hat{o}u\rangle$ in the normalized state $u = u(x, t)$ ($\Rightarrow u \in \mathcal{L}^2(\Omega)$), which evolves in time according to the Schrödinger equation $\partial u/\partial t = -i\hat{h}u/\hbar$ (the Hamiltonian operator is

$$\hat{h} = -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} + v(x), \tag{42}$$

and $v(x)$ is the external potential inside the box), can be calculated as follows:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{o}\rangle_u &= \left\langle\frac{\partial u}{\partial t}, \hat{o}u\right\rangle + \left\langle u, \hat{o}\frac{\partial u}{\partial t}\right\rangle = \frac{i}{\hbar}\langle\hat{h}u, \hat{o}u\rangle - \frac{i}{\hbar}\langle u, \hat{o}\hat{h}u\rangle \\ &= \frac{i}{\hbar}\Big(\langle\hat{h}u, \hat{o}u\rangle - \langle u, \hat{h}\hat{o}u\rangle\Big) + \frac{i}{\hbar}\langle u, [\hat{h}, \hat{o}]u\rangle,\end{aligned} \tag{43}$$

where $[\hat{h}, \hat{o}] = \hat{h}\hat{o} - \hat{o}\hat{h}$, as usual. When $\hat{o} = \hat{x}$, we can write

$$\begin{aligned}\langle\hat{h}u, \hat{x}u\rangle - \langle u, \hat{h}\hat{x}u\rangle &= \left[-\frac{\hbar^2}{2M}\int_\Omega \mathrm{d}x\, x\frac{\partial^2 u^*}{\partial x^2}u + \int_\Omega \mathrm{d}x\, xvu^*u\right] \\ &\quad - \left[-\frac{\hbar^2}{2M}\int_\Omega \mathrm{d}x\, u^*\frac{\partial^2}{\partial x^2}(xu) + \int_\Omega \mathrm{d}x\, xvu^*u\right].\end{aligned}$$

By developing this expression and using the relation

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

we obtain [13,17]

$$\langle\hat{h}u, \hat{x}u\rangle - \langle u, \hat{h}\hat{x}u\rangle = -\frac{\hbar^2}{2M}\left[x\left(\frac{\partial u^*}{\partial x}u - u^*\frac{\partial u}{\partial x}\right) - u^*u\right]\Bigg|_0^a. \tag{44}$$

Moreover,

$$\langle u, [\hat{h}, \hat{x}]u\rangle = -\frac{\hbar^2}{2M}\int_\Omega \mathrm{d}x\, u^* \frac{\partial^2}{\partial x^2}(xu) + \frac{\hbar^2}{2M}\int_\Omega \mathrm{d}x\, xu^* \frac{\partial^2 u}{\partial x^2}.$$

By developing this expression, we obtain

$$\langle u, [\hat{h}, \hat{x}]u\rangle = -\frac{i\hbar}{M}\langle \hat{p}\rangle_u. \tag{45}$$

For the particle-in-a-box, we take $v(x) = 0$ and the Dirichlet boundary condition, $u(0,t) = u(a,t) = 0$. The latter implies that the boundary term in (44) is zero. It should be noted that with this boundary condition, in addition to $\hat{x}$, the operators $\hat{p}$ and $\hat{h}$ are Hermitian (although $\hat{h}$ is also self-adjoint) [14,17]. After substituting eqs (44) and (45) into eq. (43) (with $\hat{o} = \hat{x}$), we obtain the expected result:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \hat{x}\rangle_u = \frac{1}{M}\langle \hat{p}\rangle_u. \tag{46}$$

Likewise, when $\hat{o} = \hat{p}$, we can write

$$\langle \hat{h}u, \hat{p}u\rangle - \langle u, \hat{h}\hat{p}u\rangle = \left[i\hbar\frac{\hbar^2}{2M}\int_\Omega \mathrm{d}x\, \frac{\partial^2 u^*}{\partial x^2}\frac{\partial u}{\partial x} - i\hbar\int_\Omega \mathrm{d}x\, vu^*\frac{\partial u}{\partial x}\right]$$
$$- \left[i\hbar\frac{\hbar^2}{2M}\int_\Omega \mathrm{d}x\, u^*\frac{\partial^2}{\partial x^2}\left(\frac{\partial u}{\partial x}\right) - i\hbar\int_\Omega \mathrm{d}x\, vu^*\frac{\partial u}{\partial x}\right].$$

By integrating by parts the first integral in $\langle u, \hat{h}\hat{p}u\rangle$, we obtain the result [13,17]:

$$\langle \hat{h}u, \hat{p}u\rangle - \langle u, \hat{h}\hat{p}u\rangle = i\hbar\frac{\hbar^2}{2M}\left(\frac{\partial u^*}{\partial x}\frac{\partial u}{\partial x} - u^*\frac{\partial^2 u}{\partial x^2}\right)\Bigg|_0^a. \tag{47}$$

Moreover,

$$\langle u, [\hat{h}, \hat{p}]u\rangle = -i\hbar\frac{\hbar^2}{2M}\int_\Omega \mathrm{d}x\, u^*\frac{\partial}{\partial x}\left(\frac{\partial^2 u}{\partial x^2}\right) + i\hbar\int_\Omega \mathrm{d}x\, u^*\frac{\partial}{\partial x}(vu).$$

By developing the derivative in the last integral above and simplifying, we obtain the result:

$$\langle u, [\hat{h}, \hat{p}]u\rangle = i\hbar\left\langle\frac{\mathrm{d}v}{\mathrm{d}x}\right\rangle_u = -i\hbar\langle \hat{f}\rangle_u, \tag{48}$$

where $\hat{f} = -\mathrm{d}v(x)/\mathrm{d}x$ is the external classical force upon the particle inside the box. By substituting eqs (47) and (48) into eq. (43) (with $\hat{o} = \hat{p}$) and after imposing $v(x) = 0$ ($\Rightarrow \hat{f} = 0$), and the Dirichlet boundary condition, we obtain the following result:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \hat{p}\rangle_u = -\frac{\hbar^2}{2M}\left|\frac{\partial u}{\partial x}\right|^2\Bigg|_0^a. \tag{49}$$

Note that the right-hand side of eq. (49) can be written as the mean value of the quantum force (the latter is a non-local quantity in the sense that it is not a given function of the coordinates, but is dependent of the total quantum state of the system)

$$f_\mathrm{B} = f_\mathrm{B}(x,t) \equiv -\frac{\hbar^2}{2M}\frac{1}{|u|^2}\frac{\partial}{\partial x}\left|\frac{\partial u}{\partial x}\right|^2, \tag{50}$$

in the normalized state $u \in \mathcal{L}^2(\Omega)$, which satisfies the Dirichlet boundary condition. This is so because, $\langle f_\mathrm{B}\rangle_u = \int_\Omega \mathrm{d}x\, f_\mathrm{B}(x,t)\,|u(x,t)|^2$. Hence, $\langle f_\mathrm{B}\rangle_u$ is always equal to a boundary term and $f_\mathrm{B}$ can be considered a boundary quantum force. Thus, in this case, the Ehrenfest theorem consists of eq. (46) and the following expression:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \hat{p}\rangle_u = \langle f_\mathrm{B}\rangle_u. \tag{51}$$

Note that for a particle-in-an-infinite-square-well-potential ($u \to \Psi$, $0 \to -\infty$, $a \to +\infty$), the boundary term in (47) is zero, i.e., $\langle f_\mathrm{B}\rangle_\Psi = 0$. In fact, in the open interval $\Omega = (-\infty, +\infty)$, $\Psi$ and its derivative $\partial\Psi/\partial x$ tend to zero for $x \to \pm\infty$.

If we consider a (normalized) complex general state $u = u(x,t)$ of the form

$$u(x,t) = \sum_{n=1} A_n\, u_n(x) \exp\left(-i\frac{E_n}{\hbar}t\right), \quad 0 \le x \le a, \tag{52}$$

where the eigenfunctions $u_n(x)$ are given in eq. (29), then the general state $\Psi(x,t)$ in eq. (27) can be written as follows:

$$\Psi(x,t) = u(x,t)\,[\Theta(x) - \Theta(x-a)]\,. \tag{53}$$

Therefore, the mean values calculated above for a particle-in-an-infinite-square-well-potential (§4), $\langle \hat{X}\rangle_\Psi$ and $\langle \hat{P}\rangle_\Psi$, are equal to $\langle \hat{x}\rangle_u$ and $\langle \hat{p}\rangle_u$, respectively. Hence, eqs (40) and (46) are fully equivalent. Likewise, the mean value $\langle f_\mathrm{B}\rangle_u$ at time $t$ in the general state given in eq. (52) can be obtained simply by substituting the latter solution into the right-hand side of eq. (49). In this way we obtain the following result:

$$\langle f_\mathrm{B}\rangle_u = -\frac{2}{a}\sum_{n,m=1} A_n^* A_m \sqrt{E_n E_m}\left[(-1)^{n+m} - 1\right] \exp\left[i\frac{(E_n - E_m)}{\hbar}t\right], \tag{54}$$

which precisely coincides with the mean value $\langle \hat{F}\rangle_\Psi$ given in eq. (33) for a particle-in-an-infinite-square-well-potential. This is a significant result of the present paper. Thus, eqs (41) and (51) are also equivalent, i.e., they give the same results, although these are not the same problems.

## 6. Conclusions

To summarize, we have investigated the equations of motion for the mean values of the position and momentum operators (Ehrenfest's theorem) and the average forces for a particle (ultimately) confined in one spatial dimension. We have noted two ways to achieve the confinement in a finite region: one of these leads us to the particle-in-an-infinite-square-well-potential and the other to the particle-in-a-box. In the former case, we necessarily have the Dirichlet boundary condition at the boundaries of the region, but in the latter case this boundary condition is just one more condition. In fact, there are an infinite number of boundary conditions for a quantum particle-in-a-box. For example, we have a one-parameter family of boundary conditions for the self-adjoint operator $\hat{p}$ [6], and some further conditions arise (as the Dirichlet boundary condition) if $\hat{p}$ is only a Hermitian operator. Likewise, we have a four-parameter family of boundary conditions for the self-adjoint operator $\hat{h}$ [6]. Moreover, the (relevant) force for a particle-in-an-infinite-square-well-potential, $\hat{f}$, is not the same (pertinent) force as that for a particle-in-a-box with the Dirichlet boundary condition, $f_{\mathrm{B}}$. In fact, the mean value of $f_{\mathrm{B}}$ depends only on the value of the first derivative of the wave function (more specifically, on its modulus squared) at the boundary. However, in both cases, the particle can only move between the impenetrable barriers located at the points $x = 0$ and $x = a$. Finally, and most importantly, in each case we have an Ehrenfest theorem that makes sense. We really hope that our article will be of interest to all those who are interested in the fundamental aspects of quantum mechanics.

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