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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)

Salvatore De Vincenzo[1]

Escuela de Física, Facultad de Ciencias, Universidad Central de Venezuela, Caracas, Venezuela
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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

[1]E-mail: salvatore.devincenzo@ucv.ve.

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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 $x(t \leq 0) = 0$. 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 $0 \leq x \leq a$ 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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