

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 e a frequência mecânica clássica do τ -ésimo harmônico do movimento da partícula. Depois de usar a regra de quantização de Bohr-Sommerfeld-Wilson, foram obtidos as respectivas amplitudes e frequências 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 $j(x) = (\hbar/m)\text{Im}(\psi(x)\psi'(x))$ 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 $n \rightarrow m = n - \tau$). 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

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

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 $nT \leq t \leq (n+1)T$, 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 $0 \leq t \leq T$ ($n = 0$) is $x(t) = f_0(t)$; thus, $x(t) = vt$ for $0 \leq t \leq T/2$ and $x(t) = vT - vt$ for $T/2 \leq t \leq T$. 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

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

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

The classical amplitude, a_τ , takes on the following values

$$a_\tau = -\frac{2vT}{\pi^2\tau^2}, \quad \tau = 1, 3, 5, \dots \quad (3)$$

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

$$\omega_\tau = \tau\omega, \quad (4)$$

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

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

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 $x(t \leq 0) = 0$. Clearly, the periodic function $x(t)$ in Eq. (5) (with $t \in (-\infty, +\infty)$) can be expanded into a Fourier series

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

The classical amplitude, c_τ , has the following values

$$c_\tau = i\frac{vT}{2\pi\tau}, \quad \tau = \pm 1, \pm 2, \dots \quad (7)$$

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

$$\omega_\tau = \tau\omega, \quad (8)$$

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

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

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 $x(t\pm) \equiv \lim_{\epsilon \rightarrow 0} x(t \pm \epsilon)$ 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])

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

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)

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

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

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

where, in this case, $n = 1, 2, \dots$. 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

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

Moreover, $a_\tau(n) = 0$, where $\tau = 2, 4, 6, \dots$ 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

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

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

$$x(t, n) = a_0(n) + a_1(n) \cos(\omega(n)t) + a_3(n) \cos(3\omega(n)t) + \dots \quad (15)$$

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 $n \rightarrow m$) to x , where the transition amplitude $c_{n,m} = \langle \psi_n | x | \psi_m \rangle$ is a measure of the intensity of light, and $x_{n,m} = \langle \Psi_n | x | \Psi_m \rangle$ (where $\Psi_n(x, t) = \psi_n(x) \exp(-iE_n t/\hbar)$ are solutions to the time-dependent Schrödinger equation). In the transition $n \rightarrow n - \tau$, where $n \gg \tau$, the quantized Fourier amplitude $c_\tau(n)$ must be equal to the Heisenberg amplitude $c_{n,n-\tau}$

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

Equivalently,

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

because the coefficients of the cosine Fourier series $a_\tau(n)$ with $\tau = 1, 3, 5, \dots$ 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

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

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

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

where $\tau = 1, 3, 5, \dots$, $a_\tau(n) = 0$ with $\tau = 2, 4, \dots$ 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]

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

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

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

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

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

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

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

In this case, $n = 0, 1, 2, \dots$. 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

$$c_\tau(n) = i \frac{L}{2\pi\tau}, \quad \tau = \pm 1, \pm 2, \dots \quad (24)$$

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

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

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 $c_\tau \rightarrow c_\tau(n)$ and $\omega_\tau \rightarrow \tau\omega(n)$

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

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

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

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

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

In this case, $\tau = \pm 1, \pm 2, \dots$ 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)

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

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

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

where $n = 0, 1, 2, \dots$ 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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