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Calculation of energy spectrum and eigenstates of 1D time-independent short-range potentials

Y. Ashkenazy^{a,b,*}, L.P. Horwitz^{c,d}

^a*Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel*

^b*Center for Polymer Studies and Department of Physics, Boston University, Boston, MA 02215, USA*

^c*Institute for Advanced Study, Princeton, NJ, 08540, USA*

^d*Raymond and Beverly Sackler Faculty of Exact Sciences School of Physics, Tel Aviv University, Ramat Aviv 69978, Israel*

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Abstract

We show that it is possible to approximate 1D time-independent short-range potentials by a sum of δ function potentials. By the use of transfer matrix techniques it is possible to calculate the total transfer matrix as well as the S matrix which connects the incoming waves to the outgoing waves. The transmission coefficient and the resonance states can be evaluated by the δ function approximation. Using the same approach in potential wells, the energy spectrum, as well as the eigenfunctions of the well, can be constructed. We examine the approximation, successfully, on two well-known potentials, the square-well and the harmonic oscillator. © 2001 Published by Elsevier Science B.V.

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1. Introduction

The numerical calculation of the time-independent Schrödinger equation has been of interest since the early days of quantum mechanics [1]. There are few models which have exact analytical solution and for this reason, methods such as time-independent perturbation theory were developed [1]. However, nowadays computer capability is

* Corresponding author.

E-mail address: ashkenaz@argento.bu.edu (Y. Ashkenazy).

very high, and it is possible to use them for many complicated tasks as well as simple assignments such as the integration of the Schrödinger equation [2–8]. The major aim of the present study is to give a simple, easy to use, tool which can be implemented for arbitrary potentials (with or without analytic definition). We confine ourselves to one-dimensional, real, short-range potentials, although the method can be extended to higher dimensions.

The one-dimensional time-independent Schrödinger equation can be written as

$$H|n\rangle = (H_0 + V)|n\rangle = E|n\rangle, \quad (1)$$

where

$$H_0 = p^2/2m + V_0 \quad (2)$$

has well-known solutions. V_0 usually chosen (if possible) such that the effect of V is small compared to V_0 . The basic numerical approach of solving Eq. (1), is to calculate the matrix elements of the operator H using the known eigenstates of H_0 (denoted as $|n_0\rangle$). A diagonalization of the matrix $H_{n_0 m_0}$ leads to the spectrum and the eigenstates of the Hamiltonian H . One has to diagonalize an $n \times n$ matrix where $n \rightarrow \infty$ [1]. However, usually just part of the spectrum is required and it is possible to increase the matrix dimension until the desired convergence of the needed levels is achieved. This method is applicable for spatially bounded potentials.

Other numerical methods are the iterative methods which require repeated numerical integrations of the Schrödinger equation, accompanied by adjustments of energy eigenvalues. Usually, an eigenvalue is estimated initially, and then the corresponding eigenfunction is computed by numerical integration. This eigenfunction enables one to improve the choice of the eigenvalue for the next iteration and so on.

Some new techniques use a general algorithm of the time-dependent Schrödinger equation in order to calculate the energy spectrum of the time-independent Hamiltonian [2–8]. Starting from a localized wave packet which evolves with time, the time correlation between the initial state and the later state, $\langle\psi(0)|\psi(t)\rangle$ can be calculated. The Fourier transform of the correlation function shows sharp peaks at the eigenvalue locations [2]. In other studies, it was shown that it is better to use the Chebyshev series for this propose [3,4]. All the above techniques use the fast Fourier transform (FFT) algorithm, which assumes periodic boundary conditions. Later it was shown that one can use different grid spacings which are changed according to the complexity of the motion, a procedure which can speed up the numerical calculation [5].

For spatially unbounded or semi-bounded potentials, the energy spectrum may be continuous, and the relations between the incoming and outgoing waves have to be carefully investigated. A basic assumption in scattering theory is that the potential is limited in space, and that far from the influence of the potential, the wave function behaves like a free wave [9]. In three dimensions the scheme is as follows: a plane wave collides with the potential and is then scattered to all space; the

scattered wave is a spherical wave, and the scattering amplitude for solid angle is calculated. For potentials with spherical symmetry phase shifts can be defined; they depend only on ℓ , the angular momentum, and the energy E [9]. Numerical integration of such a situation is usually done by expanding the outgoing wave into a Born series. The more elements which are considered the more accurate the result is.

In one-dimensional systems there are just two directions, left and right. The relation between incident (incoming waves) and reflected waves (outgoing waves) gives the S matrix [1]. The essential quantities are the transmission coefficient and the reflection coefficient. There are several numerical approaches for finding those coefficients. First, one can embed a localized potential in an infinite well (with or without periodic boundary conditions). If the well is wide enough the level spacing is small and, from a practical point of view, the spectrum can be considered as a continuum. The transmission coefficient of the localized wave packet which collides with the potential is similar to that of an infinite system. However, there are a few difficulties using such a method. Since one starts from a wave packet, a range of energy levels are involved, and one cannot know exactly the transmission and reflection coefficients of specific energy. In order to improve the calculation it is necessary to start from a wider wave packet which is more localized in the momentum space, a fact which requires additional computer operations. Additionally, since the space is confined, after a certain time interference between reflected and transmitted waves may occur. For this reason, an absorption potential should be added in the boundaries and the flux through it should be calculated [3,6]. In order to speed up the numerical calculation one can use the FFT which assumes periodic boundary conditions.

In contrast to the above-mentioned methods we will not use the dynamical evolution of the wave packet in order to find the energy spectrum or the transmission probability. Our approach is based on the fact that the situation is stationary; a steady incident current collides with the potential and a stationary flux emerges to the left and to the right. The energy of the incident particle is well defined. Far from the potential range the particle behaves as a free particle. We approximate the potential as a sum of δ function potentials. A transfer matrix from one side of each δ potential to other side of the potential can be calculated; the product of all those transfer matrices yields the total transfer matrix. Then, the S matrix can be obtained (the S matrix is the essential property of the solution of the problem). This idea can be extended to time periodic potentials, as will be discussed elsewhere [10].

Although we focus in this paper on one-dimensional spatially bounded potentials, this approach can be used in three-dimensional potentials which have spherical symmetry. In this case the one-dimensional Schrödinger equation can be written for the r coordinate, and can be dealt with by the present approach.

2. Method

The basic idea of this study is the approximation of a potential as a sum of δ function potentials

$$V(x) = \sum_{n=0}^N V(x_n)\delta(x - x_n)\Delta x, \tag{3}$$

where $\Delta x = (b - a)/N$ and the range $x = [a, b]$ is the effective range of the potential (see Fig. 1 for an illustration). It is clear that when $N \rightarrow \infty$ the area under the potential $V(x)$ is equal to the area under the approximated potential (3). The Fourier transform of Eq. (3)

$$\int V(x)e^{ikx} dx = \sum V(x_n) \left[\int e^{ikx} \delta(x - x_n) dx \right] \Delta x = \sum V(x_n)e^{ikx_n} \Delta x \tag{4}$$

is another justification for the use of Eq. (3).

2.1. One-dimensional scattering

In the approximation (3), one can assume that the wave function between two consecutive δ potentials in (3) is a free-particle wave function,

$$\psi_n(x) = A_n e^{ikx} + B_n e^{-ikx}, \tag{5}$$

where $\psi_n(x)$ corresponds to the wave function in the space between the $(n - 1)$ th δ and the n th δ . The wave momentum is $\hbar k = \sqrt{2mE}$. At the δ function locations, the wave function has to satisfied two conditions:

- (a) continuity of the wave function, and
- (b) the jump of the derivative of the wave function has to fulfill the Schrödinger equation.

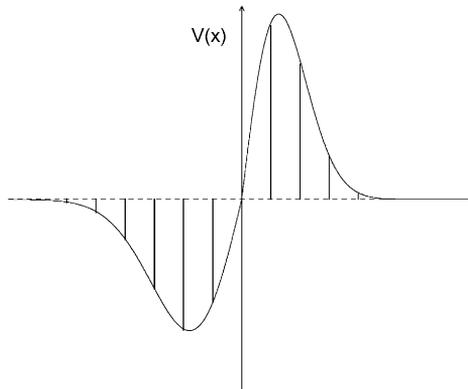


Fig. 1. An illustration of the approximation of a well-localized potential by δ potentials. The wider lines represent the infinite δ potentials and the finite height of those lines represent the coefficients which multiply the δ potentials.

These conditions lead to a transfer matrix from the left-hand side of the $V(x_n)\delta(x - x_n)$ potential to the right-hand side of it

$$T_n = \begin{pmatrix} 1 - \frac{i}{2k} \frac{2m}{\hbar^2} V(x_n) \Delta x & -\frac{i}{2k} \frac{2m}{\hbar^2} V(x_n) \Delta x e^{-2ikx_n} \\ \frac{i}{2k} \frac{2m}{\hbar^2} V(x_n) \Delta x e^{2ikx_n} & 1 + \frac{i}{2k} \frac{2m}{\hbar^2} V(x_n) \Delta x \end{pmatrix}. \tag{6}$$

The total transfer matrix is the multiplication of all transfer matrices, T_n ,

$$T = T_N T_{N-1} \cdots T_1 T_0. \tag{7}$$

The determinate of the total T matrix is 1 since the determinate of each local T_n matrix (6) is 1.

At this stage the connection between the left-hand side wave function and the right-hand side wave function is made by the use of the T matrix,

$$\begin{pmatrix} A_{N+1} \\ B_{N+1} \end{pmatrix} = T \begin{pmatrix} A_0 \\ B_0 \end{pmatrix}. \tag{8}$$

One can use the relation between the incoming wave and outgoing wave in order to define the S matrix

$$\begin{pmatrix} A_{N+1} \\ B_0 \end{pmatrix} = \frac{1}{T_{22}} \begin{pmatrix} T_{11} T_{22} - T_{12} T_{21} & T_{12} \\ -T_{21} & 1 \end{pmatrix} \begin{pmatrix} A_0 \\ B_{N+1} \end{pmatrix}. \tag{9}$$

It is clear from Eq. (6) that for each transfer matrix the diagonal elements are complex conjugate pair, as well as, the off diagonal elements. These properties hold also for the total transfer matrix, T ,

$$T_{12} = T_{21}^*, \tag{10}$$

$$T_{11} = T_{22}^*. \tag{11}$$

Together with the fact that

$$\det T = 1, \tag{12}$$

the S matrix becomes

$$S = \frac{1}{T_{22}} \begin{pmatrix} 1 & T_{12} \\ -T_{12}^* & 1 \end{pmatrix}. \tag{13}$$

Using Eqs. (10)–(12) it can be easily verified that the S matrix is a unitary matrix

$$SS^\dagger = S^\dagger S = I. \tag{14}$$

The resonance state occurs whenever the left incoming wave remains unchanged and equal to the right outgoing wave. It follows that in the resonance case the S matrix is a unit matrix. By the use of Eqs. (10)–(12), the conclusion is that the condition for a resonance state is

$$T_{22} = 1. \tag{15}$$

In a non-resonance state T_{22} is a complex number and its absolute value is greater than one.

Usually, in one-dimensional scattering problems, one considers a current of free-particle waves coming from the left, $\exp(ikx)$, which collide with the potential, and split to a left-hand side reflected wave, $r \exp(-ikx)$, and to a right-hand side transmitted wave, $t \exp(ikx)$. Using the above terminology, if we take, $A_{N+1} = t$, $B_0 = r$, $A_0 = 1$, and $B_{N+1} = 0$, the transmission and reflection coefficients are

$$t = \frac{1}{T_{22}}, \quad (16)$$

$$r = -\frac{T_{12}^*}{T_{22}} \quad (17)$$

and they satisfy the current normalization $|t|^2 + |r|^2 = 1$.

The state itself can be evaluated in the following way. Knowing the incoming and outgoing coefficients, one can compute the local coefficients A_n and B_n , by multiplying the T matrix with the left-hand side coefficients A_0 and B_0 . In the case of a resonance state, it is possible to identify a quasi-state in the potential range, and usually a normalization is required (which can be done by a division by $\int_a^b |\psi(x)|^2 dx$, where a and b are the potential boundaries).

2.2. Potential with periodic boundary conditions

The above method can be implemented in order to find the spectrum and the eigenstates of a potential embedded on a ring (i.e., periodic boundary conditions). The periodic boundary conditions imply (where x_L and x_R denote the left and right boundaries)

$$A_0 e^{ikx_L} = A_{N+1} e^{ikx_R}, \quad (18)$$

$$B_0 e^{-ikx_L} = B_{N+1} e^{-ikx_R}. \quad (19)$$

Using Eqs. (9), (13), (18), and (19) one obtains

$$\begin{pmatrix} A_{N+1} \\ B_0 \end{pmatrix} = \frac{e^{ik(x_R-x_L)}}{T_{22}} \begin{pmatrix} 1 & T_{12} \\ -T_{12}^* & 1 \end{pmatrix} \begin{pmatrix} A_{N+1} \\ B_0 \end{pmatrix} = e^{ik(x_R-x_L)} S \begin{pmatrix} A_{N+1} \\ B_0 \end{pmatrix}. \quad (20)$$

The eigenvalues may be found by the use of the function

$$f(E) = \det(e^{ik(x_R-x_L)} S - I). \quad (21)$$

A nontrivial solution for Eq. (20) occurs when $f(E) = 0$ yielding the energy spectrum. The solution leads to a certain ratio between A_{N+1} and B_0 . Using Eqs. (18) and (19), it is possible to find the ratio between A_0 and B_0 . To find the eigenstate itself it is necessary to choose initial values for either A_0 or B_0 , and then, by the use of the transfer matrix, any local coefficients (i.e., A_n and B_n) can be found. A normalization of the eigenstate can be performed by dividing by $\int_{x_L}^{x_R} |\psi(x)|^2 dx$.

2.3. Bound states of potential wells

Another class of potentials that can be treated by the δ approximation is the potential well class. In order to find the spectrum of the potential well, it is more convenient to use a negative potential that can be expanded as a sum of negative δ functions.¹ The wave function between two neighboring δ functions, can be chosen to be a combination of decaying functions

$$\psi_n(x) = A_n e^{\kappa x} + B_n e^{-\kappa x}, \tag{22}$$

where $\kappa = \sqrt{-2mE}/\hbar$ ($E < 0$), and $\psi_n(x)$ correspond to the space between the $(n-1)$ th δ and the n th δ . The transfer matrix which connects ψ_{n-1} to ψ_n space is

$$T_n = \begin{pmatrix} 1 + \frac{1}{2\kappa} \frac{2m}{\hbar^2} V(x_n) \Delta x & \frac{1}{2\kappa} \frac{2m}{\hbar^2} V(x_n) \Delta x e^{-2\kappa x_n} \\ -\frac{1}{2\kappa} \frac{2m}{\hbar^2} V(x_n) \Delta x e^{2\kappa x_n} & 1 - \frac{1}{2\kappa} \frac{2m}{\hbar^2} V(x_n) \Delta x \end{pmatrix}. \tag{23}$$

Also here $\det T_n = 1$, and the total T matrix is $T = T_N T_{N-1} \cdots T_1 T_0$, thus $\det T = 1$. From the relation

$$\begin{pmatrix} A_{N+1} \\ B_{N+1} \end{pmatrix} = T \begin{pmatrix} A_0 \\ B_0 \end{pmatrix} \tag{24}$$

one can find the matrix which connects the decaying coefficients (A_0 and B_{N+1}) to the diverging coefficients (A_{N+1} and B_0),

$$\begin{pmatrix} A_{N+1} \\ B_0 \end{pmatrix} = \frac{1}{T_{22}} \begin{pmatrix} 1 & T_{12} \\ -T_{21} & 1 \end{pmatrix} \begin{pmatrix} A_0 \\ B_{N+1} \end{pmatrix} = S \begin{pmatrix} A_0 \\ B_{N+1} \end{pmatrix}. \tag{25}$$

Because of physical reasons A_{N+1} and B_0 must vanish, and thus, in order to obtain nontrivial solution the following condition has to be fulfilled:

$$\det S = \frac{T_{11}}{T_{22}} = 0. \tag{26}$$

Since $T_{11} \neq T_{22}$ the requirement (26) is simply

$$T_{11} = 0. \tag{27}$$

Thus, when Eq. (27) has achieved, an eigenvalue has been located.

The eigenstate itself can be found by starting from an arbitrary A_0 ($B_0 = 0$); consecutive multiplication by the local T_n matrix will lead to the unnormalized state. A normalization can be performed then.

The above description is suitable also for unbounded potentials (i.e., $V(x) \rightarrow \infty$ when $x \rightarrow \infty$ or $x \rightarrow -\infty$). For that, the left and right boundaries have to be sufficiently large compared to the present energy level, such that the decaying functions drop very sharply to 0, and additional extension of the δ function approximation, either to the left or to the right, will lead to a slightly different answer.

¹ In fact, it is possible to expand also a positive potential as a sum of negative δ functions; it is necessary to shift the potential such that it will be negative.

3. Results

In this section the δ potential approximation will be worked out on two well-known potentials, the square well and the harmonic oscillator. Both examples show almost perfect correspondence between the δ function approximation and the analytical solution.

The square well potential is formulated by

$$V_1(x) = \begin{cases} 0 & \text{when } -a \leq x \leq a, \\ V_0 & \text{otherwise.} \end{cases} \quad (28)$$

Deep in the well, the energy levels are approximately the same as in the infinite well case. Then, the approximated spectrum of $V_1(x)$ is

$$E_n = \frac{n^2 \pi^2 \hbar^2}{4a^2 2m}, \quad n = 1, 2, 3, \dots \quad (29)$$

In our calculations we used $\hbar = 1$ and $2m = 1$. The number of δ functions that were used in the approximation is 10 000. In Fig. 2(a) the parameter values are $V_0 = 100$ and $a = \pi/2$. In that case, the energy spectrum Eq. (28) becomes $E_n = n^2$. The positions of E_n are indicated by a dashed line, and they coincide with the vanishing of the diverging parameter, $|T_{11}|$ (see Eq. (27)).

In Fig. 2(b) we present the transmission coefficient $T = |t|^2$ above the well height. Also here, the results that were calculated by the δ approximation coincide with the exact transmission coefficient. The difference between the two curves is not visible by eye. An enlargement of the third minima of the figure is shown in the inset; the difference between the exact transmission coefficient and the approximated one is visible now. Increasing the number of δ function potentials in the δ approximation will yield better correspondence.

The second example we shall consider here is the harmonic oscillator

$$V_2(x) = \begin{cases} V_0 x^2 / a^2 & \text{when } -a \leq x \leq a, \\ V_0 & \text{otherwise.} \end{cases} \quad (30)$$

Deep in the well the spectrum of the finite harmonic oscillator can be approximated by the exact spectrum of the harmonic oscillator

$$E_n = \hbar \sqrt{\frac{2V_0}{a^2 m}} \left(n + \frac{1}{2} \right), \quad n = 0, 1, 2, \dots \quad (31)$$

The parameter values were chosen to be $V_0 = 16$ and $a = 8$. The spectrum then becomes, $E_n = n + \frac{1}{2}$. In Fig. 3(a), the analytical results (which are indicated by the dashed lines) coincide (with high accuracy) with the δ potential approximated spectrum. In Fig. 3(b) we have calculated the eigenfunctions of the first 4 states. In the upper panel the analytical eigenfunctions and the approximated ones are presented; the difference between the two is not visible by eye. In the lower panel we have plot the actual difference between the analytical eigenfunction (of the harmonic oscillator), $\phi_n(x)$, and the one that was obtained by the δ approximation, $\phi_{\delta,n}(x)$. These differences have

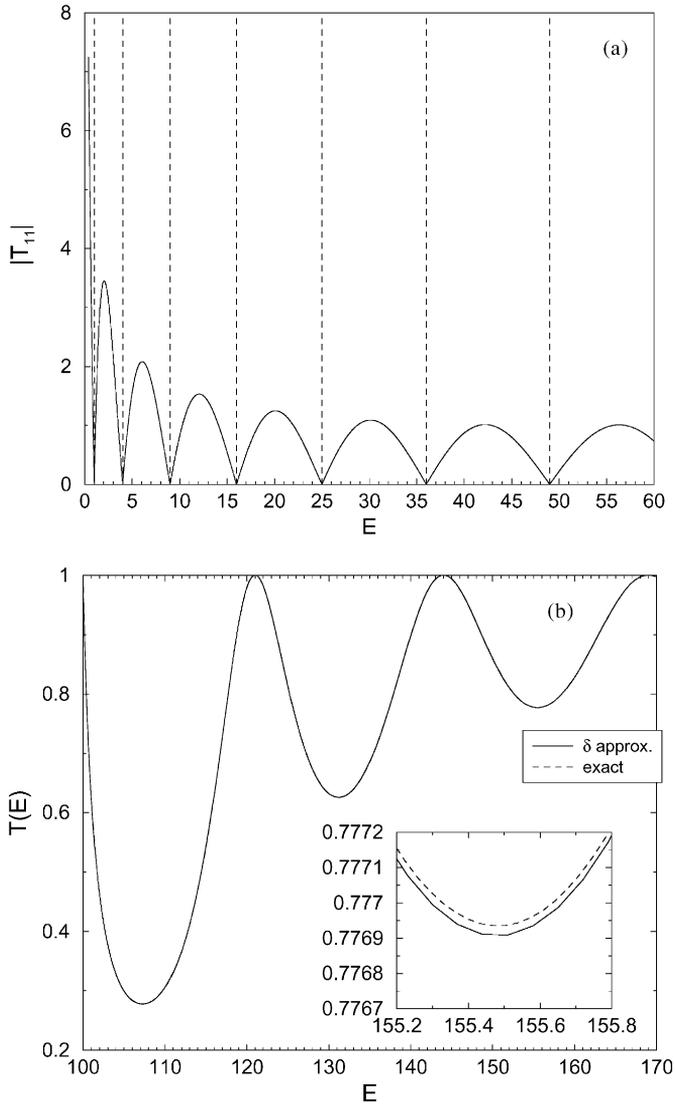


Fig. 2. (a) $|T_{11}|$ coefficient as a function of E for a square well. The analytical energy spectrum (dashed lines) coincides with the numerical results (solid line when $|T_{11}| = 0$); (b) The transmission coefficient, T , above a square-well as a function of E . An enlargement of the third minima is shown the inset. The exact solution is represented by the dashed line while the approximated solution is indicated by the solid line.

systematic structure, i.e.,

$$\phi_n(x) - \phi_{n,\delta}(x) \approx C\phi_{n+2}(x), \tag{32}$$

where C is a very small constant ($C \ll 1$). Larger number of δ functions in the δ function approximation will lead to the same behavior; the order of the difference between the two results will become smaller.

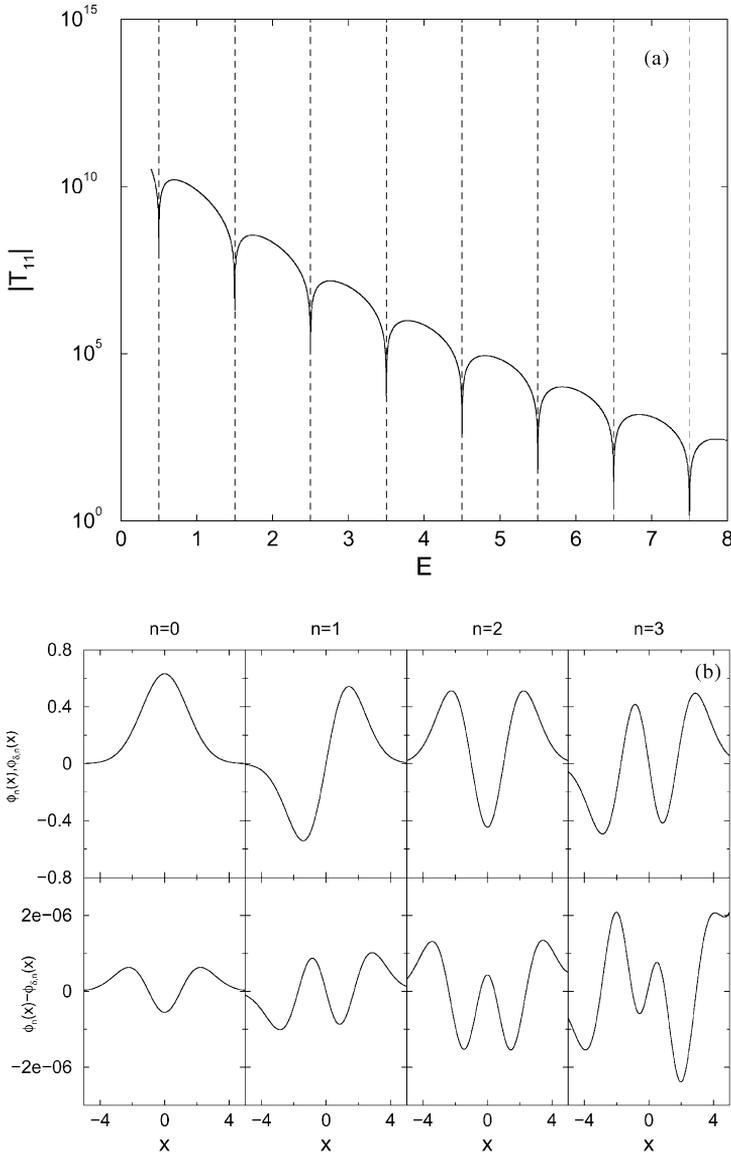


Fig. 3. (a) The energy spectrum of an harmonic oscillator potential. The dashed line indicate the positions of the exact solution and it coincides with the approximated solution curves (solid line). (b) The eigenfunctions of an harmonic oscillator. In the top panel the first four eigenfunctions are shown; the difference between the analytical eigenfunctions $\phi_n(x)$ and the approximated eigenfunctions, $\phi_{\delta,n}(x)$, is not visible by eye. In the bottom panel the difference between the analytical and the approximated eigenfunctions is shown. As seen, this difference is very small ($(\phi_n(x) - \phi_{\delta,n}(x)) \ll 1$) and has a special form, namely, $\phi_n(x) - \phi_{\delta,n}(x) \approx C\phi_{n+2}(x)$.

4. Summary

In the present study we have shown that it is possible to use a sum of δ function potentials in order to approximate 1D potentials. By the use of transfer matrices from one side of the δ potential to the other side, the transfer matrix which connects the left-hand side of the potential wave functions to the right-hand side wave functions is found. The S matrix, which connects the incoming waves to outgoing waves, is built from the total transfer matrix T . By the use of the S matrix the transmission coefficient, as well as the reflection coefficient can be calculated. Moreover, the same approach can be used to calculate the energy spectrum in a potential well (by assuming that the wavefunctions between the δ potentials are exponentially decaying functions). Resonance states above the potential well, as well as the eigenfunctions in the potential well can be found as well. The δ function approximation was examined on two well known examples, the square-well and the harmonic oscillator potentials.

It should be noted that the computation time of calculating transmission coefficients, as well as, energy spectra and eigenfunctions is small (order of seconds on a Pentium II 350 MHz PC) even when using a large number of δ functions in the approximation.

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