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Semiclassically weak reflections above analytic and non-analytic potential barriers

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Abstract. The coefficient r for reflection above a barrier $V(x)$ is computed semiclassically (i.e. as $\hbar \to 0$) employing an exact multiple-reflection series whose mth term is a $(2m+1)$-fold integral. If $V(x)$ is analytic, all terms have the same semiclassical order $(\exp(-\hbar^{-1}))$; the multiple integrals are evaluated exactly and the series summed. If $V(x)$ has a discontinuous Nth derivative, the term $m=1$ dominates semiclassically and gives $r \sim \hbar^N$. If $V(x)$ has all derivatives continuous but possesses an essential singularity on the real axis, the term $m=1$ again dominates semiclassically, and for $V \sim \exp(-|x|^{-n})$ gives $r \sim \exp(-\hbar^{-n/(n+1)})$ with an oscillatory factor corresponding to transmission resonances. The formulae are illustrated by computations of $|r|^2$ for four potentials with different continuity properties and show the limiting asymptotics emerging only when the de Broglie wavelength is less than 1% of the barrier width and $|r|^2 \sim 10^{-1000}$.

1. Introduction

Consider a beam of quantum-mechanical particles with energy E and mass μ incident from $x=-\infty$ above a one-dimensional continuous potential barrier $V(x)$ possessing a single maximum of height $V_0(<E)$ at $x=0$ (figure 1). In the classical limit, i.e. when Planck's constant $\hbar$ equals zero, there is no reflection from such a barrier. In the *semiclassical limit*, i.e. as $\hbar$ tends to zero, there is weak reflection, and this paper is devoted to studying in leading-order asymptotics precisely how the reflection coefficient r vanishes with $\hbar$.

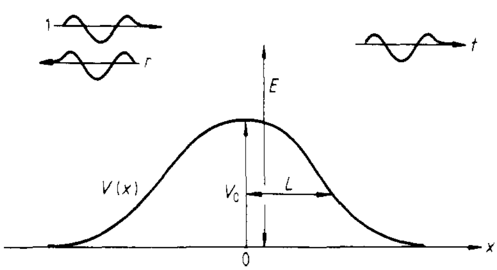

Figure 1. Scattering geometry and notation.

Two contributions are made to this venerable problem by employing an exact representation of r (§ 2) as a convergent multiple-reflection series whose terms are multiple integrals. Firstly, for the case where $V(x)$ is analytic, it is shown (§ 3) that

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all terms of the series are of the same order in $\hbar$ (i.e. $\exp(-\hbar^{-1})$), and the multiple integrals are evaluated and summed explicitly. Although the resulting 'WKB reflection formula' is well known (see e.g. Fröman and Fröman (1965), Pokrovskii and Khalatnikov (1961) or the review by Berry and Mount (1972, hereinafter called BM)), it is instructive and novel to see an asymptotic result emerging from a convergent series. Pokrovskii *et al* (1958), employing a slightly different formalism, were the first to point out that the asymptotic r can be expanded in this way, but they failed to evaluate the multiple integrals involved.

Secondly, for the non-analytic case it is shown how r depends on the continuity class of $V(x)$. Two situations are examined in §§ 4 and 5: where the Nth derivative of $V(x)$ (and none lower) is discontinuous (in which case $r \sim \hbar^N$), and where all derivatives are continuous but $V(x)$ has an essential singularity at its maximum (in which case r depends on the type of singularity, but is smaller than $\hbar^N$ for any N though greater than $\exp(-\hbar^{-1})$). This dependence on continuity class was conjectured by Mahony (1967) and proved by Meyer (1975, 1976), but these authors did not give explicit formulae for r for non-analytic potentials. This asymptotic dependence of r on continuity class arises because in the semiclassical limit the de Broglie wavelength is vanishingly small and discriminates fine details of $V(x)$.

The different reflection formulae are illustrated in § 6 by computations for four potentials with different continuity properties.

To avoid confusion it is worth mentioning that I shall not consider the high-energy limit (which is different from the semiclassical limit—see BM), the higher-order corrections to asymptotic formulae for r (see Lundborg 1979), or the 'barrier-skimming' behaviour of r as E approaches V_0 (see BM).

2. Convergent multiple-reflection expansion

It is convenient to work with the momentum function

$$p(x) \equiv [2\mu(E - V(x))]^{1/2} \tag{1}$$

defined as positive for real x. Then Schrödinger's equation for the wavefunction $\psi(x)$ is

$$\mathrm{d}^2\psi/\mathrm{d}x^2 + (p^2(x)/\hbar^2)\psi = 0. \tag{2}$$

To lowest order in $\hbar$ (BM) this has the 'WKB' solutions

$$\psi \sim \mathrm{e}^{\pm \mathrm{i}W(x)}/(p(x))^{1/2} \tag{3}$$

where W is the phase integral defined as

$$W(x) \equiv \frac{1}{\hbar}\int_0^x \mathrm{d}x'\, p(x'). \tag{4}$$

The plus and minus signs in (3) correspond to waves travelling in the positive and negative x directions, and in this approximation there is no coupling between these waves and hence no reflection. In reality, of course, there is reflection, and this indicates the inadequacy of (3).

To obtain a more useful formalism, ψ is written exactly as

$$\psi = b_+(W(x))\,\mathrm{e}^{\mathrm{i}W(x)}(p(x))^{-1/2} + b_-(W(x))\,\mathrm{e}^{-\mathrm{i}W(x)}(p(x))^{-1/2}. \tag{5}$$

The coefficients $b_\pm$ will be considered as functions of W rather than x, and this is possible because the mapping (4) between W and x is one-to-one on the real axis. At $|x| = \pm\infty$, $V \to 0$ and $p(x) = (2\mu E)^{1/2}$ = constant and the solutions (3) are exact, so that $b_\pm(\pm W) \to$ constant as $W \to \pm\infty$. The scattering geometry of figure 1 corresponds to

$$b_+(-\infty) = 0 \qquad b_-(+\infty) = 0 \tag{6}$$

and the reflection and transmission coefficients may be defined as

$$r = b_-(-\infty) \qquad t = b_+(+\infty).$$

In the decomposition (5), the single unknown function ψ has been replaced by the two unknown functions $b_\pm$, and a subsidiary condition is necessary in order for the $b_\pm$ to be defined uniquely. For present purposes the simplest condition (but not the only one) is

$$\frac{\mathrm{d}\psi}{\mathrm{d}x} = \frac{\mathrm{i}}{\hbar}(p(x))^{1/2}(b_+(W)\,\mathrm{e}^{\mathrm{i}W} - b_-(W)\,\mathrm{e}^{-\mathrm{i}W}). \tag{7}$$

Then the Schrödinger equation (2) gives, for the equations satisfied by b_+ and b_-,

$$\mathrm{d}b_\pm(W)/\mathrm{d}W = S(W) b_\mp(W)\,\mathrm{e}^{\mp 2\mathrm{i}W} \tag{8}$$

where

$$S(W) = \tfrac{1}{2}\frac{\mathrm{d}}{\mathrm{d}W}\ln p(x(W)) \tag{9a}$$

$$= \frac{\hbar}{2p^2(x(W))}\frac{\mathrm{d}}{\mathrm{d}x}p(x(W)) \tag{9b}$$

$$= \frac{-\hbar}{4p(x(W))(E - V(x(W)))}\frac{\mathrm{d}}{\mathrm{d}x}V(x(W)). \tag{9c}$$

In this maximally simple representation it is clear that coupling between b_+ and b_-, and hence reflection, arises from variations in $p(x)$ and hence of the potential $V(x)$, i.e. from forces acting on the particles, as embodied in the function $S(W)$.

It is natural to integrate both sides of (8) and solve for $b_\pm$ by iteration using the boundary conditions (6). For the reflection coefficient r this gives, on using (7), the infinite series

$$\begin{aligned} r &= -\int_{-\infty}^{\infty}\mathrm{d}W_0\, S(W_0)\,\mathrm{e}^{2\mathrm{i}W_0} + \int_{-\infty}^{\infty}\mathrm{d}W_0\, S(W_0)\,\mathrm{e}^{2\mathrm{i}W_0} \\ &\quad\times \int_{-\infty}^{W_0}\mathrm{d}V_1\, S(V_1)\,\mathrm{e}^{-2\mathrm{i}V_1}\int_{V_1}^{\infty}\mathrm{d}W_1\, S(W_1)\,\mathrm{e}^{2\mathrm{i}W_1} - \dots \\ &= -\sum_{m=0}^{\infty}(-1)^m \int_{-\infty}^{\infty}\mathrm{d}W_0\, S(W_0)\,\mathrm{e}^{2\mathrm{i}W_0}\prod_{n=1}^{m}\int_{-\infty}^{W_{n-1}}\mathrm{d}V_n\, S(V_n)\,\mathrm{e}^{-2\mathrm{i}V_n} \\ &\quad\times\int_{V_n}^{\infty}\mathrm{d}W_n\, S(W_n)\,\mathrm{e}^{2\mathrm{i}W_n} \end{aligned} \tag{10}$$

where the product is defined as unity for $m = 0$. Bremmer (1951) and Landauer (1951) (see also BM) obtained this series by considering the potential as the limit of a 'staircase' in which $V(x)$ is approximated as piece-wise constant with tiny discontinuities. The mth term in r then acquires a physical interpretation, as the wave arriving at $x=-\infty$ after all combinations of $2m+1$ reflections at the steps of the potential.

Atkinson (1960) proved that the series (10) is convergent provided

$$\int_{-\infty}^{\infty} \mathrm{d}x \left| \frac{\mathrm{d}p(x)/\mathrm{d}x}{p(x)} \right| \leqslant 2\pi. \tag{11}$$

For potential barriers with a single hump as in figure 1 this implies

$$E \geqslant V_0/(1-\mathrm{e}^{-2\pi}) \simeq 1.00187\, V_0 \tag{12}$$

and this not very restrictive condition will henceforth be assumed.

The task now is to find semiclassical approximations to the terms in the exact series (10). These terms are $(2m+1)$-fold multiple oscillatory integrals, whose asymptotics are dominated by the singularities of the functions $S(W)$. For analytic potentials, to be considered first, the singularities lie in the complex planes of the variables $W_0 \ldots V_m$. For non-analytic potentials the singularities are real.

3. Analytic barriers

If $V(x)$ is analytic on the real axis, then so are the functions $p(x)$, $W(x)$ and $S(W)$ defined by (1), (4) and (9). Contributions to the integrals in (10) arise from points W^* in the complex planes of $W_0 \ldots V_n$ at which $S(W)$ is singular. The commonest such singularities are the complex first-order turning points x^* where

$$E = V(x^*) \tag{13}$$

at which $p^2(x)$ has a simple zero, but it causes no difficulty to consider the more general case where, close to x^*,

$$p(x) \approx A(x-x^*)^{\nu/2} \tag{14}$$

corresponding to a turning point of order ν if $\nu>0$ and a pole or branch point of order ν in $V(x)$ if $\nu<0$. It is easy to show from (4) and (9b) that at any of these singularities $S(W)$ has a simple pole, whose residue depends on the order ν, as

$$S(W) \approx \frac{\nu}{2(\nu+2)(W-W^*)}. \tag{15}$$

By considering the alternating signs of the phases in (10) it appears that the contours can be deformed so as to extract the contribution of W^* only if W^* lies in the upper half-plane. It now follows that

$$r \approx -2\pi \mathrm{i}\, \mathrm{e}^{2\mathrm{i}W^*} \sum_{m=0}^{\infty} \left(\frac{\nu}{2(\nu+2)}\right)^{2m+1} (-1)^m I_m \tag{16}$$

where

$$I_m \equiv \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\xi_0\, \mathrm{e}^{\mathrm{i}\xi_0}}{\xi_0 - \mathrm{i}\varepsilon} \prod_{n=1}^{m} \int_{-\infty}^{\xi_{n-1}} \frac{\mathrm{d}\eta_n\, \mathrm{e}^{-\mathrm{i}\eta_n}}{\eta_n - \mathrm{i}\varepsilon} \int_{\eta_n}^{\infty} \frac{\mathrm{d}\xi_n\, \mathrm{e}^{\mathrm{i}\xi_n}}{\xi_n - \mathrm{i}\varepsilon} \tag{17}$$

in which ε is a positive infinitesimal.

In these formulae, Planck's constant appears only in W^*, which is defined by the complex integral

$$W^* = \frac{1}{\hbar}\int_0^{x^*} \mathrm{d}x\, p(x). \tag{18}$$

Because Im $W^* > 0$, the dominant contribution to r comes from the singularity closest to the real axis. The I_m in (17) are pure numbers, so that all terms in the multiple-reflection expansion do indeed have the same order of magnitude, as asserted.

It is shown in appendix 1 that

$$I_m = \frac{\pi^{2m}}{(2m+1)!}. \tag{19}$$

Now the series (16) can be summed to give

$$r \approx -2\mathrm{i}\, \mathrm{e}^{2\mathrm{i}W^*} \sin\left(\frac{\pi\nu}{2(\nu+2)}\right). \tag{20}$$

This is the semiclassical limit of the reflection coefficient from a νth-order turning point, previously obtained either by analytic continuation of basic WKB solutions (3) across Stokes' lines (BM) (e.g. by Pokrovskii and Khalatnikov 1961) or by comparison with the known solutions of appropriately chosen model equations (Langer 1937).

The commonest case is $\nu = 1$, for which the reflected intensity is

$$|r|^2 \approx \exp\left(-\frac{4}{\hbar}\,\mathrm{Im}\int_0^{x^*} \mathrm{d}x\, p(x)\right). \tag{21}$$

The multiple-reflection series (16) converges very rapidly in this case: the coefficient unity of the semiclassical exponential for $|r|$ is approximated by 1.047 for one reflection, 0.9993 for three reflections, and 1.000004 for five reflections. Higher-order turning points can be produced by the coalescence of lower-order ones by varying E or parameters in $V(x)$. For example, if

$$V = V_0 \exp[-(x^4 + 2a^2x^2)/L^4] \tag{22}$$

then for $E > V_0 \exp(a^4/L^4)$ there are two first-order turning points with the same positive value of Imx^* and for $E < V_0 \exp(a^4/L^4)$ there are two first-order turning points on the positive imaginary x axis with different values of Imx^*. These coalesce when $E = V_0 \exp(a^4/L^4)$ to give a second-order turning point at $x^* = \mathrm{i}a$.

4. Barriers with Nth derivative discontinuous

It is simplest and causes no essential loss of generality to let the discontinuity in the Nth derivative of the potential lie at $x = 0$, i.e. $W = 0$. Define

$$p_0 \equiv p(0) = [2\mu(E - V_0)]^{1/2} \tag{23}$$

and

$$p_n(x) \equiv \frac{\mathrm{d}^n}{\mathrm{d}x^n}\, p(x) \tag{24}$$

and realise that close to the discontinuity the mapping (4) gives

$$W(x) \approx p_0 x/\hbar. \tag{25}$$

By Taylor expansion in powers of W, the singular part of the function $S(W)$ (equation (9)), which is what contributes to the asymptotic r in the representation (10), is easily found to be

$$S_{\text{sing}}(W) = \lim_{\varepsilon \to 0} \left(\frac{\hbar^N W^{N-1}}{2p_0^{N+1}(N-1)!} \right) (p_N(+\varepsilon)\Theta(W) + p_N(-\varepsilon)\Theta(-W)) \tag{26}$$

where Θ denotes the unit step function.

On substituting S_{sing} into (10) it is clear that the mth multiple integral contributes a term of order to $\hbar^{(2m+1)N}$ to r. Therefore the semiclassical reflection is dominated by the first term, in contrast to analytic barriers, for which all terms have the same order. The first integral in (10) is easily evaluated, with the result (valid if $N>0$)

$$r \approx \lim_{\varepsilon \to 0} \left(\frac{-\mathrm{i}^N \hbar^N}{2^{N+1} p_0^{N+1}} \right) (p_N(+\varepsilon) - p_N(-\varepsilon)). \tag{27}$$

The procedure employed here, of replacing S by S_{sing}, is precisely equivalent to asymptotically evaluating the integrals for r by repeated integration by parts.

In appendix 2 it is shown how the formula (27) can be alternatively obtained by matching Nth order semiclassical approximations across the singularity.

5. Essentially singular barriers with all derivatives continuous

It will obviously not be possible to give an explicit general formula for r covering all conceivable varieties of non-analyticity. Therefore attention will be restricted to potentials having a single essential singularity at $x=0$, of the type

$$V(x) = V_0(1 - \exp(-L'^n/|x|^n)) \qquad (n>0) \tag{28}$$

where L' is a scale length. Close to the singularity, $S(W)$ takes the form (using (9) and (25))

$$S(W) \approx \frac{n}{4[(E/V_0)-1]} \left(\frac{L' p_0}{\hbar} \right)^n \exp[-(L' p_0/\hbar |W|)^n] \frac{\operatorname{sgn}(W)}{|W|^{n+1}}. \tag{29}$$

This vanishes as $\hbar \to 0$ so that (just as for potentials with a discontinuous derivative) the semiclassical reflection coefficient arises from the first integral in the series (10).

After the elementary change of variable $s \equiv (L' p_0/\hbar)^{n^2/(n+1)} W^{-n}$, r becomes

$$r \approx \frac{-\mathrm{i}(L' p_0/\hbar)^{n/(n+1)}}{2[(E/V_0)-1]} \operatorname{Im} \int_0^\infty \mathrm{d}s \exp\left[\left(\frac{L' p_0}{\hbar} \right)^{n/(n+1)} \left(-s + \frac{2\mathrm{i}}{s^{1/n}} \right) \right]. \tag{30}$$

The integral is dominated by an isolated stationary point of the exponent, at $s = s^*$, where

$$s^* = \left(\frac{2}{n} \right)^{n/(1+n)} \exp\left(\frac{-\mathrm{i}\pi n}{2(n+1)} \right) \tag{31a}$$

i.e.

$$W^* = \left(\frac{L' p_0}{\hbar}\right)^{n/(n+1)} \left(\frac{n}{2}\right)^{1/(n+1)} \exp\left(\frac{\mathrm{i}\pi}{2(n+1)}\right) \tag{31b}$$

or from (25)

$$x^* = L' \left(\frac{\hbar}{p_0 L'}\right)^{1/(n+1)} \left(\frac{n}{2}\right)^{1/(n+1)} \exp\left(\frac{\mathrm{i}\pi}{2(n+1)}\right). \tag{31c}$$

This lies in the upper half-plane of W and approaches the origin in the x plane as $\hbar \to 0$. The method of steepest descent now gives the semiclassical reflection coefficient as

$$\begin{aligned} r \approx \frac{-\mathrm{i}n}{2[(E/V_0)-1]} \left(\frac{\pi}{n+1}\right)^{1/2} \left(\frac{2}{n}\right)^{(n+1/2)/(n+1)} \left(\frac{L' p_0}{\hbar}\right)^{n/2(n+1)} \\ \times \exp\left[-\left(\frac{L' p_0}{\hbar}\right)^{n/(n+1)} \left(2+\frac{2}{n}\right)\left(\frac{n}{2}\right)^{1/(n+1)} \cos\left(\frac{\pi n}{2(n+1)}\right)\right] \\ \times \sin\left[\left(\frac{L' p_0}{\hbar}\right)^{n/(n+1)} \left(2+\frac{2}{n}\right)\left(\frac{n}{2}\right)^{1/(n+1)} \sin\left(\frac{\pi n}{2(n+1)}\right) - \frac{\pi}{4(n+1)}\right]. \end{aligned} \tag{32}$$

When $n=1$ this formula may alternatively be derived by evaluating (30) exactly in terms of a modified Bessel function.

Two things are evident from the formula (32). Firstly, the reflection is indeed transcendentally small as $\hbar \to 0$ but nevertheless greater than the reflection ((20) and (18)) from an analytic barrier. Secondly, as E and hence p_0 vary, r oscillates and repeatedly vanishes. These zeros can be thought of as coming from destructive interference between waves reflected by the 'shoulders' where $V(x)$ descends from its flat top, or, mathematically, between contributions from the stationary point W^* in (31) and a similar one symmetrically disposed about the imaginary W axis.

6. Numerical illustrations and discussion

It is instructive to compare reflection coefficients for four barriers with different continuity properties, all constructed so as to have height V_0 (i.e. $V(0)=V_0$) and thickness scale L (i.e. $V(L)=V_0/\mathrm{e}$). In each case $|r|^2$ will be computed from the foregoing formulae for energy $E=2V_0$ and expressed in terms of a parameter K, which is semiclassically large, defined as

$$K \equiv p_0 L/\hbar. \tag{33}$$

K is 2π times the number of de Broglie wavelengths (at the barrier top) in the barrier thickness L.

The first barrier $V_a(x)$ is analytic:

$$V_a(x) \equiv V_0 \exp(-x^2/L^2). \tag{34}$$

From (21), its reflection is

$$|r_a|^2 = \exp\left(-K \times 4(\ln 2)^{1/2} \int_0^1 \mathrm{d}t (2-2^{t^2})^{1/2}\right) = \exp(-2.7234K). \tag{35}$$

The second and third barriers $V_1(x)$ and $V_3(x)$ have discontinuous first and third derivatives respectively:

$$V_1(x) \equiv V_0 \exp(-|x|/L) \qquad V_3(x) \equiv V_0 \exp(-|x|^3/L^3). \tag{36}$$

From (27), these produce reflections

$$|r_1|^2 = 1/16K^2 \qquad |r_3|^2 = 9/64K^6. \tag{37}$$

The fourth barrier $V_e(x)$ has an essential singularity of the type (28) with $n = 1$ and L' chosen to make $V_e(L) = 1/e$:

$$V_e(x) = V_0\left(1 - \exp\left(\frac{-\alpha L}{|x|}\right)\right) \qquad \alpha = \ln[(1-e^{-1})^{-1}] = 0.458675.$$

From (32), its reflection is

$$|r_e|^2 = \tfrac{1}{2}\pi\,(\tfrac{1}{2}K\alpha)^{1/2} \exp[-4(K\alpha)^{1/2}] \sin^2(2(K\alpha)^{1/2} - \tfrac{1}{8}\pi). \tag{38}$$

Graphs of these four potentials are shown in figure 2. Note the large magnifications necessary to reveal the different behaviours at the maximum, especially the fact that V_e is flatter than V_a and V_3, and also the fact that V_e plunges rapidly downwards from a shoulder at $x \sim 0.04L$.

The corresponding reflection coefficients are shown in figure 3 as functions of the semiclassical parameter. Note that it was necessary to plot $-\lg|\lg|r|^2|$ against $\lg K$ in order to accommodate the large variations in $|r|^2$ required to display the limiting asymptotics, for which $|r_1|^2 > |r_3|^2 > |r_e|^2 > |r_a|^2$. The limiting forms are clearly attained

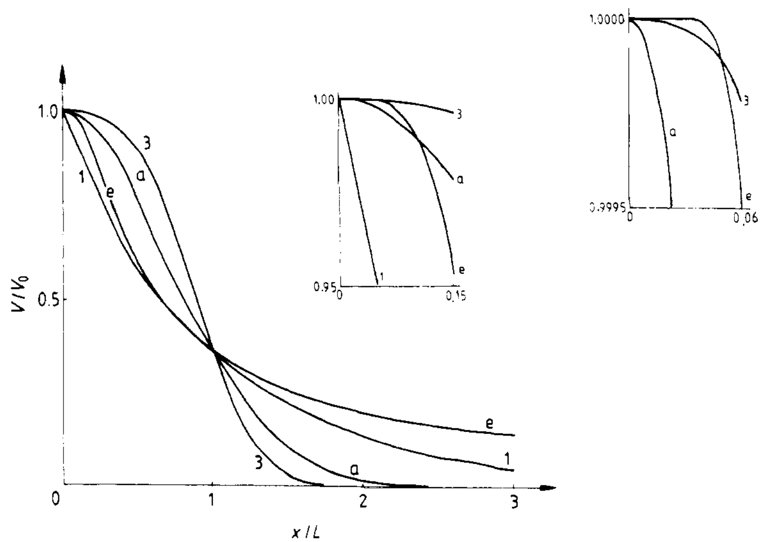

Figure 2. Four barrier potentials with different continuity properties. a, analytic potential $V_a(x)$; 1, potential $V_1(x)$ with first derivative discontinuous; 3, potential $V_3(x)$ with third derivative discontinuous; e, essentially singular potential $V_e(x)$ with all derivatives continuous.

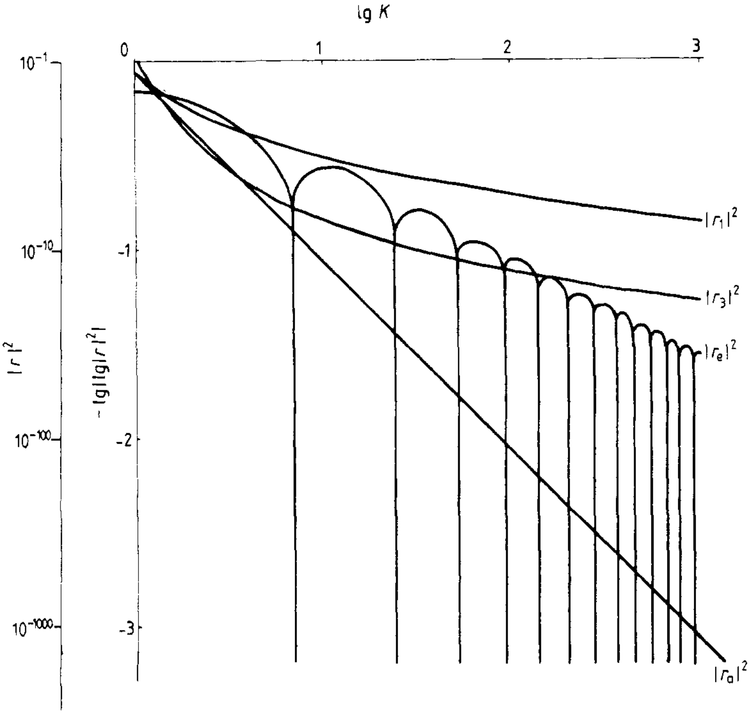

Figure 3. Graph of reflection coefficients for $E = 2V_0$ as a function of the semiclassical parameter K, for the four potentials depicted in figure 2.

only when $\lg K \sim 3$, i.e. $K \sim 1000$ and $|r_a|^2 \sim 10^{-1000}$. The curve for $|r_e|^2$ crosses that for $|r_3|^2$ when $\lg K \sim 2.2$; this corresponds to a de Broglie wavelength $2\pi L/K \sim 0.4L$, which is just where the shoulder in V_e occurs (figure 2).

Of these four asymptotic reflection coefficients, only $|r_e|^2$ has zeros as K (or E) varies. However, it is easy to devise cases where potentials which do not possess essential singularities can produce asymptotically perfect transmission as the result of reflections interfering destructively. Such behaviour can arise, for example, if $V(x)$ has two Nth order discontinuities, or is analytic with two complex turning points having the same values of Im W^* (e.g. $V(x) = V_0 \exp(-x^4/L^4)$). The following question naturally arises: are these zeros, predicted by the asymptotic formulae, approximations to zeros of the exact reflection coefficient, or do they correspond to reflection minima at which $|r|^2$ attains some higher order of semiclassical smallness without actually vanishing? The answer, which I do not know, must surely involve the fact that r is an analytic function of E (or $\hbar$) which even for symmetric potentials has a complicated phase structure on the real axis (see e.g. BM). This suggests that the zeros might move off the real E or $\hbar$ axis under the perturbation from approximation to exactness. On the other hand, the rectangular barrier does have exact transmission resonances.

Finally, it is worth pointing out that the calculation of the exceedingly small reflection coefficients in figure 3 was possible only by means of asymptotic formulae; it is a challenge to numerical analysts to produce comparable curves by 'exact' computation based directly on Schrödinger's equation.

Acknowledgments

Dr J H Hannay provided several crucial steps in the argument contained in appendix 1. This research was not supported by any military agency.

Appendix 1. Evaluation of multiple-reflection integrals

A first step in simplifying (17) is to write

$$\frac{1}{\xi_n - \mathrm{i}\varepsilon} = \mathrm{i}\int_0^\infty \mathrm{d}s_n \exp[-\mathrm{i}s_n(\xi_n - \mathrm{i}\varepsilon)] \qquad \frac{1}{\eta_n - \mathrm{i}\varepsilon} = \mathrm{i}\int_0^\infty \mathrm{d}t_n \exp[-\mathrm{i}t_n(\eta_n - \mathrm{i}\varepsilon)] \tag{A1}$$

in which the ε ensure convergence at $s_n \to \infty$ and $t_n \to \infty$. The ξ_n and η_n integrations may be performed successively, starting with ξ_n, to give

$$I_m = \frac{1}{2\pi}\int_{-\infty}^\infty \mathrm{d}\xi_0 \int_0^\infty \mathrm{d}s_0 \prod_{n=1}^\infty \int_0^\infty \mathrm{d}s_n \int_0^\infty \mathrm{d}t_n \left[\left(1 - \sum_{j=1}^n s_j - \sum_{j=1}^{n-1} t_j\right)\left(\sum_{j=1}^n (s_j + t_j)\right)\right]^{-1}$$
$$\times \exp\left[-\mathrm{i}\xi_0\left(s_0 - 1 + \sum_{n=1}^m (s_n + t_n)\right)\right]. \tag{A2}$$

Integrating over ξ_0 gives a delta function in s_0 provided $s_0 > 0$ and this restricts the range of the subsequent s and t integrations to the unit m-dimensional simplex. A slight change of notation now gives

$$I_m = \int \mathrm{d}x_1 \ldots \int \mathrm{d}x_{2m} \left[\prod_{n=1}^m \left(\sum_{j=1}^{2n} x_j\right)\left(1 - \sum_{j=1}^{2n-1} x_j\right)\right]^{-1} \tag{A3}$$

with

$$\sum_1^{2m} x_n \leq 1 \qquad x_n \geq 0.$$

The domain of integration, written explicitly, is

$$\int_0^1 \mathrm{d}x_1 \int_0^{1-x_1} \mathrm{d}x_2 \int_0^{1-x_1-x_2} \mathrm{d}x_3 \ldots \int_0^{1-x_1 \ldots x_{2m-1}} \mathrm{d}x_{2m} \tag{A4}$$

and this suggests changing variables to $\zeta_1 \ldots \zeta_{2m}$ defined by

$$x_j \equiv \zeta_{j-1} - \zeta_j \qquad (\zeta_0 \equiv 1). \tag{A5}$$

Thus (A3) becomes

$$I_m = \int_0^1 \mathrm{d}\zeta_1 \int_0^{\zeta_1} \mathrm{d}\zeta_2 \ldots \int_0^{\zeta_{2m-1}} \mathrm{d}\zeta_{2m} \left(\prod_{n=1}^m (1 - \zeta_{2n})\zeta_{2n-1}\right)^{-1}. \tag{A6}$$

The final substitution

$$\zeta_j \equiv \exp\left(-\sum_{n=1}^j y_n\right) \tag{A7}$$

gives

$$I_m = \int_0^\infty \mathrm{d}y_1 \ldots \int_0^\infty \mathrm{d}y_{2m} \left[\prod_{n=1}^m \left(\exp\left(\sum_{j=1}^{2n} y_j\right) - 1\right)\right]^{-1}. \tag{A8}$$

Expansion of the m factors using

$$\frac{1}{e^z-1}=\sum_{k=1}^{\infty} e^{-kz} \tag{A9}$$

enables the integrals to be evaluated and leads to

$$I_m=\sum_{k_1=1}^{\infty}\ldots\sum_{k_m=1}^{\infty}[k_1^2(k_1+k_2)^2\ldots(k_1+\ldots+k_m)^2]^{-1} \tag{A10}$$

which can be written

$$I_m=\sum_{0<n_1<n_2\ldots<n_m<\infty}\ldots\sum\left(\prod_{j=1}^{m}n_j^2\right)^{-1}. \tag{A11}$$

But this is

$$\begin{aligned} I_m &= \text{coefficient of } x^{2m} \text{ in } \prod_{n=1}^{\infty}\left(1+\frac{x^2}{n^2}\right) \\ &= \text{coefficient of } x^{2m} \text{ in } (\sinh \pi x)/\pi x \\ &= \pi^{2m}/(2m+1)! \end{aligned} \tag{A12}$$

Appendix 2. *N*th order semiclassical wave matching

In the case considered in § 4, where the Nth derivative of $V(x)$ is discontinuous at $x=0$, let the exact wavefunction for $x \gtrless 0$ be represented as

$$\begin{aligned} \psi &= \exp\left(\frac{i}{\hbar}\int_0^x P_+(x')\,dx'\right)+r\exp\left(\frac{-i}{\hbar}\int_0^x P_-(x')\,dx'\right) \qquad (x<0) \\ \psi &= t\exp\left(\frac{i}{\hbar}\int_0^x P_+(x')\,dx'\right) \qquad (x>0). \end{aligned} \tag{A13}$$

From the Schrödinger equation (2), $P_\pm(x)$ satisfy

$$(P_\pm(x))^2=p^2(x)\pm i\hbar\, dP_\pm(x)/dx. \tag{A14}$$

Matching ψ and $d\psi/dx$ at $x=0$ gives

$$r=-\frac{(P_+(+\varepsilon)-P_+(-\varepsilon))}{(P_-(+\varepsilon)+P_+(+\varepsilon))}. \tag{A15}$$

To lowest order in $\hbar$,

$$P_\pm(\pm\varepsilon)\approx p_0 \tag{A16}$$

and (A15) gives $r\approx 0$. But (A14) shows that successive higher-order approximations in $\hbar$ involve successive derivatives of $p(x)$, so that the problem now is to approximate the function P_+ to the lowest order in which it involves the Nth derivative of $p(x)$. To this end, write

$$P_+(x)=\sum_{j=0}^{\infty}\hbar^j P_j(x) \tag{A17}$$

where the terms P_j satisfy the following recursion relation obtained from (A14):

$$P_j(x)=\frac{\mathrm{i}}{2p(x)}\frac{\mathrm{d}P_{j-1}(x)}{\mathrm{d}x}-\frac{1}{2p(x)}\sum_{k=1}^{j-1}P_k(x)P_{j-k}(x). \tag{A18}$$

Therefore, using the notation (24),

$$P_j(x)=(\mathrm{i}/2p(x))^j p_j(x)+\text{lower derivatives of } p(x) \tag{A19}$$

so that to lowest order the numerator of (A15) is

$$P_+(+\varepsilon)-P_+(-\varepsilon)\approx(\mathrm{i}\hbar/2p_0)^N(p_N(+\varepsilon)-p_N(-\varepsilon)). \tag{A20}$$

Together with (A16) for the denominator of (A15) this gives precisely the formula (27) for r obtained from the first term of the multiple reflection series.

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