Modified Hamiltonian for a particle in an infinite box that includes wall effects

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We give a modified Hamiltonian for a particle in a box with infinite potential walls that takes into account wall effects. The Hamiltonian is expressed in both the position and momentum representation. In the momentum representation the eigenvalue problem for energy is an integral equation.

Keywords: particle in a box; modified Hamiltonian

1. Introduction

The usual textbook approach for solving the eigenvalue problem for energy for a particle in a box with infinite potential at the walls

\[ H u(x) = E u(x) \] (1)

is to write the Hamiltonian,

\[ H = \frac{p^2}{2m} \] (2)

and in the position representation, the eigenvalue problem is taken to be

\[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} u(x) = E u(x) \] (3)

and the “solution” is then written as

\[ u(x) = A \sin \sqrt{\frac{2mE}{\hbar^2}} x + B \cos \sqrt{\frac{2mE}{\hbar^2}} x \] (4)

Upon imposing the usual boundary conditions

\[ u(0) = u(L) = 0 \] (5)

one obtains the normalized eigenfunctions

\[ u_n(x) = \sqrt{\frac{2}{L}} \sin \left( \frac{n\pi}{L} x \right) \quad 0 \leq x \leq L \] (6)
with eigenvalues
\[ E_n = \frac{\pi^2 h^2}{2mL^2} n^2 \quad n = 1, 2, \ldots \]  
(7)
The \( u_n(x) \)'s are normalized and orthonormal
\[ \int_0^L u_n(x) u_m(x) dx = \delta_{nm} \]  
(8)
Writing the solutions and Hamiltonian and hence the eigenfunctions in the above forms leads to many difficulties. There is a vast literature on the subject and here we just touch on some of the issues [1-12]. If the Hamiltonian is given by Eq. (2), it would seem that \( \mathbf{H} \) and the momentum operator, \( \mathbf{p} \), commute and would hence have the same eigenfunctions, which is clearly not the case. Also, for any particular state of energy we have that \( \langle \mathbf{H}^2 \rangle = \langle \mathbf{H} \rangle^2 \) which of course is correct. However, if one substitutes Eq. (2) into this one obtains that \( \langle \mathbf{p}^4 \rangle \) is equal to \( \langle \mathbf{p}^2 \rangle^2 \) which is incorrect since \( \langle \mathbf{p}^2 \rangle \) is finite but \( \langle \mathbf{p}^4 \rangle = \infty \) [11]. Additionally, some have argued that \( \langle \mathbf{p} \rangle = \pm \sqrt{2mE_n} \) and sometimes this is interpreted as that the particle moves to the right or left with one of these values. This is false, since all values of momentum are possible. [1, 8, 10]

These difficulties and others are resolved by a modified Hamiltonian that takes into account the wall effects.

2. Modified Hamiltonian

We consider the following modified Hamiltonian, \( \mathbf{H}_M \), in the position representation
\[ \mathbf{H}_M = \frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{\hbar^2}{2m} \left[ \delta(x) - \delta(x - L) \right] \frac{d}{dx} \]  
(9)
where
\[ \Theta(x) = \begin{cases} 0 & \text{if } x < 0, \\ 1 & \text{if } x \geq 0. \end{cases} \]  
(10)
The eigenvalue problem for \( \mathbf{H}_M \), is
\[ \mathbf{H}_M v_n(x) = E_n v_n(x) \]  
(11)
where \( v_n(x) \) are the eigenfunctions. Explicitly
\[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} v_n + \frac{\hbar^2}{2m} \left[ \Theta(x) - \Theta(x - L) \right] \frac{d}{dx} v_n = E_n v_n \]  
(12)
The solutions, that is the eigenfunctions, are
\[ v_n(x) = \left[ \Theta(x) - \Theta(x - L) \right] \sqrt{\frac{2}{L}} \sin \left( \frac{n\pi}{L} x \right) \]  
(13)
\[ = \left[ \Theta(x) - \Theta(x - L) \right] u_n(x) \]  
(14)
with \( E_n \) given by Eq. (7).
Also, we point out that the operator defined by
\[ \mathbf{H}_{M'} = \frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{\hbar^2}{2m} [\delta(x) - \delta(x - L)] \frac{d}{dx} \]  
when operating on an eigenfunction, \( v_n(x) \), is equivalent to \( \mathbf{H}_M \) operating on \( v_n(x) \), that is \( \mathbf{H}_M v_n(x) = \mathbf{H}_{M'} v_n(x) \).

In the momentum representation the eigenvalue problem becomes an integral equation
\[ \frac{p^2}{2m} \varphi_n(p) + \frac{i}{2m} \int_{-\infty}^{\infty} (1 - e^{-iL(p - p')/\hbar}) p' \varphi_n(p') dp' = E_n \varphi_n(p) \]  
(16)
where
\[ \varphi_n(p) = \frac{1}{\sqrt{2\pi \hbar}} \int_{-\infty}^{\infty} v_n(x) e^{-ixp/\hbar} dx \]  
(17)
\[ v_n(x) = \frac{1}{\sqrt{2\pi \hbar}} \int_{-\infty}^{\infty} \varphi_n(p) e^{ixp/\hbar} dp \]  
(18)

The solution to Eq. (16), are found to be
\[ \varphi_n(p) = \frac{n}{L \sqrt{\pi \hbar L}} \left[ 1 - (-1)^n e^{-ipL/\hbar} \right] \]  
(19)
which may be obtained directly from Eq. (17) \[1, 8\]. An alternative expression for \( \varphi_n(p) \) is
\[ \varphi_n(p) = \frac{1}{2i} \sqrt{\frac{L}{\pi \hbar}} \left\{ e^{-iL(\xi - n\pi)/2} \sin \left( \frac{L(\xi - n\pi)/2}{L} \right) - e^{-iL(\xi + n\pi)/2} \sin \left( \frac{L(\xi + n\pi)/2}{L} \right) \right\} \]  
(20)
The probability distribution for momentum, \( |\varphi_n(p)|^2 \), is given by
\[ |\varphi_n(p)|^2 = \frac{4n^2 \pi L/\hbar}{((n\pi)^2 - (pL/\hbar)^2)^2} \left\{ \begin{array}{ll} \sin^2 \frac{2\pi}{2n} & n = \text{even} \\ \cos^2 \frac{2\pi}{2n} & n = \text{odd} \end{array} \right. \]  
(21)
or
\[ |\varphi_n(p)|^2 = \frac{8mE_n}{\pi L} \frac{1}{(p^2 - 2mE_n)^2} \left\{ \begin{array}{ll} \sin^2 \frac{2\pi}{2n} & n = \text{even} \\ \cos^2 \frac{2\pi}{2n} & n = \text{odd} \end{array} \right. \]  
(22)

3. Discussion and Conclusion

The results presented in the last section resolve the difficulties discussed in the introduction and they also resolve other issues. This will be discussed in an expanded version of this paper. We point out here that since the Hamiltonian is no longer given by Eq. (2) we can no longer conclude that \( \langle \mathbf{p}^4 \rangle \) is equal to \( \langle \mathbf{p}^2 \rangle^2 \). Calculation of \( \langle \mathbf{p}^2 \rangle \) using Eq. (13) does give the correct answer while calculation of \( \langle \mathbf{p}^4 \rangle \) with Eq. (13) does indeed give infinity. Note, too, that since the modified Hamiltonian \( \mathbf{H}_M \) and \( \mathbf{p} \) do not commute one can not use \( \langle \mathbf{H}_M^k \rangle \) to calculate \( \langle \mathbf{p}^{2k} \rangle \), but direct calculation of \( \langle \mathbf{p}^{2k} \rangle \) with the new eigenfunctions, \( v_n \), does give the correct answers, namely
\[ \langle \mathbf{p}^{2k} \rangle = \int v_n(x) \mathbf{p}^{2k} v_n(x) dx = \left\{ \begin{array}{ll} 2mE_n & \text{for } k = 1, \\ \infty & \text{for } k \geq 2. \end{array} \right. \]  
(23)
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