

A split kinetic energy solution scheme applied to various delta potentials in quantum mechanical systems

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Abstract. In this work, we extend the previously developed split kinetic energy (dubbed KEP) method by Mineo and Chao (2012) by modifying the mass parameter to include the negative mass. We first show how to separate the total system into the subsystems with 3 attractive delta potentials by using the KEP method. For repulsive delta potentials, we introduce “negative” mass terms. Two cases are demonstrated using the “negative” mass terms for repulsive delta potential problems in quantum mechanics. Our work shows that the KEP solution scheme can be used to obtain not only the exact energies but also the exact wavefunctions very precisely.

Keywords: kinetic energy partition; Schrodinger equation; negative mass; zero-range potential

1. Introduction

Zero-range potentials have been used for many decades to simplify the true complicated interactions among quantum particles and fields (Demkov and Ostrovski 1988, Yakovlev and Gradusdov 2013, Holden *et al.* 2005). In particular, delta functional potentials, due to their mathematical utilities, have shown to be very useful to help gaining physical pictures for quantum strong-coupling systems (Fermi 1936, Dirac 1958, Mineo and Chao 2012). However, in actual applications of such simplifications in solving quantum eigenvalue problems, two difficulties remain. First, for systems with many delta potentials, the resulting secular equations are very complicated transcendental algebraic equations with a high possibility of degeneracy. Therefore, independent eigenvectors are not always easily found. Second, if there are repulsive type potentials involved, such as strong Coulomb repulsion modeled by repulsive delta functions, the solution scheme by traditional methods often becomes very tedious and unstable. To solve these problems, in this paper we apply the recently developed kinetic energy partition method by Mineo and Chao (2012, 2014) to solve the many-delta-potential eigenvalue problems and two systems with repulsive delta potentials. For the latter type problems, we will use “negative” mass terms to treat properly the repulsive interactions. We will show that not only the eigenenergies, but also the eigenfunctions can be obtained very efficiently and precisely by using the KEP method.

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2. Theory

2.1 Partition with positive mass terms

In this section we introduce the basic KEP method with positive mass terms. The Hamiltonian of a system where one particle of mass m is under the action of N interaction potentials is written as

$$\hat{H} = \hat{T} + V_1 + V_2 + \cdots + V_N = \hat{T} + \sum_{i=1}^N V_i \quad (1)$$

where \hat{T} is the kinetic energy operator

$$\hat{T} = \frac{\hat{p}^2}{2m} \quad (2)$$

and V_i , $i=1,2,3,\dots,N$ are the potentials. We separate the kinetic energy into N terms

$$\hat{T} = \hat{T}_1 + \hat{T}_2 + \cdots + \hat{T}_N \quad (3)$$

where

$$\hat{T}_i = \frac{\hat{p}^2}{2m_i} \quad (4)$$

with

$$\sum_{i=1}^N \frac{1}{m_i} = \frac{1}{m} \quad (5)$$

With this partition, the total Hamiltonian can be written as

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \cdots + \hat{H}_N = \sum_{i=1}^N \hat{H}_i \quad (6)$$

where the subsystem Hamiltonians are

$$\hat{H}_i = \hat{T}_i + V_i \quad (7)$$

The corresponding Schrödinger equation for the i -th subsystem is

$$\hat{H}_i \psi_i = E_i \psi_i \quad (8)$$

where $i=1,2,3,\dots,N$ is the respective subsystem quantum number. We now assume the total wave-function is represented by a linear combination of subsystem wave-function

$$\Psi = C_1 \psi_1 + C_2 \psi_2 + \cdots + C_N \psi_N = \sum_{i=1}^N C_i \psi_i \quad (9)$$

where C_i is the expansion coefficient. The Schrödinger equation of the total system is

$$\hat{H}\Psi = E\Psi \quad (10)$$

Substituting Eq. (6) and Eq. (9) into the total Schrodinger Eq. (10), we obtain

$$\left(\sum_{i=1}^N \hat{H}_i \right) \left(\sum_{j=1}^N C_j \psi_j \right) = E \left(\sum_{j=1}^N C_j \psi_j \right) \quad (11)$$

Multiplying ψ_k^* with Eq. (11) and integrating over the coordinate space, we have

$$C_k (E_k - E) + \sum_{j=1}^N \sum_{i \neq k}^N C_j \langle \psi_k | \hat{H}_i | \psi_j \rangle + \sum_{j \neq k}^N C_j (E_k - E) \langle \psi_k | \psi_j \rangle = 0 \quad (12)$$

Notice that

$$\hat{H}_i = \left(\frac{m_j}{m_i} \right) \hat{H}_j + V_i - \left(\frac{m_j}{m_i} \right) V_j \quad (13)$$

Therefore, Eq. (12) can be rewritten as

$$C_k (E_k - E) + \sum_{j=1}^N \sum_{i \neq k}^N C_j \xi_{kij} + \sum_{j=1}^N \sum_{i \neq k}^N C_j \left(\frac{m_j}{m_i} \right) E_j \eta_{kj} + \sum_{j \neq k}^N C_j (E_k - E) \eta_{kj} = 0 \quad (14)$$

where the variable ξ_{kij} and η_{kj}

$$\xi_{kij} \equiv \langle \psi_k | V_i - \left(\frac{m_j}{m_i} \right) V_j | \psi_j \rangle \quad (15)$$

$$\eta_{kj} \equiv \langle \psi_k | \psi_j \rangle \quad (16)$$

Simplifying Eq. (14), we obtain

$$C_k \left\{ \left[1 + \sum_{i \neq k}^N \left(\frac{m_k}{m_i} \right) \right] E_k - E \right\} + \sum_{j=1}^N \sum_{i \neq k}^N C_j \xi_{kij} + \sum_{j \neq k}^N C_j \left[E_k + \sum_{i \neq k}^N \left(\frac{m_j}{m_i} \right) E_j - E \right] \eta_{kj} = 0 \quad (17)$$

Eq. (17) is the KEP coupling equation by solving which we can obtain the KEP energy.

2.2 Partition with negative mass terms

Consider a two-potential system. The Hamiltonian of the system can be written as

$$\hat{H} = \hat{T} + V_1 + V_2 \quad (18)$$

We can split the kinetic energy as

$$\hat{T}_1 = \frac{\hat{p}^2}{2m} s \quad (19)$$

$$\hat{T}_2 = \frac{\hat{p}^2}{2m}(1-s) \quad (20)$$

where s is an adjustable parameter. We then distribute the kinetic energy term to each potential and combine them to form a subsystem.

$$\hat{H}_1 = \hat{T}_1 + V_1 = \frac{\hat{p}^2}{2m}s + V_1 \quad (21)$$

$$\hat{H}_2 = \hat{T}_2 + V_2 = \frac{\hat{p}^2}{2m}(1-s) + V_2 \quad (22)$$

Accordingly, the total Hamiltonian is

$$\hat{H} = \hat{H}_1 + \hat{H}_2 \quad (23)$$

The Schrodinger equations of the two subsystems can be represented as

$$\hat{H}_1\psi_{1n} = E_{1n}\psi_{1n} \quad (24)$$

$$\hat{H}_2\psi_{2k} = E_{2k}\psi_{2k} \quad (25)$$

where n and k are the corresponding system's quantum numbers of the ranges $n=1,2,3,\dots,N$ and $k=1,2,3,\dots,K$, respectively. We use the linear combination for the total wavefunction

$$\Psi = \sum_{n=1}^N C_{1n}\psi_{1n} + \sum_{k=1}^K C_{2k}\psi_{2k} \quad (26)$$

The two sets of the coefficients C_{1n} and C_{2k} can be obtained by imposing the boundary conditions and the normalization condition. The total Schrodinger equation is

$$\hat{H}\Psi = E\Psi \quad (27)$$

Substituting Eq. (23) and Eq. (26) into Eq. (27) we obtain

$$\left(\hat{H}_1 + \hat{H}_2\right)\left(\sum_{n=1}^N C_{1n}\psi_{1n} + \sum_{k=1}^K C_{2k}\psi_{2k}\right) = E\left(\sum_{n=1}^N C_{1n}\psi_{1n} + \sum_{k=1}^K C_{2k}\psi_{2k}\right) \quad (28)$$

Multiplying ψ_{1m}^* and ψ_{2l}^* respectively with Eq. (28) and integrating over the coordinate space, we have

$$C_{1m}(E_{1m} - E) + \sum_{n=1}^N C_{1n}\langle\psi_{1m}|\hat{H}_2|\psi_{1n}\rangle + \sum_{k=1}^K C_{2k}(E_{2k} + E_{1m} - E)\langle\psi_{1m}|\psi_{2k}\rangle = 0 \quad (29)$$

$$C_{2l}(E_{2l} - E) + \sum_{k=1}^K C_{2k}\langle\psi_{2l}|\hat{H}_1|\psi_{2k}\rangle + \sum_{n=1}^N C_{1n}(E_{1n} + E_{2l} - E)\langle\psi_{2l}|\psi_{1n}\rangle = 0 \quad (30)$$

Notice that

$$\hat{H}_1 = \left(\frac{s}{1-s} \right) \hat{H}_2 + V_1 - \left(\frac{s}{1-s} \right) V_2 \quad (31)$$

$$\hat{H}_2 = \left(\frac{1-s}{s} \right) \hat{H}_1 + V_2 - \left(\frac{1-s}{s} \right) V_1 \quad (32)$$

Therefore, the coupled Eq. (29) and Eq. (30) can be written as

$$C_{1m} \left(\frac{E_{1m}}{s} - E \right) + \sum_{n=1}^N C_{1n} \langle \psi_{1m} | V_2 - \left(\frac{1-s}{s} \right) V_1 | \psi_{1n} \rangle + \sum_{k=1}^K C_{2k} (E_{2k} + E_{1m} - E) \langle \psi_{1m} | \psi_{2k} \rangle = 0 \quad (33)$$

$$C_{2l} \left(\frac{E_{2l}}{1-s} - E \right) + \sum_{k=1}^K C_{2k} \langle \psi_{2l} | V_1 - \left(\frac{s}{1-s} \right) V_2 | \psi_{2k} \rangle + \sum_{n=1}^N C_{1n} (E_{1n} + E_{2l} - E) \langle \psi_{2l} | \psi_{1n} \rangle = 0 \quad (34)$$

Eq. (33) and Eq. (34) are the KEP coupling equations. If we assign the parameter $s=-1$, we obtain the “negative” mass term that can apply to quantum systems with repulsive potentials.

3. Models with various delta potentials

3.1 Triple delta function

In this section, we will show how to apply the KEP method to solving the quantum problems with three delta potentials. The subsystem Hamiltonian can be written as three parts

$$\hat{H}_1 = \frac{\hat{p}^2}{2m_1} + V_1, \quad \hat{H}_2 = \frac{\hat{p}^2}{2m_2} + V_2, \quad \hat{H}_3 = \frac{\hat{p}^2}{2m_3} + V_3 \quad (35)$$

Where $V_1 = -\lambda\delta(x+a)$, $V_2 = -\lambda\delta(x)$ and $V_3 = -\lambda\delta(x-a)$ are the delta potentials with the same well depth λ at position $x=0, \pm a$, respectively. The subsystem ground state energies are easily obtained, respectively,

$$E_1 = -\frac{m_1\lambda^2}{2\hbar^2}, \quad E_2 = -\frac{m_2\lambda^2}{2\hbar^2}, \quad E_3 = -\frac{m_3\lambda^2}{2\hbar^2} \quad (36)$$

The subsystems masses m_1 , m_2 and m_3 are selected to be the same $m_1=m_2=m_3=3m$. The subsystem’s wave-functions are

$$\psi_1(x) = \begin{cases} \sqrt{k}e^{k(x+a)} & x < -a \\ \sqrt{k}e^{-k(x+a)} & x > -a \end{cases} \quad (37)$$

$$\psi_2(x) = \begin{cases} \sqrt{k}e^{kx} & x < 0 \\ \sqrt{k}e^{-kx} & x > 0 \end{cases} \quad (38)$$

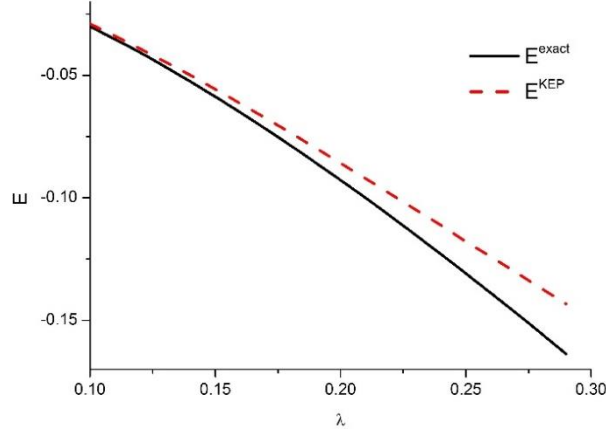


Fig. 1 The triple delta energy solution: Comparison of the KEP energy and the exact energy as the parameter of the well depth λ varies from 0.10 to 0.30. Here we introduce the dimensionless units $m=h=a=1$

$$\psi_3(x) = \begin{cases} \sqrt{k}e^{k(x-a)} & x < a \\ \sqrt{k}e^{-k(x-a)} & x > a \end{cases} \quad (39)$$

where the wave number k is

$$k = \frac{(3m)\lambda}{\hbar^2} \quad (40)$$

Applying the KEP coupling equation, i.e., Eq. (17), we obtain the algebraic equations

$$\begin{cases} C_1(3E_1 + \xi_{121} + \xi_{131} - E) + C_2[(E_1 + 2E_2 - E)\eta_{12} + \xi_{132}] + C_3[(2E_1 + E_3 - E)\eta_{13} + \xi_{123}] = 0 \\ C_1[(E_2 + 2E_1 - E)\eta_{21} + \xi_{231}] + C_2(3E_2 + \xi_{212} + \xi_{232} - E) + C_3[(E_2 + 2E_3 - E)\eta_{23} + \xi_{213}] = 0 \\ C_1[(E_3 + E_1 - E)\eta_{31} + \xi_{321}] + C_2[(E_3 + E_2 - E)\eta_{32} + \xi_{312}] + C_3(3E_3 + \xi_{313} + \xi_{323} - E) = 0 \end{cases} \quad (41)$$

Because the coefficients C_1 , C_2 and C_3 cannot all be zero, we solve the determinant equation to obtain the KEP energies

$$\begin{vmatrix} 3E_1 + \xi_{121} + \xi_{131} - E & (E_1 + 2E_2 - E)\eta_{12} + \xi_{132} & (2E_1 + E_3 - E)\eta_{13} + \xi_{123} \\ (E_2 + 2E_1 - E)\eta_{21} + \xi_{231} & 3E_2 + \xi_{212} + \xi_{232} - E & (E_2 + 2E_3 - E)\eta_{23} + \xi_{213} \\ (E_3 + E_1 - E)\eta_{31} + \xi_{321} & (E_3 + E_2 - E)\eta_{32} + \xi_{312} & 3E_3 + \xi_{313} + \xi_{323} - E \end{vmatrix} = 0 \quad (42)$$

We then compare the KEP results with the exact energies as shown in Fig. 1. In Fig. 1 the KEP energy for the triple delta potentials systems is less than 5% error from the exact result.

Total wave-function can be formed by three subsystem's ground state wave-functions

$$\Psi = C_1\psi_1 + C_2\psi_2 + C_3\psi_3 \quad (43)$$

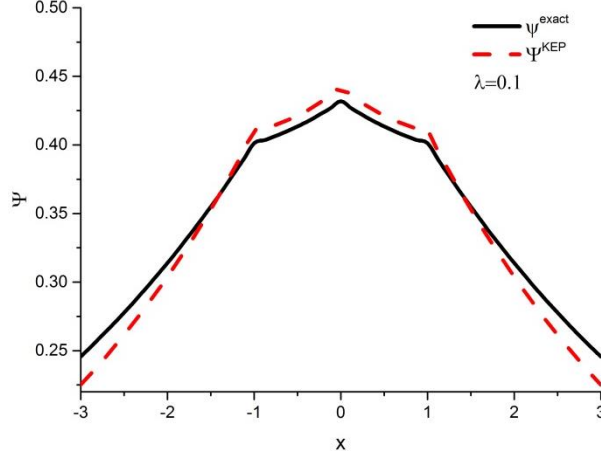


Fig. 2 The triple delta wavefunction solution: Comparison of the KEP result and the exact wavefunction for $\lambda=0.1$ utilizing the dimensionless units as in Fig. 1

Using the normalization condition of wave-function and the coupling KEP equation Eq. (41), we can obtain the expansion coefficients. In Fig. 2 the KEP wave-functions are compared with the exact wave-functions to a high level of consistency and the error is only 0.03% error. This means the KEP energy solution as well as the KEP wave-functions are very precise in reproducing the exact solutions.

3.2 Repulsive delta potentials

In this section, we illustrate the solution procedure for the antisymmetric delta potentials, using the negative mass scheme. The subsystem Hamiltonian can be respectively written as

$$\hat{H}_1 = \frac{\hat{p}^2}{2m} s + V_1 \quad (44)$$

$$\hat{H}_2 = \frac{\hat{p}^2}{2m} (1-s) + V_2 \quad (45)$$

where $V_1(x)=\lambda\delta(x-a)$ and $V_2(x)=-\lambda\delta(x+a)$ are antisymmetric delta potentials. Consider the Schrodinger equation with \hat{H}_1

$$\left(-\frac{\hbar^2}{2m/s} \frac{d^2}{dx^2} + \lambda\delta(x-a) \right) \psi_1(x) = E_1 \psi_1(x) \quad (46)$$

Because $s < 0$, Eq. (46) can be rewritten as

$$\left(-\frac{\hbar^2}{2m/|s|} \frac{d^2}{dx^2} - \lambda\delta(x-a) \right) \psi_1(x) = -E_1 \psi_1(x) \quad (47)$$

Clearly, the eigenenergy and eigenfunction of Eq. (47) are

$$E_1 = \frac{m_1 \lambda^2}{2\hbar^2}, \quad \psi_1(x) = \begin{cases} \sqrt{k_1} e^{-k_1(x-a)} & x > a \\ \sqrt{k_1} e^{k_1(x-a)} & x < a \end{cases} \quad (48)$$

where

$$m_1 = m / |s| \quad (49)$$

$$k_1 = \sqrt{2mE_1 / \hbar^2} \quad (50)$$

Similarly, the Schrödinger equation for \hat{H}_2

$$\left(-\frac{\hbar^2}{2m/(1-s)} \frac{d^2}{dx^2} - \lambda \delta(x) \right) \psi_2(x) = E_2 \psi_2(x) \quad (51)$$

The energy and wavefunction of Eq. (51) are

$$E_2 = -\frac{m_2 \lambda^2}{2\hbar^2}, \quad \psi_2(x) = \begin{cases} \sqrt{k_2} e^{-k_2(x+a)} & x > a \\ \sqrt{k_2} e^{k_2(x+a)} & x < a \end{cases} \quad (52)$$

where

$$m_2 = m / (1-s) \quad (53)$$

$$k_2 = \sqrt{2mE_2 / \hbar^2} \quad (54)$$

Using the KEP negative mass partition method, Eq. (33) and Eq. (34), with one basis set from each subsystem the KEP coupling equations are

$$C_1 \left(\frac{1}{s} E_1 + \xi_1 - E \right) + C_2 (E_1 + E_2 - E) \eta = 0 \quad (55)$$

$$C_1 (E_1 + E_2 - E) \eta + C_2 \left(\frac{1}{1-s} E_2 + \xi_2 - E \right) = 0 \quad (56)$$

The necessary matrix elements can be calculated analytically

$$\xi_1 = \langle \psi_1 | V_2 + \left(\frac{s-1}{s} \right) V_1 | \psi_1 \rangle \quad (57)$$

$$\xi_2 = \langle \psi_2 | V_1 + \left(\frac{s}{s-1} \right) V_2 | \psi_2 \rangle \quad (58)$$

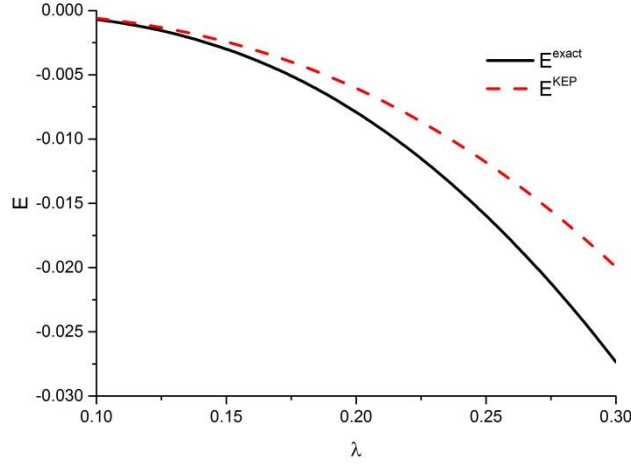


Fig. 3 The repulsive delta energy solution: Comparison of the KEP and the exact results, by varying the parameter λ

and

$$\eta = \langle \psi_1 | \psi_2 \rangle \quad (59)$$

The KEP solution can be written as

$$E_{\pm}^{KEP} = \frac{\left[\left(\frac{1}{s} - 2\eta^2 \right) E_1 + \left(\frac{1}{1-s} - 2\eta^2 \right) E_2 + \xi_1 + \xi_2 \right] \pm \sqrt{D}}{2(1-\eta^2)} \quad (60)$$

with

$$D = \left[\left(\frac{1}{s} - 2\eta^2 \right) E_1 + \left(\frac{1}{1-s} - 2\eta^2 \right) E_2 + \xi_1 + \xi_2 \right]^2 - 4(1-\eta^2) \left[\left(\frac{E_1}{s} + \xi_1 \right) \left(\frac{E_2}{1-s} + \xi_2 \right) - \eta^2 (E_1 + E_2)^2 \right] \quad (61)$$

In Fig. 3, we show the comparison of the KEP energy with the exact result. We see the overall trend is very similar and the largest error is 14%. Although the error seems to be large, this is a pretty new and novel approach which offers a perspective and may shed light on the even bigger question of how to use the negative mass idea in quantum mechanics.

3.3 Delta potential in the box

Now, we consider a distinctive delta potential confined in a one-dimensional (1D) box, where the box width is a and the range is $-a < x < a$. Using the same method as shown in Section 2.2, the subsystem Hamiltonians can be written as

$$\hat{H}_1 = \frac{\hat{p}^2}{2m} s + V_1 \quad (62)$$

$$\hat{H}_2 = \frac{\hat{p}^2}{2m}(1-s) + V_2 \quad (63)$$

where $V_1(x)=\lambda\delta(x)$ and V_2 is the infinite well potential. The energies and wave-functions of the two subsystems are well known

$$E_1 = \frac{m_1\lambda^2}{2\hbar^2}, \quad \psi_1(x) = \begin{cases} \sqrt{k}e^{-kx} & x < 0 \\ \sqrt{k}e^{kx} & x > 0 \end{cases} \quad (64)$$

$$E_2 = \frac{\hbar^2}{2m_2} \left(\frac{\pi}{2a} \right)^2, \quad \psi_2(x) = \frac{1}{\sqrt{a}} \sin \left[\frac{\pi}{2a} (x+a) \right] \quad (65)$$

where

$$m_1 = m/|s| \quad (66)$$

$$m_2 = m/(1-s) \quad (67)$$

$$k = \sqrt{2mE/\hbar^2} \quad (68)$$

The KEP energy can be obtained by Eq. (60)

$$E_{\pm}^{KEP} = \frac{\left[\left(\frac{1}{s} - 2\eta^2 \right) E_1 + \left(\frac{1}{1-s} - 2\eta^2 \right) E_2 + \xi_1 + \xi_2 \right] \pm \sqrt{D}}{2(1-\eta^2)} \quad (69)$$

As shown in Fig. 4 the KEP solution is very close to the exact energy and the error for the KEP energy is less than 1%. These results demonstrate the utility of using the “negative” mass in quantum mechanics. Subsequently, the total wave-function can be formed by the two subsystem’s ground state wave-functions

$$\Psi = C_1\psi_1 + C_2\psi_2 \quad (70)$$

Normalizing Eq. (70), together with Eq. (33) we can solve the coefficient C_1 and C_2

$$C_1 = \sqrt{\frac{1}{\Delta_1^2 + 2\eta_{12}\Delta_1 + 1}} \quad (71)$$

$$C_2 = \Delta_1 C_1 = \pm \Delta_1 \sqrt{\frac{1}{\Delta_1^2 + 2\eta_{12}\Delta_1 + 1}} \quad (72)$$

where Δ_1 is

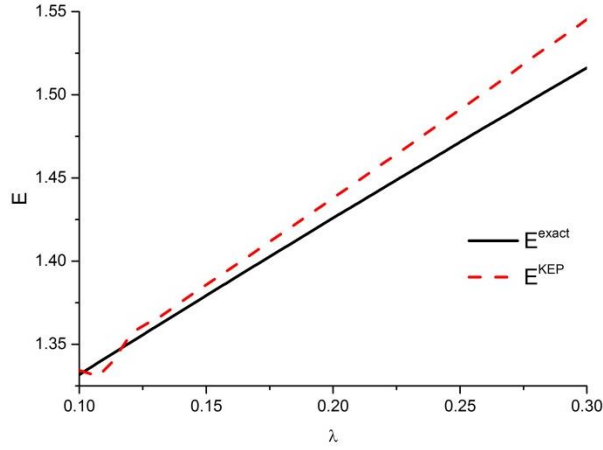


Fig. 4 The delta potential in 1D box energy solution: Comparison of the KEP and the exact results, by varying the parameter λ

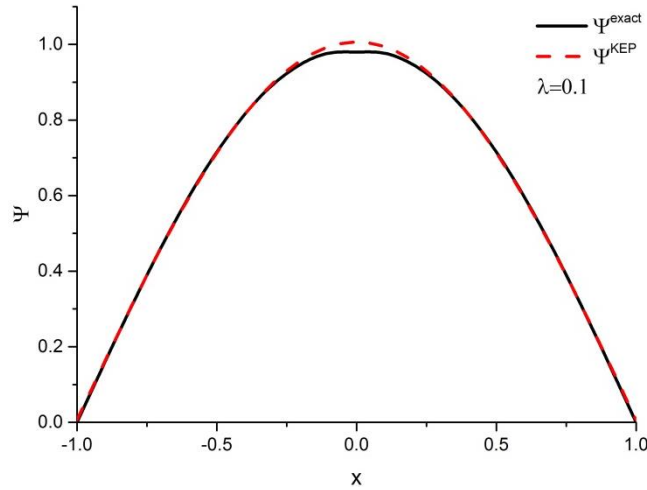


Fig. 5 The delta potential in 1D box wavefunction solution: Comparison of the KEP and the exact wavefunctions for $\lambda=0.1$ utilizing the dimensionless units as in Fig. 4

$$\Delta_1 \equiv -\frac{E_1 + \xi_{121} - E}{(E_1 + E_2 - E)\eta_{12}} \quad (73)$$

The KEP wave-function can then be rewritten as

$$\Psi = \sqrt{\frac{1}{\Delta_1^2 + 2\eta_{12}\Delta_1 + 1}} (\psi_1 + \Delta_1\psi_2) \quad (74)$$

In Fig. 5 the KEP wavefunction and the exact result are compared. In this case, no matter what is the value for the delta potential parameter λ , the KEP energy and wavefunction are precisely close to the exact solutions in which the wavefunction error is only 0.01%.

4. Conclusions

In summary, we demonstrate in this paper how to apply the KEP method to solving quantum eigenvalue problems with many delta potentials. For the cases studied in this paper, the KEP method obtains the energy and wavefunction precisely. It is an extremely useful idea that using the negative mass can cope with quantum problems with repulsive interactions. We are able to conclude that the KEP scheme to solve the quantum delta potentials is very successful. Admittedly, at the present time the negative mass has not been observed in the real world; however, the KEP method can apply to separated subsystems with Dirac delta potentials and yield accurate exact solutions with the help of negative mass terms.

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