

## Reflection from an interface

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2000 J. Phys. A: Math. Gen. 33 3161

(<http://iopscience.iop.org/0305-4470/33/16/308>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

### Download details:

IP Address: 171.66.16.118

The article was downloaded on 02/06/2010 at 08:05

Please note that [terms and conditions apply](#).

## Reflection from an interface

Zafar Ahmed

Nuclear Physics Division, Bhabha Atomic Research Centre, Bombay 400 085, India

E-mail: zahmed@apsara.barc.ernet.in

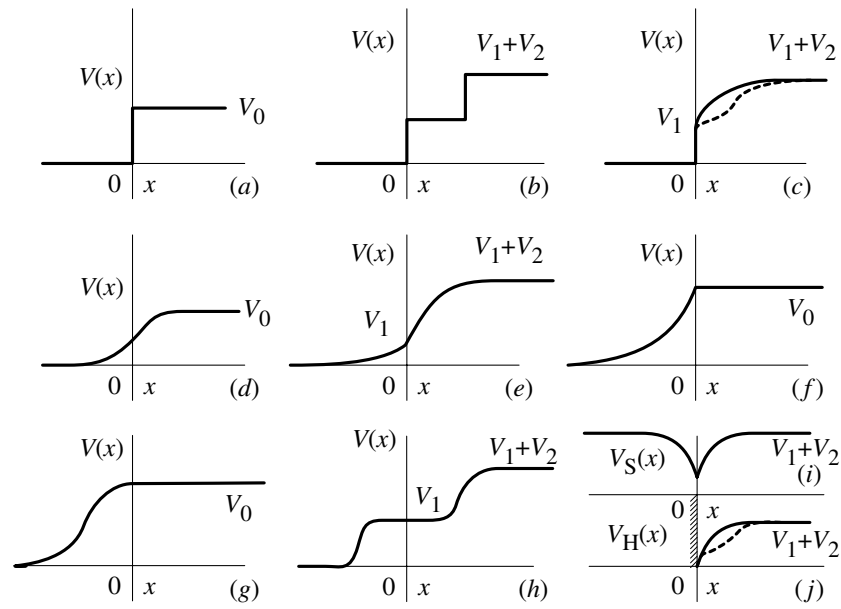
Received 9 August 1999, in final form 25 January 2000

**Abstract.** A slight mismatch of left and right derivatives at the junction of a semi-infinite potential step is shown to cause dramatic changes in above-the-step reflectivity as a function of incident energy. Firstly, the reflectivity becomes enhanced remarkably at energies much above the step. Secondly, depending on the parameters, there exists a pronounced single minimum in the reflectivity at an energy slightly above-the-step height. Several methods and interfacial profiles have been employed to verify the claimed behaviour of the reflectivity.

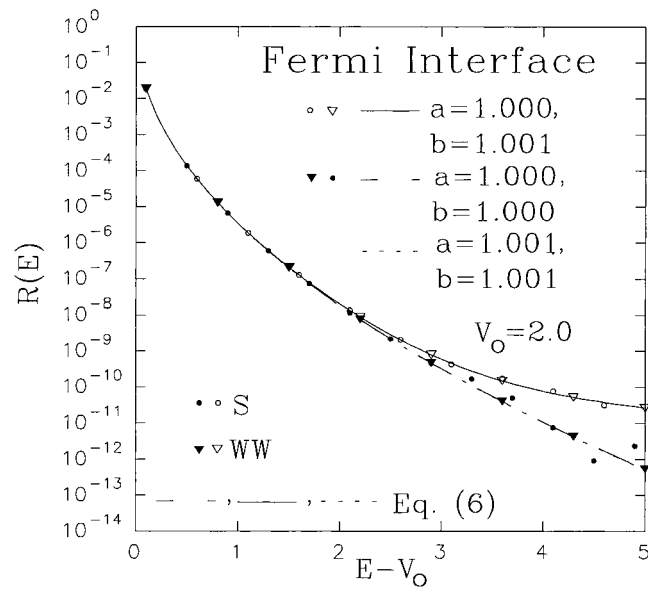
### 1. Introduction

An interface indicates separation of two mediums and its physical properties differ remarkably from these two composite mediums. Experiments involving the scattering of particles or radiation from an interface enrich the understanding of an interface. In liquid–air or liquid–vapour interfaces it is the concentration profile along the normal to the interface that changes. This change in the profile may be abrupt or gradual. Additionally, it will necessarily entail a non-differentiability in the profile at the junction. It is the non-differentiability that distinguishes an interface from an inhomogeneity of a medium. For instance, equation (5) given below schematically represents an interfacial profile if  $a \neq b$  and an inhomogeneous medium when  $a = b$ . An interesting question arising here is whether a scattering experiment done on an interfacial profile and an inhomogeneous medium would yield qualitatively disparate results. In this work, we report a dramatic change in quantal reflection probability for the two cases when: (i)  $a = 1.000$ ,  $b = 1.001$  and (ii)  $a = b = 1.000$  (see figure 2).

During the current decade, the studies of neutron and x-ray reflectometry [1] from novel kinds of interfaces [2–5] has given rise to an interesting phenomenon, namely a pronounced minimum in reflectivity. A study [6] of reflectometry of polarized neutrons from a magnetized superconductor revealed this phenomenon. In fact, for a more general appeal, this new feature has been stated in terms of quantum mechanics of one-dimensional potentials. Thus, it was found that the reflectivity as a function of energy,  $R(E > V_1 + V_2)$ , for the sharp (abrupt, discontinuous) exponential step, namely  $V(x < 0) = 0$ ,  $V(x \geq 0) = V_1 + V_2 - V_2 \exp(-\frac{x}{a})$  (see the solid curve in figure 1(c)) entails a surprising minimum. Note that  $V_1, V_2 > 0$ . Since the reflectivity of the two well known step potentials (the sharp step and the round-edged step, namely the Fermi profile (figure 1(d)) are generally known [7] to be monotonically decreasing functions of energy, the new type of reflectivity was actually surprising. Nevertheless, it was misinterpreted to be akin to the reflectivity of the well known sharp double step (figure 1(b)). It may be recalled that the simple double-step potential [13] is a practical model for growing anti-reflecting optical coatings.



**Figure 1.** A schematic depiction of the various types of semi-infinite potential steps (a)–(h). Figures (i) and (j) display the hypothetical symmetric well and half-a-well which could be associated with the two-piece (interfacial) potential (e).



**Figure 2.** Reflectivity as a function of energy for the Fermi interface (equation (5)). Note the enhancement in reflectivity for the two-piece step (solid curve) as compared with the reflectivity of the one-piece step (dotted and dashed curves) when  $E > 3$ . S stands for numerical integration of the Schrödinger equation and WW stands for equation (7).

Later, in a more general and rigorous analysis [8], it was critically emphasized that the minimum in the case of exponential potential is strictly *single*, whereas the reflectivity for a simple double step entails multiple minima as a function of energy. It is now known [8] that a sharp (abrupt) semi-infinite potential (steps) of the type

$$V(x) = \left( V_1 + V_2 \left[ 1 - f \left( \frac{x}{a} \right) \right] \right) \Theta(x) \tag{1}$$

where  $f(z) \geq 0$ ,  $f(0) = 1$ ,  $f(\infty) = 0$ ,  $\Theta(x < 0) = 0$ ,  $\Theta(x \geq 0) = 1$ , gives rise to single-minimum in  $R(E)$ . A large assortment of such potential profiles were reported to have a pronounced, parameter-dependent, *single* minimum in the reflectivity at an energy slightly above-the-step height. Moreover, an analytically tractable potential model, the sharp Eckart potential step (see the dotted curve in figure 1(c)), has been proposed [8] which demonstrates the phenomenon of the single dip in reflectivity rather clearly. The single minimum in reflectivity turned out to be an unusual feature, which on the one hand is experimentally valuable [1–6] and on the other theoretically curious [8, 9]. It may be noted here that many authors [1–6, 9] have used various phrases such as reflectivity singularity, reflectivity discontinuity, reflectivity zeros and reflectivity resonances, however, the phrase ‘single minimum/dip in reflectivity’ presently used here can be seen to be most general of all.

Recently, above-the-step quantal reflection from a variety of semi-infinite potential profiles (one-piece and two-piece) has been studied [10]. The one-piece profiles are both continuous and differentiable, e.g., see equations (3) and (13) below and figure 1(d). The two-piece semi-infinite profiles (interfaces, see figure 1(e)) are given as

$$V(x) = V_1 g \left( \frac{x}{b} \right) \Theta(-x) + \left( V_1 + V_2 \left[ 1 - f \left( \frac{x}{a} \right) \right] \right) \Theta(x) \tag{2}$$

where  $g(z)$ ,  $f(z) \geq 0$ ,  $f(0) = 1$ ,  $g(0) = 1$ ,  $f(\infty) = 0$ ,  $g(-\infty) = 0$ . These are continuous at the junction ( $x = 0$ ) but piece-wise differentiable as left and right derivatives do not match at the junction. We would like to emphasize here that one-piece profile represents an inhomogeneous medium and the two-piece profile (see profiles in figure 1(a), (c), (e)–(g)) is a simple visualization of an *interface*. It has been concluded that  $R(E)$ , in general, for the one-piece steps is always a monotonically decreasing function of energy. However, in the case of two-piece steps there exists a pronounced, *single* minimum in  $R(E)$  when an effective parameter assumes a value in a certain domain. Otherwise, the usual monotonic fall-off in  $R(E)$  persists.

In this work, we bring out the crucial role played by the non-differentiability of the potential profile in giving rise to the new type of reflectivity. We show that even a slight non-differentiability at the junction of the semi-infinite potential step causes dramatic change in the reflectivity at energy above the step. Firstly,  $R(E)$  becomes enhanced remarkably at energies much above the step. Secondly, at an energy slightly above the step there may occur the claimed dip in  $R(E)$  depending upon the parameters of the potential.

## 2. An exactly solvable interface

The Fermi step potential (figure 1(d)) is expressed as [7]

$$V(x) = \frac{V_0}{1 + \exp(-\frac{x}{a})} \tag{3}$$

the reflectivity of this step when  $E > V_0$  is given as [7]

$$R(E) = \left( \frac{\sinh \pi a(k - K)}{\sinh \pi a(k + K)} \right)^2 \tag{4}$$

where  $k = \sqrt{\frac{2mE}{\hbar^2}}$ ,  $K = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$ . The Fermi-type interface (figure 1(e)) can be realized as

$$V(x) = \frac{V_0}{1 + \exp(-\frac{x}{b})} \Theta(-x) + \frac{V_0}{1 + \exp(-\frac{x}{a})} \Theta(x). \tag{5}$$

This is a two-piece function which is non-differentiable at  $x = 0$  and the value of the mismatch of the derivative at  $x = 0$  is given as  $\Delta = \frac{V_0}{2} |\frac{1}{a} - \frac{1}{b}|$ . The reflectivity of this potential step can be obtained by transforming [7] the Schrödinger equation to the Gauss hypergeometric equation as

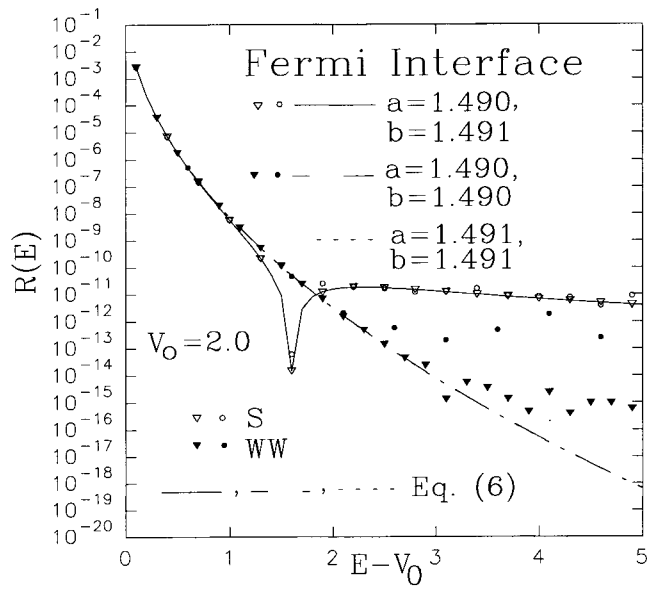
$$r = -(-2)^{-2i\beta_1} \frac{bZ'_1Z_5 + aZ_1Z'_5}{bZ'_1Z_6 + aZ_1Z'_6 - 4iabkZ_1Z_6} \tag{6}$$

where  $k = \sqrt{\frac{2mE}{\hbar^2}}$ ,  $K = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$ ,  $\alpha_1 = ka$ ,  $\alpha_2 = Ka$ ,  $\beta_1 = kb$ ,  $\beta_2 = Kb$ .  $Z_1(\alpha_1, \alpha_2) = {}_2F_1[i(\alpha_1 - \alpha_2), 1 + i(\alpha_1 - \alpha_2), 1 - 2i\alpha_2; \frac{1}{2}]$ ,  $Z_5(\beta_1, \beta_2) = {}_2F_1[i(\beta_1 - \beta_2), 1 + i(\beta_1 - \beta_2), 1 + 2i\beta_1; \frac{1}{2}]$ ,  $Z_6(\beta_1, \beta_2) = Z_5(-\beta_1, \beta_2)$  and  $Z'_i$  implies the differentiation of the corresponding Gauss hypergeometric function (GHF), i.e.  $Z'_i = \frac{LM}{N} {}_2F_1[L+1, M+1, N+1; \frac{1}{2}]$ . The reflection amplitude (6) is easily calculable as the GHFs appearing here are all rapidly converging series. The series representation for a GHF is given as

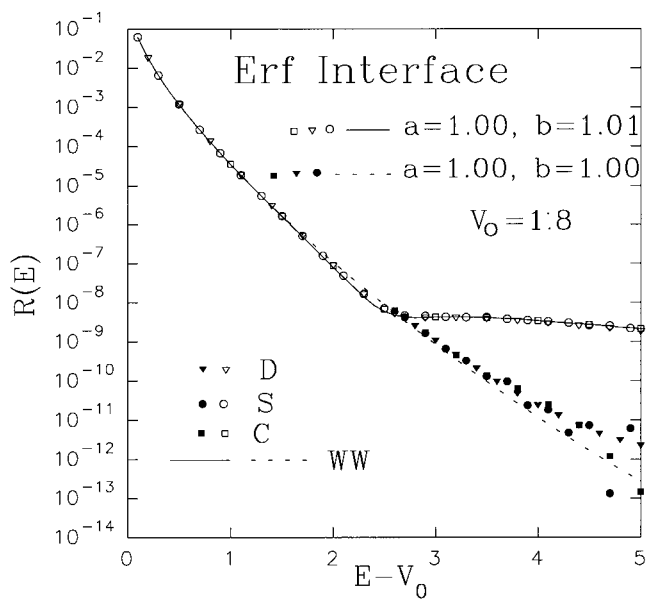
$${}_2F_1(L, M, N; U) = 1 + \frac{LM}{N} \frac{U}{1!} + \frac{L(L+1)M(M+1)}{N(N+1)} \frac{U^2}{2!} + \dots$$

We calculate the reflectivity for the Fermi interface potential (5) by assuming  $\hbar^2 = 1 = 2m$ ,  $V_0 = 2.0$ ,  $a = 1.000$ ,  $b = 1.001$  and employ formula (6). In figure 2, notice a remarkable enhancement of reflectivity (solid curve) at energy much above the step ( $E > 3.0$ ). On the other hand, when the Fermi step is single piece ( $a = 1.000 = b$ ) the reflectivity is rapidly falling as shown by the dashed curve. The reflectivity for the single piece step ( $a = 1.001 = b$ ) is shown by dotted curve which almost coincides with the dashed curve. When  $a = 1.490$  and  $b = 1.491$  giving rise to a slight mismatch of the first-derivative at the junction of the step potential, the reflectivity shows (solid curve) a *single* pronounced minimum at  $E = 1.600$  in figure 3. Above this energy a remarkable enhancement in reflectivity can be observed on comparing the solid curve with the dashed ( $a = 1.490 = b$ ) or the dotted ( $a = 1.491 = b$ ) curves (equation (6)). Though presently for the sake of only a slight mismatch in the derivatives ( $\Delta$ ), we have chosen  $a$  and  $b$  nearly equal, however, in the vicinity of these values of  $a$  and  $b$  the reflectivity dip can be observed, for example, when  $a = 1.500$ ,  $b = 1.600$ . Several other slightly unequal values of  $a, b$  may be found (for instance  $a = 2.600, b = 2.601$ ;  $a = 3.000, b = 3.001$ ) that give rise to the dip in reflectivity. Notably, in the last two cases (when values of  $a$  and  $b$  increase) the dip becomes less prominent to make way for a seemingly sharp bend (figure 6) in  $R(E)$  at the energy where the dip is expected. For the abrupt exponential step, such a bend in reflectivity for large values the slope parameter  $a$  is shown [9] to occur and it has been termed as discontinuity in  $R(E)$ .

The circles (open and filled) in figures 2 and 3 represent the calculations due to the numerical (Runge–Kutta) integration of the Schrödinger equation; this has been done to ensure the correctness of equation (6) and also to verify the claimed variation of the reflectivity. In figure 2 the filled circles show deviation from the dashed curve. This exposes the limitations (instability and inaccuracy) of the method employing the numerical integration of the Schrödinger equation for the calculation of  $R(E > 3)$ . Interestingly, even the changes in asymptotic distance ( $x_L$ ) and mesh-size ( $\Delta x$ ) do not improve the calculations either. In fact, for a given one-piece step, we find that the numerical integration of the Schrödinger equation yields unreliable values of the reflectivity below a certain order ( $10^{-M}$ ). For example, for the



**Figure 3.** The scenario of the occurrence of the single minimum in reflectivity due to even a slight non-differentiability in the Fermi potential (equation (5)). Note the disparate variation of  $R$  by comparing the solid curve with the dashed or the dotted curves.



**Figure 4.** The same as in figure 2 for the error-function interface (equation (12)). C and D stand for equations (10) and (8) respectively.

Fermi step, we find that the values of  $R(E)$  ( $< 10^{-11}$ ) in figure 2 are not reliable. For the case in figure 3 the values of  $R(E)$  below  $10^{-12}$  are not reliable. However, since  $R(E)$  of a step potential with even a slight non-differentiability becomes enhanced by orders of magnitude,

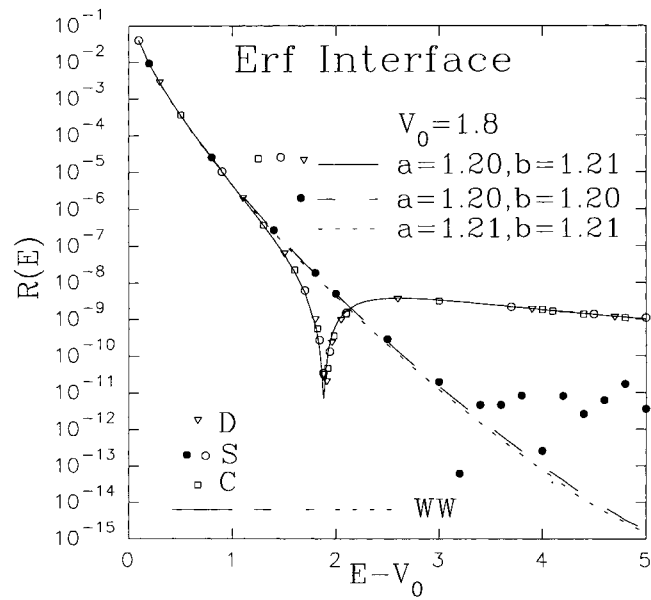


Figure 5. The same as in figure 3 for the error-function profile (equation (12)).

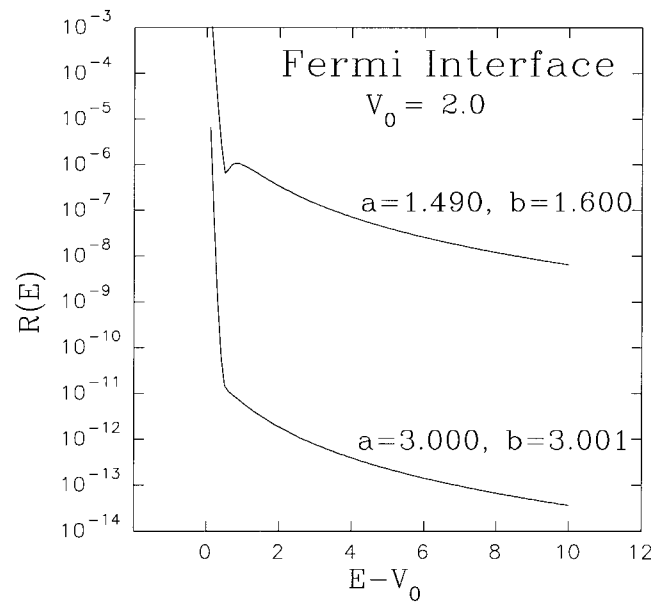


Figure 6. An example of a marginal dip and a bend in the reflectivity of the Fermi interface.

at energies much above the step, the numerical integration of the Schrödinger equation yields them correctly—compare the open circles with the solid curves in figures 2–5. We would like to caution here that evaluation of  $R(E)$  in equation (6) at much higher energies also requires high precision in the computations.

Qualitatively disparate behaviour of reflectivity (figures 3 and 5) for two so closely resembling step potentials, of which one is non-differentiable, may be taken with some suspicion. For instance, it may be suspected to arise from a consistent commitment of a certain mistake while solving the Schödinger equation both numerically and analytically. In order to be sure, we propose to employ various other methods which have apparently independent origins. These methods consist in obtaining  $R(E)$  by solving various Riccati equations for the reflection amplitude.

### 3. Verification of the new type of reflectivity using various Riccati equations

The Riccati equation is a first-order nonlinear differential equation introduced in wave propagation [12, 13] as an alternative to solving the second-order wave equation, hence it is adaptable in quantum mechanics. The main benefit in using a Riccati equation lies in its ability to yield the quantity of interest directly. In the literature we find three Riccati equations derived for the reflection amplitude. In principle, since the Riccati equations are first order and direct-yielding one would expect them to be more accurate than using the Schrödinger equation. The quantal version of the first ever Riccati equation for reflection amplitude,  $r$ , proposed by Walker and Wax [12], is given as

$$\frac{dr}{dx} = -2ir \sqrt{\frac{2m}{\hbar^2} [E - V(x)]} + \frac{\frac{\hbar}{\sqrt{2m}} \frac{dV}{dx}}{4[E - V(x)]} (1 - r^2) \quad (7)$$

where one has to evaluate  $r(-L)$  subject to the initial condition that  $r(+L) = 0$ . If the potential converges on both the sides asymptotically then  $L = \infty$ . If the potential is of finite support (truncated at  $x = \pm a$ ) then  $L = a$ . The potential need not be a symmetric function of  $x$ . We find that equation (7) also works for semi-infinite potentials ( $V(+\infty) = \text{constant}$ ,  $V(-\infty) = 0$ ; steps) in obtaining the reflectivity,  $R(= |r|^2)$ , at energies above-the-step height. But at energies below the step it fails. This failure of (7) is not really a serious one since we know that for semi-infinite potentials  $R(E \leq V_0) = 1$ , so the calculations are not required in this energy regime. Interestingly, equation (7) has a serious limitation for a potential barrier, the sub-barrier reflectivity cannot be obtained from equation (7). Since for a potential well the scattering states only exist at energies above the well, this Riccati equation works.

Interestingly we found that De'Souza has claimed another [14] Riccati equation

$$\frac{dr}{dx} = \frac{i}{2k} \left[ \frac{2m}{\hbar^2} V(x)(1 + r^2) - \frac{4m}{\hbar^2} r[V(x) - 2E] \right]. \quad (8)$$

In distinction to equation (7) note that equation (8) does not contain  $\frac{dV}{dx}$  and also it looks entirely different. As earlier, we use  $r(L) = 0$  as the initial condition to find that this equation works correctly only for finite potential wells and barriers. These potentials on both the sides are either of finite support or vanish asymptotically.

We find that the initial condition that

$$r(+L) = \frac{K - k}{K + k} \quad (9)$$

can enable equation (8) to work correctly for semi-infinite potentials at both the energies below and above-the-step height. The potential is such that  $V(\infty) = \text{constant} > 0$ ,  $V(-\infty) = 0$ .

A third Riccati equation for reflection amplitude has been given by Calogero which reads as [15]

$$\frac{dr}{dx} = (2ik)^{-1} \frac{2m}{\hbar^2} V(x) [\exp(-ikx) + r \exp(ikx)]^2 \quad (10)$$



with the condition that  $r(\infty) = 0$ . Once again, we find that equation (10) works for potential barriers and wells which converge at  $x = \pm\infty$  and fails for semi-infinite potentials. Later Rozman *et al* [16] independently derived an equation identical to equation (10) and suggested a crucial initial-value condition as

$$r(+L) = \frac{k - K}{k + K} \exp(-2ikL) \quad (11)$$

to be imposed on equation (10), if  $V(\infty) = \text{constant}$  and  $V(-\infty) = 0$ .

The failure of (8) and (10) without imposition of (9) and (11) is of the common nature. The Riccati equations (8) and (10) are obtained from the Schrödinger equation after discretizing a potential function (well/barrier) into infinitesimally thin rectangles [14, 16]. Note that these potentials have been assumed to be of finite support or asymptotically converging type, the first rectangle on the left and the last rectangle on the right (though almost of zero height) remain rectangular potentials. Consequently, then the reflection amplitude of the infinitesimally small rectangular potential is used in the analysis [14, 16]. But the situation for the semi-infinite potential differs as on the right-hand side ( $x \rightarrow \infty$ ) the last part of the potential ceases to be rectangular (having some width), this instead is a simple step (of infinite width). Thus, the imposition of the reflection amplitudes (9) and (11) as boundary conditions enable equations (8) and (9), respectively, to work for semi-infinite potentials.

Having described three Riccati equations (7), (8) and (10), we now employ them to confirm the claimed variation of reflectivity that arises due to even a slight non-differentiability in the step potential. Also, we would like to check the performance of these Riccati equations at energies much above the step. In the figures presented here, we denote equation (7) by WW, equation (8) by D, equation (10) by C, and S denotes integration of the Schrödinger equation.

In figures 2–5, one can see a good agreement between open characters (squares, circles, triangles) with the solid curves. This confirms the claimed variations of the reflectivity that are caused by even a slight non-differentiability in the step potential at the junction point. The single minimum in reflectivity is parameter-dependent which may also be found for some other values of  $V_0$ ,  $a$ ,  $b$ . The excursions of the filled characters (circles, squares, triangles) from the dashed/dotted curves at the higher energies in figures 2 and 5 indicate the inaccuracies and instabilities of the various numerical methods (D, S, C), when the semi-infinite potential is one piece. In this case, the reflectivity decreases more rapidly and after a value of  $10^{-11}$  the results become unreliable. Of all the methods, we find that equation (7) works the best.

In figures 4 and 5, we have used error-function profile for an interface, i.e.,

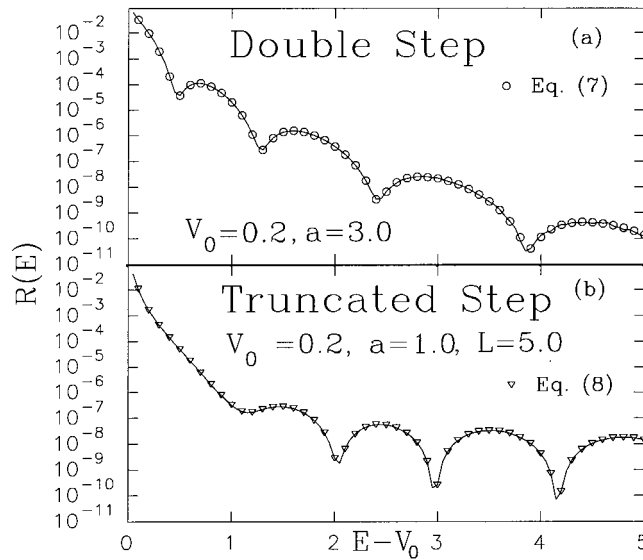
$$V(x) = \frac{V_0}{2} \left[ 1 + \operatorname{erf}\left(\frac{x}{b}\right) \right] \Theta(-x) + \frac{V_0}{2} \left[ 1 + \operatorname{erf}\left(\frac{x}{a}\right) \right] \Theta(x) \quad (12)$$

which gives the one-piece erf semi-infinite profile when  $a = b$  as

$$V(x) = \frac{V_0}{2} \left[ 1 + \operatorname{erf}\left(\frac{x}{a}\right) \right]. \quad (13)$$

This is an analytically unamenable instance, we have compared the reflectivities due to various methods against the values obtained by equation (7). Figures 4 and 5 support the findings of figures 2 and 3. We have also used several other step profiles to verify the robustness of the new variations in reflectivity as caused by even a slight non-differentiability in the step potential. One interesting aspect of the computation of reflectivity using any of the above-mentioned methods including equation (6) is that they yield erratic oscillations (see filled characters in figures 2–5) of  $R(E)$ , in case they fail due to numerical limitations.

The usual (general) variations of  $R(E)$  are presented for (i) a smooth double step i.e.,  $V(x) = \frac{V_0}{1 + \exp(-\frac{x^3}{a^3})}$  in figure 7(a) and for (ii) a truncated (three-piece) potential step i.e.,



**Figure 7.** The usual multiple minima in reflectivity for a double step (see the text and figure 1(h)) and a truncated step (three piece, see the text). The solid curves are due to numerical integration of the Schrödinger equation and the open triangles are due to equation (7) in (a) and due equation (8) in (b).

$V(x < -L) = 0, V(-L \leq x \leq L) = \frac{V_0}{1 + \exp(-\frac{x}{a})}, V(x > L) = V_0$  in figure 7(b). Note the occurrence of multiple minima in the reflectivity. The solid curves are obtained from numerical integration of the Schrödinger equation and the open triangles are due to equation (7). For a truncated three-piece step, we find that the Riccati equation (7) yields the values of reflectivity which disagree with those due to methods D, C and S, here the unusability of equation (7) for such cases should be noted. For the truncated step we have used equation (8) to generate the open triangles in figure 7(b). We re-emphasize that multiple minima in  $R(E)$  is a common feature of reflectivity of several potentials, but it is the single minimum that is experimentally promising and theoretically intriguing.

**4. Reflection from non-differentiable potential wells**

Earlier, it was important to note that in [11] the non-differentiable potential wells of the type  $V_S(x)$  (figure 1(i)) have been found to yield the reflectivity which either falls-off monotonically or entails a single minimum. The non-differentiability of  $V_S(x)$  (at  $x = 0$ ) has been held [11] crucially responsible for the single minimum in the reflectivity, for a variety of such potential wells. Here, we would like to give two more examples:  $R(E)$  for  $V(x) = -V_0[\text{sech}(\frac{x}{b})\Theta(-x) + \text{sech}(\frac{x}{a})\Theta(x)]$  entails a pronounced minimum when  $a = 2.21, b = 1.59, V_0 = 1.00, E = 0.24$ . More interestingly, the asymmetric Eckart well,  $V(x) = -V_0[\text{sech}^2(\frac{x}{b})\Theta(-x) + \text{sech}^2(\frac{x}{a})\Theta(x)]$ , holds a pronounced minimum in  $R(E)$  when  $a = 2.40, b = 3.10, V_0 = 1.00, E = 0.56$ . Compare this scenario with the case of the symmetric Eckart well ( $-V_0\text{sech}^2(\frac{x}{a})$ ) also called the soliton potential [15] that always gives rise to a monotonically decreasing  $R(E)$  which becomes reflectionless at any energy, when  $\frac{2mV_0a^2}{\hbar^2} = n(n + 1), n = 0, 1, 2, 3, \dots$ . Note that for these two potential wells, it is the second derivative which is discontinuous at  $x = 0$ . If  $R(E)$  is the reflectivity of the step (figure 1(c))

and  $R_S(E)$  is for the corresponding  $V_S(x)$  (figure 1(i)) then in [9] Abeles' connection [20] between  $R(E)$  and  $R_S(E)$  has been invoked to explain the zero in  $R(E)$  it is inferred that a zero in  $R(E)$  would correspond to a zero in  $R_S(E)$ . However, the Abeles connection only shifts the question instead of answering it. The question then arises is as to what causes a zero in  $R_S(E)$ . In the light of the discussion in this section and in [11], the non-differentiability in the potential well emerges to be a strong cause.

## 5. Hypothesizing a well in the semi-infinite potential

All these developments give rise to an inevitable question: what causes this pronounced, parameter-dependent, single minimum in reflectivity? Whether it is due to the non-differentiability of the potential profile or some known spectral property of the possible binding potentials such as the non-differentiable and symmetric one:  $V_S(x) = V_1 + V_2[1 - f(\frac{|x|}{a})]$  (figure 1(i)) [9, 11] or the hard-walled potential (half-a-well):  $V_H(x < 0) = \infty, V_H(x \geq 0) = V_1 + V_2[1 - f(\frac{x}{a})]$  (figure 1(j)) [8] which, in an imaginative way, is a part of the total potential step. Such semi-infinite potential steps have been termed 'attractive' in [9]. Note that the condition that  $f(z) \geq 0$  [8] essentially gives rise to a hypothetical half-a-well in the step (figure 1(j)), in absence of which the claimed minimum in  $R(E)$  *does not occur* [9]. For instance, the semi-infinite profiles given in figures 1(f) and (g) are non-differentiable at  $x = 0$ , containing 'half-a-barrier' instead of 'half-a-well' (hence they are exceptions for the single-dip type of reflectivity). On the other hand, the Fermi step (figure 1(d)) despite being 'attractive' (containing half-a-well, for  $x > 0$ ), as per equation (4) supports only a monotonic behaviour of  $R(E)$  and this, we claim, is true of any one-piece step (e.g. equations (3) and (13)) of arbitrary profile which is differentiable everywhere. Such profiles being differentiable and one piece do not entail a junction point and therefore the search for half-a-well becomes redundant. It is not really possible to closely fit a two-piece profile by a one-piece profile over the whole domain of  $x$ , therefore, the Fermi interface with  $a = 1.490, b = 1.491$  can be assumed to be close enough to the Fermi step ( $a = b = 1.490$  or  $a = b = 1.491$ ) wherein the disparate behaviour of  $R(E)$  has been observed in figure 3. Thus, both the conditions, i.e. the attractiveness and the non-differentiability of the semi-infinite profiles, can be adjudged to be crucially responsible in giving rise to the claimed single dip in the reflectivity which is displayed in figures 3 and 5. Next, the question of whether any known spectral property of the non-differentiable (at  $x = 0$ ) binding potentials ( $V_S(x)$ , figure 1(i) or  $V_H(x)$ , figure 1(j)) can help *a priori* to determine the condition on potential parameters and the energy at which the minimum in reflectivity would exist, deserves investigation.

The potential  $V_S(x)$  (figure 1(i)) can support bound states of definite parity (even/odd). Consequently, the potential  $V_H(x)$  will hold only half the number of bound states which will be of odd parity and the wavefunction will vanish at  $x = 0$  (at the hard wall). Incidentally, we note that for two abrupt steps the exponential step (the solid curve in figure 1(c)) [6] and Eckart step (the dotted curve in figure 1(c)) [8], the condition of finding the minima in reflectivity coincided with that of finding a bound level at the edge, i.e.  $E = V_1 + V_2$  in  $V_H(x)$  (figure 1(j)). This interesting coincidence is slightly approximate for the exponential step but exact (analytic) for the Eckart step. However, for several other abrupt steps of arbitrary profiles, we do not find this correspondence as remarkable. More so, in the light of the Fermi interface (5), we realize that the other part of the potential,  $V(x < 0)$ , does play an interesting role through the parameter  $b$ .

## 6. Conclusion

We would like to remark that the singleness of the zero of the reflectivity of an abrupt step (1) has sometimes gone unheeded. For instance, while re-describing the reflection from the abrupt exponential step of [6], through equation (4.5) in [9], multiple zeros in the reflectivity have been argued. Strangely enough, in [9], impressions/statements have been given implying that in 1953 Morse and Feshbach [18, pp 1670–2] already explained/predicted the physical origin/occurrence of the reflectivity-zero(s) as quasi-bound state(s) in  $V_S$  (figure 1(i)). In fact, Morse and Feshbach only worked out the s-wave bound states of the exponential well, without any mention of the quasibound states. It is indeed important to assert that, to the best of our knowledge, the single zero in the reflectivity, including the one described here in section 4 and in [11], is a phenomenon that has gone unnoticed until the beginning of the current decade.

To sum up, we have shown that even a slight mismatch of derivative at the junction of the potential step causes a much less rapid variation of reflectivity at energy much above the step. More interestingly, the reflectivity entails a pronounced, parameter-dependent, *single* minimum. Since a non-differentiable potential step essentially represents an interface, these could also be seen as essential features of quantal reflection from an interface. We have solved various Riccati equations (7), (8) and (10) as a means to re-confirm our results in that it is amusing to note that these seemingly different equations yield essentially the same results apart from their inherent individualistic numerical errors. Our listing of discussions regarding the usage of Riccati equations for various types of one-dimensional potentials may be found instructive. Here we have extended the use of (8) for semi-infinite potentials by imposing (9) as a necessary boundary condition.

Though, presently, we do not have a proof, however, the contention that non-differentiability is crucially important in giving rise to the remarkable enhancement and a single minimum in reflectivity for an attractive type of semi-infinite potential step has been strongly supported here. A physical explanation of this phenomenon which could also be termed as a *single* destructive interference of multiply scattered waves in the interfacial potential may turn out to be very inspiring. In that, it is interesting to recall the more familiar and the closely related phenomenon of the Ramsauer–Townsend (RT) effect [17–19]. As per this effect, an attractive potential may be ‘strong enough’ to pass-off the s-wave phase shift through  $\pi$  at a very low energy, to yield, in turn, a dramatically low cross-section. This happens in electron scattering from inert-gas atoms. Despite a long history of research, one cannot actually predict whether a given form of the potential well will exhibit the RT effect. However, there are potential wells of both kinds—finite support [17, 18] and infinite range [19]—that model the RT effect.

## References

- [1] Zhou X-L and Chen S-H 1995 *Phys. Rep.* **257** 223
- [2] Jannink G, Farnoux B and des Cloizeaux J 1989 *J. Phys. Colloq. C* **50** 67
- [3] Guiselin O 1989 *J. Physique* **50** 3407
- [4] Guiselin O 1992 *Europhys. Lett.* **17** 57
- [5] Zhao H, Pennincks-Sans A, Lee L T, Beysens D and Jannink G 1995 *Phys. Rev. Lett.* **75** 1977
- [6] Zhang H and Lynn J W 1993 *Phys. Rev. Lett.* **70** 77  
Zhang H and Lynn J W 1993 *Phys. Rev. B* **38** 15 893
- [7] Landau L D and Lifshitz E M 1965 *Quantum Mechanics* (London: Pergamon)
- [8] Ahmed Z 1996 *Phys. Lett. A* **210** 1
- [9] Geoghegan M and Jannink G 1998 *Proc. R. Soc. A* **454** 659
- [10] Ahmed Z 1999 *J. Phys. A: Math. Gen.* **32** 2767
- [11] Ahmed Z 1997 *Phys. Lett.* **236** 289

- Ahmed Z 1998 *Phys. Lett.* **239** 411
- [12] Walker L R and Wax N 1946 *J. Appl. Phys.* **17** 1043
- [13] Lekner J 1987 *Theory of Reflection* (Boston: Martinus Nijhoff)
- [14] De'Souza P 1987 *Pramana J. Phys.* **29** 121
- [15] Calogero F and degasperis A 1982 *Spectral Transforms and Solitons* (Amsterdam: North-Holland)
- [16] Rozman M G, Reineker P and Tehver R 1994 *Phys. Rev.* **49** 3310
- [17] Schiff L I 1968 *Quantum Mechanics* 3rd edn (New York: McGraw-Hill)
- [18] Morse P M and Feshbach H 1953 *Methods of Theoretical Physics* (New York: McGraw-Hill)
- [19] Morse P M, Allis W P and Lammer E S 1935 *Phys. Rev.* **48** 412
- [20] Abeles F 1950 *Ann. Phys., Paris* **5** 596