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2001 J. Phys. A: Math. Gen. 34 5041

(http://iopscience.iop.org/0305-4470/34/24/303)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL
J. Phys. A: Math. Gen. **34** (2001) 5041–5057 www.iop.org/Journals/ja PII: S0305-4470(01)21877-0

Asymptotic Green functions: a generalized semiclassical approach for scattering by multiple barrier potentials

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Received 8 February 2001, in final form 27 April 2001

Abstract
We show how quantum mechanical barrier reflection and transmission coefficients $\mathcal{R}$ and $\mathcal{T}$ can be obtained from asymptotic Green functions. We exemplify our results by calculating such coefficients for the Rosen–Morse (RM) potential. For multiple barrier potentials, $V(x) = \sum_j V^{(j)}(x)$, where each $V^{(j)}$ goes to zero for $x \to \pm\infty$, we derive the asymptotic Green functions by a generalized semiclassical approximation, which is based on the usual sum over classical paths considered only in the classically allowed regions and includes local quantum effects through the individual $\mathcal{R}^{(j)}$ and $\mathcal{T}^{(j)}$. The approach is applied to double RM potentials and to Woods–Saxon barriers. We obtain analytical expressions for the transmission and reflection probabilities of these potentials which are very accurate when compared with exact numerical calculations, being much better than the usual WKB approximation. Finally we briefly discuss how to extend the present method to other kinds of potential.

PACS numbers: 0365S, 0230G, 8530

1. Introduction

Scattering by multiple barrier potentials, $V = \sum_j V^{(j)}(x)$ where each individual $V^{(j)}$ goes to zero asymptotically, is a most topical problem. It turns up in the description [1] of resonant tunnelling diode devices, disordered one-dimensional lattices and realistic one-dimensional solid-state systems such as quantum wells, junctions and superlattices. This problem also plays a role [2, 3] in the study of electronic transport in polymers and the effect of intermolecular potential barriers in chemical reactions.

The goal of this paper is to calculate the energy-dependent Green function and from it to derive, for any range of energy, analytical expressions for the transmission and reflection amplitudes of multiple barrier potentials. Obviously, in general we cannot find closed exact solutions for such potentials and some kind of approximation is in order. Therefore, here we consider a generalized semiclassical approach for the problem.

Semiclassical approximations are very valuable tools to solve quantum mechanical systems. However, some phenomena, such as tunnelling, cannot be properly described by the usual semiclassical approach, i.e. to consider only the classically allowed paths for the particle, the real (valued) trajectories. In fact, these trajectories cannot deal with the possibility of the particle being found in different (dynamically disconnected) regions of the phase space. There are ways to overcome this difficulty: for instance, to use complex trajectories, formally extending classical variables (momentum or time) into the complex plane. In this way one obtains complex (valued) trajectories inside the classical forbidden regions [4]. Recently, multi-dimensional tunnelling [5] and chaotic tunnelling [6] were discussed in this fashion. Alternatively, we consider a semiclassical version of the Heisenberg matrix mechanics, which in some sense 'avoids' the problem of connecting the distinct classical regions [7]. Furthermore, specialized extensions of the WKB approximation are also possible when one is concerned with specific situations such as reflection above barriers [8, 9], tunnelling near the base of barriers [10] and tunnelling in the limit of long waves [11].

Due to the characteristics of our V, complex valued trajectories inside the classically prohibited regions can be very cumbersome to obtain [3]. Thus, in contrast to the methods mentioned above, to calculate the asymptotic Green functions we solve the tunnelling regions quantum mechanically, taking explicitly into account their wave aspects through local quantum amplitudes. In the regions where the classical dynamics is well defined, we consider the usual sum over paths, the Van Vleck–Gutzwiller formula [12], for the approximated G. To do so we follow [13] and incorporate non-classical effects into the semiclassical formula through generalized semiclassical amplitudes W, in substitution of the usual $|\dot{x}_f \dot{x}_i|^{-1/2}$ (which diverges at the classical turning points), writing $G(x_{\mathrm{f}}, x_{\mathrm{i}}; E) = \sum_{\mathrm{cl}} W \exp[\mathrm{i}S/\hbar]$. As we are going to see, the approach requires one to determine the quantum amplitudes of the individual $V^{(j)}$ (which will yield the W), but in general this is a much easier task than to calculate numerically propagation along the whole $V(x)$. We should observe that this kind of approach has already been successfully used in the study of propagators [14], and in the exact calculation of Green functions [15] for segmented potentials, a class of potentials which includes, for instance, piecewise constant potentials, well known to have a poor WKB approximation.

The paper is arranged as follows. In section 2 we show how to obtain a Green function in the above generalized semiclassical form for a general decaying potential and also how to extract from it the transmission and reflection quantum amplitudes. In section 3 we exemplify our general results discussing the Rosen–Morse (RM) potential. In section 4 we use an extended version of a calculation developed in [15] and the results of section 2 to obtain the asymptotic Green functions for a potential which is a sum of an arbitrary number of decaying potentials. In section 5 we show that the method gives very good results by applying it for a double RM barrier and a Woods–Saxon (WS) barrier, being a sensible improvement when compared with the usual WKB solution. Finally, we make some remarks and draw some conclusions in section 6.

2. Asymptotic Green functions

We consider a generic one-dimensional potential for which $V(|x| \to \infty) \to 0$. If $\{\varphi_n, \varphi_\lambda\}$ forms the complete set of solutions for the Schrödinger equation (φ_n and φ_λ representing, respectively, bound and scattering states with energies E_n and $\hbar^2\lambda^2/(2m)$), the Green function

$G(x_f, x_i; E)$ for the problem can be written as

$$G = G^{(\mathrm{b.s.})}(x_f, x_i; E) + G^{(\mathrm{s.s.})}(x_f, x_i; E) = \sum_n \frac{\varphi_n(x_f)\varphi_n^*(x_i)}{E - E_n} + \int_0^\infty \mathrm{d}\lambda\, \frac{\varphi_\lambda(x_f)\varphi_\lambda^*(x_i)}{E - \frac{\hbar^2\lambda^2}{2m}}. \quad (1)$$

For convergence in calculations, we assume for the above expression the energy $E + \mathrm{i}\eta$ (with $\eta > 0$), and afterwards take the limit $\eta \to 0^+$. When necessary we consider this procedure, but for simplicity of notation we do not write this explicitly.

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

$$\varphi_k^{(\pm)} \approx \frac{1}{\mathcal{N}} \begin{cases} \exp[\pm\mathrm{i}kx] + \mathcal{R}^{(\pm)}(k)\exp[\mp\mathrm{i}kx] & x \to \mp\infty \\ \mathcal{T}(k)\exp[\pm\mathrm{i}kx] & x \to \pm\infty. \end{cases} \quad (2)$$

Note that $\mathcal{T}^{(+)} = \mathcal{T}^{(-)} = \mathcal{T}$ [16]. Also the normalization constant is independent of V, with $\mathcal{N} = \sqrt{2\pi}$ [17].

The asymptotic Green functions are obtained by inserting (2) into (1). If we denote $G_{\pm\mp}(x_f, x_i; E)$ for $x_f \to \pm\infty$, $x_i \to \mp\infty$, and $G_{\pm\pm}(x_f, x_i; E)$ for $x_f, x_i \to \pm\infty$, then $(E = \hbar^2 k^2/(2m))$

$$G_{\pm\mp} = G_{\pm\mp}^{(\mathrm{b.s.})}(x_f, x_i; E) + \frac{m}{\pi\hbar^2}\int_{-\infty}^{+\infty} \mathrm{d}\lambda\, \frac{\mathcal{T}(\lambda)}{k^2 - \lambda^2}\exp[\mathrm{i}\lambda|x_f - x_i|] \quad (3)$$

and

$$G_{\mp\mp} = G_{\mp\mp}^{(\mathrm{b.s.})}(x_f, x_i; E) + \frac{m}{\pi\hbar^2}\int_{-\infty}^{+\infty} \mathrm{d}\lambda\, \frac{1}{k^2 - \lambda^2}\big\{\exp[\mathrm{i}\lambda(x_f - x_i)] + \mathcal{R}^{(\pm)}(\lambda)\exp[\mp\mathrm{i}\lambda(x_f + x_i)]\big\}. \quad (4)$$

In deriving the above equations we have used the general relations [16] $\mathcal{T}^*(k) = \mathcal{T}(-k)$ and $\mathcal{R}^{(\pm)*}(k)\,\mathcal{T}(k) + \mathcal{R}^{(\mp)}(k)\,\mathcal{T}^*(k) = 0$ for equation (3), and $|\mathcal{R}|^2 + |\mathcal{T}|^2 = 1$, $\mathcal{R}^{(\pm)*}(k) = \mathcal{R}^{(\pm)}(-k)$ for equation (4). Obviously, if there are no bound states for the system we just set $G^{(\mathrm{b.s.})} = 0$.

The integral involving $\exp[\mathrm{i}\lambda(x_f - x_i)]$ in (4) leads to a free particle Green function. For the other integrals we consider contour integration along the real axis closed by an infinite semicircle in the upper half of the complex plane. The pole contributions in the integrations are due to the denominator $k^2 - \lambda^2$ and possible singularities of $\mathcal{R}(\lambda)$ and $\mathcal{T}(\lambda)$. Concerning the poles of the quantum coefficients in the upper half of the complex plane λ we note the following. For V non-negative everywhere, for example barriers, the poles [18] (i) are absent when V has either a compact support or a Gaussian-like decay and (ii) exist when V decreases exponentially, appearing at a finite distance to the real axis. If the potential has bound states, say V is a well, besides the results above we also (iii) have poles corresponding to bound energies which are on the positive imaginary axis [16].

For a very large number of cases (see, for instance, [15] and references therein) the terms in the integrations resulting from the bound energy poles exactly cancel $G^{(\mathrm{b.s.})}$. In fact, such cancellations may happen in general as has been argued in [15]. However, if the conjecture is not true, we observe that if a scattering wavefunction is properly extended to the k-complex plane (at the position of a bound energy), the result is proportional to the bound state wavefunction [19]. Thus, $G^{(\mathrm{b.s.})}$ and these terms decrease exponentially as $x \to \pm\infty$ since bound states are localized, so they can be disregarded. For the other poles of $\mathcal{R}$ and $\mathcal{T}$, which are related to the asymptotic decreasing of V (see (i) and (ii) above), it is easy to see that they will lead to terms of the form $C\exp[-c(|x_{\mathrm{f}}|+|x_{\mathrm{i}}|)]$, with C bounded and $c>0$. So, they can also be dropped in the asymptotic limit.

With all this in mind, the remaining steps in the calculations of (3) and (4) are quite straightforward. Thus, we finally find

$$G_{\pm\mp}(x_{\mathrm{f}},x_{\mathrm{i}};E)=\frac{m}{\mathrm{i}\hbar^2 k}\mathcal{T}(k)\exp[\mathrm{i}k|x_{\mathrm{f}}-x_{\mathrm{i}}|] \tag{5}$$

and

$$G_{\mp\mp}(x_{\mathrm{f}},x_{\mathrm{i}};E)=\frac{m}{\mathrm{i}\hbar^2 k}\big\{\exp[\mathrm{i}k|x_{\mathrm{f}}-x_{\mathrm{i}}|]+\mathcal{R}^{(\pm)}(k)\exp[\mp\mathrm{i}k(x_{\mathrm{f}}+x_{\mathrm{i}})]\big\}. \tag{6}$$

The above expressions are deduced for potentials which in the asymptotic limit go to zero at least exponentially. Although there are studies of the continuous spectrum of slowly decaying potentials [20] (for instance, having power law tails), as far as we know there are no general results regarding the pole structures of their quantum amplitudes. Therefore, in principle we cannot assure that (5) and (6) are also valid for this kind of problem. However, we recall that the main point in the previous derivations is to have all the pole contributions from $\mathcal{R}$ and $\mathcal{T}$ vanishing exponentially as $|x|\to\infty$. Thus, our asymptotic Green functions hold for any V for which this is the case.

3. An explicit case, the Rosen–Morse barrier

In this section we exemplify our general results by analysing a specific case, the RM potential $V_{\pm}^{(\mathrm{RM})}(x)=V_0/\cosh^2[\alpha(x\pm c)]$ (for V_{+}^{RM} see figure 1(*a*)). We derive its exact Green function and show that in the asymptotic limit G is given by our previous expressions. We observe that different approximations [8, 21] have been used in the study of this barrier.

Here, for simplicity, we set $\alpha=1$ and $c=0$. The exact Green function $G^{(\mathrm{RM})}(x_{\mathrm{f}},x_{\mathrm{i}};E)$ is given by the differential equation ($U_0=2mV_0/\hbar^2$)

$$\frac{\hbar^2}{2m}\left[-\frac{\partial^2}{\partial x_{\mathrm{f}}^2}+\frac{U_0}{\cosh^2[x_{\mathrm{f}}]}-k^2\right]G^{(\mathrm{RM})}=-\delta(x_{\mathrm{f}}-x_{\mathrm{i}}). \tag{7}$$

Kleinert and Mustapic [22] found the following exact solution for (7) (valid for any value of E):

$$\begin{aligned}G^{(\mathrm{RM})}=&-\frac{m}{\hbar^2}\,\Gamma(n(E)-s)\,\Gamma(n(E)+s+1)\\&\times\big[\Theta(x_{\mathrm{f}}-x_{\mathrm{i}})P_s^{-n(E)}(\tanh[x_{\mathrm{f}}])P_s^{-n(E)}(-\tanh[x_{\mathrm{i}}])+\{x_{\mathrm{f}}\leftrightarrow x_{\mathrm{i}}\}\big]\end{aligned} \tag{8}$$

where $P_a^b(z)$ is the associated Legendre function, $\Gamma(z)$ is the gamma function, $\Theta(z)$ is the Heaviside function, $s=(-1+\sqrt{1-4U_0})/2$ and $n(E)=\sqrt{-2mE/\hbar^2}$. In [22] the authors are interested in boundary conditions such that $G^{(\mathrm{RM})}$ vanishes for $x\to\pm\infty$. For this, they consider $\mathrm{Re}\,[n(E)]>0$ and write $n(E)=+\mathrm{i}k$. However, our interest is in the scattering states, i.e. $G^{(\mathrm{RM})}\neq 0$ for $x\to\pm\infty$. Thus, observing that $n(E)=-\mathrm{i}k$ in (8) is also a solution for (7), and then the condition $\mathrm{Re}\,[n(E)]>0$ (following the assumptions in [22]) is no longer satisfied, we can rewrite equation (8) for $x_{\mathrm{f}}>x_{\mathrm{i}}$ as ($t_{\pm}(x)=(1\pm\tanh[x])/2$)

$$\begin{aligned}G^{(\mathrm{RM})}=&-\frac{m}{\hbar^2}\,\frac{\Gamma(-\mathrm{i}k-s)\,\Gamma(-\mathrm{i}k+s+1)}{\Gamma(-\mathrm{i}k+1)\,\Gamma(-\mathrm{i}k+1)}\exp[\mathrm{i}k(x_{\mathrm{f}}-x_{\mathrm{i}})]\\&\times F(-s,s+1;1-\mathrm{i}k;t_{-}(x_{\mathrm{f}}))\,F(-s,s+1;1-\mathrm{i}k;t_{+}(x_{\mathrm{i}})).\end{aligned} \tag{9}$$

In deriving (9), we have used the identity (9) of [22], relating the associated Legendre functions to the hypergeometric functions $F(a,b;c;z)$ (see [23]). The above Green function can also be

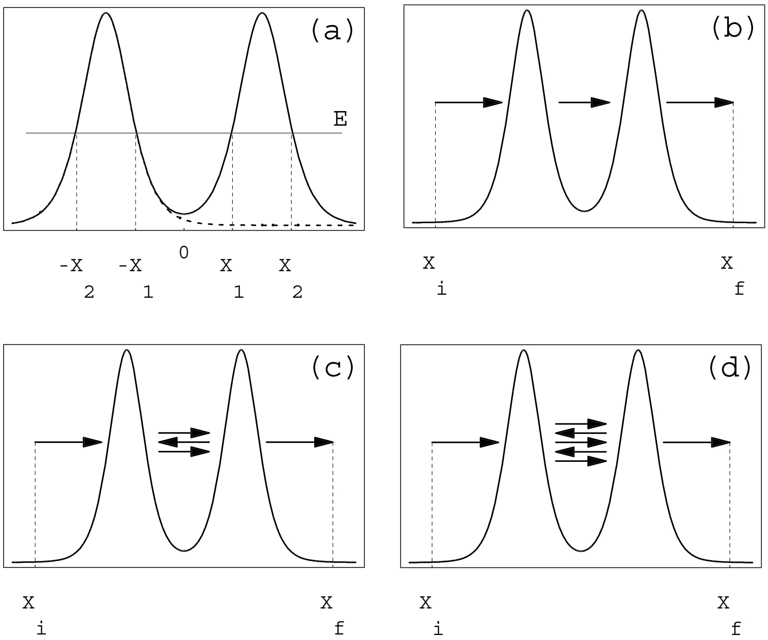

Figure 1. (*a*) The single RM potential $V_+^{\mathrm{RM}}(x)$ (dashed curve) and the double RM potential $V^{\mathrm{d.RM}}(x) = V_+^{\mathrm{RM}} + V_-^{\mathrm{RM}}$. For $V^{\mathrm{d.RM}}$, the classical turning points are four in number if $V^{\mathrm{d.RM}}(0) < E < V^{\mathrm{d.RM}}(\pm c)$ and two (only the external ones, $\pm x_2$) if $E < V^{\mathrm{d.RM}}(0)$. Here, $\alpha = 1/20$ and $c = 50$, so the RM barrier V_+^{RM} practically does not overlap significantly with V_-^{RM}. Figures (*b*)–(*d*) show three examples of scattering paths for the double RM potential. The particle tunnels V_+^{RM}, suffers (*b*) zero, (*c*) one and (*d*) two multiple reflections in between the two single RM barriers and finally tunnels V_-^{RM}.

written in a different form, useful to analyse the reflection case. Applying the identity 9.131-2 of [23] to the hypergeometric function with argument x_{f} in (9), we find

$$\begin{aligned} G^{(\mathrm{RM})} = \frac{m}{\mathrm{i}k\hbar^2}\, & F(-s, s+1; 1-\mathrm{i}k; t_+(x_{\mathrm{i}})) \\ & \times\Bigg\{ \exp[\mathrm{i}k(x_{\mathrm{f}} - x_{\mathrm{i}})]\, F(-s, s+1; 1+\mathrm{i}k; t_+(x_{\mathrm{f}})) \\ & + \frac{\Gamma(-\mathrm{i}k - s)\,\Gamma(-\mathrm{i}k + s + 1)\,\Gamma(\mathrm{i}k)}{\Gamma(-s)\,\Gamma(s+1)\,\Gamma(-\mathrm{i}k)} \exp[-\mathrm{i}k(x_{\mathrm{f}} + x_{\mathrm{i}})]\; (1 + \exp[2x_{\mathrm{f}}])^{\mathrm{i}k} \\ & \times F(1 - \mathrm{i}k + s, -\mathrm{i}k - s; 1 - \mathrm{i}k; t_+(x_{\mathrm{f}}))\Bigg\}. \end{aligned} \tag{10}$$

Now, we consider the asymptotic limit for the exact Green functions (9) and (10). If $x_{\mathrm{f}} \to \infty$ and $x_{\mathrm{i}} \to -\infty$ in (9), then $t_-(x_{\mathrm{f}})$ and $t_+(x_{\mathrm{i}})$ go to zero. Since for the hypergeometric functions $F(a, b; c; 0) = 1$ [23], we find

$$G_{+-}^{(\mathrm{RM})}(x_{\mathrm{f}}, x_{\mathrm{i}}; E) = \frac{m}{\mathrm{i}k\hbar^2}\, \mathcal{T}^{(\mathrm{RM})} \exp[\mathrm{i}k(x_{\mathrm{f}} - x_{\mathrm{i}})] \tag{11}$$

with

$$\mathcal{T}^{(\mathrm{RM})} = \frac{k}{\mathrm{i}}\, \frac{\Gamma(-\mathrm{i}k - s)\,\Gamma(-\mathrm{i}k + s + 1)}{\Gamma(-\mathrm{i}k + 1)\,\Gamma(-\mathrm{i}k + 1)}. \tag{12}$$

In the same way, considering in (10) $x_{\rm f}, x_{\rm i} \to -\infty$, we obtain

$$G_{--}^{(\rm RM)}(x_{\rm f}, x_{\rm i}; E) = \frac{m}{{\rm i}k\hbar^2}\big\{\exp[{\rm i}k(x_{\rm f} - x_{\rm i})] + \mathcal{R}^{(\rm RM,+)}\exp[-{\rm i}k(x_{\rm f} + x_{\rm i})]\big\} \quad (13)$$

where

$$\mathcal{R}^{(\rm RM,+)} = \frac{\Gamma(-{\rm i}k - s)\,\Gamma(-{\rm i}k + s + 1)\Gamma({\rm i}k)}{\Gamma(-s)\,\Gamma(s+1)\Gamma(-{\rm i}k)}. \quad (14)$$

$\mathcal{T}^{(\rm RM)}$ and $\mathcal{R}^{(\rm RM,+)}$ are the correct transmission and reflection coefficients for the RM barrier [24, 25].

Thus, we see from (11)–(14) that the asymptotic Green functions for the RM potential are exactly in the general forms discussed in section 2. Finally, we mention that the pole structures for the quantum amplitudes (12) and (14) are analysed in [18].

4. Multiple-barrier case

Suppose the Hamiltonian $H = H^{(0)} + V$, with $G^{(0)}$ being the Green function for $H^{(0)}$. We can obtain G for H from

$$G(x_{\rm f}, x_{\rm i}; E) = \sum_{j=0}^{\infty}\int_{-\infty}^{+\infty} {\rm d}x_1 \ldots {\rm d}x_j\, V(x_1)\ldots V(x_j) G^{(0)}(x_1, x_{\rm i}; E)\ldots G^{(0)}(x_{\rm f}, x_j; E). \quad (15)$$

Now we assume $V = \sum_{j=1}^{N} V^{(j)}(x)$, with $V^{(j)}(|x| \to \infty) \to 0$ for all j and no appreciable overlapping between the $V^{(j)}$ (see, for instance, figure 1(a)). From the above expansion and the results in section 2 we construct the asymptotic Green function for this multiple barrier potential.

Since we shall derive a semiclassical formula for the problem, which includes, for example, multiple propagation between the $V^{(j)}$, we need to consider the classical actions of the corresponding trajectories. Thus, instead of the expressions for the G derived in section 2, we use the slightly modified asymptotic Green functions (see appendix A)

$$G_{\mp\mp}(x_{\rm f}, x_{\rm i}; k) = \frac{m}{{\rm i}\hbar^2 k}\left\{\exp\left[\frac{\rm i}{\hbar}S_k(x_{\rm f}, x_{\rm i})\right] + R^{(\pm)}(k)\exp\left[\mp\frac{\rm i}{\hbar}(S_k(x_{\rm f}, x_0) + S_k(x_{\rm i}, x_0))\right]\right\}$$
$$G_{\pm\mp}(x_{\rm f}, x_{\rm i}; k) = \frac{m}{{\rm i}\hbar^2 k}\,T^{(\pm)}(k)\exp\left[\frac{\rm i}{\hbar}(S_k(x_{\rm f}, x_0^{(\pm)}) + S_k(x_{\rm i}, x_0^{(\mp)}))\right]. \quad (16)$$

In (16), S_k is the classical action, x_0 are just reference points (chosen according to convenience, see the next section) and R and T are related to the amplitudes $\mathcal{R}$ and $\mathcal{T}$ by energy-dependent phases (equation (31) in appendix A).

The procedure to follow now is completely analogous to that in [15], where the lengthy calculations are performed in detail, so here we just outline the main steps and the final results. For a given energy, we assume that the end points $x_{\rm i}$ and $x_{\rm f}$ are outside the classically prohibited regions; for instance, for the case shown in figure 1(a), the prohibited regions are $(-x_2, -x_1)$ and (x_1, x_2). First, we consider $H^{(0)}(x) = -\frac{\hbar^2}{(2m)}{\rm d}^2/{\rm d}x^2$ ($G^{(0)}$ being then the free Green function) and set $V(x)$ equal to a single $V^{(j)}$, say $V^{(1)}$. From (15) we have $G^{(1)}$ given as a series, whose terms are given by integrals over the classical actions and $V^{(1)}$, but since $G^{(j)}$, for any j, must be given as in (16), we can formally associate for $V^{(j)}$ its corresponding $T^{(j)}$ and $R^{(j)}$ through such series. Thus, we end up with $G^{(1)}$ in the appropriate form (16). Next we proceed by assuming $H^{(0)}(x) = -\frac{\hbar^2}{(2m)}{\rm d}^2/{\rm d}x^2 + V^{(1)}$, where this time the unperturbed Green function is $G^{(1)}$ calculated in the previous step. For $V(x)$ we take the single potential

$V^{(2)}$. Equation (15) now leads to a series involving $T^{(1)}$, $R^{(1)}$, classical actions and $V^{(2)}$. Again, we can identify from the series expressions corresponding to the coefficients $R^{(2)}$ and $T^{(2)}$. After this identification, the series reduces to an infinite sum comprising only the four quantum amplitudes, but which can be performed exactly since it is a geometric series. The resulting Green function is once more given by a formula like equation (16), but now with the amplitudes being functions of $R^{(1)}$, $T^{(1)}$, $R^{(2)}$ and $T^{(2)}$. The process thus can be recursively repeated until all the N potentials $V^{(j)}$ are included [15]. This yields

$$G^{(\mathrm{gcl})} = \frac{m}{\mathrm{i}\hbar^2 k} \sum_{\mathrm{s.p.}} W_{\mathrm{s.p.}} \exp\left[\frac{\mathrm{i}}{\hbar} S_{\mathrm{s.p.}}(x_\mathrm{f}, x_\mathrm{i}; E)\right]. \tag{17}$$

Here, s.p. stands for 'scattering path', and $S_{\mathrm{s.p.}}$ and $W_{\mathrm{s.p.}}$ are, respectively, its corresponding classical action and amplitude. A 'scattering path' represents a trajectory where the particle starts from x_i, suffers multiple reflections and transmissions between the $V^{(j)}$, and finally arrives at x_f. In an s.p. however, the particle never goes into a classically forbidden region; it reflects from or tunnels these regions instead (this point will become clearer in the applications in the next section). The weights $W_{\mathrm{s.p.}}$ are constructed as follows: each time the particle hits a classical turning point associated with $V^{(j)}$, it can be reflected or transmitted by the potential. In the first case W gains a factor $R^{(j)}$, and in the second it gains a factor $T^{(j)}$. The total W is then the product of all the partial amplitudes for that particular s.p.

For segmented potentials, i.e., potentials written as a sum of non-overlapping $V^{(j)}$ of compact support, expressions such as (17) lead to exact Green functions [15]. In the present case equation (17) is an approximation, because to derive it we (i) use the asymptotic Green functions (16) and (ii) consider that in the region between the classical turning points of $V^{(j)}$ the total $V(x)$ is practically well described by $V^{(j)}$ alone, i.e. the contribution of the other $V^{(i)}$ to V in such a region is not very important (e.g. see figure 1(*a*)). So, we can use the transmission and reflection coefficients $T^{(j)}$ and $R^{(j)}$ at these classical turning points to construct W. Thus, if the individual potentials become closer and closer we expect to have a less accurate approximation from our method. However, as we will see from the next examples, the $V^{(j)}$ can be fairly close to each other and yet we obtain good results from $G^{(\mathrm{gcl})}$. We leave to the last section the discussion of ways to overcome the difficulties when the $V^{(j)}$ are too close together.

Finally, we can derive the quantum coefficients for multiple barrier potentials from the Green function by (a) setting $x_\mathrm{i} \to \pm\infty$ and $x_\mathrm{f} \to \pm\infty$ (reflection case) or $x_\mathrm{i} \to \mp\infty$ and $x_\mathrm{f} \to \pm\infty$ (transmission case), (b) taking the appropriate asymptotic limit for the $S(x_\mathrm{f}, x_\mathrm{i})$ and (c) performing the sum in (17). The final result must have exactly the same form as the asymptotic Green functions from section 2. Therefore, by a direct inspection we obtain the desired quantum amplitudes. We illustrate this procedure in the examples in the next section.

5. Examples

5.1. Double Rosen–Morse potential

The double RM potential is given by $V^{(\mathrm{d.RM})}(x) = V_+^{(\mathrm{RM})}(x) + V_-^{(\mathrm{RM})}(x)$. We discuss only the transmission case; the reflection case follows in a similar fashion.

We need to consider all the scattering trajectories joining the end points. Each particular trajectory can be described as follows. The particle leaves the initial position $x_\mathrm{i} < -x_2$ (see figure 1) and goes to $-x_2$. In $-x_2$, the particle tunnels to $-x_1$ (in this step the path's contribution to the semiclassical propagator gains a factor $T^{(\mathrm{RM})}$). Between the classical turning points, $-x_1$ and x_1, the particle suffers n multiple reflections (gaining a factor $[R^{(\mathrm{RM})}]^{2n}$). Then the particle tunnels to x_2 (the contribution again gaining a factor $T^{(\mathrm{RM})}$). Finally, it travels to the final position $x_{\rm f} > x_2$. Figures 1(*b*)–(*d*) show schematically three examples of these 'classical paths'.

The generalized semiclassical Green function is written as

$$\begin{aligned} G_{+-}^{(\rm gcl)} &= \frac{m}{{\rm i}k\hbar^2}\left\{T^{(\rm RM)}\exp\left[\frac{\rm i}{\hbar}S(-x_2, x_{\rm i})\right]\sum_{n=0}^{\infty}\left[R^{(\rm RM)}\right]^{2n}\exp[{\rm i}k(2n+1)\phi(k)]\right.\\ &\qquad\left.\times T^{(\rm RM)}\exp\left[\frac{\rm i}{\hbar}S(x_{\rm f}, x_2)\right]\right\}\\ &= \frac{m}{{\rm i}k\hbar^2}\,T_{(\rm gcl)}^{(\rm d.RM)}\exp\left[\frac{\rm i}{\hbar}\left\{S(x_{\rm f}, x_2)+S(-x_2, x_{\rm i})\right\}\right]. \end{aligned} \tag{18}$$

The expressions for the action S and the amplitudes $T^{(\rm RM)}$ and $R^{(\rm RM)}$ are presented in appendix B. The generalized semiclassical transmission coefficient for the double RM barrier is then

$$T_{\rm gcl}^{(\rm d.RM)} = \left(\frac{[T^{(\rm RM)}]^2}{1-\left[R^{(\rm RM)}\right]^2\exp[2{\rm i}k\phi(k)]}\right)\exp[{\rm i}k\phi(k)] \tag{19}$$

where ($\varepsilon = V_0/E$)

$$\phi(k) = \int_{-x_1}^{+x_1}{\rm d}x\sqrt{1-\left(\frac{\varepsilon}{\cosh^2[\alpha(x+c)]}+\frac{\varepsilon}{\cosh^2[\alpha(x-c)]}\right)}. \tag{20}$$

In (20), if $E < V^{(\rm d.RM)}(0)$, we take $x_1 = 0$, so $\phi = 0$. On the other hand, if $E > V^{(\rm d.RM)}(c)$, then $x_1 = c$ (see figure 1(*a*)). Depending on the distance between the two barriers, the above integral can be approximated by (with I defined in appendix B)

$$\begin{aligned} \phi(k) &\approx 2\int_{-c+{\rm arccosh}[\sqrt{\varepsilon}]/\alpha}^{0}{\rm d}x\sqrt{1-\frac{\varepsilon}{\cosh^2[\alpha(x+c)]}}\\ &\approx \frac{1}{\alpha}\times\begin{cases} 2I(\alpha c)-\ln[|\varepsilon-1|] & \text{if}\quad \varepsilon\neq 1\\ 2\ln[\cosh[\alpha c]] & \text{if}\quad \varepsilon = 1. \end{cases} \end{aligned} \tag{21}$$

It is worth recalling that equations (18) and (19) are valid for any value of E.

In order to test how accurate the method is, we numerically integrate the Schrödinger equation for this potential using the split-operator approach. We evolve a Gaussian wavepacket initially localized well to the left of the potential. After sufficient evolution time the packet is split into the reflected and transmitted parts. By choosing a very broad Gaussian the average momentum and consequently the energy are well defined, so its transmission can quite fairly be compared with the steady-state plane wave transmission probability [14], which in our case is $|T_{\rm gcl}^{(\rm d.RM)}|^2$ (we note that T and $\mathcal{T}$ differ only by a global phase).

For the parameters we choose typical values for heterostructures in GaAs [26]; the particle's mass is $m = 0.07 \times$ electron mass, $V_0 = 0.23$ eV, $\alpha^{-1} = 20$ Å and $c = 50$ and 25 Å. The transmission probability $|\mathcal{T}_{\rm gcl}^{(\rm d.RM)}|^2$ is displayed in figures 2(*a*) and (*b*) and shows a very good agreement with the exact numerical calculations[1]. We observe that this is also the case even when the individual barriers are close to each other, as for $c = 25$ Å, figure 2(*b*). For this last case we have integrated (20) numerically.

[1] Figure 2(*a*) differs from figure 9 of [14], which in principle corresponds to the same calculations. We were able to exactly reproduce the graph of Kira *et al* by using a barrier height of $0.23\ {\rm eV}/2 = 0.115$ eV, so there may be a misprint in [14] regarding the value of V_0 for that plot.

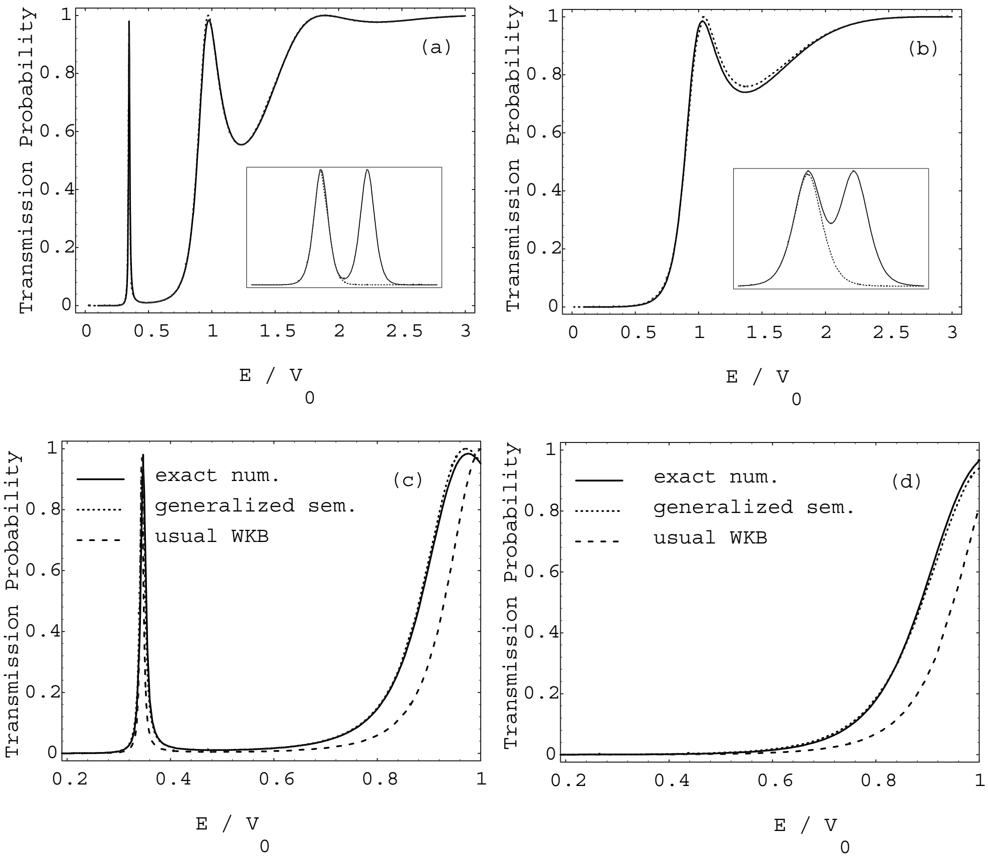

Figure 2. (*a*) Comparison between the transmission probability, for the parameters as in the text and $c = 50$ Å, for the double RM potential calculated exact numerically (solid curve) and by using our generalized semiclassical approximation (dotted curve). In the inset is shown the double RM potential and the single $V_+^{\mathrm{RM}}(x)$ barrier (dotted curve). (*b*) The same as in (*a*) but with $c = 25$ Å. For $E < V_0$ we also plot the usual WKB approximation, equation (22) (which is valid only in this region of energy), with (*c*) $c = 50$ Å and (*d*) $c = 25$ Å.

We also compare our approach with the usual WKB approximation. In [27] (p 86, problem 12) the authors discuss the WKB wavefunction for a general double barrier potential. Specializing their expressions for our system, we obtain the following transmission probability:

$$|T_{\mathrm{WKB}}^{(\mathrm{d.RM})}|^2 = \left(4\exp\left[4\pi\frac{k}{\alpha}(\sqrt{\varepsilon}-1)\right]\cos^2[k\phi(k)] + \sin^2[k\phi(k)]\right)^{-1} \tag{22}$$

valid only for $E < V_0$ (for $E > V_0$ the above expression rapidly increases to values greater than unity, losing its physical meaning). In figures 2(*c*) and (*d*) equation (22) is compared with our results. We see that our generalized semiclassical method is really better than the WKB approximation and, in contrast to (22), valid for the whole energy range.

5.2. *Woods–Saxon barrier*

The method can also be applied to potentials having asymmetric asymptotic behaviour. As an example we consider the WS steps $V_{(\pm)}^{(\mathrm{WS})} = V_0/(1 + \exp[\pm\alpha(x \mp c)])$, which go to 0 for

$x \to \pm\infty$ and to V_0 for $x \to \mp\infty$. Their quantum mechanical amplitudes are presented in appendix C.

It is straightforward to extend the results in section 2 to this case. Indeed, the asymptotic Green functions, say, for $V_{(-)}^{(\mathrm{WS})}$ with $c = 0$, are easily obtained as (valid for any value of E)

$$\begin{aligned} G_{\pm\mp} &= \frac{m}{\mathrm{i}\hbar^2\sqrt{k\mu}} \mathcal{T}_{(-)}^{(\mathrm{WS},\pm)} \exp[\pm\mathrm{i}(k_\mp x_\mathrm{f} - k_\pm x_\mathrm{i})] \\ G_{\mp\mp} &= \frac{m}{\mathrm{i}\hbar^2 k_\pm} \left\{ \exp[\mathrm{i}k_\pm|x_\mathrm{f} - x_\mathrm{i}|] + \mathcal{R}_{(-)}^{(\mathrm{WS},\pm)} \exp[\mp\mathrm{i}k_\pm(x_\mathrm{f} + x_\mathrm{i})] \right\} \end{aligned} \tag{23}$$

where $k_+ = k$ and $k_- = \mu = \sqrt{2m(E - V_0)/\hbar^2}$.

We construct a WS barrier by writing $V^{(\mathrm{WSb.})}(x) = V_0/(1 + \exp[-\alpha(x + c)]) - V_0/(1 + \exp[-\alpha(x - c)])$, figure 3($a$). This barrier can be treated as a composition [28] of the two potential steps $V_{(-)}^{\mathrm{WS}}$ and $V_{(+)}^{\mathrm{WS}}$, so we can derive the Green function and consequently the transmission and the reflection amplitudes by following the same steps as those for the double RM potential. We illustrate this by discussing in detail the reflection case. Suppose $E > V_0$, then there is a direct path (the particle goes straight from x_i to x_f without hitting the barrier) and a whole class of indirect paths. For the indirect paths the particle leaves $x_\mathrm{i} \ll -c$ and can either (i) be reflected at $-c$ (gaining a factor $R_{(-)}^{(\mathrm{WS},+)}$) coming back to $x_\mathrm{f} \ll -c$, or (ii) cross the point $-c$ (gaining a factor $T_{(-)}^{(\mathrm{WS},+)}$), suffer n multiple scatterings within the region $(-c, c)$ (gaining a factor $[R_{(-)}^{(\mathrm{WS},-)}]^{2n-1}$, note that $R_{(-)}^{(\mathrm{WS},-)} = R_{(+)}^{(\mathrm{WS},+)}$) and finally cross $-c$ (gaining a factor $T_{(-)}^{(\mathrm{WS},-)}$) arriving at $x_\mathrm{f} \ll -c$. Examples of such paths are displayed in figures 3(b), (d). Here we take the reference points x_0 in equation (16) as being $\pm c$, but it is easy to show that the final results do not depend on any particular choice for them. Thus, we find that the Green function is (for S, the quantum amplitudes and the function J see appendix C)

$$\begin{aligned} G_{--}^{(\mathrm{gcl})} &= \frac{m}{\mathrm{i}k\hbar^2} \Bigg\{ \exp\left[\frac{\mathrm{i}}{\hbar} S(x_\mathrm{f}, x_\mathrm{i})\right] + R_{(-)}^{(\mathrm{WS},+)} \exp\left[\frac{\mathrm{i}}{\hbar}\{S(-c, x_\mathrm{i}) + S(x_\mathrm{f}, -c)\}\right] \\ &\quad + T_{(-)}^{(\mathrm{WS},+)} R_{(-)}^{(\mathrm{WS},-)} \exp\left[\frac{\mathrm{i}}{\hbar} S(-c, x_\mathrm{i})\right] \sum_{n=0}^{\infty} \left[R_{(-)}^{(\mathrm{WS},-)}\right]^{2n} \exp[2(n+1)\mathrm{i}k\phi(k)] \\ &\quad \times T_{(-)}^{(\mathrm{WS},-)} \exp\left[\frac{\mathrm{i}}{\hbar} S(x_\mathrm{f}, +c)\right] \Bigg\} \\ &= \frac{m}{\mathrm{i}k\hbar^2} \left\{ \exp\left[\frac{\mathrm{i}}{\hbar} S(x_\mathrm{f}, x_\mathrm{i})\right] + R_{\mathrm{gcl}}^{(\mathrm{WS\,b.},+)} \exp\left[\frac{\mathrm{i}}{\hbar}\{S(x_\mathrm{f}, -c) + S(-c, x_\mathrm{i})\}\right] \right\} \end{aligned} \tag{24}$$

with

$$R_{\mathrm{gcl}}^{(\mathrm{WS\,b.},+)} = R_{(-)}^{(\mathrm{WS},+)} + \frac{T_{(-)}^{(\mathrm{WS},+)} T_{(-)}^{(\mathrm{WS},-)} R_{(-)}^{(\mathrm{WS},-)} \exp[2\mathrm{i}k\phi(k)]}{1 - \left[R_{(-)}^{(\mathrm{WS},-)}\right]^2 \exp[2\mathrm{i}k\phi(k)]} \tag{25}$$

where ($\varepsilon = V_0/E$)

$$\begin{aligned} \phi(k) &= \int_{-c}^{+c} \mathrm{d}x \sqrt{1 - \left(\frac{\varepsilon}{1 + \exp[-\alpha(x + c)]} - \frac{\varepsilon}{1 + \exp[-\alpha(x - c)]}\right)} \\ &\approx 2\int_0^c \mathrm{d}x \sqrt{1 - \frac{\varepsilon}{1 + \exp[-\alpha x]}} \\ &= \frac{2}{\alpha}(J(\exp[-\alpha c]) - J(1)). \end{aligned} \tag{26}$$

The approximation made in the above integration is valid for large values of c.

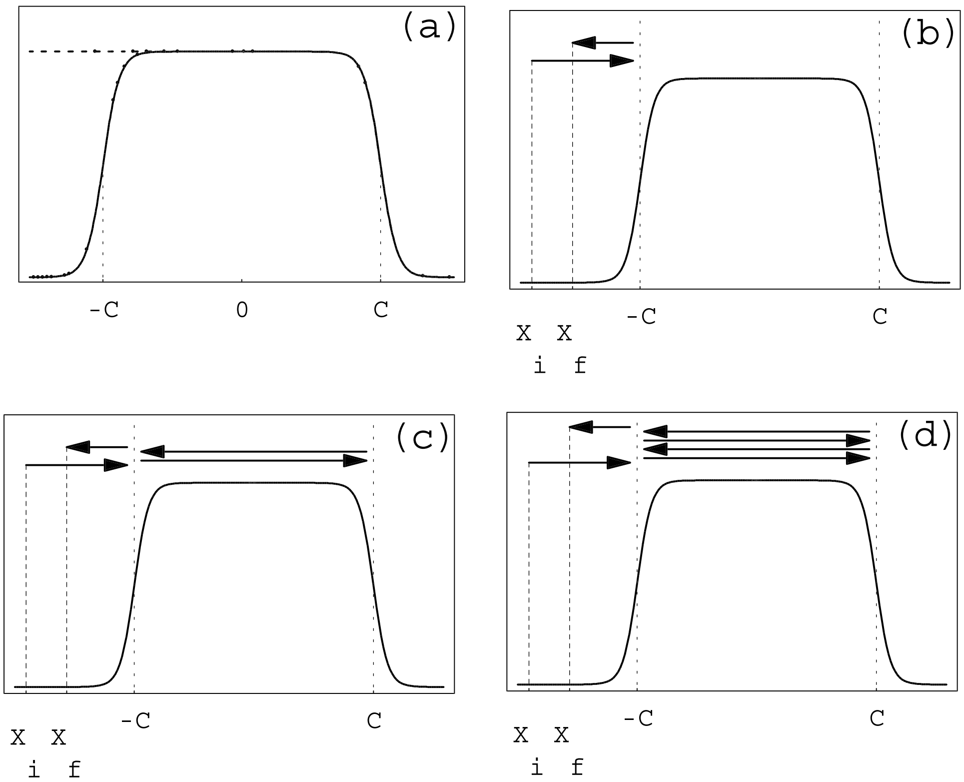

Figure 3. (*a*) The potential step $V_+^{(\mathrm{WS})}$ (dashed line) and the WS barrier $V^{(\mathrm{WS\,b.})}(x) = V_0/(1+\exp[-\alpha(x+c)]) - V_0/(1+\exp[-\alpha(x-c)])$. The barrier can be viewed as a composition of $V_+^{(\mathrm{WS})}$ and $V_-^{(\mathrm{WS})}$. Three examples of scattering paths for the WS barrier for $E > V_0$ are displayed in (*b*)–(*d*). (*b*) A single reflection at $-c$. (*c*) Transmission at $-c$, reflection at $+c$ and transmission at $-c$. (*d*) The same as in (*c*) but now with an extra bouncing between $-c$ and $+c$.

As discussed before, the relation between R and $\mathcal{R}$ is established by taking explicitly the limit of $x_{\mathrm{f}}, x_{\mathrm{i}} \to -\infty$ and then comparing (24) with the general form of the Green function in (6). From the results in appendix C it is straightforward to show that $\mathcal{R}_{\mathrm{gcl}}^{(\mathrm{WS\,b.},+)} = R_{\mathrm{gcl}}^{(\mathrm{WS\,b.},+)} \exp[\mathrm{i} f_R^{(+)}]$. For the transmission case ($x_{\mathrm{f}} \to +\infty$, $x_{\mathrm{i}} \to -\infty$) a similar analysis gives

$$T_{\mathrm{gcl}}^{(\mathrm{WS\,b.})} = \left(\frac{T_{(-)}^{(\mathrm{WS},+)} T_{(-)}^{(\mathrm{WS},-)}}{1 - \left[R_{(-)}^{(\mathrm{WS},-)}\right]^2 \exp[2\mathrm{i}k\phi(k)]} \right). \qquad (27)$$

We derived all these expressions assuming $E > V_0$, but, as in a full quantum mechanical calculation, they are equally valid for $E < V_0$.

To test the above expressions we consider the same values of V_0 and mass as used for the double RM potential and set $c = 40$ Å, with $\alpha^{-1} = 5$ Å (figure 4(*a*)) and $\alpha^{-1} = 0.2$ Å (figure 4(*b*)). Figure 4(*a*) shows a very good agreement between the generalized semiclassical transmission and reflection probabilities and the exact numerical calculations. For the values of α in figure 4(*b*) the smooth barrier practically becomes the usual rectangular barrier (see the inset). We compare our results with the analytical transmission and reflection probabilities for the rectangular barrier and the agreement is quite good. In fact, one can easily show that in the

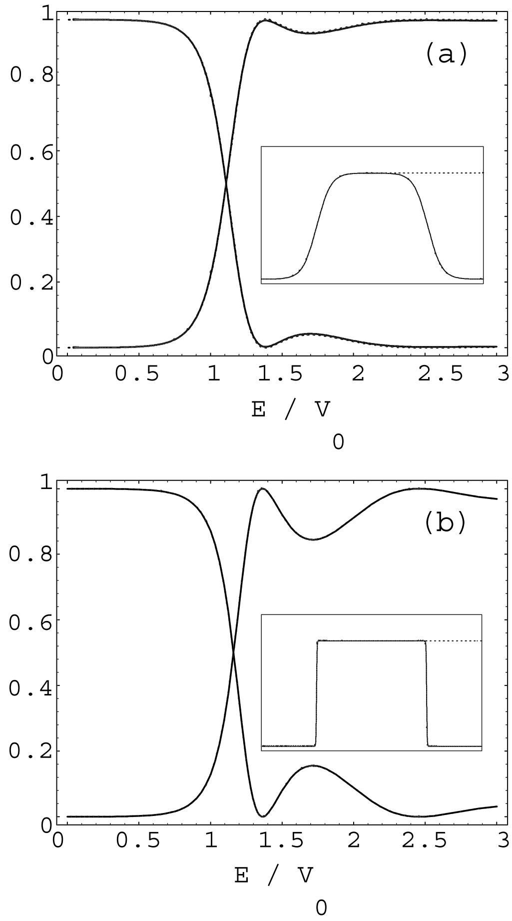

Figure 4. (*a*) Reflection and transmission probabilities from our method (dotted curves) compared with exact numerical calculations (solid curves). The parameters are as in the text and $\alpha^{-1} = 5$ Å. In the inset is shown the WS barrier, where for reference is also plotted the $V_+^{(\mathrm{WS})}$ step (dotted curve). (*b*) The same parameters as in (*a*) but with $\alpha^{-1} = 0.2$ Å. Since in this case the WS barrier (inset) is practically a rectangular barrier we compare our generalized semiclassical approximation (dotted line) with the results of an equivalent rectangular barrier (solid line). The agreement is such that we cannot distinguish between the curves.

limit of $\alpha \to \infty$ equations (25) and (27) give the exact quantum amplitudes for the rectangular barrier.

6. Discussion and conclusions

Throughout this paper we have discussed an improved semiclassical approach to calculate Green functions for multiple barrier potentials. We showed how asymptotic semiclassical Green functions can lead to transmission and reflection amplitudes of decaying potentials. In particular, we emphasized the problem of barrier tunnelling. Two cases, double symmetric RM and WS barriers, were explicitly calculated. Good analytical results were obtained for their transmission and reflection probabilities.

The generalized semiclassical approximation presented here is a mixed approach. Only the usual sum over classical trajectories is used to construct the Green functions (in contrast with situations where purely non-classical paths are necessary to describe the system evolution [29]). However, local quantum effects due to each barrier are fully treated in terms of quantum coefficients which contribute as amplitudes (or weights) for the classical paths. Global transmission and reflection amplitudes are obtained by just composing semiclassically the 'parts' (the $V^{(j)}$) of the whole potential. Thus, our method can be regarded as a semiclassical version of a quantum multiple-scattering theory [30].

To illustrate our results we discussed two examples for which the number of single barriers is $N = 2$. One may think that for a large N the sum in (17) would be hard to carry out. However, this is not the case. First we observe that the series in (17) is always a geometric series, so it can be performed exactly. Second, to identify all the scattering paths may seem difficult, but in [15] a simple method is derived that allows one to classify and to sum up all the scattering paths in a straightforward way.

Although the potentials discussed here are already of interest, one may want to extend the present method to other situations, for example if the individual $V^{(j)}$ decay exponentially and are very close to each other, if they have power-law decay and, finally, if the whole V is not written as $\sum_j V^{(j)}(x)$, but still has successive 'valleys' and 'hills' in a certain region and then decays asymptotically. We can apply our method in all these cases. The semiclassical Green function is again given by (17), with the actions given by $\int \mathrm{d}x\, \sqrt{2m[E - V(x)]}$ in the classically allowed regions. But now the R and T are constructed as follows. We fit each hill by a single barrier which falls off exponentially but locally has the same shape as the hill. Then, the transmission and reflection amplitudes to be considered are those of the fitted barriers. Obviously, the difficulties in implementing such a decomposition will depend on each system considered.

Finally, we would like to comment on the energy-dependent phases, which connect the usual reflection and transmission amplitudes $\mathcal{R}$ and $\mathcal{T}$ with our R and T (see appendix A). If we reorganize all these phases, written $W = w \exp[\mathrm{i}\mu(E)]$, we have from (17) $G^{(\mathrm{gcl})} = m/(\mathrm{i}\hbar^2 k) \sum w \exp[\mathrm{i}(S/\hbar + \mu(E))]$. Thus, $\mu(E)$ can be considered as a generalized Maslov index. Recently [31], modifications in the usual Maslov index have led to nice improved semiclassical results for barrier scattering and for the bound state energy spectrum. Following this line, one could try, from the WKB quantization rule [12] $\oint p(x)\,\mathrm{d}x = \hbar\pi(n + \mu/4)$, with μ calculated as in the present approach, to obtain the eigenenergies for confined systems. Indeed, this prescription gives accurate bound energies for quantum wells as will be reported elsewhere.

Acknowledgments

We would like to thank N T Maitra for bringing to our knowledge important features about the RM potential and J A Freire for help with the numerics. We also acknowledge computational facilities provided by PADCT (project no 620081/97-0).

Appendix A

The Schrödinger equation can be written as [32]

$$\varphi_k^{(\pm)}(x) = \frac{C}{\sqrt{p(x)}} \left\{ A^{(\pm)}(x) \exp\left[\pm\frac{\mathrm{i}}{\hbar}\int_{x_0}^{x} \mathrm{d}y\, p(y)\right] + B^{(\pm)}(x) \exp\left[\mp\frac{\mathrm{i}}{\hbar}\int_{x_0}^{x} \mathrm{d}y\, p(y)\right]\right\} \quad (28)$$

with $p(x) = \sqrt{2m[E_k - V(x)]}$, $E_k = \hbar^2 k^2/(2m)$, C the normalization constant and $(f'(x) \equiv \mathrm{d}f(x)/\mathrm{d}x)$

$$\begin{aligned} A'^{(\pm)}(x) &= \frac{p'(x)}{2p(x)} B^{(\pm)}(x) \exp\left[\mp \frac{2\mathrm{i}}{\hbar} \int_{x_0}^{x} \mathrm{d}y\, p(y)\right] \\ B'^{(\pm)}(x) &= \frac{p'(x)}{2p(x)} A^{(\pm)}(x) \exp\left[\pm \frac{2\mathrm{i}}{\hbar} \int_{x_0}^{x} \mathrm{d}y\, p(y)\right]. \end{aligned} \tag{29}$$

We note that x_0 is just a reference point and can be chosen arbitrarily. Different solutions for the wavefunctions are obtained by considering different boundary conditions. For scattering states, the appropriate boundary conditions for waves incoming from the left (+) and right (−) are $A^{(\pm)}(\mp\infty) = 1$ and $B^{(\pm)}(\pm\infty) = 0$. So, we can rewrite (29) as

$$\begin{aligned} A^{(\pm)} &= 1 + \int_{\mp\infty}^{x} \mathrm{d}y\, \frac{p'(y)}{2p(y)} B^{(\pm)}(y) \exp\left[\mp \frac{2\mathrm{i}}{\hbar} \int_{x_0}^{y} \mathrm{d}z\, p(z)\right] \\ B^{(\pm)} &= -\int_{x}^{\pm\infty} \mathrm{d}y\, \frac{p'(y)}{2p(y)} A^{(\pm)}(y) \exp\left[\pm \frac{2\mathrm{i}}{\hbar} \int_{x_0}^{y} \mathrm{d}z\, p(z)\right]. \end{aligned} \tag{30}$$

Usually, we can solve (30) only by using some kind of approximation. For instance, if we assume $p'/(2p) \approx 0$, we obtain the usual WKB solution [32]. Better expressions are, in general, derived with the help of recurrence procedures [33].

Suppose that for $x > x_+$ and $x < x_-$, $p'/2p$ in (30) is small and so we can approximate $A^{(\pm)}(x \gtrless x_\pm) \approx A^{(\pm)}(\pm\infty)$ and $B^{(\pm)}(x \lessgtr x_\mp) \approx B^{(\pm)}(\mp\infty)$. In this limit we can identify the amplitudes A and B with the usual reflection and transmission amplitudes

$$\begin{aligned} A^{(\pm)}(\pm\infty) &= T^{(\pm)} = \mathcal{T} \exp[\mathrm{i}\phi_T^{(\pm)}] \\ B^{(\pm)}(\mp\infty) &= R^{(\pm)} = \mathcal{R}^{(\pm)} \exp[\mathrm{i}\phi_R^{(\pm)}] \end{aligned} \tag{31}$$

and write for (28) (with $C/p \approx 1/\mathcal{N}$ and $S_k(x, x_0) = \int_{x_0}^{x} \mathrm{d}y\, p(y) = \hbar k \int_{x_0}^{x} \mathrm{d}y\, \sqrt{1 - V(y)/E_k}$)

$$\begin{aligned} \varphi_k^{(\pm)}(x) &= \frac{1}{\mathcal{N}} \left\{ \exp\left[\pm \frac{\mathrm{i}}{\hbar} S_k(x, x_0)\right] + R^{(\pm)} \exp\left[\mp \frac{\mathrm{i}}{\hbar} S_k(x, x_0)\right] \right\} \qquad \text{for} \quad x \lessgtr x_\mp \\ \varphi_k^{(\pm)}(x) &= \frac{1}{\mathcal{N}} T^{(\pm)} \exp\left[\pm \frac{\mathrm{i}}{\hbar} S_k(x, x_0)\right] \qquad \text{for} \quad x \gtrless x_\pm. \end{aligned} \tag{32}$$

The phases in (31) are obtained through a direct comparison between the asymptotic wavefunctions (2) and (32) (for which the limit of $S_k(x \to \pm\infty, x_0)$ must be explicitly taken). Observe that the wavefunctions (2) and (32) may differ by a physically irrelevant overall phase.

Now, the Green function outside the region (x_-, x_+) is obtained by using (32) into (1). All the assumptions made in section 2 are also valid here. So, following the same steps and noticing that $-S_k(x_\mathrm{f}, x_\mathrm{i}) = S_{-k}(x_\mathrm{f}, x_\mathrm{i})$ we finally obtain the asymptotic Green function (16).

Appendix B

Here we consider the classical action S for the single RM potential $V(x) = V_0/\cosh^2[\alpha x]$. We define $\varepsilon = V_0/E$ and identify the x_0 in (16), for $\varepsilon \geqslant 1$, as the classical turning points $\pm x_t = \pm\mathrm{arccosh}[\sqrt{\varepsilon}]/\alpha$ and, for $\varepsilon \leqslant 1$, as $x_t = 0$. S is given by

$$\begin{aligned} S(x_\mathrm{f}, x_\mathrm{i}) &= \int_{x_\mathrm{i}}^{x_\mathrm{f}} \mathrm{d}x \sqrt{2m\left(E - \frac{V_0}{\cosh^2[\alpha x]}\right)} \\ &= \hbar \frac{k}{\alpha} \{\mathrm{sign}(x_\mathrm{f}) I(\alpha|x_\mathrm{f}|) - \mathrm{sign}(x_\mathrm{i}) I(\alpha|x_\mathrm{i}|)\} \end{aligned} \tag{33}$$

with (for $\varepsilon \neq 1$)

$$I(x) = \ln\left[\sinh[x] + \sqrt{\cosh^2[x] - \varepsilon}\right] + \frac{\sqrt{\varepsilon}}{4}\ln\left[\left(\frac{\sqrt{\varepsilon}\sinh[x] - \sqrt{\cosh^2[x] - \varepsilon}}{\sqrt{\varepsilon}\sinh[x] + \sqrt{\cosh^2[x] - \varepsilon}}\right)^2\right] \tag{34}$$

and (for $\varepsilon = 1$)

$$I(x) = \ln[\cosh[x]]. \tag{35}$$

We now shall analyse different asymptotic limits of S. For this we set $S_{\pm\mp} = \pm S(\mp x_t, x_\mathrm{i} \to \mp\infty) \pm S(x_\mathrm{f} \to \pm\infty, \pm x_t)$ and $S_{\mp\mp} = \pm S(\mp x_t, x_\mathrm{i} \to \mp\infty) \mp S(x_\mathrm{f} \to \mp\infty, \mp x_t)$ (the signs in front the S are to take into account the correct directions of movement). From (34) and (35) we derive the following important relations:

$$\begin{aligned} I(\alpha x_t) &= \begin{cases} \frac{1}{2}\ln[|\varepsilon - 1|] & \varepsilon \neq 1 \\ 0 & \varepsilon = 1 \end{cases} \\ I(x \to \infty) &= x + \begin{cases} \dfrac{\sqrt{\varepsilon}}{2}\ln[|\sqrt{\varepsilon} - 1|/(\sqrt{\varepsilon} + 1)] & \varepsilon \neq 1 \\ -\ln[2] & \varepsilon = 1. \end{cases} \end{aligned} \tag{36}$$

Then, with the help of (36) we find

$$\begin{aligned} S_{\pm\mp} &= \hbar k(|x_\mathrm{f} - x_\mathrm{i}| - L(k)) \\ S_{\mp\mp} &= \hbar k(|x_\mathrm{f} + x_\mathrm{i}| - L(k)) \end{aligned} \tag{37}$$

where

$$L(k) = \alpha^{-1}\{2\sqrt{\varepsilon}\ln[\sqrt{\varepsilon} + 1] + (1 - \sqrt{\varepsilon})\ln[|\varepsilon - 1|]\} \tag{38}$$

is valid for any ε including the limit of $\varepsilon \to 1$, which gives $L(k) = 2\ln[2]/\alpha$.

From equations (37), (38) and the discussion in section 4 we can directly identify the quantum amplitudes R and T to be used in the generalized semiclassical Green function for the RM potential. They are

$$\begin{aligned} T^{(\mathrm{RM})} &= \mathcal{T}^{(\mathrm{RM})}\exp[\mathrm{i}kL(k)] \\ R^{(\mathrm{RM})} &= \mathcal{R}^{(\mathrm{RM})}\exp[\mathrm{i}kL(k)]. \end{aligned} \tag{39}$$

We should observe that one can incorporate the parameter α in all the expressions in section 3 (including in $\mathcal{R}$ and $\mathcal{T}$ above) by rescaling: $k \to k/\alpha$, $V_0 \to V_0/\alpha^2$ and $x \to x \times \alpha$.

Appendix C

For the WS step $V_0/(1 + \exp[-\alpha x])$ the quantum amplitudes can be obtained with the help of the results in [25], which lead after a little lengthy but straightforward calculation to ($\mu = \sqrt{2m(E - V_0)/\hbar^2}$)

$$\begin{aligned} \mathcal{R}_{(-)}^{(\mathrm{WS},+)} &= \frac{\Gamma(2\mathrm{i}k/\alpha)\Gamma(-\mathrm{i}(k+\mu)/\alpha)\Gamma(1 - \mathrm{i}(k+\mu)/\alpha)}{\Gamma(-2\mathrm{i}k/\alpha)\Gamma(\mathrm{i}(k-\mu)/\alpha)\Gamma(1 + \mathrm{i}(k-\mu)/\alpha)} \\ \mathcal{T}_{(-)}^{(\mathrm{WS},+)} &= \frac{\Gamma(-\mathrm{i}(k+\mu)/\alpha)\Gamma(1 - \mathrm{i}(k+\mu)/\alpha)}{\Gamma(-2\mathrm{i}k/\alpha)\Gamma(1 - 2\mathrm{i}\mu/\alpha)}. \end{aligned} \tag{40}$$

The superscript + represents an incident wave from the left. The case of an incoming wave from the right (−) is given by $k \leftrightarrow \mu$ in (40).

The classical action is ($\varepsilon = V_0/E$)

$$S(x_\mathrm{f}, x_\mathrm{i}) = \int_{x_\mathrm{i}}^{x_\mathrm{f}} \mathrm{d}x \sqrt{2m\left(E - \frac{V_0}{1+\exp[-\alpha x]}\right)}$$
$$= \hbar\frac{k}{\alpha}\{J(\exp[-\alpha x_\mathrm{f}]) - J(\exp[-\alpha x_\mathrm{i}])\} \tag{41}$$

with

$$J(u) = \sqrt{1-\varepsilon}\,\ln\left[-2\frac{(1+u)}{u}\sqrt{1-\varepsilon}\left(\sqrt{1-\varepsilon}+\sqrt{1-\frac{\varepsilon}{1+u}}\right)-\varepsilon\right]$$
$$-\ln\left[2(1+u)\left(1+\sqrt{1-\frac{\varepsilon}{1+u}}\right)-\varepsilon\right]. \tag{42}$$

For our purposes we define $S_{\pm\mp} = \pm S(x_\mathrm{f}\to\pm\infty, x_\mathrm{i}\to\mp\infty)$ and $S_{\mp\mp} = \pm S(0, x_\mathrm{i}\to\mp\infty) \mp S(x_\mathrm{f}\to\mp\infty, 0)$ (again the signs in front of the S are to take into account the correct directions of movement). Using (41) and (42) one can show that ($k_+ = k, k_- = \mu$)

$$\begin{aligned} S_{\pm\mp} &= \hbar(\pm(k_\mp x_\mathrm{f} - k_\pm x_\mathrm{i}) - f_T) \\ S_{\mp\mp} &= \hbar(\mp k_\pm(x_\mathrm{f}+x_\mathrm{i}) - f_R^{(\mp)}) \end{aligned} \tag{43}$$

where

$$\begin{aligned} f_T &= \frac{k}{\alpha}\ln\left[\frac{2-\varepsilon+2\sqrt{1-\varepsilon}}{4}\right] + \frac{\mu}{\alpha}\ln\left[\frac{2-\varepsilon+2\sqrt{1-\varepsilon}}{4(1-\varepsilon)}\right] \\ f_R^{(+)} &= 2\frac{k}{\alpha}\ln\left[\frac{2(1+\sqrt{1-\varepsilon})-\varepsilon}{4(1+\sqrt{1-\varepsilon/2})-\varepsilon}\right] + 2\frac{\mu}{\alpha}\ln\left[\frac{4(1-\varepsilon+\sqrt{(1-\varepsilon)(1-\varepsilon/2)})+\varepsilon}{4(1-\varepsilon)}\right] \\ f_R^{(-)} &= 2\frac{k}{\alpha}\ln\left[1+\sqrt{1-\varepsilon/2}-\varepsilon/4\right] + 2\frac{\mu}{\alpha}\ln\left[\frac{2-\varepsilon+2\sqrt{1-\varepsilon}}{4(1-\varepsilon+\sqrt{(1-\varepsilon)(1-\varepsilon/2)})+\varepsilon}\right]. \end{aligned} \tag{44}$$

From equations (43) and (44) and the discussion in section 4 the quantum amplitudes R and T for the WS barrier follow:

$$\begin{aligned} T_{(-)}^{(\mathrm{WS},\pm)} &= \mathcal{T}_{(-)}^{(\mathrm{WS},\pm)}\exp[\mathrm{i}f_T] \\ R_{(-)}^{(\mathrm{WS},\pm)} &= \mathcal{R}_{(-)}^{(\mathrm{WS},\pm)}\exp[\mathrm{i}f_R^{(\pm)}]. \end{aligned} \tag{45}$$

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