Particle in a box with a $\delta$-function potential: strong and weak coupling limits

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Abstract

A particle in a one-dimensional $\delta$-function potential and particle in a box are two well-known pedagogical examples; their combination, particle in a box with a $\delta$-function potential $V_\lambda(x) = \lambda \delta(x - x_0)$, too, has been recently explored. We point out that it provides a unique example that is solvable in the weak ($\lambda \to 0^\pm$) and the strong ($1/\lambda \to 0^\pm$) coupling limits. In either limit, the attractive and repulsive potentials lead to identical spectra, with the possible exception of a single negative-energy state that is present when $1/\lambda \to 0^-$. We numerically obtain the spectra near the strong-coupling limit and discuss the consequences of the degeneracy that arises when $1/\lambda \to 0^\pm$. 
I. INTRODUCTION

A particle in a $\delta$-function potential $V_\lambda(x) = \lambda \delta(x - x_0)$ and particle in a box of size $a$ that runs from $x = 0$ to $x = a$ are two pedagogical examples discussed in introductory quantum mechanics. The first is often used to model short-ranged, elastic impurities whereas the second serves as a model for semiconductor quantum dots and quantum wells at low temperatures. In the first case, when $\lambda < 0$, the spectrum develops a single bound state with negative energy $E_b = -\frac{\lambda^2 m}{2\hbar^2}$ where $m$ is the mass of the particle, and the continuous spectrum at positive energies remains unchanged. In the second case, all states are localized within the box and have discrete energy eigenvalues given by $E_n = (n\pi)^2 E_0$ where $E_0 = \frac{\hbar^2}{2ma^2}$ is the characteristic energy scale for the box. The problem of particle in a box with a $\delta$-function potential has been recently investigated using perturbative expansion in the strength of the $\delta$-function potential $\lambda$. One salient feature of this problem is that the perturbation affects the energies of all eigenfunctions that do not vanish at $x_0$; this is in marked contrast to a particle in $\delta$-function potential.

We point out in this note that the aforementioned problem is solvable in both, weak coupling $\lambda \to 0^\pm$ and strong coupling $1/\lambda \to 0^\pm$, limits. In either limit the attractive and repulsive potentials have identical spectra except for a single bound-state that appears for the attractive potential; identical spectra are naturally expected when the $\delta$-function perturbation vanishes, $\lambda \to 0^\pm$. The strong-coupling result raises a question regarding the completeness of eigenfunctions in these two cases; the attractive potential has one more eigenstate - the bound state - in the spectrum compared to the repulsive potential. We show that the contribution of the bound state to the completeness relation vanishes when $1/\lambda \to 0^-$. We numerically obtain the spectra for intermediate values of $|\lambda|$ and compare them with perturbative corrections to the strong-coupling results.

II. PARTICLE IN A BOX WITH A $\delta$-FUNCTION POTENTIAL

Let us consider a particle in a box with $\delta$-function potential inside it, $V_\lambda(x) = \lambda \delta(x - x_0) = \lambda \delta(x - pa)$ where $0 \leq p \leq 1$. The time-dependent Schrödinger equation implies that the eigenvalues $E_n$ and eigenfunctions $\psi_n(x)$ satisfy

$$-rac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_n(x) + \lambda \delta(x - pa) \psi_n(x) = E_n \psi_n(x).$$ (1)
The eigenfunctions $\psi_n(x)$ are continuous and vanish outside the box. At positive energies, the (unnormalized) eigenfunctions are given by $\psi_n(x) = \sin(k_n x_\text{<}) \sin[k_n a - (x_\text{<})]$ where $x_\text{<(>)}$ is the smaller (greater) of $(x, x_0)$, and the eigenenergies are $E_n = (k_n a)^2 E_0 > 0$. When $E < 0$ the corresponding eigenfunction is $\psi_n(x) = \sinh(\kappa x_\text{<}) \sinh[\kappa(a - x_\text{>})]$ and $E = -(\kappa a)^2 E_0$. Integrating Eq.(1) over a small interval $(x_0 - \epsilon, x_0 + \epsilon)$ gives the quantization conditions

$$u_n \sin(u_n) + \Lambda \sin(pu_n) \sin[(1 - p)u_n] = 0,$$

$$v \sinh(v) + \Lambda \sinh(pv) \sinh[(1 - p)v] = 0,$$

where we have defined (dimensionless) $u_n = k_n a$, $v = \kappa a$, and the dimensionless $\delta$-function strength $\Lambda = 2ma\lambda/\hbar^2 = \lambda/(E_0 a)$.

First we will discuss the negative-energy solution. Eq.(3) has no nonzero solution if $\lambda > 0$. For $\lambda < 0$, a small-$v$ and large-$v$ expansion shows that it has exactly one nonzero solution when $|\lambda| > \lambda_\text{c}(p) = (E_0 a)/p(1 - p)$. The critical strength $\lambda_\text{c}(p)$ required for the negative-energy state increases as the $\delta$-function is moved closer to one of the walls. For a “strong” attractive potential, $|\lambda| \gg \lambda_\text{c}(p)$, we recover the result for a free-particle with $\delta$-function perturbation, $\kappa a = -\Lambda/2$ and $E = -\lambda^2 m/2\hbar^2$. Fig. 1 shows the spectra $\kappa(p)$ for different strengths of the attractive potential obtained by numerically solving Eq.(3), and verifies the results we have derived analytically.

Next we will focus on the (more interesting) positive energy solutions. When $E > 0$ the eigenvalues $u_n$ are determined by Eq.(2). In the weak coupling limit $\lambda \to 0^\pm$ we recover the well-known result, $k_n = n\pi/a$. In the strong coupling limit $1/\lambda \to 0^\pm$, the solutions of Eq.(2) are given by

$$k_\nu(p) = \left\{ \frac{n\pi}{ap}, \frac{m\pi}{a(1 - p)} : m, n = 1, 2, \ldots \right\}.$$  

This spectrum is the same irrespective of the sign of the potential and it is symmetric in $p \leftrightarrow (1 - p)$. We note that the strong-coupling limit corresponds to two infinite wells with widths $pa$ and $(1 - p)a$ respectively. Figure 2 shows the spectra for both attractive (blue-solid) and repulsive (red-dotted) potential when $1/|\Lambda| = 0.02$. Recall that the spectrum for particle in a box is horizontal lines at $k_\nu(p) = n\pi/a$. In the strong-coupling limit, we see that the $(j + 1)$-state for attractive potential (blue-solid) and the $j$-state for the repulsive potential (red-dotted) approach each other. To better understand Eq.(4), let us consider the spectrum for a specific case, say $p = 2/5$. In Fig. 2 the low-lying states $m = 1, n = 1, m = 2$ are marked by the circles. The rectangle in Fig. 2 shows the states with $m = 3$ and...
\[ n = 2. \] Since either gives the same value of \( k_\nu \), the degeneracy in the strong-coupling limit is doubled. In general, a double-degeneracy at \( k_\nu = N\pi/a \ (N \geq 2) \) arises when \( p = \alpha/N \ (\alpha = 1, \ldots, N-1) \). In particular, at the symmetric point \( p = 1/2 \) the entire spectrum, given by \( k_n = 2n\pi/a \), is doubly-degenerate and represents the symmetric and antisymmetric states in a double quantum well. For a finite \( 1/\lambda \), Eqs. (2) and (4) give the following perturbative correction

\[ \begin{align*}
    k_\nu(p, 1/\lambda) &= \frac{n\pi}{ap} \left[ 1 - \frac{1}{\Lambda p} \right] \quad \text{(5)}
\end{align*} \]

when \( k_\nu(p) = n\pi/ap \) and a corresponding expression with \( p \leftrightarrow (1 - p) \) provided \( k_\nu(p) = m\pi/a(1 - p) \). Eq. (5) shows that near the strong-coupling limit, the repulsive potential suppresses the energy and attractive potential raises it. This is in stark contrast with the weak-coupling limit where the first order perturbative correction is given by

\[ \begin{align*}
    k_n(p, \lambda) &= \frac{n\pi}{a} \left[ 1 + \Lambda \frac{\sin^2(n\pi x_0/a)}{(n\pi)^2} \right] \quad \text{(6)}
\end{align*} \]

This unusual behavior arises because, in contrast to all other potentials, the \( \delta \)-function spectrum is well-defined in the strong-coupling limit, and is the same irrespective of the sign of the potential.

We conclude the note with a comment on the completeness relation. The completeness of eigenfunctions in the attractive and repulsive cases implies that

\[ \begin{align*}
    \sum_\nu \phi_{k_\nu}(x)\phi^*_{k_\nu}(x') &= \delta(x - x') \quad (\lambda > 0), \quad \text{(7)} \\
    \phi_\kappa(x)\phi_\kappa(x') + \sum_\nu \phi_{k_\nu}(x)\phi^*_{k_\nu}(x') &= \delta(x - x') \quad (\lambda < 0). \quad \text{(8)}
\end{align*} \]

where \( 0 \leq x, x' \leq a \), \( \phi_{k_\nu} \) are the normalized positive-energy eigenfunctions, and the normalized negative-energy eigenfunction is given by \( \phi_\kappa(x) = A\psi_\kappa(x) \) with

\[ \begin{align*}
    A^{-2} &= \frac{1}{4\kappa} \left\{ \sinh^2[(1 - p)\kappa a] \left[ \sinh(2p\kappa a) - (2p\kappa a) \right] + [p \to (1 - p)] \right\}. \quad \text{(9)}
\end{align*} \]

In the strong-coupling limit, \( \kappa a \gg 1 \) and Eq. (9) implies that \( A \sim 4\sqrt{\kappa} \exp(-\kappa a) \). Therefore, the contribution to Eq. (8) from the negative-energy state vanishes in the strong-coupling limit, as the two spectra at positive energies converge.
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4 In the strong-coupling limit, the ground state (j = 1) for attractive potential is at negative energy, and we do not consider it in the spectrum presented in Fig. 2.

5 This expression is valid provided sin(ka) ≠ 0.

6 This contribution also vanishes in the weak-coupling limit, κa ≪ 1 and is consistent with the results in Ref. 3.
FIG. 1: The spectrum of the negative-energy state $\kappa(p)$ for different strengths of the attractive potential. For $|\Lambda| \geq 4$, a single state occurs in the interval of width $\Delta p = \sqrt{1 - 4/|\Lambda|}$ around $p = 1/2$. Note that, as discussed in the text, $\kappa a(p) \to |\Lambda|/2$ for large $|\Lambda|$ over the interval where $|\Lambda| \gg 1/p(1 - p)$. 
FIG. 2: The spectra $k_n(p)$ for attractive (blue-solid) and repulsive (red-dotted) potential in the strong coupling limit, $1/|\Lambda| = 0.02$. Apart from the $j = 1$ state pulled down to negative energy (bottom-blue-solid), we see that the $(j+1)$-state for $\Lambda < 0$ (blue-solid) and the $j$-state for $\Lambda > 0$ (red-dotted) become degenerate as $1/|\Lambda| \to 0$. The circles show the $m = 1$, $n = 1$, and $m = 2$ states from the $p = 2/5$ spectrum. The $m = 3$ and $n = 2$ states, shown in the rectangle, become doubly-degenerate in the strong-coupling limit $1/|\Lambda| \to 0$. 