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Exact Treatment of the Infinite Square Well in One Dimension with $\lambda\delta'(x)$ Potential

M. A. Dalabeeh

Department of Physics, Faculty of Science, Al-Balqa Applied University, Al-Salt, Jordan.

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Abstract: This work considered the infinite square well in one dimension with a contact potential. The Dirac delta derivative function potential $\lambda\delta'$ where λ is a coupling constant was used to represent the contact potential. Using Green's function technique, exact implicit expressions of the energy eigenvalues and eigenfunctions were obtained. The energy eigenvalues were expressed using a transcendental equation. The energy eigenfunctions satisfy the Schrödinger equation and the infinite square well boundary conditions. Also, the eigenfunctions and their first derivative were shown to be discontinuous. The values of these discontinuity jumps agreed with the required conditions for a self-adjoint extension Hamiltonian. In the weak coupling region, the energy eigenvalues are close to that of the even parity solution before adding the contact potential. The energy eigenvalues in the strong coupling regime reveal the energy eigenvalues of the odd parity solution.

Keywords: Point interactions, Infinite square well, Green's function technique.

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1. Introduction

The problem of the infinite square well is so prevalent in quantum mechanics textbooks, especially at the undergraduate level. This popularity is because it represents a simple, analytically solvable model without approximations [1]. Many properties in quantum mechanics can be introduced and verified using this model. These properties include discreteness of the energy eigenvalues, orthogonality, normalization, and completeness of the solutions. It also has many applications in real quantum mechanics problems where it can be used as a model or as an approximation to the problem. For example, the infinite square well model was used in modeling quantum well lasers [2]. These laser diodes comprise one semiconductor material representing the well, with two other semiconductor layers of different materials surrounding it. This configuration is represented by a double quantum dot, which allows quantized energy states that enable complete control of the electron's energy, resulting in a laser beam. Because of the small size of the quantum dot, they represent quantum confinement, where the electron is trapped within the dot. The gap between the two quantum dots in this representation is around $100A^0 \simeq 200a_0$, representing the well's width.

Contact potentials are usually represented by the Dirac delta function potential or its derivatives because of the simplicity of their solutions. The interest in this model of contact potential goes back to the early days of quantum mechanics [3]. Many problems in quantum mechanics, nuclear physics, and material science have been modeled or approximated using such potential since then. The Dirac delta derivative potential has many exciting features, such as admitting continuum and bound state solutions. Also, these solutions were discontinuous at the

Corresponding Author: M. A. Dalabeeh **Email**: madalabeeh@bau.edu.jo

singular points [4]. This short-range interaction was used to examine novel physical concepts for more realistic problems. The mathematical methods used to manipulate such potential include regularization, distribution theory, Green's functions technique, and self-adjoint extensions.

Gadella et al. [5] studied the one-dimensional infinite square well with added singular potential given by $-a\delta(x) + b\delta'(x)$ where $a, b > 0$. The authors used the Lippman-Schwinger Green function technique to find the energy eigenvalues. Many interesting works, based on the physical applications and models related to this type of potential, have been raised since then [6-13]. In this work, the singular potential is given by $\lambda\delta'(x)$ alone. Even though this potential is a part of the more general potential $-a\delta(x) + b\delta'(x)$, still, it is a well-known fact that problems with such potential are sensitive to the choice of the parameters involved and the used techniques as well. For example, many examples in the literature demonstrate that the results depend on the methods used to deal with such potential, especially when using the regularization technique [14]. Also, it is not usually possible to turn off such potential. For example, we cannot claim that by letting $a \to 0$ in the results obtained for the general expression $a\delta(x) + b\delta'(x)$ we will get the result for $b\delta'(x)$ alone, this ambiguity can be related to the Klauder phenomenon [15], where $H = H_0 + \lambda H'$ does not converge to H_0 when λ is set to be zero.

In this work, Green's functions technique is used. Atkinson and Crater followed this technique [16] to get the energy eigenvalues for systems with Dirac delta function potential in the form $\lambda\delta(x)$ where λ is a coupling constant. Recently, this method was used to obtain the energy eigenvalues, and the exact solution to a problem involving $\lambda\delta'(x)$ [17]. Using the fact that the energy eigenfunctions of the problem without the Dirac delta function potential are complete, the authors [17] obtain the solution as a linear superposition of these eigenfunctions. The presence of the $\lambda\delta'(x)$ potential in the Schrödinger equation implies the discontinuity of the wave function and its first derivative. This behavior of the wave function was proven to be required to ensure the self-adjointness of the Hamiltonian operator [4]. The conditions to have a self-adjoint operator are $A = A^\dagger$ and the domain of A and $A^\dagger$ match. In one dimension, the operator A is self-adjoint if

$$\int_{-\infty}^{\infty} \psi^* A\phi dx - \int_{-\infty}^{\infty} \left(A^\dagger \psi^*\right)\phi dx = 0, \tag{1}$$

endures for any pair of wave functions ϕ and ψ in the same domain. In the case of one-dimensional problems, the Hamiltonian in the form $-\frac{d^2}{dx^2} + \lambda\delta'(x)$ is self-adjoint provided that the following boundary conditions at the origin are satisfied:

$$\begin{pmatrix} \psi_+ \\ \psi'_+ \end{pmatrix} = \begin{pmatrix} \frac{2+\lambda}{2-\lambda} & 0 \\ 0 & \frac{2-\lambda}{2+\lambda} \end{pmatrix} \begin{pmatrix} \psi_- \\ \psi'_- \end{pmatrix}. \tag{2}$$

These boundary conditions determine the values of the discontinuity jumps $\Delta\psi$ and $\Delta\psi'$ at $x = 0$ to be equal to the average value of the wave function and its first derivative as $x \to 0$ multiplied by the coupling constant namely $\lambda\overline{\psi}(0)$ and $\lambda\overline{\psi'}(0)$ respectively.

2. General Outline of the Solution of the One-Dimensional Schrödinger Equation in the Presence of $\lambda\delta'(x)$ Potential

This section presents a general outline of Green's function technique. Using this technique, the problem of the infinite square well with $\lambda\delta'(x)$ potential will be solved. This technique enables us to get the .energy eigenvalues and the exact solutions to the problem. The technique is applied whenever the problem with $\lambda = 0$ has a complete orthonormal set of eigenfunctions. The Schrödinger equation with general potential $U(x)$ in the presence of $\lambda\delta'(x)$ potential is given by:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x) + \lambda\delta'(x)\right]\psi(x) = \epsilon\psi(x). \tag{3}$$

where m is the particle's mass, $\hbar$ is the reduced Planck constant, and ϵ is the energy eigenvalue. If the solution for this equation when $\lambda = 0$ is known and forms a complete set of orthonormal eigenfunctions $\psi_n(x)$ corresponding to the eigenvalues ϵ_n, then the solution $\psi(x)$ to the problem with $\lambda \neq 0$ can be written as a linear superposition of the eigenfunctions $\psi_n(x)$, since they provide the appropriate expansion basis, that is:

$$\psi(x) = \sum_{n\geq 0} c_n \psi_n(x). \tag{4}$$

Substituting this expansion into the Schrödinger Eq. (3) gives:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x) + \lambda\delta'(x)\right]\sum_{n\geq 0} c_n\,\psi_n(x) = \epsilon\sum_{n\geq 0} c_n\,\psi_n(x). \quad (5)$$

Since the eigenfunctions $\psi_n(x)$ satisfy the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)\right]\psi_n(x) = \epsilon_n\psi_n(x), \quad (6)$$

one obtains:

$$\sum_{n\geq 0} c_n\,\epsilon_n\psi_n(x) + \lambda\delta'(x)\psi(x) = \epsilon\sum_{n\geq 0} c_n\,\psi_n(x). \quad (7)$$

Multiplying both sides of the Eq. (7) by $\psi_m(x)$ and integrate over x, then using the fact that the eigenfunctions $\psi_n(x)$ are orthonormal

$$\int_{-\infty}^{\infty}\psi_n(x)\psi_m^*(x)dx = \delta_{nm}, \quad (8)$$

and the following property of the $\delta'(x)$ multiplied with discontinuous functions $f(x), g(x)$

$$\int_{-\infty}^{\infty} f(x)g(x)\delta'(x)dx = -\left[\overline{f}'(0)\overline{g}(0) + \overline{g}'(0)\overline{f}(0)\right], \quad (9)$$

where $\overline{f}(0), \overline{g}(0)$ and $\overline{f}'(0), \overline{g}'(0)$ are the averages of the function $f(x), g(x)$ and their first derivative at the origin, respectively. Notice here that this property recovers the well-known property if $f(x), g(x)$ are continuous functions

$$\int_{-\infty}^{\infty} f(x)g(x)\delta'(x)dx = -\frac{d}{dx}[f(x)g(x)]_{x=0}. \quad (10)$$

Using Eqs. (9) and (8), then from Eq. (7) the expansion coefficients c_n in Eq. (4) now are given by:

$$c_n = \lambda\frac{\left[\overline{\psi}'(0)\psi_n^*(0) + \overline{\psi}(0)\psi_n'^*(0)\right]}{\epsilon_n - \epsilon}. \quad (11)$$

Substituting for c_n in Eq. (4), the solution of the Schrödinger Eq. (7) in the presence of the Dirac delta derivative potential is given by the following sum over all the eigenfunctions $\psi_n(x)$ of the problem when $\lambda = 0$:

$$\psi(x) = \lambda\sum_{n\geq 0}\frac{\left[\overline{\psi}'(0)\psi_n^*(0) + \overline{\psi}(0)\psi_n'^*(0)\right]}{\epsilon_n - \epsilon}\psi_n(x). \quad (12)$$

Provided that the sum is convergent for all values of $x \neq 0$, and converges to $\overline{\psi}(0)$ as $x \to 0$, then the limit $x \to 0$ can be taken, and one obtains the following implicit equation for the eigenvalues of the problem under consideration:

$$\frac{1}{\lambda} = \frac{\overline{\psi}'(0)}{\overline{\psi}(0)}\sum_{n\geq 0}\frac{|\psi_n(0)|^2}{\epsilon_n - \epsilon} + \sum_{n\geq 0}\frac{\psi_n'^*(0)\psi_n(0)}{\epsilon_n - \epsilon}. \quad (13)$$

Obtaining the eigenvalues λ from the above Eq. (13), the corresponding eigenfunctions can be found by substituting the appropriate eigenvalues ϵ into Eq. (12). The values of the scales $\overline{\psi}(0)$ and $\overline{\psi}'(0)$ can be determined by normalizing the wave function $\psi(x)$

$$\int_{-\infty}^{\infty}|\psi(x)|^2 dx = 1, \quad (14)$$

together with the derivative of the obtained solution evaluated at the origin. This procedure will be used in the following section to find the solution to the infinite square well with $\lambda\delta'(x)$.

3. The Infinite Square Well with $\lambda\delta'(x)$ Potential

3.1 The Infinite Square Well

The infinite quantum square well centered at the origin of width $2b$ is defined by the potential:

$$V(x) = \begin{cases} 0 & -b < x < b \\ \infty & \text{otherwise.} \end{cases} \quad (15)$$

The Schrödinger equation for this potential is similar to the free particle wave function on the interval $-b < x < b$. By setting $\frac{\hbar^2}{2m} = 1$, the Schrödinger equation for this system reads

$$-\frac{d^2}{dx^2}\psi_n(x) = \epsilon_n\psi_n(x), \quad (16)$$

with boundary conditions given by $\psi_n(\pm b) = 0$. The following eigenfunctions give the solution to this system (18)

$$\psi_n(x) = \frac{1}{\sqrt{b}}\sin(n\pi x/b), -b < x < b \text{(odd parity)}, \quad (17)$$

$$\psi_n(x) = \frac{1}{\sqrt{b}}\cos\left(n + \frac{1}{2}\right)(\pi x/b), -b < x < b \text{(even parity)}. \quad (18)$$

Outside this region, the solution is $\psi_n(x) = 0$. The energy eigenvalues ϵ_{n_o} for the odd parity solution is given by:

$$\epsilon_{n_o} = \frac{n^2\pi^2}{b^2}, \quad (19)$$

while the energy eigenvalues ϵ_{n_e} for the even parity solution is:

$$\epsilon_{n_e} = \frac{\left(n + \frac{1}{2}\right)^2\pi^2}{b^2}, \quad (20)$$

where $n = 0,1,2,3,4,\cdots$. We note here that the $n = 0$ case for the odd parity solution is not allowed since the solution, in this case, is $\psi_0(x) = ax + c$, which cannot satisfy the boundary conditions; on the other hand, the negative integer solutions $n = -1, -2, -3, \cdots$ will give the same solution up to a phase factor with the same energy eigenvalues. Also, the first derivative of the solutions is discontinuous at the boundaries of the well. These solutions are complete and orthonormal, which means that they can be used as an expansion basis (see section (2)) to find the solution to the problem with added $\lambda\delta'(x)$ potential.

3.2. The Infinite Square Well with $\lambda\delta'(x)$ Potential

The Schrödinger equation for a particle in the infinite square well with $\lambda\delta'(x)$ potential is given by:

$$\left[-\frac{d^2}{dx^2} + \lambda\delta'(x)\right]\psi(x) = \epsilon\psi(x), \quad (21)$$

with boundary conditions $\psi(\pm b) = 0$ as before. From section (2), the solution to this problem is a superposition of the odd and the even parity solutions that is:

$$\psi(x) = \sum_{n\geq 0} a_n \cos\left(n + \frac{1}{2}\right)(\pi x/b) + \sum_{n>0} b_n \sin(n\pi x/b). \quad (22)$$

Using the orthonormality of $\psi_n(x)$ Eq. (8) together with the properties of the delta derivative integral Eq. (9), the solution to the Schrödinger Eq (21) is given by:

$$\psi(x) = \lambda \frac{\overline{\psi}'(0)}{b} \sum_{n\geq 0} \frac{\cos\left(\left[n+\frac{1}{2}\right]\pi x/b\right)}{\epsilon_{n_e} - \epsilon} + \lambda \frac{\pi\overline{\psi}(0)}{b^{3/2}} \sum_{n>0} \frac{n\sin(n\pi x/b)}{\epsilon_{n_o} - \epsilon}. \quad (23)$$

To get the energy eigenvalues for this system, one uses the Eq. (13). From this equation, the sum over the odd parity solution will give zero contribution when setting $x = 0$, and hence the energy eigenvalues are given by the following infinite sum:

$$\frac{1}{\lambda} = \frac{\overline{\psi}'(0)}{\overline{\psi}(0)} \frac{1}{b} \sum_{n\geq 0} \frac{1}{\frac{\left(n+\frac{1}{2}\right)^2 \pi^2}{4b^2} - \epsilon}, \epsilon > 0. \quad (24)$$

To evaluate this sum, one can refer to Gradshteyn and Ryzhik [19]. The result is:

$$\sqrt{\epsilon} = \lambda \frac{\overline{\psi}'(0)}{2\overline{\psi}(0)} \tan\left(b\sqrt{\epsilon}\right). \quad (25)$$

It is clear from this equation that the energy eigenvalues recover that of the even parity solution for small $\lambda \ll 1$; this can be seen by implying that relation (25) is finite in this regime, so $\tan\left(b\sqrt{\epsilon}\right) \to \infty$. This can be satisfied by setting $\epsilon = \frac{\left(n+\frac{1}{2}\right)^2 \pi^2}{b^2}$ and this is the energy eigenvalues of the even parity solution. For large coupling $\lambda \gg 1$ the energy eigenvalues Eq. (25) tends to the odd parity solution where $\tan\left(b\sqrt{\epsilon}\right)$ should tend to zero to maintain the expansion (25) finite, that leads to $\epsilon = \frac{n^2\pi^2}{b^2}$ wich is the energy eigenvalues of the odd parity solutions.

4. The Energy Eigenvalues

The energy eigenvalues can be determined using the transcendental Eq. (25). In Fig. 1, the energy eigenvalues ϵ are illustrated as a function of the scaled coupling constant $\lambda_s = \lambda \frac{\overline{\psi}'(0)}{2\overline{\psi}(0)}$.

The following tables show the values of the energy eigenvalues of the infinite square well with Dirac delta derivative function potential. Table 1 gives the energy eigenvalues for different values of the negative coupling constant λ,, while Table 2 provides the energy eigenvalues for the positive coupling constant. In both tables, the weak and strong coupling regions are included.

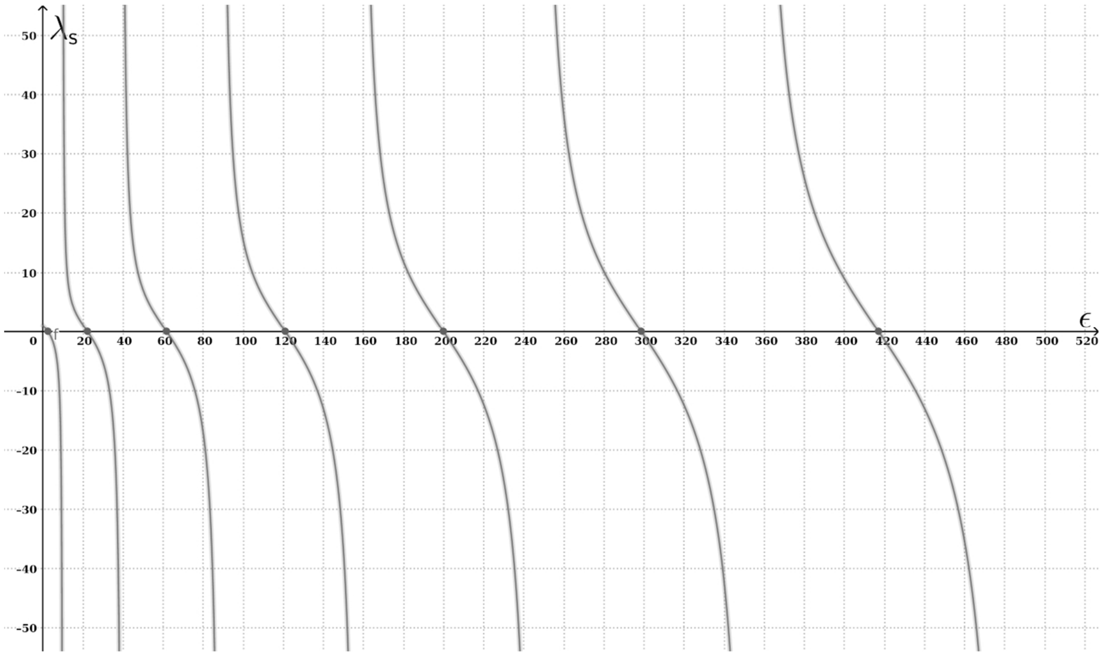

FIG 1. A plot of the transcendental equation (25) with the coupling constant λ replaced by the scaled coupling constant $\lambda_s = \lambda \frac{\overline{\psi'}(0)}{2\overline{\psi}(0)}$ and the width of the well is se equal to one.

TABLE 1. Energy eigenvalues of the infinite square well in the presence of $\lambda\delta'(x)$ potential for different values of the negative scaled coupling constant $\lambda_s = \lambda \frac{\overline{\psi'}(0)}{2\overline{\psi}(0)}$.

λ_s	ϵ_0	ϵ_1	ϵ_2	ϵ_3	ϵ_4	ϵ_5
-0.0001	2.4676	22.206	61.685	120.90	199.85	298.22
-0.1	2.6634	22.406	61.884	121.10	200.05	298.75
-1	4.1158	24.139	63.659	122.89	201.85	300.54
-2	5.2391	25.877	65.547	124.83	203.81	302.81
-4	6.6071	28.665	68.938	128.47	207.58	306.37
-8	7.8648	32.113	74.012	134.54	214.25	313.40
-10	8.1954	33.184	75.834	136.95	217.07	316.51
-15	8.6881	34.904	79.028	141.51	222.75	323.07
-20	8.9583	35.905	81.033	144.60	226.87	328.10

TABLE 2. Energy eigenvalues of the infinite square well in the presence of $\lambda\delta'(x)$ potential for different values of the positive scaled coupling constant $\lambda_s = \lambda \frac{\overline{\psi'}(0)}{\overline{\psi}(0)}$.

λ_s	ϵ_0	ϵ_1	ϵ_2	ϵ_3	ϵ_4	ϵ_5
0.0001	2.4672	22.064	61.684	120.90	199.85	298.55
0.1	2.2632	22.006	61.484	120.70	199.65	298.35
1	-	20.190	59.679	118.89	197.85	296.55
2	-	18.273	57.707	116.91	195.86	294.56
4	-	15.338	54.109	113.12	191.99	290.64
8	-	12.675	49.030	106.85	185.11	283.42
10	-	12.083	47.420	104.47	182.24	280.23
15	-	11.303	44.936	100.26	176.66	273.64
20	-	10.235	43.586	97.688	172.86	268.73

The figure and tables serve as a clue to investigate the behaviors of the energy eigenvalues ϵ in the weak and strong coupling. For weak coupling, the energy eigenvalues are like the energy eigenvalues of the original infinite square well for the ground state $n = 0$ and $n = 1,2,3,4,\cdots$ of the even parity solution; this is in agreement with the discussion provided after Eq. (25) in the case of small coupling. By increasing λ, the energy eigenvalues start to deviate from their original values. This deviation has two schemes. The first one corresponds to positive λ where the energy eigenvalues are decreased toward the energy eigenvalues of the odd parity energy eigenvalues such that

$$\epsilon \simeq \epsilon_{n_e}(|\lambda| \ll 1) \to \epsilon \simeq \epsilon_{n_o}(|\lambda| \gg 1), n_e = n_o = 1,2,3,\cdots.$$

The other scheme corresponds to negative λ where the energy eigenvalues are increased to the successive energy eigenvalues of the odd parity energy eigenvalues such that

$$\epsilon \simeq \epsilon_{n_e}(|\lambda| \ll 1) \to \epsilon \simeq \epsilon_{n_o+1}(|\lambda| \gg 1), n_e = n_o = 1,2,3,\cdots.$$

Finally, this conclusion is valid for different values of the well-width $2b$ since the width of the well affects only the number of states within the energy interval.

5. The Energy Eigenstates

Using Eq. (23), we can obtain the wave function of the infinite square well. The sum over cosine can be computed exactly using the following sum (19)

$$\sum_{n=1}^{\infty} \frac{\cos nx}{n^2-\alpha^2} = \frac{1}{2\alpha^2} - \frac{\pi}{2}\frac{\cos\alpha[(2m+1)\pi-x]}{\alpha\sin\alpha\pi}, 2m\pi \leq x \leq (2m+2)\pi, \alpha \text{ not an integer} \quad (26)$$

splitting the sum into summation over odd and even n, we obtain:

$$\sum_{n=1}^{\infty} \frac{\cos nx}{n^2-\alpha^2} = \sum_{n=0}^{\infty} \frac{\cos(2n+1)x}{(2n+1)^2-\alpha^2} + \sum_{n=1}^{\infty} \frac{\cos 2nx}{4n^2-\alpha^2} \quad (27)$$

The second sum on the right-hand side is similar to the cosine sum in Eq. (26) with α replaced by $\alpha/2$ and x by $2x$ so

$$\sum_{n=0}^{\infty} \frac{\cos(2n+1)x}{(2n+1)^2-\alpha^2} = \frac{\pi}{2}\left[\frac{\cos\left(\alpha\left[\frac{(2m+1)\pi}{2}-x\right]\right)}{2\alpha\sin\left(\frac{\alpha\pi}{2}\right)} - \frac{\cos(\alpha[(2m+1)\pi-x])}{\alpha\sin\left(\frac{\alpha\pi}{2}\right)}\right], \quad (28)$$

$m\pi < x < (m+1)\pi, \alpha$ not an integer.

The sum over sine can be done using the identity (19) given by:

$$\sum_{n=1}^{\infty} \frac{n\sin nx}{n^2-\alpha^2} = \pi\frac{\sin(\alpha[(2m+1)\pi-x])}{2\sin(\alpha\pi)}, \quad (29)$$

$2m\pi < x < (2m+2)\pi, \alpha$ not an integer,

if $x = 0$, the sum is zero. From Eqs. (28) and (29) the infinite sum appears in the expression of the wave function $\psi(x)$ Eq. (23) can be computed exactly and the result is

$$\psi(x) = \frac{\lambda\overline{\psi}'(0)}{\sqrt{\epsilon}}\left[\frac{\cos(\sqrt{\epsilon}[(2m+1)b-x])}{2\sin(b\sqrt{\epsilon})} - \frac{\cos(\sqrt{\epsilon}[(4m+2)b-x])}{\sin(2b\sqrt{\epsilon})}\right] + \lambda\overline{\psi}(0)\frac{\sin(\sqrt{\epsilon}[(2m+1)b-x])}{2\sin(b\sqrt{\epsilon})}, \quad (30)$$

$mb \leq x \leq (m+1)b$, $\frac{b\sqrt{\epsilon}}{\pi}$ not an integer,

Choosing $m = 0, -1$ to meet the boundaries of the infinite square well gives:

$$\psi(x) = \begin{cases} \frac{\lambda\overline{\psi}'(0)}{\sqrt{\epsilon}}\left[\frac{\cos(\sqrt{\epsilon}[b+x])}{2\sin(b\sqrt{\epsilon})} - \frac{\cos(\sqrt{\epsilon}[2b+x])}{\sin(2b\sqrt{\epsilon})}\right] - \lambda\overline{\psi}(0)\frac{\sin(\sqrt{\epsilon}[b+x])}{2\sin(b\sqrt{\epsilon})}, -b < x < 0, \\ \frac{\lambda\overline{\psi}'(0)}{\sqrt{\epsilon}}\left[\frac{\cos(\sqrt{\epsilon}[b-x])}{2\sin(b\sqrt{\epsilon})} - \frac{\cos(\sqrt{\epsilon}[2b-x])}{\sin(2b\sqrt{\epsilon})}\right] + \lambda\overline{\psi}(0)\frac{\sin(\sqrt{\epsilon}[b-x])}{2\sin(b\sqrt{\epsilon})}, 0 < x < b, \\ \frac{b\sqrt{\epsilon}}{\pi} \text{not an integer.} \end{cases} \quad (31)$$

This wave function solves the problem under consideration. We can check that this solution is indeed the required solution by substituting it back into the Schrödinger equation of the infinite square well in the presence of $\lambda\delta'(x)$, to do that, we first rewrite the solution in terms of the Heaviside function $\theta(x)$ given by:

$$\theta(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{if } x < 0 \end{cases} \quad (32)$$

as follows

$$\psi(x) = \left[\frac{\lambda\overline{\psi}'(0)}{\sqrt{\epsilon}}\left[\frac{\cos(\sqrt{\epsilon}[b+x])}{2\sin(b\sqrt{\epsilon})} - \frac{\cos(\sqrt{\epsilon}[2b+x])}{\sin(2b\sqrt{\epsilon})}\right] - \lambda\overline{\psi}(0)\frac{\sin(\sqrt{\epsilon}[b+x])}{2\sin(b\sqrt{\epsilon})}\right]\theta(-x) + \left[\frac{\lambda\overline{\psi}'(0)}{\sqrt{\epsilon}}\left[\frac{\cos(\sqrt{\epsilon}[b-x])}{2\sin(b\sqrt{\epsilon})} - \frac{\cos(\sqrt{\epsilon}[2b-x])}{\sin(2b\sqrt{\epsilon})}\right] + \lambda\overline{\psi}(0)\frac{\sin(\sqrt{\epsilon}[b-x])}{2\sin(b\sqrt{\epsilon})}\right]\theta(x). \quad (33)$$

The first derivative of $\psi(x)$ is given by:

$$\begin{aligned}\psi'(x) = &\left[\frac{\lambda\overline{\psi'}(0)}{\sqrt{\epsilon}}\left[\frac{-\sqrt{\epsilon}\sin(\sqrt{\epsilon}[b+x])}{2\sin(b\sqrt{\epsilon})}+\frac{\sqrt{\epsilon}\sin(\sqrt{\epsilon}[2b+x])}{\sin(2b\sqrt{\epsilon})}\right]-\lambda\overline{\psi}(0)\frac{\sqrt{\epsilon}\cos(\sqrt{\epsilon}[b+x])}{2\sin(b\sqrt{\epsilon})}\right]\theta(-x)\\ &+\left[\frac{\lambda\overline{\psi'}(0)}{\sqrt{\epsilon}}\left[\frac{\sqrt{\epsilon}\sin(\sqrt{\epsilon}[b-x])}{2\sin(b\sqrt{\epsilon})}-\frac{\sqrt{\epsilon}\sin(\sqrt{\epsilon}[2b-x])}{\sin(2b\sqrt{\epsilon})}\right]-\lambda\overline{\psi}(0)\frac{\sqrt{\epsilon}\cos(\sqrt{\epsilon}[b-x])}{2\sin(b\sqrt{\epsilon})}\right]\theta(x)\\ &-\left[\frac{\lambda\overline{\psi'}(0)}{\sqrt{\epsilon}}\left[\frac{\cos(\sqrt{\epsilon}[b+x])}{2\sin(b\sqrt{\epsilon})}-\frac{\cos(\sqrt{\epsilon}[2b+x])}{\sin(2b\sqrt{\epsilon})}\right]-\lambda\overline{\psi}(0)\frac{\sin(\sqrt{\epsilon}[b+x])}{2\sin(b\sqrt{\epsilon})}\right]\delta(x)\\ &+\left[\frac{\lambda\overline{\psi'}(0)}{\sqrt{\epsilon}}\left[\frac{\cos(\sqrt{\epsilon}[b-x])}{2\sin(b\sqrt{\epsilon})}-\frac{\cos(\sqrt{\epsilon}[2b-x])}{\sin(2b\sqrt{\epsilon})}\right]+\lambda\overline{\psi}(0)\frac{\sin(\sqrt{\epsilon}[b-x])}{2\sin(b\sqrt{\epsilon})}\right]\delta(x).\end{aligned} \tag{34}$$

Where we use $\frac{d}{dx}\theta(x)=\delta(x)$. the second derivative can be obtained similarly, and the result is:

$$\psi''(x) = \begin{aligned}&-\epsilon\psi(x)-\left[\frac{\lambda\overline{\psi'}(0)}{\sqrt{\epsilon}}\left[\frac{\cos(\sqrt{\epsilon}[b+x])}{2\sin(b\sqrt{\epsilon})}-\frac{\cos(\sqrt{\epsilon}[2b+x])}{\sin(2b\sqrt{\epsilon})}\right]-\lambda\overline{\psi}(0)\frac{\sin(\sqrt{\epsilon}[b+x])}{2\sin(b\sqrt{\epsilon})}\right]\delta'(x)\\ &+\left[\lambda\overline{\psi'}(0)\left[\frac{-\sin(\sqrt{\epsilon}[b+x])}{2\sin(b\sqrt{\epsilon})}+\frac{\sin(\sqrt{\epsilon}[2b+x])}{\sin(2b\sqrt{\epsilon})}\right]-\lambda\overline{\psi}(0)\frac{\cos(\sqrt{\epsilon}[b+x])}{2\sin(b\sqrt{\epsilon})}\right]\delta'(x)\\ &-2\left[\lambda\overline{\psi'}(0)\left[\frac{-\sin(\sqrt{\epsilon}[b+x])}{2\sin(b\sqrt{\epsilon})}+\frac{\sin(\sqrt{\epsilon}[2b+x])}{\sin(2b\sqrt{\epsilon})}\right]-\lambda\overline{\psi}(0)\frac{\cos(\sqrt{\epsilon}[b+x])}{2\sin(b\sqrt{\epsilon})}\right]\delta(x)\\ &2\left[\lambda\overline{\psi'}(0)\left[\frac{\sin(\sqrt{\epsilon}[b-x])}{2\sin(b\sqrt{\epsilon})}-\frac{\sin(\sqrt{\epsilon}[2b-x])}{\sin(2b\sqrt{\epsilon})}\right]-\lambda\overline{\psi}(0)\frac{\cos(\sqrt{\epsilon}[b-x])}{2\sin(b\sqrt{\epsilon})}\right]\delta(x).\end{aligned} \tag{35}$$

Applying the following property (20) to the terms containing $\delta'(x)$

$$f(x)\delta'(x) = -\overline{f}'(0)\delta(x)+\overline{f}(0)\delta'(x), \tag{36}$$

and

$$f(x)\delta(x)=\overline{f}(0)\delta(x), \tag{37}$$

leads to

$$\psi''(x) = -\epsilon\psi(x)-\lambda\overline{\psi'}(0)\delta(x)+\lambda\overline{\psi}(0)\delta'(x). \tag{38}$$

Using relation (36) and rearranging the terms leads to:

$$\left[-\frac{d^2}{dx^2}+\lambda\delta'(x)\right]\psi(x)=\epsilon\psi(x), \tag{39}$$

This is the Schrödinger equation for the infinite square well with $\lambda\delta'(x)$ potential. The solution also satisfies the boundary conditions at $x=\pm 0$ that is $\psi(\pm b)=0$; this can be checked by direct substitution of the boundaries where:

$$\psi(-b)=\frac{\lambda\overline{\psi'}(0)}{\sqrt{\epsilon}}\left[\frac{1}{2\sin(b\sqrt{\epsilon})}-\frac{\cos(b\sqrt{\epsilon})}{\sin(2b\sqrt{\epsilon})}\right]= \frac{\lambda\overline{\psi'}(0)}{\sqrt{\epsilon}}\left[\frac{\sin(2b\sqrt{\epsilon})-2\cos(b\sqrt{\epsilon})\sin(b\sqrt{\epsilon})}{2\sin(b\sqrt{\epsilon})\sin(2b\sqrt{\epsilon})}\right]=0, \tag{40}$$

and similarly, for $x=b$. Furthermore, the required conditions on the set of the eigenstates to have a self-adjoint extension Hamiltonian are also satisfied. The first condition is the requirement that the discontinuity jumps in the wave function equal to the average of the wave function multiplied by the coupling constant λ. This can be verified using Eq. (33) as follows:

$$\psi(0^+)=\left[\frac{\lambda\overline{\psi'}(0)}{\sqrt{\epsilon}}\left[\frac{\cos(b\sqrt{\epsilon})}{2\sin(b\sqrt{\epsilon})}-\frac{\cos(2b\sqrt{\epsilon})}{\sin(2b\sqrt{\epsilon})}\right]+ \lambda\overline{\psi}(0)\frac{\sin(b\sqrt{\epsilon})}{2\sin(b\sqrt{\epsilon})}\right], \tag{41}$$

and

$$\psi(0^-)=\left[\frac{\lambda\overline{\psi'}(0)}{\sqrt{\epsilon}}\left[\frac{\cos(b\sqrt{\epsilon})}{2\sin(b\sqrt{\epsilon})}-\frac{\cos(2b\sqrt{\epsilon})}{\sin(2b\sqrt{\epsilon})}\right]- \lambda\overline{\psi}(0)\frac{\sin(b\sqrt{\epsilon})}{2\sin(b\sqrt{\epsilon})}\right], \tag{42}$$

and hence

$$\Delta\psi(0)=\psi(0^+)-\psi(0^-)=\lambda\overline{\psi}(0). \tag{43}$$

It is crucial to mention here that the average $\overline{\psi}(0)$ in the case of a discontinuous function is defined in a distributional sense, that is:

$$\int_{-\infty}^{\infty}\psi(x)\delta(x)=\overline{\psi}(0). \tag{44}$$

The second condition to have a self-adjoint extension Hamiltonian $\Delta\psi'(0)=-\lambda\overline{\psi'}(0)$ can be checked to be satisfied using Eq. (34) as follows:

$$\psi'(0^+) = -\frac{\lambda\overline{\psi'}(0)}{2} + \lambda\overline{\psi}(0)\frac{\sqrt{\epsilon}\cos(b\sqrt{\epsilon})}{2\sin(b\sqrt{\epsilon})}, \quad (45)$$

and

$$\psi'(0^-) = \frac{\lambda\overline{\psi'}(0)}{2} - \lambda\overline{\psi}(0)\frac{\sqrt{\epsilon}\cos(b\sqrt{\epsilon})}{2\sin(b\sqrt{\epsilon})}, \quad (46)$$

Then $\Delta\psi'(0) = \psi'(0^+) - \psi'(0^-) = \lambda\overline{\psi'}(0)$ as it should be.

Conclusion

The energy eigenfunctions and eigenvalues of the infinite square well with $\lambda\delta'(x)$ potential have been obtained precisely using Green's function technique. This method was shown to be valid, powerful, and simple to apply when dealing with contact potential. In this work, the energy eigenvalues of the system were obtained as a transcendental equation. The values of these eigenvalues were determined for weak and large λ. The energy eigenvalues were close to those of the odd parity solution in the large λ scheme. For very small λ, the system energy tends to be the energy eigenvalues of the even parity solution. The exact solution was shown to satisfy the Schrödinger equation together with the boundary conditions of the infinite square well. Furthermore, the solution meets the required boundary conditions to have a self-adjoint Hamiltonian. That is, both the wave function and its first derivative should be discontinuous at the origin with discontinuity jumps equal to the coupling constant times their averages, respectively.

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