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# On the Ehrenfest theorem in a one-dimensional box(*)

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**Summary.** — The Ehrenfest theorem for a non-relativistic particle in a one-dimensional box is studied. By considering the cases of confined and "free" particle, the domains of the involved operators in this theorem are obtained. It is shown that the usual form of the Ehrenfest theorem is not valid.

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## 1. – Introduction

In classical mechanics the dynamical state of each particle is defined by their position and momentum, at a given instant. In quantum mechanics the dynamical state of the system is represented by its wave function $\Psi(x,t)$. One can attempt to recover the classical picture in terms of the position and momentum mean values in the corresponding quantum state, that is $\langle X\rangle = (\Psi, X\Psi)$ and $\langle P\rangle = (\Psi, P\Psi)$. In fact, the Ehrenfest theorem [1, 2] states that the equations of motion of these mean values are formally identical to the Hamiltonian equations of classical mechanics, except that the quantities which occur on both sides of the classical equations must be replaced by their corresponding operator mean values. In fact, if there exists a potential energy, the mean values $\langle X\rangle$ and $\langle P\rangle$ follow the laws of classical mechanics; but, this holds rigorously only when $U(x)$ is a polynomial of almost second degree in $x$. For example, with $U(x) \sim x^2$ (harmonic oscillator), $U(x) \sim x$ (charged particle in a constant electric field) and when $U(x) = 0$ (free particle) [3]. Otherwise $U(x)$ must vary sufficiently slow over a distance of the order of the extension of the wave packet, in which case the time derivative of the mean value of the momentum operator is almost equal to the mean value of a local "force".

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In model problems the potential may become infinite in some region or points, as for example in the case of the infinite square well or with point interaction potentials. In these cases, it is more appropriate to substitute the potential by fixed boundary conditions for which the Hamiltonian operator without the potential operator is self-adjoint. Then, the time derivative of the mean value of the momentum operator is equal to the mean value of Bohm's "non local quantum force" [4]; but interpreted as acting on the particle described by $\Psi(x,t)$ statistically or probabilistically. These interesting aspects of the problem will be considered in a forthcoming publication.

Important quantities in quantum mechanics, such as momentum and energy, are represented by linear and self-adjoint operators defined on a Hilbert space. But the domain of every operator is not always the whole space, which is the case for bounded operators. Most useful operators in quantum mechanics are unbounded and are defined as self-adjoint operators only on a smaller set of vectors called its domain. For that reason, formal calculations may be misleading if we are not careful about domains.

For the particle in the infinite potential well, or rather, in a one-dimensional box, the Ehrenfest theorem has been studied [5-7]; however, some important aspects were not properly considered. The usual requirement that the wavefunction vanish at the two walls (Dirichlet boundary condition) is not the most general one. In fact, there is a four-parameter family of boundary conditions (or equivalently different self-adjoint extensions of the free Hamiltonian with) each of which leads to unitary time evolution [8, 9]. For each of these boundary conditions there is a different Green's function, which determines the time evolution of any state in the box. A four-parameter family of functional integrals, which is associated with the four-parameter family of Green's functions, has been constructed [8]. All this illustrates to some extent the equivalence of the operator and functional integral approaches in quantum mechanics for a particle in a box. In this paper, we emphasize that for the most general family of self-adjoint extensions of the Hamiltonian operator $H$ for a particle in a box, the time evolution of the mean values of the operators $X$ and $P$ may be easily obtained just by being careful with the involved operators domains. However, the Ehrenfest theorem does not hold for any of the above-mentioned self-adjoint extensions of $H$. We specify the domains on which this theorem holds without any modification.

In sect. **2**, we summarize some general features of the operators position, momentum and Hamiltonian for a particle in a box, in particular, of their domains. In sect. **3**, we present the extended Ehrenfest theorem for a particle in a box. In sect. **4**, we apply this extended theorem to three types of boundary conditions, which describe a confined particle, *i.e.* with vanishing current $j(0) = j(L) = 0$ at the walls.

In sect. **5**, we consider a "free" particle, *i.e.* in a box but not confined in it, so, $j(0) = j(L) \neq 0$. Conclusions are presented in sect. **6**.

## 2. – Observables in a box

Let us consider a particle in a one-dimensional box in the interval $\Omega = [0, L]$. The Hilbert space of the system is $\mathcal{H} = \mathcal{L}^2(\Omega)$, with the scalar product denoted by $(\Psi_1, \Psi_2) = \int_0^L \overline{\Psi}_1 \Psi_2 \mathrm{d}x$, where $\bar{\Psi}$ is the complex conjugate of $\Psi$. In this Hilbert space we shall define the operators position, momentum and Hamiltonian.

The position observable $X$ is a multiplicative operator defined by

$$X\Psi(x,t) = x\Psi(x,t)\,, \tag{1}$$

$X$ is a bounded operator, therefore its domain is the whole space, that is

$$\mathrm{Dom}(X) = \{\Psi/\Psi \in \mathcal{H}, X\Psi \in \mathcal{H}\}\,. \tag{2}$$

However, the momentum operator $P$ is unbounded. It is defined by

$$P\Psi(x,t) = \left(-i\hbar\frac{\partial}{\partial x}\right)\Psi(x,t) \tag{3}$$

and its domain is [12]

$$\mathrm{Dom}(P) = \{\Psi/\Psi \in \mathcal{H}, \text{a.c. in } \Omega, P\Psi \in \mathcal{H}, \Psi \text{ fulfils } \Psi(L) = \Psi(0)\}\,, \tag{4}$$

where hereafter a.c. mean absolutely continuous functions. There exists a one-parameter family of boundary conditions for which $P$ is self-adjoint [10, 11]; but it has been shown that only for periodic boundary condition the operator $P$ transforms as a vector, and the parity symmetry operation of the Hamiltonian, $P^2/2m$ is not spontaneously broken [12]. Therefore, this is the physical momentum operator in the interval $\Omega$.

The Hamiltonian operator $H$ is defined by

$$H\Psi(x,t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\Psi(x,t)\,, \tag{5}$$

$H$ is also unbounded and the most general domain for which it is self-adjoint is [9]

$$\mathrm{Dom}(H) = \left\{ \begin{matrix} \Psi/\Psi \in \mathcal{H}, \;\; \Psi \text{ and } \Psi' \text{ a.c. in } \Omega, H\Psi \in \mathcal{H}, \Psi \text{ fulfils} \\ \begin{pmatrix} \Psi(L)-i\lambda\Psi'(L) \\ \Psi(0)+i\lambda\Psi'(0) \end{pmatrix} = U\begin{pmatrix} \Psi(L)+i\lambda\Psi'(L) \\ \Psi(0)-i\lambda\Psi'(0) \end{pmatrix}, \;\; U^{-1} = U^{\dagger} \end{matrix} \right\}. \tag{6}$$

The primes, hereafter, mean differentiation with respect to $x$, the parameter $\lambda$ is inserted for dimensional reasons and the symbol $\dagger$ denotes the adjoint of a vector or a matrix. The unitary matrix $U$ may be written as $U = \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)$ where $a = e^{i\mu}e^{i\tau}\cos\theta$, $b = e^{i\mu}e^{i\gamma}\sin\theta$, $c = e^{i\mu}e^{-i\gamma}\sin\theta$ and $d = -e^{i\mu}e^{-i\tau}\cos\theta$, with $0 \le \theta < \pi$, $0 \le \mu, \tau, \gamma < 2\pi$. We see that there is a four-parameter family of boundary conditions, each of which leads, for a fixed set of parameters $\theta$, $\mu$, $\tau$, $\gamma$, to a unitary time evolution. It is worth noting that with this parametrization the self-adjoint extensions are not labeled in a single form, that is to say, the same boundary condition may be given by a sub-family of parameters. The probability current density at the walls is

$$j(0) = j(L) = -\frac{\hbar}{2im}\frac{\sin\theta}{(\sin\mu - \sin\tau\cos\theta)}[\bar{\Psi}(L)\Psi(0)e^{i\gamma} - \Psi(L)\bar{\Psi}(0)e^{-i\gamma}]\,, \tag{7}$$

where $\sin\mu - \sin\tau\cos\theta \neq 0$ and $\Psi(0)$ and $\Psi(L)$ are related by (6). By making $\theta = 0$ in (6), we obtain the sub-family of boundary conditions for which $j(0) = j(L) = 0$,

$$\begin{aligned} \cos\left(\frac{\mu-\tau}{2}\right)\Psi(0) &= -\lambda\sin\left(\frac{\mu-\tau}{2}\right)\Psi'(0)\,, \\ \sin\left(\frac{\mu+\tau}{2}\right)\Psi(L) &= -\lambda\cos\left(\frac{\mu+\tau}{2}\right)\Psi'(L)\,. \end{aligned} \tag{8}$$

These boundary conditions include

– Dirichlet condition ($\theta = 0, \mu = \tau = \pi/2$):

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

– Neumann condition ($\theta = 0, \mu = \pi/2, \tau = 3\pi/2$):

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

– Non-relativistic MIT bag-like condition ($\theta = 0, \mu = 0, \tau = \pi/2$):

$$\frac{\Psi'(L)}{\Psi(L)} = -\frac{\Psi'(0)}{\Psi(0)} = -\frac{1}{\lambda}.$$

Among the boundary conditions which satisfy $j(0) = j(L) \neq 0$, we have

– Periodic condition ($\theta = \pi/2, \mu = \gamma = 0, \pi$):

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

## 3. – The Ehrenfest theorem

In the Schrödinger representation, the time derivative of the mean value of a given explicitly time-independent self-adjoint operator $A$ in the normalized state $\Psi = \Psi(x,t)$ is

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = \left(\frac{\partial \Psi}{\partial t}, A\Psi\right) + \left(\Psi, A\frac{\partial \Psi}{\partial t}\right).$$

Taking into account the Schrödinger evolution equation, $i\hbar\frac{\partial\Psi}{\partial t} = H\Psi$, one has

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = \frac{i}{\hbar}[(H\Psi, A\Psi) - (\Psi, AH\Psi)]\,, \tag{9}$$

where, for all $t$ we must have $\Psi \in \mathrm{Dom}(A) \cap \mathrm{Dom}(H)$ and $H\Psi \in \mathrm{Dom}(A)$. Since the operator $A$ is self-adjoint: $(\Psi, AH\Psi) = (A\Psi, H\Psi)$, and we write

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = \frac{i}{\hbar}[(H\Psi, A\Psi) - (A\Psi, H\Psi)] \equiv -\frac{2}{\hbar}\Im\,(H\Psi, A\Psi)\ , \tag{10}$$

where $\Im$ denotes the imaginary part of complex number.

With the above requirements on $\Psi(x,t)$, this equation is always true and may be used to calculate the time derivative of $\langle A\rangle$. One might have $\mathrm{Ran}(A) \cap \mathrm{Dom}(H) = \{0\}$, where $\mathrm{Ran}(A)$ is the range of $A$, in which case $HA$ and $[H, A]$ are meaningless, by the way, this is just the case which will be considered in the following sections with $A = X$ or $P$. However, if $A\Psi \in \mathrm{Dom}(H)$, the commutator $[H, A]$ may be introduced, and eq. (9) may be written as

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = \frac{i}{\hbar}[(H\Psi, A\Psi) - (\Psi, HA\Psi)] + \left(\Psi, \frac{i}{\hbar}[H, A]\Psi\right). \tag{11}$$

The Hamiltonian operator is self-adjoint, so $(H\Psi, A\Psi) = (\Psi, HA\Psi)$, then

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = \frac{i}{\hbar}\langle [H, A]\rangle\,. \tag{12}$$

It is worth pointing out that eq. (12) makes sense only in those cases where $A\Psi \in \mathrm{Dom}(H)$. In particular, for the operators $X$ and $P$,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle &= \frac{i}{\hbar}\langle [H, X]\rangle = \frac{1}{m}\langle P\rangle\,,\\ \frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle &= \frac{i}{\hbar}\langle [H, P]\rangle\,,\end{aligned} \tag{13}$$

where we have assumed that $X\Psi$ and $P\Psi$ both belong to $\mathrm{Dom}(H)$. These two equations constitute the Ehrenfest theorem. It is important to note that eq. (12) cannot be obtained just by taking the mean value of the analogous evolution equation in the Heisenberg picture, unless the domain problems be considered. On the other hand, if both $X\Psi$ and $P\Psi$ do not belong to $\mathrm{Dom}(H)$, the time derivative of the mean value of the position and momentum operators must be written as

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle &= -\frac{2}{\hbar}\Im\,(H\Psi, X\Psi)\,,\\ \frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle &= -\frac{2}{\hbar}\Im\,(H\Psi, P\Psi)\,.\end{aligned} \tag{14}$$

In the following, this theorem for Dirichlet, MIT bag model-like, Neumann and periodic boundary conditions, is considered. The commutator $[H, A]$ will be introduced wherever be possible.

## 4. – Confined particle

Let $H \equiv H_\mathrm{D}$ be the Dirichlet Hamiltonian operator given by (5) whose domain is

$$\mathrm{Dom}(H_\mathrm{D}) = \left\{ \begin{matrix} \Psi/\Psi \in \mathcal{H}, \Psi \text{ and } \Psi' \text{ a.c. in } \Omega, H_\mathrm{D}\Psi \in \mathcal{H} \\ \Psi \text{ fulfils } \Psi(L) = \Psi(0) = 0 \end{matrix} \right\}\,. \tag{15}$$

It can be easily checked that $X\Psi \in \mathrm{Dom}(H_\mathrm{D})$, in fact, $(X\Psi)(0, t) = (X\Psi)(L, t)$. In order that $P\Psi \in \mathrm{Dom}(H_\mathrm{D})$, $\Psi'(x, t)$ must additionally satisfy $\Psi'(L, t) = \Psi'(0, t) = 0$ for all $t$; but this is not compatible with the other requirements on $\Psi(x, t)$. So, we write

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle &= -\frac{2}{\hbar}\Im\,(H_\mathrm{D}\Psi, X\Psi) = \frac{i}{\hbar}\langle [H_\mathrm{D}, X]\rangle = \frac{1}{m}\langle P\rangle\,,\\ \frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle &= -\frac{2}{\hbar}\Im\,(H_\mathrm{D}\Psi, P\Psi)\,.\end{aligned} \tag{16}$$

Let us consider, without loss of generality, a simple example where the wave function $\Psi(x, t)$ is a linear combination of the first two stationary states

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

where the normalized $H_D$-eigenfunctions are $\psi_N(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{N\pi x}{L}\right)$ with eigenvalues $E_N = \frac{\hbar^2}{2m}\left(\frac{N\pi}{L}\right)^2$. Note that $\Psi(x,t) \in \mathrm{Dom}(P) \cap \mathrm{Dom}(H_D)$ and $H_D\Psi(x,t) \in \mathrm{Dom}(P)$. In fact, $\Psi(L,t) = \Psi(0,t) = 0$ and $\Psi''(L,t) = \Psi''(0,t)$. The mean values of $X$ and $P$ are

$$\langle X\rangle = \frac{L}{2} - \frac{16L}{9\pi^2}\cos(\omega_{21}t) \ ,$$
$$\langle P\rangle = \frac{8\hbar}{3L}\sin(\omega_{21}t)$$

with $\omega_{21} \equiv \frac{E_2-E_1}{\hbar} = \frac{3\hbar\pi^2}{2mL^2}$ . The time derivatives of the mean values are

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle = \frac{8\hbar}{3mL}\sin(\omega_{21}t) \ ,$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle = \frac{8E_1}{L}\cos(\omega_{21}t)$$

which coincide with the right-hand side of eqs. (16). Let us point out that in order to calculate the right-hand side of the equation for the time derivative of $\langle P\rangle$, we do not have to worry about the mean value of this force as in ref. [5], we simply calculate it through $\Im(H\Psi, P\Psi)$.

Another boundary condition, which describes a confined particle, is the non-relativistic limit of the boundary condition used in the relativistic MIT bag model of quarks confinement [13]. This relativistic boundary condition is $C\Pi T$ invariant (charge conjugation, parity and time-reversal invariant) for a particle in a box [9]. In the following, we consider a non-relativistic Hamiltonian $H \equiv H_M$ with a non-relativistic MIT bag-like condition. The domain of $H \equiv H_M$ is given by

$$\mathrm{Dom}(H_M) = \left\{ \begin{array}{c} \Psi/\Psi \in \mathcal{H},\ \Psi \text{ and } \Psi' \text{ a.c. in } \Omega,\ H_M\Psi \in \mathcal{H} \\ \Psi \text{ fulfils } \frac{\Psi'(L)}{\Psi(L)} = -\frac{\Psi'(0)}{\Psi(0)} = -\frac{1}{\lambda} \end{array} \right\} , \tag{17}$$

Equations (14) are satisfied if

$$\Psi(L,t) = \Psi(0,t), \quad \Psi'(L,t) = -\Psi'(0,t), \quad \Psi''(L,t) = \Psi''(0,t) . \tag{18}$$

Clearly, $X\Psi(x,t) \notin \mathrm{Dom}(H_M)$, furthermore $P\Psi(x,t) \in \mathrm{Dom}(H_M)$ if $\lambda^2\Psi''(L,t) = \Psi(L,t)$ and $\lambda^2\Psi''(0,t) = \Psi(0,t)$, but this is not compatible with the other requirements for a fixed $\lambda$, then $P\Psi(x,t) \notin \mathrm{Dom}(H_M)$. It follows that the evolution equations are those of (14).

As a simple check of eqs. (14), let us consider a wave packet $\Psi(x,t)$ superposition of the first two odd eigenstates of $H_M$ with domain given by (17), whose eigenvalues are obtained from the transcendental equation: $\tan(kL) = \frac{2k\lambda}{(k\lambda)^2-1}$, where $k = \frac{\sqrt{2mE}}{\hbar}$. Choosing the natural scale $\lambda = L$, we obtain $E_1 \approx 1.7069\frac{\hbar^2}{2mL^2}$ and $E_3 \approx 43.3570\frac{\hbar^2}{2mL^2}$. The corresponding normalized eigenfunctions are $\psi_1(x) \approx \frac{1.0725}{\sqrt{L}}\cos\left(\frac{1.3065x}{L} - 0.6533\right)$ and $\psi_3(x) \approx \frac{1.3834}{\sqrt{L}}\cos\left(\frac{6.5846x}{L} - 3.2923\right)$. Then

$$\Psi(x,t) = \frac{2}{\sqrt{2}}\left[\psi_1(x)e^{-i\frac{E_1}{\hbar}t} + \psi_3(x)e^{-i\frac{E_3}{\hbar}t}\right] ,$$

which satisfy the MIT bag-like condition for all $t$. Likewise, the boundary conditions in (18) are also satisfied for all $t$. Then, the mean values of $X$ and $P$ are

$$\langle X \rangle \approx \frac{L}{2} - 0.5199L\cos(\eta_{31}t)\,,$$
$$\langle P \rangle \approx 0$$

with $\eta_{31} \equiv \frac{E_3 - E_1}{\hbar} = \frac{41.6501\hbar}{2mL^2}$. From (14), the time derivatives of these mean values are

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle X \rangle \approx \frac{10.8269\hbar}{mL}\sin(\eta_{31}t) \neq \frac{1}{m}\langle P \rangle\,,$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\langle P \rangle \approx 0\,.$$

Let us point out that in spite of having a vanishing probability current at the walls, the mean value of the "quantum force" vanishes, but the wave packet is reflected by the walls [14]. The interference between this reflected packet and the incident one produces oscillations of the probability density.

Finally, we consider the Hamiltonian $H \equiv H_{\mathrm{N}}$ with the Neumann boundary condition. The domain of $H_{\mathrm{N}}$ is given by

$$\mathrm{Dom}(H_{\mathrm{N}}) = \left\{ \begin{matrix} \Psi/\Psi \in \mathcal{H},\ \Psi \text{ and } \Psi' \text{ a.c. in } \Omega,\ H_{\mathrm{N}}\Psi \in \mathcal{H} \\ \Psi \text{ fulfils } \Psi'(L) = \Psi'(0) = 0 \end{matrix} \right\}. \tag{19}$$

It can be shown that $X\Psi \in \mathrm{Dom}(H_{\mathrm{N}})$ if $\Psi(L,t) = \Psi(0,t) = 0$, and $P\Psi(x,t) \in \mathrm{Dom}(H_{\mathrm{N}})$ if $\Psi''(L,t) = \Psi''(0,t) = 0$, nevertheless, both conditions are not compatible with the other requirements on $\Psi(x,t)$. So, the time derivatives of $\langle X \rangle$ and $\langle P \rangle$ must be also written as in eq. (14).

Let us consider, without loss of generality, a wave function $\Psi(x,t)$, linear combination of two stationary states

$$\Psi(x,t) = \frac{1}{\sqrt{2}}[\psi_2(x)e^{-i\frac{E_2}{\hbar}t} + \psi_4(x)e^{-i\frac{E_4}{\hbar}t}]\,,$$

where the normalized $H_{\mathrm{N}}$-eigenfunctions are $\psi_n(x) = \sqrt{\frac{2}{L}}\cos\left(\frac{n\pi x}{L}\right)$ with eigenvalues $E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$. Clearly $\Psi(x,t) \in \mathrm{Dom}(P) \cap \mathrm{Dom}(H_{\mathrm{N}})$ and $H_{\mathrm{N}}\Psi(x,t) \in \mathrm{Dom}(P)$. The mean values of $X$ and $P$ are

$$\langle X \rangle = \frac{L}{2}\,, \qquad \langle P \rangle = 0\,,$$

consistently, the time derivatives of the mean values are

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle X \rangle = 0\,, \qquad \frac{\mathrm{d}}{\mathrm{d}t}\langle P \rangle = 0$$

which coincide with the right-hand side of eqs. (14).

## 5. – "Free" particle

A necessary condition in order to have a "free" particle in $\Omega$ is: $j(0) = j(L) \neq 0$. The Hamiltonian operator for a "free" particle $H \equiv H_{\rm F}$ must be a function of $P$ in the interval $\Omega$, *i.e.*

$$H_{\rm F}(P) = \frac{P.\,P}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\,. \tag{20}$$

Therefore its domain is

$$\mathrm{Dom}(H_{\rm F}) = \left\{ \begin{array}{c} \Psi/\Psi \in \mathcal{H},\ \Psi \text{ and } \Psi' \text{ a.c. in } \Omega,\ H_{\rm F}\Psi \in \mathcal{H} \\ \Psi \text{ fulfils } \Psi(L) = \Psi(0) \neq 0,\ \Psi'(L) = \Psi'(0) \neq 0 \end{array} \right\}, \tag{21}$$

which is one of the above-mentioned self-adjoint extensions (periodic boundary condition). $H_{\rm F}$ is the kinetic energy operator in the one-dimensional box, that is, this Hamiltonian operator is the only self-adjoint extension which is a function of the momentum operator $P$ in $\Omega$. Equations (14) are satisfied by requiring

$$\Psi(L,t) = \Psi(0,t) \neq 0; \quad \Psi'(L,t) = \Psi'(0,t) \neq 0; \quad \Psi''(L,t) = \Psi''(0,t) \neq 0\,. \tag{22}$$

Since $X\Psi$ does not satisfy the periodicity condition in (21), $X\Psi \notin \mathrm{Dom}(H_{\rm F})$. On the other hand, $\Psi'(L,t) = \Psi'(0,t) \neq 0$, therefore $P\Psi \in \mathrm{Dom}(H_{\rm F})$. Then, the evolution equations for the mean values $\langle X\rangle$ and $\langle P\rangle$ are

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle &= -\frac{2}{\hbar}\Im\left(H_{\rm F}\Psi, X\Psi\right)\,, \\ \frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle &= -\frac{2}{\hbar}\Im\left(H_{\rm F}\Psi, P\Psi\right) = \frac{i}{\hbar}\langle [H_{\rm F}, P]\rangle = 0\,. \end{aligned} \tag{23}$$

Likewise, it can be shown that for this case, since $\mathrm{Ran}(X) \cap \mathrm{Dom}(P) = \{0\}$, the canonical commutation relation has not a meaning [15], neither the corresponding uncertainty relation [12]. This peculiarity also arises when one attempts to introduce an operator $\phi$ conjugate to the angular momentum $L_z = -i\hbar\frac{\partial}{\partial\phi}$ [16]. Recently, it has been mentioned that the same difficulty appears in large systems with periodic boundary conditions, as is usual in condensed matter physics [17].

Let us also perform a simple check of eqs. (23) by using a linear combination of the two $P$-eigenfunctions $\phi_n(x) = \frac{1}{\sqrt{L}}e^{i\frac{2n\pi}{L}x}$ with $n = 1, 2$, which satisfy the periodic boundary conditions $\Psi(L,t) = \Psi(0,t) \neq 0$, $\Psi'(L,t) = \Psi'(0,t) \neq 0$ and $\Psi''(L,t) = \Psi''(0,t) \neq 0$. Let

$$\Psi(x,t) = \frac{1}{\sqrt{2}}[\phi_1(x)e^{-i\frac{E_1}{\hbar}t} + \phi_2(x)e^{-i\frac{E_2}{\hbar}t}]\,,$$

where $E_n = \frac{\hbar^2}{2m}\left(\frac{2n\pi}{L}\right)^2$. One obtains

$$\langle X\rangle = \frac{L}{2} - \frac{L}{2\pi}\sin\left(\nu_{21}t\right)\,, \qquad \langle P\rangle = \frac{3\pi\hbar}{L}\,,$$

where $\nu_{21} \equiv \frac{E_2 - E_1}{\hbar} = \frac{6\hbar\pi^2}{mL^2}$. Finally,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle = -\frac{3\pi\hbar}{mL}\cos(\nu_{21}t) \neq \frac{1}{m}\langle P\rangle\,, \qquad \frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle = 0\,.$$

Hence, the Ehrenfest equation for the time derivative of the mean position does not hold due to the fact that $X\Psi \notin \mathrm{Dom}(H_{\mathrm{F}})$ and, as opposed to what was assumed in ref. [6], the commutator $[H_{\mathrm{F}}, X]$ is meaningless. It is worth pointing out that for a particle described by the wave packet $\Psi(x,t)$, the evolution of its probability density shows that the particle does not "interact" with the walls. On the other hand, since $H$ is a function of $P$, then they commute [18], consistently with the vanishing of the time derivative of $\langle P\rangle$.

## 6. – Conclusions

We have made some precisions about the domains on which the Ehrenfest theorem holds for a particle in a box. A common feature of all self-adjoint extensions of the Hamiltonian operator for a particle in a box, is that the Ehrenfest theorem does not hold as is usually written in the literature. In fact, for every $H$ one has $\mathrm{Ran}(A) \cap \mathrm{Dom}(H) = \{0\}$ for $A = X$ or $P$, or for both of them. But for all self-adjoint extensions for which $j(0) = j(L) = 0$, corresponding to the boundary conditions given in (8), $\mathrm{Ran}(P) \cap \mathrm{Dom}(H) = \{0\}$; so that the commutator $[H, P]$ cannot be defined because $P\Psi \notin \mathrm{Dom}(H)$. Moreover, the operator $P^2$ in these Hamiltonians is not really defined as $P.\,P$ [19].

By considering various examples of Hamiltonians for a confined particle, *i.e.* with vanishing probability current density at the walls, the law of motion of the mean values of $X$ and $P$ was obtained, pointing out that these mean values do not follow the usual Ehrenfest theorem (13).

On the other hand, for a "free" particle with a non-vanishing probability current density at the walls, the Ehrenfest theorem does not hold because $X\Psi \notin \mathrm{Dom}(H_{\mathrm{F}})$; nevertheless, the time derivatives of $\langle X\rangle$ and $\langle P\rangle$ may be calculated using (14). It is worth to emphasize that the "free" particle in a box is analogous to the free particle in the real line $\mathbb{R}$ only in the sense that formally its Hamiltonian operator is the kinetic energy operator. Nevertheless, the free particle in $\mathbb{R}$ verifies the usual form of the Ehrenfest theorem, the canonical commutation relation and the uncertainty relation, which are not satisfied for a "free" particle in a box.

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## APPENDIX

If the formal steps that yield to eq. (11) for the operator $X$ are written out explicitly in coordinate representation, one has

$$\text{(A.1)} \qquad \frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle = -\frac{i\hbar}{2m}\left[x\left(\Psi\frac{\partial\overline{\Psi}}{\partial x} - \overline{\Psi}\frac{\partial\Psi}{\partial x}\right) - \overline{\Psi}\Psi\right]\Bigg|_0^L + \frac{i}{\hbar}\langle[H, X]\rangle\,,$$

where $\Psi \in \mathrm{Dom}([H,X])$ for all $t$. Only if additionally $\Psi \in \mathrm{Dom}(P)$, then $\frac{i}{\hbar}\langle[H,X]\rangle = \frac{\langle P\rangle}{m}$. Since the corresponding Hamiltonian operator is self-adjoint, the integral by part term in (A.1) is automatically null and we obtain eq. (12) for $X$. Likewise, we can write eq. (11) for the operator $P$

$$\text{(A.2)} \qquad \frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle = -\frac{\hbar^2}{2m}\left(\frac{\partial\Psi}{\partial x}\frac{\partial\overline{\Psi}}{\partial x} - \overline{\Psi}\frac{\partial^2\Psi}{\partial x^2}\right)\Bigg|_0^L + \frac{i}{\hbar}\langle[H,P]\rangle\,,$$

where $\Psi \in \mathrm{Dom}([H,P])$ for all $t$. As the corresponding Hamiltonian operator is self-adjoint, the integral by part term in (A.2) is null, and we obtain eq. (12) for $P$. The pair of eqs. (A.1) and (A.2) are simultaneously satisfied only if $\Psi \in \mathrm{Dom}([H,X])\cap\mathrm{Dom}([H,P])$. Finally, it can be seen that either $\mathrm{Dom}([H,X])$ or $\mathrm{Dom}([H,P])$ is empty, or both of them (owing to that the boundary conditions are too restrictive for the solutions of the Schrödinger equation). When it is possible to write some of eqs. (A.1) or (A.2), then the integral by parts terms are automatically nulls. In fact, for the dynamics studied in sects. **4** and **5** this can be verified.

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