Exact solutions of a particle in a box with a delta function potential: The factorization method

Pouria Pedram

*Plasma Physics Research Center, Science and Research Campus, Islamic Azad University, Tehran, Iran**

M. Vahabi

Department of Physics, Shahid Beheshti University, G. C., Evin, Tehran 19839, Iran

Abstract

We find the exact eigenvalues and eigenfunctions for the problem of a particle in a box with a delta function potential $V(x) = \lambda\delta(x - x_0)$ using the factorization method. We show that the presence of the delta function potential results in the discontinuity of the corresponding ladder operators. More importantly, the presence of the delta function potential allows us to obtain the full spectrum of the problem in the first step of the factorization procedure *even* for the weak coupling limit ($\lambda \to 0$).

I. INTRODUCTION

Schrödinger equation is the basic equation for the non-relativistic quantum mechanics. The time-independent form of this equation in the presence of a potential V can be written as[1]

$$H\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi, \tag{1}$$

where H is the Hamiltonian operator of the system, ψ is the wave function, m is the mass of the particle and E is the eigenenergy. This eigenvalue equation can be solved exactly only for a few number of potentials.

A particle in a box and a particle in a $\delta-$function potential are two well-known, instructive, and exactly solvable examples in quantum mechanics textbooks.[1] The former can be used to describe the semiconductor quantum dots and quantum wells at low temperatures[2,3] and the later can be used as a model for atoms and molecules.[4]

The problem of a particle in a box with a delta function potential has been recently investigated using a perturbative expansion in the strength of the delta function potential λ.[5] Moreover, the exact solutions has also been obtained by Joglekara for the weak ($\lambda \to 0$) and the strong ($1/\lambda \to 0$) coupling limits.[6]

In this paper, we discuss the problem of a particle in a box with a delta function potential using the factorization method. We obtain the energy spectrum and the corresponding ladder operators. We show that, contrary to the first anticipation, the presence of the delta function potential simplifies the factorization procedure more. In this respect, we find the full spectrum of the Hamiltonian in the first step of the factorization method. Furthermore, we show that this result is also true for the weak coupling limit ($\lambda \to 0$).

II. PARTICLE IN A BOX WITH A DELTA FUNCTION POTENTIAL

Let us consider a particle in a one-dimensional box of size a with a delta function potential, $V(x) = \lambda\,\delta(x-x_0) = \lambda\,\delta(x-pa)$ where $0 < p < 1$. Now, the corresponding time-independent Schrödinger equation takes the following form

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2} + \lambda\delta(x-pa)\psi_n(x) = E_n\psi_n(x), \tag{2}$$

where $\psi_n(x)$ and E_n are the corresponding eigenfunctions and eigenvalues, respectively. Because of the boundary conditions ($\psi_n(x) = 0$ for $x \le 0$ or $x \ge a$) the eigenfunctions take the following form inside the box

$$\psi_n(x) = \begin{cases} A\sin(k_n x), & 0 \le x \le pa, \\ B\sin[k_n(x-a)], & pa \le x \le a, \end{cases} \tag{3}$$

where $k_n = \sqrt{\frac{2mE_n}{\hbar^2}}$. Moreover, the continuity condition of the wave function at $x = pa$ gives $\frac{A}{B} = \frac{\sin[(p-1)k_n a]}{\sin(pk_n a)}$. Since the delta function potential is infinite at the point $x = pa$, the first derivative of the wave function is not continuous and the relation between the left and right derivatives of the wave function can be obtained by integrating the Schrödinger equation (2) over a small interval $(x_0 - \epsilon, x_0 + \epsilon)$

$$\begin{aligned} \frac{d\psi_n(x)}{dx}|_{pa+\epsilon} - \frac{d\psi_n(x)}{dx}|_{pa-\epsilon} &= \frac{2m}{\hbar^2}\int_{pa-\epsilon}^{pa+\epsilon} V(x)\,\psi_n(x) \\ &= \frac{2m\lambda}{\hbar^2}\psi_n(pa). \end{aligned} \tag{4}$$

Substituting above eigenfunctions (3) in the discontinuity condition (4) results in the following quantization condition[5,6]

$$k_n \sin(k_n a) = \frac{2m\lambda}{\hbar^2}\sin(pk_n a)\sin[(p-1)k_n a]. \tag{5}$$

The solutions to above equation give us the energy spectrum of the Hamiltonian, $E_n = \frac{\hbar^2 k_n^2}{2m}$.

III. PARTICLE IN A BOX WITH A DELTA FUNCTION POTENTIAL REVISITED: THE FACTORIZATION METHOD

To calculate the eigenvalues and eigenfunctions of a Hamiltonian operator H, we can use a general operational procedure so called the factorization method. In this method, the Hamiltonian of the system is written as the multiplication of two ladder operators. Then, we use these operators to obtain the Hamiltonian's eigenfunctions. In general, in contrast to the case of a simple harmonic oscillator, one ladder operator is not enough to form all the Hamiltonian's eigenfunctions and for each eigenfunctions a ladder operator is needed.

This method was first introduced by Schrödinger[7–9] and Dirac[10] and was further developed by Infeld and Hull[11] and Green[12]. The spirit of the factorization method is to write the second-order differential operator H as the product of two first order differential operators a and $a^\dagger$, plus a real constant E. The form of these operators depends on the form of the potential $V(x)$ and the factorization energy.

The procedure of finding the ladder operators and the eigenfunctions consists of some steps;[13] We find operators $a_1, a_2, a_3, ...$ and real constants $E_1, E_2, E_3, ...$ from the following recursive relations

$$\begin{aligned} a_1^\dagger a_1 + E_1 &= H, \\ a_2^\dagger a_2 + E_2 &= a_1 a_1^\dagger + E_1, \\ a_3^\dagger a_3 + E_3 &= a_2 a_2^\dagger + E_2, ... \end{aligned} \tag{6}$$

or generally

$$a_{n+1}^\dagger a_{n+1} + E_{n+1} = a_n a_n^\dagger + E_n, \qquad j = 1, 2, ..., \tag{7}$$

where the real constants E_n's are the Hamiltonian's eigenvalues and the operators a_n's are the ladder operators used to form the eigenfunctions. Also, assume that there exists a null eigenfunction $|\xi_n\rangle$ with zero eigenvalue for each a_n, namely

$$a_n|\xi_n\rangle = 0. \tag{8}$$

Hence, E_n is the n^{th} eigenvalue of the Hamiltonian with the following corresponding eigenfunction[13] (up to a normalization coefficient)

$$|E_n\rangle = a_1^\dagger a_2^\dagger ... a_{j-1}^\dagger |\xi_n\rangle. \tag{9}$$

Because of Eq. (6), it would be useful to consider the following form of ladder operators

$$a_n = \frac{1}{\sqrt{2m}}(P + if_n(x)), \tag{10}$$

where P is the momentum operator and $f_n(x)$ is a real function of x. Although these operators are not hermitian ($a_n^\dagger = \frac{1}{\sqrt{2m}}(P - if_n(x)) \neq a_n$), their product will be hermitian

$$a_n^\dagger a_n = \frac{1}{2m}P^2 + \frac{1}{2m}f_n^2 + \frac{\hbar}{2m}\frac{df_n}{dx}. \tag{11}$$

Now, we are ready to find the ladder operators and eigenenergies of our problem. First, let us consider Eq. (6) for $n = 1$

$$a_1^\dagger a_1 + E_1 = H. \tag{12}$$

Because of the form of the Hamiltonian (2) and the ladder operators (11), we can rewrite above equation as

$$\frac{P^2}{2m} + \frac{1}{2m}f_1^2 + \frac{\hbar}{2m}\frac{df_1}{dx} + E_1 = \frac{P^2}{2m} + \lambda\delta(x - pa), \tag{13}$$

or equivalently

$$\frac{1}{2m}f_1^2 + \frac{\hbar}{2m}\frac{df_1}{dx} + E_1 = \lambda\delta(x - pa). \tag{14}$$

Note that, contrary to the case of Schrödinger equation (2), above equation is a non-linear first-order differential equation. To solve Eq. (14), let us consider the left-hand and right-hand sides of the delta function potential separately. For these regions, above equation reduces to

$$\frac{1}{2m}f_1^2 + \frac{\hbar}{2m}\frac{df_1}{dx} + E_1 = 0, \qquad\qquad x \neq pa, \tag{15}$$

which has the following solution

$$f_1 = \sqrt{2mE_1}\cot[\frac{\sqrt{2mE_1}}{\hbar}(x - b)], \tag{16}$$

where b is the constant of integration. We insist that f_1 be finite in the range $0 < x < a$, where it is the answer to our problem. Knowing that the singularities of cotangent function are π radian apart, we choose the points $x = 0$ and $x = a$ as the singularity points of the f_1. Since at these points the potential and hence the Hamiltonian are infinite, f_1 could be infinite at the boundaries. So we have

$$f_1(x) = \begin{cases} \sqrt{2mE_1}\cot[\frac{\sqrt{2mE_1}}{\hbar}x], & x < pa, \\ \sqrt{2mE_1}\cot[\frac{\sqrt{2mE_1}}{\hbar}(x - b)], & x > pa, \end{cases} \tag{17}$$

where $\frac{\sqrt{2mE_1}}{\hbar}(a - b) = \pi$. In order to fix the value of b, we need to use the discontinuity relation of ladder operators which can be obtained by integrating Eq. 14 over the small interval $(pa - \epsilon, pa + \epsilon)$

$$f_1(pa + \epsilon) - f_1(pa - \epsilon) = \frac{2m\lambda}{\hbar}. \tag{18}$$

This relation shows that the presence of the delta function potential results in the discontinuity of $f_1(x)$ at $x = pa$. Now, using Eq. 17 and $b = -\frac{\pi\hbar}{\sqrt{2mE_1}} + a$, Eq. 18 reduces to

$$\sqrt{2mE_1}\left\{\cot[\frac{\sqrt{2mE_1}}{\hbar}(pa + \frac{\pi\hbar}{\sqrt{2mE_1}} - a)] - \cot[\frac{\sqrt{2mE_1}}{\hbar}(pa)]\right\} = \frac{2m\lambda}{\hbar}. \tag{19}$$

Also, using the fact that $\cot(\pi + \alpha) = \cot\alpha$, the above result will be written in the following form

$$k_1\left\{\cot[(p - 1)k_1 a] - \cot(k_1 a)\right\} = \frac{2m\lambda}{\hbar^2}, \tag{20}$$

or

$$k_1 \sin(k_1 a) = \frac{2m\lambda}{\hbar^2} \sin(pk_1 a) \sin[(p-1)k_1 a], \tag{21}$$

where $k_1 = \frac{\sqrt{2mE_1}}{\hbar}$. This equation is similar to Eq. (5) which has previously been obtained using the explicit form of the Schrödinger equation. It is interesting to note that, although we were looking for the ground state energy of the Hamiltonian in the first step of the factorization method, this result gives us the full spectrum of the model. Moreover, this conclusion is also true for the case of weak coupling limit ($\lambda \to 0$). At this limit, from Eq. (21) we have $\sin(k_1 a) = 0$ which results in the full spectrum of a particle in a box $k_1 = \frac{n\pi}{a}$. This result has an interesting consequence; If we use the factorization method to calculate the energy levels of a particle in a box with $\lambda = 0$, we cannot find all of them in the first step of the procedure. In fact, we should continue the recursion relations to find one of the eigenvalues in each step[13]. Thus, contrary to the case of Schrödinger equation, the presence of the delta function potential simplifies the problem more from the factorization method point of view. So, it is not necessary to continue the recursion relations and we only need to replace index 1 with n in Eqs. (17,21).

Now, in order to obtain the eigenfunctions we rewrite Eq. (8) as

$$\left(\frac{\hbar}{i}\frac{d}{dx} + i\hbar k_n \cot(k_n x)\right)\xi_n(x) \ = \ 0, \qquad x < pa, \tag{22}$$

$$\left(\frac{\hbar}{i}\frac{d}{dx} + i\hbar k_n \cot[k_n(x-b)]\right)\xi_n(x) \ = \ 0, \qquad x > pa, \tag{23}$$

where $\xi_n(x) \equiv \langle x|\xi_n\rangle$. It can be easily checked that the following solution satisfy above equations

$$\xi_n(x) = \begin{cases} \sin(k_n x), & x < pa, \\ \sin[k_n(x-b)], & x > pa. \end{cases} \tag{24}$$

It is obvious that this result is similar to Eq. (3) for $x < pa$. Moreover, since $k_n b = k_n a - \pi$ we have $\sin[k_n(x-b)] = \sin[k_n(x-a)+\pi] = -\sin[k_n(x-a)]$. So, these eigenfunctions are equal to Eq. (3) up to normalization coefficients.

IV. CONCLUSION

We have considered the problem of a particle in a box in the presence of a delta function potential using the factorization method. We obtained the energy eigenvalues and eigenfunctions and their corresponding ladder operators. We showed that the presence of the delta function potential results in the discontinuity of the ladder operators. More importantly, we obtained all solutions in the first step of the factorization method even for the weak coupling limit ($\lambda \to 0$). So, the presence of the delta function potential much more simplifies the factorization procedure with respect to its absence.

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* Electronic address: pouria.pedram@gmail.com

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