On the functional form of the infinite square well model

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The original model of the infinite square well contains a vague notation $\infty$ and therefore results in some ambiguities. We investigate to obtain a functional form for the potential energy $V(x)$. This is done by substituting back the original energy eigenstates and eigenvalues into the Schrödinger equation. We then obtain a precise functional form of the $V(x)$. From this reformed model, we show that energy eigenstates and eigenvalues can directly be obtained without the need of imposing boundary condition, Ehrenfest’s theorem can directly be confirmed, and ambiguities in the original model can be resolved.

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I. INTRODUCTION

The infinite square well is a model using infinitely high potential barrier to confine particles inside a well. We also have other models using infinitely large potential energy, such as the Dirac delta function potential. Recently, Belloni and Robinett have given a review on these models [1]. The potential energy $V(x)$ of the infinite square well is described by

$$V(x) = \begin{cases} 0, & 0 < x < L, \\ \infty, & \text{otherwise}. \end{cases}$$ (1)

The notation $\infty$ is used in Eq. (1). Such a form of potential energy does not have a precise functional form. In what follows, we investigate to reform above potential energy in terms of established functions so that $V(x)$ has a precise functional form, and therefore avoid some ambiguities which will be discussed below.

The time independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\Psi''(x) + V(x)\Psi(x) = E\Psi(x).$$ (2)

For $V(x)$ defined in Eq. (1), the energy eigenfunctions $\Psi_n(x)$ and the eigenvalues $E_n$ of Eq. (2) are well-known [2-8]. We have

$$\Psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin(k_n x), & 0 < x < L, \\ 0, & \text{otherwise}. \end{cases}$$ (3)

$$E_n = \frac{\hbar^2 k_n^2}{2m},$$ (4)

where $k_n = n\pi/L$, $n = 1, 2, 3,...$. These solutions are obtained by imposing boundary conditions at the two sides of the well. The boundary condition imposed is that we require and only require the continuity of $\Psi(x)$ at the two sides of the well. This then yields the solutions described in Eqs. (3-4). If we also impose the continuity of $\Psi'(x)$, then we only obtain a trivial solution $\Psi(x) = 0$. We can only impose boundary conditions, because the form of the $V(x)$ in Eq. (1) does not allow us to determine the boundary condition from Schrödinger equation. [7, 8].

Although we have obtained solutions by imposing boundary conditions, nevertheless, it seems dangerous in physics using a quantity such as infinity. There is no controversy over the delta function potential, because we know how to handle the infinity; we have the formula as

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\[
\int_{-\infty}^{\infty} \delta(x)dx = 1. \tag{5}
\]

This is a specification formula showing how to handle the infinity. And this results that boundary conditions can be derived from Schrödinger equation for the delta function potential. In contrast, the quantity \(\infty\) in Eq. (11) is quite a vague notation. It lacks a specification formula like that in Eq. (5). We therefore have no guide on how to deal with it. And for this reason, we have to impose extra boundary conditions to obtain solutions. Also, there are ambiguities resulted from straightforwardly using this notation of \(\infty\). These are described as follows:

1. The first ambiguity is: what is the value of \(V(x)\Psi_n(x)\) outside the well, where \(V(x) = \infty\) and \(\Psi_n(x) = 0\)? We would encounter the problem as \(V(x)\Psi_n(x) = \infty \times 0 = ?\) \(\delta \Psi(x) = 0\) and \(\Psi''(x) = 0\) outside the well, therefore from the Schrödinger equation, Eq. (2), we need \(V(x)\Psi_n(x) = \infty \times 0 = 0\).

2. The second ambiguity is: what is the value of \(V(x)\Psi_n(x)\) at the sides of the well, where again \(V(x) = \infty\) and \(\Psi_n(x) = 0\)? However, in this case, we need \(V(x)\Psi_n(x) = \infty \times 0 = \infty\). This had already been pointed out that \(V(x)\Psi_n(x)\) should have a delta function at each side of the well \(\infty\).

3. The third ambiguity concerns the manifestation of Ehrenfest’s theorem. We note that the term \(-dV(x)/dx\) represents a force, which is zero inside the well but is infinite at the sides. Yet, the probability density \(\Psi^*(x)\Psi(x)\) is zero at the two sides. Hence, calculating the expectation value of the force, we encounter the problem at the edges that \(dV(x)/dx \Psi^*(x)\Psi(x) = \infty \times 0 = ?\) \(\infty\).

We have different ways for solving these ambiguities. The first is an indirect way; that is, we consider the infinite square well potential as a limiting case of a finite well potential \(\infty\). Seki and Rokhsar calculated quantities in a finite well, and followed by taking the limit \(V_0 \to \infty\). In this way, we can calculate the value of \(V(x)\Psi(x)\) and also the expectation values to confirm Ehrenfest theorem in the infinite square well \(\infty\).

The second is a direct way. The above ambiguities shows that we need a more precise functional form for the potential energy. Therefore, it is interesting and worth to investigate the limit of the functional form of the potential energy. This is quite similar to the definition of Dirac delta function \(\delta(x)\), which usually is defined as

\[
\delta(x) = \begin{cases} 
0, & x \neq 0, \\
\infty, & x = 0.
\end{cases} \tag{6}
\]

We may consider it as the limit of the finite square step function, defined as:

\[
f(x, \epsilon) = \begin{cases} 
\frac{1}{\epsilon}, & -\frac{\epsilon}{2} < x < \frac{\epsilon}{2}, \\
0, & \text{otherwise}.
\end{cases} \tag{7}
\]

Simply taking the limit \(\epsilon \to 0\) leads directly to Eq. (6). But, on the hand, we do have a functional form to this limit, that is

\[
\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ixy}dy. \tag{8}
\]

This is a very useful formula for describing the delta function.

In the same spirit, we seek a functional form of \(V(x)\) for the original infinite square well model. The potential energy of a finite well may also be described as: \(V(x) = V_0[\theta(x - L)]\). Taking the limit \(V_0 \to \infty\) simply leads to the \(V(x)\) in Eq. (11). This is not the functional form we are looking for. Instead, we are looking for an approach to study the limit of a finite square well physically.

To explore such a functional form physically, we work in an opposite way. That is, from \(\Psi(x)\) to determine \(V(x)\). By taking \(V(x)\) as an unknown, and substituting back a wave function \(\Psi(x)\) into the Schrödinger equation, we can then determine the corresponding potential energy. We confirm this method in the Appendix I for the case of the finite well.

For the infinite square well, the wave function in Eq. (3) can be rewritten in a more compact form as

\[
\Psi_n(x) = \sqrt{\frac{2}{L}} \sin(k_n x) \theta(x) \theta(L - x). \tag{9}
\]

The term \(\theta(x)\theta(L - x)\) can also be expressed as \([\theta(x) - \theta(L - x)]\) \(\infty\). We then substitute this form of \(\Psi_n(x)\) into the Schrödinger equation, Eq. (2). This then yields

\[
V(x)\Psi_n(x) = \sqrt{\frac{2}{L}} \frac{\hbar^2}{2m} k_n \left[\delta(x) - \cos(k_n L)\delta(L - x)\right]. \tag{10}
\]
The derivation is shown in Sec. II. Eq. (10) shows the required delta functions that are inherent in the values of $V(x)\Psi_n(x)$.

Eq. (11) is an important result. We show in Sec. IV that Eq. (11) enables us to directly resolve all the ambiguities mentioned above. That is, we need not solve these ambiguities by means of finite well. More importantly, Eq. (11) shows the property of the functional form of the $V(x)$ in the infinite square well. The $V(x)$ containing the notation $\infty$ in Eq. (11) is now replaced by a functional form. If we are to confine particles inside a well with $\Psi_n(x)$ as the energy eigenstates, then the potential energy should have such a property described in Eq. (11). We note that $\Psi_n(x)$ contains the factor $\theta(x)\theta(L - x)$. Because the divergence nature in the $V(x)$ of the infinite square well, this factor shows how to handle the infinity in the $V(x)$. From this formula, we can go on to investigate a more precise functional form of $V(x)$.

In Sec. II, we show the derivation of the functional form of $V(x)$ from the known eigenfunctions $\Psi_n(x)$ and eigenvalues $E_n$. We call the system defined by this $V(x)$ the reform model. In Sec. III, we show that the energy eigenstates and eigenvalues of the reformed model are the same as those in the original model. In Sec. IV, we show that above ambiguities can be resolved by the reformed model. In Sec. V, we have a conclusion. In Appendix I, we show that the functional form of the potential energy of a finite well can be obtained by the solutions of the finite well.

II. THE DERIVATION OF THE FUNCTIONAL FORM OF $V(x)$ FROM $\Psi_n(x)$

We here show the derivation of the functional form of $V(x)$ from the energy eigenstates $\Psi_n(x)$ described in Eq. (6). As we are to derive the form of $V(x)$ from the wave function, we then rewrite the Schrödinger equation as:

$$V(x)\Psi(x) = \frac{\hbar^2}{2m} \Psi''(x) + E\Psi(x).$$

(11)

The $\Psi''(x)$ can be calculated by the following formula

$$\Psi(x) = D(x)\theta(x)\theta(L - x)$$

$$\Psi''(x) = D''(x)\theta(x)\theta(L - x) + D'(x)\delta(x) - D'(x)\delta(L - x).$$

(12)

Substituting this formula of $\Psi''(x)$ into the right side of Eq. (11) and replacing $\Psi(x)$ by $\Psi_n(x)$, energy $E$ by $E_n$, and $D(x)$ by $D_n(x)$ where

$$D_n(x) = \sqrt{\frac{2}{L}} \sin(k_nx),$$

(13)

this then yields

$$V(x)\Psi_n(x) = \frac{\hbar^2}{2m} \left[\delta(x) - \delta(L - x)\right]D'_n(x).$$

(14)

Such a form is not symmetrical with respect to the two edges. We need a more symmetrical one. Substituting Eq. (13) into Eq. (14), we have

$$V(x)\Psi_n(x) = \sqrt{\frac{2}{L}} \frac{\hbar^2}{2m} k_n \cos(k_nx) \left[\delta(x) - \delta(L - x)\right].$$

$$= \sqrt{\frac{2}{L}} \frac{\hbar^2}{2m} k_n \left[\delta(x) - \cos(k_nL)\delta(L - x)\right].$$

(15)

This is the formula we state in Eq. (10). In what follows, we try to obtain a functional form of $V(x)$ from Eq. (15). We need to rearrange the right side of Eq. (15). Using the result that $\lim_{x \to 0} \sin(k_nx)/x = k_n$, the first term, $\sqrt{2/L} k_n\delta(x)$, can simply be written as $[D(x)/x]\delta(x)$. We also need to rewrite the second term, $-\sqrt{2/L} k_n \cos(k_nL)\delta(L - x)$, in a similar way. This can be done, as $D_n(x)$ can also be written as

$$D_n(x) = \sqrt{\frac{2}{L}} \sin(k_nx) = \sqrt{\frac{2}{L}} \sin[k_n(x - L)] \cos(k_nL).$$

(16)
Above, we have used $\sin(k_n L) = 0$ and $\cos(k_n L) = \pm 1$. Using $\lim_{x \to L} \sin[k_n(x - L)]/(x - L) = k_n$, Then we have: $-\sqrt{2/E} k_n \cos(k_n L) \delta(L - x) = [D_n(x)/(L - x)] \delta(L - x)$. Finally, Eq. (15) can be rewritten, together with the formula for $\Psi_n(x)$, as follows

$$\Psi_n(x) = D_n(x) \theta(x) \theta(x - L), \quad (17)$$
$$V(x) \Psi_n(x) = \frac{\hbar^2}{2m} \left[ \delta(x) + \frac{\delta(L - x)}{(L - x)} \right] D_n(x). \quad (18)$$

Dividing both sides of Eq. (18) by $D_n(x)$, we have

$$V(x) \theta(x) \theta(L - x) = \frac{\hbar^2}{2m} \left[ \frac{\delta(x)}{x} + \frac{\delta(L - x)}{(L - x)} \right]. \quad (19)$$

Eq. (19) defines the infinite square well with a precise functional form. The factor $\theta(x) \theta(L - x)$ seems unavoidable. This factor is in fact needed, due to the divergence nature of the $V(x)$ outside the well. We may wonder how to describe the divergence in Eq. (19) may then be viewed as a specification formula for $V(x)$. Because $V(x)$ is divergent outside the well, Eq. (19) shows that this divergence is eliminated when multiplied by the function $\theta(x) \theta(L - x)$. Thus, the $\theta(x) \theta(L - x)$ term is needed to accompany with the $V(x)$ in order to have a regular result. In other words, the $\theta(x) \theta(L - x)$ factor shows how to handle the infinity in the $V(x)$. This is then interesting to note that to define the $V(x)$ of an infinite square well, the $V(x)$ cannot be defined alone, it must be accompanied with the factor $\theta(x) \theta(L - x)$; a step better than using the notation $\infty$.

We may naively divide both sides of Eq. (19) by $\theta(x) \theta(L - x)$ to obtain a functional form of $V(x)$, but this is not formal, and in fact is not necessary. The formula in Eq. (19) is enough for discussing the infinite square well model. Multiplying both sides of Eq. (19) by an arbitrary function $F(x)$, we obtain a regular form of $V(x) \Psi(x)$, with $\Psi(x) = F(x) \theta(x) \theta(L - x)$. Thus a particle confined inside an infinite square well with a wave function $\Psi(x)$, then the wave function and the potential energy should be described as follows

$$\Psi(x) = F(x) \theta(x) \theta(L - x), \quad (20)$$
$$V(x) \Psi(x) = \frac{\hbar^2}{2m} \left[ \frac{\delta(x)}{x} + \frac{\delta(L - x)}{(L - x)} \right] F(x). \quad (21)$$

Eqs. (20)–(21) are a consequence of Eq. (19). Eq. (20) describes the wave function in an infinite square well, and Eq. (21) describes the functional form of the potential energy term in the Schrödinger equation. We see that $V(x) \Psi(x)$ is well defined. That $V(x) \Psi(x)$ is well defined is important, because it is $V(x) \Psi(x)$, not $V(x)$, that appears in the Schrödinger equation. A well defined $V(x) \Psi(x)$ then enables us to go on to solve energy eigenstates and eigenvalues of the Schrödinger equation, and to calculate expectation values, etc.

We conclude that Eq. (19) defines the infinite square well. Or, equivalently, Eqs. (20)–(21) define the infinite square well. We call Eq. (19) or Eqs. (20)–(21) the reformed model of the infinite square well. We will see the advantage of this form in the following two sections.

III. THE ENERGY EIGENSTATES AND EIGENVALUES OF THE REFORMED MODEL

We here solve the energy eigenstates and eigenvalues of the system defined in Eqs. (20)–(21). The results can be obtained by the following two methods.

Method (1)

case (I) , $E > 0$

We write the energy as $E = \hbar^2 k^2/(2m)$, where $k > 0$. Substituting the wave function $\Psi(x)$ in Eq. (20), and the $\Psi''(x)$ formulated in Eq. (12) into the Schrödinger equation in Eq. (2), we then obtain an equation of the following form:

$$C_0(x) \theta(x) \theta(L - x) + C_1(x) \delta(x) + C_2(x) \delta(x - L) = 0. \quad (22)$$
It then needs

\[ C_0(x) = F''(x) + k^2 F(x). \]  \hspace{1cm} (23)

\[ C_1(x) = \frac{F(x)}{x} - F'(x). \]  \hspace{1cm} (24)

\[ C_2(x) = \frac{F(x)}{L-x} + F'(x). \]  \hspace{1cm} (25)

Eq. (22) requires that \( C_0(x) = 0, \lim_{x \to 0} C_1(x) = 0 \) and \( \lim_{x \to L} C_2(x) = 0 \). From \( C_0(x) = 0 \), we obtain

\[ F(x) = A \sin(kx) + B \cos(kx). \]  \hspace{1cm} (26)

Substituting this \( F(x) \) into Eq. (24) yields

\[ \lim_{x \to 0} C_1(x) = \lim_{x \to 0} \frac{B}{x} = 0. \]  \hspace{1cm} (27)

Thus, it needs \( B = 0 \). Therefore,

\[ F(x) = A \sin(kx). \]  \hspace{1cm} (28)

Substituting Eq. (28) into Eq. (25) then yields

\[ \lim_{x \to L} C_2(x) = A \lim_{x \to L} \left[ k \cos(kL) + \frac{\sin(kx)}{L-x} \right] = 0. \]  \hspace{1cm} (29)

It then needs

\[ \sin(kL) = 0. \]  \hspace{1cm} (30)

Eq. (30) implies \( \cos(kL) = \pm 1 \). We can then use the identity, \( \sin(kx) = \sin(k(x-L)) \cos(kL) \). This shows that the term, \( k \cos(kL) + \sin(kx)/(L-x) \) in the bracket of Eq. (29) is indeed approaching zero when \( x \) approaches \( L \).

From Eqs. (28) and (30), we see that we have reproduced the solutions in Eq. (3-4). We obtain these solutions by only using the precise form of \( V(x) \Psi(x) \); we need not put in by hand boundary conditions. That is, the precise form of \( V(x) \Psi(x) \) and the Schrödinger equation determine all.

Case (II) \( , E = 0 \)

In this case, \( k = 0 \). From Eq. (23), we have \( F(x) = Ax + B \) \cite{12}. From Eqs. (24), we have \( \lim_{x \to 0} C_1(x) = \lim_{x \to 0} (B/x) = 0 \), therefore \( B = 0 \). And then from Eqs. (25), we obtain \( \lim_{x \to L} C_2(x) = \lim_{x \to L} AL/(L-x) = 0 \). This requires that \( A = 0 \). Thus, for \( E = 0 \), we only have the trivial solution, \( \Psi(x) = 0 \).

Case (III) \( , E < 0 \)

In this case, \( E = -\hbar^2 k^2/(2m) \). We then have \( F(x) = Ae^{kx} + Be^{-kx} \). From Eq. (24), we have \( \lim_{x \to 0} C_1(x) = \lim_{x \to 0} (A + B)/x = 0 \); therefore \( B = -A \). And then from Eq. (25), we obtain \( \lim_{x \to L} C_2(x) = \lim_{x \to L} A[\sinh(kL)/(L-x) + k \cosh(kL)] = 0 \). This requires that \( A = 0 \). Thus, for \( E < 0 \), we again only have the trivial solution, \( \Psi(x) = 0 \).

Method-2

We may also solve this system by the usual way, that is, we separately solve \( \Psi(x) \) in different regions and then connect these solutions at the boundaries. We consider here only the case for positive energy. From Eq. (21), \( V(x) \Psi(x) = 0 \), inside the well. We then easily obtain

\[ \Psi(x) = A \sin(kx) + B \cos(kx), \quad 0 < x < L. \]  \hspace{1cm} (31)

We need to connect this solution with \( \Psi(x) \) outside, which is \( \Psi(x) = 0 \). The boundary condition can only be derived from the Schrödinger equation, which tells us the information about \( \Delta \Psi(x) \), where we let \( \Delta \Psi(x) \) represent the amount of change of \( \Psi(x) \) in the infinitesimal interval \( [x-\epsilon, x+\epsilon] \). That is: \( \Delta \Psi(x) = \lim_{\epsilon \to 0} (\Psi(x+\epsilon) - \Psi(x-\epsilon)) \). Thus

\[ \Delta \Psi(x) = \lim_{\epsilon \to 0} \int_{x-\epsilon}^{x+\epsilon} \Psi''(y) \, dy. \]  \hspace{1cm} (32)
From Eq. (2), $\Psi''(y)$ can be replaced by $V(y)\Psi(y)$ and $E\Psi(y)$. The $E\Psi(y)$ term makes no contribution to the integration. We then have

$$\Delta\Psi'(x) = \lim_{\varepsilon \to 0} \frac{2m}{\hbar^2} \int_{x-\varepsilon}^{x+\varepsilon} V(y)\Psi(y) \, dy.$$  

(33)

Eq. (33) shows that the continuity of $\Psi'(x)$ is determined by $V(x)\Psi(x)$. For $x = 0$, substituting Eqs. (21), (31) into Eq. (33), we then have

$$\Delta\Psi'(0) = \lim_{x \to 0} (Ak + \frac{Bx}{x}).$$  

(34)

Thus, it needs $B = 0$. Then $\Psi(x) = A\sin(kx)$. Eq. (34) shows that $\Delta\Psi'(0) = Ak$, therefore $\Psi'(x)$ is not continuous at $x = 0$. For $x = L$, we have

$$\Delta\Psi'(L) = \lim_{x \to L} \frac{A\sin(kx)}{L-x}.$$  

(35)

It then needs

$$\sin(kL) = 0.$$  

(36)

And then $\Delta\Psi'(L) = -Ak \cos(kL)$.

In conclusion, we obtain $\Psi(x) = A\sin(kx)$, and the value of $k$ is determined by $\sin(kL) = 0$. We then have reproduce the solutions in Eqs. (3)-(4). It is interesting to note that, for the reformed model, the boundary conditions derived are concerning about the values of $\Delta\Psi'(x)$, not $\Psi(x)$. And the values of $\Delta\Psi'(0)$ and $\Delta\Psi'(L)$ can be determined from Schrödinger equation.

In what follows, we discuss ambiguities in the original infinite square well model, and we show that they can be resolved by the formula in Eq. (10).

IV. RESOLVING THE AMBIGUITIES

A. The value of $V(x)\Psi_n(x)$ outside the well

From Eq. (10), we have $V(x)\Psi_n(x) = 0$ outside the well. We thus resolve the ambiguity of $V(x)\Psi_n(x) = \infty \times 0 = ?$ in the original model. Actually, we see that $V(x)\Psi_n(x) = 0$ everywhere, except at the two sides. The two delta functions in $V(x)\Psi_n(x)$ are important, discussed below.

B. The value of $V(x)\Psi_n(x)$ at the edges of the well

From Eq. (10), due to the delta function, we also have $V(x)\Psi_n(x) = \infty$ at the two edges of the well. The need of delta function at sides had been pointed out in Ref. [9, 10]. We thus also resolve the ambiguity of $V(x)\Psi_n(x) = \infty \times 0 = ?$ in the original model. We can calculate the values of $\Delta\Psi_n'(0)$ and $\Delta\Psi_n'(L)$ from Eq. (10). By the solutions in Eq. (3), we know that $\Psi'(x)$ is discontinuous at $x = 0$ and $x = L$, and we obtain

$$\Delta\Psi_n'(0) = \sqrt{\frac{2}{L}} k_n,$$  

(37)

$$\Delta\Psi_n'(L) = -\sqrt{\frac{2}{L}} k_n \cos(k_n L).$$  

(38)

These results can not be checked from Eq. (33) for the original model, due to the vague notation $\infty$. For the reformed model, from Eqs. (10), (33), we have:

$$\Delta\Psi_n'(0) = \frac{2m}{\hbar^2} \int_{-\varepsilon}^{\varepsilon} \sqrt{\frac{2}{L}} \frac{\hbar^2}{2m} k_n \delta(y)dy = \sqrt{\frac{2}{L}} k_n,$$  

(39)

$$\Delta\Psi_n'(L) = \frac{2m}{\hbar^2} \int_{L-\varepsilon}^{L+\varepsilon} \sqrt{\frac{2}{L}} \frac{\hbar^2}{2m} k_n [-\cos(k_n L)\delta(L-y)]dy$$

$$= -\sqrt{\frac{2}{L}} k_n \cos(k_n L).$$  

(40)
These results in Eqs. (39-40) are consistent with those in Eqs. (37-38). From Eqs. (39-40), we note that if there were no delta functions, but only ordinary functions in $V(x)\Psi_n(x)$, then $\Delta \Psi'_n(0) = 0$ and $\Delta \Psi'_n(L) = 0$. That means $\Psi'(x)$ is continuous at the two sides of the well, and we will only obtain a trivial solution, $\Psi(x) = 0$. The two delta functions in the $V(x)\Psi_n(x)$ in Eq. (10) are therefore important, as they change a trivial solution to a non-trivial solution.

C. The manifestation of Ehrenfest’s theorem

The third puzzle concerns about the manifestation of Ehrenfest’s theorem for time-evolved wave packets in the infinite square well. The time evolution of a general wave packet $\Psi(x, t)$ is as follows

$$\Psi(x, t) = \sum_{n=1}^{\infty} a_n \Psi_n(x)e^{-i\omega_n t}. \quad (41)$$

where $\omega_n = E_n/\hbar$. To verify Ehrenfest’s theorem, we need to verify the following formula:

$$\frac{d}{dt} \langle \Psi(t) | \hat{p} | \Psi(t) \rangle = -\langle \Psi(t) | \frac{dV(x)}{dx} | \Psi(t) \rangle. \quad (42)$$

The calculation of the right side of Eq. (42) is related to the calculation of $\Psi_n(x)(dV(x)/dx)\Psi_j(x)$. We note that

$$\Psi_n(x)\frac{dV(x)}{dx}\Psi_j(x) = \frac{d}{dx} [\Psi_n(x)V(x)\Psi_j(x)] - \frac{d\Psi_n(x)}{dx}[V(x)\Psi_j(x)] - [\Psi_n(x)V(x)]\frac{d\Psi_j(x)}{dx}. \quad (43)$$

For the right side of Eq. (43), the first term makes no contribution in the calculation of integration. Using Eq. (10), the other two terms can be calculated, and we obtain

$$\frac{d\Psi_n(x)}{dx}V(x)\Psi_j(x) = \frac{\hbar^2}{2mL} k_n k_j \theta(x)\theta(L-x) [\delta(x) - (-1)^{n+j}\delta(L-x)]. \quad (44)$$

And then we have

$$\int_{-\infty}^{\infty} \frac{d\Psi_n(x)}{dx}V(x)\Psi_j(x)dx = \frac{\hbar^2}{2mL} k_n k_j \int_{0}^{L} [\delta(x) - (-1)^{n+j}\delta(L-x)]dx$$

$$= \frac{\hbar^2}{2nL} k_n k_j \beta_{nj}. \quad (45)$$

where $\beta_{nj} = 1 - (-1)^{n+j}$. Above, we have used the following results

$$\int_{0}^{L} \delta(x) dx = \frac{1}{2}, \quad (46)$$
$$\int_{0}^{L} \delta(L-x) dx = \frac{1}{2}. \quad (47)$$

These results are due to the even function property of the delta function, so that the integration of $x$, over the range, $[0, L]$, is equal to one half of that over the range, $[-L, L]$. We whence obtain the final result

$$\langle \Psi(t) | \frac{dV(x)}{dx} | \Psi(t) \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t)\frac{dV(x)}{dx}\Psi(x, t)dx$$

$$= -\frac{\hbar^2}{mL} \sum_{n=1}^{\infty} \sum_{j=1}^{\infty} a_n^* a_j k_n k_j \beta_{nj} e^{i(\omega_n - \omega_j)t}. \quad (48)$$
We also have
\[
\langle \Psi(t) | \hat{p} | \Psi(t) \rangle = (-i\hbar) \frac{2}{L} \sum_{n=1}^{\infty} \sum_{j \neq n} a_n a_j \frac{k_n k_j}{k_n^2 - k_j^2} \beta_{nj} e^{i(\omega_n - \omega_j)t}.
\]
(49)

And then, we have
\[
\frac{d}{dt} \langle \Psi(t) | \hat{p} | \Psi(t) \rangle = \frac{\hbar^2}{mL} \sum_{n=1}^{\infty} \sum_{j=1}^{\infty} a_n a_j k_n k_j \beta_{nj} e^{i(\omega_n - \omega_j)t}.
\]
(50)

Comparing Eqs. (48) and (50), we see that Ehrenfest’s theorem is confirmed. The calculations are done directly using the function \( V(x)\Psi_n(x) \) in Eq. (10). We need not first do those calculations in the finite square well and then take the limit, \( V_0 \to \infty \). It had been argued that the infinite potential cannot be simply described as the limit of a finite one \[13\]. The potential energy \( V(x) \) in a finite well is well defined, see Eq. (51). Simply taking the limit \( V_0 \to \infty \) results the potential energy \( V(x) \) defined in Eq. (11), which does not have a well defined functional form. It turns out that the limit should not be taken in the potential energy \( V(x) \). Instead, our results show that the limit should be taken in the potential energy term \( V(x)\Psi(x) \).

V. CONCLUSION

Infinite square well model is a model using infinite large potential barrier to confine particles inside a well. In this paper, we show that we need to avoid using the notation \( \infty \), because it requires imposing extra boundary condition and it also brings in ambiguities. Somehow this means that using the notation \( \infty \) does not define the system precisely; there is some degree of freedom remained, and it needs extra boundary condition to fix the solution.

To investigate a more precise form of the potential energy, we start from the well-known solutions of the infinite square well, and go back to determine the corresponding potential energy. The derived potential energy \( V(x) \) is described in Eq. (19). We can have an understanding of the divergence of the potential energy term \( V(x)\Psi(x) \) by noting that the \( V(x) \) is needed to be accompanied with the function \( \theta(x)\theta(L - x) \). In another point of view, what we have done is to showing the specification of the infinity in Eq. (11) such that it results the known solutions of \( \Psi_n(x) \) and \( E_n \). That is, the derived functional form of the \( V(x) \) gives a specification or a description about how to handle the infinity in the original model.

Such an infinite large barrier, however, is not enough to confine particles inside a well. To confine particles inside a well, we also need delta functions, \( \delta(x) \) and \( \delta(L - x) \) in the form of \( V(x) \). These two delta functions are needed for constructing non-trivial solutions.

We show that the energy eigenfunctions and eigenvalues of this reformed model are the same as the original ones. The difference between the original and the reformed model in obtaining solutions is that, for the reformed model, we need not impose boundary conditions at the two sides, we need only use the precise functional form of \( V(x)\Psi(x) \). Readers, who are interested in other type of solutions of the infinite square well, in which the continuity of \( \Psi(x) \) at boundaries is not required, may refer to Ref. [14].

Besides without the need of imposing boundary conditions, we show that the reformed model enables us to calculate quantities directly and precisely, such as the values of \( \Delta \Psi'(0), \Delta \Psi'(L) \), the expectation values \( \langle \Psi(t) | d\hat{V}(x)/dx | \Psi(t) \rangle \), and Ehrenfest’s theorem can be confirmed directly. Finally, for discussing the time evolution of the wave function \( \Psi(x,t) \) in the reformed model, we need only replace the \( F(x) \) in Eqs. (20)–(21) by \( F(x,t) \).

APPENDIX I

In this appendix, we drive the functional form of the potential energy \( V(x) \) for a finite well from the known solutions of \( \Psi(x) \). The potential energy \( V(x) \) of the finite square well is described by

\[
V(x) = \begin{cases} 
0, & 0 < x < L, \\
V_0, & \text{otherwise},
\end{cases}
\]
(51)
where \( V_0 > 0 \). We set the energy \( E = \hbar^2 k^2 / 2m \), and let \( V_0 - E = \hbar^2 q^2 / 2m \). The wave number \( k > 0 \) is determined by:

\[
\tan(kL) = \frac{2kq}{k^2 - q^2}. \tag{52}
\]

or,

\[
\begin{align*}
\sin(kL) &= a \frac{2kq}{k^2 + q^2}, \\
\cos(kL) &= a \frac{k^2 - q^2}{k^2 + q^2},
\end{align*} \tag{53}
\]

where \( a = \pm 1 \); which value of \( a \) should be chosen depends on the value of \( kL \) in Eq. \( \text{(53)} \). The energy eigenfunction is known to be

\[
\Psi(x) = \begin{cases} 
A e^{qx}, & x < 0, \\
A D(x), & 0 < x < L, \\
A e^{-qx}, & x > L.
\end{cases} \tag{54}
\]

where \( A \) is the normalization constant, and \( D(x) = \frac{1}{\sqrt{2}} \sin(kx) + \cos(kx) \). We have

\[
A = \sqrt{\frac{2k}{Lq} \frac{1}{(1 + \frac{q^2}{L^2})(1 + \frac{k^2}{q^2})}}. \tag{55}
\]

We now write the \( \Psi(x) \) in Eq. \( \text{(54)} \) as:

\[
\Psi(x) = A \left[ e^{qx} \theta(-x) + D(x) \theta(x) \theta(L-x) + a e^{-qx} \theta(x-L) \right]. \tag{56}
\]

To determine \( V(x) \) from the Schrödinger equation in Eq. \( \text{(2)} \), we rewrite the equation as

\[
V(x)\Psi(x) = \frac{\hbar^2}{2m} \Psi''(x) + E\Psi(x). \tag{57}
\]

Substituting the \( \Psi(x) \) in Eq. \( \text{(56)} \) into the right side of Eq. \( \text{(57)} \), we can then read out the form of \( V(x)\Psi(x) \). After some calculation, we obtain

\[
V(x)\Psi(x) = V_0 \theta(-x) A e^{qx} + V_0 \theta(x-L) a A e^{-qx}. \\
= V_0 \theta(-x) \Psi(x) + V_0 \theta(x-L) \Psi(x) \tag{58}
\]

This yields that

\[
V(x) = V_0 \theta(-x) + V_0 \theta(x-L). \tag{59}
\]

This is just the potential energy defined in Eq. \( \text{(51)} \). Thus, we have derived \( V(x) \) from \( \Psi(x) \).

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