

Exact Green's function for the step and square-barrier potentials

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We calculate both the exact retarded and advanced Green's function for the one-dimensional step and square-barrier potentials in the space-energy representation. Some of the results for the square barrier are also extended to general symmetric potentials of finite range.

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I. INTRODUCTION

The space-time propagator contains all the information about a quantum system. Although in several specific problems one is interested only in the spectrum and eigenfunctions, and these are more easily obtained by a direct solution of the time-independent Schrödinger equation, a number of very important questions have been raised recently in which the propagator enters in a crucial way. One of these questions concerns the problem of dissipation in quantum tunneling. The pioneering work of Caldeira and Leggett [1] introduced a formalism in which a subsystem in a metastable state is coupled to a bath of oscillators and the equilibrium density operator is calculated as a path integral [2]. Taking the trace over the bath variables results in a reduced density for the subsystem from which the tunneling rate can be extracted in the semiclassical limit. A second approach, particularly suited to treat Brownian motion in the classically accessible region, was also discussed by the abovementioned authors [3]. In that case, the time-dependent propagator for the "universe" (subsystem plus oscillators) is written in terms of the uncoupled propagators using the Feynman-Vernon theory [4]. As emphasized in Ref. [3], this method cannot be applied directly to the study of tunneling through a barrier. The main reason for this restriction is that the time-dependent propagator for scattering (unbounded) problems is very hard to obtain. If this difficulty could be overcome the effects of dissipation in quantum tunneling could be studied in a very detailed fashion. The two simplest problems where these effects could be observed are the one-dimensional step and square-barrier potentials. However, although these are very simple systems, only very recently [5] the space-time propagator for the first case was derived in terms of integrals of simpler propagators. Besides, as far as the author knows, the space-time propagator for the square barrier has not yet been computed.

The space-time propagator $K(x, x', t)$ is related to the space-energy propagator, or Green's function, $G(x, x', E)$ by a Fourier transform. In this paper we show that, although the space-time representation of the Green's function for the step and square-barrier potentials may be very complicated, its space-energy representation can be calculated in closed (and very simple) form. In a

recent paper [6] $G(x, x', E)$ was partially computed for the square barrier and some semiclassical results concerning group velocity and tunneling time were derived. In this paper we present a complete and exact calculation of the space-energy Green's function for both the step and square-barrier potentials. We also generalize some of these results for general symmetric potentials of finite range. The expressions for $G(x, x', E)$ turn out to be very simple and allow for interpretations in terms of classical paths.

Therefore, the basic motivation for the present calculation is the possibility of coupling the square-barrier potential to other degrees of freedom, such as free particles, and eventually to study the limit of many such freedoms. This study, now under current investigation, has become possible due to the very simple structure of the Green's function. As a final remark we should point out that the use of square-barrier and square-well potentials as simple models for more realistic physical problems has also a long history in the theory of heterostructures in solid-state physics [7] and the development of techniques to perform time propagation of wave packets has become of great importance [8]. We discuss the advantages of using the Green's function as an intermediate step for the time propagation in the Conclusion.

The calculations presented here are based on the spectral decomposition of $G(x, x', E)$. They are lengthy and sometimes tedious. Therefore, this paper is organized in such a way that the results and discussions come before the calculations. In Sec. II we review the basic definitions of time and energy representations of the Green's function and their connections. In Sec. III we compute the energy Green's function for the step potential. The results of this computation are given by Eqs. (3.3)–(3.6). In Sec. IV we do the same calculations for the square barrier, with results given by Eqs. (4.3)–(4.6). In Sec. V we generalize some results of Sec. IV for symmetric potentials of finite range and Sec. VI is devoted to some concluding remarks.

II. ENERGY AND TIME REPRESENTATIONS

Let us consider a one-dimensional system described by the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi, \quad (2.1)$$

where the Hamiltonian operator H has a continuum spectrum in the interval $0 < E < \infty$. The Green's function $K(t)$ associated with (2.1) satisfies the equation

$$i\hbar \frac{\partial K}{\partial t} - HK = \delta(t) \quad (2.2)$$

and has two formal solutions given by [9]

$$K^+(t) = \begin{cases} -\frac{i}{\hbar} e^{-iHt/\hbar}, & \text{for } t > 0, \\ 0, & \text{for } t < 0, \end{cases} \quad (2.3a)$$

and

$$K^-(t) = \begin{cases} 0, & \text{for } t > 0, \\ \frac{i}{\hbar} e^{-iHt/\hbar}, & \text{for } t < 0. \end{cases} \quad (2.3b)$$

From now on we shall refer to the time-dependent Green's functions as *propagators*, reserving the name *Green's function* for the energy-dependent operator $G(E)$ to be defined below. The operators K^+ and K^- are called the *retarded* and *advanced* propagators, respectively.

The coordinate representation of $K^\pm(t)$ is

$$K^\pm(x, x', t) \equiv \langle x | K^\pm(t) | x' \rangle = \mp \frac{i}{\hbar} \int_0^\infty \psi_E^*(x') \psi_E(x) e^{-iEt/\hbar} dE, \quad (2.4)$$

where it is implicit that the above expression is valid for $K^+(x, x', t)$ only if $t > 0$ and for $K^-(x, x', t)$ only if $t < 0$. The functions $\psi_E(x)$ are normalized eigenfunctions of H with eigenvalue E satisfying

$$\int_{-\infty}^{+\infty} \psi_E^*(x) \psi_{E'}(x) dx = \delta(E - E'). \quad (2.5)$$

The (energy-dependent) Green's functions associated with the propagators $K^+(t)$ and $K^-(t)$ are defined by their Fourier transform:

$$G^\pm(E) = \int_{-\infty}^{+\infty} K^\pm(t) e^{iEt/\hbar} dt. \quad (2.6)$$

As usual, a convergence factor $e^{\mp \epsilon t/\hbar}$ has to be inserted in the integral. When this is done, a formal solution can be obtained with the help of Eq. (2.3):

$$G^\pm(E) = \frac{1}{E - H \pm i\epsilon} = \mathcal{P} \left[\frac{1}{E - H} \right] \mp i\pi \delta(E - H), \quad (2.7)$$

where \mathcal{P} stands for the Cauchy principal values.

The coordinate representation of $G^\pm(E)$ is, therefore, given by

$$\begin{aligned} G^\pm(x, x', E) &= \langle x | G^\pm(E) | x' \rangle = \int_0^\infty \frac{\psi_E^*(x') \psi_E(x)}{E - E' \pm i\epsilon} dE' \\ &= \mathcal{P} \int_0^\infty \frac{\psi_E^*(x') \psi_E(x)}{E - E'} dE' \mp i\pi \psi_E^*(x') \psi_E(x). \end{aligned} \quad (2.8)$$

Defining [10]

$$\begin{aligned} DG(x, x', E) &= G^+(x, x', E) - G^-(x, x', E) \\ &= -2\pi i \psi_E^*(x') \psi_E(x), \end{aligned} \quad (2.9)$$

we may write the inverse of (2.6) as

$$\begin{aligned} K^\pm(x, x', t) &= \frac{1}{2\pi\hbar} \int_0^\infty G^\pm(x, x', E) e^{-iEt/\hbar} dE \\ &= \pm \frac{1}{2\pi\hbar} \int_0^\infty DG(x, x', E) e^{-iEt/\hbar} dE, \end{aligned} \quad (2.10)$$

where the time domains for $K^\pm(t)$ are again implicit. The last equality, which is the spectral decomposition of the propagator [see Eq. (2.4)], follows from the fact that the integral over G^- (G^+) vanishes for positive (negative) times.

III. GREEN'S FUNCTION FOR THE STEP POTENTIAL

A. Summary of results and discussion

The step potential $V(x)$ is defined by

$$V(x) = \begin{cases} V_0, & \text{if } x \geq 0, \\ 0, & \text{if } x < 0. \end{cases} \quad (3.1)$$

We divide the Green's function $G(x, x', E)$ in four parts and introduce the following notation:

$$G(x, x', E) = \begin{cases} G_{--}(x, x', E) & \text{if } x' < 0 \text{ and } x < 0, \\ G_{-+}(x, x', E) & \text{if } x' < 0 \text{ and } x > 0, \\ G_{+-}(x, x', E) & \text{if } x' > 0 \text{ and } x < 0, \\ G_{++}(x, x', E) & \text{if } x' > 0 \text{ and } x > 0. \end{cases} \quad (3.2)$$

A discussion of the main steps involved in the calculation of each part is presented in the next section. Here we only list and discuss the results:

$$G_{\pm-}(x, x', E) = \begin{cases} \pm \frac{m}{ik\hbar^2} [e^{\pm ik|x-x'|} + a(\pm k) e^{\mp ik(x+x')}] & \text{if } k < k_0, \\ \pm \frac{m}{ik\hbar^2} [e^{\pm ik|x-x'|} + r(k) e^{\mp ik(x-x')}] & \text{if } k > k_0, \end{cases} \quad (3.3)$$

$$G_{\pm+}^{\pm}(x, x', E) = \begin{cases} \pm \frac{m}{ik\hbar^2} b(\pm k) e^{-vx \mp ikx'} & \text{if } k < k_0, \\ \pm \frac{m}{ik\hbar^2} t(k) e^{\pm i(\mu x - kx')} & \text{if } k > k_0, \end{cases} \quad (3.4)$$

$$G_{+-}^{\pm}(x, x', E) = G_{-+}^{\pm}(x', x, E), \quad (3.5)$$

$$G_{++}^{\pm}(x, x', E) = \begin{cases} -\frac{m}{v\hbar^2} [e^{-v|x-x'|} - a(\pm k) e^{-v(x+x')}] & \text{if } k < k_0, \\ \pm \frac{m}{i\mu\hbar^2} [e^{\pm i\mu|x-x'|} - r(k) e^{\pm i\mu(x+x')}] & \text{if } k > k_0, \end{cases} \quad (3.6)$$

where the coefficients $a(k)$, $b(k)$, $r(k)$, and $t(k)$ are given by Eqs. (3.7c) and (3.8b) and are related to the reflexion and transmission coefficients.

It is interesting to observe that all the above expressions have a very simple semiclassical interpretation. G_{--} , for instance, consists of the contribution of a direct path connecting x to x' , the first term, plus the contribution of a path from x' to the barrier at 0 and then back to x , weighed by the reflexion amplitude $r(k)$ or $a(k)$. Notice, however, that the second path (of length $|x+x'|$)

corresponds to a classical path only if $k < k_0$. The expression for G_{++} has a structure very similar to that of G_{--} , as it should be, with the roles of k and μ interchanged.

Even the *tunneling terms* G_{-+} and G_{+-} can be interpreted classically: only the direct path from x' to x , with total action $\int_{x'}^x p dx = \hbar(\mu x - kx')$, contributes to G_{-+} with weight $t(k)$.

It can be checked by direct computation that

$$(1) G_{--}(0, x', E) = G_{-+}(0, x', E)$$

$$(2) G_{++}(x, 0, E) = G_{-+}(x, 0, E)$$

$$(3) \lim_{k_0 \rightarrow \infty} G_{--}^{\pm}(x, x', E) = \pm \frac{m}{ik\hbar^2} [e^{\pm ik|x-x'|} - e^{\pm ik|x+x'|}], \quad \text{for } k < k_0,$$

which is the result for a infinite wall at $x=0$

$$(4) \lim_{k_0 \rightarrow 0} G_{--}^{\pm}(x, x', E) = \pm \frac{m}{ik\hbar^2} e^{-ik|x-x'|}, \quad \text{for } k > k_0,$$

which is the result for the free particle.

For $k_0/k \ll 1$ the formulas for $G(x, x', E)$ can be expanded in a Taylor series, giving corrections for the free-particle limit. These expansions may be useful to obtain approximate expressions for the time-dependent propagator.

B. The calculation of the Green's function

The Schrödinger equation for the step potential

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x) \psi = E \psi$$

with $V(x)$ given by Eq. (3.1), has, for $E > V_0$, two normalized degenerate solutions $\psi_E^A(x)$ and $\psi_E^B(x)$ given by

$$\psi_E^A(x) = A \begin{cases} e^{ikx} + e^{-ikx} & \text{for } x < 0, \\ e^{i\mu x} + e^{-i\mu x} & \text{for } x > 0, \end{cases} \quad (3.7a)$$

and

$$\psi_E^B(x) = B \begin{cases} e^{ikx} - e^{-ikx} & \text{for } x < 0, \\ \frac{k}{\mu} (e^{i\mu x} - e^{-i\mu x}) & \text{for } x > 0, \end{cases} \quad (3.7b)$$

where

$$\begin{aligned} |A|^2 &= \frac{1}{2\pi\hbar^2} \left[\frac{m}{k+\mu} \right], \\ |B|^2 &= \frac{1}{2\pi\hbar^2} \left[\frac{m\mu}{k(k+\mu)} \right], \\ k &= \sqrt{2mE/\hbar^2}, \\ \mu &= \sqrt{2m(E-V_0)/\hbar^2}, \\ r &= \frac{k-\mu}{k+\mu}, \quad t = \frac{2k}{k+\mu}, \quad v = \frac{2\mu}{k+\mu}. \end{aligned} \quad (3.7c)$$

For $E < V_0$ the normalized function

$$\psi_E^C(x) = C \begin{cases} e^{ikx} + ae^{-ikx} \\ be^{-vx} \end{cases} \quad (3.8a)$$

with

$$\begin{aligned} |C|^2 &= \frac{m}{2\pi k \hbar^2}, \\ a &= \frac{k - i\nu}{k + i\nu}, \\ b &= \frac{2k}{k + i\nu}, \\ \nu &= \sqrt{2m(V_0 - E)/\hbar^2} \end{aligned} \quad (3.8b)$$

satisfies

$$\int_{-\infty}^{+\infty} \psi_E^{C*}(x) \psi_{E'}^C(x) dx = \delta(E - E') + \frac{1}{2\pi E} \frac{k}{\nu} \delta_{EE'}. \quad (3.9)$$

The Kronecker δ function in the above expression is an interesting mark of the infinitely long classically forbidden region of the step potential, although it has no effect when integrated over.

Once the normalized wave functions are known, the calculation of the Green's function is straightforward but lengthy. Consider, for instance, G_{--} ; using the spectral decomposition, Eq. (2.8), G_{--} reads as

$$\begin{aligned} G_{--}(x, x', E) &= \int_0^{V_0} \frac{\psi_E^{C*}(x') \psi_E^C(x)}{E - E'} dE' + \int_{V_0}^{\infty} \frac{\psi_E^{A*}(x') \psi_E^A(x)}{E - E'} dE' + \int_{V_0}^{\infty} \frac{\psi_E^{B*}(x') \psi_E^B(x)}{E - E'} dE' \\ &\equiv G_{--}^C + G_{--}^A + G_{--}^B. \end{aligned} \quad (3.10)$$

Changing variables from E to $k = \sqrt{2mE/\hbar^2}$ we observe that the integrals above contain terms of the form $e^{ik\Delta}/(k^2 - k'^2)$, with poles at $k' = \pm k$: The best way to compute these integrals is, therefore, by the method of residues. With the poles shifted to $k' = \pm(k + i\epsilon)$ or $k' = \pm(k - i\epsilon)$ we obtain G_{--}^+ or G_{--}^- , respectively. However, the way it stands, the integrals in (3.14) run from 0 to $k_0 \equiv \sqrt{2mV_0/\hbar^2}$ or from k_0 to ∞ . Therefore, the main usage of the calculation consists of manipulating these limits in order to write (3.14) as an integral in the complex k' plane running from $-\infty$ to $+\infty$. This can be achieved after some algebra using simple properties such as $a^*a = 1$ and $a(-k) = a(k^*)$.

Notice also that the presence of $\mu(k) = \sqrt{k^2 - k_0^2}$ in the wave functions introduces branch cuts in the complex plane [11]. The account of the correct signs of $\mu(k)$ above and below the branch lines are of fundamental importance in the calculation. The explicit calculation of the integrals in (3.10) is quite tedious and will not be carried out here. Also, the calculation of G_{-+} and G_{++} follows about the same scheme and, from the definition, $G_{+-}(x, x', E) = G_{-+}(x', x, E)$.

IV. GREEN'S FUNCTION FOR THE SQUARE-BARRIER POTENTIAL

The calculation of the Green's function for the square-barrier potential,

$$G_{--}^{\pm}(x, x', E) = \frac{m}{ik\hbar^2} [e^{\pm ik|x-x'|} + R_a(\pm k) e^{\mp ik(x+x'+2a)}], \quad (4.3)$$

$$G_{-+}^{\pm}(x, x', E) = \pm \frac{m}{ik\hbar^2} e^{\pm ik(x-x'-2a)} T_a(\pm k), \quad (4.4)$$

$$G_{00}^{\pm}(x, x', E) = \begin{cases} \pm \frac{m}{ik\hbar^2} e^{\mp ikx'} [e^{\pm i\mu x} \alpha_{\pm}(\pm k) + e^{\mp i\mu x} \alpha_{\mp}(\pm k)], & \text{if } k < k_0, \\ \pm \frac{m}{ik\hbar^2} e^{\mp ikx'} [e^{-\nu x} \beta_{-}(\pm k) + e^{\nu x} \beta_{+}(\pm k)], & \text{if } k > k_0, \end{cases} \quad (4.5)$$

$$V(x) = \begin{cases} 0 & \text{if } x < -a, \\ V_0 & \text{if } -a < x < a, \\ 0 & \text{if } x > a, \end{cases} \quad (4.1)$$

goes through the same steps of previous section, namely, finding normalized eigenfunctions and constructing, via Eq. (2.8), integrals in the complex plane. These integrals are then solved by the method of residues. Again the explicit computation of these integrals will not be carried out here.

As in Sec. III we divide the Green's function $G(x, x', E)$ into separate pieces according to the position of x and x' relative to the barrier:

$$G(x, x', E) = \begin{cases} G_{--} & \text{if } x \text{ and } x' < -a, \\ G_{-0} & \text{if } x' < -a \text{ and } -a < x < a, \\ G_{-+} & \text{if } x' < -a \text{ and } x > a, \\ G_{00} & \text{if } -a < x, x' < a. \end{cases} \quad (4.2)$$

Other situations, such as G_{+-} or G_{+0} can be obtained from the above functions by symmetry properties. The results of the calculations are now summarized as follows:

$$G_{00}(x, x', E) = \begin{cases} \pm \frac{m}{ik\hbar^2} e^{\pm ika} \left[\left[1 + \frac{k}{\mu} \right] e^{\mp i\mu(x'+a)} + \left[1 - \frac{k}{\mu} \right] e^{\pm i\mu(x'+a)} \right] \\ \quad \times \left[\frac{\alpha_{\pm}(\pm k)e^{\pm i\mu x} + \alpha_{\mp}(\pm k)e^{\mp i\mu x}}{2} \right], & \text{if } k > k_0, \\ \pm \frac{m}{ik\hbar^2} e^{\pm ika} \left[\left[1 \mp \frac{ik}{\nu} \right] e^{\nu(x'+a)} + \left[1 \pm \frac{ik}{\nu} \right] e^{-\nu(x'+a)} \right] \\ \quad \times \left[\frac{\beta_{-}(\pm k)e^{-\nu x} + \beta_{+}(\pm k)e^{\nu x}}{2} \right], & \text{if } k < k_0. \end{cases} \quad (4.6)$$

The indices a and b in Eqs. (4.3) and (4.4) refer to above ($k > k_0$) and below ($k < k_0$) the barrier, respectively. The coefficients T, R are the transmission and reflexion amplitudes, given by Eq. (4.11) and α and β , given by Eq. (4.10), are amplitudes of the plane waves entering in the scattering solutions in the region $-a < x < a$.

The result for G_{--} is essentially identical to G_{--} for the step potential, Eq. (3.3), since $x + x' + 2a$ represents the length of a classical path from x' to $-a$ and the back to x .

The expression for G_{-+} is at the same time simple and interesting. In words G_{-+} has the form of a free-particle Green's function weighted by the transmission amplitude T_a or T_b depending on whether $E > V_0$ or $E < V_0$, which is quite natural to expect. However, the length of the "classical path" contributing to G_{-+} is $x - x' - 2a$, and not just $x - x'$. Therefore, it works as if the particle had

tunneled through the barrier region instantaneous even if $E > V_0$. Of course this is just a "classical" interpretation of (4.4) and, in fact, the concept of instantaneity has no real meaning in an energy representation.

The formulas for G_{-0} and G_{00} are more complicated and do not have a direct interpretation in terms of classical paths, since they involve points *inside* the barrier.

It can be checked that the expressions (4.3)–(4.6) satisfy the continuity conditions at the boundary of their respective domains, such as

$$G_{--}(x', -a, E) = G_{-0}(x', -a, E),$$

$$G_{-0}(-a, x, E) = G_{00}(-a, x, E), \text{ etc.}$$

It can also be checked whether in the limit of a δ potential, $V_0 \rightarrow \infty$, $a \rightarrow 0$ with $2aV_0 = 1$, the results for G_{--} and G_{-+} tend to

$$\lim_{\substack{a \rightarrow 0 \\ (2V_0 a = 1)}} G_{--}(x, x', E) = \pm \frac{m}{ik\hbar^2} \left[e^{\pm ik|x-x'|} + \frac{1}{\frac{ik\hbar^2}{m} - 1} e^{\mp ik(x+x')} \right],$$

$$\lim_{\substack{a \rightarrow 0 \\ (2V_0 a = 1)}} G_{-+}(x, x', E) = \pm \frac{m}{ik\hbar^2} \left[\frac{1}{1 - \frac{m}{ik\hbar^2}} \right] e^{\pm ik(x-x')},$$

which are well known in the literature [12].

The coefficients appearing in the above expressions are related to the symmetrized wave functions ψ_0 and ψ_1 and to the "scattering" solutions ψ^+ and ψ^- [13]. For $E > V_0$ the even solution, for instance, is given by

$$\psi_0 = C \begin{cases} \cos(kx + \delta_0), \\ A_0 \cos(\mu x), \\ \cos(kx - \delta_0). \end{cases} \quad (4.7)$$

The odd solution is identical with the cosines replaced by sines and the index 0 by 1. For $E < V_0$ we replace the trigonometric functions by their hyperbolic counterparts ($\cos \rightarrow \cosh$, etc.) and the phase shifts δ_i by γ_i . In all cases

$$|C|^2 = \left[\frac{m}{2\pi\hbar^2 E} \right]^{1/2}. \quad (4.8)$$

The scattering solutions ψ^+ and ψ^- are given by

$$\psi^{\pm} = \psi_0 e^{i\delta_0} \pm i \psi_1 e^{i\delta_1}, \quad (4.9)$$

and ψ^+ for $E > V_0$, for instance, is given explicitly by

$$\psi^+ = \begin{cases} t_a e^{ikx}, & \text{if } x > a, \\ \alpha_+ e^{i\mu x} + \alpha_- e^{-i\mu x}, & \text{if } -a < x < a, \\ e^{ikx} + r_a e^{-ikx}, & \text{if } x < -a. \end{cases} \quad (4.10)$$

For $E < V_0$ we substitute the subscripts a into b and α

into β . The incoming solutions ψ^- are given by similar expressions.

The "phase shifts" δ_0 , δ_1 , γ_0 , and γ_1 and the amplitudes A_0 , A_1 , B_0 , and B_1 are obtained by direct imposition of continuity of $\psi(x)$ and $\partial\psi/\partial x$ at $x=-a$ and $x=a$. The explicit relations between the coefficients of the symmetrized wave functions (4.7) and those of the scattering wave functions (4.10) can be found easily [13]. Finally, we have defined T and R as

$$\begin{aligned} t_i &\equiv T_i e^{-2ika}, \\ r_i &\equiv R_i e^{-2ika}, \end{aligned} \quad (4.11)$$

where i can be either a (for "above barrier") or b (for "below barrier").

V. GENERALIZATION FOR FINITE-RANGE SYMMETRIC POTENTIALS

The results obtained for the square barrier can actually be generalized for symmetric potentials with compact support, i.e., potentials of the form

$$V(x) = \begin{cases} 0, & \text{if } x < -a, \\ v(x), & \text{if } -a < x < a, \\ 0, & \text{if } x > a, \end{cases} \quad (5.1)$$

where $v(x)$ is any bounded even function of x . In this case the Schrödinger equation admits solutions of the form

$$\begin{aligned} \psi_0(x) &= C \begin{cases} \cos(kx + \delta_0) & \text{for } x > a, \\ g_k(x) & \text{for } -a < x < a, \\ \cos(kx - \delta_0) & \text{for } x < -a, \end{cases} \\ \psi_1(x) &= C \begin{cases} \sin(kx + \delta_0) & \text{for } x > a, \\ h_k(x) & \text{for } -a < x < a, \\ \sin(kx - \delta_0) & \text{for } x < -a, \end{cases} \end{aligned} \quad (5.2)$$

where $g_k(x)$ is even and $h_k(x)$ is odd. The transmission and reflexion amplitudes are given again by

$$\begin{aligned} t &= \frac{e^{2i\delta_0} + e^{2i\delta_1}}{2}, \\ r &= \frac{e^{2i\delta_0} - e^{2i\delta_1}}{2}, \end{aligned} \quad (5.3)$$

where δ_0 and δ_1 follow from

$$\tan(k_0 + \delta_0) = -\frac{g'_k(a)}{kg_k(a)}$$

and

$$\tan(ka + \delta_1) = \frac{kh_k(a)}{h'_k(a)}, \quad (5.4)$$

where the prime means $\partial/\partial x$.

It is interesting that the normalization constant C does not depend on the function v and is given by Eq. (4.3):

$$|C|^2 = \left[\frac{m}{2\pi\hbar^2 E} \right]^{1/2}. \quad (5.5)$$

Therefore, expressions (4.3) and (4.4) for G_{--} and G_{-+} can be applied directly:

$$G_{--}^{\pm}(x, x', E) = \pm \frac{m}{ik\hbar^2} [e^{\pm ik|x-x'|} + R(\pm k)e^{\mp ik(x+x'+2a)}], \quad (5.6)$$

$$G_{-+}^{\pm}(x, x', E) = \pm \frac{m}{ik\hbar^2} e^{\pm ik(x-x'-2a)} T(\pm k), \quad (5.7)$$

where

$$T(k) = \frac{1}{2} \left[\frac{k - ig'_k(a)/g_k(a)}{k + ig'_k(a)/g_k(a)} - \frac{kh_k(a)/h'_k(a) - i}{kh_k(a)/h'_k(a) + i} \right] \quad (5.8)$$

and

$$R(k) = \frac{1}{2} \left[\frac{k - ig'_k(a)/g_k(a)}{k + ig'_k(a)/g_k(a)} + \frac{kh_k(a)/h'_k(a) - i}{kh_k(a)/h'_k(a) + i} \right] \quad (5.9)$$

follow from (5.4) and (5.3).

The form of G_{-0} and G_{00} of course depends explicitly on $v(x)$.

VI. CONCLUSIONS

In this paper we have computed the Green's function in the space-energy representation for three physically important one-dimensional situations, namely, the step potential, and the square-barrier and general symmetric finite-range potentials. We have shown that the parts of $G(x, x', E)$ that are relevant for tunneling, G_{-+} (where x' is at the left of the barrier and x is at the right) and G_{--} (where both x' and x are at the left) can be written in a very simple and general form [Eqs. (5.6)–(5.9)] where the basic ingredients are the reflection and transmission amplitudes. The most interesting feature of G_{-+} is that it can be interpreted as a free-particle Green's function weighted by the transmission amplitude and whose action corresponds to a path connecting x' to x but with the

barrier subtracted, i.e., with an action $\hbar k(x - x' - 2a)$.

The form of Eqs. (5.6) and (5.7) for G_{--} and G_{-+} also answer the following question: how does one extract the reflection and transmission coefficients from a time-dependent propagator? Certainly one should not attempt to propagate wave packets, due to the uncertainty introduced in the energy of the packet and also due to broadening effects during the propagation. Therefore, as suggested by (5.7), the formally correct procedure is to take its Fourier transform:

$$\lim_{\substack{x' \rightarrow -\infty \\ x \rightarrow +\infty}} \int_0^\infty K(x, x', t) e^{iEt/\hbar} dt = T(E) \frac{m}{ik\hbar^2} e^{ik(x - x' - 2a)}.$$

The limits $x' \rightarrow -\infty$ and $x \rightarrow +\infty$ are not necessary for finite-range potentials but they might make the calculation easier. The reflection amplitude $R(E)$ can be extracted in a similar way. It should be noticed, however, that in a few cases, such as in the coupling of a square well with a uniform laser field [14], exact solutions of the time-dependent Schrödinger equation are known and the scattering problem can be solved by appropriate matching conditions.

Finally, we point out the advantages of using the Green's function as an intermediate step in the propagation of wave packets. Given a wave packet $\varphi(x)$ at $t=0$, its time evolution is given by

$$\varphi(x, t) = i\hbar \int K(x, x', t) \varphi(x') dx'.$$

Fourier transforming both sides of this equation leads to

$$\phi(x, E) = i\hbar \int G(x, x', E) \varphi(x') dx',$$

where $\phi(x, E)$ is the Fourier transform of $\varphi(x, t)$. For Gaussian or square-shaped wave packets, the last integral can be performed analytically, since the x and x' dependence of G is trivial. Therefore, the discontinuities of the potential are taken care of analytically and the numerical calculation is reduced to an inverse Fourier transform.

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