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The Quantum Harmonic Oscillator with λδ' (x) Potential

M. A. Dalabeeh

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

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Abstract: In this work, the problem of the quantum harmonic oscillator with a delta-derivative potential $\lambda\delta'(x)$, where λ is a coupling constant, is solved using the Green's function technique. A transcendental equation that governs the energy eigenvalues of the problems for each coupling constant is obtained. The eigenfunctions and their first derivative are proved to be discontinuous at the origin. The values of the discontinuity jumps are found to agree with the requirements of having a self-adjoint extension Hamiltonian. In the large coupling limit, the even energy eigenvalues and eigenfunctions for the quantum harmonic oscillator are annihilated, and only the odd parts survive. The dependence of the energy eigenvalues and eigenfunctions on the sign of λ was made clear. A mapping between the sign of λ and the positions of the particle was used to explain the discontinuity of the solution. In the large-λ regime, an educated guess for the wave functions was proposed. The proposed solutions led to the correct energy eigenvalues and obeyed the required conditions to have a self-adjoint extension Hamiltonian.

Introduction

The quantum harmonic oscillator potential is among the most popular and important potentials in quantum mechanics; this comes from the fact that it is an approximate solution to many systems around their minimum potential. Moreover, the simplicity of obtaining its exact solution using various approaches, such as the analytic and algebraic techniques, is useful in presenting quantum mechanics ideas and formalisms [1]. On the other hand, the Dirac delta derivative potential describes a point-like or contact interactions that appear in many applications in physics. The interest in this model of contact potential goes back to the early days of quantum mechanics. After the pioneering paper of Berezin and Faddeev [2], a lot of works on this subject have been published. It was shown that contact or singular potential of different physical systems could be represented using the Dirac delta function and its derivatives, such as spectral filters [3, 4], supersymmetry [5], quantum waveguides [6, 7], thin sheets [8, 9], an entanglement of polymers [10], Bose-Einstein condensation in a harmonic trap [11], and propagation of a light [12]. Also, this contact potential is of particular importance in the nanoscale quantum devices [13].

The interpretation of the $\delta'(x)$ potential is unclear, and there are many discussions about its physical meaning. For example, in many works [14–19], this potential is used as boundary conditions on the wave function or its first derivative; in other works [20, 21], it is considered as a dipole-dipole interaction [22–24], or as a zero limit of a smooth potential [25, 26]. A discussion of these interpretations can be found in [27].

Solving the Schrödinger equation for a Hamiltonian with a contact potential is usually challenging compared to other regular Hamiltonians and has attracted considerable attention, including some controversy. One difficulty related to this potential is that the

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

Hamiltonian is not self-adjoint unless the solutions are allowed to be discontinuous, with specific discontinuity jumps required to ensure self-adjointness.

Janev *et al.* [28] determined the perturbed spectrum of a three-dimensional harmonic oscillator potential with an added singular δ-type potential centered at the origin. In the work of Gadella *et al.* [29], the authors studied the one-dimensional harmonic oscillator with a singular potential given in terms of the Dirac delta function and its first derivative, namely, $-a\delta(x)+b\delta'(x)$, where $a,b>0$. They used the Lippman-Schwinger Green's function technique to obtain the energy eigenvalues for the problem. Many interesting works, based on the physical applications and models related to this type of potential, have been published since then [30–37].

In our work, we deal with a closely related singular potential, namely, $\lambda\delta'(x)$, which uses part of the potential studied by Gadella *et al.* [29]. The motivation behind this is that problems involving singular potentials are susceptible to our choice of the involved parameters and the applied techniques as well. For example, we can find many examples in the literature where the obtained results directly depend on the way the authors followed in dealing with the singular potential, especially in the regularization technique [38]. On the other hand, it is not straightforward to simply set $a=0$ in the general expression $a\delta(x)+b\delta'(x)$ to obtain the correct result for $b\delta'(x)$ alone. This ambiguity is particularly evident in the Klauder phenomenon [39], where $H=H_0+\lambda H'$ does not converge to H_0 when the positive real parameter λ of the singular perturbation H' tends to zero.

In contrast, the Green's function approach used in this work is independent of the specific potential of the problem as long as the solutions without the contact potential are known. This method was followed by Atkinson [40] and Chair [41] to obtain the solution and the exact eigenvalues for problems involving contact potential. In this method, the completeness and the orthonormality properties of the exact solutions are used as an expansion basis for the solution of the problem with the $\lambda\delta'(x)$ potential. For the Hamiltonian operator to be self-adjoint, both $H^\dagger=H$ and the domains of $H^\dagger$ and H should be equal, that is:

$$<\phi|H\psi>-<H^\dagger\phi|\psi>=0 \qquad (1)$$

is satisfied for all ϕ and ψ in the same domain. In the one-dimensional case, the Hamiltonian is given by

$$H=-\frac{d^2}{dx^2}+\lambda\delta'(x) \qquad (2)$$

Kurasov's theorem states that there is a one-to-one correspondence between the set of self-adjoint extensions of such Hamiltonians and the wave functions' boundary conditions [42]. For the harmonic oscillator with a Dirac delta-derivative potential Hamiltonian, namely, $H=-\frac{d^2}{dx^2}+x^2+\lambda\delta'(x)$, we adopt Griffiths' [43] method to find the boundary conditions on the solutions to ensure the self-adjointness of the Hamiltonian.

General Outline

The bound state problem in one dimension with a potential that involves a delta function derivative $\lambda\delta'(x)$, where λ is a coupling constant, has an exact solution whenever the exact solutions to the problem without $\lambda\delta'(x)$ potential are known and complete. In the following, we will outline the procedure, then apply it to the problem under consideration. The Schrödinger equation in the presence of $\delta'(x)$ is given by:

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

If for $\lambda=0$ the set of eigenfunctions $\psi_n(x)$ corresponding to the energy eigenvalues ϵ_n, that is

$$[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+U(x)]\psi_n(x)=\epsilon_n\psi_n(x), \qquad (4)$$

are complete

$$\sum_n \psi\,(x)_n^*\psi_n(x')=\delta(x-x') \qquad (5)$$

and orthonormal

$$\int \psi(x)_n^*\psi_m(x)dx=\delta_{nm}, \qquad (6)$$

then we can expand the solution $\psi(x)$ using these eigenfunctions

$$\psi(x)=\sum_{n=0} c_n\,\psi_n(x). \qquad (7)$$

Substituting this into Eq. (3), we obtain

$$\sum_{n\geq 0}[\,c_n\epsilon_n\psi_n(x)+\lambda\delta'(x)c_n\psi_n(x)]=\epsilon\sum_{n\geq 0} c_n\,\psi_n(x). \qquad (8)$$

Using the orthonormality of the eigenfunctions $\psi_n(x)$

$$\int_{-\infty}^{\infty} \psi_n(x)\psi_m(x)dx = \delta_{nm} \quad (9)$$

and the following property of the $\delta'(x)$ proposed by Kurasov [44] when applied to a function with discontinuity jump at the origin and a discontinuity jump in its first derivative at the origin,

$$f(x)\delta'(x) = \bar{f}(0)\delta'(x) - \bar{f}'(0)\delta(x), \quad (10)$$

where

$$\bar{f}(0) = \frac{f(+0)+f(-0)}{2}, \bar{f}'(0) = \frac{f'(+0)+f'(-0)}{2} \quad (11)$$

are the averages of the function and its first derivative at $x = 0$, respectively[1], leads to the following expression of the expansion coefficient c_n:

$$c_n = \lambda \frac{[\overline{\psi'}(0)\psi_n^*(0)+\bar{\psi}(0)\psi_n'^*(0)]}{\epsilon_n-\epsilon}. \quad (12)$$

From Eq. (7), the solution $\psi(x)$ now is given by:

$$\psi(x) = \lambda \sum_{n\geq 0} \frac{[\overline{\psi'}(0)\psi_n^*(0)+\bar{\psi}(0)\psi_n'^*(0)]}{\epsilon_n-\epsilon} \psi_n(x). \quad (13)$$

The assumption that the sum is convergent for all values of $x \neq 0$, while for $x \to 0$ it converges to $\bar{\psi}(0)$, leads us to an implicit equation for the eigenvalues ϵ and the coupling constant λ:

$$\frac{1}{\lambda} = \frac{\overline{\psi'}(0)}{\bar{\psi}(0)} \sum_{n\geq 0} \frac{|\psi_n(0)|^2}{\epsilon_n-\epsilon} + \sum_{n\geq 0} \frac{\psi_n'^*(0)\psi_n(0)}{\epsilon_n-\epsilon}. \quad (14)$$

After obtaining the energy eigenvalues ϵ, the corresponding eigenfunctions $\psi(x)$ can be found using Eq. (13). The ratio $\frac{\overline{\psi'}(0)}{\bar{\psi}(0)}$ can be determined by normalizing the wave function $\psi(x)$ using:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1, \quad (15)$$

and by implying that the first derivative of the wave function $\psi'(x)$ can be obtained using Eq. (13), that is:

$$\psi'(x) = \lambda \sum_{n\geq 0} \frac{[\overline{\psi'}(0)\psi_n^*(0)+\bar{\psi}(0)\psi_n'^*(0)]}{\epsilon_n-\epsilon} \psi_n'(x). \quad (16)$$

In the following, we are going to apply this technique to the quantum harmonic oscillator problem $U(x) = \frac{1}{2}m\omega^2x^2$ to solve the Schrödinger equation with the added delta-derivative potential.

Schrödinger Equation for the Harmonic Oscillator with $\lambda\delta'(x)$

The Schrödinger equation for the harmonic oscillator with a delta-derivative potential is given by:

$$[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2 + \lambda\delta'(x)]\psi(x) = \epsilon\psi(x), \quad (17)$$

where m is the particle's mass, $\omega = \sqrt{\frac{k}{m}}$ is the angular frequency of the oscillator, and k is the force constant. By applying the Green's function technique [45, 46], we obtain the solutions in the following linear combination:

$$\psi(x) = \sum_{n\geq 0} c_n \psi_n(x), \quad (18)$$

where $\psi_n(x)$ are the eigenfunctions of the problem with $\lambda = 0$, that is:

$$[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2]\psi_n(x) = \epsilon_n\psi_n(x). \quad (19)$$

The energy eigenvalues in this case are given by $\epsilon_n = (n + \frac{1}{2})\hbar\omega$. The eigenfunctions of $\psi_n(x)$ are given explicitly by:

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}}(\frac{mw}{\pi\hbar})^{1/4} e^{-mwx^2/2\hbar} H_n(\sqrt{\frac{mw}{\hbar}}x). \quad (20)$$

Here, $H_n(x)$ are the Hermite polynomials [47]. To simplify the calculations, we will use the following scale for length and energy. In this scale, the energy is measured in units of $\hbar\omega/2$ while the length is measured in units of $\sqrt{\hbar/m\omega}$. Using this scale, the Schrödinger equation for the harmonic oscillator becomes:

$$[-\frac{d^2}{dx^2} + x^2]\psi_n(x) = \epsilon_n\psi_n(x), \quad (21)$$

and the eigenvalues ϵ_n are given by $\epsilon_n = 2n + 1$.

[1]For a continuously differentiable function $f(x)$, the equation $f(x)\delta'(x) = f(0)\delta'(x) - f'(0)\delta(x)$ holds. This equation can be extended to discontinuous functions. In Kurasov [44], the values and derivatives at $x = 0$ were replaced with the average values of the left- and right-hand limits at the discontinuity point, using the generalized definition of the δ function $\int \delta(x-a)f(x)dx = \frac{f(a-0)+f(a+0)}{2}$.

The Self-Adjoint Extension of the Hamiltonian

The presence of the contact potential $\lambda\delta'(x)$ in the Hamiltonian

$$H = -\frac{d^2}{dx^2} + x^2 + \lambda\delta'(x) \quad (22)$$

requires imposing additional conditions on the domain of H, such that the domains of H and its hermitian conjugate $H^\dagger$ coincide. In one dimension, the self-adjointness of a Hermitian operator requires that

$$\int_{-\infty}^{\infty}\psi^* H\phi dx - \int_{-\infty}^{\infty}(H^\dagger\psi^*)\phi dx = 0, \quad (23)$$

hold for any pair of functions ψ and ϕ sharing the same domain. The process of adding the required conditions to the domain of a Hermitian operator to ensure that Eq. (23) is satisfied is called self-adjoint extension. In the case of the one-dimensional Hamiltonian given by $H = -\frac{d^2}{dx^2} + \lambda\delta'(x)$, the wave function and its first derivative according to Kurasov's theorem [42] should satisfy the following boundary conditions at the origin

$$\begin{pmatrix}\psi(+0)\\ \psi'(+0)\end{pmatrix} = \begin{pmatrix}\frac{2+\lambda}{2-\lambda} & 0\\ 0 & \frac{2-\lambda}{2+\lambda}\end{pmatrix}\begin{pmatrix}\psi(-0)\\ \psi'(-0)\end{pmatrix}. \quad (24)$$

Now these boundary conditions require that the discontinuity jumps $\Delta\psi = \psi(+0) - \psi(-0)$ and $\Delta\psi' = \psi'(+0) - \psi'(-0)$ are equal to $\lambda\overline{\psi}(0)$ and $-\lambda\overline{\psi'}(0)$, respectively. In our case, we can find the conditions on the wave function and its first derivative by following the procedure used by Griffiths [43]. First, we integrate the Shrödinger equation for the harmonic oscillator in the presence of $\lambda\delta'(x)$ from η to $-\eta$:

$$-\int_{-\eta}^{\eta}\frac{d^2}{dx^2}\psi(x)dx + \lambda\int_{-\eta}^{\eta}\delta'(x)\psi(x)dx + \int_{-\eta}^{\eta}x^2\psi(x)dx = \epsilon\int_{-\eta}^{\eta}\psi(x)dx. \quad (25)$$

The first integral gives $\psi'(+\eta) - \psi'(-\eta)$, which is the discontinuity jump at $x = 0$ of the first derivative that is $\Delta\psi'$ when we take the limit $\eta \to 0$. The second integral can be computed using integration by parts:

$$\lambda\int_{-\eta}^{\eta}\delta'(x)\psi(x)dx = \lambda\delta(x)\psi(x)|_{-\eta}^{\eta} - \lambda\int_{-\eta}^{\eta}\delta(x)\psi'(x)dx. \quad (26)$$

The term $\delta(x)\psi(x)|_{-\eta}^{\eta}$ is zero, while the integral $\int_{-\eta}^{\eta}\delta(x)\psi'(x)dx$ can be computed by considering $\delta(x)$ and $\psi'(x)$ as distributions [42], and the result is:

$$\int_{-\eta}^{\eta}\delta(x)\psi'(x)dx = \bar{\psi}'(0). \quad (27)$$

The integrals $\int_{-\eta}^{\eta}\psi(x)dx$ and $\int_{-\eta}^{\eta}x^2\psi(x)dx$ in Eq. (25) vanish in the limit $\eta \to 0$, and we end up with the following boundary condition:

$$\Delta\psi' = -\lambda\bar{\psi}'(0). \quad (28)$$

This matches the boundary condition on the first derivative of the eigenfunctions obtained in [43] and [42] for the simpler Hamiltonian $H = -\frac{d^2}{dx^2} + \lambda\delta'(x)$. To obtain the second boundary condition, we integrate the Schrödinger equation from $-l$ to x with l positive this time:

$$-\int_{-l}^{x}\frac{d^2}{dy^2}\psi(y)dy + \lambda\int_{-l}^{x}\delta'(y)\psi(y)dy + \int_{-l}^{x}y^2\psi(y)dy = \epsilon\int_{-l}^{x}\psi(y)dy. \quad (29)$$

The first integral gives $\psi'(x) - \psi'(l)$. The second, via integration by parts, yields

$$\int_{-l}^{x}\delta'(y)\psi(y)dy = \delta(y)\psi(y)|_{-l}^{x} - \int_{-l}^{x}\delta(y)\psi'(y)dy, \quad (30)$$

Now, for $x < 0$, the integral $\int_{-l}^{x}\delta(y)\psi'(y)dy$ is zero. For $x \geq 0$ the integral can be found as before by regarding $\delta(y)$ and $\psi'(y)$ as distributions:

$$\int_{-l}^{x}\delta'(y)\psi(y)dy = \delta(x)\psi(x)|_{-l}^{x} - \theta(x)\bar{\psi}'(0) = \delta(x)\psi(x) - \theta(x)\bar{\psi}'(0), \quad (31)$$

where $\theta(x)$ is the Heaviside step function given by:

$$\theta(x) = \begin{cases}0 & x < 0\\ 1 & x \geq 0\end{cases}$$

Substituting these results into Eq. (29), then integrating again from $-\eta$ to η, we obtain:

$$-\int_{-\eta}^{\eta}(\psi'(x) - \psi'(l))dx, + \lambda\int_{-\eta}^{\eta}(\delta(x)\psi(x) - \theta(x)\bar{\psi}'(0))dx = \int_{-\eta}^{\eta}\Big(\int_{-l}^{x}(\epsilon - y^2)\psi(y)dy\Big)dx \quad (32)$$

integrating the left-hand side and taking the limit $\eta \to 0$ yields $-\Delta\psi + \lambda\bar{\psi}(0)$. As the right-hand side integral is zero in the limit $\eta \to 0$, we conclude that the wave function $\psi(x)$ is discontinuous and the discontinuity jump is

$$\Delta\psi = \lambda\bar{\psi}(0). \quad (33)$$

This is again the same condition found for the kinetic energy operator with a singular potential $\lambda\delta'(x)$.

The Energy Eigenvalues

The energy eigenvalues ϵ for the quantum harmonic oscillator with $\lambda\delta'(x)$ are determined using Eq. (14), which gives

$$\frac{1}{\lambda} = \frac{\overline{\psi'}(0)}{\bar{\psi}(0)}\sum_{n\geq 0}\frac{|\psi_{2n}(0)|^2}{\epsilon_{2n}-\epsilon}, \quad (34)$$

where the second term in Eq. (14) has no contribution to ϵ since $\psi_n(0) = 0$ for odd n, while $\psi_n'(0) = 0$ for even n. By a process of analytic continuation, this sum can be found as follows. First, note that $\psi_{2n}(0)$ is given by [48]:

$$\psi_{2n}(0) = (-1)^n\sqrt{\frac{(2n)!}{\pi^{1/2}2^{2n}(n!)^2}} = (-1)^n\sqrt{\frac{1}{\pi}\frac{\Gamma(n+\frac{1}{2})}{\Gamma(n+1)}}. \quad (35)$$

If we assume temporarily that $\epsilon < 1$, the following integral representation can be used to evaluate the sum

$$\frac{1}{\lambda} = -\frac{\overline{\psi'}(0)}{4\pi\bar{\psi}(0)}\int_0^1 x^{-(\epsilon+3)/4}\sum_{n\geq 0} x^n\frac{\Gamma(n+\frac{1}{2})}{\Gamma(n+1)}dx. \quad (36)$$

The asymptotic behavior of the ratio of gamma functions $\frac{\Gamma(n+\frac{1}{2})}{\Gamma(n+1)}$ can be obtained using Stirling's formula

$$\Gamma(az+b) \sim \sqrt{2\pi}e^{-az}(az)^{az+b-(1/2)}, a > 0,\ b \in C, \quad (37)$$

then

$$\frac{\Gamma(n+\frac{1}{2})}{\Gamma(n+1)} \sim n^{-1/2}, n \to \infty. \quad (38)$$

This ensures the convergence of the series that appeared in Eq. (36) (after doing the integration). Using the Taylor series expansion of the function $\frac{1}{\sqrt{1-x}}$, the sum can be found as

$$\sum_{n\geq 0} x^n\frac{\Gamma(n+\frac{1}{2})}{\Gamma(n+1)} = \frac{\pi^{1/2}}{(1-x)^{1/2}}. \quad (39)$$

Substituting this back into Eq. (36), the integral can be easily computed using the beta functions expressed in terms of gamma functions:

$$\int_0^1\frac{x^{-(\epsilon+3)/4}}{(1-x)^{1/2}}dx = B(\tfrac{1}{4}-\tfrac{\epsilon}{4},\tfrac{1}{2}) = \frac{\Gamma(\frac{1}{4}-\frac{\epsilon}{4})\Gamma(\frac{1}{2})}{\Gamma(\frac{3}{4}-\frac{\epsilon}{4})}. \quad (40)$$

where $\Gamma(\frac{1}{2}) = \sqrt{\pi}$. By analytic continuation, we can extend the result of Eq. (40) for small ϵ to include all values of $\epsilon \neq 4n+1$. Using Eq. (34), the energy eigenvalues are determined by the following transcendental equation:

$$\frac{1}{\lambda} = -\frac{\overline{\psi'}(0)}{4\bar{\psi}(0)}\frac{\Gamma(1/4-\epsilon/4)}{\Gamma(3/4-\epsilon/4)}. \quad (41)$$

The scale $\frac{\overline{\psi'}(0)}{\bar{\psi}(0)}$ may be computed numerically using the normalization condition together with Eq. (16) evaluated at $x = 0$. Using the transcendental equation, exact numerical values of the energy eigenvalue ϵ of the problem can be obtained. For each given λ, an infinite set of eigenvalues ϵ exists. In Tables 1 and 2, the ground state and the first five excited-state energy eigenvalues for different positive and negative coupling constant is given. The purpose of the figure and tables is to provide an outline of the general behavior of the energy spectrum. The $\lambda = 0$ case recovers the eigenvalues energy for the even states of the original problem without $\lambda\delta'(x)$.

TABLE 1. Energy eigenvalues of the harmonic oscillator in the presence of the $\lambda\delta'(x)$ potential for different values of the negative scaled coupling constant $\lambda_s = \lambda\frac{\overline{\psi'}(0)}{4\bar{\psi}(0)}$.

λ_s	E_0	E_2	E_4	E_6	E_8	E_{10}
0	1	5	9	13	17	21
-0.1	0.75577	4.88620	8.91510	12.9293	16.9382	20.9111
-0.2	0.47073	4.77166	8.83015	12.8587	16.8765	20.8889
-0.5	-	4.44153	8.58245	12.6515	16.6946	20.7248
-0.8	-	4.16109	8.35827	12.4588	16.5229	20.5684
-1	-	4.0095	8.22685	12.3419	16.4166	20.4703
-2	-	3.57029	7.77759	11.9073	16.0006	20.0724
-5	-	3.23098	7.33826	11.4155	15.4776	19.5301
- 10	-	3.12994	7.17024	11.2116	15.2457	19.2753

TABLE 2. Energy eigenvalues of the harmonic oscillator in the presence of the $\lambda\delta'(x)$ potential for different values of the positive scaled coupling constant $\lambda_s = \lambda\frac{\overline{\psi'}(0)}{4\overline{\psi}(0)}$.

λ_s	E_0	E_2	E_4	E_6	E_8	E_{10}
0.1	0.75577	4.88620	8.91510	12.9293	16.9382	20.9111
0.2	1.38757	5.21886	9.16676	13.1397	17.1225	21.1105
0.5	1.78548	5.50928	9.40039	13.3398	17.3001	21.2717
0.8	2.04393	5.74525	9.60541	13.5219	17.4652	21.4235
1	2.16779	5.87417	9.72459	13.6313	17.5664	21.5180
2	2.50638	6.28378	10.1423	14.0407	17.9627	21.9001
5	2.78401	6.67640	10.5984	14.5357	18.4826	22.4365
10	2.88937	6.83036	10.7922	14.7581	18.7284	22.6962

From Fig. 1, we notice that the energy eigenvalues increase with increasing λ in the positive region. For negative λ, however, the energy decreases as the magnitude of λ increases. For sufficiently large λ, these energy eigenvalues converge to the energy eigenvalues of the odd states of the original problem without the contact interaction $\lambda\delta'(x)$. The convergence depends on the sign of λ. If λ is positive, the energy converges to the next odd state energy, whereas for negative λ, it converges to the odd eigenvalue of the previous state. In the first table, we neglected the values of ϵ in the negative region, since the transcendental equation is derived for positive values of ϵ.

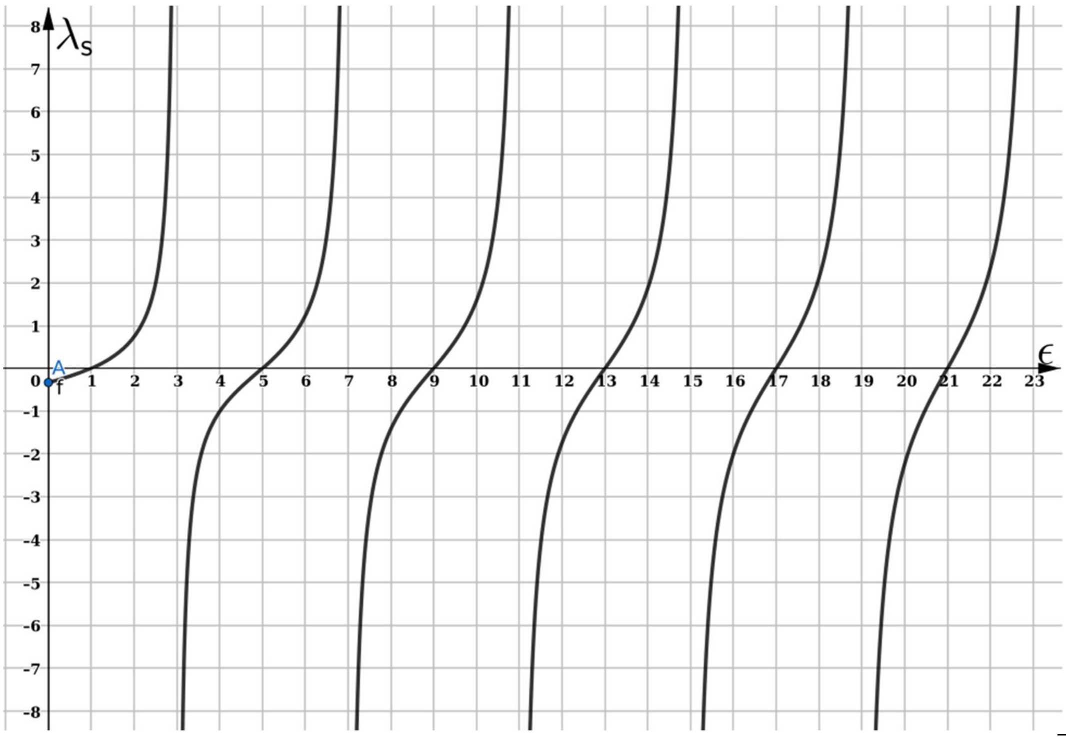

FIG. 1. A plot of Eq. (41) with the coupling constant λ replaced by the scaled coupling constant $\lambda_s = \lambda\frac{\overline{\psi'}(0)}{4\overline{\psi}(0)}$.

The behavior of the energy eigenvalues can be explained using the gamma function identity

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin(\pi z)} \quad (42)$$

together with Stirling's formula

$$\Gamma(az+b) \sim \sqrt{2\pi}e^{-az}(az)^{az+b-(1/2)}, a > 0,\ b \in C. \quad (43)$$

For large ϵ, the ratio that appears in Eq. (40) can be written as:

$$\frac{\Gamma(\frac{1}{4}-\frac{\epsilon}{4})}{\Gamma(\frac{3}{4}-\frac{\epsilon}{4})} = \frac{\Gamma(\frac{1}{4}+\frac{\epsilon}{4})\sin\pi(\frac{3}{4}-\frac{\epsilon}{4})}{\Gamma(\frac{3}{4}+\frac{\epsilon}{4})\sin\pi(\frac{1}{4}-\frac{\epsilon}{4})} \sim \frac{\sqrt{\epsilon}}{2}\tan\frac{\pi}{4}(\epsilon-1). \quad (44)$$

This asymptotic behavior is periodic under the shift $\epsilon \rightarrow \epsilon + 4$. Moreover, as $\epsilon \rightarrow 2n+1$, the ratio diverges to infinity. This behavior is clearly reflected in Tables 1 and 2 and in Fig. 1.

The Energy Eigenfunctions

The Green's function technique is used to obtain exact implicit results concerning the energy eigenvalues of the system under consideration. Using this technique, we can go further and try to get the energy eigenfunctions of the system. From Eq. (13) and the transcendental Eq. (41), the solution to the Schrödinger equation of the quantum harmonic oscillator in the presence of the Dirac delta derivative potential can be written as an infinite sum:

$$\psi(x) = \frac{4\overline{\psi}(0)}{\psi'(0)} \frac{\Gamma\left(\frac{3}{4}-\frac{\epsilon}{4}\right)}{\Gamma\left(\frac{1}{4}-\frac{\epsilon}{4}\right)} \times \sum_{n\geq 0} \frac{[\overline{\psi'}(0)\psi_n^*(0)+\overline{\psi}(0)\psi_n'^*(0)]}{\epsilon-\epsilon_n}\psi_n(x). \quad (45)$$

Since $\psi_{2n+1}(0)$ and $\psi'_{2n}(0)$ are both zeros, we can simplify the sum above by splitting it into two sums, one over the odd values of n and another over even n as follows:

$$\psi(x) = \frac{4\Gamma\left(\frac{3}{4}-\frac{\epsilon}{4}\right)}{\Gamma\left(\frac{1}{4}-\frac{\epsilon}{4}\right)} \times \begin{bmatrix} \overline{\psi}(0)\sum_{n\geq 0}\frac{\psi_{2n}^*(0)}{\epsilon-\epsilon_{2n}}\psi_{2n}(x) \\ +\frac{\overline{\psi}^2(0)}{\psi'(0)}\sum_{n\geq 0}\frac{\psi_{2n+1}'^*(0)}{\epsilon-\epsilon_{2n+1}}\psi_{2n+1}(x)\end{bmatrix}. \quad (46)$$

Using the recursion relation

$$\psi_n'(x) = \sqrt{\frac{n}{2}}\psi_{n-1}(x) - \sqrt{\frac{n+1}{2}}\psi_{n+1}(x) \quad (47)$$

together with the identity Eq. (35), the wave function can be written as:

$$\psi(x) = \frac{4\Gamma(3/4-\epsilon/4)}{\sqrt{\pi}\Gamma(1/4-\epsilon/4)}\sum_{n\geq 0}(-1)^n\frac{\sqrt{\Gamma(n+\frac{1}{2})}}{\sqrt{\Gamma(n+1)}} \times \left[\frac{\overline{\psi}(0)\psi_{2n}(x)}{(\epsilon-\epsilon_{2n})} + \sqrt{4n+2}\frac{\frac{\overline{\psi}^2(0)}{\overline{\psi'}(0)}\psi_{2n+1}(x)}{(\epsilon-\epsilon_{2n+1})}\right]. \quad (48)$$

This wave function is supposed to be discontinuous at the origin. We can check this by noting that there is a one-to-one correspondence between the solution in the positive and the negative regions and the sign of the coupling constant λ. Specifically, the solution in the positive region, $\psi_+(x)$, is equal to the solution in the negative region, $\psi_-(x)$, with λ replaced by $-\lambda$. To see this, we write the Shrödinger equation in the positive and the negative regions:

$$[-\frac{d^2}{dx^2} + x^2 + \lambda\delta'(x)]\psi(x) = \epsilon\psi(x), x > 0 \quad (49)$$

$$[-\frac{d^2}{dx^2} + x^2 + \lambda\delta'(x)]\psi(x) = \epsilon\psi(x), x < 0 \quad (50)$$

Since the Hamiltonian $-\frac{d^2}{dx^2} + x^2 + \lambda\delta'(x)$ is odd only on $\delta'(x)$, Eq. (50) can be rewritten as:

$$[-\frac{d^2}{dx^2} + x^2 - \lambda\delta'(|x|)]\psi(x) = \epsilon\psi(x), x < 0. \quad (51)$$

This equation is similar to Eq. (49) with the opposite sign of λ. This means that the solution in the negative region can be obtained by solving the Schrödinger equation in the positive region for the opposite sign of λ. This one-to-one correspondence is transitive to the energy eigenvalues. Let us denote the roots of the transcendental Eq. (41) for $\pm\lambda$ by $\epsilon_{m_\pm}$. Then the solutions in both regions are related to each other by replacing the energy eigenvalues from $\epsilon_{m_+} \to \epsilon_{m_-}$. In the case of $\lambda = 0$, the energy eigenvalues satisfy $\epsilon_{m_+} = \epsilon_{m_-}$, and the solutions in both regions are the same. This recovers the original solution of the quantum harmonic oscillator. Our solution now can be rewritten in a way that emphasizes its discontinuity as follows:

$$\psi_m(x) = \begin{cases} \frac{4\Gamma(3/4-\epsilon_{m_+}/4)}{\sqrt{\pi}\Gamma(1/4-\epsilon_{m_+}/4)}\sum_{n\geq 0}(-1)^n\frac{\sqrt{\Gamma(n+\frac{1}{2})}}{\sqrt{\Gamma(n+1)}}\left[\frac{\overline{\psi}(0)\psi_{2n}(x)}{(\epsilon_{m_+}-\epsilon_{2n})} + \frac{\sqrt{4n+2}\frac{\overline{\psi}^2(0)}{\psi'(0)}\psi_{2n+1}(x)}{(\epsilon_{m_+}-\epsilon_{2n+1})}\right], & x > 0 \\ \frac{4\Gamma(3/4-\epsilon_{m_-}/4)}{\sqrt{\pi}\Gamma(1/4-\epsilon_{m_-}/4)}\sum_{n\geq 0}(-1)^n\frac{\sqrt{\Gamma(n+\frac{1}{2})}}{\sqrt{\Gamma(n+1)}}\left[\frac{\overline{\psi}(0)\psi_{2n}(x)}{(\epsilon_{m_-}-\epsilon_{2n})} + \frac{\sqrt{4n+2}\frac{\overline{\psi}^2(0)}{\psi'(0)}\psi_{2n+1}(x)}{(\epsilon_{m_-}-\epsilon_{2n+1})}\right], & x < 0. \end{cases} \quad (52)$$

Using Cramér's inequality [49]

$$|\psi_n(x)| \leq \pi^{1/4}, \quad (53)$$

we notice that the sums in the wave function $\psi_m(x)$ depend critically on the denominators $\epsilon_{m_\pm} - \epsilon_{2n}$ and $\epsilon_{m_\pm} - \epsilon_{2n+1}$. Thus, the dominant sum is chosen regarding the eigenvalues $\epsilon_{m_\pm}$. For small λ, the values of $\epsilon_{m_\pm}$ lie between the odd and even original eigenvalues of the problem (without the added contact interaction), namely, $\epsilon_{2m+1} > \epsilon_{m_+} > \epsilon_{2m}$, and $\epsilon_{2m+1} < \epsilon_{m_-} < \epsilon_{2m}$. So for small λ, both the even and the odd sums contribute to the wave function $\psi_m(x)$. On the other hand, for a large value of λ, the eigenvalues $\epsilon_{m_\pm}$ tend to $\epsilon_{2m\pm1}$ as we can see from Eq. (44), so the odd part of the sums above will dominate the even contribution and hence, the solution will be represented by the odd wave function of the problem before adding the contact interaction. In the following section, we will give an educated solution for the large λ situation.

Large Coupling Constant Solutions

The asymptotic behavior of the energy eigenvalues, as given in Eq. (44) and shown in Fig. 1, motivates us to write the solutions in the large coupling constant regime. Since the eigenvalues in this limit shift to the odd energy levels of the quantum harmonic oscillator, we suggest that the eigenfunctions approach the odd oscillator wave functions $\psi_{2n\pm1}(x)$. The shift in ϵ, evident from Fig. 1, depends on the sign of λ. Since $\delta'(x)$ is an odd function of x, the sign of λ can be transferred to the variable x. Hence, the behavior of the energy eigenvalues ϵ now depends on the sign of x. This implies that the wave functions differ on either side of the singular point $x = 0$, consistent with the discontinuity condition established in Sec. IV and the discussion in Sec. VI. Taking these facts into account, we propose the following form for the wave functions in the large-λ region.

$$\psi_n(x) = \begin{cases} \psi_{2n+1}(x) + \phi_+(x) & \text{if } x > 0, n = 0,1,2,3\cdots \\ \psi_{2n-1}(x) + \phi_-(x) & \text{if } x < 0, n = 1,2,3\cdots \\ \phi_-(x) & \text{if } x < 0, n = 0 \end{cases} \quad (54)$$

Since the eigenfunctions $\psi_{2n\pm1}(x)$ are zeros at $x = 0$, we add the functions $\phi_\pm(x)$. The functions $\phi_\pm(x)$ are chosen to decay rapidly and to satisfy both the boundary conditions on the wave function and its derivative. Moreover, for $x << 1$, they must satisfy the Schrödinger equation, where the harmonic potential x^2 can be neglected. A good choice of $\phi_\pm(x)$ comes from the bound-state solution of the Schrödinger equation in the presence of the $\lambda\delta'(x)$ potential:

$$[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \lambda\delta'(x)]\phi(x) = \epsilon\phi(x), \quad (55)$$

The solutions to this problem, for the bound state case, were obtained in [41] and are given by:

$$\phi_\pm(x) = \frac{\lambda}{2}(\frac{\overline{\psi'}(0)}{\kappa} \pm \overline{\psi}(0))e^{\mp\kappa x}. \quad (56)$$

The $\pm$ stands for the solution on the positive (negative) x-axis. The eigenvalue κ is related to the coupling constant λ by:

$$\frac{1}{\lambda} = \frac{\overline{\psi'}(0)}{2\kappa\overline{\psi}(0)}. \quad (57)$$

The solutions $\phi_\pm$ were shown to satisfy the required boundary conditions on the wave function and its first derivative. As $\psi_{2n\pm1}(x)$ are zero at the origin and as the boundary conditions on our work are similar to the conditions on the solution $\phi_\pm$, we conclude that Eq. (54) provides valid approximate solutions for the Schrödinger equation of the harmonic oscillator with the additional $\lambda\delta'(x)$ potential in the large coupling region.

Conclusion

In this work, we found that exact solutions of the quantum harmonic oscillator with the addition of a point interaction represented by the $\lambda\delta'(x)$ centred at the origin can be obtained using Green's method. The values of the energy eigenvalues are determined using a transcendental equation. The numerical values of the energy eigenvalues can be determined exactly whenever the solutions are normalized. We showed that, for a large coupling constant, the energy eigenvalues tend to be the odd eigenvalues of the quantum harmonic oscillator. The conditions required for a self-adjoint extension of the Hamiltonian were obtained following the method of Griffiths. Both the wave function and its first derivative were found to be discontinuous at the singular point $x = 0$, with discontinuity jumps consistent with the results previously derived by Kurasov and Griffiths for simpler Hamiltonians. These boundary conditions appear to be a general feature whenever such contact potentials are present. The results in the large coupling constant region show that only the odd solutions of the harmonic oscillator were available. Furthermore, for large λ, it was easy to guess the solution that meets the behavior of the energy eigenvalues and the conditions on the solution. Finally, expressing the exact solutions, which are represented as infinite series, in terms of elementary functions remains a challenging mathematical problem. Successfully doing so would enable full normalization of the wave functions, exact computation of energy eigenvalues, and deeper physical insight into the problem.

The authors have no conflicts to disclose.

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