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ALGUNOS RESULTADOS ASOCIADOS A PROBLEMAS MODÉLICOS EN LA MECÁNICA CUÁNTICA UNIDIMENSIONAL

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Algunos Resultados Asociados a Problemas Modélicos en la Mecánica Cuántica Unidimensional

(Trabajo de ascenso presentado por el Profesor Asociado,
Dr. Salvatore De Vincenzo,
para optar a la categoría de Profesor Titular)

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MEMORIA

Resultados clasico-cuánticos versus resultados cuánticos exactos para una partícula en una caja

La llamada partícula en una caja unidimensional, o en un intervalo, es uno de los sistemas modélicos que pueden usarse para ilustrar aspectos y conceptos importantes de la mecánica cuántica elemental. Como es sabido, el correspondiente operador Hamiltoniano (auto-adjunto) posee un dominio general que involucra un número infinito de condiciones de frontera; de hecho, ese dominio podría incluir hasta una familia de cuatro parámetros de condiciones de frontera. Es de destacar que cada una de estas condiciones de frontera lleva a la conservación de la densidad de corriente de probabilidad $j(x) = (\hbar/m)\,\mathrm{Im}(\bar{\psi}(x)\psi'(x))$ en los extremos de la caja, es decir, $j(a) = j(b)$ (para una caja en el intervalo $x \in [a, b] \equiv \Omega$). Sin embargo, solo para algunas de estas condiciones de frontera se tiene que $j(a) = j(b) = 0$. A pesar de la gran variedad de condiciones de frontera, o de extensiones auto-adjuntas del Hamiltoniano, clasicamente solo se pueden distinguir dos situaciones o casos: (i) una partícula que rebota entre dos paredes rígidas, y (ii) una partícula que desaparece una vez que alcanza una pared y entonces aparece en la otra pared (o equivalentemente, una partícula que se mueve a lo largo de un círculo con rapidez constante). Por supuesto, en estos dos problemas la partícula lleva a cabo un movimiento periódico, y esta periodicidad, junto con una regla de cuantización, nos puede llevar a resultados que coinciden con los que se obtienen al usar la mecánica cuántica moderna. Especificamente, a partir de la serie de Fourier de la posición de la partícula para cada problema podemos identificar tanto a la amplitud clásica (o de Fourier) como a la frecuencia mecánica del armónico τ-ésimo, luego podemos expresar estas cantidades en función de la etiqueta cuántica n haciendo uso de una regla de cuantización como la de Bohr-Sommerfeld-Wilson. Pues bien, en el límite $n \gg \tau$ estas cantidades coinciden, respectivamente, con la amplitud de Heisenberg y la frecuencia espectral asociada a la transición $n \to n - \tau$, ambas obtenidas usando la mecánica cuántica moderna. Estos resultados indican que, el caso clásico (i) mencionado antes corresponde al de una partícula cuántica descrita por el Hamiltoniano con la condición de frontera de Dirichlet, es decir, $\psi(a) = \psi(b) = 0$; mientras que el caso (ii) corresponde al de una partícula cuántica descrita por el Hamiltoniano con la condición de frontera periódica, es decir, $\psi(a) = \psi(b)$ y $\psi'(a) = \psi'(b)$ (vea la Ref. [1]).

La partícula en un pozo infinito versus la partícula en una caja

Para forzar a una partícula cuántica a permanecer en el interior de una caja, hemos identificado dos casos o modos de confinamiento: (i) si la partícula (libre) se esta moviendo sobre toda la linea real, es decir, si suponemos que la partícula se mueve en el interior de un pozo de potencial finito, basta hacer muy grande al potencial en la regiones externas al segmento de linea donde finalmente estará la partícula. Este caso se puede llamar "la partícula en un pozo de potencial cuadrado infinito" (y la respectiva función de onda satisface la condición de frontera de Dirichlet en toda la región exterior, es decir, se anula allí). (ii) Si la partícula (libre) ha estado moviéndose dentro de la caja, un potencial externo no es necesario para confinar la partícula, solo condiciones de frontera. Este caso se puede llamar "la partícula en la caja" (y la respectiva función de onda -si se habla de confinamiento- debe anular a la densidad de corriente de probabilidad en los extremos de la caja, siendo la condición de frontera de Dirichlet solo una de las infinitas condiciones de frontera que podemos usar). En el caso (i), el teorema de Ehrenfest puede verificarse para un estado general que es combinación lineal de autoestados y que pertenece a $\mathcal{L}^2(\mathbb{R})$. Es decir, $d\langle \hat{X}\rangle/dt = \langle \hat{P}\rangle/M$, y $d\langle \hat{P}\rangle/dt = \langle \hat{F}\rangle$, pero el cálculo de $\langle \hat{F}\rangle$ debe hacerse con cuidado ya que $\hat{F} = F(x) = -dV(x)/dx$, y el potencial $V(x)$ es un pozo de potencial (cuadrado) infinito (lo que conduce a deltas de Dirac con intensidades infinitas en las paredes del pozo, que están presentes en $\hat{F}$). En el caso (ii), el teorema de Ehrenfest puede también verificarse, por ejemplo, para estados que pertenecen a $\mathcal{L}^2(\Omega)$ y que satisfacen la condición de frontera de Dirichlet en los extremos de Ω. En efecto, se obtiene lo siguiente: $d\langle \hat{x}\rangle/dt = \langle \hat{p}\rangle/M$, y $d\langle \hat{p}\rangle/dt = \langle \hat{f}\rangle + \langle f_B\rangle = \langle f_B\rangle$, donde $\hat{f} = f(x) = -dv(x)/dx = 0$ ($v(x)$ es el potencial dentro de la caja), y $f_B = f_B(x,t) = (-\hbar^2/2M) \mid u \mid^{-2} \partial_x \mid \partial u/\partial x \mid^2$ es una fuerza cuántica no-local en el sentido que es dependiente del estado cuántico en cuestión $u = u(x,t)$ (y por lo tanto $\langle f_B\rangle$ es un término de frontera, es decir, es un término que se obtiene evaluando una cierta cantidad en cada frontera de la caja y luego restando los dos resultados). Por supuesto, las ecuaciones de Ehrenfest en los dos casos mencionados son equivalentes, es decir, ellas dan los mismos resultados. En conclusión, tanto en (i) como en (ii) la partícula solo puede moverse entre dos paredes, y en cada caso se tiene un teorema de Ehrenfest que tiene sentido (vea la Ref. [2]).

Sobre el cálculo formal de $d\langle \hat{x}\rangle/dt$ y $d\langle \hat{p}\rangle/dt$ para la partícula en una caja

La demostración usual de las ecuaciones de Ehrenfest en la representación de coordenadas con $x \in \mathbb{R}$ no parece tener problemas, sin embargo, la forma típica que tienen estas ecuaciones no siempre se mantiene cuando la partícula se encuentra en el interior de una caja. Es decir, la demostración de estas ecuaciones en este último caso puede llevar a resultados inesperados. De hecho, en el cálculo formal de las derivadas con respecto al tiempo de $\langle \hat{x}\rangle$ y $\langle \hat{p}\rangle$ surgen ciertos términos de frontera que no necesariamente se anulan (aquí llamamos formal al hecho que no nos restringimos a los dominios de los operadores auto-adjuntos involucrados, ni nos preocupamos por la apropiada clase de funciones sobre las cuales estos operadores y algunos de sus productos deben actuar). Puede demostrarse que estos términos de frontera se pueden hacer depender solo de los valores que toman en los extremos de la caja la densidad de probabilidad, su derivada espacial, la densidad de corriente de probabilidad, y el potencial externo. Si el término de frontera en $d\langle \hat{x}\rangle/dt$ no se anula, se tiene en general que $d^2\langle \hat{x}\rangle/dt^2 \neq \langle \hat{f}\rangle/M$. Si la partícula se encuentra -digamos- en una caja del tamaño de la recta real, pero con una probabilidad baja de encontrarse justamente en el infinito, las derivadas con respecto al tiempo de $\langle \hat{x}\rangle$ y $\langle \hat{p}\rangle$ obedecen las relaciones de Ehrenfest usuales. Puede también mostrarse que $d\langle \hat{p}\rangle/dt$ es igual a $\langle \hat{f}\rangle + \langle f_Q\rangle + \text{término de frontera}$ (aquí $\hat{f} = f(x) = -dv(x)/dx$, como se dijo antes, $f_Q = -\partial Q/\partial x$ es la llamada fuerza cuántica, siendo Q el potencial cuántico de Bohm, y el término de frontera depende esencialmente de los valores que allí toman la densidad de probabilidad y de corriente de probabilidad). Además, $\langle f_Q\rangle$ puede siempre escribirse como un término de frontera, y la cantidad que se evalua en los extremos de la caja, en casos particulares, es proporcional a la llamada cantidad de información de Fisher. Desde luego, el término $\langle f_B \rangle$ mencionado en el párrafo anterior es precisamente $\langle f_Q \rangle$. Puede notarse, en general, que $\langle f_Q \rangle$ tiene un rol significativo en situaciones en las cuales la partícula esta confinada a una región, incluso si $\hat{f} = 0$ en esa región, por ejemplo, cuando la partícula (libre) se encuentra confinada a una caja con la condición de frontera de Dirichlet (vea la Ref. [3]).

La partícula en un salto infinito versus la partícula en una semi-línea

Así como pueden identificarse dos modos de confinamiento para una partícula cuántica (libre) en un intervalo finito [2], pueden considerarse también dos tipos de confinamiento al restringir la partícula a un intervalo semi-infinito: (i) el que nos lleva a la llamada "partícula libre en un potencial salto infinito" (y la respectiva función de onda satisface inevitablemente la condición de frontera de Dirichlet en toda la región externa al intervalo semi-infinito), y (ii), el que nos lleva a la llamada "partícula libre sobre una semi-línea" (y la condición de frontera de Dirichlet para la correspondiente función de onda es solo una condición de frontera más). De nuevo puede demostrarse que, en cada caso, los valores medios de la posición, el momentum y la correspondiente fuerza, como funciones del tiempo, verifican el teorema de Ehrenfest. Sin embargo, la fuerza involucrada no es la misma en cada caso. De hecho, uno tiene la fuerza clásica externa usual en el primer caso, y una fuerza cuántica de frontera (no-local) en el segundo caso. A pesar de esta diferencia, los correspondientes valores medios de estas cantidades dan los mismos resultados. En consecuencia, las ecuaciones de Ehrenfest en las dos situaciones son equivalentes, y la consistencia interna del formalismo de la mecánica cuántica se ratifica (vea la Ref. [4]).

La trayectoria clásica a partir del movimiento cuántico para la partícula en una caja (transparente)

Como se establece usualmente, la mecánica clásica se puede extraer de la mecánica cuántica imponiendo límites matemáticos. Este resultado general es llamado el principio de correspondencia, y se puede expresar haciendo $\hbar \to 0$ y $n \to \infty$ junto con la restricción $n\hbar = \mathrm{constante}$ (n es un número cuántico típico). El teorema de Ehrenfest, bajo ciertas condiciones, proporciona una relación general formal entre la dinámica clásica y la cuántica. En particular, bajo las condiciones del principio de correspondencia, los valores medios $\langle \hat{x} \rangle(t)$ y $\langle \hat{p} \rangle(t)$ (en un estado general complejo, normalizado, y dependiente del tiempo) deben ser iguales a la posición y al momentum clásicos, $x(t)$ y $p(t)$. Especificamente, se puede probar que, en el caso de una partícula en una caja penetrable (o una caja con paredes transparentes), la función del tiempo $\langle \hat{x} \rangle(t)$ se reduce a la trayectoria newtoniana, $x(t)$, haciendo (esencialmente) la aproximación de números cuánticos altos sobre el valor medio, es decir, imponiendo las condiciones del principio de correspondencia. Es de mencionarse que, en este problema, la conexión clasico-cuántica pudo verificarse porque se pudo calcular la serie de Fourier asociada a la posición de la partícula, sin embargo, este no es siempre el caso (vea la Ref. [5]).

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Notas e Discussões

Classical-quantum versus exact quantum results for a particle in a box

(Resultados clássico-quânticos versus resultados quânticos exatos para uma partícula em uma caixa)

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The problems of a free classical particle inside a one-dimensional box: (i) with impenetrable walls and (ii) with penetrable walls, were considered. For each problem, the classical amplitude and mechanical frequency of the τ-th harmonic of the motion of the particle were identified from the Fourier series of the position function. After using the Bohr-Sommerfeld-Wilson quantization rule, the respective quantized amplitudes and frequencies (i.e., as a function of the quantum label n) were obtained. Finally, the classical-quantum results were compared to those obtained from modern quantum mechanics, and a clear correspondence was observed in the limit of $n \gg \tau$.
Keywords: classical mechanics, particle in a box, Fourier harmonics, Heisenberg harmonics.

Foram considerados os problemas de uma partícula livre clássica dentro de uma caixa unidimensional: (i) com paredes impenetráveis e (ii) com paredes penetráveis. Para cada problema, foram identificados a partir da série de Fourier da função de posição, a amplitude clássica ea freqüência mecânica clássica do τ-ésimo harmônico do movimento da partícula. Depois de usar a regra de quantização de Bohr-Sommerfeld-Wilson, foram obtidos a respectivas amplitudes e freqüências quantizadas (isto é, como uma função do rótulo quantum n). Finalmente, os resultados clássico-quânticos foram comparados com aqueles obtidos a partir da moderna mecânica quântica, e uma clara correspondência foi observada no limite de $n \gg \tau$.
Palavras-chave: mecânica clássica, partícula em uma caixa, harmônicos de Fourier, harmônicos de Heisenberg.

1. Introduction

The quantum particle in a box ($0 \leq x \leq L$) is one of the best systems to illustrate important aspects and key concepts of elementary quantum mechanics [1–3]. The domain of the corresponding self-adjoint Hamiltonian operator involves an infinite number of boundary conditions. Specifically, the domain includes a four-parameter family of boundary conditions, and each of the conditions leads to the conservation of the probability current density $j(x) = (\hbar/m)\mathrm{Im}\left(\bar{\psi}(x)\psi'(x)\right)$ at the ends of the box (*i.e.*, $j(0) = j(L)$). However, for several boundary conditions, the current is equal to zero ($j(0) = j(L) = 0$) [4–7]. When a finite square well potential tends toward infinity in the regions outside of the box (to confine the particle inside the box), only the Dirichlet boundary conditions are recovered [4,8]. Similarly, the solutions to Heisenberg's equations of motion obtained from the respective classical equations for a particle bouncing between two rigid walls, lead to only one of the extensions of the Hamiltonian operator (the extension that contains the Dirichlet boundary conditions [9]). However, in the classical discussion, another case must be considered. Namely, the case where the particle disappears upon reaching a wall and then appears at the other end must be considered. This type of movement (which is very unusual because the particle is not actually trapped between the two walls) corresponds to that of a quantum particle described by the Hamiltonian operator under periodic boundary conditions. Although there are an infinite number of quantum self-adjoint Hamiltonian operators, all of the operators do not correspond to a different classical system. In our cases, each Hamiltonian operator is defined by a specific boundary condition (rather than the form of each Hamiltonian). However, if a classical expression is dependent on the canonical variables, the corresponding quantum operator is not unique because the canonical operators can be ordered in various ways (see Ref. [9] and references therein).

The problem of a classical particle confined to an impenetrable box has been considered in several specific contexts [9–14]. In contrast, except for Ref. [9] and brief comments in Refs. [5, 15, 16], the problem of a classical particle inside a penetrable box is rarely discussed. Clearly, in each of these problems, the particle

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carries out a periodic motion. In this short paper, we wish to illustrate the connection between the periodicity of particle motion and quantum jumps. First, the so-called classical amplitude and mechanical frequency of the τ-th harmonic of the motion of the particle were identified from the Fourier series of each position function ($x(t)$). Next, the Bohr-Sommerfeld-Wilson quantization rule was used to obtain the respective quantized amplitudes and frequencies, *i.e.*, the classical amplitudes and frequencies as a function of the quantum label n. Subsequently, these classical-quantum quantities were compared to the respective transition amplitudes ($c_{n,n-\tau}$) and transition frequencies ($\omega_{n,n-\tau}$) obtained from modern quantum mechanics (Heisenberg-Schrödinger's quantum mechanics). In fact, these quantum quantities are the elements that constitute the matrix of Heisenberg's harmonics $x_{n,m} \equiv c_{n,m} \exp(i\omega_{n,m} t)$ (in this case, the matrix is associated with transitions $n \to m = n - \tau$). As a result, the classical-quantum quantities are equal to the exact quantum quantities for small jumps ($n \approx n - \tau$ or $n \gg \tau$). We believe that the present manuscript (which is somewhat inspired by the excellent paper by Fedak and Prentis [13]) may be of genuine interest to teachers and students of physics because the two simple examples described herein (in particular, the particle inside a penetrable box, which is discussed in the present article for the first time) illustrate the deep connection between classical and quantum mechanics.

2. Classical results

Let us begin by considering the motion of a free particle with a mass of m, which is confined to a one-dimensional region of length L that contains rigid walls at $x = 0$ and $x = L$ (the potential $U(x)$ is zero inside the box). The particle moves back and forth between these two points forever. The extended position function versus time, $x(t)$ (which is periodic for all times $t \in (-\infty, +\infty)$ with a period of T), can be written as

$$x(t) = \sum_{n=-\infty}^{+\infty} f_n(t)\Theta_n(t), \tag{1}$$

where $f_n(t) = (vT/2) - v\,|t - nT - (T/2)|$, $v > 0$ is the speed of the particle, $\Theta_n(t) \equiv \Theta(t-nT)-\Theta(t-(n+1)T)$ ($\Theta(y)$ is the Heaviside unit step function, $\Theta(y > 0) = 1$ and $\Theta(y < 0) = 0$) and $vT/2 = L$. In the time interval $nT \le t \le (n + 1)T$, the zigzag solution (1) is equal to $x(t) = f_n(t)$, where n is an integer, and verifies $x(nT) = 0$ and $x((n+(1/2))T) = L$). For example, the solution at $0 \le t \le T$ ($n = 0$) is $x(t) = f_0(t)$; thus, $x(t) = vt$ for $0 \le t \le T/2$ and $x(t) = vT - vt$ for $T/2 \le t \le T$. In contrast, the sum in Eq. (1) should begin at $n = 0$ if the particle starts from $x = 0$ at $t = 0$. In fact, under these circumstances, the solution of the equation of motion, $x(t)$, verifies the condition $x(t \le 0) = 0$. Because the position as a function of time given in Eq. (1) is periodic in $t \in (-\infty, +\infty)$, the formula can be expanded into a Fourier series

$$x(t) = \sum_{\tau=0}^{+\infty} a_\tau \cos(\omega_\tau t)\,. \tag{2}$$

The classical amplitude, a_τ, takes on the following values

$$a_\tau = -\frac{2vT}{\pi^2\tau^2}, \quad \tau = 1, 3, 5, \ldots. \tag{3}$$

Moreover, $a_\tau = 0$ with $\tau = 2, 4, 6, \ldots$ and $a_0 = vT/4$. The mechanical frequency of the (permitted) τ-th harmonic of the motion of the particle is

$$\omega_\tau = \tau\omega, \tag{4}$$

where $\omega = 2\pi/T$ is the fundamental frequency of periodic motion.

Let us now consider the motion of a free particle with a mass of m in a one-dimensional box. The particle is not confined to the box, and the walls at $x = 0$ and $x = L$ are transparent (in this problem, the potential $U(x)$ is zero inside the box). Under these circumstances, the particle starts from $x = 0$ (for example), reaches the wall at $x = L$ and reappears at $x = 0$ again (and it does so forever). The extended position as a function of time ($x(t)$) is periodic and discontinuous and can be written as

$$x(t) = \sum_{n=-\infty}^{+\infty} g_n(t)\Theta_n(t), \tag{5}$$

where $g_n(t) = vt - nvT$, $v > 0$ is the speed of the particle and T is the period ($\Theta_n(t)$ was introduced after Eq. (1)). In each time interval $nT < t < (n + 1)T$, the (extended) position is $x(t) = g_n(t)$, where n is an integer (as a result, all the discontinuities occur at $t = nT$). For example, the solution at $t \in (0, T)$ ($n = 0$) is $x(t) = g_0(t)$; thus, $x(t) = vt$. To be more precise, if the particle starts from $x = 0$ at $t = 0$ (and it begins to move towards $x = L$), then the sum in Eq. (5) should begin at $n = 0$. In that case, the solution of the equation of motion ($x(t)$) verifies the condition $x(t \le 0) = 0$. Clearly, the periodic function $x(t)$ in Eq. (5) (with $t \in (-\infty, +\infty)$) can be expanded into a Fourier series

$$x(t) = \sum_{\tau=-\infty}^{+\infty} c_\tau \exp(i\omega_\tau t)\,. \tag{6}$$

The classical amplitude, c_τ, has the following values

$$c_\tau = i\frac{vT}{2\pi\tau}, \quad \tau = \pm1, \pm2, \ldots. \tag{7}$$

Moreover, $c_0 = vT/2$. Once again, the mechanical frequency of the (permitted) τ-th harmonic of the motion of the particle is

$$\omega_\tau = \tau\omega, \tag{8}$$

where $\omega = 2\pi/T$ is the fundamental frequency of periodic motion. *Note:* if the particle is moving from right to left (starting at $x = L$, for example) the Fourier series associated to $x(t)$ is the Eq. (6), but the classical amplitude is the complex conjugate of c_τ. The series in Eq. (6) appears to be complex but is actually real. In fact, because $c_\tau = -c_{-\tau}$ ($\tau \neq 0$), $x(t)$ can be written as

$$x(t) = \frac{vT}{2} - \frac{vT}{\pi}\sum_{\tau=1}^{+\infty}\frac{1}{\tau}\sin(\omega_\tau t)\,. \tag{9}$$

Thus, the extended function ($x(t)$) given in Eq. (5) is discontinuous at $t = nT$, where n is an integer. Nevertheless, if one wants to assign a value to $x(nT)$, then a value must be assigned to $\Theta(0)$. At $t = nT$, the Fourier series (6) (or (9)) converges to $x(t) \equiv (x(t+) + x(t-))/2$, where $x(t\pm) \equiv \lim_{\epsilon\to 0} x(t \pm \epsilon)$ and $\epsilon > 0$ (as usual). Thus, in this case, the definition $\Theta(0) \equiv 1/2$ must be applied; therefore (from Eq. (5)), $x(nT) = vT/2$. Clearly, the latter choice is not physically satisfactory because the particle always reaches $x = L$ (it is moving from $x = 0$). Thus, we may prefer to choose $\Theta(0) \equiv 0$, which implies that $x((n+1)T) = vT = L$, where n is an integer (more precisely, $n \geq 0$). Clearly, when $\Theta(0) \equiv 0$ is selected, the time at which the particle passes through $x = 0$ cannot be obtained. This situation is unavoidable; thus, the best that we can do is to assume that the motion of the particle in each time interval $nT \leq t \leq (n+1)T$ is independent of the other intervals. Therefore, we must also add (by definition) the condition $x(nT) = 0$.

3. Classical-quantum versus exact quantum results

Thus, we have seen that the classical particle confined to a box and the particle inside a penetrable box display periodic motion (between the walls of the box). This is precisely the type of motion considered by Heisenberg in his famous paper published in 1925 [17] (For an english translation of the article, see Ref. [18]. For a delicious discussion on the ideas expressed in Heisenberg's article, see Ref. [19]). To illustrate the important connection between the periodic motion of a classical particle (its classical harmonics) and quantum jumps, the problem of a particle confined to a box (as described in Ref. [13]) was considered in the present study. Moreover, for the first time, the problem of a particle inside a box with penetrable walls was also considered herein.

A condition that quantizes the classical states of a one-dimensional periodic system is the Bohr-Sommerfeld-Wilson (BSW) quantization rule (see Refs. [13, 20])

$$\frac{1}{2\pi}\oint dx\, mv(x) = n\hbar, \tag{10}$$

where $\hbar$ is Planck's constant and n are quantum labels. Integration is conducted over the entire period of motion. From Eq. (10), the (constant) speed of the particle ($v > 0$) was obtained as a function of n (*i.e.*, the speed of the particle in quantum state n)

$$v \equiv v(n) = \frac{\pi\hbar}{mL}n. \tag{11}$$

Moreover, by substituting $v(n)$ into the classical mechanical energy equation $E = mv^2/2$, the same quantum energy spectrum given by modern quantum mechanics was obtained

$$E \equiv E(n) = \frac{\pi^2\hbar^2}{2mL^2}n^2 = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2, \tag{12}$$

where, in this case, $n = 1, 2, \ldots$. Similarly, the expression for the quantized speed (11) could be substituted into Eq. (3) and Eq. (4) to obtain the quantized amplitude and quantized frequency, respectively. In the former case, substitution was not necessary because $vT/2 = L$. Therefore

$$a_\tau(n) = -\frac{4L}{\pi^2\tau^2}, \quad \tau = 1, 3, 5, \ldots. \tag{13}$$

Moreover, $a_\tau(n) = 0$, where $\tau = 2, 4, 6, \ldots$ and $a_0(n) = L/2$. Thus, $a_\tau(n)$ is independent of the quantum state (n). In the latter case, Eq. (11) was substituted into Eq. (4), and the quantized frequency was obtained

$$\omega_\tau(n) = \tau\frac{2\pi}{T} = \tau\frac{2\pi v(n)}{2L} = \tau\frac{\pi^2\hbar}{mL^2}n \equiv \tau\omega(n). \tag{14}$$

Clearly, the Fourier series for $x(t)$ can also be quantized by replacing $a_\tau \to a_\tau(n)$ and $\omega_\tau \to \tau\omega(n)$ in Eq. (2). Thus, we can write

$$\begin{aligned} x(t,n) &= a_0(n) + a_1(n)\cos(\omega(n)t) + \\ &a_3(n)\cos(3\omega(n)t) + \cdots. \end{aligned} \tag{15}$$

Equation (15) describes the classical motion of the particle in quantum state n. Clearly, these results are classical-quantum mechanical because they were obtained by supplementing the classical Fourier analysis with a simple quantization condition.

Now a question arises: how (and under which conditions) can we generate Eq. (13) and (14) using modern quantum theory? In his paper published in 1925, Heisenberg assigned a matrix of harmonics $x_{n,m} \equiv c_{n,m}\exp(i\omega_{n,m}t)$ (associated with transition $n \to m$) to x, where the transition amplitude $c_{n,m} = \langle\psi_n \mid x \mid \psi_m\rangle$ is a measure of the intensity of light, and $x_{n,m} = \langle\Psi_n \mid x \mid \Psi_m\rangle$ (where $\Psi_n(x,t) = \psi_n(x)\exp(-iE_nt/\hbar)$ are solutions to the time-dependent Schrödinger equation). In the transition $n \to n - \tau$, where $n \gg \tau$, the quantized Fourier amplitude $c_\tau(n)$ must be equal to the Heisenberg amplitude $c_{n,n-\tau}$

$$c_\tau(n) = c_{n,n-\tau}. \tag{16}$$

Equivalently,

$$a_\tau(n) = 2c_{n,n-\tau}, \tag{17}$$

because the coefficients of the cosine Fourier series $a_\tau(n)$ with $\tau = 1, 3, 5, \ldots$ in Eq. (15) are always twice that of the exponential Fourier series $\sum_\tau c_\tau(n) \exp(\tau\omega(n)t)$ [13] (nevertheless, $a_\tau(n) = c_\tau(n)$ with $\tau = 0$). The stationary states of a quantum particle to a box with a width of L under Dirichlet boundary conditions ($\psi_n(0) = \psi_n(L) = 0$) are characterized by the energies given in Eq. (12) ($E(n) = E_n$) and the following eigenfunctions

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right),\ n = 1, 2, \ldots. \tag{18}$$

If $c_{n,n-\tau} = \langle \psi_n \mid x \mid \psi_{n-\tau} \rangle = \int_0^L dx\, \psi_n(x)\, x\, \psi_{n-\tau}(x)$ is calculated, and the result are substituted into Eq. (17), we obtain

$$a_\tau(n) = -\frac{4L}{\pi^2\tau^2} \frac{1 - \frac{\tau}{n}}{\left(1 - \frac{\tau}{2n}\right)^2} \underset{n\gg\tau}{\longrightarrow} -\frac{4L}{\pi^2\tau^2}, \tag{19}$$

where $\tau = 1, 3, 5, \ldots$, $a_\tau(n) = 0$ with $\tau = 2, 4, \ldots$ and $a_0(n) = L/2$. Clearly, the quantized Fourier amplitude $a_\tau(n)$ (Eq. (13)) can also be obtained from Heisenberg-Schrödinger's quantum mechanics.

Likewise, the quantized frequency $\omega_\tau(n)$ must be equal to the transition (or spectral) frequency $\omega_{n,n-\tau} = (E_n - E_{n-\tau})/\hbar$ for $n \gg \tau$ [13]

$$\omega_\tau(n) = \omega_{n,n-\tau}. \tag{20}$$

In fact, for the particle confined to the box, $\omega_{n,n-\tau}$ was calculated from Eq. (12) with $E(n) = E_n$. Using Eq. (20), we can write

$$\omega_\tau(n) = \tau\frac{\pi^2\hbar}{mL^2} n\left(1 - \frac{\tau}{2n}\right) \underset{n\gg\tau}{\longrightarrow} \tau\frac{\pi^2\hbar}{mL^2} n. \tag{21}$$

Clearly, the same result given in Eq. (14) was obtained in the limit $n \gg \tau$.

Next, a particle inside a box with transparent walls was considered. Using the BSW rule in Eq. (10), the speed of the particle as a function of n was obtained

$$v \equiv v(n) = \frac{2\pi\hbar}{mL} n. \tag{22}$$

By substituting Eq. (22) into $E = mv^2/2$, we obtain

$$E \equiv E(n) = \frac{2\pi^2\hbar^2}{mL^2} n^2 = \frac{\hbar^2}{2m}\left(\frac{2n\pi}{L}\right)^2. \tag{23}$$

In this case, $n = 0, 1, 2, \ldots$. The quantum energy spectrum given by modern quantum mechanics (with the exception of the ground state) is degenerate (see Eq. (27)), and the complex eigenfunctions corresponding to the negative sign ($-$) are plane waves propagating to the left (they are also eigenfunctions of the momentum operator $\hat{p} = -i\hbar d/dx$ with negative eigenvalues). Because the classical motion of the particle moving to the right is under consideration, a positive sign ($+$) must be used. Clearly, each state ($n > 0$) with the positive sign in Eq. (27) corresponds to a one-dimensional trip in which the particle is moving inside the box from left to right at a constant speed.

Because $vT = L$, Eq. (22) does not have to be substituted into Eq. (7); therefore, the quantized amplitude is independent of n

$$c_\tau(n) = i\frac{L}{2\pi\tau}, \quad \tau = \pm1, \pm2, \ldots. \tag{24}$$

Moreover, $c_0(n) = L/2$. Alternatively, by substituting Eq. (22) into Eq. (8), the following quantized frequency was obtained

$$\omega_\tau(n) = \tau\frac{2\pi}{T} = \tau\frac{2\pi v(n)}{L} = \tau\frac{4\pi^2\hbar}{mL^2} n \equiv \tau\omega(n). \tag{25}$$

This frequency must be positive if it corresponds to the frequency of light emitted as the particle jumps from level n to level $n - \tau < n$. Finally, the quantized Fourier series $x(t, n)$ was obtained from $x(t)$ (Eq. (6)) by replacing $c_\tau \to c_\tau(n)$ and $\omega_\tau \to \tau\omega(n)$

$$x(t,n) = \cdots + c_{-1}(n) \exp(-i\omega(n)t) + c_0(n) + c_1(n) \exp(i\omega(n)t) + \cdots. \tag{26}$$

For a free particle in a box with a width of L and transparent walls, the periodic boundary condition $\psi_n(x) = \psi_n(x + L)$ is physically adequate. The exact energy eigenvalues are given in Eq. (23) ($E(n) = E_n$), and the eigenfunctions are

$$\psi_n(x) = \frac{1}{\sqrt{L}} \exp\left(\pm i\frac{2n\pi}{L}x\right),\ n = 0, 1, 2, \ldots. \tag{27}$$

Nevertheless, only the positive sign must be employed. By calculating $c_{n,n-\tau} = \int_0^L dx\, \bar{\psi}_n(x)\, x\, \psi_{n-\tau}(x)$ and substituting the result into Eq. (16) (the bar represents complex conjugation), we obtain

$$c_\tau(n) = i\frac{L}{2\pi\tau}. \tag{28}$$

In this case, $\tau = \pm1, \pm2, \ldots$ and $c_0(n) = L/2$. To obtain Eq. (28), the limit $n \gg \tau$ was not applied. Clearly, the quantized Fourier amplitude $c_\tau(n)$ (Eq. (24)) was obtained from Heisenberg-Schrödinger's quantum mechanics. *Note:* for a particle moving from right to left we must take the negative sign in Eq. (27); therefore, the corresponding Heisenberg amplitude is the complex conjugate of $c_\tau(n)$ in Eq. (28). Similarly, Eq. (20) was verified. In fact, $\omega_{n,n-\tau} = (E_n - E_{n-\tau})/\hbar$ was calculated from Eq. (23) using $E(n) = E_n$. Thus, in the limit $n \gg \tau$, the results were identical to those of Eq. (25)

$$\omega_\tau(n) = \tau \frac{4\pi^2\hbar}{mL^2} n \left(1 - \frac{\tau}{2n}\right) \underset{n\gg\tau}{\longrightarrow} \tau \frac{4\pi^2\hbar}{mL^2} n. \tag{29}$$

4. Final notes

In some cases, the BSW quantization rule (Eq. (10)) may fail [20,21]; however, in the two problems considered in the present study, this rule provides the correct quantum mechanical energy values. A more flexible formula that fixes problems associated with the BSW rule is the Einstein-Brillouin-Keller (EBK) quantization rule. For one-dimensional problems, this formula presents the following form

$$\frac{1}{2\pi} \oint dx\, mv(x) = \left(n + \frac{\mu}{4}\right) \hbar, \tag{30}$$

where $n = 0, 1, 2, \ldots$ and μ is the Maslov index [20,21]. This index is essentially "a detailed accounting of the total phase loss during one period in units of $\pi/2$" [20]. In general, each classical turning point and each reflection gives one unit to μ. For example, for a confined particle in a box, $\mu = 4$ (because two turning points and two hard reflections are observed). Alternatively, for a particle in a transparent box, $\mu = 0$ (because there are no turning points or reflections). The latter motion is pretty similar to that of a particle moving freely on a circle, which corresponds to the familiar plane rigid rotator problem. Clearly, our results (Eq. (12) and Eq. (23)) coincide with those provided by the EBK quantization rule. To conclude, in the approximation $n \gg \tau$, the classical-quantum results agree with the exact quantum results. Nevertheless, the quantum-classical calculations are easier to perform. Moreover, the classical-quantum mechanical and exact quantum energies perfectly match in both problems. Lastly, for the particle in the open box, the quantized Fourier and Heisenberg amplitudes are identical and independent of n.

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

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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_{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_{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:

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

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:

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

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:

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

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

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

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 κ 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 $x \le 0$ and $x \ge a$ (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 $0 \le x \le a$ (see eqs (11) and (14)), with $k \to n\pi/a$ and $\varepsilon \to E_n$, we obtain the following equation:

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

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 $\psi_n(x \leq 0) = \psi_n(x \geq a) = 0$. 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 $\psi(x \leq 0) = \psi(x \geq a) = 0$ [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:

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

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:

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

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_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_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_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 Ψ 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

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

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, $\langle f_{\rm B}\rangle_u = \int_\Omega {\rm d}x\; f_{\rm B}(x,t)\,|u(x,t)|^2$. Hence, $\langle f_{\rm B}\rangle_u$ is always equal to a boundary term and $f_{\rm B}$ can be considered a boundary quantum force. Thus, in this case, the Ehrenfest theorem consists of eq. (46) and the following expression:

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

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., $\langle f_{\rm B}\rangle_\Psi = 0$. In fact, in the open interval $\Omega = (-\infty, +\infty)$, Ψ and its derivative $\partial\Psi/\partial x$ tend to zero for $x \to \pm\infty$.

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 $\langle f_{\rm B}\rangle_u$ 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:

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

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_B. In fact, the mean value of f_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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The formula that follows Eq. (47) was incorrectly written:

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

This formula must be written as follows:

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

That's all!

Salvatore De Vincenzo.

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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])

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

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

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

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

$$\rho = \bar{\Psi}\Psi. \qquad (11)$$

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

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

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

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

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

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

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))

$$\rho|_a^b = 0. \qquad (14)$$

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 $\hat{A} = \hat{x}$):

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

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

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

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:

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

By developing this expression, we obtain

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

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

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

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

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

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])

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

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:

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

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

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

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

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

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

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

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

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 $v=j/\rho$):

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

(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:

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

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

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

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

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

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

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

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:

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

(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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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 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 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:

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

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

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

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

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 $\psi_k(x\ge 0)=0$.

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

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

(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:

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

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

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

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

$$u_k(x) = 2i\,\sin(kx). \qquad (13)$$

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:

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

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)):

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

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:

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

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

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

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 $\hat{X}$:

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

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:

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

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

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

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:

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

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:

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

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

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

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

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

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:

$$\frac{d}{dt}\langle\hat{p}\rangle_u = \langle f_B\rangle_u. \tag{41}$$

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:

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

$$(-\infty < x \leq 0), \tag{42}$$

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:

$$\langle f_B\rangle_u = -4\int_0^\infty\int_0^\infty \frac{dk\,dk'}{2\pi}\,\bar{A}(k)A(k')$$

$$\times\sqrt{E_k E_{k'}}\,\exp\left[i\frac{(E_k - E_{k'})}{\hbar}t\right]. \tag{43}$$

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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Classical path from quantum motion for a particle in a transparent box

(Trajetória clássica a partir do movimento quântico para uma partícula em uma caixa transparente)

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We consider the problem of a free particle inside a one-dimensional box with transparent walls (or equivalently, along a circle with a constant speed) and discuss the classical and quantum descriptions of the problem. After calculating the mean value of the position operator in a time-dependent normalized complex general state and the Fourier series of the function position, we explicitly prove that these two quantities are in accordance by (essentially) imposing the approximation of high principal quantum numbers on the mean value. The presentation is accessible to advanced undergraduate students with a knowledge of the basic ideas of quantum mechanics.
Keywords: correspondence principle, classical limit, Ehrenfest theorem.

Consideramos o problema de uma partícula livre no interior de uma caixa unidimensional com paredes transparentes (ou equivalentemente, ao longo de um círculo com uma velocidade constante) e discutimos as descrições clássica e quântica do problema. Depois de calcular o valor médio do operador da posição num estado geral complexo normalizado dependente do tempo e a série de Fourier da função de posição, provamos explicitamente que estas duas quantidades estão em correspondência se (essencialmente) impusermos sobre o valor médio a aproximação dos números quânticos principais elevados. A apresentação é acessível a alunos de graduação avançados com conhecimento das idéias básicas da mecânica quântica.
Palavras-chave: princípio da correspondência, limite clássico, teorema de Ehrenfest.

1. Introduction

As typically stated in the field of quantum physics, classical mechanics can be obtained from quantum mechanics by imposing mathematical limits. This general statement is called the correspondence principle. Two different formulations or (non-equivalent) limits that give form to the aforementioned principle are commonly found in the literature: (i) the Planck formulation employs the classical or quasi-classical limit $\hbar \to 0$, and (ii) in the Bohr formulation, the large principal quantum number limit $n \to \infty$ is applied. Some physicists believe (and we agree) that the most meaningful principle is the combination of (i) and (ii) together with the restriction $n\hbar =$ constant. In fact, according to the Bohr-Sommerfeld-Wilson (BSW) quantization rule, the latter constant is proportional to the classical action J

$$n\hbar = \frac{1}{2\pi} \oint dx\, p(x) = \frac{J}{2\pi}, \tag{1}$$

(where $p(x)$ is the classical momentum, and the integral is obtained over the entire period of motion). Some particularly useful descriptions of these fundamental issues are provided in Refs. [1–6] (to mention only a few).

As is well known, the Ehrenfest theorem states that the mean values of the position and momentum operators (in the time-dependent normalized complex general state $\Psi = \Psi(x,t)$) $\langle \hat{x} \rangle(t) = \langle \Psi, \hat{x}\Psi \rangle$ and $\langle \hat{p} \rangle(t) = \langle \Psi, \hat{p}\Psi \rangle$ satisfy (essentially) the same equations of motion that the classical position and momentum ($x(t)$ and $p(t)$, respectively) satisfy. This theorem can be properly verified in a straightforward manner when the potential energy function is well behaved. The most common example is the potential energy of the simple harmonic oscillator [7]. In other cases, such as the infinite well and infinite step potentials, verification is problematic [8–11]. Although the Ehrenfest theorem provides a (formal) general relationship between classical and quantum dynamics, it does not necessarily (neither sufficiently) characterize the classical regime [12]. Certainly, using only the aforementioned theorem, one cannot state that the mean values $\langle \hat{x} \rangle(t)$ and $\langle \hat{p} \rangle(t)$ are always equal to the functions $x(t)$ and $p(t)$; however, this statement does hold true in the limit $n \to \infty$ (for a general discussion of the behaviour of a physical quantity for high values of the quantum number n, see, for example, Ref. [13]). In fact, this specific aspect of the relationship between classical and quantum motion has

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been considered to some extent in a few cases, such as the free particle and the particle in the harmonic oscillator potential [14]. The case of the free particle inside an impenetrable box (or in an infinite potential well) has also been treated [15–17]. Specifically, Ref. [15] explicitly proved that the mean value $\langle\hat{x}\rangle(t)$ matches the classical path $x(t)$ in the approximation of high principal quantum numbers.

Inspired by the results provided in Ref. [15] (and by the general procedure discussed in Ref. [13]), the aim of the present paper is to explicitly prove that, in the case of a particle in a penetrable box (or a box with transparent walls), the functions of time, $\langle\hat{x}\rangle(t)$ and $x(t)$, are in agreement when n is high (we must also appeal to some semi-classical arguments, of course). In this problem, the classical particle disappears upon reaching a wall (say, at $x = a$) and then appears at the other end (say, at $x = 0$), and it does so without changing its velocity. This situation could be physically achieved if the movement is more like that of a particle along a circle with radius a and a constant speed (this is true because a circle can be considered an interval with its ends glued together). The latter two classical movements (in a box or in a circle) correspond to that of a quantum particle described by the free Hamiltonian operator (i.e., the kinetic energy operator) with standard periodic boundary conditions (which are imposed at the ends of the box or at any point along the circle). The quantum case of a particle in a transparent box has been previously considered to some extent. For example, briefly in an interesting study on Heisenberg's equations of motion for the particle confined to a box [18]; as an example to illustrate the agreement between the periodic motion of classical particles and quantum jumps for large principal quantum numbers [19] (to mention only two examples). The present article is organized as follows: in section 2, we introduce and discuss the classical and quantum versions of the problem at hand. In section 3, we explicitly prove that $\langle\hat{x}\rangle(t)$ and $x(t)$ are in agreement by imposing the approximation of high principal quantum numbers on the mean value. Finally, we present concluding remarks in section 4.

2. Classical and quantum descriptions

Let us begin by considering classical motion: we have a free particle of mass μ that resides in a one-dimensional box but is not confined to the box, i.e., the walls at $x = 0$ and $x = a$ are transparent (the potential, $U(x)$, is zero inside the box). In this situation, we assume that the particle starts from $x = 0$ (for example), reaches the wall at $x = a$ and then reappears at $x = 0$ (with the same velocity throughout). The extended position as a function of time $x(t)$ is periodic and discontinuous and can be written as:

$$x(t) = \sum_{r=-\infty}^{+\infty} (vt - rvT)\left[\Theta(t - rT) - \Theta(t - (r+1)T)\right]. \tag{2}$$

Here, $\Theta(y)$ is the Heaviside unit step function ($\Theta(y > 0) = 1$ and $\Theta(y < 0) = 0$), $v > 0$ is the speed of the particle and T is the period. In each time interval ($rT < t < (r+1)T$), the extended position is simply $x(t) = vt - rvT$, where r is an integer (thus, all discontinuities occur at $t = rT$). For example, the solution at $t \in (0, T)$ ($r = 0$) is $x(t) = vt$. At the end of each time interval, we must also enforce (i.e., when r is given), the conditions $x(rT) = 0$ and $x((r+1)T) = vT = a$. Moreover, if the particle starts at $t = 0$ from $x = 0$ (and begins to move towards $x = a$), then the sum in Eq. (2) should begin at $r = 0$. In this case, the solution of the equation of motion, $x(t)$, satisfies the condition $x(t \le 0) = 0$. Clearly, the periodic function $x(t)$ in Eq. (2) (with $t \in (-\infty, +\infty)$) can be expanded in a Fourier series

$$x(t) = \frac{a}{2} + i\frac{a}{2\pi} \sum_{(0\neq)\tau=-\infty}^{+\infty} \frac{1}{\tau} \exp\left(i\frac{2\pi\tau}{T}t\right). \tag{3}$$

The series in Eq. (3) seems complex but is actually real-valued (of course, a complex solution $x(t)$ is not entirely acceptable as a classical trajectory). Moreover, if the particle is moving from right to left instead of moving from left to right (say, starting at $x = a$), the Fourier series associated with the corresponding extended position is given by Eq. (3), but the (classical) amplitude (for $\tau \neq 0$) of $ia/2\pi\tau$ changes to $-ia/2\pi\tau$.

The quantum results that are relevant to the discussion at hand include the following: first, for a free particle in a transparent box with a width of a, the Hamiltonian operator is

$$\hat{H} = \frac{\hat{p}^2}{2\mu} = \frac{1}{2\mu}\left(-i\hbar\frac{\partial}{\partial x}\right)^2 = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2}. \tag{4}$$

This operator (essentially) acts on functions $\Psi = \Psi(x,t)$, which belong to the Hilbert space of square-integrable functions on the interval $0 \le x \le a$ and whose derivatives are absolutely continuous. It is natural to include the periodic boundary condition, $\Psi(0,t) = \Psi(a,t)$ and $\Psi_x(0,t) = \Psi_x(a,t)$ (where, as usual, $\Psi_x \equiv \partial\Psi/\partial x$) in the domain of $\hat{H}$. With these boundary conditions, the Hamiltonian is self-adjoint, its spectrum is purely discrete and doubly degenerate (with the exception of the ground state), and their eigenfunctions form an orthonormal basis [20, 21]. Precisely, the (complex) orthonormalized eigenfunctions of $\hat{H}$ are also eigenfunctions of the momentum operator $\hat{p}$, and can be written separately as follows:

(i) Eigenfunctions of $\hat{p}$ with eigenvalues $p_n =$

$2\pi\hbar n/a$

$$\phi_n(x) = \frac{1}{\sqrt{a}} \exp\left(i\frac{2\pi n}{a}x\right),$$
$$E_n = \frac{\hbar^2}{2\mu}\left(\frac{2\pi n}{a}\right)^2, \quad n = 1, 2, 3, \ldots. \tag{5}$$

Each function $\phi_n(x)$ is a stationary plane wave propagating to the right.

(*ii*) Eigenfunctions of $\hat{p}$ but with eigenvalues $p_n = -2\pi\hbar n/a$

$$\chi_n(x) = \frac{1}{\sqrt{a}} \exp\left(-i\frac{2\pi n}{a}x\right),$$
$$E_n = \frac{\hbar^2}{2\mu}\left(\frac{2\pi n}{a}\right)^2, \quad n = 1, 2, 3, \ldots. \tag{6}$$

Each function $\chi_n(x)$ is a stationary plane wave propagating to the left.

Finally, the eigenfunction of $\hat{H}$ to the ground state can be expressed as

$$\psi_0(x) = \frac{1}{\sqrt{a}}, \quad E_0 = 0. \tag{7}$$

This is also an eigenfunction of $\hat{p}$ with an eigenvalue of $p_0 = 0$. All of these eigenfunctions specifically verify the following orthonormality relationships: $\langle\phi_n, \phi_m\rangle = \delta_{n,m}$, $\langle\chi_n, \chi_m\rangle = \delta_{n,m}$, $\langle\psi_0, \psi_0\rangle = 1$, and $\langle\phi_n, \chi_m\rangle = \langle\phi_n, \psi_0\rangle = \langle\chi_n, \psi_0\rangle = 0$. Let us note in passing that in this problem, the BSW quantization rule (given by Eq. (1)) also provides the exact quantum mechanical energies (see, for example, Ref. [19]).

3. Approximation of high principal quantum number to $\langle\hat{x}\rangle(t)$

Let us now consider the following complex general state $\Psi = \Psi(x, t)$, which is assumed to be normalized

$$\Psi(x,t) = \sum_{n=1}^{\infty} A_{-n}\chi_n(x) \exp\left(-i\frac{E_n}{\hbar}t\right) +$$
$$A_0\psi_0(x) \exp\left(-i\frac{E_n}{\hbar}t\right)$$
$$+\sum_{n=1}^{\infty} A_n\phi_n(x) \exp\left(-i\frac{E_n}{\hbar}t\right). \tag{8}$$

Precisely, due to the normalization condition, $\| \Psi \|^2 = \langle\Psi, \Psi\rangle = 1$, the (complex) constant coefficients of the Fourier expansion in Eq. (8) (A_{-n}, A_0 and A_n) must satisfy the following relation

$$\sum_{n=1}^{\infty} | A_{-n} |^2 + | A_0 |^2 + \sum_{n=1}^{\infty} | A_n |^2 = 1. \tag{9}$$

Now, by calculating the mean value of the position operator, $\hat{x} = x$, in the general state given in Eq. (8),

$$\langle\hat{x}\rangle(t) = \langle\Psi, \hat{x}\Psi\rangle = \int_0^a dx\, \bar{\Psi}(x,t) x \Psi(x,t) = \int_0^a dx\, x \mid \Psi(x,t) \mid^2, \tag{10}$$

we obtain the following expression (throughout the article, the horizontal bar represents complex conjugation)

$$\langle\hat{x}\rangle(t) = \frac{a}{2} + i\frac{a}{2\pi} \sum_{(m\neq)n=0}^{\infty} \sum_{m=0}^{\infty} \bar{A}_n A_m \frac{1}{n-m} \exp\left[i\frac{(E_n - E_m)}{\hbar}t\right] - i\frac{a}{2\pi} \sum_{(m\neq)n=0}^{\infty} \sum_{m=0}^{\infty} \bar{A}_{-n} A_{-m} \frac{1}{n-m} \exp\left[i\frac{(E_n - E_m)}{\hbar}t\right]$$
$$- i\frac{a}{2\pi} \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \bar{A}_{-n} A_m \frac{1}{n+m} \exp\left[i\frac{(E_n - E_m)}{\hbar}t\right] + i\frac{a}{2\pi} \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} A_{-n} \bar{A}_m \frac{1}{n+m} \exp\left[-i\frac{(E_n - E_m)}{\hbar}t\right]. \tag{11}$$

In the latter expression, we made use of Eq. (9). Also note that the last two terms in Eq. (11) are complex conjugate of each other.

Because we consider that the classical particle is moving from left to right, we must choose the part of $\langle\hat{x}\rangle(t)$ that corresponds to the quantum motion of plane waves propagating to the right. Hence, in the expansion given in Eq. (8), we must impose the condition $A_{-n} = 0$, where $n = 1, 2, 3, \ldots$. Therefore, the infinite series for $\langle\hat{x}\rangle(t)$ takes the form

$$\langle\hat{x}\rangle(t) = \frac{a}{2} + i\frac{a}{2\pi} \sum_{(m\neq)n=0}^{\infty} \sum_{m=0}^{\infty} \bar{A}_n A_m \frac{1}{n-m} \exp\left[i\frac{(E_n - E_m)}{\hbar}t\right]. \tag{12}$$

Now, the constants A_n satisfy the following relation (see Eq. (9))

$$| A_0 |^2 + \sum_{n=1}^{\infty} | A_n |^2 = \sum_{n=0}^{\infty} \bar{A}_n A_n = 1. \tag{13}$$

By introducing $\tau \equiv n - m$ ($\Rightarrow m = n - \tau$) and changing the sum over m in Eq. (12) to a sum over τ (note that, because $n = 1, 2, 3, \ldots$ and $m = 1, 2, 3, \ldots$ with $n \neq m$, then $\tau = \ldots -2, -1, +1, +2, \ldots$. Thus, $\tau \neq 0$), we can write $\langle \hat{x} \rangle(t)$ as follows:

$$\langle \hat{x} \rangle(t) = \frac{a}{2} + i\frac{a}{2\pi} \sum_{(0\neq)\tau=-\infty}^{+\infty} \frac{1}{\tau} \sum_{n=0}^{\infty} \bar{A}_n A_{n-\tau} \exp\left[i\frac{(E_n - E_{n-\tau})}{\hbar}t\right]. \tag{14}$$

In the latter expression, we also changed the order of the sums.

Using the expression for the allowed energy values given in Eq. (5), we obtained the following result

$$\frac{E_n - E_{n-\tau}}{\hbar} = 2\pi \frac{1}{\frac{\mu a^2}{2\pi n\hbar}} \tau \left(1 - \frac{\tau}{2n}\right). \tag{15}$$

Clearly, when $n \gg 1$ or equally when $n \approx n - \tau$ or $n \gg \tau$, the following approximation can be obtained

$$\frac{E_n - E_{n-\tau}}{\hbar} \approx 2\pi \frac{1}{\frac{\mu a^2}{2\pi n\hbar}} \tau = \frac{2\pi\tau}{T(n)}. \tag{16}$$

Thus, we identified $T(n)$ as the period of the classical particle (as a function of n). In fact, from the BSW quantization rule (see Eq. (1)), the following result was obtained

$$\oint dx\, p(x) = \mu v a = \frac{\mu a^2}{T(n)} = 2\pi n\hbar. \tag{17}$$

Note that, strictly speaking, in the limit as $n \to \infty$, one obtains $(E_n - E_{n-\tau})/\hbar \to \infty$ (the same applies to the model of the particle in the box with rigid walls [17]). In other words, the separation between two neighbouring energy levels does not become small as n becomes large. However, the results expressed in Eq. (16) make sense because $n\hbar$ = constant (and we are assuming that $\hbar \to 0$). Nevertheless, the relative spacing satisfies $(E_{n+1} - E_n)/E_n \to 0$ for large E_n. This (apparently) explains why cuantization is not observed at high energies [22]. On the other hand, we may assume that the sum over n in Eq. (14) is significant only around (say) $n = N$, such that $N \gg 1$. By substituting Eq. (16) into Eq. (14) (and using the approximation $n - \tau \approx n$), we obtain

$$\langle \hat{x} \rangle(t) \approx \frac{a}{2} + i\frac{a}{2\pi} \sum_{(0\neq)\tau=-\infty}^{+\infty} \frac{1}{\tau} \sum_{n \text{ around } N} \bar{A}_n A_n \exp\left[i\frac{2\pi\tau}{T(n)}t\right]. \tag{18}$$

However, in the interval of n (in the neighbourhood of N), we assumed that $T(n)$ did not change significantly (in fact, $T(n) \approx T = a\sqrt{\mu/2E}$, where E is the energy of the classical particle). Therefore the exponential in Eq. (18) can be separated from the sum. Precisely, due to the restriction given by Eq. (13), the sum takes on a value of one; thus, we recovered the expected classical result

$$\langle \hat{x} \rangle(t) \approx \frac{a}{2} + i\frac{a}{2\pi} \sum_{(0\neq)\tau=-\infty}^{+\infty} \frac{1}{\tau} \exp\left(i\frac{2\pi\tau}{T}t\right) = x(t). \tag{19}$$

4. Concluding remarks

Although the separation between the eigenvalues of energy tends to increase with an increase in the value of n, the semi-classical arguments we used to obtain the result given in Eq. (19) appear to be physically reasonable. In fact, we explicitly proved that the quantum average, $\langle \hat{x} \rangle(t)$, and the classical path, $x(t)$, are in agreement. The mean value, $\langle \hat{x} \rangle(t)$, was initially calculated in a state that included the general superposition of energy eigenstates but was finally converted (using the applied approximation) into a state formed by a number of stationary states with quantum numbers n in a band with a narrow width around $n = N \gg 1$ (a semiclassical state, of course). Certainly, for the problem at hand, classical-quantum correspondence was easy to verify because the Fourier series associated with the position of the particle was easy to calculate. Unfortunately, this is not always the case. We believe that the issues presented herein will be attractive to advanced undergraduate students, as well as to teachers and lecturers.

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