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Determinable solutions for one-dimensional quantum potentials: scattering, quasi-bound and bound-state problems

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Abstract

We derive analytic expressions of the recursive solutions to Schrödinger's equation by means of a cutoff-potential technique for one-dimensional piecewise-constant potentials. These solutions provide a method for accurately determining the transmission probabilities as well as the wavefunction in both classically accessible regions and inaccessible regions for any barrier potentials. It is also shown that the energy eigenvalues and the wavefunctions of bound states can be obtained for potential-well structures by exploiting this method. Calculational results of illustrative examples are shown in order to verify this method for treating barrier and potential-well problems.

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1. Introduction

Quantum-mechanical tunnelling and quantum-well problems have attracted more interest, due to recent advances in the fabrication of semiconductor layers and the development of high-speed and novel devices [1]. In order to better understand the physical properties of a device, it is important that one can accurately solve and analyse the one-dimensional potential problems. A number of methods for solving Schrödinger's equation and for locating the bound states and resonances generated by one-dimensional potentials have been developed over the past decades [2–6]. Most of them are based on the so-called transfer-matrix approach. There are also some methods that are cumbersome to implement, for instance, the Monte Carlo method [7] and the finite element method (FEM) [8].

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In contrast to those numerical methods, a limited number of exact analytic solutions are available only for simple potential structures; analytic solutions are preferred due to its simple form and clear interpretation of the physics underlying the process. The WKB method, as an approximate analytic approach, has been widely used but it is restricted to slowly varying potential profiles that are continuous. Improved methods such as the modified conventional WKB (MWKB) [9] and the modified Airy functions (MAF) [10] still fail to provide perfect results.

Tikochinsky [11] has derived two nonlinear first-order equations replacing the second-order linear Schrödinger's equation in a cutoff-potential method for one-dimensional scattering amplitudes. In this paper, we solve these nonlinear first-order equations analytically and obtain recursive solutions of Schrödinger's equation for multi-step barrier potentials. We intend to find a method providing a general analysis of the one-dimensional problem for both classically accessible region and inaccessible region. In fact, arbitrarily accurate solutions including the scattering amplitudes and the wavefunctions are obtainable with these recursive solutions for any potential profile by dividing it into many segments, since any continuous potential problem can be recovered as the segments become finer and finer.

Using the recursive solutions, we will also determine the wavefunctions of quasi-bound and bound states. We can solve a potential-well problem by evenly uplifting the potential function restricted on the potential-well region and its surroundings to construct a resonant-barrier potential that can readily be handled as a model potential. The resonant-barrier potential constitutes a quasi-bound-state problem; therefore each sharp tunnelling resonance is locatable so that a quasi-bound-state eigenvalue can be determined which immediately leads to a bound-state eigenvalue being sought for the original potential well. Then, we can determine the eigenfunction belonging to the quasi-bound-state eigenvalue by means of the recursive solutions.

In section 2, we review the basic formalism for the one-dimensional problems that allows two nonlinear first-order equations to replace the linear second-order Schrödinger's equation. In section 3, we derive analytic expressions with recursive coefficients by solving the nonlinear equations for the transmission amplitudes, reflection amplitudes and the wavefunctions for piecewise-constant potentials. In section 4, a quasi-bound potential profile which characterizes a resonant tunnelling is considered as the model potential of a potential well in order to treat bound-state problems. In sections 5 and 6, we demonstrate the validity of the method by taking some examples, and discuss the calculational results.

2. Basic formalism

The one-dimensional Schrödinger equation for a particle with mass m incident upon a potential energy $U(z)$ that asymptotically vanishes can be written as

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k^2\right)\psi(x) = V(x)\psi(x), \tag{1}$$

where $x = z\sqrt{2m\epsilon/\hbar^2}$, $k^2 = K/\epsilon$ and $V(x) = U(z)/\epsilon$ with a certain unit energy ϵ chosen for convenience. Here, z is the position of the particle in the one-dimensional coordinate, K is the energy of the particle, and $\hbar = h/2\pi$, h being Planck's constant. Thus, the coordinate x, the wave number k and the potential $V(x)$ are all dimensionless. The dimensionless energy E is defined by

$$E = k^2. \tag{2}$$

Now, we introduce a cutoff potential that was used in [11–14]. The cutoff potential is defined by

$$V_c(y, x) = V(x)\theta(x - y), \tag{3}$$

where $\theta(x - y)$ is the step function. If $V(x)$ is replaced by the cutoff potential, equation (1) has the formal solution

$$\psi_E(y, x) = A\,\mathrm{e}^{\mathrm{i}kx} + \frac{1}{2\mathrm{i}k}\int \mathrm{e}^{\mathrm{i}k|x-x'|} V_c(y, x')\psi_E(y, x')\,\mathrm{d}x'. \tag{4}$$

Then, the cutoff-reflection and cutoff-transmission amplitudes for this problem can, respectively, be written as

$$R_E(y) = \frac{1}{2\mathrm{i}kA}\int \mathrm{e}^{\mathrm{i}kx'} V_c(y, x')\psi_E(y, x')\,\mathrm{d}x' \tag{5}$$

and

$$T_E(y) = 1 + \frac{1}{2\mathrm{i}kA}\int \mathrm{e}^{-\mathrm{i}kx'} V_c(y, x')\psi_E(y, x')\,\mathrm{d}x'. \tag{6}$$

In [11], it has been shown that the problem can be stated as two nonlinear first-order equations given by

$$\frac{\mathrm{d}R_E(y)}{\mathrm{d}y} = -\frac{1}{2\mathrm{i}k}V(y)[\mathrm{e}^{\mathrm{i}ky} + \mathrm{e}^{-\mathrm{i}ky}R_E(y)]^2 \tag{7}$$

and

$$\frac{\mathrm{d}T_E(y)}{\mathrm{d}y} = -\frac{\mathrm{e}^{-\mathrm{i}ky}}{2\mathrm{i}k}V(y)[\mathrm{e}^{\mathrm{i}ky} + \mathrm{e}^{-\mathrm{i}ky}R_E(y)]T_E(y), \tag{8}$$

with the boundary conditions, $R_E(\infty) = 0$ and $T_E(\infty) = 1$. Schrödinger's equation, which is a second-order differential equation, has been disassembled through the cutoff-potential manipulation into two first-order equations, equations (7) and (8). Integration of equation (8) immediately leads to

$$T_E(x) = \exp\left(\int_x^{\infty} \frac{\mathrm{e}^{-\mathrm{i}ky}}{2\mathrm{i}k}V(y)[\mathrm{e}^{\mathrm{i}ky} + \mathrm{e}^{-\mathrm{i}ky}R_E(y)]\,\mathrm{d}y\right). \tag{9}$$

The reflection amplitude R_E and the transmission amplitude T_E for the potential $V(x)$ are $R_E = R_E(-\infty)$ and $T_E = T_E(-\infty)$ in terms of which the reflection and transmission probabilities are, respectively, given as

$$P_R = |R_E|^2 \tag{10}$$

$$P_T = \frac{k_f}{k}|T_E|^2, \tag{11}$$

where $k_f = \sqrt{E - V(\infty)}$.

3. The piecewise-constant potential problem

We want to find analytic expressions of the transmission amplitude, reflection amplitude and the wavefunction for a multi-step potential profile which contains n layers of constant potential in the zero-potential environment, as shown in figure 1. Let us solve equation (7) for $R_E(x)$ in the jth-step region ($b_{j-1} < x < b_j$) for $V(x) = V_j \neq 0$, where V_j is a constant for $j = 1, \ldots, n$. By defining

$$Q_E(x) = R_E(x)\,\mathrm{e}^{-2\mathrm{i}kx} + 1 - \frac{2k^2}{V_j}. \tag{12}$$

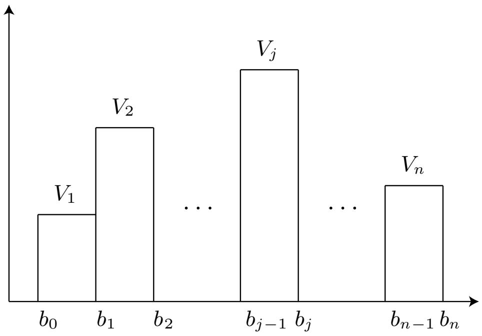

Figure 1. A multi-step potential profile consisting of n steps in the zero-potential environment.

Equation (7) can be rewritten as

$$\frac{\mathrm{d}Q_E(x)}{\mathrm{d}x} = \mathrm{i}\frac{V_j}{2k}\left[(Q_E(x))^2 + \left(\frac{4k^2}{V_j^2}(V_j - k^2)\right)\right] \tag{13}$$

to which the solution is

$$Q_E(x) = \mathrm{i}2k\frac{p_j}{V_j}\left(\frac{1 + A_j\,\mathrm{e}^{-2p_j x}}{1 - A_j\,\mathrm{e}^{-2p_j x}}\right), \tag{14}$$

with a constant A_j to be determined by a boundary condition. Here, p_j is defined by

$$p_j = \begin{cases} \sqrt{V_j - k^2} & \text{for} \quad V_j > k^2, \\ i\sqrt{k^2 - V_j} & \text{for} \quad V_j < k^2. \end{cases} \tag{15}$$

Then, we obtain the cutoff-reflection amplitude in the jth-step region:

$$R_E(x) = \left[\frac{2k^2}{V_j} - 1 + \mathrm{i}2k\frac{p_j}{V_j}\left(\frac{1 + A_j\,\mathrm{e}^{-2p_j x}}{1 - A_j\,\mathrm{e}^{-2p_j x}}\right)\right]\mathrm{e}^{2\mathrm{i}kx}. \tag{16}$$

On the other hand, the solution of equation (7) for $V_j = 0$ in the jth-step region is

$$R_E(x) = C_j, \tag{17}$$

which can be determined by the continuity condition of $R_E(x)$ at the boundary $x = b_j$.

If $V_{j+1} = 0$, $R_E(x) = C_{j+1}$ in the region $b_j < x < b_{j+1}$, the continuity of $R_E(x)$ at the boundary $x = b_j$ leads to

$$A_j = \left(\frac{V_j(C_{j+1}\,\mathrm{e}^{-2\mathrm{i}kb_j} + 1) - 2k^2 - \mathrm{i}2kp_j}{V_j(C_{j+1}\,\mathrm{e}^{-2\mathrm{i}kb_j} + 1) - 2k^2 + \mathrm{i}2kp_j}\right)\mathrm{e}^{2p_j b_j}. \tag{18}$$

But, if $V_{j+1} \neq 0$, the boundary condition gives

$$A_j = \left(\frac{D_j - V_{j+1}p_j + \mathrm{i}k(V_{j+1} - V_j)}{D_j + V_{j+1}p_j + \mathrm{i}k(V_{j+1} - V_j)}\right)\mathrm{e}^{2p_j b_j}, \tag{19}$$

where

$$D_j = V_j p_{j+1}\left(\frac{1 + A_{j+1}\,\mathrm{e}^{-2p_{j+1}b_j}}{1 - A_{j+1}\,\mathrm{e}^{-2p_{j+1}b_j}}\right). \tag{20}$$

Let us take the index $j = n + 1$ for the region $x > b_n$. Since $V_{n+1} = 0$ and $p_{n+1} = \mathrm{i}k$, we obtain $A_{n+1} = 0$ from (18). A_j is related to A_{j+1} through equation (19) if $V_{j+1} \neq 0$, while it is related to the constant reflection amplitude C_{j+1} through equation (18) if $V_{j+1} = 0$. Therefore, all A_js for $j = 1, \ldots, n$ can be determined recursively from the starting value $A_{n+1} = 0$.

The cutoff transmission amplitude $T_E(x)$ can be obtained in the jth-step region $(b_{j-1} < x < b_j)$ from equation (9) by the help of (16):

$$T_E(x) = T_E(b_j)\exp[(p_j - \mathrm{i}k)(b_j - x)]\left(\frac{1 - A_j\,\mathrm{e}^{-2p_jb_j}}{1 - A_j\,\mathrm{e}^{-2p_jx}}\right), \tag{21}$$

where

$$T_E(b_j) = \prod_{l=j+1}^{n}\exp[(p_l - \mathrm{i}k)(b_l - b_{l-1})]\left(\frac{1 - A_l\,\mathrm{e}^{-2p_lb_l}}{1 - A_l\,\mathrm{e}^{-2p_lb_{l-1}}}\right). \tag{22}$$

Therefore, the analytic expression of the transmission amplitude is

$$T_E = T_E(-\infty) = \prod_{l=1}^{n}\exp[(p_l - \mathrm{i}k)(b_l - b_{l-1})]\left(\frac{1 - A_l\,\mathrm{e}^{-2p_lb_l}}{1 - A_l\,\mathrm{e}^{-2p_lb_{l-1}}}\right). \tag{23}$$

From equations (4) and (5)

$$\psi_E(y, y) = A[\mathrm{e}^{\mathrm{i}ky} + \mathrm{e}^{-\mathrm{i}ky}R_E(y)] \tag{24}$$

and by differentiating equation (4) in the region $y < x$ one has the relation

$$\frac{\partial\psi_E(y, x)}{\partial y} = -\frac{\mathrm{e}^{-\mathrm{i}ky}V(y)}{2\mathrm{i}k}\psi_E(y, y)\,\mathrm{e}^{\mathrm{i}kx} + \frac{1}{2\mathrm{i}k}\int \mathrm{e}^{\mathrm{i}k|x-x'|}V_c(y, x')\frac{\partial\psi_E(y, x')}{\partial y}\,\mathrm{d}x'. \tag{25}$$

Equations (4) and (25) both are the solutions of equation (1) with the cutoff potential $V_c(y, x)$ but have different amplitudes. Their amplitudes differ by a factor $-\mathrm{e}^{-\mathrm{i}ky}V(y)\psi_E(y, y)/2\mathrm{i}kA$, thus in the region $y < x$,

$$\frac{\partial\psi_E(y, x)}{\partial y} = -\frac{\mathrm{e}^{-\mathrm{i}ky}V(y)}{2\mathrm{i}k}[\mathrm{e}^{\mathrm{i}ky} + \mathrm{e}^{-\mathrm{i}ky}R_E(y)]\psi_E(y, x). \tag{26}$$

Integration of equation (26) in the region $y < x$ leads to

$$\begin{aligned}\frac{\psi_E(x, x)}{\psi_E(x)} &= \frac{\psi_E(x, x)}{\psi_E(-\infty, x)} \\ &= \exp\left(-\int_{-\infty}^{x}\frac{\mathrm{e}^{-\mathrm{i}ky}}{2\mathrm{i}k}V(y)[\mathrm{e}^{\mathrm{i}ky} + \mathrm{e}^{-\mathrm{i}ky}R_E(y)]\,\mathrm{d}y\right),\end{aligned} \tag{27}$$

which can be rewritten, with the aid of equation (9), as

$$\psi_E(x) = A\frac{T_E}{T_E(x)}[\mathrm{e}^{\mathrm{i}kx} + \mathrm{e}^{-\mathrm{i}kx}R_E(x)]. \tag{28}$$

One can imagine the insertion of an infinitesimally thin virtual layer of zero potential at x, and consider the wavefunction $\psi_E(x)$ to be the superposition of the forward travelling wave $\mathrm{e}^{\mathrm{i}kx}$ and the backward travelling wave $R_E(x)\,\mathrm{e}^{-\mathrm{i}kx}$ reflected upon the potential on the right side of the virtual layer, multiplied by the factor $AT_E/T_E(x)$ which is fathomable to be the correct amplitude for the superposed wavefunction at x.

Substituting (21) and (23) into equation (28), we write the wavefunction for the energy E in the jth layer $(b_{j-1} < x < b_j)$ as

$$\begin{aligned}\psi_{jE}(x) = A\prod_{l=1}^{j}&\exp[(p_l - \mathrm{i}k)(b_l - b_{l-1})]\left(\frac{1 - A_l\,\mathrm{e}^{-2p_lb_l}}{1 - A_l\,\mathrm{e}^{-2p_lb_{l-1}}}\right) \\ &\times\exp[(p_j - \mathrm{i}k)(x - b_j)]\left(\frac{1 - A_j\,\mathrm{e}^{-2p_jx}}{1 - A_j\,\mathrm{e}^{-2p_jb_j}}\right)[\mathrm{e}^{\mathrm{i}kx} + \mathrm{e}^{-\mathrm{i}kx}R_E(x)]\end{aligned}$$

$$= A \prod_{l=1}^{j} \exp[(p_l - \mathrm{i}k)(b_l - b_{l-1})] \left(\frac{1 - A_l\, \mathrm{e}^{-2p_l b_l}}{1 - A_l\, \mathrm{e}^{-2p_l b_{l-1}}} \right)$$
$$\times \frac{2\mathrm{i}k \exp[(\mathrm{i}k - p_j)b_j]}{V_j[1 - A_j \exp(-2p_j b_j)]}[(-\mathrm{i}k + p_j)\,\mathrm{e}^{p_j x} + A_j(\mathrm{i}k + p_j)\,\mathrm{e}^{-p_j x}]. \qquad (29)$$

Equation (29) is an analytic expression for the recursive solution of the Schrödinger equation. It is simple and fast to calculate A_js for any multi-step potential. Also, any continuous potential problem may be considered to be a multi-step potential problem by dividing the non-zero potential region into a lot of small segments such that the potential in each segment can be approximated to a specific value, for instance, the average value of the continuous potential within the segment. Thus, the analytic expression of the wavefunction given by equation (29) can be used for obtaining an arbitrarily accurate solution for any one-dimensional potential.

In passing, let us check that equation (29) is consistent with the travelling plane waves which are expected in the regions $x < b_0$ and $x > b_n$, where $V(x) = 0$. Without loss of generality, one may take the first-step region ($b_0 < x < b_1$) such that $V_1 = 0$. Then, the wavefunction in the region $x < b_1$ becomes

$$\psi_{1E}(x) = \lim_{V_1 \to 0} A(\mathrm{e}^{\mathrm{i}kx} + \mathrm{e}^{-\mathrm{i}kx} R_E(x)) \exp[(p_1 - \mathrm{i}k)(x - b_0)] \frac{1 - A_1 \mathrm{e}^{-2p_1 x}}{1 - A_1 \mathrm{e}^{-2p_1 b_0}}$$
$$= A[\mathrm{e}^{\mathrm{i}kx} + R_E\, \mathrm{e}^{-\mathrm{i}kx}], \qquad (30)$$

since $A_1 = -(V_1/4k^2)R_E$ from equation (16) for the limit $V_1 \to 0$. On the other hand, if we take the last-step region $b_{n-1} < x < b_n$ such that $V(x) = V_n = 0$, the wavefunction in the region $x > b_{n-1}$ becomes

$$\psi_{nE}(x) = A T_E\, \mathrm{e}^{\mathrm{i}kx}, \qquad (31)$$

since $R_E(x) = 0$ and $A_n = -(V_n/4k^2)R_E(x)$ from equations (16) and (23) in the limit $V_n \to 0$. Equations (30) and (31) show that equation (29) is consistent as the solution of equation (1) in the zero-potential region.

4. Quasi-bound states

We consider a resonant-barrier structure that consists of n layers of piecewise-constant potential. Resonances are supposed to occur at energies less than both V_1 and V_n which are potential values of the end steps so that quasi-bound states are involved. The wavefunction $\psi_{jE}(x)$ in the jth layer for this structure can be obtained with the calculated A_js which are dependent on E. A_n, in the last layer, can be evaluated from (18) with the cutoff-reflection amplitude $C_{n+1} = 0$. Inserting the evaluated A_n into (29), we find in the last layer for $E < V_n$,

$$\psi_{nE}(x) \propto (-\mathrm{i}k + p_n)\,\mathrm{e}^{p_n x} + \frac{V_n - 2k^2 - 2\mathrm{i}kp_n}{V_n - 2k^2 + 2\mathrm{i}kp_n}(\mathrm{i}k + p_n)\,\mathrm{e}^{p_n(2b_n - x)}, \qquad (32)$$

where the first term exponentially increases with increasing x, while the second term exponentially decreases. One can see that if $p_n(b_n - b_{n-1})$ is large enough, the first term is negligible in magnitude compared with the second term, so the wavefunction exponentially damps with increasing x in the region $b_{n-1} < x < b_n$.

Now, let us consider the wavefunction in the first layer which is given from (29) by

$$\psi_{1E}(x) = A \frac{2\mathrm{i}k\, \mathrm{e}^{\mathrm{i}kb_0}}{V_1(\mathrm{e}^{p_1 b_0} - A_1 \mathrm{e}^{-p_1 b_0})}[(-\mathrm{i}k + p_1)\,\mathrm{e}^{p_1 x} + (\mathrm{i}k + p_1)A_1 \mathrm{e}^{-p_1 x}], \qquad (33)$$

where A_1 is obtained through the step potential profile of the resonant-barrier structure. The wavefunction given by equation (33) exponentially increases with increasing x when $|A_1| = 0$;

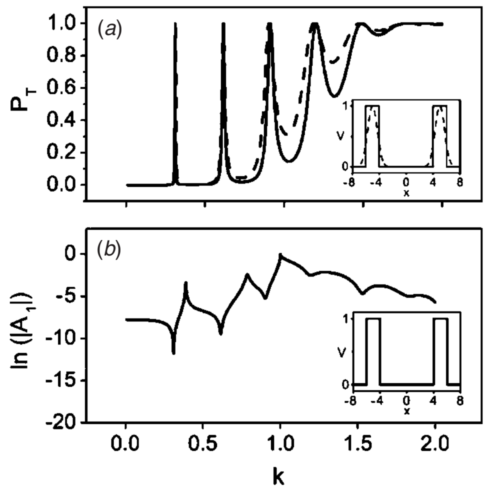

Figure 2. (a) Transmission probabilities of double-barrier potentials: the solid line and the dashed line are for the square and the Gaussian double-barrier potential, respectively. Their potential profiles are shown in the inset graph. (b) The curve of $\ln(|A_1|)$ for the double square-barrier potential. Its profile is in the inset graph. Each dip of the $\ln(|A_1|)$ curve below the barrier exactly agrees with the resonant peak of transmission probability shown in (a).

A_1 vanishes at the energies of quasi-bound states. $|A_1| = 0$ may be used as the quantization condition for the energy levels of a particle confined in a potential well. In the practical calculations, transmission resonances occur at the energies where $|A_1|$ takes a minimum value in a sudden dip, if $b_1 - b_0$ and $b_n - b_{n-1}$ are large enough. Such resonances indicate quasi-bound states.

Now, a potential well can be treated by uplifting the potential function restricted on the region of the well and its surroundings to form a resonant-barrier structure that can be handled in our approach. This resonant structure is used as a model potential of the potential well under consideration. Then, each resonance occurred in this model-potential problem corresponds to an energy eigenvalue for the potential well, and the real part or the imaginary part of the quasi-bound-state function obtained for a resonant energy is the eigenfunction of the bound state belonging to the corresponding eigenvalue for the potential well within a normalization constant.

5. Some examples

In order to demonstrate the validity of our method, we consider quantum barriers and quantum-well potentials. Here, we examine the derived recursive expressions of the transmission amplitude and the state wavefunction given by equations (23) and (29), respectively, by calculating A_js for several potentials.

First, we consider rectangular and Gaussian double-barrier potentials which are shown in the inset of figure 2(a). Here, the unit energy ϵ is chosen to be the maximum potential energy of the barrier. Since the rectangular double-barrier structure consists of three layers of constant potential, the analytic expression of the recursive solution $\psi_{jE}(x)$ for this structure can be obtained with calculated A_js which are dependent on E. One can determine A_3 from equation (18) with the cutoff-reflection amplitude $C_4 = R_E(x) = 0$ in the region $x > b_3$,

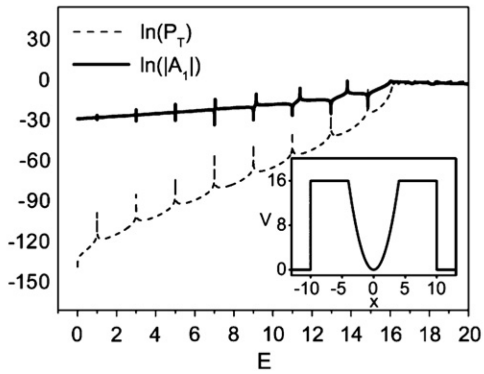

Figure 3. Resonances for a model potential of harmonic oscillator given by equation (34). Each sharp dips on the solid line of the curve $\ln(|A_1|)$ exactly agrees with a resonant peak on the dashed line of the curve $\ln(P_T)$.

and determine C_2 for the step region of $j = 2$, where $V_2 = 0$ by evaluating $R_E(x)$ at $x = b_2$ in the step region of $j = 3$ through equation (16). Then, A_1 can also be obtained through equation (18) using the value of C_2. Figure 2(*b*) shows the curve of $\ln(|A_1|)$ for the rectangular double-barrier structure. Each dip of the curve coincides with a transmission resonance for the energy below the barrier ($k < 1$) as shown in figure 2. Such a sharp dip of A_1 indicates that an exponentially increasing term of the wavefunction is dominant in the first barrier region due to a negligibly small $|A_1|$ as was considered below equation (33), so that the transmission probability becomes large in the narrow energy region. The resultant transmission probabilities for the two barrier profiles have similar resonance patterns as shown in figure 2(*a*). We have confirmed that the solid line for the rectangular double barrier perfectly agrees with the result obtained by the traditional method for solving Schrödinger's equation for step potential problems with boundary conditions imposed.

Next, we consider a potential model by which one can obtain eigenvalues and eigenfunctions for a harmonic oscillator. We take the unit energy to be $\epsilon = \hbar\omega/2$, where ω is the characteristic angular frequency of the harmonic oscillator. Then, the dimensionless potential in equation (1) is $V_{\text{ho}} = x^2$ for the harmonic oscillator. In order to apply our method to the harmonic oscillator in an energy range $0 < E < 16$, we employ a model potential

$$V_{\text{HO}}(x) = \begin{cases} x^2 & \text{for} \quad |x| < 4 \\ 16 & \text{for} \quad 4 < |x| < 10 \\ 0 & \text{for} \quad |x| > 10, \end{cases} \tag{34}$$

as shown in the inset of figure 3. This model has a double-barrier structure and represents a quasi-bound problem in which the transmission of a particle through the model potential reaches its peak when the energy is resonant with one of the energy levels of the quasi-bound states in the region between the two potential barriers. The potential in equation (34) is expected to involve low quasi-bound-state energies that approximately equal the bound-state energies of the harmonic oscillator, respectively. Each sharp dip of $\ln(|A_1|)$ suppresses the term exponentially decreasing with increasing x in the wavefunction in equation (29) allowing the exponentially increasing term to be dominant in the first barrier, and thus occurs at the same energy as a resonance peak which locates a quasi-bound state, as shown in figure 3. Energies of the quasi-bound states have been determined very accurately to fit in the exact eigenvalues of the harmonic oscillator $E_n = 2n + 1$ with $n = 0, 1, 2, \ldots$ for the low-lying

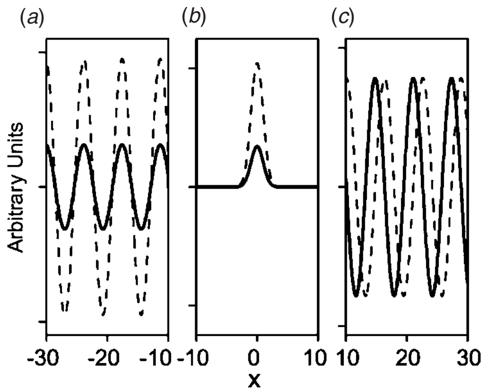

Figure 4. The wavefunction of the lowest quasi-bound state ($E = 1.0$) for the potential given by equation (34) for three regions with different units. The solid line and dashed line are the real and imaginary parts of the wavefunction, respectively.

states. However, there are very small errors for the upper levels, for instance, $n = 5, 6, 7$, because the model potential in equation (34) is different from the potential of the harmonic oscillator for the region $|x| > 4$.

Once a quasi-bound-state eigenvalue is determined, the wavefunction of the state can be obtained from equation (29). The lowest quasi-bound state for the model potential in equation (34) corresponds to the ground state for the harmonic oscillator. The wavefunction of the state is separately shown in figure 4 for the regions, $-30 < x < -10$, $-10 < x < 10$ and $10 < x < 30$ with different units. The solid and dashed lines are, respectively, the real and imaginary parts of the wavefunction. The forward and reflected plane waves are superposed in the region $x < -10$, and only the transmitted forward plane-wave propagates in the region $x > 10$. One can see in figure 4(*b*) that the wavefunction exponentially increases with increasing x in the first barrier region at the resonance energy but exponentially decreases in the second barrier region which is sufficiently wide as explained earlier, forming the lowest quasi-bound-state wavefunction in the binding potential region between the two barriers. Wavefunctions of the next three quasi-bound states for the same model potential that correspond to the three lowest excited states in the harmonic-oscillator problem are also shown in figure 5. Either the real part or the imaginary part of a quasi-bound-state wavefunction can be taken as the wavefunction of the corresponding bound state for the harmonic oscillator.

For our final example, we consider a symmetric double-well potential given by

$$V_{\mathrm{dw}}(x) = \begin{cases} x^2(x^2 - 16) & \text{for} \quad |x| < 4, \\ 0 & \text{for} \quad |x| > 4. \end{cases} \tag{35}$$

For treating this problem with our methods, we take a model potential of V_{dw} by uplifting the potential function on the region $|x| < 6$ by 64:

$$V_{\mathrm{DW}}(x) = \begin{cases} x^2(x^2 - 16) + 64 & \text{for} \quad |x| < 4, \\ 64 & \text{for} \quad 4 < |x| < 6, \\ 0 & \text{for} \quad |x| > 6, \end{cases} \tag{36}$$

which is shown in the inset of figure 6(*a*). The local maximum of the model potential located at $x = 0$ is 64, and the two local minima are located at $x = 2\sqrt{2}$. The calculated curve for $\ln P_T$ is plotted in figure 6(*a*). As is well known, each peak comprises a pair of states, an even state and an odd state, whose energies are the very same especially for a peak of lower

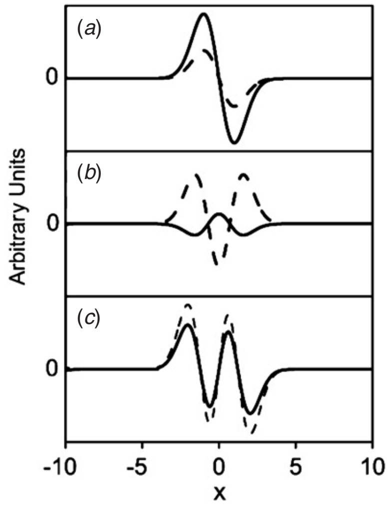

Figure 5. The wavefunctions of three quasi-bound states of energies, (*a*) $E = 3.0$, (*b*) $E = 5.0$ and (*c*) $E = 7.0$, for the potential given by equation (34). The solid lines and dashed lines are the real and imaginary parts of the wavefunctions, respectively.

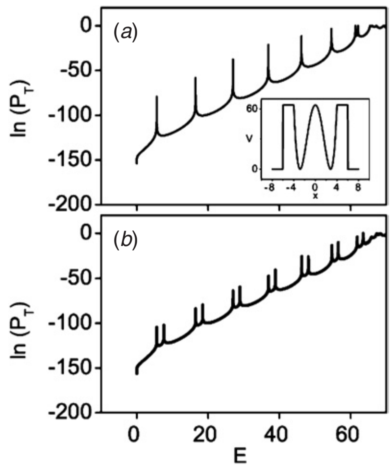

Figure 6. Logarithmic transmission probabilities for double-well model potentials given by (*a*) equation (36) and (*b*) equation (37). Each peak represents transmission resonance.

energy. But they are not perfectly degenerate, since a particle in one potential well can tunnel into the other well through the middle barrier which is finite. The energy difference of two states comprised in a peak increases with increasing energy, and thus the seventh pair of states which is just below the barrier appears to be separated.

In order to confirm that two states are comprised in a peak, we add a small asymmetric potential function to the potential in equation (36):

$$V'_{\mathrm{DW}}(x) = V_{\mathrm{DW}}(x) + V'(x) = V_{\mathrm{DW}}(x) + \tanh x + 1. \qquad (37)$$

Using this potential, we obtain a curve of $\ln|P_T|$ in which there are seven pairs of quasi-bound states as shown in figure 6(*b*). Each pair is split into two peaks due to the perturbing

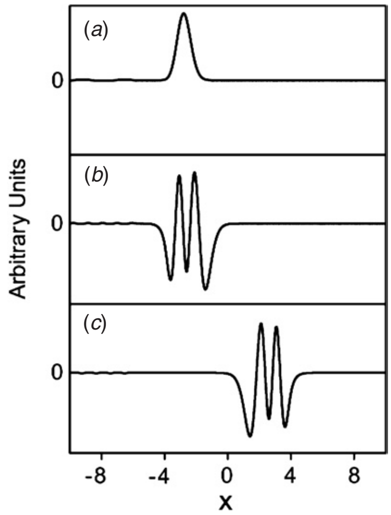

Figure 7. The wavefunctions of three bound states for the double-well potential, $V(x) = x^2(x^2 - 16) + \tanh x$; ($a$) the ground state, ($b$) the eighth excited state, and (c) the ninth excited state. These wavefunctions have been obtained by using the model potential given by equation (37) as explained in the text.

potential $V'(x)$ from a peak containing two states for the double-well potential V_{DW} shown in figure 6(a). The lower and higher states in each pair are expected to be confined in the left well and the right well, respectively.

In order to find bound-state wavefunctions for the double-well potential given as $V(x) = x^2(x^2 - 16) + \tanh x$, one may take either the real parts or imaginary parts of quasi-bound-state wavefunctions determined from equation (29) for an appropriate model potential such as equation (37). The real parts (or imaginary parts) can be considered as the bound-state eigenfunctions within a normalization constant. Real parts of the wavefunction of the lowest ($n = 0$), the ninth ($n = 8$), and the tenth ($n = 9$) quasi-bound states, which are taken to be the wavefunctions of corresponding bound states, are plotted in figures 7(a), (b) and (c), respectively. Figure 7 shows that the particle which occupies the lowest state or the ninth state stays in the left potential well, while the particle occupying the tenth state stays in the right potential well, as expected.

6. Discussions and conclusion

Analytically solving two nonlinear first-order differential equations equivalent to Schrödinger's equation, we have obtained the recursive solutions of the cutoff-reflection amplitude $R_E(x)$, the cutoff transmission amplitude $T_E(x)$ and the state wavefunction $\psi_E(x)$ for a multi-step potential. One can use the recursive solutions in equations (23) and (29) for any piecewise-constant potential to obtain transmission amplitudes and eigenfunctions, respectively. If an approximate multi-step potential consisting of sufficiently many layers is substituted for a smooth potential profile, calculations with the recursive solutions are accurate and fast.

For treating a potential well, we take a model potential with two side barriers, which contains a partial profile identical to the profile of the potential well in the region between the side barriers. In the model potential problem, resonance occurs at the energy of a quasi-bound state, so the energies can be determined by locating the transmission resonances. Once a quasi-bound-state energy is known, the eigenfunction for the energy can also be determined. However, the real and the imaginary parts of the wavefunction of a quasi-bound state exponentially increase at a same rate in the first barrier and exponentially decrease in the last barrier as explained earlier, and are the same within a factor $\tan\phi$ in the region between two side barriers, ϕ being a phase angle. Therefore, either the real or the imaginary part can be taken for the wavefunction of the corresponding bound state with a normalization constant.

We have considered several examples to demonstrate the validity of our method with the recursive solutions. First, we have calculated the transmission probabilities of a particle incident upon a rectangular and a Gaussian double-barrier potentials which show typical features of resonant tunnelling in figure 2(*a*). The rectangular double barrier simply consists of three layers, the left barrier being the first potential step, and the feature of resonant tunnelling can be explained by the calculational results of A_1 in which information of the barrier structure is included. If $A_1 = 0$ for an energy lower than the barriers, the wavefunction does not contain exponentially decreasing term with increasing x in the first barrier region so that it exponentially increases in the region, and thus the transmission probability reaches maximum at the energy. Practically, the sharp dips of the $\ln|A_1|$ curve in figure 2(*b*) represent the resonances associated with quasi-bound states in the rectangular well between the barriers.

The harmonic-oscillator problem can be dealt with by solving a quasi-bound-state problem with the model potential given by equation (34). The calculational results for $\ln|A_1|$ and $\ln P_T$ are shown in figure 3, so the quasi-bound-state energies which may be regarded as the energy eigenvalues of the harmonic oscillator can readily be determined by locating the resonance peaks of $\ln P_T$ or the sharp dips of $\ln|A_1|$. The resultant peaks perfectly agree with the exact eigenvalues for low energy states, but deviate a little from the exact values for high energy states; $E_0 = 1.000$, $E_1 = 3.000$, $E_2 = 5.000$, $E_3 = 6.9999$ $E_4 = 8.999$, $E_5 = 10.994$, $E_6 = 12.970$, and $E_7 = 14.857$. Since the deviation originates from the approximated model potential which does not agree with the harmonic-oscillator potential on the high potential region $|x| > 4$, one may get more accurate eigenvalues for higher states by using a larger model potential which coincides with the harmonic-oscillator potential in a wider region.

We have applied our method to a symmetric double-well potential given by equation (35), using equation (36) as its model potential. It is well known that an even state and an odd state are folded together belonging closely to an eigenvalue if they are deeply bound in a symmetric double well whose middle barrier is strong enough so that the wavefunctions nearly vanish in the barrier region. The even and odd states belonging to the same eigenvalue can be combined to constitute two bound states that are localized in the left well and right well with the same eigenvalue, respectively. Thus, one may consider each resonance peak to correspond to a pair of states confined in one and the other well, as well as a pair of even and odd states. When an asymmetric perturbing potential is added to the double-well potential, each resonance peak has been split into two peaks, as shown in figure 6(*b*). Since the potential is not symmetric due to the perturbation, even and odd states cannot be sustained. Therefore, each resonance peak in figure 6(*b*) represents a state confined in one of the two wells. As expected, figure 7 shows that among the two states separated from each other due to the perturbation, the lower energy state is confined in the left well which is a little deeper than the right well, while the higher energy state is confined in the right-well region. The ninth ($n = 8$) and tenth ($n = 9$) states are the fifth states in the left well and the right well, respectively, so the numbers of nodes in their wavefunctions are identically four as in figure 7(*b*) and (*c*).

Here, more accurate determination of quasi-bound-state energies is required to obtain eigenfunctions of the lower quasi-bound state confined in the right well, because the resonance is sharper for the particle tunnelling into a deeper quasi-bound state or a state confined in the right well through the stronger barrier or two barriers (the first barrier and the middle barrier); for instance, the determined eigenvalues $E_0 = 5.601849104$, $E_1 = 7.583\,423\,678\,569\,52$, $E_8 = 46.290\,706$ and $E_9 = 48.153\,853\,6$ should be used in obtaining the wavefunctions, where E_1 is required to be the most accurate. Here, each bound-state energy for $V(x) = x^2(x^2 - 16) + \tanh x$ is the corresponding quasi-bound-state energy for $V'_{\rm DW}$ minus 65. Unlike the model potential of the harmonic oscillator, no approximation is involved in the calculation with the model potential of this double-well potential.

Although here we have presented results for double barriers, a harmonic-oscillator, and double-well potentials, the analysis can easily be applied for accurate calculations to general potential barrier and quantum-well structures. The analysis could be extended to the one-dimensional problem of a particle that has a coordinate-dependent mass, by imposing the boundary conditions on the step potential structure. In addition, the three-dimensional Schrödinger equation for a spherically symmetric potential can also be solved using the present method because such a three-dimensional problem can be reduced to a one-dimensional problem.

In conclusion, we have described a method for solving the one-dimensional Schrödinger equation by means of the analytic expressions of recursive solutions derived for piecewise-constant potentials. The recursive solutions provide a general analysis of one-dimensional scattering, quasi-bound and bound-state problems. We have demonstrated the validity of the method by taking some examples to show consistent and predictable calculational results. The calculations with the recursive solutions were rapid and accurate even for smoothly varying potentials.

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