Transmission, reflection, and resonance formation in one-dimensional systems

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A method is developed that treats on equal footing bound states, resonance formation, and scattering problems in one-dimensional systems. The approach allows one to deal with nonlocal, energy-dependent potentials and is conceptually analogous to the variable phase method where the role of the scattering phase and the amplitude functions is played by nonlocal reflection and transmission functions. The formal results are illustrated and analyzed by simple examples and the physical significance of these examples is pointed out.

I. INTRODUCTION

The question of how a quantum particle penetrates, being trapped or ejected from a potential barrier, has been the subject of intensive research since the early days of quantum physics. The interest in this problem is rooted in its ubiquitous occurrence in various physical, chemical, and biological processes [1–4]. To name just but few examples, the key ingredient of scanning tunneling spectroscopy of surface-deposited molecules is the tunneling of the tip electrons to the conduction band of the surface through the molecular (tunneling) region where the electrons can be back reflected, resonantly transmitted or captured [5]. Furthermore, constrictions in a quasi-one-dimensional quantum wire, that act as tunneling barriers, can nowadays be engineered with an impressive accuracy [9]. The transmittance through the constrictions governs the transport properties of the wire; hence the central question to be addressed by theory is how the barrier characteristics affect the transmission and reflection coefficients. Having this kind of problems in mind we set out to reconsider the quantum tunneling from nonlocal energy-dependent potentials. The nonlocality can be brought about by various factors; perhaps the most widely known case occurs when an electronic system is described within a mean-field approach such as the Hartree-Fock theory. Due to the exchange (Fock) term the single particle potentials are inherently nonlocal. The aim of the present work is to treat on the same footing bound, scattering, and resonant states in one-dimensional systems in the presence of a nonlocal energy-dependent potential, V. The method is the one-dimensional (1D) analogue to the variable phase method (VPA) [6,7], which is well-known in the three-dimensional case. Recently we have generalized the VPA as to include nonlocal interactions [8]. The method relies on introducing, instead of the wave function, the so-called transmission $T(x)$ and reflection functions $R(x)$ that depend on the distance x. The asymptotic $(x \rightarrow \infty)$ values of these functions tend to the physical transmission and reflection coefficients for the potential V. At the finite distance x the transmission and the reflection functions can also be interpreted as the transmission and the reflection *coefficients* for the potential $V_{x_{cut}}(x)$ obtained by appropriately cutting-off $V(x)$ at x_{cut}. As demonstrated below, the reflection function $R(x)$ thus contains the essential information pertinent to bound, scattering, and resonant states for a whole class of potentials $V_{x_{cut}}$, $\forall x_{cut} \in (-\infty, +\infty)$.

II. GENERAL DEFINITIONS AND OUTLINE

We consider the time-independent, nonrelativistic scattering of a particle with the energy k^2 impinging on a 1D nonlocal potential from the left to the right. We use units in which $2m = 1 = \hbar$, $Z = 1$, where m and Z are the mass and the charge of the particle. The nonlocal potential is introduced as an integral operator $\hat{V}$ acting along the entire x axis ($\hat{V}$ may well have a local component), i.e., the particle wave function ψ satisfies

$$\left[\frac{d^2}{dx^2} + k^2 \right] \psi(x) = \hat{V}\psi = \int_{-\infty}^{+\infty} V(x,x') \psi(x') dx'. \quad (1)$$

The derivation given below is valid as it stands in case the potential $V(x,x')$ is energy-dependent. To simplify notation we will suppress however this energy dependence in the equations. The key idea of the present work, pointed out by Calogero and Babikov [6,7] for the general case, is to re-express the wave function ψ in terms of observable quantities. To do that one converts the second-order differential Schrödinger equation into two (coupled) first-order differential equations. This is achieved by casting ψ as a superposition of transmitted and reflected plane waves weighted with the position dependent amplitudes $T(x)$ and $R(x)$,

$$\psi(x) = T(x)\left[e^{ikx} + R(x)e^{-ikx} \right]. \quad (2)$$

In addition, for a unique representation we make furthermore the ansatz

$$\frac{d}{dx}\psi(x) = T(x)\left[\frac{d}{dx}e^{ikx} + R(x)\frac{d}{dx}e^{-ikx} \right]$$
$$= ikT(x)\left[e^{ikx} - R(x)e^{-ikx} \right]. \quad (3)$$

Instead of solving for $\psi(x)$ one determines the amplitudes $T(x)$ and $R(x)$. The advantage of doing this becomes obvious by inspecting the properties of these functions, in particular those of the function R. To this end we derive at first the differential equations governing $T(x)$ and $R(x)$ and inspect the mathematical structure and the symmetry properties of these equations. We then illustrate the various features of the reflection and transmission amplitudes, R and T, by some numerical examples. We start our analysis by an interpretation of the physical sense of $R(x)$ and $T(x)$ and show how

these functions are connected to the reflection and transmission coefficients. As shown below, the knowledge of the spatial behavior of $R(x)$ and $T(x)$ may be exploited as a guide for the construction of one-dimensional structures with desired reflection properties. We will also explore the parametrical dependence of $R(x;\mathbf{k})$ on the complex wave vector $\mathbf{k}$ with the following results: the dependence on a *real positive* wave vector $\mathrm{Re}(\mathbf{k})=k>0$ allows one to address questions arising in scattering problems such as the energetic conditions for the resonant penetration of a particle through a potential barrier. These conditions are extracted from the zeros of $R(\mathbf{k})$. The eigenvalue problem is formulated and resolved by considering the reflection function $R(x;\mathbf{k})$ that depends on a *pure imaginary* wave vector $\mathbf{k}=i\kappa$. Finally, operating in the whole complex $\mathbf{k}$ plane we utilize the reflection amplitude for the description of quantum decay or fusion of compound systems via quasibound states with a finite lifetime.

III. DETERMINING EQUATIONS FOR THE REFLECTION TRANSMISSION FUNCTIONS

To illustrate the physical properties of the complex functions $T(x)$ and $R(x)$ we consider a particle that impinges from $x\to-\infty$ to $x\to+\infty$ onto a localized potential. At $x\to-\infty$ the function $T(x)$ is determined by the normalization of the flux of the incident particles and can thus be normalized to unity $T(x\to-\infty)=1$ [16]. The absence of the reflection behind the potential at $x\to+\infty$ is signaled by the condition $R(x\to+\infty)=0$.

To obtain the determining equations for $T(x)$ and $R(x)$ we transform by means of Eqs. (2) and (3) the second-order Schrödinger equation (1) for the wave function to an equivalent set of two coupled first-order differential equations for the functions $T(x)$ and $R(x)$ (details of the derivation are given in the Appendix). The results are

$$\frac{d}{dx}R(x) = -\frac{1}{ik}F^2(x)V(x), \tag{4}$$

$$\frac{1}{T(x)}\frac{dT}{dx} = +\frac{1}{ik}F(x)e^{-ikx}V(x). \tag{5}$$

The function $V(x)$ is given by

$$V(x) = \int_x^{+\infty} V(x,x')\cosh\left\{ik\int_x^{x'}\frac{G(x'')}{F(x'')}dx''\right\}dx'. \tag{6}$$

As stated above the initial integration conditions are $R(x\to+\infty)=0$, $T(x\to-\infty)=1$. Here we introduced the auxiliary functions

$$F(x) = e^{ikx} + R(x)e^{-ikx}, \quad G(x) = e^{ikx} - R(x)e^{-ikx}.$$

A key element of the above relations is the independence of the determining equation for $R(x)$ on the transmission function T. This property is important insofar as a number of physical quantities follow solely from R (for example, eigenenergies), without the need to calculate T. This reduces substantially the computational efforts.

In case $T(x)$ (or the wave function ψ) is required, one evaluates at first the function $R(x)$, inserts it into Eq. (5) and then performs the integration

$$T(x) = \exp\left(\frac{1}{ik}\int_{-\infty}^x dx'\left[1 + R(x')e^{-2ikx'}\right]V(x')\right). \tag{7}$$

The case of a local potential can be retrieved from the above equations upon the assumption $V(x,x')=V(x')\delta(x-x')$ which leads to the following relations:

$$\frac{d}{dx}R(x) = -\frac{V(x)}{2ik}\left[e^{ikx} + R(x)e^{-ikx}\right]^2, \tag{8}$$

$$\frac{1}{T(x)}\frac{dT}{dx} = +\frac{V(x)}{2ik}\left[1 + R(x)e^{-2ikx}\right]. \tag{9}$$

We note that for *nonlocal* potentials the equations for R and T fulfill the particle conservation law at the asymptotical spatial points $x\to\pm\infty$ only. In contrast, for local potentials the probability flux density

$$j(x) = 2k|T(x)|^2[1 - |R(x)|^2] \tag{10}$$

is conserved at each point x because $(d/dx)j(x)=0$ provided the potential is real. In the case of a complex potential $U(x)=V(x)+iW(x)$ the change of the flux is determined by the imaginary part $W(x)$ only. A positive (negative) sign of this part describes the gain (loss) of particles when scattering off the potential. This is evident by casting the gradient of the flux density in the form

$$\frac{d}{dx}j(x) = \frac{W(x)}{k}\left\{1 + |R(x)|^2 + 2\mathrm{Re}\left[R(x)e^{-2ikx}\right]\right\} \tag{11}$$

and noting that the expression in the curly braces is nonnegative [17].

In the derivation of the reflection-transmission equations we introduced the wave vector k as an arbitrary free parameter. For dealing with continuum state problems the wave vector is real. For the description of bound systems such as the solution of eigenvalue problems and the treatment of the decay or fusion of composite systems, we analytically continue the reflection amplitude to the complex plane of the wave vector $\mathbf{k}=k+i\kappa$; $k,\kappa\in\mathbb{R}$. To do that we consider at first the symmetry properties of the function R, as dictated by Eq. (4) for complex wave vectors. The general solution of this equation possesses two symmetry properties: First, the replacement of the parameter $\mathbf{k}$ by $-\mathbf{k}$ leads to the following relation for the inverse reflection function $1/R(x)$, i.e.,

$$\frac{d}{dx}R(x,-\mathbf{k}) = -\frac{1}{-i\mathbf{k}}\left[e^{-ikx} + R(x)e^{ikx}\right]^2 V(x) = \frac{d}{dx}\left(\frac{1}{R(x,\mathbf{k})}\right). \tag{12}$$

Therefore, we conclude that

$$R(x,-\mathbf{k}) = R^{-1}(x,\mathbf{k}). \tag{13}$$

The origin of this property is the quadratic dependence of the Schrödinger equation on the wave vector. The second property of the general solution is
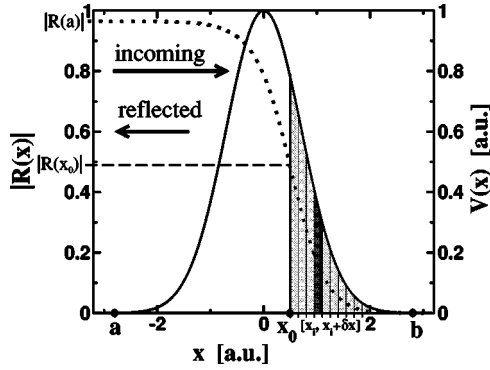
FIG. 1. The spatial variation of the modulus of the reflection function $R(x)$ (dashed curve) describing the scattering of a particle impinging on the Gaussian barrier $V(x)=e^{-x^2}$ (black curve). The particle has the positive real wave vector $k=0.3$ a.u. The zeros value $|R(b)|=0$ indicates the absence of reflection of the incident wave "behind" the barrier. The squared value of $R(x)$ at the point a "before" potential hill coincides with the reflection coefficient $|R(a)|^2=R_c$ for the whole barrier. The value $|R(x_0)|^2$ yields the co-efficient of the reflection from the cut-off potential part (dashed area, see the text for details). Note that $R(x)$ is a dimensionless quantity, whereas the potential is plotted in atomic hartree units.

$$R^*(x,\mathbf{k}^*) = R^{-1}(x,\mathbf{k}) \tag{14}$$

and it follows from the Hermiticity of the potential $V^+=V$ which dictates that

$$\frac{d}{dx}R^*(x,\mathbf{k}^*) = \left(\frac{d}{dx}R(x,\mathbf{k}^*)\right)^*$$

$$= -\frac{1}{-i(\mathbf{k}^*)^*}\left[e^{-i(\mathbf{k}^*)^*x} + R(x)e^{i(\mathbf{k}^*)^*x}\right]^2\hat{V}(x)$$

$$= \frac{d}{dx}\left(\frac{1}{R(x,\mathbf{k})}\right).$$

The initial condition $R(+\infty,k)=0$ for the integration and the two properties stated by Eqs. (13) and (14) require a mirror symmetry of the amplitude $R(x,\mathbf{k})$ with respect to the imaginary axis in the complex wave vector plane, i.e.,

$$R(x,k+i\kappa) = R(x,-k+i\kappa). \tag{15}$$

It is important to note that these arguments are valid for any value of the spacial variable x. Furthermore, the mirror symmetry restricts the calculations to only one half of the **k** plane.

IV. PHYSICAL SIGNIFICANCE OF THE REFLECTION AMPLITUDE AND SPATIALLY MANIPULATED RESONANT TUNNELING

To elucidate the physical meaning of the amplitudes R and T we discuss numerical results for some simple examples; we note however that the interpretation given below does not depend on the shape of the barrier or whether the potential is local or not. The results depicted in Fig. 1 are for a particle with a *positive real* wave vector which impinges from the left onto a Gaussian potential barrier $V(x)=e^{-x^2}$ localized at $x=0$. We assume that at some points a and b the potential becomes negligible and its tails play no role. The complex function $R(x)$ is to be calculated opposite to the direction of incidence, i.e., from the right side of the x axis to the left side. In the spatial regions where the potential vanishes the particle is not reflected and hence $R(x)$ is zero or constant, i.e., $R(x)=0$, $x\in[b,+\infty)$ and $R(x)=$ const, $x\in(-\infty,a]$. In the region where the potential is localized the influence on the impinging particle can be viewed as the cumulative action of a set of infinitely thin slices of the potential. Each slice (the black area on Fig. 1) is defined by the domains $[x_i,x_i+\delta x]$. The potential part $V(x_i)$ contributes to the reflection by the amount $\delta R \sim V(x)\delta x$ [cf. Eqs. (4) and (9)]. Thus, the reflection amplitude at a given point x_0 is an integral sum over these slices lying to the right side from x_0 (shaded area). At the very left point a, when the potential becomes negligible, or where its influence is marginal, the reflection function $R(a)$ and the amplitude of the outgoing wave coincide, i.e., $|\psi(a)|^2=|R(a)|^2$ (and from Eq. (2) follows $T(a)=1$). Thus, $|R(a)|^2$ is the physically observable reflection *coefficient* R_c. For a potential with infinitely extended tails the points a and b tend to $-\infty$ and $+\infty$. We find then that

$$|R(-\infty)|^2 = R_c; \quad R(+\infty) = 0.$$

The transmission coefficient T_c can be found from the conservation condition: $T_c=1-R_c$.

Figure 1 represents the spatial behavior of the function $|R(x)|$, which characterizes the reflection of a particle incident with a wave vector $k=0.3$ a.u.. For real wave vector values $k\in\mathbb{R}$ the modulus of the reflection amplitude is bound to the interval $|R|\in[0,1]$ and is a measure for the potential reflectivity (or opacity). When it is about unity the potential reflects the incident particle almost completely. If $|R|\sim 0$, the wave is fully transmitted through the barrier. We remark that in Fig. 1 the potential is symmetrically located at $x=0$. Due to the specific initial conditions, this symmetry is however not reflected in the potential influence on the function $R(x)$: half of the reflection function magnitude is determined by the small right-side part of the potential, whereas the second half is due to the large left-side.

The above analysis makes clear that the present method for dealing with tunneling problems allows an insight into the influence of various parts of the potential on the reflection coefficients. Such a knowledge is valuable when dealing with more complex potentials in which case $R(x)$ is not a uniform function of x. An example is shown in Fig. 2 where the function $|R(x)|$ (dashed curves) has been calculated for four different potentials, as shown in the figures. From the right to the left we add successively $n=1,2,3,4$ Gaussian barriers (solid curves) located at the positions inferred from the figures. The physical situation we have in mind is the following. The situation depicted in Fig. 2(a) corresponds to a system of independent electrons a 1D wire with one constriction (cf. Ref. [9] for an experimental realization), whereas in (b), (c), and (d) the wire contains, respectively, two, three, or four constrictions. These act as tunneling bar-
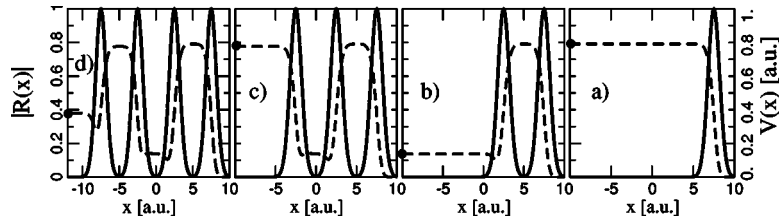
FIG. 2. The behavior of the reflection function (dashed curves) plotted for a series of n spatially separated Gaussian potential barriers. The solid curve on each plot shows the potentials. The dashed curve stands for the modulus of the reflection function $|R(x)|$ for the respective potential. The full dots at the left side of each graph indicate the asymptotic values of $|R(-\infty)|$ which also dictate the reflection coefficients values $R_c = |R(-\infty)|^2$. The particle energy of $E = 0.34$ a.u. (hartree) is chosen to be below the top of the Gaussians ($V_{max} = 1$ a.u.).

riers and are located at the positions of the peak value of the potentials. Furthermore, we assume that a small voltage bias is applied to the wire (small with respect to the Fermi energy) which drives the electrons from the left to the right. In the regime of a linear response (linear with respect to the applied bias) the conductance of the wire is governed by the transmission function (which can be retrieved from the reflection function) (see, e.g., Refs. [10,11], and references therein). The black dots on the vertical axis of each of the plots in Fig. 2 mark the asymptotic values of $|R(x \to -\infty)|$. It is interesting to note that, in fact, the reflection coefficient $R_c = |R(x \to -\infty)|^2$ oscillates with the number of constrictions in the system. In particular, the reflection from the fourfold barrier potential is several times smaller than the reflection even from the single Gaussian. Furthermore, the physical interpretation of $R(x)$ is readily observed when comparing Figs. 2(a)–2(d). The reflection coefficient in (a) is 0.8. Therefore, in (b) the reflection function rise to the value 0.8 at $x \approx 5$ a.u., i.e., after passing the first Gaussian; meaning that $R(x=0.5$ a.u.$)$ in (b) is equal to $R(x=-\infty$ a.u.$)$ in (a). The same observation is also made by considering analogously (c) and (d). From Fig. 2 it is also clear that any value of the reflection coefficients which is between approximately 0.8 and 0.1 can be realized by designing one of the cut potentials $V_{x_{cut}}$.

A further interesting issue concerns the question of how the conductance of the wire is modified when the distance between the constrictions is varied. This situation is shown in Fig. 3. At a certain separation (for a fixed particle energy) the reflection drops to zero and the constrictions become transparent to the traversing particle. The oscillations occurring in the reflection coefficients in Figs. 2 and 3 are of a ubiquitous nature and appear due to the formation of resonant states in the tunneling structure, a fact which is well documented in the literature [12]. The useful aspect about the present method is that it provides direct information on which part of the potential yields a desired reflection (or transmission) coefficients. Such information is highly useful for controlling the conductance of the quantum wire. We note in this context that tunneling barrier can nowadays be engineered accurately [9,13].

V. BOUND STATES

The dependence on the *real positive* wave vector k allows one to address questions arising in scattering problems [14],

such as the energetic conditions for the resonant penetration of the particles through the potential barriers. These conditions are set by the zeros of R. Now we turn to the analytical continuation of R to the complex plane of wave vector **k**. In the three-dimensional (3D) case the scattering amplitude as a function of the complex wave vector gives not only the magnitude of the cross section but also describes the stationary or quasistationary (quasibound) states. In particular, the positions of the poles of the scattering amplitude on the imaginary wave vector axis mark the values of the eigenenergies of the Hamiltonian [1].

In the 1D case the asymptotic value of the reflection function $R(x \to -\infty, k)$ is the analogue of the 3D-scattering amplitude [6]. Therefore, the transmission-reflection equations can also be utilized for solving the eigenvalue problem, when the particle energy is negative and the wave vector is pure imaginary $\mathbf{k} = i\kappa$, $\kappa \in \mathbb{R}^+$. While for real wave vectors the modulus of the reflection function $|R(k)|$ never exceeds unity, for certain complex wave vector values it can be arbitrary large. In fact, at each (complex) wave vector that corresponds to a bound state of the system $R(x \to -\infty, \mathbf{k})$ has a simple pole, i.e., the modulus of R tends to infinity. From these imaginary wave vectors $\mathbf{k} = i\kappa$ we infer the energies of the bound states. For complex **k** the determining equation for $R(x, k \to i\kappa)$ has the form
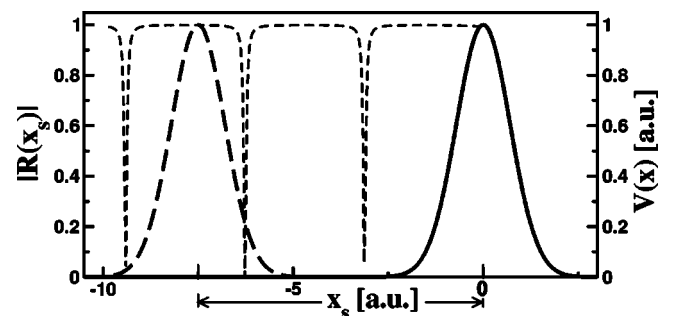

FIG. 3. The dependence of the reflection coefficient R_c on the separation distance x_s between two Gaussian barriers. The solid curve shows the fixed potential part whereas the dashed curve stands for the "variable" part of the potential. The coordinate x_s refers to the relative distance between the positions of the peak values of the Gaussian potentials. The dotted curve shows to reflection coefficient $|R_c|$ calculated as a function of the separation distance x_s. The particle energy is small ($E = 0.17$ a.u. $\ll V_{max} = 1$ a.u.).

$$\frac{d}{dx}R(x,\kappa) = \frac{1}{2\kappa}\left[e^{-\kappa x} + R(x,\kappa)e^{\kappa x}\right]^2 V(x). \qquad (16)$$

The potential function $V(x)$ possesses the structure

$$V(x) = \int_x^{+\infty} V(x,x')\cosh\left\{-\kappa\int_x^{x'}\frac{e^{-\kappa x''} - R(x'')e^{+\kappa x''}}{e^{-\kappa x''} + R(x'')e^{+\kappa x''}}dx''\right\}dx'.$$

The initial condition for the integration are $R(\infty,\kappa)=0$, whereas the condition for the occurrence of the eigenvalues E_n is for $E_n=(i\kappa_n)^2<0$ the relation $|R(x\rightarrow-\infty,\kappa_n)|\rightarrow\infty$ holds. Each pole of $R(x\rightarrow-\infty)$ on the positive semiaxis of κ marks the existence of bound states. It is interesting to note that, although R is generally a complex function, the real right-hand side of Eq. (16) together with the initial integration condition require that the solution is real for any negative energy of the particle. Moreover, for a strictly attractive (repulsive) potential the solution is monotonously decreasing (increasing) with x.

In case the eigenfunctions need to be determined, in addition to the eigenenergies one has to solve for $T(x)$ by carrying out the integral

$$T(x,\kappa_n) = \exp\left\{-\int_{-\infty}^x dx'\frac{1}{2\kappa_n}\left[1 + R(x',\kappa_n)e^{-2\kappa_n x'}\right]\hat{V}(x')\right\}. \qquad (17)$$

Having calculated both amplitudes $R(x,\kappa_n)$ and $T(x,\kappa_n)$ one substitutes in Eq. (2) and obtains the wave function.

For a numerical realization, the equation for $R(x)$ has to be regularized. This can be done, for example, by introducing the tangent of the reflection function, i.e.,

$$R(x,\kappa) = \tan\rho(x,\kappa),$$

$$\frac{d}{dx}\rho(x,\kappa) = \frac{1}{2\kappa}\left[e^{-\kappa x}\cos\rho(x,\kappa) + e^{\kappa x}\sin\rho(x,\kappa)\right]^2 V(x),$$

$$\rho(+\infty,\kappa) = 0. \qquad (18)$$

The eigenvalue conditions and the potential function $V(x)$ attain then the form

$$\rho(-\infty,\kappa_n) = \left(n+\tfrac{1}{2}\right)\pi, \quad n=0,1,\ldots,$$

$$V(x) = \int_x^{+\infty} V(x,x')$$

$$\times\cosh\left\{-\kappa\int_x^{x'}\frac{e^{-\kappa x}\cos\rho(x,\kappa) - e^{\kappa x}\sin\rho(x,\kappa)}{e^{-\kappa x}\cos\rho(x,\kappa) + e^{\kappa x}\sin\rho(x,\kappa)}dx''\right\}$$

$$\times dx'. \qquad (19)$$

Note that according to the Levinson theorem the difference between the tangent values calculated for $\kappa=0$ and $\kappa\rightarrow\infty$ can be used to evaluate the total number N of bound states in the system, i.e.,
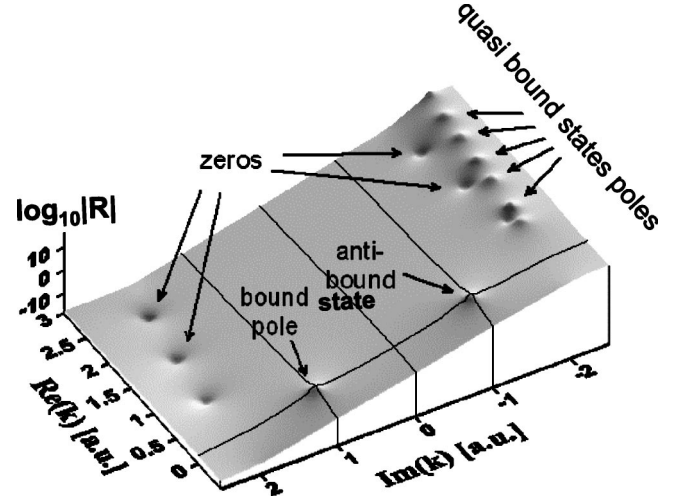

FIG. 4. The logarithm of the modulus of the reflection function $\log|R(k+i\kappa)|$ as a function of the real and the imaginary part of the wave vector. The calculations are done for a Morse potential. The maxima on the imaginary wave vector axis indicate the positions of the bound (on the positive imaginary semiaxis $\kappa>0$) and antibound states (on the negative imaginary semiaxis). Other peaks (poles) mark the positions of the quasibound states that have a finite lifetime. The zeros (minima) located symmetrically with respect to real k axis are the signature of resonant transmission through the potential.

$$\tan\rho(\kappa\rightarrow\infty) - \tan\rho(\kappa=0) = \pi(N-1/2).$$

An example of the behavior of the amplitude of the reflection function $R(-\infty,\mathbf{k})$ in the complex $\mathbf{k}$-plane is shown in Fig. 4. The function is evaluated numerically for the symmetric Morse potential $V(x)=-V_0/\cosh^2(\alpha x)$. The logarithm of the modulus of $R(-\infty,\mathbf{k})$ is depicted in Fig. 4. The finite extremal values of $|R|$ at the eigenenergies are due to the finite difference smoothing. We recall that the energies E_n of the states associated with the Morse potential are known in closed analytical form, namely

$$E_n = -\frac{\alpha^2}{4}\left[\sqrt{1+\frac{4V_0}{\alpha^2}} - (1+2n)\right]^2$$

[15]. For the parameter values $V_0=3$ a.u. and $\alpha=2$ a.u. there is a single eigenenergy $E_0=-1$ a.u. The wave vector is then imaginary positive and has the value $\kappa_0=1$ a.u.) The pole on the negative imaginary axis appears due to the so-called antibound state; it is not permitted physically but it may change the observable spectra [1].

VI. QUASIBOUND STATES

As previously mentioned, the poles of the amplitude $R(x\rightarrow-\infty,\mathbf{k}=k+i\kappa)$; $k,\kappa\in\mathbb{R}$ for wave vectors (or energies) correspond to the stationary or quasistationary states of the system. The conventional understanding of such a state $\psi_\mathbf{k}$ is that the real part of the energy $E_\mathbf{k}=\varepsilon_\mathbf{k}+i\Gamma_\mathbf{k}/2=k^2-\kappa^2+2ik\kappa$ describes the position of the resonance in the spectra (the observable energy of the state) whereas the imaginary part is related to the resonance half-width $\Gamma_\mathbf{k}/2$ or to the lifetime

$\tau_{\mathbf{k}} = 2/\Gamma_{\mathbf{k}}$ of the state. A vanishing value of the imaginary energy $\Gamma_{\mathbf{k}} = 0$ occurs for bound states and corresponds to an infinite lifetime of the states. We note that in the literature the term "quasibound" is used to refer only to those states which satisfy the condition $\Gamma_{\mathbf{k}}/2 \ll \varepsilon_{\mathbf{k}}$, i.e., for states with a lifetime large enough for a unique experimental identification of the resonance. The example shown in Fig. 4 illustrates how quasibound states appear as peaks located in the complex $\mathbf{k}$ plane. There are no poles on the real axis which indicates the absence of bound, square integrable states embedded in the continuum. There are poles on the lower half of $\mathbf{k}$ plane. The positions of these poles mark the resonance energies ε_q with $\varepsilon_q = k_q^2 - \kappa_q^2$. The inverse lifetimes of the states are $\Gamma_q/2 = k_q \kappa_q$. The zeros of the reflection function $R(k)$ are positioned symmetrically with respect to the real wave-vector axis, which is consistent with the spatial symmetry of the Morse potential. With increasing values of the real part of the wave vector the positions of the zeros approach the real k axis. Note that both the poles and the zeros have to be located symmetrically with respect to imaginary axis κ.

VII. CONCLUSIONS

In this work we presented a method capable of dealing with scattering, bound and resonant problems in one-dimensional systems involving energy-dependent, nonlocal potentials. We illustrated how the contributions to reflection coefficient of various parts of the potentials can be visualized and how bound and quasibound states are manifested in the present approach.

APPENDIX

This appendix provides a detailed account on the derivation of the determining equations for $R(x)$ and $T(x)$. The method relies on converting the second-order differential Schrödinger equation

$$\left[\frac{d^2}{dx^2} + k^2 \right] \psi(x) = \int_{-\infty}^{+\infty} V(x,x')\psi(x')dx' \quad (A1)$$

into two (coupled) first-order differential equations. This is achieved by making the ansatz

$$\psi = T(x)\left[e^{+ikx} + R(x)e^{-ikx} \right], \quad (A2)$$

$$\frac{d\psi}{dxF} = ikT(x)\left[e^{+ikx} - R(x)e^{-ikx} \right]. \quad (A3)$$

The aim is then to determine the functions $T(x)$ and $R(x)$ chosen appropriate for the problems under study. From the condition (A3) it follows that

$$\frac{d^2\psi}{dx^2} = ik\frac{dT}{dx}\left[e^{+ikx} - Re^{-ikx} \right] + (ik)^2 T\left[e^{+ikx} + Re^{-ikx} \right]$$

$$- ikT\frac{dR}{dx}e^{-ikx}. \quad (A4)$$

Noting that $k^2\psi = k^2 T[e^{+ikx} + Re^{-ikx}]$ we can recast the kinetic

part of the Schrödinger equation into the form

$$\frac{d^2\psi}{dx^2} + k^2\psi = ik\frac{dT}{dx}\left[e^{+ikx} - Re^{-ikx} \right] - ikT\frac{dR}{dx}e^{-ikx}. \quad (A5)$$

Now we evaluate the derivative of the wave function [Eq. (A2)] and compare with Eq. (A3). By doing so we conclude that the quantity dT/dx is expressible as

$$\frac{dT}{dx} = -T\frac{dR}{dx}\frac{e^{-ikx}}{e^{+ikx} + Re^{-ikx}}. \quad (A6)$$

Upon substitution into the kinetic energy term (A5) we conclude that

$$\frac{d^2\psi}{dx^2} + k^2\psi = -ikT\frac{dR}{dx}e^{-ikx}\frac{[e^{+ikx} - Re^{-ikx}]}{[e^{+ikx} + Re^{-ikx}]} - ikT\frac{dR}{dx}e^{-ikx}$$

$$= -\frac{2ik}{[e^{+ikx} + Re^{-ikx}]}T\frac{dR}{dx}. \quad (A7)$$

The potential part of the Schrödinger equation possesses the form

$$\int_{-\infty}^{+\infty} V(x,x')\psi(x')dx' = \int_{-\infty}^{+\infty} V(x,x')T(x')$$

$$\times \left[e^{+ikx'} + R(x')e^{-ikx'} \right] dx'. \quad (A8)$$

Combining the potential and the kinetic energy parts (A5) and (A8) leads to the desired determining equation for the reflection function which reads

$$\frac{d}{dx}R(x) = -\frac{1}{2ik}\left[e^{+ikx} + R(x)e^{-ikx} \right]$$

$$\times \int_{-\infty}^{+\infty} V(x,x')\left[e^{+ikx'} + R(x')e^{-ikx'} \right]$$

$$\times \exp\left\{ -\int_x^{x'} \frac{e^{-ikx''}}{e^{+ikx''} + R(x'')e^{-ikx''}}\frac{dR(x'')}{dx''}dx'' \right\} dx'. \quad (A9)$$

An important point is that $T(x)$ does not depend on $R(x)$, i.e., for the calculations of the reflection coefficients and the related physical quantities only the integration of a first-order differential equation is required. Using the identity $e^{-ikx}dR = d(e^{+ikx} + e^{-ikx}R(x)) - ik(e^{+ikx} - e^{-ikx}R(x))dx$, Eq. (A9) can be recast in the form

$$\frac{d}{dx}R(x) = -\frac{1}{2ik}\left[e^{+ikx} + R(x)e^{-ikx} \right]^2 \int_{-\infty}^{+\infty} V(x,x')$$

$$\times \exp\left\{ ik\int_x^{x'} \frac{e^{ikx''} - R(x'')e^{-ikx''}}{e^{ikx''} + R(x'')e^{-ikx''}}dx'' \right\} dx'. \quad (A10)$$

Finally we recall that the transmission-reflection problem is formulated as a Cauchy problem on the differential equations with the initial conditions in the spatial regions $\pm\infty$. This means that the numerical integration of the equation for

the reflection function $R(x)$ has to be performed starting from the right side of the x axis and propagating to the left side. The opposite applies for the transmission function $T(x)$. Now we assume for simplicity that the nonlocal potential is Hermitian [18]. Upon symmetrizing the exponential term in the integrand occurring in Eq. (A10) the integration region can be restricted to $[x, +\infty)$ [instead of $(-\infty, +\infty)$]. This is because, for an arbitrary symmetric function $S(x,x')=S(x',x)$ the rule $\int_a^b S(x,x')dx' = 2\int_x^b S(x,x')dx' = 2\int_a^x S(x,x')dx'$ applies. Thus, for a Hermitian potential the equation for $R(x)$ can be recast as

$$\frac{d}{dx}R(x) = -\frac{1}{ik}\left[e^{+ikx}+R(x)e^{-ikx}\right]^2 \int_x^{+\infty} V(x,x')$$

$$\times \cosh\left\{ik\int_x^{x'} \frac{e^{ikx''}-R(x'')e^{-ikx''}}{e^{ikx''}+R(x'')e^{-ikx''}}dx''\right\}dx' \tag{A11}$$

with the initial condition $R(k;+\infty)=0$.

If we are dealing with an eigenvalue problem we replace the real wave vector $k>0$ by a pure imaginary one $\mathbf{k}=i\kappa$. Then, the equation for the eigenvalues follows as

$$\frac{d}{dx}R(x) = \frac{1}{\kappa}\left[e^{-\kappa x}+R(x)e^{+\kappa x}\right]^2 \int_x^{+\infty} V(x,x')$$

$$\times \cosh\left\{-\kappa\int_x^{x'} \frac{e^{-\kappa x''}-R(x'')e^{+\kappa x''}}{e^{-\kappa x''}+R(x'')e^{+\kappa x''}}dx''\right\}dx' \tag{A12}$$

with the same initial condition as in Eq. (A11).

The differential equation for the function $T(x)$ is retrieved upon substitution of the derivative dR/dx, as given by Eq. (A11) or (A12) into Eq. (A6).

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[16] In general, the normalization of this function can be defined at an arbitrary point x which is convenient for the particular problem under study. The condition $T(x \to -\infty)=1$ is generally valid for any potentials that vanish asymptotically.

[17] That the expression in the square brackets in Eq. (10) is nonnegative can be seen from the following relations $1+|R(x)|^2 +2\,\mathrm{Re}\,[R(x)e^{-2ikx}] = 1+[\mathrm{Re}(R)]^2 + [\mathrm{Im}(R)]^2 + 2\,\mathrm{Re}(R)\cos 2kx +2\mathrm{Im}(R)\sin 2kx = [\mathrm{Re}(R)+\cos 2kx]^2 + [\mathrm{Im}(R)+\sin 2kx]^2 \geq 0$.

[18] If the potential is not Hermitian we can always divide it in two parts which are symmetric and antisymmetric with respect to an interchange of the variables x and x'.