One-dimensional scattering: Recurrence relations and differential equations for transmission and reflection amplitudes

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A recurrence method for analytical and numerical evaluation of tunneling, transmission, and reflection amplitudes is developed. As the first step, a rule for composition of two arbitrary scatterers separated by a region of constant potential is obtained. Transmission and reflection amplitudes for this double-barrier potential are expressed in terms of transmission and reflection amplitudes for its subparts. As the length of the constant-potential region can be arbitrary and the subparts of a potential may, in turn, be arbitrary segmented potentials, one obtains recurrence formulas which express the scattering amplitudes for the arbitrary segmented potential via the scattering amplitudes for the subparts into which the complete potential can be divided. The efficiency of the method is demonstrated by solving analytically the problem of scattering from locally periodic potentials. Since an arbitrary potential can be approximated by a set of infinitely narrow rectangular barriers, the recurrence formulas can be applied to any potential, giving, in the limit of zero-width segments, differential equations for transmission, and reflection amplitudes.

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I. INTRODUCTION

In many actual physical problems, such as resonant tunneling in semiconductor junctions and superlattices [1], conductivity of one-dimensional random scatterers [2,3], time analysis of tunneling processes [4,5], and tunneling of systems with internal degrees of freedom through potential barriers [6], one deals with one-dimensional quantum-mechanical potentials of the following general type: regions of arbitrary complicated variation of a potential are separated by regions where the scattering potential is constant (see Fig. 1, in this paper we call potentials of this type "segmented").

The transfer-matrix technique is the standard method of solving the Schrödinger equation for such systems. The approach has, however, several inherent deficiencies. One deals with elements of the transfer matrix, but not directly with observable quantities such as scattering (transmission and reflection) coefficients. The amount of computational work required grows linearly with increasing number of segments in a potential, which can become a problem for sufficiently complicated potentials. The transfer-matrix technique runs into loss-of-significant-digits problem when opaque barriers are investigated because of round-off error in sums of different in magnitudes numbers with opposite signs.

One of the goals of the present work is to develop a method of solving the Schrödinger equation for segmented potentials, dealing directly with observable quantities and convenient for the analytical and numerical investigation of complicated barrier structures. We start from the simplest case of double-barrier scattering and obtain an expression for the reflection and transmission amplitudes of segmented potentials in terms of the corresponding amplitudes for its subparts. As the subparts of a potential may, in turn, be complicated multisegmented potentials, the formulas obtained recurrently determine the scattering amplitudes for a complete potential from the scattering amplitudes of its elementary subparts into which the potential can be divided.

The formulas obtained are convenient both for analytical (including the usage of systems of symbolical computations) and numerical calculation of scattering data. The amount of computations only increases logarithmically as the number of potential segments increases.

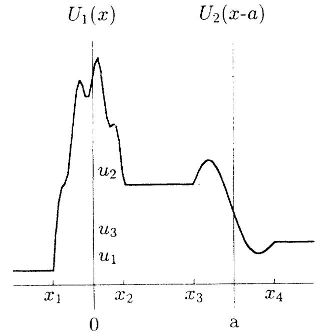

FIG. 1. Schematic representation of a segmented potential. The two-segment case is shown.

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The lengths of the constant-potential regions of a segmented potential can be arbitrary, and, in particular, zero. Since an arbitrary potential can be approximated by a set of infinitely narrow adjacent rectangular barriers, the basic formulas can also be applied to an arbitrary potential. In the limit of the barrier segment width going to zero, differential equations for amplitudes are deduced from the recurrence relations. The problem of solving the Schrödinger equation in scattering geometry and extracting scattering amplitudes from the wave function is therefore replaced by a boundary-value problem, which is simpler for numerical solution.

The present article is organized as follows. In Sec. II A we review the basic facts of one-dimensional scattering. In Sec. II B the recurrence formulas expressing the scattering amplitudes of a segmented barrier in terms of scattering amplitudes of its subparts are derived. In Sec. III several applications are considered. In Sec. III A, due to the importance of rectangular potentials, we apply the general formulas to this particular case. In Sec. III B the analytical solution of the problem of scattering from an arbitrary finite periodic chain [7–12] is obtained. Section IV is devoted to the differential equations that can be derived from the recurrence relations. In Sec. IV A differential equations for transmission and reflection amplitudes and in Sec. IV B differential equations for the transfer matrix are obtained. Analytical solutions of the equations are considered in Sec. IV C. Numerical solutions of the differential equations are discussed in Sec. IV D. A final discussion is given in Sec. V.

II. BASIC FORMULAS

A. Theory of one-dimensional scattering

In this section we summarize the necessary results from the theory of one-dimensional scattering [13].

For a quantum-mechanical potential $U(x)$ such that

$$U(x) = \begin{cases} u_1, & x \to -\infty \\ u_2, & x \to +\infty, \end{cases} \tag{1}$$

where the constants u_i, the asymptotics of the general solution of the Schrödinger equation are

$$\psi = \begin{cases} A_1 e^{ik_1 x} + B_1 e^{-ik_1 x}, & x \to -\infty \\ A_2 e^{ik_2 x} + B_2 e^{-ik_2 x}, & x \to +\infty. \end{cases} \tag{2}$$

Here

$$k_i = \frac{1}{\hbar}\sqrt{2m(E-u_i)}, \tag{3}$$

$\hbar$ is Planck's constant, m is the mass of a particle, and E is its energy.

Between the amplitudes A_i and B_i of (2) there are linear homogeneous relations:

$$A_2 = \alpha A_1 + \beta B_1, \tag{4}$$

$$B_2 = \beta^* A_1 + \alpha^* B_1, \tag{5}$$

conveniently expressed in terms of a transfer matrix

$$M = \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix}, \tag{6}$$

where α and β are generally complex and depend on the potential $U(x)$:

$$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = M \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}. \tag{7}$$

The conservation of the probability current leads to the following relation for the matrix elements of (6):

$$\frac{k_1}{k_2} = |\alpha|^2 - |\beta|^2. \tag{8}$$

The transmission (reflection) amplitudes T (R) are defined as the ratio of the amplitude of the transmitted (reflected) wave and the amplitude of the incoming wave.

For a wave incident from the left, $B_2 = 0$ and the reflection amplitude becomes

$$R_L \equiv \frac{B_1}{A_1} = -\frac{\beta^*}{\alpha^*}. \tag{9}$$

The transmission amplitude is

$$T_L \equiv \frac{A_2}{A_1} = \frac{k_1}{k_2}\frac{1}{\alpha^*}. \tag{10}$$

The last equalities in (9), (10) were obtained using (4), (5), and (8). The subscripts L (R) here and below denote the physical quantities of the particles incident from the left (right).

Analogously, for the wave incident from the right, $A_1 = 0$ and

$$R_R \equiv \frac{A_2}{B_2} = \frac{\beta}{\alpha^*}, \tag{11}$$

$$T_R \equiv \frac{B_1}{B_2} = \frac{1}{\alpha^*}. \tag{12}$$

From (10), (12) and (9), (11) it follows that

$$T_R = \frac{k_2}{k_1} T_L, \tag{13}$$

and in general $R_L \neq R_R$ although $|R_L| = |R_R|$.

Transmission (reflection) coefficients $\mathcal{T}$ ($\mathcal{R}$) are defined as the transmitted (reflected) probability current divided by the incident probability current.

For the particle incident from the left ($B_2 = 0$)

$$\mathcal{T}_L \equiv \frac{k_2}{k_1}\frac{|A_2|^2}{|A_1|^2} = \frac{k_2}{k_1}|T_L|^2 = \frac{k_1}{k_2}\left|\frac{1}{\alpha}\right|^2, \tag{14}$$

$$\mathcal{R}_L = \frac{|B_1|^2}{|A_1|^2} = 1 - \frac{k_2}{k_1}\frac{|A_2|^2}{|A_1|^2} = 1 - \mathcal{T}_L, \tag{15}$$

$$\mathcal{R}_L = |R_L|^2 = \left|\frac{\beta}{\alpha}\right|^2. \tag{16}$$

Similarly, for the particle incident from the right ($A_1 = 0$)

$$\mathcal{T}_R \equiv \frac{k_1}{k_2}\frac{|B_1|^2}{|B_2|^2} = \frac{k_1}{k_2}|T_R|^2 = \frac{k_1}{k_2}\left|\frac{1}{\alpha}\right|^2, \tag{17}$$

$$\mathcal{R}_R = \frac{|A_2|^2}{|B_2|^2} = 1 - \frac{k_1}{k_2}\frac{|B_1|^2}{|B_2|^2} = 1 - \mathcal{T}_R, \tag{18}$$

$$\mathcal{R}_R = |R_R|^2 = \left|\frac{\beta}{\alpha}\right|^2. \tag{19}$$

The transmission and reflection coefficients are independent of the direction of the wave: $\mathcal{R}_L = \mathcal{R}_R = \mathcal{R}$ and $\mathcal{T}_L = \mathcal{T}_R = \mathcal{T}$,

$$\mathcal{T} = \frac{k_2}{k_1}|T_L|^2 = \frac{k_1}{k_2}|T_R|^2. \tag{20}$$

B. Scattering from segmented potentials

In this section we obtain the law of composition of two scatterers in series expressing the scattering amplitudes for a two-segment barrier in terms of scattering amplitudes for the individual sections.

Let us assume that the stationary scattering problem for the two potentials $U_1(x)$ and $U_2(x)$ such that

$$U_1(x) = \begin{cases} u_1, & x \to -\infty \\ u_2, & x \to +\infty, \end{cases} \tag{21}$$

$$U_2(x) = \begin{cases} u_2, & x \to -\infty \\ u_3, & x \to +\infty \end{cases} \tag{22}$$

has been solved exactly. Here u_i =const, $i = 1,2,3$. The origin $x = 0$ of the coordinate systems of each potential we call reference point of the potential. Let us consider scattering for the following combination of the $U_1(x)$ and $U_2(x)$ (see Fig. 1):

$$U(x) = \begin{cases} u_1, & x < x_1 \\ U_1(x), & x_1 < x < x_2 \\ u_2, & x_2 < x < x_3 \\ U_2(x), & x_3 < x < x_4 \\ u_3, & x > x_4, \end{cases} \tag{23}$$

such that the distance between the reference points of the two potentials is a.

The wave function has the form

$$\psi = \begin{cases} A_1 e^{ik_1 x} + B_1 e^{-ik_1 x}, & x \to -\infty \\ A_2 e^{ik_2 x} + B_2 e^{-ik_2 x}, & x_2 < x < x_3 \\ A_3 e^{ik_3 x} + B_3 e^{-ik_3 x}, & x \to +\infty, \end{cases} \tag{24}$$

where the k_i are determined by (3). This can also be rewritten with respect to the reference point $x = a$ as

$$\psi = \begin{cases} A_1 e^{ik_1 x} + B_1 e^{-ik_1 x}, & x \to -\infty \\ A_2' e^{ik_2(x-a)} + B_2' e^{-ik_2(x-a)}, & x_2 < x < x_3 \\ A_3' e^{ik_3(x-a)} + B_3' e^{-ik_3(x-a)}, & x \to +\infty, \end{cases} \tag{25}$$

where

$$A_l' = A_l e^{ik_l a}, \quad B_l' = B_l e^{-ik_l a}, \quad l = 2,3. \tag{26}$$

We denote by α_i, β_i, $T_{i(R,L)}$, $R_{i(R,L)}$ the scattering parameters introduced in Sec. II A corresponding to the potential $U_i(x)$, $i = 1,2$.

Writing down Eqs. (4) and (5) for the right barrier, we obtain for a particle incident from the left

$$B_3' = \alpha_2^* B_2' + \beta_2^* A_2' = 0, \tag{27}$$

$$A_3' = \alpha_2 A_2' + \beta_2 B_2'. \tag{28}$$

Using (8) we get

$$B_2' = -\beta_2^* \frac{k_3}{k_2} A_3', \tag{29}$$

$$A_2' = \alpha_2^* \frac{k_3}{k_2} A_3'. \tag{30}$$

Similarly, for the left barrier

$$A_2 = A_1\alpha_1 + \beta_1 B_1 = A_2' e^{-ik_2 a}, \tag{31}$$

$$B_2 = \alpha_1^* B_1 + A_1 \beta_1^* = B_2' e^{ik_2 a}. \tag{32}$$

Substituting (29) and (30) into (31) and (32) we get

$$\frac{A_3'}{A_1} = e^{ik_2 a} \frac{\frac{k_1}{k_3}\frac{1}{\alpha_1^*\alpha_2^*}}{1 + \frac{\beta_1\beta_2^*}{\alpha_1^*\alpha_2^*} e^{2ik_2 a}}. \tag{33}$$

Using the relations (9)–(12) this can be written as

$$\frac{A_3'}{A_1} = e^{ik_2 a} \frac{T_{1L} T_{2L}}{1 - R_{2L} R_{1R} e^{2ik_2 a}}. \tag{34}$$

The total transmission amplitude of the segmented potential (23) can be finally expressed as follows:

$$T_L = \frac{A_3}{A_1} = e^{-ik_3 a}\frac{A_3'}{A_1} = e^{i(k_2 - k_3)a} \frac{T_{1L} T_{2L}}{1 - R_{2L} R_{1R} e^{2ik_2 a}}. \tag{35}$$

Similarly, one gets from (32), (29)

$$\frac{B_1}{A_1} = (B_2' e^{ik_2 a} - \beta_1^*)\frac{1}{\alpha_1^*} = \frac{1}{\alpha_1^*}\left(-\beta_2^* \frac{k_3}{k_2} A_3' e^{ik_2 a} - \beta_1^*\right)$$

$$= e^{2ik_2 a} \frac{R_{2L} T_{1R}}{T_{2L}} A_3 + R_{1L}. \tag{36}$$

Using (9)–(12) we get the reflection amplitude for the segmented potential (23):

$$R_L = R_{1L} + e^{2ik_2 a} \frac{T_{1L} R_{2L} T_{1R}}{1 - R_{2L} R_{1R} e^{2ik_2 a}}. \tag{37}$$

One can find similarly the scattering amplitudes for a particle incident from the right:

$$T_R = e^{i(k_2 - k_3)a} \frac{T_{2R} T_{1R}}{1 - R_{1R} R_{2L} e^{2ik_2 a}}, \tag{38}$$

$$R_R = R_{2R}e^{-2ik_3a} + e^{2i(k_2-k_3)a}\frac{T_{2R}R_{1R}T_{2L}}{1-R_{1R}R_{2L}e^{2ik_2a}}. \quad (39)$$

Formulas (35) and (37)–(39) solve the problem under study.

Similar expressions have been obtained earlier by different methods for the particular cases of symmetric rectangular [14] and double δ barriers [15], respectively. The scaling theory of localization in disordered one-dimensional lattices [2,3] was based on heuristically derived expressions of type (35) for the case $u_i = 0$.

A clear physical interpretation can be given to formulas (35)–(39) using the multiple scattering approach [14]. (See also [8,15].) In this approach the scattering process is viewed as consisting of a sequence of reflections and transmissions occurring at each barrier. The total scattering amplitude is given by a coherent sum of individual scattering amplitudes representing different possible paths leading to transmission.

Consider, for example, (35). Expanding (35) in series we get

$$T_L = e^{i(k_2-k_3)a}(T_{1L}T_{2L} + T_{1L}R_{2L}R_{1R}e^{2ik_2a}T_{2L} + T_{1L}R_{2L}R_{1R}e^{2ik_2a}R_{2L}R_{1R} \times e^{2ik_2a}T_{2L} + \cdots). \quad (40)$$

The nth term in this series can be interpreted as the amplitude corresponding to the possible path when the incident wave $\sim e^{ik_1x}$ transmitted through the first barrier from the left with the amplitude T_{1L} is n times reflected both by the second barrier with the amplitude R_{2L} and by the first barrier with the amplitude R_{1R}, before it is transmitted through the second barrier with the amplitude T_{2L}; the additional phase shift due to going back and forth is e^{2ik_2an}.

At the end of this section we derive for future reference the transformation rule for the transfer matrix (6) and scattering amplitudes (9)–(12) under the translation of the scattering potential $U(x) \to U(x-d)$. Let us assume that the Schrödinger equation for the potential $U(x)$ located at $x = 0$ has been solved, *i.e.*, $T^0_{R,L}$, $R^0_{R,L}$, α^0, and β^0 are known. The translated potential may be formally considered as the composition of two potentials — zero-height barrier ($T = 1$, $R = 0$) located at $x = 0$ and barrier $U(x)$ located at $x = d$. Applying the composition rule (35), (37)–(39), we get the following amplitudes of scattering on the potential $U(x-d)$:

$$T^d_R = T^0_R e^{i(k_1-k_3)d}, \quad (41)$$

$$T^d_L = T^0_L e^{i(k_1-k_3)d}, \quad (42)$$

$$R^d_R = R^0_R e^{-2ik_3d}, \quad (43)$$

$$R^d_L = R^0_L e^{2ik_1d}. \quad (44)$$

From here, using the relation (12), (11) we get the relations for the transfer-matrix elements:

$$\alpha^d = \alpha^0 e^{i(k_1-k_3)d}, \quad (45)$$

$$\beta^d = \beta^0 e^{-i(k_1+k_3)d}. \quad (46)$$

III. APPLICATIONS

In this section we present several applications of formulas (35) and (37)–(39).

We start in Sec. III A considering rectangular potentials due to their importance both pedagogical and practical. Although nice formulas, useful for complicated barriers, are obtained, the principal goal of this section is to demonstrate the efficiency of the method. The simple examples are also helpful in providing better understanding of the recurrence nature of (35) and (37)–(39).

In Sec. III B we present the complete analytical solution of the problem of one-dimensional scattering by a finite periodic chain of nonoverlapping barriers or wells (see Fig. 3).

A. Rectangular potentials

An arbitrary complicated rectangular potential can be considered as a segmented potential, therefore formulas (35) and (37)–(39) give exact results for this class of barriers.

The simplest "element" from which any rectangular potential can be built is a potential step [see Fig. 2(a)]:

$$U(x) = \begin{cases} u_1, & x < 0 \\ u_2, & x > 0. \end{cases} \quad (47)$$

The scattering amplitudes for the potential (47) are as follows:

$$T^{(1)}_L = \frac{2k_1}{k_1+k_2}, \quad R^{(1)}_L = \frac{k_1-k_2}{k_1+k_2}, \qquad T^{(1)}_R = \frac{2k_2}{k_1+k_2}, \quad R^{(1)}_R = \frac{k_2-k_1}{k_2+k_1}, \quad (48)$$

where k_i are determined by (3). (In this section the superscripts of the scattering amplitudes denote the number of jumps of the potential.) In accordance with (20)

$$\mathcal{T}^{(1)} = |T^{(1)}_L|^2\frac{k_2}{k_1} = |T^{(1)}_R|^2\frac{k_1}{k_2},$$

$$\mathcal{R}^{(1)} = |R^{(1)}_L|^2 = |R^{(1)}_R|^2.$$

For later convenience we rewrite Eqs. (48) as follows:

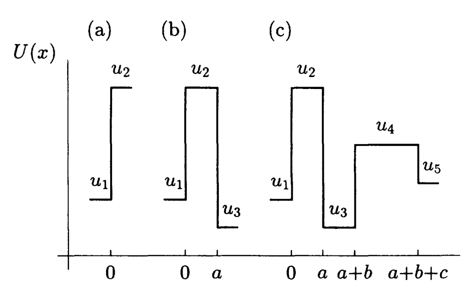

FIG. 2. Rectangular potentials: (a) Potential step, (b) asymmetric rectangular barrier, (c) double asymmetric barrier.

$$T_L^{(1)} = e^{-ik_2 0}\frac{2k_1}{D^{(1)}(k_1k_2)}, \tag{49}$$

$$T_R^{(1)} = e^{-ik_2 0}\frac{2k_2}{D^{(1)}(k_1k_2)}, \tag{50}$$

$$R_L^{(1)} = \frac{N^{(1)}(k_1k_2)}{D^{(1)}(k_1k_2)}, \tag{51}$$

$$R_R^{(1)} = -e^{-2ik_2 0}\frac{[N^{(1)}(k_1k_2)]^*}{D^{(1)}(k_1k_2)}, \tag{52}$$

where $N^{(1)}(k_1k_2) = k_1 - k_2$, and $D^{(1)}(k_1k_2) = k_1 + k_2$.

1. Asymmetric rectangular barrier

An asymmetric rectangular barrier of a width a [see Fig. 2(b)]:

$$U(x) = \begin{cases} u_1, & x<0 \\ u_2, & 0<x<a \\ u_3, & x>a, \end{cases} \tag{53}$$

can be considered as a combination of two potential steps (possibly of different heights) located at a distance a from each other.

Substituting the scattering amplitudes for a potential step (48) into the basic formulas (35) and (37)–(39) we get the following expression for the amplitudes of scattering on the asymmetric barrier:

$$T_L^{(2)} = \frac{2k_1k_2e^{-ik_3a}}{(k_1k_2+k_2k_3)\cos k_2a - i(k_2^2+k_1k_3)\sin k_2a} = e^{-ik_3a}\frac{2^2k_1k_2}{D^{(2)}(a;k_1k_2k_3)}, \tag{54}$$

$$R_L^{(2)} = \frac{(k_1k_2-k_2k_3)\cos k_2a + i(k_2^2-k_1k_3)\sin k_2a}{(k_1k_2+k_2k_3)\cos k_2a - i(k_2^2+k_1k_3)\sin k_2a} = \frac{N^{(2)}(a;k_1k_2k_3)}{D^{(2)}(a;k_1k_2k_3)}, \tag{55}$$

$$T_R^{(2)} = \frac{2k_2k_3e^{-ik_3a}}{(k_1k_2+k_2k_3)\cos k_2a - i(k_2^2+k_1k_3)\sin k_2a} = e^{-ik_3a}\frac{2^2k_2k_3}{D^{(2)}(a;k_1k_2k_3)}, \tag{56}$$

$$R_R^{(2)} = e^{-2ik_3a} \times\frac{(k_3k_2-k_2k_1)\cos k_2a + i(k_2^2-k_1k_3)\sin k_2a}{(k_1k_2+k_2k_3)\cos k_2a - i(k_2^2+k_1k_3)\sin k_2a} = -e^{-2ik_3a}\frac{[N^{(2)}(a;k_1k_2k_3)]^*}{D^{(2)}(a;k_1k_2k_3)}. \tag{57}$$

In formulas (54)–(57) we used

$$D^{(2)}(a;k_1k_2k_3) = e^{-ik_2a}D^{(1)}(k_2k_3)D^{(1)}(k_1k_2) + e^{ik_2a}N^{(1)}(k_2k_3)[N^{(1)}(k_1k_2)]^*, \tag{58}$$

$$N^{(2)}(a;k_1k_2k_3) = e^{-ik_2a}D^{(1)}(k_2k_3)N^{(1)}(k_1k_2) + e^{ik_2a}N^{(1)}(k_2k_3)[D^{(1)}(k_1k_2)]^*. \tag{59}$$

For the transmission and reflection coefficients of an asymmetric barrier we get

$$\mathcal{T}^{(2)} = \frac{4k_1k_2^2k_3}{(k_1^2-k_2^2)(k_2^2-k_3^2)\cos^2 k_2a + (k_1k_3+k_2^2)^2}, \tag{60}$$

$$\mathcal{R}^{(2)} = \frac{(k_1^2-k_2^2)(k_2^2-k_3^2)\cos^2 k_2a + (k_1k_3-k_2^2)^2}{(k_1^2-k_2^2)(k_2^2-k_3^2)\cos^2 k_2a + (k_1k_3+k_2^2)^2}. \tag{61}$$

For later reference we present expressions for the scattering amplitudes on a symmetric rectangular barrier. In this case $u_3 = u_1$, and therefore $k_3 = k_1$. From (54) and (61) we find

$$T = e^{-ik_1a}\frac{2k_1k_2}{2k_1k_2\cos k_2a - i(k_2^2+k_1^2)\sin k_2a}, \tag{62}$$

$$R_L = \frac{i(k_2^2-k_1^2)\sin k_2a}{2k_1k_2\cos k_2a - i(k_2^2+k_1^2)\sin k_2a}, \tag{63}$$

$$R_R = e^{-2ik_1a}R_L. \tag{64}$$

2. Double rectangular barrier

Pursuing one step further we investigate a double rectangular barrier [see Fig. 2(c)]

$$u(x) = \begin{cases} u_1, & x<0 \\ u_2, & 0<x<a \\ u_3, & a<x<a+b \\ u_4, & a+b<x<a+b+c \\ u_5, & x>a+b+c. \end{cases} \tag{65}$$

It can be considered, in turn, as a combination of two rectangular barriers of widths a and c located at some distance b.

Substituting the expressions for scattering amplitudes for a single barrier (54)–(57) into (35), (37)–(39) yields

$$T_L^{(4)} = e^{-ik_5(a+b+c)}\frac{2^4k_1k_2k_3k_4}{D^{(4)}(a,b,c;k_1k_2k_3k_4k_5)}, \tag{66}$$

$$T_R^{(4)} = e^{-ik_5(a+b+c)}\frac{2^4k_2k_3k_4k_5}{D^{(4)}(a,b,c;k_1k_2k_3k_4k_5)}, \tag{67}$$

$$R_L^{(4)} = \frac{N^{(4)}(a,b,c;k_1k_2k_3k_4k_5)}{D^{(4)}(a,b,c;k_1k_2k_3k_4k_5)}, \tag{68}$$

$$R_R^{(4)} = -e^{-2ik_5(a+b+c)}\frac{[N^{(4)}(a,b,c;k_1k_2k_3k_4k_5)]^*}{D^{(4)}(a,b,c;k_1k_2k_3k_4k_5)}. \tag{69}$$

Here

$$D^{(4)}(a,b,c;k_1k_2k_3k_4) = e^{-ik_3b}D^{(2)}(a;k_1k_2k_3)D^{(2)}(c;k_3k_4k_5) + e^{ik_3b}N^{(2)}(c;k_3k_4k_5)[N^{(2)}(a;k_1k_2k_3)]^*, \quad (70)$$

$$N^{(4)}(a,b,c;k_1k_2k_3k_4) = e^{-ik_3b}N^{(2)}(a;k_1k_2k_3)D^{(2)}(c;k_3k_4k_5) + e^{ik_3b}N^{(2)}(c;k_3k_4k_5)[D^{(2)}(a;k_1k_2k_3)]^*, \quad (71)$$

and $N^{(2)}$ and $D^{(2)}$ are determined by (59) and (58). In the particular case of a symmetric double barrier ($u_1 = u_3 = u_5 = 0$, $u_2 = u_4 = u$, $k_1 = k_3 = k_5 = k$, $k_2 = k_4 = q$, $a = c$) this expression simplifies and, for example, for the transmission amplitude we have

$$T_L = \frac{16k^2q^2e^{-2ika}}{[4qk\cos qa - 2i(q^2+k^2)\sin qa]^2 + 4(k^2-q^2)^2\sin^2 qa\, e^{2ikb}}. \quad (72)$$

The remarkable symmetry of the scattering amplitudes $T^{(n)}_{R,L}$ and $R^{(n)}_{R,L}$ expressed through $D^{(n)}$ and $N^{(n)}$ [compare (49)–(52), (54)–(57) together with (58), (59), and (66)–(69) together with (70), (71)] allows us to write analytical expressions for more complicated rectangular barriers by inspection.

B. Scattering by a locally periodic potential

The problem of one-dimensional scattering by a finite periodic chain of nonoverlapping barriers or wells (see Fig. 3) is of significant interest because it exhibits the important features of quantum mechanics: tunneling and interference [8,9]. The solution of the problem manifests the origin of the band energy spectrum of periodic potentials — Brillouin zones and forbidden energy gaps — as the number of scattering centers grows, making thus a bridge between atomic scattering (one center) and solid-state physics ($n \to \infty$, semi-infinite periodic chain). It is also of practical interest for the physics of superlattice electronic devices.

This problem was discussed in [7–12] but only the analytical solution for a finite Dirac comb was obtained.

Let us consider scattering from n equally spaced non-overlapping potentials, centered at the positions 0, x_0, $2x_0$, $\ldots$, $(n-1)x_0$. Let $t \equiv t_R = t_L$ and $r_{R,L}$ be the transmission and reflection amplitudes for the single potential. Denote by $T^{(n)} \equiv T^{(n)}_R = T^{(n)}_L$ and $R^{(n)}_{R,L}$ the total transmission and reflection amplitudes for the potential chain with n sites.

The chain containing n sites may be considered as a composition of two potentials — a finite chain of $(n-1)$ sites and a single scatterer.

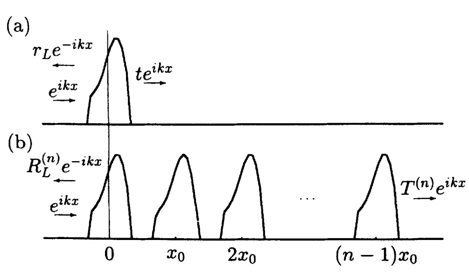

FIG. 3. Sketch of the potentials and scattering geometry: (a) single scatterer $U(x)$, (b) finite periodic potential $U^{(n)}(x) = \sum_{k=0}^{n-1} U(x - kx_0)$.

General formulas (35), (37)–(39) applied to the case under study give the following recurrence relations for $T^{(n)}$ and $R^{(n)}_{R,L}$:

$$\begin{aligned} T^{(n)} &= \frac{T^{(n-1)}t}{1 - R^{(n-1)}_L r_R e^{2ikx_0}}, \\ R^{(n)}_L &= r_L + e^{2ikx_0}\frac{t^2 R^{(n-1)}_L}{1 - R^{(n-1)}_L r_R e^{2ikx_0}}, \\ R^{(n)}_R &= e^{-2ikx_0}R^{(n-1)}_R + \frac{T^{(n-1)}_R T^{(n-1)}_L r_R}{1 - R^{(n-1)}_L r_R e^{2ikx_0}}, \end{aligned} \quad (73)$$

with the natural "boundary" conditions

$$T^{(0)} = 1, \quad R^{(0)}_{R,L} = 0, \quad T^{(1)} = t, \quad R^{(1)}_{R,L} = r_{R,L}. \quad (74)$$

Introducing a notation

$$T^{(n)} = \tilde{T}^{(n)}e^{-ikx_0n}, \qquad R^{(n)}_R = \tilde{R}^{(n)}_R e^{-2ikx_0n}, \quad R^{(n)}_L = \tilde{R}^{(n)}_L \quad (75)$$

from where one can get for the single potential

$$\tilde{t} = te^{ikx_0}, \quad \tilde{r}_R = r_Re^{2ikx_0}, \quad \tilde{r}_L = r_L, \quad (76)$$

we get the following system of equations for $\tilde{T}^{(n)}$ and $\tilde{R}^{(n)}_{L,R}$:

$$\begin{aligned} \tilde{T}^{(n)} &= \frac{\tilde{T}^{(n-1)}\tilde{t}}{1 - \tilde{R}^{(n-1)}_L\tilde{r}_R}, \\ \tilde{R}^{(n)}_L &= \tilde{r}_L + \frac{\tilde{t}\tilde{R}^{(n-1)}_L\tilde{t}}{1 - \tilde{R}^{(n-1)}_L\tilde{r}_R}, \\ \tilde{R}^{(n)}_R &= \tilde{R}^{(n-1)}_R + \frac{\tilde{T}^{(n-1)}_R\tilde{T}^{(n-1)}_L\tilde{r}_R}{1 - \tilde{R}^{(n-1)}_L\tilde{r}_R}. \end{aligned} \quad (77)$$

The solutions of system (77), satisfying the conditions (74), are of the form

$$\begin{aligned} \tilde{T}^{(n)} &= \frac{1}{U_n(z) - \frac{1}{\tilde{t}^*}U_{n-1}(z)}, \\ \tilde{R}^{(n)}_{R,L} &= \frac{\frac{\tilde{r}_{R,L}}{\tilde{t}}U_{n-1}(z)}{U_n(z) - \frac{1}{\tilde{t}^*}U_{n-1}(z)}, \end{aligned} \quad (78)$$

where

$$z = \frac{1}{2}\left(\frac{1}{t} + \frac{1}{t^*}\right) = \frac{1}{2}\left(\frac{e^{-ikx_0}}{t} + \frac{e^{ikx_0}}{t^*}\right) \tag{79}$$

is a real quantity and U_n are the Chebyshev polynomials of the second kind, satisfying the recurrence relations

$$U_{n+1}(z) - 2zU_n(z) + U_{n-1}(z) = 0 \tag{80}$$

and boundary conditions

$$U_{-1}(z) = 0, \qquad U_0(z) = 1. \tag{81}$$

For proving the validity of (78) the identity

$$U_n^2(z) + U_{n+1}^2(z) - 2zU_n(z)U_{n+1}(z) = 1 \tag{82}$$

can be used.

Finally, the scattering amplitudes for the finite periodic chain of n sites,

$$\begin{aligned} T^{(n)} &= \frac{1}{U_n(z) - \frac{e^{ikx_0}}{t^*}U_{n-1}(z)} e^{-ikx_0 n}, \\ R_L^{(n)} &= \frac{\frac{r_L}{t}U_{n-1}(z)}{U_n(z) - \frac{e^{ikx_0}}{t^*}U_{n-1}(z)} e^{-ikx_0}, \\ R_R^{(n)} &= \frac{\frac{r_R}{t}U_{n-1}(z)}{U_n(z) - \frac{e^{ikx_0}}{t^*}U_{n-1}(z)} e^{-ikx_0(2n-1)}. \end{aligned} \tag{83}$$

Using the identity (82), we get for the transmission and reflection coefficients

$$|T^{(n)}|^2 = \frac{1}{1 + \frac{|r|^2}{|t|^2}U_{n-1}^2(z)}, \tag{84}$$

$$|R_L^{(n)}|^2 \equiv |R_R^{(n)}|^2 = \frac{\frac{|r|^2}{|t|^2}U_{n-1}^2(z)}{1 + \frac{|r|^2}{|t|^2}U_{n-1}^2(z)}, \tag{85}$$

where $r \equiv |r_L| = |r_R|$.

The transmission resonances $|T^{(n)}|^2 = 1$ occur when either $|r| = 0$ or $U_{n-1}(z) = 0$. The former case may happen when the single potential has an internal (for example, double-barrier) structure and therefore is transparent at some energies of the incident particles [16]. In the latter case the energies of the incident particles are solutions of the equation

$$z = \cos\left(m\frac{\pi}{n}\right), \quad m = 1, \ldots, n-1. \tag{86}$$

In the limit $n \to \infty$ the system of scatterers becomes a semi-infinite periodic chain. For this limiting case the potential must be opaque, i.e., $T^{(\infty)} = 0$, when the energies of the scattered particles fall into the forbidden energy gaps of the periodic potential. Indeed, $\lim_{n\to\infty} U_n^2(z) = \infty$, whenever the argument of the Chebyshev polynomial is outside the range $(-1, 1)$. Therefore $T^{(\infty)} = 0$, for $|z| > 1$. The equation ($|z| = 1$)

$$\left|\frac{e^{-ikx_0}}{t} + \frac{e^{ikx_0}}{t^*}\right| = 2 \tag{87}$$

determines the edges of allowed and forbidden energy bands for the infinite periodic chain.

The calculated transmission coefficient for a chain of three inverted parabolic barriers are depicted in Fig. 4, together with the solutions of (86), (87). The scattering potential is of the form

$$U(x) = \begin{cases} U_0 - \frac{1}{2}m\omega^2x^2, & |x| < \sqrt{\frac{2U_0}{\hbar\omega}}\,\delta \\ 0, & |x| \geq \sqrt{\frac{2U_0}{\hbar\omega}}\,\delta, \end{cases} \tag{88}$$

where m is the mass of the incident particle, ω is the angular frequency, and $\delta = \sqrt{\hbar/m\omega}$ is the characteristic linear size of the ground state of the particle in the harmonic potential $\frac{1}{2}m\omega^2x^2$. Parameters for numerical calculations were chosen as follows: $x_0 = 8\delta$, $U_0 = 2\hbar\omega$.

The scattering amplitudes for the single inverted parabolic barrier are calculated by the numerical method described in Sec. IV. This combination of the numerical method of Sec. IV with the analytical solutions (84) and (85) has the following advantages: (a) the positions of narrow resonance peaks, where calculations have to be carried out very carefully, are known for chains of arbitrary length after the solution of the scattering problem

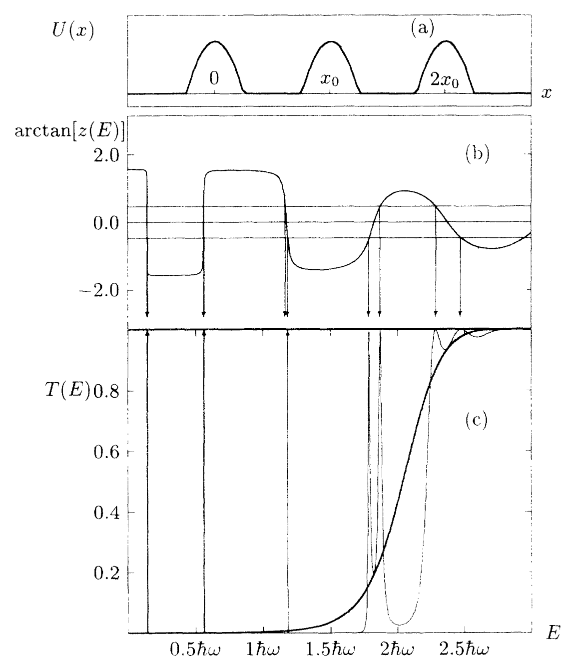

FIG. 4. Transmission coefficient for the periodic chain of three inverted parabolic barriers of frequency ω. (a) Sketch of the potential. (b) Function $z(E)$ determined by Eq. (79) of the text. Points of intersection of the $z(E)$ graph with thin lines marked by vertical arrows are the graphical solutions of Eq. (86) and determine the positions of the transparency resonances. Points of intersection with dotted lines are the graphical solutions of Eq. (87) for the gap edges of semi-infinite chain. (c) Transmission coefficient $T(E)$ for single barrier (bold line) and periodic chain (thin line). Resonances too narrow to be drawn on the figure are marked by vertical arrows.

(96)–(99) for a single barrier only; (b) the computational time does not depend on the size of the chain.

IV. DIFFERENTIAL EQUATIONS FOR SCATTERING AMPLITUDES AND THE TRANSFER MATRIX

In Sec. II B of this article we obtained formulas allowing us to calculate the scattering from a two-segment potential barrier. Developing this approach further, we added a third barrier to the progression of the previous two in Sec. III B, and then a fourth to the progression of the previous three, and an nth to the progression of the previous $(n-1)$. In the same way, as when deriving formulas (35), (37)–(39), we put limits neither on the width of the segments nor on the distances between them. Therefore one can use the formulas also to combine arbitrary rectangular potentials with vanishing distance between them.

Any potential may be considered as a limit of a set of rectangular barriers, with the width of the barriers tending to zero. Therefore recurrence formulas (35), (37)–(39) can be modified, allowing us to calculate the transmission and reflection amplitudes (and therefore also the coefficients) for *any* potential. We will see below that in the case of a nonsegmented potential the recurrence relations are transformed to ordinary differential equations.

To obtain the differential equations we use the "truncated potentials" as an intermediate tool.

The potential $U(x)$ truncated at $x = x_0$ is defined as

$$U^\tau(x) = U(x)\theta(x_0 - x), \tag{89}$$

where $\theta(x)$ is the unit step function:

$$\theta(x) = \begin{cases} 0, & x < 0 \\ 1, & x > 0. \end{cases} \tag{90}$$

Solutions of the Schrödinger equation with truncated potentials are investigated in [13], Sec. 2.9.

The idea is to put in series a potential truncated at the point x_0 and a narrow rectangular potential of width Δx and height $U(x_0)$, such that the distance between two segments is zero, obtaining thus a potential truncated at the point $x_0 + \Delta x$ (see Fig. 5). By taking the limit $\Delta x \to 0$, the recurrence relations are converted to a system of differential equations, such that all derivatives are taken with respect to the truncation coordinate x_0. Scattering coefficients and elements of the transfer matrix for the nontruncated potential $U(x)$ are then the solutions of these equations with appropriate boundary conditions in the limit $x_0 \to +\infty$.

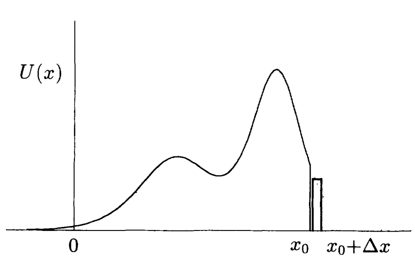

FIG. 5. Arbitrary potential $U(x)$ (dotted line), associated truncated potential $U^\tau(x_0)$ (thin line), and narrow rectangular potential of height $U(x_0)$ (bold line).

A. Differential equations for reflection and transmission amplitudes

Let us denote the transmission and reflection amplitudes for a potential truncated at the point x_0 by $T_{R,L}(x_0)$ and $R_{R,L}(x_0)$. Using the composition law (35), (37)–(39) we add an infinitely narrow rectangular barrier of width Δx and height $U(x_0)$ to a truncated potential at $x = x_0$ so that the distance between the two barriers is zero (see Fig. 5), obtaining thus $T_{R,L}(x_0 + \Delta x)$ and $R_{R,L}(x_0 + \Delta x)$.

From (62) and (63) we have the following expressions for a narrow rectangular barrier of width Δx ($\Delta x \to 0$, $\sin \Delta x \approx \Delta x$, $\cos \Delta x \approx 1$) located at the origin $x = 0$ of the coordinate axis:

$$T_L^\Delta = T_R^\Delta = \frac{1 - ik_1 \Delta x}{1 - \frac{i}{2k_1}\Delta x (k_1^2 + k_2^2)} = 1 + a(x)\Delta x, \tag{91}$$

$$R_L^\Delta = R_R^\Delta = \frac{\frac{i}{2k_1}\Delta x (k_2^2 - k_1^2)}{1 - \frac{i}{2k_1}\Delta x (k_1^2 + k_2^2)} = a(x)\Delta x, \tag{92}$$

where

$$a = \frac{i}{2k_1}(k_2^2 - k_1^2). \tag{93}$$

Let us choose the origin of the energy axes such that $\lim_{x\to\infty} U(x) = 0$. Then, $k_1 = k$, $k_2^2 = k^2 - (2m/\hbar^2)U(x)$, and

$$a(x) = -\frac{i}{k}\frac{m}{\hbar^2}U(x). \tag{94}$$

Taking into account that the distance between the reference points of the truncated and the narrow rectangular potential is x_0, from (35) we have for $T_L(x_0 + \Delta x)$

$$T_L(x_0 + \Delta x) = T_L(x_0) + T_L(x_0)\Delta x a(x_0)\left(1 + R_R e^{2ikx_0}\right). \tag{95}$$

Here (91), (92) are used, and only terms linear in Δx are kept.

Carrying out the limit $\Delta x \to 0$ we get an ordinary differential equation for $T_L(x_0)$:

$$T_L'(x_0) = a(x_0)T_L(x_0)\left(1 + R_R e^{2ikx_0}\right). \tag{96}$$

Here and below the prime denotes differentiation with respect to the truncation position x_0.

Similarly, from the recurrence relation (37)

$$T_R'(x_0) = a(x_0)T_R(x_0)\left(1 + R_R e^{2ikx_0}\right), \tag{97}$$

from (38)

$$R_L'(x_0) = a(x_0)T_L(x_0)T_R(x_0)e^{2ikx_0}, \tag{98}$$

and from (39)

$$R_R'(x_0) = a(x_0)e^{-2ikx_0}\left(1 + R_R e^{2ikx_0}\right)^2. \tag{99}$$

Let us discuss now the boundary conditions for the system of ordinary differential equations (96)–(99). If the potential $U(x)$ is localized, i.e., $\lim_{x\to\pm\infty} U(x) = 0$, then the associated potential, truncated at $x = -\infty$, is $U^\tau(x) \equiv 0$. Therefore the boundary conditions imposed at the point $x_0 = -\infty$ are as follows:

$$\begin{aligned} R_L(-\infty) = R_R(-\infty) = 0, \\ T_L(-\infty) = T_R(-\infty) = 1. \end{aligned} \tag{100}$$

If the potential $U(x)$ is not localized, i.e., $U(-\infty) = u_- \neq 0$ [let us remember that by convention $U(+\infty) = 0$], then associated potential $U^\tau(x)$ truncated at some point x_τ sufficiently far to the left, is the potential step of height u_-. Therefore the boundary conditions for this case are as follows:

$$T_L(x_\tau) = \frac{2k_1}{k_1 + k_2} e^{i(k_1-k_2)x_\tau}, \tag{101}$$

$$R_L(x_\tau) = \frac{k_1 - k_2}{k_1 + k_2} e^{2ik_1 x_\tau}, \tag{102}$$

$$T_R(x_\tau) = \frac{2k_2}{k_1 + k_2} e^{i(k_1-k_2)x_\tau}, \tag{103}$$

$$R_R(x_\tau) = \frac{k_2 - k_1}{k_2 + k_1} e^{-2ik_2 x_\tau}, \tag{104}$$

where $k_1 = \frac{1}{\hbar}\sqrt{2m(E-u_-)}$, $k_2 = \frac{1}{\hbar}\sqrt{2mE}$, and the relations (48), (41)–(44) were used. These conditions are imposed at the arbitrary point x_τ in the region, where the scattering potential $U(x)$ reaches its left asymptotic value.

B. Differential equations for the transfer matrix

Let us denote by $\alpha(x_0)$ and $\beta(x_0)$ elements of the transfer matrix, corresponding to a scattering potential $U(x)$, truncated at the point x_0:

$$M^t(x_0) = \begin{pmatrix} \alpha(x_0) & \beta(x_0) \\ \beta^*(x_0) & \alpha^*(x_0) \end{pmatrix}. \tag{105}$$

The transfer matrix of this potential truncated at the point $x_0 + \Delta x$ is

$$M^t(x_0 + \Delta x) = \begin{pmatrix} \alpha(x_0+\Delta x) & \beta(x_0+\Delta x) \\ \beta^*(x_0+\Delta x) & \alpha^*(x_0+\Delta x) \end{pmatrix}. \tag{106}$$

The transfer matrices of two truncated potentials are connected by the relation

$$M(x_0 + \Delta x) = M^\Delta M(x_0), \tag{107}$$

where M^Δ is the transfer matrix of the narrow rectangular barrier. From Eqs. (91), (92) using (11), (12) we get

$$M^\Delta = \begin{pmatrix} 1 + a(x_0)\Delta x & a(x_0)\Delta x e^{-2ikx_0} \\ -a(x_0)\Delta x e^{2ikx_0} & 1 - a(x_0)\Delta x \end{pmatrix}, \tag{108}$$

where $a(x)$ is determined by (93), (94). Substituting (105), (106), and (108) into (107) and taking the limit $\Delta x \to 0$, we get the following linear differential equations for the matrix elements of the transfer matrix:

$$\frac{d\alpha(x_0)}{dx_0} = a(x_0)\left[\alpha(x_0) + e^{-2ikx_0}\beta^*(x_0)\right], \tag{109}$$

$$\frac{d\beta^*(x_0)}{dx_0} = -a(x_0)\left[\alpha(x_0)e^{2ikx_0} + \beta^*(x_0)\right]. \tag{110}$$

In the case of scattering on a localized potential, the boundary conditions for (109), (110) are as follows:

$$\alpha(-\infty) = 1, \quad \beta^*(-\infty) = 0. \tag{111}$$

If the potential $U(x)$ is not localized, similarly to the case of differential equations for the scattering amplitudes we get

$$\alpha(x_\tau) = \frac{k_1 + k_2}{2k_2} e^{i(k_1-k_2)x_\tau}, \tag{112}$$

$$\beta(x_\tau) = \frac{k_1 - k_2}{2k_2} e^{i(k_1+k_2)x_\tau}. \tag{113}$$

These conditions are imposed at an arbitrary point x_τ in the region where the scattering potential $U(x)$ reaches its left asymptotic value.

C. Analytical solution of the differential equations

The simplest case for an analytical solution of Eqs. (96)–(99) or (109), (110) is the symmetric rectangular barrier. The potential may be considered as a truncated potential associated with a wider rectangular barrier of the same height. It is easy to check that the scattering amplitudes (62)–(64), where the coordinate of the right border of the barrier is now the truncation parameter, indeed are the solution of Eqs. (96)–(99).

As a somewhat more elaborate example, consider scattering on the following reflectionless potential:

$$U(x) = -\frac{\hbar^2}{m}\frac{1}{\cosh^2(x)}. \tag{114}$$

The solutions of Eqs. (96)–(99) are

$$T(x_0) = \frac{2k(k+i)}{k^2 + 1 + (k - i\tanh x_0)^2}, \tag{115}$$

$$R_L(x_0) = e^{2ikx_0}\frac{k+i}{k-i}\frac{1/\cosh^2(x_0)}{k^2 + 1 + (k - i\tanh x_0)^2}, \tag{116}$$

$$R_R(x_0) = -e^{-2ikx_0}\frac{1/\cosh^2(x)}{k^2 + 1 + (k - i\tanh x_0)^2}. \tag{117}$$

Similarly, the solutions of Eqs. (109), (110) are

$$\alpha(x) = \frac{k^2 + 1 + (k + i\tanh x)^2}{2k(k-i)}, \tag{118}$$

$$\beta^*(x) = -\frac{e^{2ikx}}{2k(k-i)\cosh^2(x)}. \tag{119}$$

Taking the limit $x_0 \to +\infty$ we get the correct scattering amplitudes for the reflectionless potential (114):

$$T = \frac{k+i}{k-i}, \quad R = 0. \tag{120}$$

It is possible to establish general relations between the solutions of (96)–(99), (109), (110), and the Schrödinger equation. Let us use the following ansatz for the solutions of the differential equations (109) and (110):

$$\alpha(x) = -\frac{e^{-2ikx}}{2ik}\frac{d}{dx}\left[\psi(x)e^{ikx}\right], \tag{121}$$

$$\beta(x) = \frac{e^{2ikx}}{2ik}\frac{d}{dx}\left[\psi(x)e^{-ikx}\right]. \tag{122}$$

Substituting the ansatz (121) and (122) into the first differential equation (109) we find that $\psi(x)$ is the solution of the following equation:

$$\frac{d^2}{dx^2}\psi(x) + \left(k^2 - \frac{2m}{\hbar^2}U(x)\right)\psi(x) = 0, \tag{123}$$

i.e., $\psi(x)$ is the solution of the Schrödinger equation for the potential $U(x)$.

From this result we conclude that the system of equations (96)–(99), and (109) and (110) has analytical solutions for all potentials $U(x)$ which lead to analytical solutions of the Schrödinger equation.

D. Numerical solution of the differential equations

In the general case Eqs. (96)–(99), (109) and (110) cannot be integrated analytically and have to be solved numerically. The algorithm for the numerical solution is as follows: Eq. (99) is an ordinary differential equation of the Riccati type, it can be integrated numerically and R_R can be calculated. If only scattering probabilities are required, this is the only equation to be solved, because the transmission and reflection coefficients are connected by relation (15). If the complete solution of the scattering problem is required, i.e., scattering phases are also of interest, one gets $T_{R,L}$ directly from (96) and (97), respectively. Substituting then $T_{R,L}$ into (98), one can find R_L. Finally, the wave function may be obtained integrating the relations (121), (122).

Formulas (96)–(99) not only allow one to find the reflection and transmission amplitudes directly, instead of extracting them from the wave function, but rather the eigenvalue problem of the Schrödinger equation is replaced by a boundary-value problem, much easier to deal with, especially in numerical calculations.

In the present work two examples demonstrating the numerical solutions of the differential equations are presented. As the first example we consider the periodic chain of inverted parabolic barriers [see Fig. 4(a)]. The scattering potential is localized and differential equations are solved using the boundary conditions (100). The results of the calculations are depicted in Fig. 4 and have been discussed already in Sec. III B. They may be compared with similar ones obtained by a different method in [9].

As the second example we consider the resonant tunneling diode having a parabolic profile. The energy diagrams for zero and for nonzero voltage applied across the diode are depicted in Figs. 6(a) and 6(b), respectively. This system is expected to have equally spaced (unlike the rectangular double-barrier diode) transmission resonances and hence peaks in current-voltage characteristics. It can have therefore a potential application as a quantum electron device, and was studied experimentally [1].

The scattering potential is of the form

$$U(x) = U_0(x) + U_\Delta(x), \tag{124}$$

where (see Fig. 6)

$$U_0(x) = \begin{cases} 0, & |x| > (a+b) \\ u_0, & a \le |x| \le (a+b) \\ \frac{m\omega^2 x^2}{2}, & |x| \le a \end{cases} \tag{125}$$

is the zero-voltage potential, m is the (effective) electron mass, ω is the frequency, corresponding to the parabolic well, $u_0 = \frac{1}{2}m\omega^2 a^2$,

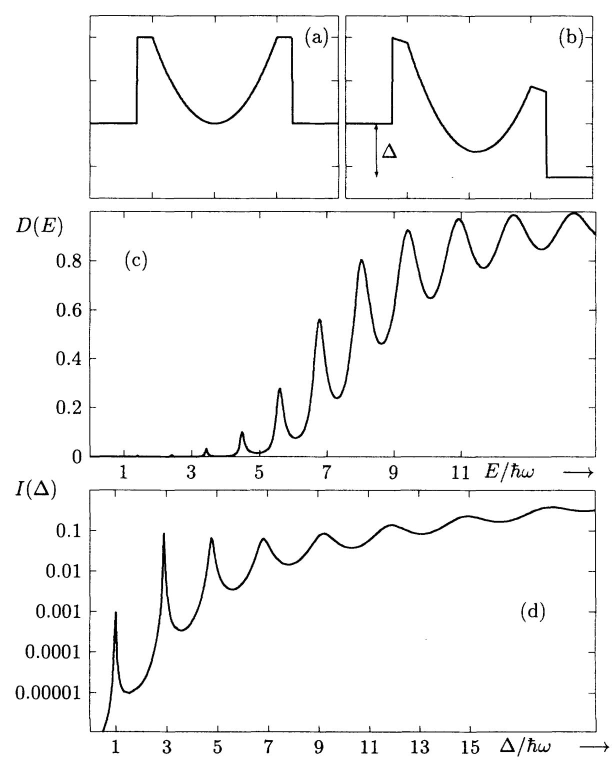

FIG. 6. Resonant-tunneling diode having a parabolic profile. Energy diagrams with no voltage bias (a) and with voltage bias Δ (b) across the diode. (c) Transmission probability vs energy of incident particles, $\Delta = 6\hbar\omega$. (d) Current (arbitrary units) vs voltage across the parabolic-well diode, $E = 3\hbar\omega$.

$$U_\Delta(x) = \begin{cases} \Delta, & x < -(a+b) \\ \frac{\Delta}{2}\left(1 - \frac{x}{a+b}\right), & -(a+b) \le x \le (a+b) \\ 0, & x > (a+b) \end{cases} \tag{126}$$

is the voltage applied across the barrier. (Here we neglect effects connected with the accumulation and redistribution of charges across the barrier.)

In contrast to the first example, the scattering potential for nonzero voltage Δ applied across the barrier is not localized $[\lim_{x\to-\infty} U(x) \neq \lim_{x\to+\infty} U(x)]$ and differential equations (96)–(99) or (109) and (110) must be solved with the boundary conditions (101)–(104) or (112) and (113), respectively.

Numerical calculations are carried out for the following parameters of the parabolic barrier: $a = 4\delta$, $b = 0.3\delta$, where $\delta = \sqrt{\hbar/m\omega}$ is the characteristic size of the ground state in the parabolic potential. The results of the calculations are presented in Fig. 6. The probability of transmission through the tunneling diode versus the kinetic energy of the incident particle is presented in Fig. 6(c). The approximately equally spaced progression of transmission resonances corresponds to equidistant virtual levels in the potential (124).

Figure 6(d) presents the calculated current-voltage characteristics $I(\Delta)$ of the tunneling diode:

$$I(\Delta) = cg(\Delta)\Delta, \tag{127}$$

where the factor c depends on the system of units used, and the dimensionless conductance $g(\Delta)$ is expressed through the amplitudes of scattering on the potential barrier via the relation [2,3] (see Appendix for details)

$$g(\Delta) = \frac{|T|^2}{1 - |T|^2}. \tag{128}$$

In spite of the crudeness of the approximation (126) the results are in good qualitative agreement with the experimental data [1].

V. CONCLUDING REMARKS

In the present work interesting results for the theory of one-dimensional scattering are obtained. We have developed a method which deals directly with scattering amplitudes without introducing any auxiliary objects.

In Sec. II B the algebraic recurrence approach to the one-dimensional scattering is developed. The formulas obtained are convenient both for analytical (including the usage of computer algebra systems) and numerical calculation of scattering data. In the proposed method one deals directly with probability amplitudes, i.e., with the complex numbers with the absolute value less than one. Therefore the method is free from the numerical problem of the loss of significant digits arising from the cancellation in sums of different in magnitudes numbers with the opposite signs. The outstanding feature of the recurrence approach is the fact that computational effort scales logarithmically with the number of subparts of the potential. Indeed, if optimal order of the potential decomposition is selected, after the nth step of the iteration process 2^n subparts of the potential are combined, as it was demonstrated in Sec. III A. The method is most suitable for the calculation of reflection and transmission amplitudes for complicated potential structures.

The system of differential equations derived in Sec. IV is expected to be suitable for the numerical calculation of scattering amplitudes for electrons in semiconductor electron devices or light in thin-film coatings and for the determination of tunneling times [4,5] in complicated barriers. The linear differential equations for the transfer matrix (109) and (110) may be useful in investigating properties of one-dimensional disordered systems.

Our interest is concentrated on the scattering states, however, the method can be applied to investigate bound and resonant states, considering the poles of the transmission amplitude. Another approach to the numerical determination of the energies of bound states is to convert formally a bound potential $U(x)$ into scattering one [for example into $U(x)e^{-ax^2}$ with sufficiently small a], and determine the positions of narrow scattering resonances.

Although in the present work only quantum-mechanical systems are considered, the formulas obtained are also applicable for the description of the scattering of electromagnetic or elastic waves in one dimension.

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APPENDIX

In this appendix, following Refs. [2,3], we present the derivation of Eq. (128),

$$g(\Delta) = \frac{|T|^2}{1 - |T|^2}$$

for the conductivity of a potential barrier.

The two following assumptions are natural for the investigation of quantum electron devices.

The temperature is low enough so that one deals with a degenerate Fermi gas and only electrons with the energy close to the Fermi level make a contribution to the electric current.

The thermodynamic reservoirs at the two ends of the barrier destroy the coherence between waves incident on the barrier from the left and from the right such that their *incoherent* superposition has to be considered (i.e., one has to add not amplitudes but probabilities and probability currents).

We imagine that the Fermi level of the reservoir on the left from the barrier is raised by Δ relative to that on the right.

By definition the conductance G is

$$G = \frac{I}{\Delta}, \tag{A1}$$

where I is the electric current through the barrier. The idea is to express I and Δ through the probability currents and changes in the density of electrons on both sides of the barrier.

Let the probability currents of electrons incident on the barrier from the left and from the right be j_l and j_r, respectively. Then the electric current through the barrier is

$$I \sim (j_l - j_r)|T|^2. \tag{A2}$$

The density of electrons on the left from the barrier is the total probability current on the left divided by the speed of electrons:

$$n_l \sim j_l + j_l(1 - |T|^2) + j_r|T|^2, \tag{A3}$$

where we add the current incident on the barrier from the left, the current reflected from the barrier, and the current transmitted through the barrier from the right. The averaging over a space of several wavelengths is assumed in (A3).

Similarly, the density of electrons on the right from the barrier is

$$n_r \sim j_r + j_r(1 - |T|^2) + j_l|T|^2. \tag{A4}$$

The extra density of electrons on the left from the barrier is

$$\delta n = n_l - n_r \sim (j_l - j_r)(1 - |T|^2). \tag{A5}$$

At the same time

$$\delta n = \rho\Delta \sim \Delta, \tag{A6}$$

where ρ is the density of states.

Substituting (A6) and (A2) into (A1) and using (A5) we get

$$G \sim \frac{|T|^2}{1 - |T|^2}. \tag{A7}$$

As it was shown in [3] the exact coefficient in this equation is $e^2/\pi\hbar$. Finally for the dimensionless conductance

$$g = \frac{\pi\hbar}{e^2}G \tag{A8}$$

we get the expression (128).

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