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Exact form of Green functions for segmented potentials

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Abstract. We derive the exact Green functions for segmented potentials, i.e. for potentials of the form $V(x) = \sum_{j=1}^{N} V^{(j)}(x)$, where each $V^{(j)}(x)$ has compact support. The expressions depend explicitly on the wavefunctions' quantum amplitudes (e.g. transmission and reflection coefficients) for the individual $V^{(j)}$'s. We also show that the exact Green functions are in fact generalizations of the usual semiclassical formula. Finally, the possibility of applying the method to a general potential is briefly discussed.

1. Introduction

Recently there has been rapid and successful developments in obtaining exact and approximate Green functions and propagators. Indeed, in the context of path integrals formalism one can compare the state of art in 1981 [1] with the more recent progress in the subject (see, for example, the review in [2] or the book by Kleinert [3]).

Among different techniques for calculations, a very important one is the semiclassical approximation, which relies on the Van Vleck–Gutzwiller formula [4]. For n-dimensional systems the semiclassical Green function is given by

$$G_{\text{s.cl.}}(\boldsymbol{r}_f, \boldsymbol{r}_i; E) = \frac{2\pi}{(2\pi \mathrm{i}\hbar)^{\frac{n+1}{2}}} \sum_{\text{cl}} \sqrt{(-1)^{n+1} D_{\text{cl}}} \exp\left[-\mathrm{i}\frac{\pi}{2}\eta_{\text{cl}}\right] \exp\left[\frac{\mathrm{i}}{\hbar} S_{\text{cl}}(\boldsymbol{r}_f, \boldsymbol{r}_i; k)\right]. \qquad (1)$$

In (1), $S_{\text{cl}}(x_f, x_i; k)$ is the classical action and the sum is over all the trajectories with energy E, starting from $\boldsymbol{r}_i$ and arriving in $\boldsymbol{r}_f$. For each path, the Morse index η is the number of conjugate points at constant energy, and the semiclassical amplitude (or weight) is the square root of the path's density, which for $n = 1$ is given by $D_{\text{cl}} = (|\dot{x}_f||\dot{x}_i|)^{-1}$.

Very good results can be achieved from equation (1) and its trace, the Gutzwiller trace formula [4], in solving semiclassically quantum-mechanical systems, e.g. the anisotropic Kepler problem [5], the helium atom [6], etc. However, some phenomena cannot be described by purely classical orbits, i.e. by the real solutions of the Hamilton–Jacobi equation. In those cases modifications in the more primitive semiclassical approximation are necessary. For instance, the necessity of complex orbtis in the study of tunnelling [7], and the incorporation of diffractive trajectories [8] to take into account diffraction by such objects as hard walls, wedge and point scatterers.

It would be nice to improve expression (1) without drastic changes in its form. Actually, some results in the literature [9] show that non-classical effects can be incorporated into

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the semiclassical formula through a generalized semiclassical amplitude W, with the Green function then being $\sum_{\rm cl} W \exp[{\rm i}/\hbar S_{\rm cl}]$, and W more general than the path's density $D_{\rm cl}$. For some specific examples, it was shown [10] that the exact Fourier transform of G (the propagator) can be written as such a *generalized* semiclassical formulae.

The main purpose in this paper is to derive the correct Green functions for a class of one-dimensional systems, the segmented potentials, i.e. $V(x) =$ sum of potentials of compact support, and to show they are exactly of the above generalized semiclassical form. We mention that in doing so we also follow recent efforts in providing analytical results for quantum scattering in one dimension [11, 12]. Along this line a large number of works [13] address the problem of scattering by a potential $V(x) \to 0$ for $|x| \to \infty$, considering the scattering matrices for fragments of V. They obtain, for instance, the wavefunctions' reflection and transmission amplitudes, but little is said about the Green functions in terms of the fragments. It is true that for a long time the mathematical literature gave expressions relating the Green function of a barrier (or well) with the left and right Jost solutions of the Schrödinger equation (see [14, p 248]). However, the results are too general, and a direct association between the quantum amplitudes (e.g. the transmission and reflection coefficients) and the Green function is lacking, except for some particular examples [15, 16]. So, a second aim in this paper is to fulfil such a gap for the potentials discussed here.

We are interested in the Green function associated to the Schrödinger equation, $[-\frac{\hbar^2}{2m}\frac{{\rm d}^2}{{\rm d}x^2} + V(x)]\varphi(x) = E\varphi(x)$, where the segmented potential V is

$$V(x) = \sum_{j=1}^{N} V^{(j)}(x). \tag{2}$$

In (2); $V^{(j)}(x) = 0$ for $x < a_j$ or $x > b_j$ $(a_j < b_j)$; and $b_j < a_{j+1}$ $(j = 1, 2, \ldots, N-1)$.

If $\{\varphi_n, \varphi_k\}$ is the complete set of solutions for the Schrödinger equation (φ_n and φ_k standing, respectively, for the bound and scattering states with energies E_n and $\hbar^2k^2/(2m)$), the Green function can be written as [17]

$$\begin{aligned} G(x_f, x_i; E) &= G^{(\text{b.s.})}(x_f, x_i; E) + G^{(\text{s.s.})}(x_f, x_i; E) \\ &= \sum_n \frac{\varphi_n(x_f)\varphi_n^*(x_i)}{E - E_n} + \int_0^\infty {\rm d}k\, \frac{\varphi_k(x_f)\varphi_k^*(x_i)}{E - \frac{\hbar^2k^2}{2m}}. \end{aligned} \tag{3}$$

Usually, for convergence in calculations, one assumes for the above expression the energy $E + {\rm i}\varepsilon$ (with $\varepsilon > 0$), and afterwards takes the limit $\varepsilon \to 0^+$. When necessary we consider this procedure, but for simplicity of notation we do not write this explicitly.

A second way to obtain the Green function is through a perturbative expansion. Suppose we can write the Hamiltonian as $H = \tilde{H} + V$, and the Green function for $\tilde{H}$ is $\tilde{G}$. Then, the full G is given by [17]

$$\begin{aligned} G(x_f, x_i; E) = \tilde{G}(x_f, x_i; E) &+ \int {\rm d}x_1\, \tilde{G}(x_f, x_1; E)V(x_1)\tilde{G}(x_1, x_i; E) \\ &+ \iint {\rm d}x_2\, {\rm d}x_1\, \tilde{G}(x_f, x_2; E)V(x_2)\tilde{G}(x_2, x_1; E)V(x_1)\tilde{G}(x_1, x_i; E) + \cdots. \end{aligned} \tag{4}$$

This paper is organized as follows. In section 2 we derive the Green function for a single potential of compact support by summing the scattering states with the corresponding energies, equation (3). By comparing the results in section 2 with the perturbative series expansion (4), we show how to evaluate the Green function for segmented potentials in section 3. In section 4 we present a general expression for the exact Green function based on a sum over scattering paths, and show that this expression can be thought of

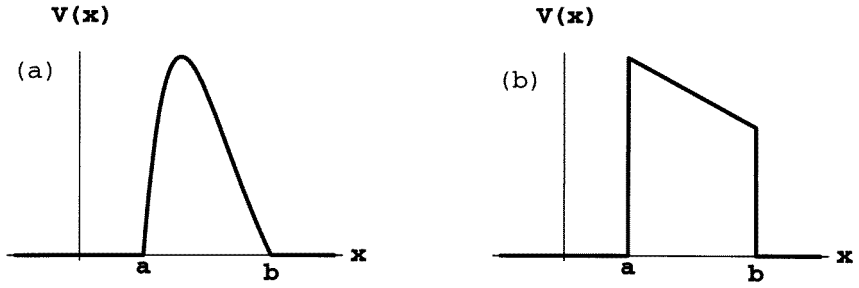


Figure 1. Examples of potentials of compact support: (*a*) continuous asymmetric barrier, (*b*) trapeze barrier.

as a modification of the usual semiclassical formula. Finally, we draw some remarks and conclusions in section 5.

2. Single compact support potentials

In this section we derive the exact Green function for a general single potential of compact support, $V(x) = V^{(1)}(x)$, as shown schematically in figure 1 (for simplicity, we drop the indices (1)). In [16] this was done for the case of a symmetric $V(x)$; here, however, such a condition is not necessary.

The scattering solutions $\varphi_k^{(\pm)}(x)$ of a plane wave incoming from the left $(+)$ and right $(-)$ are given by

$$\varphi_k^{(\pm)}(x) = \frac{1}{\mathcal{N}} \begin{cases} \exp[\pm \mathrm{i}kx] + \mathcal{R}^{(\pm)}(k) \exp[\mp \mathrm{i}kx] & \begin{cases} x < a & \text{for } (+) \\ x > b & \text{for } (-) \end{cases} \\ \mathcal{A}^{(\pm)}(k) u_k(x) + \mathcal{B}^{(\pm)}(k) s_k(x) & a < x < b \\ \mathcal{T}(k) \exp[\pm \mathrm{i}kx] & \begin{cases} x > b & \text{for } (+) \\ x < a & \text{for } (-). \end{cases} \end{cases} \tag{5}$$

Note that we have written $\mathcal{T}(k)$ instead $\mathcal{T}^{(\pm)}(k)$ since $\mathcal{T}^{(+)} = \mathcal{T}^{(-)} = \mathcal{T}$ [18]. Explicit expressions for the coefficients in (5) are given in appendix A. $u_k(x)$ and $s_k(x)$ are two independent (fundamental) solutions of the Schrödinger equation in the region where $V(x) \neq 0$, which correspond, for $E > V$ ($E < V$), to waves propagating (decaying) to the right and left, respectively. $\mathcal{N}$ is the normalization constant and is independent of $V(x)$ [16]. We can consider either p or E normalization for the φ's [19]. Choosing the former, i.e. $\int_{-\infty}^{+\infty} \mathrm{d}x\, \varphi_{k''}^{(\pm)}(x) \varphi_{k'}^{(\pm)^*}(x) = \delta(k'' - k')$, we have $\mathcal{N} = \sqrt{2\pi}$ (obviously, $\int_{-\infty}^{+\infty} \mathrm{d}x\, \varphi_{k''}^{(\pm)}(x) \varphi_{k'}^{(\mp)^*}(x) = 0$). The completeness relation yields $\sum_n \varphi_n(x)\varphi_n^*(y) + \int_0^{+\infty} \mathrm{d}k\, [\varphi_k^{(+)}(x)\varphi_k^{(+)^*}(y) + \varphi_k^{(-)}(x)\varphi_k^{(-)^*}(y)] = \delta(x - y)$. Here we should also mention that when a scattering wave function is properly extended to the k-complex plane (at the position of a bound energy) then the result is the bound-state wavefunction [20].

We now assume $G^{(\mathrm{b.s.})} = 0$ in equation (3), i.e. there are no bound states for V (we discuss the case of potentials allowing bound states in the end of this section). For convenience, we first analyse the possibilities: $(--)$ $x_i, x_f < a$; $(-+)$ $x_i < a$ and $x_f > b$; $(+-)$ $x_i > b$ and $x_f < a$; and $(++)$ $x_i, x_f > b$. Then, from (3) and (5) we have

$(E = \hbar^2\lambda^2/(2m))$

$$\begin{aligned} G_{\substack{--\\++}}(x_f, x_i; \lambda) &= \frac{2m}{\hbar^2}\frac{1}{2\pi}\int_0^\infty \mathrm{d}k\, \frac{1}{\lambda^2 - k^2}\{\exp[\mathrm{i}k(x_f - x_i)] + \exp[-\mathrm{i}k(x_f - x_i)] \\ &\quad + \mathcal{R}^{(\pm)}(k)\exp[\mp\mathrm{i}k(x_f + x_i)] + \mathcal{R}^{(\pm)^*}(k)\exp[\pm\mathrm{i}k(x_f + x_i)]\} \\ &= \frac{2m}{\hbar^2}\frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}k\, \frac{1}{\lambda^2 - k^2}\{\exp[\mathrm{i}k(x_f - x_i)] + \mathcal{R}^{(\pm)}(k)\exp[\mp\mathrm{i}k(x_f + x_i)]\} \end{aligned} \tag{6}$$

and

$$\begin{aligned} G_{\substack{-+\\+-}}(x_f, x_i; \lambda) &= \frac{2m}{\hbar^2}\frac{1}{2\pi}\int_0^\infty \mathrm{d}k\, \frac{1}{\lambda^2 - k^2}\{\mathcal{T}(k)\exp[\pm\mathrm{i}k(x_f - x_i)] \\ &\quad + \mathcal{T}^*(k)\exp[\mp\mathrm{i}k(x_f - x_i)] \\ &\quad + (\mathcal{R}^{(\pm)^*}(k)\mathcal{T}(k) + \mathcal{R}^{(\mp)}(k)\mathcal{T}^*(k))\exp[\pm\mathrm{i}k(x_f + x_i)]\} \\ &= \frac{2m}{\hbar^2}\frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}k\, \frac{1}{\lambda^2 - k^2}\mathcal{T}(k)\exp[\mathrm{i}k|x_f - x_i|]. \end{aligned} \tag{7}$$

In (6) we have used: $|\mathcal{R}|^2 + |\mathcal{T}|^2 = 1$ and $\mathcal{R}^{(\pm)^*}(k) = \mathcal{R}^{(\pm)}(-k)$; and in (7): $\mathcal{T}^*(k) = \mathcal{T}(-k)$ and $\mathcal{R}^{(\pm)^*}(k)\mathcal{T}(k) + \mathcal{R}^{(\mp)}(k)\mathcal{T}^*(k) = 0$. All these identities are well known and proven, for instance, in [18].

The above integrals are easily obtained by contour integration. Indeed, in (6), for the integral in $\exp[\mathrm{i}k(x_f - x_i)]$, a free particle, we consider a contour along the real axis closed by an infinite semicircle in the upper (if $x_b - x_a > 0$) or lower (if $x_f - x_i < 0$) half of the complex plane. For the integral in $\mathcal{R}^{(\pm)}(k)\exp[\mp\mathrm{i}k(x_f + x_i)]$, we take a contour along the real axis closed by an infinite semicircle in the upper half of the complex plane. In (7) we consider a contour in the upper half of the complex plane. Thus, we find (see appendix B)

$$G_{\substack{--\\++}}(x_f, x_i; \lambda) = \frac{m}{\mathrm{i}\hbar^2\lambda}\{\exp[\mathrm{i}\lambda|x_f - x_i|] + \mathcal{R}^{(\pm)}(\lambda)\exp[\mp\mathrm{i}\lambda(x_f + x_i)]\} \tag{8}$$

and

$$G_{\substack{-+\\+-}}(x_f, x_i; \lambda) = \frac{m}{\mathrm{i}\hbar^2\lambda}\mathcal{T}(\lambda)\exp[\mathrm{i}\lambda|x_f - x_i|]. \tag{9}$$

We now consider the Green functions for the following situations: (-0) $x_i < a$ and $a < x_f < b$; $(+0)$ $x_i > b$ and $a < x_f < b$; $(0+)$ $a < x_i < b$ and $x_f > b$; and $(0-)$ $a < x_i < b$ and $x_f < a$. From (3) and (5), we obtain

$$\begin{aligned} G_{\substack{-0\\+0}}(x_f, x_i; \lambda) &= \frac{2m}{\hbar^2}\frac{1}{2\pi}\int_0^\infty \mathrm{d}k\, \frac{1}{\lambda^2 - k^2} \\ &\quad \times\{\exp[\mp\mathrm{i}kx_i](\mathcal{A}^{(\pm)}(k)u_k(x_f) + \mathcal{B}^{(\pm)}(k)s_k(x_f)) \\ &\quad + \exp[\pm\mathrm{i}kx_i][(\mathcal{R}^{(\pm)^*}(k)\mathcal{A}^{(\pm)}(k) + \mathcal{T}^*(k)\mathcal{A}^{(\mp)}(k))u_k(x_f) \\ &\quad + (\mathcal{R}^{(\pm)^*}(k)\mathcal{B}^{(\pm)}(k) + \mathcal{T}^*(k)\mathcal{B}^{(\mp)}(k))s_k(x_f)]\}. \end{aligned} \tag{10}$$

Under the conditions discussed in appendix A (see equation (36)), we have

$$\begin{aligned} G_{\substack{-0\\+0}}(x_f, x_i; \lambda) &= \frac{2m}{\hbar^2}\frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}k\, \frac{1}{\lambda^2 - k^2}\exp[\mp\mathrm{i}kx_i](\mathcal{A}^{(\pm)}(k)u_k(x_f) + \mathcal{B}^{(\pm)}(k)s_k(x_f)) \\ &= \frac{m}{\mathrm{i}\hbar^2\lambda}\exp[\mp\mathrm{i}\lambda x_i](\mathcal{A}^{(\pm)}(\lambda)u_\lambda(x_f) + \mathcal{B}^{(\pm)}(\lambda)s_\lambda(x_f)) \end{aligned} \tag{11}$$

where again we have used contour integration (appendix B). Observe that in (11) there is no pole contribution from u_k and s_k because these functions are analytic in the k complex plane [12]. Likewise, one can show that $G\,{}^{0-}_{0+}(x_f, x_i; \lambda) = G\,{}^{-0}_{+0}(x_i, x_f; \lambda)$.

In principle, the expression for the case (00) $a < x_i, x_f < b$ can be obtained in the same fashion. However, for this case it is necessary to know the explicitly form of V. This is so because in extending integral (3) over the k real line $(-\infty, +\infty)$, we introduce in the integrand terms of the type $\mathcal{A}(\pm k)$ and $\mathcal{B}(\pm k)$. Thus, the fact of performing the integral in the upper half of the k complex plane does not prevent us knowing whether poles exist in the lower half of the k complex plane.

The above results are simple but nevertheless interesting. They inform us that if we know the quantum amplitudes for a potential of compact support, then the Green function for this system is obtained in a straightforward way. For instance, for the endpoints lying outside the potential region, G is just the combination of free particle Green functions weighted by the appropriate transmission and reflection coefficients. As a concrete example, we consider the trapeze barrier in figure 1(b). With $\mathcal{R}$ and $\mathcal{T}$ as calculated in appendix C, the exact Green functions are readily written as

$$G\,{}^{--}_{++}(x_f, x_i; k) = \frac{m}{\mathrm{i}\hbar^2 k}\{\exp[\mathrm{i}k|x_f - x_i|] + r^{(\pm)}_{\mathrm{trap.}}(k)\exp[\mp\mathrm{i}k(x_f + x_i - 2c^{\mp})]\} \tag{12}$$

and

$$G\,{}^{-+}_{+-}(x_f, x_i; k) = \frac{m}{\mathrm{i}\hbar^2 k} t_{\mathrm{trap.}}(k)\exp[\mathrm{i}k(|x_f - x_i| - (b-a))]. \tag{13}$$

The final important point we want to consider is the possibility of poles for the quantum coefficients in the upper half of the k complex plane, which correspond to the system's bound states [18]. No such poles exist if $V(x)$ does not allow bound states [12], $G^{(\mathrm{b.s.})} = 0$ (as assumed before) and equations (6)–(11) hold without problems. However, if there are bound states, the integrations in (6), (7) and (11) must include their contributions, and $G^{(\mathrm{b.s.})} \neq 0$. Nevertheless, some particular examples in the literature [21, 22] show that the contributions of these poles are exactly cancelled by $G^{(\mathrm{b.s.})}$. Actually, for symmetric potentials this result can be proved with the help of a recently derived relation between the bound and scattering wavefunctions at the bound-state poles [23]. Albeit, for the time being, we are not able to show this for asymmetric V's having bound states, we claim that our final expressions are valid in general. To support such a claim in appendix D we present a class of asymmetric potentials where these cancellations occur.

3. Segmented potentials

In view of the results of the previous section it is natural to ask how to calculate the exact Green function for the segmented potential (2). Obviously, for: $x_f, x_i < a_1$; $x_f, x_i > b_N$; and x_f $(x_i) > b_N$ and x_i $(x_f) < a_1$; the discussion in section 2 still holds (recall that by definition $V(x) = 0$ for $a_1 < x$ and $x > b_N$). In all these cases $\mathcal{R}$ and $\mathcal{T}$ are just the total quantum amplitudes for the whole $V(x)$.

To analyse the more general case, we consider the expansion of the total Green function in terms of the perturbative series (4). As we show next, the series can be summed up exactly and thus one can obtain the desired Green function in a closed form.

3.1. $V(x) = V^{(1)}(x)$

In this case $H^{(0)} = -\frac{\hbar^2}{2m}(\mathrm{d}^2/\mathrm{d}x^2)$ and $H^{(1)} = H^{(0)} + V^{(1)}(x)$. From (4) and $G^{(0)}(x_f, x_i; k) = \frac{m}{\mathrm{i}\hbar^2 k}\exp[\mathrm{i}k|x_f - x_i|]$, the Green function for a free particle, we have for $G^{(1)}$ (valid for $x_f, x_i < a_1$)

$$G^{(1)}(x_f, x_i, k) = \frac{m}{\mathrm{i}\hbar^2 k}\left\{\exp[\mathrm{i}k|x_f - x_i|] + \sum_{j=1}^{\infty} g_j^{(1,+)}(k)\exp[-\mathrm{i}k(x_f + x_i)]\right\} \tag{14}$$

where

$$g_j^{(1,\pm)}(k) = \left(\frac{m}{\mathrm{i}\hbar^2 k}\right)^j \int_{a_1}^{b_1} \mathrm{d}x_1 \ldots \mathrm{d}x_j\, V^{(1)}(x_1)\ldots V^{(1)}(x_j)\exp[\pm\mathrm{i}k(x_j + x_1)] \times \exp[\mathrm{i}k(|x_2 - x_1| + |x_3 - x_2| + \cdots + |x_j - x_{j-1}|)]. \tag{15}$$

Comparing the exact result (8) with (15) we see that formally $\mathcal{R}^{(1,+)}(k) = \sum_{j=1}^{\infty} g_j^{(1,+)}(k)$. Likewise, one can show that $\mathcal{R}^{(1,-)}(k) = \sum_{j=1}^{\infty} g_j^{(1,-)}(k)$ and $\mathcal{T}^{(1)}(k) = 1 + \sum_{j=1}^{\infty} f_j^{(1)}(k)$, where

$$f_j^{(1)}(k) = \left(\frac{m}{\mathrm{i}\hbar^2 k}\right)^j \int_{a_1}^{b_1} \mathrm{d}x_1 \ldots \mathrm{d}x_j\, V^{(1)}(x_1)\ldots V^{(1)}(x_j)\exp[\mathrm{i}k(x_j - x_1)] \times \exp[\mathrm{i}k(|x_2 - x_1| + |x_3 - x_2| + \cdots + |x_j - x_{j-1}|)]. \tag{16}$$

Also, $\mathcal{A}^{(1,\pm)}(k)u_k^{(1)}(x) + \mathcal{B}^{(1,\pm)}(k)s_k^{(1)}(x) = \exp[\pm\mathrm{i}kx] + \sum_{j=1}^{\infty} v_j^{(1,\pm)}(x; k)$, with

$$v_j^{(1,\pm)}(x; k) = \left(\frac{m}{\mathrm{i}\hbar^2 k}\right)^j \int_{a_1}^{b_1} \mathrm{d}x_1 \ldots \mathrm{d}x_j\, V^{(1)}(x_1)\ldots V^{(1)}(x_j)\exp[\mathrm{i}k(|x - x_j| \pm x_1)] \times \exp[\mathrm{i}k(|x_2 - x_1| + |x_3 - x_2| + \cdots + |x_j - x_{j-1}|)]. \tag{17}$$

We should note that relations similar to those above, but used in a different context, can be found in [12].

3.2. $V(x) = V^{(1)}(x) + V^{(2)}(x)$

Here, $H^{(1)} = -\frac{\hbar^2}{2m}(\mathrm{d}^2/\mathrm{d}x^2) + V^{(1)}(x)$ and $H^{(2)} = H^{(1)} + V^{(2)}(x)$. Now $\tilde{G}$ in (4) is the Green function given in section 2 for the potential $V^{(1)}(x)$. Thus, considering $b_1 < x_f < a_2$ and $x_i < a_1$ (see figure 2), we have ($a_2 < x_j < b_2$, for any j)

$$\begin{aligned} G^{(1)}(x_f, x_j; k) &= \frac{m}{\mathrm{i}\hbar^2 k}\{\exp[\mathrm{i}k(x_j - x_f)] + \mathcal{R}^{(1,-)}(k)\exp[\mathrm{i}k(x_f + x_j)]\} \\ G^{(1)}(x_j, x_i; k) &= \frac{m}{\mathrm{i}\hbar^2 k}\mathcal{T}^{(1)}(k)\exp[\mathrm{i}k(x_j - x_i)] \\ G^{(1)}(x_{j+1}, x_j; k) &= \frac{m}{\mathrm{i}\hbar^2 k}\{\exp[\mathrm{i}k|x_{j+1} - x_j|] + \mathcal{R}^{(1,-)}(k)\exp[\mathrm{i}k(x_{j+1} + x_j)]\} \end{aligned} \tag{18}$$

from which we obtain

$$G^{(2)}(x_f, x_i; k) = \frac{m}{\mathrm{i}\hbar^2 k}\mathcal{T}^{(1)}(k)\left\{\exp[\mathrm{i}k(x_f - x_i)] + \sum_{j=1}^{\infty} w_j(k)(\exp[-\mathrm{i}k(x_f + x_i)] + \mathcal{R}^{(1,-)}(k)\exp[\mathrm{i}k(x_f - x_i)])\right\} \tag{19}$$

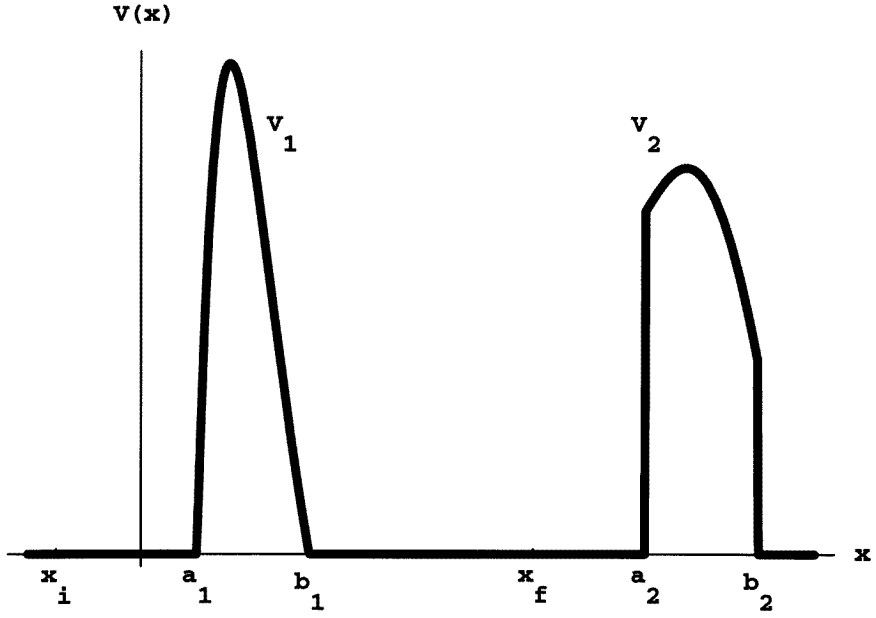


Figure 2. Schematic representation of $V(x) = V^{(1)}(x) + V^{(2)}(x)$. Here, the Green function's endpoints lie in the regions $b_1 < x_f < a_2$ and $x_i < a_1$.

with

$$w_j(k) = \left(\frac{m}{\mathrm{i}\hbar^2 k}\right)^j \int_{a_2}^{b_2} \mathrm{d}x_1 \ldots \mathrm{d}x_j \, V^{(2)}(x_1) \ldots V^{(2)}(x_j) \exp[\mathrm{i}k(x_j + x_1)]$$
$$\times \{\exp[\mathrm{i}k|x_2 - x_1|] + \mathcal{R}^{(1,-)}(k) \exp[\mathrm{i}k(x_2 + x_1)]\} \ldots$$
$$\times \{\exp[\mathrm{i}k|x_j - x_{j-1}|] + \mathcal{R}^{(1,-)}(k) \exp[\mathrm{i}k(x_j + x_{j-1})]\}. \tag{20}$$

By rearranging the above expression we obtain after lengthy but straightforward manipulations

$$\sum_{j=1}^{\infty} w_j(k) = \sum_{j=1}^{\infty} \left(g_j^{(2,+)}(k) + [\mathcal{R}^{(1,-)}(k)]^j \prod_{l=1}^{j+1} \sum_{n_l=1}^{\infty} g_{n_l}^{(2,+)}(k) \right). \tag{21}$$

Now, it is easy to see from $\mathcal{R}^{(2,+)}(k) = \sum_{j=1}^{\infty} g_j^{(2,+)}(k)$ that $\prod_{l=1}^{j+1} \sum_{n_l=1}^{\infty} g_{n_l}^{(2,+)}(k) = [\mathcal{R}^{(2,+)}(k)]^{j+1}$, so

$$G^{(2)}(x_f, x_i; k) = \frac{m}{\mathrm{i}\hbar^2 k} \mathcal{T}^{(1)}(k) \Bigg\{ \exp[\mathrm{i}k(x_f - x_i)] + \mathcal{R}^{(2,+)}(k) \sum_{j=0}^{\infty} [\mathcal{R}^{(1,-)}(k) \mathcal{R}^{(2,+)}(k)]^j$$
$$\times (\exp[-\mathrm{i}k(x_f + x_i)] + \mathcal{R}^{(1,-)}(k) \exp[\mathrm{i}k(x_f - x_i)]) \Bigg\}. \tag{22}$$

Finally, performing the geometric series in (22), we find

$$G^{(2)}(x_f, x_i; k) = \frac{m}{\mathrm{i}\hbar^2 k} \mathcal{T}^{(1)}(k) \Bigg\{ \exp[\mathrm{i}k(x_f - x_i)] + \frac{\mathcal{R}^{(2,+)}(k)}{1 - \mathcal{R}^{(1,-)}(k) \mathcal{R}^{(2,+)}(k)}$$
$$\times (\exp[-\mathrm{i}k(x_f + x_i)] + \mathcal{R}^{(1,-)}(k) \exp[\mathrm{i}k(x_f - x_i)]) \Bigg\}. \tag{23}$$

The Green function for all the other cases can be obtained in a similar way. For instance, if $b_1 < x_f, x_i < a_2$, then

$$G^{(2)}(x_f, x_i; k) = \frac{m}{\mathrm{i}\hbar^2 k}\left\{ \exp[\mathrm{i}k|x_f - x_i|] + \frac{1}{1 - \mathcal{R}^{(1,-)}(k)\mathcal{R}^{(2,+)}(k)} \times\left[+ \mathcal{R}^{(1,-)}(k)\exp[\mathrm{i}k(x_f + x_i)] + \mathcal{R}^{(2,+)}(k)\exp[-\mathrm{i}k(x_f + x_i)] + \mathcal{R}^{(2,+)}(k)\mathcal{R}^{(1,-)}(k)(\exp[\mathrm{i}k(x_f - x_i)] + \exp[-\mathrm{i}k(x_f - x_i)])\right]\right\} \tag{24}$$

and if $a_2 < x_f < b_2, x_i < a_1$, we obtain

$$G^{(2)}(x_f, x_i; k) = \frac{m}{\mathrm{i}\hbar^2 k}\frac{\mathcal{T}^{(1)}(k)}{1 - \mathcal{R}^{(1,-)}(k)\mathcal{R}^{(2,+)}(k)} \times \exp[-\mathrm{i}kx_i](\mathcal{A}^{(2,+)}(k)u_k^{(2)}(x_f) + \mathcal{B}^{(2,+)}(k)s_k^{(2)}(x_f)). \tag{25}$$

3.3. The general case

Albeit cumbersome, this procedure can be applied to any number N of $V^{(j)}(x)$'s. The approach then requires writing the series (4); identify the correct powers of $\mathcal{R}^{(j)}$'s and $\mathcal{T}^{(j)}$'s in each integral; and sum up all the terms. In doing so, one verifies that the following is always true.

- The exact Green functions $G(x_f, x_i; k)$, for x_f, x_i lying outside the $V^{(j)}$'s regions, are appropriate plane waves multiplied by factors that are functions only of series of powers of the transmission and reflection coefficients for the individual $V^{(j)}$'s.
- The series of powers are, in fact, geometric series, and therefore can be performed exactly.
- The above observations are still valid when one (both) endpoint(s) lie inside the $V^{(j)}$'s regions; however, in such cases we must replace the plane waves $\exp[\pm\mathrm{i}kx]$ by terms in the form $\mathcal{A}(k)u_k(x) + \mathcal{B}(k)s_k(x)$ (or a little more complicated linear combination of u and s), where x is x_i or (and) x_f. For instance, compare (23) with (25).

These statements are the main conclusions of this section. However, for practical purposes it is desirable to have a simpler prescription than equation (4). We present it next.

4. The exact expression: A generalized semiclassical formula

Here we want to express the Green function in a more suitable way for calculations. A careful analysis of the previous method reveals that G can be put exactly in the following form (for x_f, x_i outside the $V^{(j)}$'s regions)

$$G(x_f, x_i; k) = \frac{m}{\mathrm{i}\hbar^2 k}\sum_{\text{s.p.}} W_{\text{s.p.}}\exp\left[\frac{\mathrm{i}}{\hbar}S_{\text{s.p.}}(x_f, x_i; k)\right] \tag{26}$$

where s.p. stands for 'scattering path', and $S_{\text{s.p.}}$ and $W_{\text{s.p.}}$ are, respectively, its corresponding action and amplitude. According to section 3.3, a simple modification of (26) is necessary in order to include the case of one or both endpoints lying inside the $V^{(j)}$'s regions. Nevertheless, the study of (26) is enough to demonstrate the approach, and for the other cases one can use the same reasoning.

Before we discuss the above expression in more detail, it is instructive to compare (26) with the usual Van Vleck–Gutzwiller formula (1) with $n = 1$. We see that equations (26)

and (1) are similar, with $m/(\hbar k)W$ playing the role of $\sqrt{D}\exp[-i\pi\eta/2]$. However, as will be clarified below, W is more general than the semiclassical amplitude since it takes into account purely quantum effects such as tunnelling. Thus, segmented potentials belong to the interesting class of systems whose exact Green functions or propagators are given by generalizations of the usual semiclassical formulae [10, 16].

In (26), a 'scattering path' represents a trajectory where the particle starts from x_i, suffers multiple reflections between the $V^{(j)}$'s, and finally arrives at x_f. The weights $W_{\text{s.p.}}$ are constructed as follows. Each time the particle hits a $V^{(j)}$, it can be reflected or transmitted by the potential. In the first case, W gets a factor $r^{(j)}$ and in the second, it gets a factor $t^{(j)}$ (see appendix A for the definition of t and r in terms of $\mathcal{R}$ and $\mathcal{T}$). The total W is then the product of all the partial amplitudes for that particular scattering path. $S_{\text{s.p.}}$ is the classical action for the 'free scattering path', i.e. it is given by $S_{\text{s.p.}} = kL_{\text{s.p.}}$, where $L_{\text{s.p.}}$ is the total length of the particle's trajectory (outside the $V^{(j)}$'s). For $V(x) = V^{(1)}(x) + V^{(2)}(x) + V^{(3)}(x)$, figure 3 shows four examples of scattering paths. Their respective amplitudes and actions are; (a) $W_{\text{s.p.}} = t^{(2)}(k)$ and $S_{\text{s.p.}} = \exp[ik[(a_2 - x_i) + (x_f - b_2)]]$; (b) $W_{\text{s.p.}} = t^{(2)}(k)r^{(1,-)}(k)r^{(3,+)}(k)$ and $S_{\text{s.p.}} = \exp[ik[(x_i - b_1) + (a_2 - b_1) + (a_3 - b_2) + (a_3 - x_f)]]$; (c) $W_{\text{s.p.}} = [t^{(2)}(k)]^3 r^{(3,+)}(k)r^{(1,-)}(k)$ and $S_{\text{s.p.}} = \exp[ik[(a_2 - x_i) + 2(a_3 - b_2) + 2(a_2 - b_1) + (x_f - b_2)]]$; (d) $W_{\text{s.p.}} = t^{(2)}(k)[r^{(1,-)}(k)]^3[r^{(2,+)}(k)]^2$ and $S_{\text{s.p.}} = \exp[ik[(x_i - b_1) + 5(a_2 - b_1) + (x_f - b_2)]]$.

It remains to sum over the infinite number of 'scattering paths'. Actually, this can be done by a simple diagrammatic classification of the trajectories' splitting, which is a practical way to identify and perform the geometric series mentioned above. The paths are labelled by their sequence of pre-exponential factors. The two sets of amplitudes in each level, '{', represent the two possible paths splitting at that point of the trajectory. For each coefficient we need to add its related action corresponding to the distance covered in that step. Contributions from coefficients in the same level are summed up and from successive levels are multiplied.

As an example, let us consider a typical situation as shown in figure 4. The particle starting from x_i may (1) go straight to $x = a_2$, or (2) go to the left, hit the potential $V^{(1)}$ at $x = b_1$, and then go to the right arriving at $x = a_2$. There is an infinite set of possible paths for the particle at $x = a_2$, and we call them P_{12}. Thus, by using our scheme, the Green function can be written as

$$G^{(3)}(x_f, x_i; k) = \frac{m}{i\hbar^2 k} \begin{cases} \exp[ik(a_2 - x_i)]P_{12} \\ r^{(1,-)} \exp[ik((x_i - b_1) + (a_2 - b_1))]P_{12}. \end{cases} \tag{27}$$

Any path in P_{12} belongs to one of two possibilities: (1) transmission through $V^{(2)}$ followed by one of trajectories in the set P_{23}, or (2) reflection by $V^{(2)}$ and then by $V^{(1)}$, finally arriving again at $x = a_2$. So, P_{12} is given by

$$P_{12} = \begin{cases} t^{(2)}P_{23} \\ r^{(2,+)}r^{(1,-)} \exp[ik2(a_2 - b_1)]P_{12}. \end{cases} \tag{28}$$

Similar reasoning shows that

$$P_{23} = \begin{cases} \exp[ik(x_f - b_2)] \\ r^{(3,+)} \exp[ik(a_3 - b_2)] \begin{cases} \exp[ik(a_3 - x_f)] \\ \exp[ik(a_3 - b_2)] \begin{cases} r^{(2,-)}P_{23} \\ t^{(2)}r^{(1,-)} \exp[ik2(a_2 - b_1)]P_{12}. \end{cases} \end{cases} \end{cases} \tag{29}$$

Observe that the particle finally arrives in x_f either by the left or by the right (see figure 4). It can, once in the region $b_2 < x < a_3$, come back to the region $b_1 < x < a_2$, bouncing

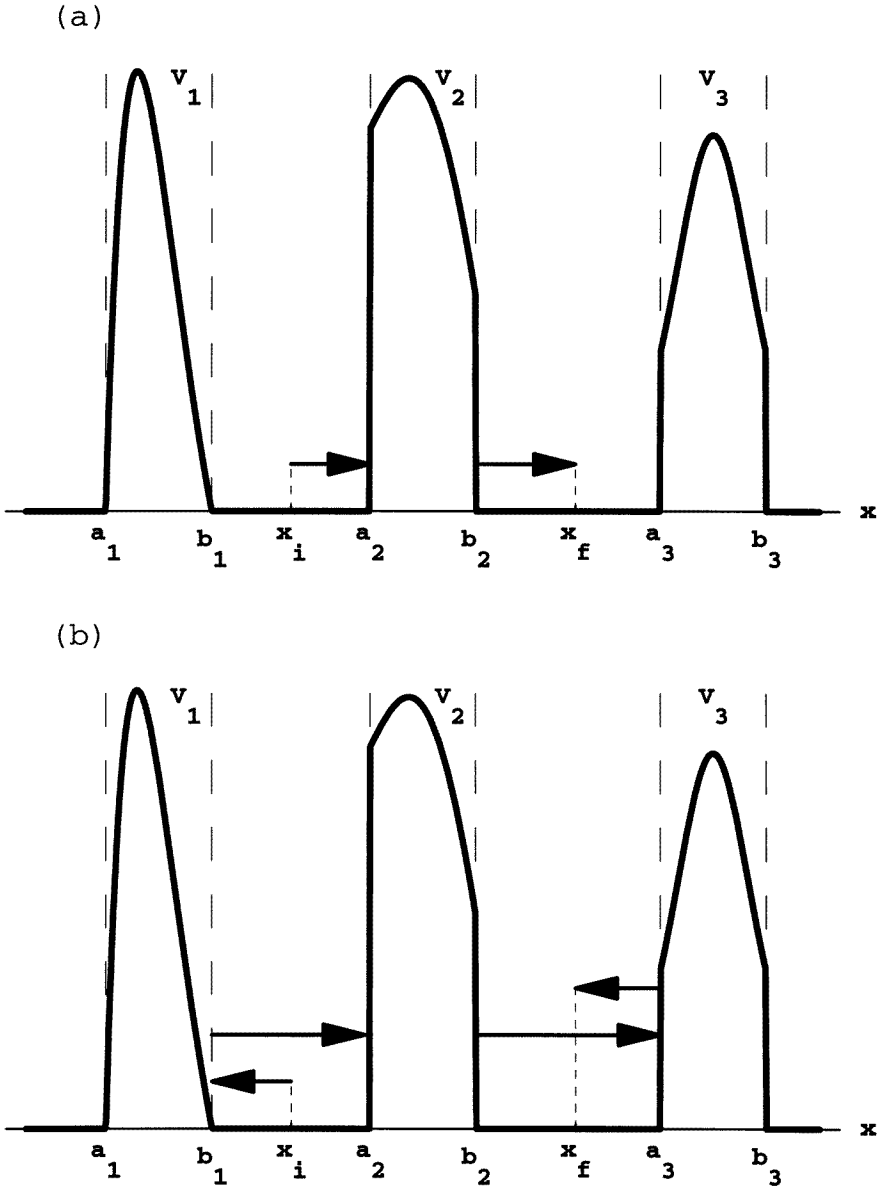


Figure 3. Four examples of 'scattering paths' for the case of $V(x) = V^{(1)}(x)+V^{(2)}(x)+V^{(2)}(x)$, and $b_2 < x_f < a_3$, $b_1 < x_i < a_2$.

back and forth. All these possibilities are taken into account in (29).

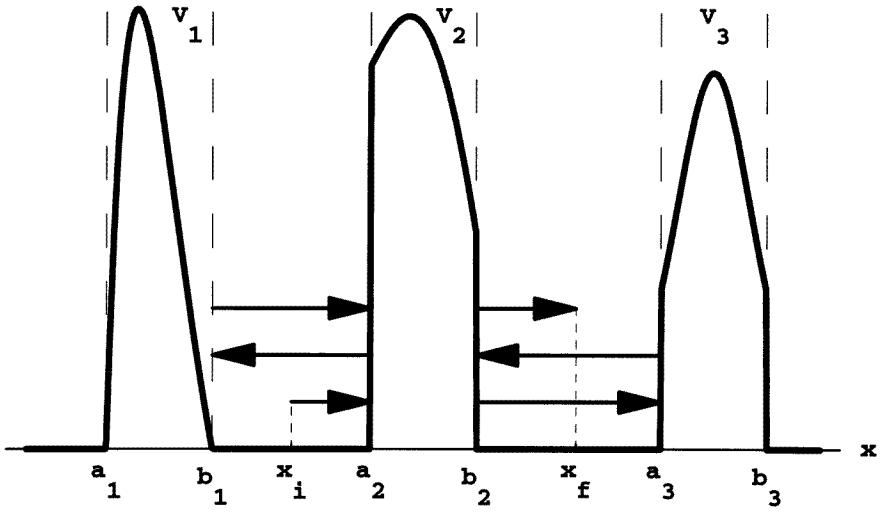
Using the previous rules, we can easily write down the equations equivalent to (27)–(29). Indeed,

$$P_{12} = t^{(2)} P_{23} + r^{(2,+)} r^{(1,-)} \exp[\mathrm{i}k2(a_2 - b_1)] P_{12} \tag{30}$$

and

$$P_{23} = \exp[\mathrm{i}k(x_f - b_2)] + r^{(3,+)} \exp[\mathrm{i}k(a_3 - b_2)]\{\exp[\mathrm{i}k(a_3 - x_f)]$$

(c)



(d)

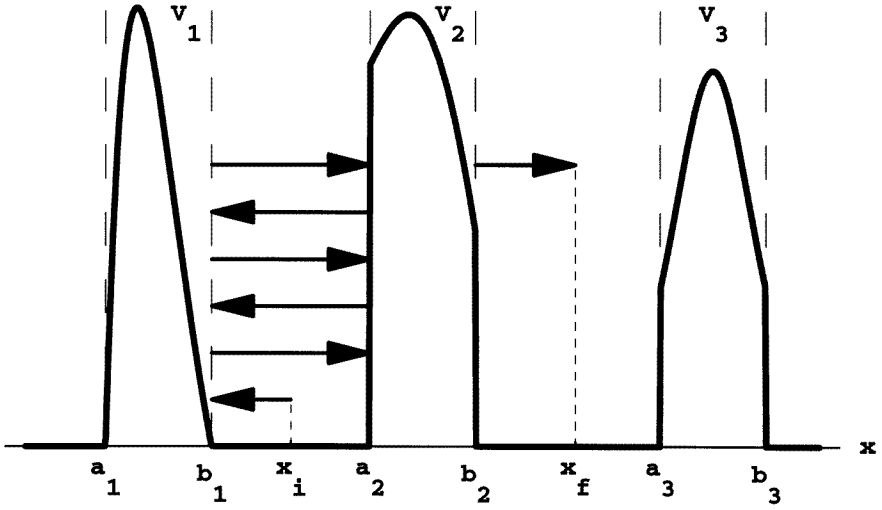


Figure 3. (Continued)

$$+\exp[\mathrm{i}k(a_3-b_2)]\{r^{(2,-)}P_{23}+t^{(2)}r^{(1,-)}\exp[\mathrm{i}k2(a_2-b_1)]P_{12}\}. \tag{31}$$

Solving (30) and (31), and putting the result into (27), we finally obtain

$$G^{(3)}(x_f,x_i;k)=\frac{m}{\mathrm{i}\hbar^2k}\frac{\mathcal{T}^{(2)}}{[1-\mathcal{R}^{(2,+)}\mathcal{R}^{(1,-)}][1-\mathcal{R}^{(2,-)}\mathcal{R}^{(3,+)}]-\mathcal{T}^{(2)^2}\mathcal{R}^{(3,+)}\mathcal{R}^{(1,-)}}$$
$$\times\{\exp[-\mathrm{i}kx_i]+\mathcal{R}^{(1,-)}\exp[\mathrm{i}kx_i]\}\{\exp[\mathrm{i}kx_f]+\mathcal{R}^{(3,+)}\exp[-\mathrm{i}kx_f]\} \tag{32}$$

which is the exact Green function for the problem.

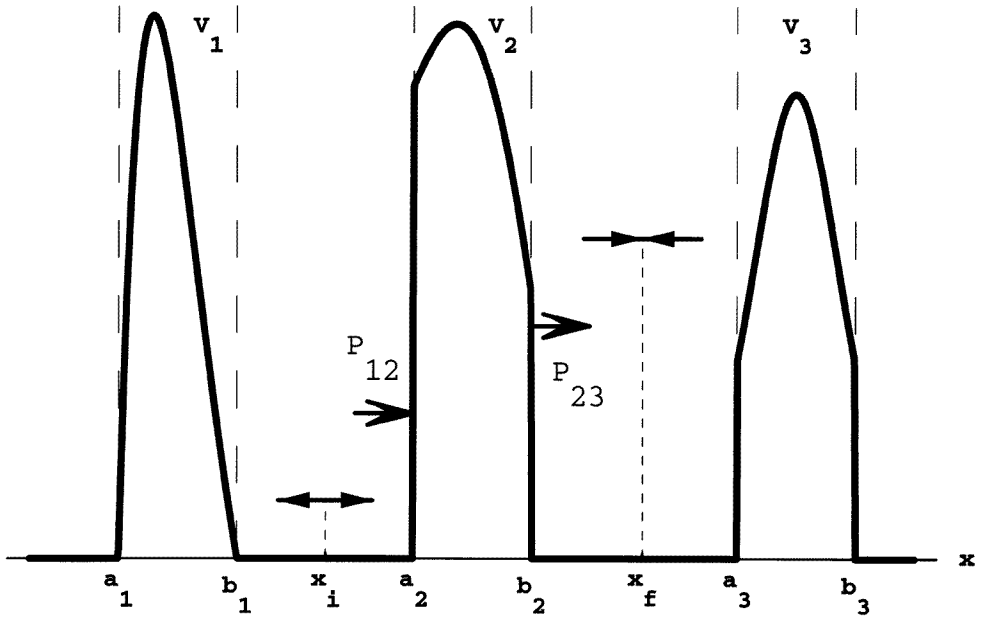


Figure 4. Typical situation for the classification of the trajectories' splitting. Observe that the particle can leave x_i to the left or right and can finally arrive in x_f from the left or right.

One can construct the diagrams for any number N of $V^{(j)}$'s. However, it is important to note that the situation in figure 4 already describes the most general case. For arbitrary N we may regroup the $V^{(j)}$'s to form blocks, with each block corresponding to the individual potentials in figure 4. The method can then be applied to this new partition of $V(x)$. This allows us to solve $V(x) =$ sum of a large number of compact support potentials, by using a recurrence procedure. Finally, we mention that in considering each block one is, in fact, calculating its exact transmission and reflection coefficients. So, our method gives an approach based on Green function (therefore alternative to the works in [13]) to obtain quantum amplitudes for segmented potentials.

5. Remarks and conclusions

In this paper we have enlarged the class of potentials whose exact Green function can be obtained in a closed form (once we know the quantum amplitudes for the parts $V^{(j)}(x)$ of the segmented $V(x)$). We have shown that the expressions for the Green functions are generalizations of the usual semiclassical formulae. Furthermore, our results, summarized in equation (26), can also be thought of as a one-dimensional multiple scattering expansion. Nevertheless, each separated term in our expansion is physically meaningful, in contrast to the usual one-dimensional multiple scattering approaches, where the individual terms may not have a clear physical interpretation [24].

We should observe that a general $V(x)$ can always be written as a segmented potential with $a_{j+1} = b_j$ $(j = 1, \ldots, N-1)$, see Aktosun in [13]. Since the derivations here are valid for any value of the d_j's (with $d_j = a_{j+1} - b_j$), they also include the case $d_j = 0$. Thus, in principle the approach can also be applied to arbitrary potentials. Obviously, the best division of $V(x)$ into 'pieces', the $V^{(j)}(x)$'s, will depend on the system considered.

An immediate consequence of this is that one can easily extend equation (26) to the case where, instead of being null, the segmented potential assumes constant values between its parts $V^{(j)}$'s and outside the region $a_1 < x < b_N$.

Finally, we emphasize a very important application for the Green functions derived in this paper, besides calculations of transmissions and reflections amplitudes. As is well known, a wavepacket propagates as $\varphi(x,t) = \int \mathrm{d}x_0\, K(x,x_0;t)\varphi_0(x_0)$, with the quantum propagator K given by the inverse Fourier transform of G. So, we have $\varphi(x,t) = \int \mathrm{d}x_0 \frac{\mathrm{i}}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}E\, \exp[-\mathrm{i}tE/\hbar]G(x,x_0;E)\varphi_0(x_0)$. Then, our Green functions are also useful for the study of the time evolution of wavepackets in segmented potentials. In particular, for the problem of disordered one-dimensional lattices, where the scaling theory of localization in [25] is based heuristically on expressions similar to ours and to those in Rozman *et al* [13]. Also, in the description of transport in solid-state systems such as quantum wells, junctions, superlattices, etc, which may be modelled by square barriers and wells [26], particular cases of the potentials discussed here.

A natural continuation for this work is to consider particular systems in order to analyse the points mentioned above. Currently, this is under investigation and the results will be reported in due course.

Acknowledgments

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Appendix A

In this appendix we write down the quantum amplitudes in (5) and discuss some properties used in section 2.

To determine the coefficients for the scattering solutions (5) we impose the usual boundary conditions of continuity of $\varphi(x)$ and $\varphi'(x)$ at $x = a$ and $x = b$. Thus, we obtain after some straightforward manipulations ($c^+ = b$ and $c^- = a$)

$$\begin{aligned}
\mathcal{A}^{(\pm)}(k) &= \pm\frac{2}{Z(k)}\left(s_k(c^\pm) \mp \frac{1}{\mathrm{i}k}s_k'(c^\pm)\right)\exp[\pm\mathrm{i}kc^\mp]\\
\mathcal{B}^{(\pm)}(k) &= \mp\frac{2}{Z(k)}\left(u_k(c^\pm) \mp \frac{1}{\mathrm{i}k}u_k'(c^\pm)\right)\exp[\pm\mathrm{i}kc^\mp]\\
\mathcal{T}(k) &= \frac{2}{Z(k)}\frac{W_k}{\mathrm{i}k}\exp[-\mathrm{i}k(b-a)]\\
\mathcal{R}^{(\pm)}(k) &= \frac{Z^{(\pm)}(k)}{Z(k)}\exp[\pm 2\mathrm{i}kc^\mp]
\end{aligned} \tag{33}$$

with

$$\begin{aligned}
W_k &= W_k(x) = s_k(x)u_k'(x) - u_k(x)s_k'(x)\\
Z(k) &= \left[u_k(a) + \frac{1}{\mathrm{i}k}u_k'(a)\right]\left[s_k(b) - \frac{1}{\mathrm{i}k}s_k'(b)\right] - \left[u_k(b) - \frac{1}{\mathrm{i}k}u_k'(b)\right]\left[s_k(a) + \frac{1}{\mathrm{i}k}s_k'(a)\right]\\
Z^{(\pm)}(k) &= \left[u_k(a) \mp \frac{1}{\mathrm{i}k}u_k'(a)\right]\left[s_k(b) \mp \frac{1}{\mathrm{i}k}s_k'(b)\right] - \left[u_k(b) \mp \frac{1}{\mathrm{i}k}u_k'(b)\right]\left[s_k(a) \mp \frac{1}{\mathrm{i}k}s_k'(a)\right].
\end{aligned} \tag{34}$$

It is interesting to note that the amplitudes in (33) are written as a *complex number* $\times$ *overall phase*. So, for convenience of notation in section 4, we define r and t as these complex numbers for $\mathcal{R}$ and $\mathcal{T}$, or

$$\begin{aligned} \mathcal{R}^{(\pm)}(k) &= r^{(\pm)}(k)\exp[\pm \mathrm{i}k2c^{\mp}] \\ \mathcal{T}(k) &= t(k)\exp[-\mathrm{i}k(b-a)]. \end{aligned} \tag{35}$$

Now, we observe the following features for the quantum amplitudes $\mathcal{A}$ and $\mathcal{B}$. By explicitly considering ${u_k}^* = u_{-k}$; ${s_k}^* = s_{-k}$; and either u_k, s_k real or ${u_k}^* = s_k$, we find from (33) and (34), after lengthy but straightforward calculations, that

$$\begin{aligned} {\mathcal{R}^{(\pm)}}^*(k)\mathcal{A}^{(\pm)}(k) + \mathcal{T}^*(k)\mathcal{A}^{(\mp)}(k) &= \begin{cases} \mathcal{B}^{(\pm)}(-k) & \text{if } {u_k}^* = s_k \\ \mathcal{A}^{(\pm)}(-k) & \text{if } u_k, s_k \text{ real} \end{cases} \\ {\mathcal{R}^{(\pm)}}^*(k)\mathcal{B}^{(\pm)}(k) + \mathcal{T}^*(k)\mathcal{B}^{(\mp)}(k) &= \begin{cases} \mathcal{A}^{(\pm)}(-k) & \text{if } {u_k}^* = s_k \\ \mathcal{B}^{(\pm)}(-k) & \text{if } u_k, s_k \text{ real} \end{cases} \end{aligned} \tag{36}$$

and also ${\mathcal{A}^{(\pm)}}^*(k) = \mathcal{A}^{(\pm)}(-k)$, ${\mathcal{B}^{(\pm)}}^*(k) = \mathcal{B}^{(\pm)}(-k)$.

Appendix B

The contour integrations in (6), (7) and (11) (all taken in the upper half of the complex plane, except by the free particle part in equation (6) when $x_f - x_i < 0$) are straightforward if we realize that the poles are only due to the denominator $\lambda^2 - k^2$ in the integrands (see the discussion at the end of section 2), and the integrals over the infinite semicircle in the upper half of the complex plane are identically zero. In this way, our calculations become similar to those in [21]. To prove the null contributions of the semicircle we observe that $r^{(\pm)}(|k| \to \infty) = 0$ (see equation (35) relating r to $\mathcal{R}$) and $\mathcal{T}(|k| \to \infty) = 1$, which are trivially derived from the results in [12] (for example, consider equation (63) and the definitions following equation (32) in that reference, and then take the limit $|k| \to \infty$ in the upper half of the k complex plane). We also note that $u_{|k|\to\infty}(x) = \exp[\mathrm{i}kx]$, and $s_{|k|\to\infty}(x) = \exp[-\mathrm{i}kx]$; and from equations (33) and (34) that $\mathcal{A}^{(+)}(|k| \to \infty) = \mathcal{B}^{(-)}(|k| \to \infty) = 1$, and $\mathcal{A}^{(-)}(|k| \to \infty) = \mathcal{B}^{(+)}(|k| \to \infty) = 0$ (vanishing as exponentially fast); furthermore, these expressions can be analytically continued into the k complex plane [12].

From the above results, a simple analysis shows that for all the integrals along the semicircle, the integrands have the asymptotic form $F(k)\exp[\mathrm{i}kd]$, with $F(k)$ a bounded function and $d > 0$. For instance, for G_{--} in (6) we have the expression $\mathcal{R}^{(+)}(k)\exp[-\mathrm{i}k(x_f + x_i)] = r^{(+)}(k)\exp[\mathrm{i}k(2a - (x_f + x_i))]$, where $d = 2a - (x_f + x_i) > 0$. Since the exponential goes to zero for $\mathrm{Im}[k] \to +\infty$, our assertion holds.

Appendix C

The potential in figure 1(b) is given by $V(x) = [-(V_a - V_b)x + (V_a b - V_b a)]/(b - a)$ for $a \leqslant x \leqslant b$ (note that $V(a) = V_a$ and $V(b) = V_b$), and $V(x) = 0$ elsewhere. For $a < x < b$, the Schrödinger equation can be written as $[\mathrm{d}^2/\mathrm{d}y^2 - y]\varphi(y) = 0$, where $y = [(\beta - k^2)/\alpha - x]\alpha^{\frac{1}{3}}$ with $\alpha = (2m/\hbar^2)(V_a - V_b)/(b-a)$ and $\beta = (2m/\hbar^2)(V_a b - V_b a)/(b-a)$. The two independent solutions are given in terms of Airy functions [27], or $u_k(x) = \mathrm{Ai}(y)$ and $s_k(x) = \mathrm{Bi}(y)$. Now, with the help of the identity $\mathrm{Ai}(y)\,\mathrm{Bi}'(y) - \mathrm{Ai}'(y)\,\mathrm{Bi}(y) = \pi^{-1}$ [27], we find from (33)–(35) (see appendix A), $t_{\mathrm{trap.}}(k) = -2\eta_k/(\pi C(k))$ and $r^{(\pm)}_{\mathrm{trap.}}(k) =$

$D^{(\pm)}(k)/C(k)$, where ($\eta_k = \mathrm{i}\alpha^{\frac{1}{3}}/k$, $y_c = y|_{x=c}$, $F'(y_c) = \mathrm{d}/\mathrm{d}y_c\, F(y_c)$)

$$\begin{aligned} C(k) &= [\mathrm{Ai}(y_a) + \eta_k\,\mathrm{Ai}'(y_a)][\mathrm{Bi}(y_b) - \eta_k\,\mathrm{Bi}'(y_b)] \\ &\quad -[\mathrm{Ai}(y_b) - \eta_k\,\mathrm{Ai}'(y_b)][\mathrm{Bi}(y_a) + \eta_k\,\mathrm{Bi}'(y_a)] \\ D^{(\pm)} &= [\mathrm{Ai}(y_a) \mp \eta_k\,\mathrm{Ai}'(y_a)][\mathrm{Bi}(y_b) \mp \eta_k\,\mathrm{Bi}'(y_b)] \\ &\quad -[\mathrm{Ai}(y_b) \mp \eta_k\,\mathrm{Ai}'(y_b)][\mathrm{Bi}(y_a) \mp \eta_k\,\mathrm{Bi}'(y_a)]. \end{aligned} \tag{37}$$

We finally observe that in (37) one can readily write the Airy functions and their derivatives in terms of Bessel functions (see, for instance, [27, p 447]).

Appendix D

Consider $V(x) = V^{(1)}(x) + V^{(2)}(x)$ (for instance, see figure 2), with $V^{(2)}(x)$ a symmetric potential not allowing bound states, and $V^{(1)}(x)$ an attractive delta function, $-\gamma\delta(x - b_1)$, $\gamma > 0$. As is well known, the Green function for V is given by [28, 2]

$$G^{(V)}(x_f, x_i; k) = G^{(2)}(x_f, x_i; k) - \frac{G^{(2)}(x_f, b_1; k)G^{(2)}(b_1, x_i; k)}{G^{(2)}(b_1, b_1; k) + 1/\gamma}. \tag{38}$$

Possible bound states are determined by the poles of G, i.e. by the equation $G^{(2)}(b_1, b_1; k) = -1/\gamma$. For brevity, we only discuss the case of $x_i < b_1$ and $x_f > b_2$. By calculating $G^{(2)}$ from our results in section 2, we obtain from (38), $G^{(V)}(x_f, x_i; k) = (m/\mathrm{i}\hbar^2 k)\mathcal{T}\exp[\mathrm{i}k(x_f - x_i)]$, where

$$\mathcal{T} = \frac{\mathcal{T}^{(\delta)}\mathcal{T}^{(2)}}{1 - \mathcal{R}^{(\delta,-)}\mathcal{R}^{(2,+)}} \tag{39}$$

is the correct transmission coefficient for the whole V. Here $\mathcal{T}^{(\delta)} = 1/(1 + \lambda)$ and $\mathcal{R}^{(\delta,-)} = -\lambda/(1 + \lambda)\exp[-2\mathrm{i}kb_1]$, with $\lambda = m\gamma/(\mathrm{i}\hbar^2 k)$, are the usual transmission and reflection amplitudes for the delta potential. Now, to have a single compact support for V, we just assume $b_1 = a_2$ (or more rigorously, take the limit $b_1 \to a_2{}^-$).

So, we end up with a class of asymmetric single potentials of compact support which may have b.s. and are exactly of the form discussed in section 2. As an example, if $V^{(2)}$ is a square barrier of high v_0, then the bound energy E_b is obtained from the pole condition mentioned above, or ($L = b_2 - a_2$, $\mu^2 = 2m|E_\mathrm{b}|/\hbar^2$, $\nu^2 = \mu_0{}^2 + \mu^2$, $\mu_0{}^2 = 2mv_0/\hbar^2$)

$$\frac{\mu\sinh[\nu L] + \nu\cosh[\nu L]}{(\mu^2 + \nu^2)\sinh[\nu L] + 2\mu\nu\cosh[\nu L]} = \frac{\hbar^2}{2m\gamma} \tag{40}$$

that always has one solution if $2m\gamma/\hbar^2 \geqslant \mu_0\tanh[\mu_0 L]$.

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