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Reflection above potential steps

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Abstract. Disparate behaviour of above-the-step quantal reflection probability for smooth and composite semi-infinite potentials is shown. For a smooth semi-infinite potential (step) the reflectivity is usually a monotonically decreasing function of energy. But the composite two-piece (non-differentiable, e.g., at $x = 0$) potential step gives rise to a parameter-dependent pronounced single minimum in the reflectivity. Three analytically solvable and several other models of composite semi-infinite (step) potentials are shown supporting such a behaviour of the quantal reflection.

1. Introduction

Broadly speaking, the potential functions in quantal description based on the Schrödinger equation of various phenomena may be of two types: smooth (one-piece) and composite (two-piece). The smooth ones are both continuous and differentiable at every point of the domain of interaction. On the other hand, the composite potentials are two-piece which are essentially continuous but not differentiable at the joining point (e.g., $x = 0$). In fact, the two-piece functions cannot have left and right derivatives of all orders matching at the junction; so they are essentially non-differentiable. In quantal calculations, we may recall that the physical condition of the continuity of the flux at each and every point in the space demands the continuity of the wavefunction and its first derivative at every point. So, without any loss of generality, the quantal calculations for both smooth and composite potentials are performed by finding the left and right wavefunctions and then by matching them and their first derivatives at a given point. When the potentials are composite, this point corresponds to the point of non-differentiability. On the other hand, if the potential is smooth this point could be any convenient point; e.g., $x = 0$, or, the classical turning point. One-dimensional potentials which are semi-infinite such that $V(+\infty) = 0$, $V(-\infty) = -V_0$ (see figure 1) are known as potential steps. Usually, the probability of quantal reflection (reflectivity, $R(E)$) from a semi-infinite potential is unity for energies below the step height and at energies above the step it falls off monotonically. The probability of reflection at energies a little above the step is quite close to unity. This feature is of current interest in the collisions of cold atoms [1, 2]. Reflectometry [3] of a polarized neutron from the magnetized super-conductors is a recent application of semi-infinite potentials. In condensed-matter physics the semi-infinite potentials represent an interface. In the propagation of waves semi-infinte potentials are analogous to an inhomogeneous dielectric medium [5]. Tunnelling of electrons from a metal to a vacuum perhaps marks the first usage of a semi-infinite potential step.

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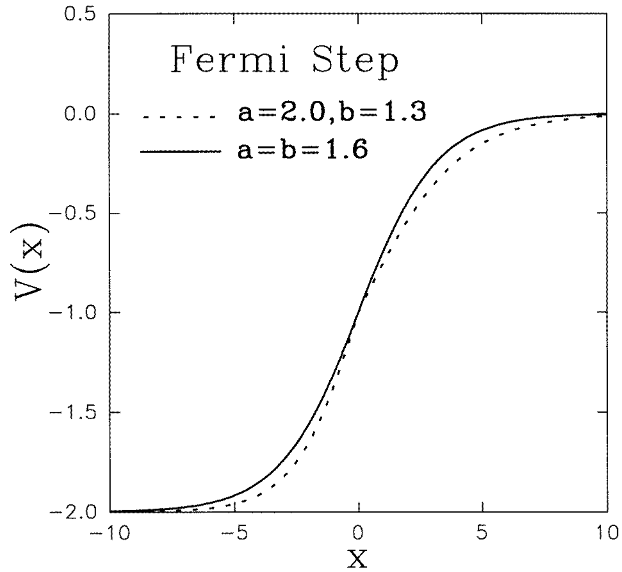

Figure 1. Fermi potential step equations (14*a*) and (14*b*) as a representative of semi-infinite potentials (potential steps). The solid curve is the smooth potential the dotted curve is the composite potential. We have taken $V_1 = V_2 = 1$.

Now consider the phenomenon of quantal reflection by two closely lying potential steps (cf figure 1: a smooth (solid curve) and composite one (dashed curve)). One would usually expect the probability of reflection as a function of energy for these steps to follow a similar *qualitative* trend, though the *quantitative* differences would, of course, persist. It is intriguing to notice the disparate behaviour of reflectivity, $R(E)$, for these two cases in figure 2. For the smooth step, $R(E)$, as stated above, it is monotonically decreasing whereas for the composite step it supports a *single* pronounced minimum. Here the smooth step is the well known Fermi or Wood–Saxon step:

$$V(x) = \frac{-V_0}{1 + \exp(x/a)} \tag{1}$$

which admits an exact analytic form for $R(E)$ namely,

$$R(E) = \frac{\sinh^2 \pi(k - k')a}{\sinh^2 \pi(k + k')a} \tag{2}$$

where $k = \sqrt{2mE/\hbar^2}$ and $k' = \sqrt{2m(E + V_0)/\hbar^2}$. Notice the monotonic behaviour of $R(E)$. Note also, that the composite step is an interesting variant of this potential, i.e. $V(x) = \frac{-V_0}{1+\exp(x/b)}\Theta(-x) + \frac{-V_0}{1+\exp(x/a)}\Theta(x)$, where $\Theta(x)$ is the Heaviside step function. This unexpected behaviour of the reflection probability above a composite step provides the motivation for this paper. Here, we present three analytically solvable models of composite potential steps and obtain the exact analytic forms for reflectivity (section 2). The formulae are new and useful in their own right in several branches of physics. However, using these results we demonstrate the unusual behaviour of the reflectivity as mentioned above. It may be mentioned that some special cases of these semi-infinite potentials wherein $V(x < 0) = 0$, the occurrence of a single dip has already been reported [3, 4]. However, in this paper we aim at reporting more general instances of unusual reflectivity.

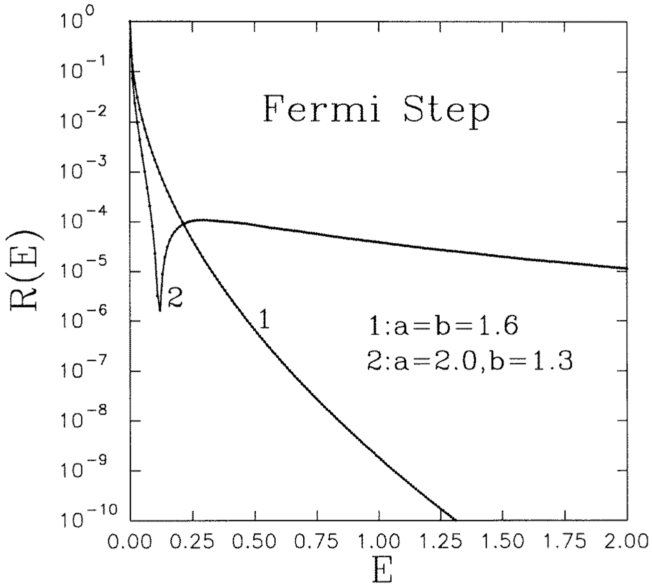

Figure 2. Disparate intriguing behaviour of the reflectivity for (1) smooth and (2) composite Fermi step: the reflectivities are calculated using equations (19) and (20), respectively. The dots denote results obtained by numerical integration of the Schrödinger equation. In all the figures in this paper we have taken $V_1 = 1$, $V_2 = 1$, $\hbar = 1 = 2m$, and energies are in arbitrary units.

2. Solvable models of composite potential steps

In the following, we propose three solvable models of the composite, semi-infinite potential (step barrier) and consider the phenomenon of quantal reflection of particle waves which impinge on the potential step from the left (see figure 1). Studies of such potential profiles would also be desired in modelling various interfaces in condensed-matter physics and wave optics e.g., metal–vacuum, metal–metal, n–p junctions etc. These models are particularly useful in neutron reflectometry [3], where the reflection amplitude for such step barriers are computed rather extensively [5]. We aim at obtaining the exact analytic reflection amplitudes for the proposed model steps in this section.

2.1. The composite Eckart step

The two-piece Eckart [7] semi-infinite potential can be constructed as

$$V(x > 0) = -V_2 \operatorname{sech}^2(x/a) \tag{3a}$$

$$V(x < 0) = -V_2 - V_1 \tanh^2(x/b). \tag{3b}$$

At $x = 0$ the potential and its first derivative are continuous but the second derivative is discontinuous. The Schrödinger equation for this potential can be written as

$$\frac{d^2\Psi_>(y)}{d^2y} + (\lambda^2 + \bar{\mu}^2 \operatorname{sech}^2 y)\Psi_>(y) = 0 \tag{4a}$$

$$\frac{d^2\Psi_<(z)}{d^2z} + (\nu^2 - \bar{\eta}^2 \operatorname{sech}^2 z)\Psi_<(z) = 0. \tag{4b}$$

Here the following substitutions have been used $\lambda = \sqrt{(E)/\Delta}$, $\bar{\mu} = \sqrt{(V_2/\Delta)}$, $\Delta = \hbar^2/(2ma^2)$, $y = x/a$ in equation (4*a*) and $\nu = \sqrt{(E + V_1 + V_2)/\Delta'}$, $\bar{\eta} = \sqrt{(V_1/\Delta')}$,

$\Delta' = \bar{h}^2/(2mb^2)$, $z = x/b$ in equation (4*b*). Using a transformation $u = (1 - \tanh y)/2$ and by defining $\mu = \sqrt{\bar{\mu}^2 + \frac{1}{4}}$ and $\eta = \sqrt{\bar{\eta}^2 - \frac{1}{4}}$ the solution of (4*a*) can be written in terms of a Gaussian hypergeometric function (GHF) as

$$\Psi_>(x) = C\ g(y) = C(\cosh y)^{\mathrm{i}\lambda}\ {}_2F_1(\tfrac{1}{2} - \mathrm{i}\lambda + \mu, \tfrac{1}{2} - \mathrm{i}\lambda - \mu, 1 - \mathrm{i}\lambda; u). \quad (5)$$

Out of several forms of the solution of equation (4*a*) available in terms of GHF [6], we have chosen one which ensures the correct asymptotic behaviour i.e., $\Psi(x \sim \infty) \sim \exp(\mathrm{i}kx)$.

Next, we employ a transformation $v = (1 + \tanh z)/2$ to obtain a solution of (4*b*) as

$$\Psi_<(x) = Af_1(x) + Bf_2(x). \quad (6)$$

The function f_1 is expressed as

$$f_1(x) = (\cosh z)^{-\mathrm{i}\nu}\ {}_2F_1(\tfrac{1}{2} + \mathrm{i}\nu + \mathrm{i}\eta, \tfrac{1}{2} + \mathrm{i}\nu - \mathrm{i}\eta, 1 + \mathrm{i}\nu; v) \quad (7)$$

and $f_2(x) = f_1^*(x)$. These forms are chosen so that $\Psi(x \sim -\infty) \sim A\exp(\mathrm{i}Kx) + B\exp(-\mathrm{i}Kx)$, where $K = \nu/b = \sqrt{2m(E + V_1 + V_2)/\bar{h}^2}$. The matching conditions at $x = 0$ give us the reflection amplitude $r(= B/A)$ as below:

$$r = -\frac{f_1(0)}{f_2(0)}\left(\frac{\left[\frac{g'(0)}{g(0)} - \epsilon\frac{f_1'(0)}{f_1(0)}\right]}{\left[\frac{g'(0)}{g(0)} - \epsilon\frac{f_2'(0)}{f_2(0)}\right]}\right). \quad (8)$$

This equation would involve GHF at arguments $u = v = \frac{1}{2}$ i.e., ${}_2F_1(L, M, (L + M + 1)/2; \frac{1}{2})$ which, fortunately, can be eliminated using a special property, namely ${}_2F_1(L, M, (L + M + 1)/2; \frac{1}{2}) = \sqrt{\pi}\frac{\Gamma[1/2+(L+M)/2]}{\Gamma[(L+1)/2]\Gamma[(M+1)/2]}$ [6]. Here, $\Gamma(z)$ are gamma functions with a complex argument. Finally, for the composite Eckart step we propose

$$r = -\exp(2\mathrm{i}\delta)\left(\frac{\epsilon\frac{\Gamma(3/4+\mathrm{i}\alpha)\Gamma(3/4+\mathrm{i}\beta)}{\Gamma(1/4+\mathrm{i}\alpha)\Gamma(1/4+\mathrm{i}\beta)} + \frac{\Gamma(3/4+\gamma)\Gamma(3/4-\omega)}{\Gamma(1/4+\gamma)\Gamma(1/4-\omega)}}{\epsilon\frac{\Gamma(3/4-\mathrm{i}\alpha)\Gamma(3/4-\mathrm{i}\beta)}{\Gamma(1/4-\mathrm{i}\alpha)\Gamma(1/4-\mathrm{i}\beta)} + \frac{\Gamma(3/4+\gamma)\Gamma(3/4-\omega)}{\Gamma(1/4+\gamma)\Gamma(1/4-\omega)}}\right). \quad (9)$$

Here, $\delta = \mathrm{Arg}(\frac{\Gamma(1+\mathrm{i}\nu)}{\Gamma(3/4+\mathrm{i}\alpha)\Gamma(3/4+\mathrm{i}\beta)})$, $\epsilon = a/b$, $\alpha = (\nu-\eta)/2$, $\beta = (\nu+\eta)/2$, and $\gamma = (\mu-\mathrm{i}\lambda)/2$, $\omega = (\mu+\mathrm{i}\lambda)/2$. When $V_2 = 0$ an interesting special case of equations (3*a*) and (3*b*) has earlier been proposed by us [4].

2.2. *The composite exponential step*

This potential is represented as

$$V(x > 0) = -V_2\exp(-x/a) \quad (10a)$$

$$V(x < 0) = -V_2 - V_1[1 - \exp(x/b)]. \quad (10b)$$

This potential is continuous but not differentiable at $x = 0$ even when $a = b$. We write the Schrödinger equation for this potential as

$$\frac{\mathrm{d}^2\Psi_>(y)}{\mathrm{d}y^2} + (\lambda^2 + \mu^2\exp(-2y))\Psi_>(y) = 0 \quad (11a)$$

$$\frac{\mathrm{d}^2\Psi_<(y)}{\mathrm{d}z^2} + (\nu^2 - \eta^2\exp(2z))\Psi_<(z) = 0. \quad (11b)$$

Here, $\lambda = \sqrt{E/\Delta}$, $\mu = \sqrt{V_2/\Delta}$, $\Delta = \bar{h}^2/(8ma^2)$, $y = x/(2a)$ and $\nu = \sqrt{(E + V_1 + V_2)/\Delta'}$, $\eta = \sqrt{V_1/\Delta'}$, $\Delta' = \bar{h}^2/(8mb^2)$, $z = x/(2b)$. Equations (11*a*) and (11*b*) are transformable to a standard cylindrical Bessel equation and hence we choose

$$\Psi_>(x) = CJ_{-\mathrm{i}\lambda}(\mu\exp(-y)) \quad (12a)$$

$$\Psi_<(x) = AI_{\mathrm{i}\nu}(\eta\exp(z)) + BI_{-\mathrm{i}\nu}(\eta\exp(z)). \quad (12b)$$

J and I are cylindrical Bessel and modified Bessel functions, respectively. By using the near-zero behaviour of the Bessel function, i.e. $J_p(\varepsilon) \approx \frac{(\varepsilon/2)^p}{\Gamma(1+p)}$, we check that $\Psi(\infty) \sim \exp(\mathrm{i}kx)$ and $\Psi(-\infty) = A\exp(\mathrm{i}Kx) + B\exp(-\mathrm{i}Kx)$. The matching conditions using equations (12*a*) and (12*b*) at $x = 0$ yield the reflection amplitude. We obtain

$$r = -\exp(2\mathrm{i}\delta)\left(\frac{\frac{\epsilon J'_{-\mathrm{i}\lambda}(\mu)}{J_{-\mathrm{i}\lambda}(\mu)} + \frac{I'_{\mathrm{i}\nu}(\eta)}{I_{\mathrm{i}\nu}(\eta)}}{\frac{\epsilon J'_{-\mathrm{i}\lambda}(\mu)}{J_{-\mathrm{i}\lambda}(\mu)} + \frac{I'_{-\mathrm{i}\nu}(\eta)}{I_{-\mathrm{i}\nu}(\eta)}}\right). \tag{13}$$

The phase δ is defined as $\delta = \mathrm{Arg}[I_{\mathrm{i}\nu}(\eta)]$, $\epsilon = \sqrt{V_2/V_1}$ and the primes here denote a derivative w.r.t. the argument. The limiting case, when $V_2 = 0$, is found useful in neutron reflectometry from the magnetized superconductor [3].

2.3. The composite Fermi step

We tailor the two-piece Fermi potential step as

$$V(x > 0) = -V_2\left[1 - \tanh\left(\frac{x}{2a}\right)\right] \tag{14a}$$

$$V(x < 0) = -V_2 + V_1\tanh\left(\frac{x}{2b}\right). \tag{14b}$$

When $V_1 = V_2$ and $a = b$, this potential becomes the well known Fermi potential step (smooth), otherwise at $x = 0$ this function is continuous but not differentiable (first derivative-mismatch). The Schrödinger equation for this potential can be written as

$$\frac{\mathrm{d}^2\Psi_>(x)}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}\left[E + \frac{2V_2}{1+\exp(x/a)}\right]\Psi_>(x) = 0 \tag{15a}$$

$$\frac{\mathrm{d}^2\Psi_<(x)}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}\left[E + V_2 - V_1 + \frac{2V_1}{1+\exp(x/b)}\right]\Psi_<(x) = 0. \tag{15b}$$

Let us define the following parameters which are useful in the following. These are $k = \sqrt{2mE}/\hbar$, $K = \sqrt{2m(E+V_1+V_2)}/\hbar$, $k_1 = \sqrt{2m(E-V_1+V_2)}/\hbar$ and $k_2 = \sqrt{2m(E+2V_2)}/\hbar$. Next we define $\alpha_1 = k_2 a$, $\alpha_2 = ka$, $\beta_1 = Kb$, and $\beta_2 = k_1 b$. Equations (15*a*) and (15*b*) can be transformed to a Gaussian hypergeometric equation by changing the variables as $y = -\exp(-x/a)$ and $z = -\exp(-x/b)$, respectively. The wavefunctions can be written as $\Psi_>(x) = Cy^{-\mathrm{i}\alpha_2}W_1(y)$ and $\Psi_<(x) = z^{-\mathrm{i}\beta_2}[AW_5(z) + BW_6(z)]$. W_i are expressible in terms of GHF as

$$W_1(y) = {}_2F_1[\mathrm{i}(\alpha_1-\alpha_2), -\mathrm{i}(\alpha_1+\alpha_2), 1-2\mathrm{i}\alpha_2; y] \tag{16a}$$

$$W_5(z) = z^{-\mathrm{i}(\beta_1-\beta_2)}\,{}_2F_1[\mathrm{i}(\beta_1-\beta_2), \mathrm{i}(\beta_1+\beta_2), 1+2\mathrm{i}\beta_1; 1/z] \tag{16b}$$

$$W_6(z) = z^{\mathrm{i}(\beta_1+\beta_2)}\,{}_2F_1[-\mathrm{i}(\beta_1+\beta_2), -\mathrm{i}(\beta_1-\beta_2), 1-2\mathrm{i}\beta_1; 1/z]. \tag{16c}$$

By matching the wavefunctions and their first derivative at $x = 0$, we obtain the reflection amplitude as

$$r = -\frac{[\mathrm{i}(k_1-k)W_1(-1)W_5(-1) + W_{51}(-1)]}{[\mathrm{i}(k_1-k)W_1(-1)W_6(-1) + W_{61}(-1)]} \tag{17}$$

where W_{51} and W_{61} are the Wronskians e.g., $W_{51} = [W_5, W_1]$ [6]. In a special case, when $V_1 = V_2$ and $a = b$ the potential in (14*a*) and (14*b*) becomes the smooth Fermi step which is single piece. Then the parameters α and β coincide and we get $r = W_{51}/W_{61}$. Also, these Wronskians in the case given are expressible in terms of gamma functions, so we write

$$r = -\frac{\Gamma(1+2\mathrm{i}\alpha_1)\Gamma[-\mathrm{i}(\alpha_1+\alpha_2)]\Gamma[1-\mathrm{i}(\alpha_1+\alpha_2)]}{\Gamma(1-2\mathrm{i}\alpha_1)\Gamma[\mathrm{i}(\alpha_1-\alpha_2)]\Gamma[1+\mathrm{i}(\alpha_1-\alpha_2)]} \tag{18}$$

which, in turn, yields the reflectivity as

$$R(E) = \left| \frac{\sinh \pi(k-K)a}{\sinh \pi(k+K)a} \right|^2. \tag{19}$$

Unfortunately, the reflection amplitude (17) for the general Fermi step is not expressible in terms of gamma functions. However, it further simplifies to

$$r = -(-2)^{-2\mathrm{i}\beta_1} \frac{[2\mathrm{i}ab(k_1 - k_2 - k + K)Z_1 Z_5 + bZ_1' Z_5 + aZ_1 Z_5']}{[2\mathrm{i}ab(k_1 - k_2 - k - K)Z_1 Z_6 + bZ_1' Z_6 + aZ_1 Z_6']} \tag{20}$$

where $Z_1(\alpha_1, \alpha_2) = {}_2F_1[\mathrm{i}(\alpha_1 - \alpha_2), 1 + \mathrm{i}(\alpha_1 - \alpha_2), 1 - 2\mathrm{i}\alpha_2; \frac{1}{2}]$, $Z_5(\beta_1, \beta_2) = {}_2F_1[\mathrm{i}(\beta_1 - \beta_2), 1 + \mathrm{i}(\beta_1 - \beta_2), 1 + 2\mathrm{i}\beta_1; \frac{1}{2}]$, $Z_6(\beta_1, \beta_2) = Z_5(-\beta_1, \beta_2)$ and Z_i' implies the differentiation of the corresponding HGF i.e., $Z_i' = \frac{LM}{N}\, {}_2F_1[L+1, M+1, N+1; \frac{1}{2}]$. The reflection amplitude (20) is easily calculable as the GHFs appearing here are all rapidly converging series. The series representation for a GHF is given as

$${}_2F_1(L, M, N; U) = 1 + \frac{LM}{N}\frac{U}{1!} + \frac{L(L+1)M(M+1)}{N(N+1)}\frac{U^2}{2!} + \cdots.$$

3. Results and discussion

We calculate $R(E) = |r|^2$ for various potential steps mentioned above. Without loss of generality we assume $V_1 = V_2 = 1$ and $\hbar = 1 = 2m$ so that $\Delta = 1/a^2$ and $\Delta' = 1/b^2$. The units for E, V_1, V_2, a and b are arbitrary. In figure 2 the reflectivity for the smooth Fermi step (14*a*) and (14*b*) ($a = b = 1.6$) is shown falling off monotonically whereas that for the closely lying composite counterpart ($a = 2.0$, $b = 1.3$) shows a marked single minimum at $E = 0.12$ arbitrary.

We calculate $R(E)$ using equation (9) for an Eckart composite step assuming $a = b$, we find usual pattern for reflectivity when $a < 2.33$. When the value of a is increased further reflectivity starts developping a minimum which becomes prominent when $a = 2.55$. When a is further increased the dip starts diminishing, eventually disappearing completely when $a = 2.78$ (see figure 3). So when $V_1 = V_2 = 1$ and $a \in (2.33, 2.78)$ the reflectivity minimum is observed. We also note that the reflectivity-minimum is sensitive to the value of V_2, whereas when $V_2 = 1$ and $a = 2.55$ several values of V_1 ($0 \leqslant V_1 \leqslant 2$) also give rise to dip in reflectivity but at some different values of energy, E. Several other sets of (V_1, V_2, a) may be found which present the scenario of single minimum in reflectivity. For the exponential step (10*a*) and (10*b*), we calculate $R(E)$ using equation (13) when $a = b$. A similar scenario emerges: when $V_1 = V_2 = 1$ and $a \in (1.27, 1.72)$ the minimum in $R(E)$ occurs which becomes prominent when $a = 1.48$ (see figure 4). We also note that for $V_2 = 1$ and $a = 1.47$ there is an interval for V_1 i.e., $0.6 \leqslant V_1 \leqslant 2.3$ for which the dip does not disappear. We find another set, namely $V_1 = 2$, $V_2 = 2$ and $a = 3.10$ where a prominent dip in reflectivity occurs.

We have also confirmed the scenario of the existence of a pronounced single minimum in reflectivity for several other analytically unamenable profiles of composite potential steps. These are $V(x > 0) = -V_2[1 - \mathrm{erf}(x/a)]$, $V(x < 0) = -V_2 + V_1 \mathrm{erf}(x/b)$; $V(x) = -\frac{V_0}{2}[1 - \tanh(\frac{-x|x|}{2a^2})]$, $V(x > 0) = -V_2 \exp(-x^2/a^2)$, $V(x < 0) = -V_2 - V_1[1 - \exp(-x^2/b^2)]$. Moreover, the usual monotonic behaviour of $R(E)$ has been confirmed very carefully for the smooth steps: error-function step namely, $V(x) = -V_0[1 - \mathrm{erf}(x/a)]$ and a more general profile of a semi-infinite potential [2]. Notice that the Schrödinger equation for all the potential profiles (functions) presented in this section is not amenable to analytic solutions. Therefore, for these profiles, we perform the numerical integration (Runge–Kutta) of the Schrödinger

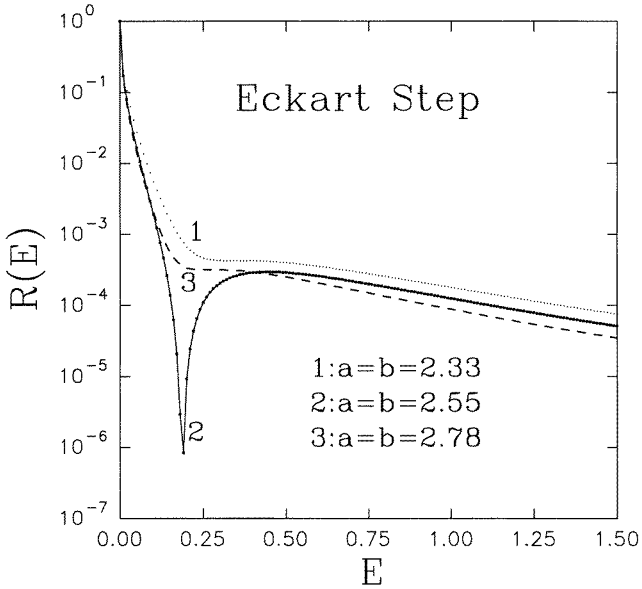

Figure 3. The scenario of the occurrence of a single minimum in the reflectivity equation (9) for the Eckart potential step equations (3*a*) and (3*b*). The dots denote the reflectivity calculated using the numerical integration of the Schrödinger equation.

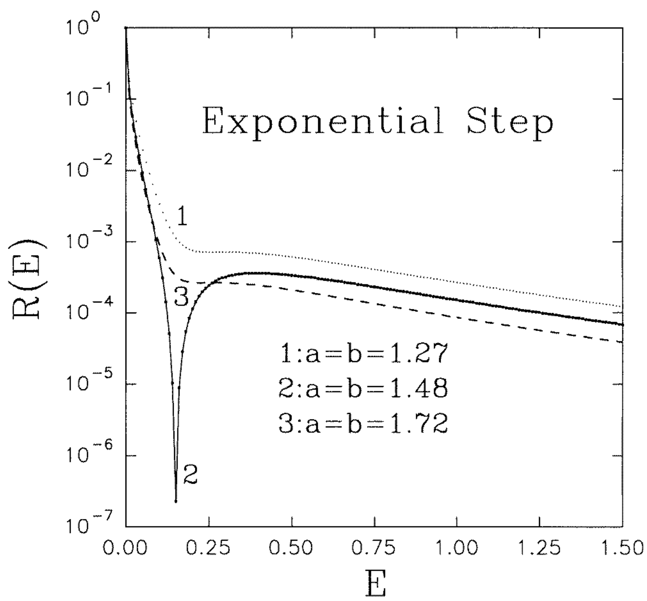

Figure 4. The same as in figure 3: for the exponential potential step (equations (10*a*) and (10*b*)) using equation (13).

equation. Results for the Gaussian step are presented in figure 5. When $V_1 = V_2 = 1$ and $a = b \in (2.21, 2.79)$ there occurs a minimum in reflectivity which becomes prominent when $a = 2.52$. The dots in figures 2–4 are due to the numerical integration method. This is done

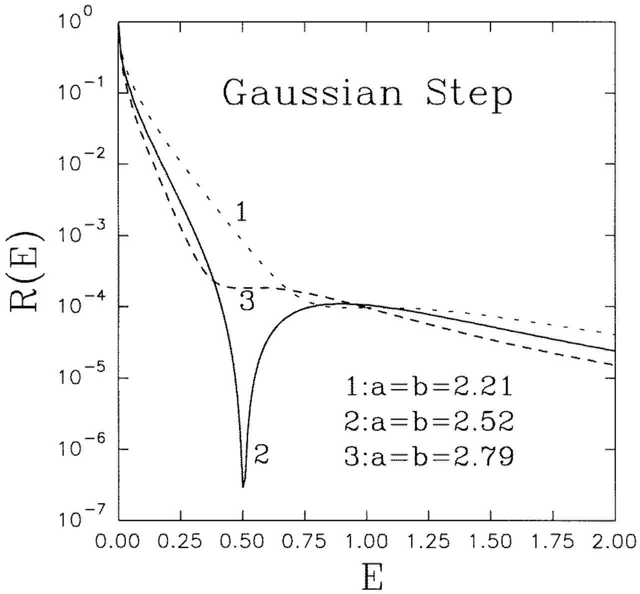

Figure 5. The similar scenario (as in figure 3) for the composite Gaussian step (see the text) which is analytically intractable.

to testify the correctness of the proposed new expressions of reflectivity in equations (9), (13) and (20).

We notice that the integration methods become unstable at energies well above the step. This is where the analytic results are most desirable. However, in this paper we have been concerned with energies little above the step. While performing these calculations, it has been very interesting to observe that for a given mesh size, Δx, and a chosen asymptotic (large) distance, x_L, the integration method is more stable for the composite potential step than for the smooth counterpart of the potential. For instance, for the Fermi potential the reflectivity (figure 6) shows a convergence to the exact analytic result (20) when we choose $\Delta x = 0.1$ and $x_L = 12.0$ for the composite step; whereas for the smooth step for which the exact result is known (19) we took $\Delta x = 0.1$ and $x_L = 20.0$, yet the numerical method yields a wrong reflectivity after about $E = 2.50$. In figure 6, one should also, once again, notice the remarkable difference between the reflectivities of the smooth ($V_1 = V_2 = 1.0$, $a = b = 1.60$ in (14*a*), (14*b*)) and the composite ($V_1 = V_2 = 1.0$, $a = 1.55$, $b = 1.60$ in (14*a*), (14*b*)) Fermi steps although they are not very different.

4. Conclusions

We have shown a surprising occurrence of a single pronounced minimum in the reflectivity for a large assortment of composite potential steps. Also we have studied several numbers of smooth potential steps and found that above the step the reflection probability is a monotonically decreasing function of energy which hitherto was supposed to have the characteristic behaviour of a semi-infinite potential step. Our analyses in this paper indicates that the non-differentiability of a semi-infinite potential step is at least a *sufficient* condition for giving rise to an unusual single pronounced minimum in the reflectivity, with the proviso that

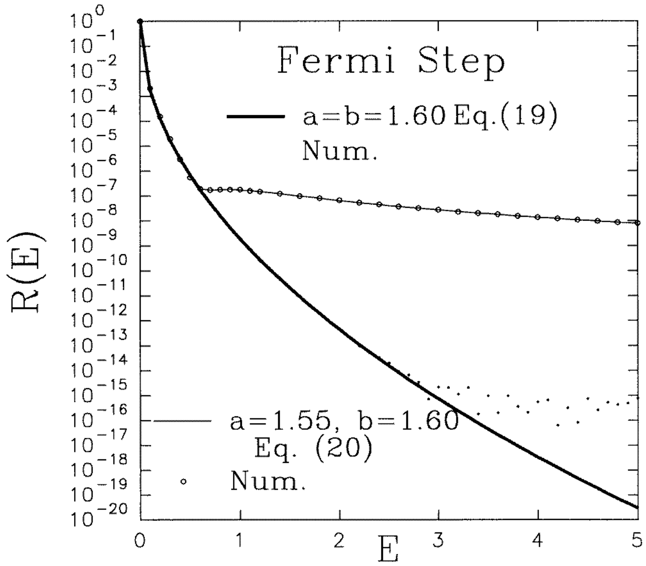

Figure 6. Display of the interesting instability of the numerical integration method when the potential step is smooth. Compare the dots and thick line after $E = 2.5$ arbitrary and observe a good matching between the thin solid curve and the open circles when the step is a closely lying composite potential. Also, notice the dramatic difference in the reflectivities for the two cases.

only some special values of V_1, V_2, a, b allow the occurrence of this minimum. When these conditions are met with, the wave of a certain wavelength (energy) gets multiply scattered in the semi-infinite medium, these multiply scattered waves then interfere destructively to produce a single minimum in the reflectivity. We would like to remark that the interesting instances of potential steps (where $V(x < 0) = 0$) reported in [4] display such unusual reflectivity because they are all essentially non-differentiable at $x = 0$. This point could not be realized in [4]. One surprising calculational feature of the semi-infinite potentials is revealed i.e., the calculation of reflectivity by numerical integration of the Schrödinger equation shows a better stability for composite step than for even a closely associated smooth partner of the step.

It may also be noted that the expressions for reflectivity proposed here in equations (9), (13) and (20) are new exactly solvable examples of quantal reflection. Since the semi-infinite potentials entail only one turning point, the usual WKB method for reflectivity becomes unusable [2]. Thus, the exact analytic expression of reflectivity becomes more important. The exact formulae given here may be useful in areas such as wave optics, neutron reflectometry and interfaces in condensed-matter physics. It may be worthwhile mentioning that we have recently discussed the occurrence of such unusual reflectivity when the scattering takes place from a composite potential well [8].

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