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Transmission probability and traversal time in scattering by a one-dimensional potential of finite range

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Abstract. Scattering by a one-dimensional potential $V = V(x)$ which is constant outside $[-a, a]$ ($a > 0$) is investigated. Exact expressions for the transmission and reflection coefficients are obtained in terms of $f_0(a)$, $f_1(a)$, $f'_0(a)$ and $f'_1(a)$, where f_0 and f_1 are the solutions in $[-a, a]$ satisfying the boundary conditions $f_0(-a) = 1$, $f'_0(-a) = 0$, $f_1(-a) = 0$ and $f'_1(-a) = 1$. These expressions are used to show that the first-order WKB approximation conserves particles. Numerical results are obtained from these expressions for the transmission and reflection probabilities by (i) using the WKB formulae and (ii) solving the time-independent Schrödinger equation numerically in $[-a, a]$. The time T for the centre of a wavepacket to traverse the interval $[-a, a]$ is also obtained in terms of $f_0(a)$, $f_1(a)$, $f'_0(a)$ and $f'_1(a)$, and some of its properties studied. In particular, it is shown that T takes the classical form in the classical limit.

1. Introduction

One-dimensional tunnelling in modern solid state devices has led to renewed interest both in the computation of tunnelling probabilities, and also in the question of the time taken for an electron to tunnel through a potential barrier. This paper is devoted to a discussion of these two problems.

The WKB method, or JWKB method, has frequently been used to calculate the tunnelling probability. The method was certainly known to Green (Farina 1976) and may be traced back even earlier (Fröman and Fröman 1965). In quantum mechanics it is often used to calculate the tunnelling coefficient τ for a one-dimensional potential barrier, which is important for applications in solid state physics, for example.

With the advent of modern computers it is now easy to calculate τ directly by numerical means (see, for example, the VL method, described in Vignerón and Lambin (1980), Lambin and Vignerón (1981) and Nguyen *et al* (1985)). We shall present a method here which, like the VL method, provides a direct numerical technique for evaluation of the tunnelling probability. However, in addition to this, it also checks the numerical accuracy by means of the Wronskian and the conservation of particles and provides a general expression for the time T taken for the centre of a wavepacket to cross the barrier. In fact, our result is valid for any piecewise continuous potential V which is constant outside some finite interval $[-a, a]$, and not just for tunnelling through a rectangular barrier, which is a special case.

In § 2 we derive expressions for the transmission and reflection coefficients in terms of the values of real functions f_0 and f_1 (defined by boundary conditions at $x = -a$) evaluated at the point $x = a$. It is then shown that particles are conserved if f_0 and f_1

are exact solutions of the time-independent Schrödinger equation in $(-a, a)$. A quantity ε is defined which measures the extent to which particle conservation is violated if approximate solutions are used for f_0 and f_1 .

In § 3 we describe the zero- and first-order wKB approximations and prove that the first-order wKB approximation conserves particles. Numerical examples, including comparison with exact calculations, are described in § 4. In the remaining sections the method is used to analyse the time taken for the centre of the wavepacket (as defined by the stationary phase approximation) to cross the interval $[-a, a]$. In particular, we show that this takes the expected form in the classical limit (§ 7), while the special case of the rectangular barrier is considered in § 8.

2. The general result

We consider the one-dimensional problem (in standard notation)

$$-\frac{\hbar^2}{2m} \psi'' + V\psi = E\psi \quad (2.1)$$

where the potential V is constant for $x < -a$ or $x > a$ ($a > 0$). Without loss of generality we can take $V = 0$ when $x < -a$; we put $V = V_0$ when $x > a$. It will be assumed that $E > 0$ and $E > V_0$, so that transmission is possible.

Equation (2.1) can be written

$$\psi'' + k^2\psi = U\psi \quad (2.2)$$

where

$$U = 2mV/\hbar^2 \quad k = (2mE/\hbar^2)^{1/2}. \quad (2.3)$$

Assuming that the particle is incident from the left

$$\psi(x) = \begin{cases} \exp(ikx) + \rho \exp(-ikx) & x < -a \\ \tau \exp(iqx) & x > a \end{cases} \quad (2.4)$$

where ρ and τ are the reflection and transmission coefficients, respectively, and the positive wavenumber q is defined by the energy conservation condition

$$\hbar^2 k^2/2m = E = \hbar^2 q^2/2m + V_0. \quad (2.5)$$

Let f_0 and f_1 be two continuously differentiable functions in $[-a, a]$ (not necessarily solutions of (2.2)) which satisfy the boundary conditions

$$f_0(-a) = 1 \quad f_0'(-a) = 0 \quad f_1(-a) = 0 \quad f_1'(-a) = 1. \quad (2.6)$$

Define a function ψ on $[-a, a]$ by

$$\psi(x) = \alpha_0 f_0(x) + \alpha_1 f_1(x). \quad (2.7)$$

α_0 and α_1 are constants which will be complex in general. Again ψ may not necessarily satisfy (2.2).

The continuity conditions on ψ and ψ' at $x = \pm a$ are easily written down using (2.4), (2.6) and (2.7); they are

$$\begin{aligned} \exp(-ika) + \rho \exp(ika) &= \alpha_0 \\ ik \exp(-ika) - ik\rho \exp(ika) &= \alpha_1 \\ \tau \exp(iqa) &= \alpha_0 f_0(a) + \alpha_1 f_1(a) \\ iq\tau \exp(iqa) &= \alpha_0 f_0'(a) + \alpha_1 f_1'(a). \end{aligned} \quad (2.8)$$

Equations (2.8) are easily solved algebraically for ρ and τ ; we get

$$\tau = 2ik \exp[-i(k+q)a] W(a) \Delta^{-1} \quad (2.9)$$

$$\rho = \exp(-2ika) \{ [kqf_1(a) + f'_0(a)] + i[kf'_1(a) - qf_0(a)] \} \Delta^{-1} \quad (2.10)$$

where

$$\Delta = kqf_1(a) - f'_0(a) + i[kf'_1(a) + qf_0(a)] \quad (2.11)$$

and the Wronskian $W(x)$ is defined by

$$W(x) = f_0(x)f'_1(x) - f'_0(x)f_1(x). \quad (2.12)$$

If $f_0(a)$, $f'_0(a)$, $f_1(a)$ and $f'_1(a)$ are computed by solving (2.2) *exactly* for f_0 and f_1 , subject to the boundary conditions (2.6), and τ and ρ are obtained from (2.9)-(2.12), then τ and ρ will be the *exact* transmission and reflection coefficients, respectively.

The condition for the conservation of particles is $k|\rho|^2 + q|\tau|^2 = k$, so if we put

$$\varepsilon = k^{-1}(k|\rho|^2 + q|\tau|^2) - 1 \quad (2.13)$$

ε is a measure of the extent to which conservation of particles is violated. Equations (2.9)-(2.13) yield

$$\varepsilon = 4kqW(a)[W(a) - 1]|\Delta|^{-2}. \quad (2.14)$$

Suppose now that f_0 and f_1 are indeed exact solutions of (2.2) in $[-a, a]$. If V is piecewise continuous in $[-a, a]$ the Wronskian is constant and then $W(a) = W(-a) = 1$, so by (2.14) $\varepsilon = 0$ and particles are conserved.

If, on the other hand, f_0 and f_1 , while satisfying (2.6), are only approximate solutions of (2.2) in $[-a, a]$, then $W(-a) = 1$ but $W(a)$ may differ from unity and ε may not vanish. ε becomes *an indicator of the accuracy of the approximation* for f_0 and f_1 .

3. Application to the wkb approximation

Define $\kappa = \kappa(x)$ by

$$\kappa(x) = \begin{cases} [U(x) - k^2]^{1/2} & \text{if } U(x) \geq k^2 \\ i[k^2 - U(x)]^{1/2} & \text{if } U(x) \leq k^2. \end{cases} \quad (3.1)$$

The differential equation (2.2) can now be written

$$\psi'' - \kappa^2 \psi = 0. \quad (3.2)$$

The basis of the wkb method is to make the substitution

$$\psi(x) = A \exp[iS(x)/\hbar] \quad (3.3)$$

where A is a (possibly complex) constant and S is a complex-valued function of x . If we substitute for ψ from (3.3) into (3.2) we obtain

$$i\hbar S'' - S'^2 - \hbar^2 \kappa^2 = 0. \quad (3.4)$$

Put $[p(x)]^2 = -\hbar^2[\kappa(x)]^2$; if $p(x)$ is real (that is, $k^2 \geq U(x)$) it is the classical momentum. Equation (3.4) can be written

$$i\hbar S'' - S'^2 + p^2 = 0. \quad (3.5)$$

Equation (3.5) is solved by expanding S in powers of \hbar (the details may be found in Schiff (1955, pp 185-7)). The results are:

$$\text{zero order: } \psi(x) = A \exp[\pm\beta(x)] \quad (3.6)$$

where

$$\beta(x) = \int_{-a}^x \kappa(y) dy \quad (3.7)$$

$$\text{first order: } \psi(x) = A[\kappa(x)]^{-1/2} \exp[\pm\beta(x)]. \quad (3.8)$$

It follows from these results that the zeroth-order wkb approximations to f_0 and f_1 are

$$f_0(x) = \cosh \beta(x) \quad f_1(x) = [\kappa(-a)]^{-1} \sinh \beta(x). \quad (3.9)$$

These are approximate solutions of (2.2) which satisfy the boundary conditions (2.6) exactly. The first-order approximations are

$$f_0(x) = A_0[\kappa(x)]^{-1/2} \cosh \beta(x) + \hat{B}_0[\kappa(x)]^{-1/2} \sinh \beta(x) \quad (3.10a)$$

$$f_1(x) = A_1[\kappa(x)]^{-1/2} \cosh \beta(x) + B_1[\kappa(x)]^{-1/2} \sinh \beta(x). \quad (3.10b)$$

The constants A_0 , B_0 , A_1 and B_1 are determined by the boundary conditions (2.6); in fact

$$A_0 = [\kappa(-a)]^{-1/2} \quad B_0 = \frac{1}{2}[\kappa(-a)]^{-3/2} \kappa'(-a) \quad (3.11a)$$

$$A_1 = 0 \quad B_1 = [\kappa(-a)]^{-1/2}. \quad (3.11b)$$

It is easy to check that these approximations to f_0 and f_1 , whether given by (3.9), or by (3.10) and (3.11), are real.

The neglect of $i\hbar S''$ in (3.4) is justified if

$$\hbar |S''(x)| \ll \hbar^2 \kappa^2. \quad (3.12)$$

The zeroth-order approximation for S is

$$S(x) = \pm i \hbar \beta(x). \quad (3.13)$$

If the approximation is consistent (3.13) should satisfy (3.12), i.e.

$$|\kappa'(x)| \ll [\kappa(x)]^2. \quad (3.14)$$

In other words, κ must be slowly varying.

In fact, (3.14) is necessary but not sufficient. For, if a is large, $\kappa(x)$ may vary significantly from $\kappa(-a)$ for values of x in $[-a, a]$. Comparison of (3.6) with (3.8) then shows that the first-order wkb approximation for $\psi(x)$ is significantly different from the zeroth-order approximation.

If we use the zeroth-order approximation for f_0 and f_1 , (2.12) gives

$$W(a) = \kappa(a)/\kappa(-a). \quad (3.15)$$

If $\kappa(a)$ is significantly different from $\kappa(-a)$, $W(a)$ becomes significantly different from unity and conservation of particles will be violated.

We can also evaluate ε , a measure of the extent to which particle conservation is violated. Substituting (3.9) into (2.11) gives

$$\Delta = \frac{kq - \kappa(a)\kappa(-a)}{\kappa(-a)} \sinh \beta(a) + i \frac{k\kappa(a) + q\kappa(-a)}{\kappa(-a)} \cosh \beta(a). \quad (3.16)$$

Substituting for $|\Delta|$ and $W(a)$ from (3.16) and (3.15) into (2.14)

$$\varepsilon = \frac{4kq\kappa(a)[\kappa(a) - \kappa(-a)]}{[kq - \kappa(a)\kappa(-a)]^2 \sinh^2 \beta(a) + [k\kappa(a) + q\kappa(-a)]^2 \cosh^2 \beta(a)}. \quad (3.17)$$

In the case of tunnelling β is a real, positive and increasing function of x and (3.17) shows that ε will, in general, be small due to the size of $\beta(a)$. However, if $\beta(a) \approx 0$, (3.17) becomes

$$\varepsilon \approx \frac{4kq\kappa(a)[\kappa(a) - \kappa(-a)]}{[k\kappa(a) + q\kappa(-a)]^2}$$

and if $\kappa(a)$ is significantly different from $\kappa(-a)$, ε may be significant.

Now consider the first-order approximation given by (3.10) and (3.11). If $W(x)$ is computed from these expressions (see the appendix) we find $W(x) \equiv 1$. It follows from (2.14) that $\varepsilon = 0$. This means that *the first-order WKB approximation conserves particles*.

4. Numerical examples

If f_0 is known f_1 may be obtained from the textbook formula

$$f_1(x) = f_0(x) \int_{-a}^x \frac{dx}{[f_0(x)]^2} \quad (4.1)$$

which is easily deduced from the constancy of the Wronskian. If we take

$$f_0(x) = 1 + h_i^2(x+a)^2 \quad (4.2)$$

where h_i is a positive constant then f_0 satisfies (2.6). It will satisfy (2.2) if

$$U = k^2 + \frac{2h_i^2}{1 + h_i^2(x+a)^2}. \quad (4.3)$$

f_1 , as calculated from (4.1), satisfies (2.2) and (2.6) also. Substitution of (4.2) into (4.1) gives

$$f_1(x) = \frac{1}{2} h_i^{-1} [1 + h_i^2(x+a)^2] \left(\tan^{-1} h_i(x+a) + \frac{h_i(x+a)}{1 + h_i^2(x+a)^2} \right). \quad (4.4)$$

The values of $|\tau|^2$, $|\rho|^2$, W and ε were obtained from (2.9)–(2.12) and (2.14). For the exact values (4.2) and (4.4) were used to find $f_0(a)$, $f_0'(a)$, $f_1(a)$ and $f_1'(a)$. $|\tau|^2$ and $|\rho|^2$ were also calculated in zero-order and first-order WKB using the formulae of § 3, with U given by (4.3). Finally they were calculated by numerically solving the differential equation (2.2) for f_0 and f_1 subject to (2.6); the numerical method used was the Taylor series method of order 4. We have called the last method the DE method—short for ‘differential equation’ method.

If U is given by (4.3), (3.1) yields

$$[\kappa(x)]^2 = \frac{2h_i^2}{1+h_i^2(x+a)^2} \tag{4.5}$$

from which we easily deduce that

$$\frac{\kappa'(x)}{[\kappa(x)]^2} = -\frac{h_i(x+a)}{\sqrt{2}[1+h_i^2(x+a)^2]^{1/2}} \tag{4.6}$$

and

$$\frac{|\kappa(x) - \kappa(-a)|}{\kappa(-a)} = 1 - [1+h_i^2(x+a)^2]^{-1/2}. \tag{4.7}$$

Our discussion in the previous section suggests that, if the quantities defined by (4.6) and (4.7) are very much less than unity, the wkb approximation should be good, but if they are comparable to, or greater than, unity then the wkb approximation may not do so well. If $a = 1$ and $h_i = 0.1$ the right-hand sides of (4.6) and (4.7) are both very much less than unity for $-a \leq x \leq a$, but if $a = 1$ and $h_i = 1$ the right-hand sides are no longer numerically small compared with unity. We therefore expect the wkb approximation to do well in the first case, but not in the second.

The results are shown in tables 1 and 2. In both cases we have taken $a = k = q = 1$, so that by (2.5) $V_0 = 0$. In table 1 $h_i = 1$, which, as we have seen, represents a situation in which the wkb method might not do so well. In table 2 $h_i = 0.1$, when the wkb approximation is expected to do better. In both cases $h = 0.01$, where h is the step length used both in the numerical evaluation of the integral (3.7) which occurs in the wkb approximation and also in the solution of the differential equation (the DE method).

The first columns in tables 1 and 2 are the results of the exact calculation where f_0 and f_1 are given by (4.2) and (4.4). It is 'exact' in the sense that, with the potential (4.3), f_0 and f_1 satisfy the differential equation (2.2) identically. The very small

Table 1. U given by (4.3), $a = k = q = h_i = 1$, $h = 0.01$.

	Exact calculation	Zero-order wkb	First-order wkb	DE method
$ \rho ^2$	$9.407\ 658\ 09 \times 10^{-1}$	$9.444\ 534\ 05 \times 10^{-1}$	$9.538\ 149\ 83 \times 10^{-1}$	$9.408\ 019\ 05 \times 10^{-1}$
$ \tau ^2$	$5.923\ 419\ 10 \times 10^{-2}$	$2.484\ 120\ 82 \times 10^{-2}$	$4.618\ 504\ 62 \times 10^{-2}$	$5.920\ 085\ 30 \times 10^{-2}$
W	$9.999\ 999\ 96 \times 10^{-1}$	$4.472\ 138\ 83 \times 10^{-1}$	1.000 000 64	1.000 046 58
ε	$-2.206\ 645\ 58 \times 10^{-10}$	$-3.070\ 538\ 64 \times 10^{-2}$	$2.959\ 304\ 62 \times 10^{-8}$	$2.757\ 508\ 25 \times 10^{-6}$

Table 2. U given by (4.3), $a = k = q = 1$, $h_i = 0.1$, $h = 0.01$.

	Exact calculation	Zero-order wkb	First-order wkb	DE method
$ \rho ^2$	$5.163\ 383\ 59 \times 10^{-1}$	$5.179\ 068\ 70 \times 10^{-1}$	$5.203\ 085\ 77 \times 10^{-1}$	$5.163\ 379\ 35 \times 10^{-1}$
$ \tau ^2$	$4.836\ 616\ 41 \times 10^{-1}$	$4.727\ 312\ 04 \times 10^{-1}$	$4.796\ 914\ 23 \times 10^{-1}$	$4.836\ 620\ 80 \times 10^{-1}$
W	1.000 000 00	$9.805\ 806\ 70 \times 10^{-1}$	1.000 000 00	1.000 000 03
ε	$-1.126\ 112\ 51 \times 10^{-10}$	$-9.361\ 925\ 78 \times 10^{-3}$	$-1.116\ 868\ 63 \times 10^{-10}$	$1.486\ 469\ 82 \times 10^{-8}$

departures of W and ε from their theoretical values of unity and zero arise only from limitations on the accuracy with which f_0, f_1, f'_0 and f'_1 can be calculated from their algebraic definitions.

As we would expect, the result for the transmission probability $|\tau|^2$ is close to the exact result even in zero-order wKB when $h_t = 0.1$, but is not so good when $h_t = 1$. The DE method, however, gives good accuracy for both reflection and transmission probabilities—the accuracy being limited only by the finite step length h .

In zero-order wKB both W and ε differ significantly from their exact values. In the case of W this is particularly so if $h_t = 1$; both W and ε improve when $h_t = 0.1$, as we should expect. In first-order wKB the values of W and ε are better than those obtained from the DE method. This, of course, is not surprising given the result proved in the last section that the first-order wKB approximation conserves particles. The differences of W and ε from their theoretical values of unity and zero arise only from the numerical integration procedure used.

The calculation was also performed with the linear potential

$$U(x) = U_0 + h_t x \tag{4.8}$$

in zero-order and first-order wKB and the DE method. The results are shown in tables 3 and 4.

The two potentials in tables 3 and 4 differ only in the value of h_t ; in table 3 $h_t = 1$ and in table 4 $h_t = 0.1$. Again the above criteria imply that we expect the wKB approximation to do better when $h_t = 0.1$; for

$$[\kappa(x)]^2 = U_0 + h_t x - k^2$$

so, using $U_0 = 3$ and $k = 1 = a$,

$$\frac{\kappa'}{\kappa^2} = \frac{\kappa \kappa'}{\kappa^3} = \frac{h_t}{2(U_0 + h_t x - k^2)^{3/2}} = \frac{h_t}{2(2 + h_t x)^{3/2}} \tag{4.9}$$

Table 3. U given by (4.8), $a = k = q = h_t = 1$, $U_0 = 3$, $h = 0.01$.

	Zero-order wKB	First-order wKB	DE method
$ \rho ^2$	$9.872\ 068\ 03 \times 10^{-1}$	$9.892\ 484\ 80 \times 10^{-1}$	$9.872\ 276\ 54 \times 10^{-1}$
$ \tau ^2$	$2.215\ 851\ 63 \times 10^{-2}$	$1.075\ 154\ 44 \times 10^{-2}$	$1.277\ 234\ 15 \times 10^{-2}$
W	1.732 054 74	1.000 002 26	$9.999\ 997\ 32 \times 10^{-1}$
ε	$9.365\ 320\ 00 \times 10^{-3}$	$2.435\ 194\ 03 \times 10^{-8}$	$-3.425\ 809\ 87 \times 10^{-9}$

Table 4. U given by (4.8), $a = k = q = 1$, $h_t = 0.1$, $U_0 = 3$, $h = 0.01$.

	Zero-order wKB	First-order wKB	DE method
$ \rho ^2$	$9.876\ 405\ 37 \times 10^{-1}$	$9.876\ 570\ 42 \times 10^{-1}$	$9.876\ 418\ 46 \times 10^{-1}$
$ \tau ^2$	$1.299\ 369\ 79 \times 10^{-2}$	$1.234\ 296\ 81 \times 10^{-2}$	$1.235\ 815\ 07 \times 10^{-2}$
W	1.051 315 81	1.000 000 83	$9.999\ 997\ 02 \times 10^{-1}$
ε	$6.342\ 358\ 60 \times 10^{-4}$	$1.029\ 976\ 66 \times 10^{-8}$	$-3.683\ 017\ 00 \times 10^{-9}$

while

$$\frac{\kappa(x) - \kappa(-a)}{\kappa(-a)} = \left(\frac{U_0 + h_r x - k^2}{U_0 - h_r a - k^2} \right)^{1/2} - 1 = \left(\frac{2 + h_r x}{2 - h_r} \right)^{1/2} - 1. \quad (4.10)$$

If the right-hand sides of (4.9) and (4.10) are very much less than unity for $x \in [-a, a] = [-1, 1]$ the wkb approximation should do well; this is the case if $h_r = 0.1$.

The above remarks are confirmed by the figures, the wkb approximation doing much better when $h_r = 0.1$ (table 4) than when $h_r = 1$ (table 3). Recalling that, in first-order wkb, $W = 1$ and $\varepsilon = 0$ the nearness of W to unity and ε to zero in the second and third columns gives a check on the numerical accuracy attained.

5. Tunnelling time

The meaning to be attached to the term 'tunnelling time' is complicated and context dependent. It may be the time a particle spends on average inside $[-a, a]$ (the 'dwell' time), or the time taken for the transmitted particle to traverse the interval ('traversal' time), or the time for a signal to be transmitted ('signal' time) (see Büttiker and Landauer 1982, Büttiker 1983, Stevens 1983). In this paper we shall consider it as the difference between the time, t_1 , when the centre of the incident wavepacket reaches the point $x = -a$ and the time, t_2 , when the centre of the transmitted wavepacket appears at $x = a$. We shall follow the heuristic method of stationary phase used by Eisenbud and Wigner in their pioneering work (Wigner 1955) and which has become standard textbook material (see, for example, Mavromatis 1987, p 79).

We shall find an expression for

$$T = t_2 - t_1 \quad (5.1)$$

in terms of $f_0(a)$, $f_1(a)$, $f'_0(a)$ and $f'_1(a)$. From this we shall show that the classical expression for T is given by the zero-order wkb approximation or classical approximation provided V is everywhere continuous.

We shall not assume that $k^2 > U(x)$; in fact, in going to the classical limit, we shall have to assume the opposite inequality. The term 'tunnelling time' is therefore inappropriate, so we shall call T the 'traversal time'.

6. Expression for the traversal time

The incoming wavepacket has the wavefunction $\psi_{\text{in}}(\cdot, t)$ where

$$\psi_{\text{in}}(x, t) = \int_{-\infty}^{\infty} \phi(k') \exp[ik'x - i\omega(k')t] dk' \quad (6.1)$$

$$\omega(k') = \hbar k'^2 / 2m. \quad (6.2)$$

ϕ is a normalisable complex-valued function of the real variable k' . We shall suppose that the incident wavepacket represents the state of a particle of well defined velocity $v_{\text{in}} > 0$, so that ϕ vanishes unless k' is in the neighbourhood of $k = mv_{\text{in}}/\hbar$. The method of stationary phase implies that $\psi_{\text{in}}(\cdot, t)$ is only significant in the neighbourhood of the point $x = x_{\text{in}}(t)$ where this is the solution of

$$\frac{d}{dk} \{ \arg \phi(k) + kx - \omega(k)t \} = 0. \quad (6.3)$$

Equations (6.2) and (6.3) give

$$x_{\text{in}}(t) = x_{\text{in}} + v_{\text{in}}t \quad (6.4)$$

where

$$v_{\text{in}} = \hbar k / m \quad (6.5)$$

$$x_{\text{in}} = -\frac{d}{dk} \arg \phi(k). \quad (6.6)$$

The transmitted wavepacket $\psi_{\text{tr}}(\cdot, t)$ is given by

$$\psi_{\text{tr}}(x, t) = \int_{-\infty}^{\infty} \tau(k') \phi(k') \exp[iq'x - i\omega(k')t] dk' \quad (6.7)$$

where q' is determined by the condition

$$\frac{\hbar^2 k'^2}{2m} = \frac{\hbar^2 q'^2}{2m} + V_0 \quad (6.8)$$

(cf (2.5)). In this case the stationary phase method shows that the transmitted wavepacket is centred on the point $x = x_{\text{tr}}(t)$ where

$$x_{\text{tr}}(t) = x_{\text{tr}} + v_{\text{tr}}t \quad (6.9)$$

$$v_{\text{tr}} = \hbar q / m \quad (6.10)$$

$$\frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 q^2}{2m} + V_0 \quad \text{so that} \quad \frac{dq}{dk} = \frac{k}{q} = \frac{v_{\text{in}}}{v_{\text{tr}}} \quad (6.11)$$

$$x_{\text{tr}} = -\frac{v_{\text{tr}}}{v_{\text{in}}} \left(\frac{d}{dk} \arg \tau(k) + \frac{d}{dk} \arg \phi(k) \right). \quad (6.12)$$

The centre of the incident wavepacket traverses the point $x = -a$ when $t = t_1$ where

$$x_{\text{in}} + v_{\text{in}}t_1 = -a. \quad (6.13)$$

The centre of the transmitted wavepacket emerges at the point $x = a$ when $t = t_2$ where

$$x_{\text{tr}} + v_{\text{tr}}t_2 = a. \quad (6.14)$$

It follows from (5.1) and the results of this section that

$$T = \frac{1}{v_{\text{in}}} \frac{d}{dk} \arg \tau(k) + \frac{a}{v_{\text{in}}} + \frac{a}{v_{\text{tr}}}. \quad (6.15)$$

If we put (2.9) into (6.15) we obtain

$$T = -\frac{1}{v_{\text{in}}} \frac{d}{dk} \arg \Delta. \quad (6.16)$$

Insertion of (2.11) into (6.16) yields

$$T = -\frac{1}{v} \frac{d}{dk} \tan^{-1} \frac{kf'_1(a) + qf_0(a)}{kf_1(a) - f'_0(a)} \quad (6.17)$$

where we have replaced v_{in} by $v = \hbar k / m$ for simplicity.

It should be noted that the phase involved here is that of the time-dependent wavefunction in k space; the wkb approximation involves the phase of the time-independent wavefunction in configuration space (see Messiah 1964, p 231).

7. The classical limit for the traversal time

We now examine the result in the classical limit $\hbar \rightarrow 0$ when the zero-order WKB approximation is applicable provided there are no classical turning points in $(-a, a)$. f_0 and f_1 are now given by (3.7) and (3.9), so (2.11) becomes

$$\Delta = \left(\frac{kq}{\kappa(-a)} - \kappa(a) \right) \sinh \beta(a) + i \left(\frac{k\kappa(a)}{\kappa(-a)} + q \right) \cosh \beta(a). \quad (7.1)$$

Discontinuities in the potential at $x = \pm a$ introduce non-classical phenomena, so we assume $|\kappa(-a)| = k$ and $|\kappa(a)| = q$. We also need to assume that $k^2 > U$ throughout, so that classical transmission time has a meaning. With these assumptions (7.1) gives, with the aid of (3.1) and (3.7),

$$\Delta = 2iq \exp\left(-i \int_{-a}^a [k^2 - U(x)]^{1/2} dx\right) \quad (7.2)$$

so that by (6.16)

$$T = \frac{1}{v_{\text{in}}} \frac{d}{dk} \int_{-a}^a [k^2 - U(x)]^{1/2} dx. \quad (7.3)$$

Differentiating under the integral sign we easily find from (7.3) that

$$T = \int_{-a}^a \frac{dx}{[v_{\text{in}}^2 - 2V(x)/m]^{1/2}}. \quad (7.4)$$

Equation (7.4) is just the classical expression for the transit time of a particle with incident velocity v_{in} .

8. The rectangular barrier

A particularly simple case is the rectangular barrier, when $V = V_1$, say, for $-a < x < a$, with $V_1 > \hbar^2 k^2 / 2m$. Thus $\kappa(x) = \text{constant} = \kappa$, say. The zeroth-order WKB approximation is now exact and so (3.9) and (3.7) give

$$f_0(x) = \cosh \kappa(x+a) \quad f_1(x) = \kappa^{-1} \sinh \kappa(x+a). \quad (8.1)$$

Applying (8.1), (6.17) becomes

$$T = -\frac{1}{v} \frac{d}{dk} \tan^{-1} \frac{(k+q) \kappa \cosh 2\kappa a}{(kq - \kappa^2) \sinh 2\kappa a}. \quad (8.2)$$

For a 'strong' barrier, when $2\kappa a \gg 1$, (8.2) approximates to

$$T = -\frac{1}{v} \frac{d}{dk} \tan^{-1} \frac{\kappa(k+q)}{(kq - \kappa^2)} \quad (8.3)$$

and the tunnelling time becomes independent of the barrier thickness, as pointed out by Franz (1967). However, (2.9) and (2.11) imply, in the strong barrier case, that

$$|\tau|^2 \approx \frac{4k^2 \kappa^2 \exp(-4\kappa a)}{(kq - \kappa^2)^2 + (k+q)^2 \kappa^2} \quad (8.4)$$

which is very small—although particles will cross the barrier quickly, few of them will, in fact, get through.

If the differentiation on the right-hand side of (8.3) is carried out we find

$$T = \frac{1}{\kappa v} (k/q + 1). \quad (8.5)$$

This is the same result as obtained by Franz (1967), but obtained from the general result (6.17), valid for any sufficiently well behaved potential V (such as a piecewise continuous one).

9. Discussion

We have described a method of calculating the tunnelling coefficients whose accuracy is limited only by the numerical accuracy with which the ordinary differential equation (2.2) can be solved in $(-a, a)$ for the fundamental solutions f_0 and f_1 . Conservation of particles is not built into the numerical procedure as in the v_L method referred to in § 1. Instead, it provides a check on the numerical accuracy by means of the quantity ε (see (2.13) and (2.14)). A further check is provided by the Wronskian W : if W is close to unity ε will, in general, be small. The converse may not be the case—for example, in tunnelling, if a is large (see § 8). However, the Wronskian still provides a useful check.

We have used our results to show that the first-order wKB approximation conserves particles. We have also expressed the traversal time T in terms of $f_0(a)$, $f'_0(a)$, $f_1(a)$ and $f'_1(a)$ (equation (6.17)). These last four numbers are determined by the numerical solution of (2.2) subject to the boundary conditions (2.6). We also used (6.16) to show that T takes the classical form (7.4) in the classical limit.

Finally we have applied our results to the special case of the rectangular barrier. This has confirmed Franz's expression in this case.

Appendix

We shall prove that, if f_0 and f_1 are calculated by means of the first-order wKB approximation, their Wronskian is unity. Equations (3.10) and (3.11) give

$$f_0 = A_0 u + B_0 v \quad f_1 = B_1 v$$

where

$$u = \kappa^{-1/2} \cosh \beta \quad v = \kappa^{-1/2} \sinh \beta \quad \kappa = \kappa(x) \quad \beta = \beta(x).$$

Hence by (2.12)

$$\begin{aligned} W &= (A_0 u + B_0 v)(B_1 v') - (A_0 u' + B_0 v')(B_1 v) \\ &= A_0 B_1 (u v' - u' v). \end{aligned}$$

Now it is easily checked from the definitions of u and v that

$$u v' - u' v = 1$$

and so

$$W = A_0 B_1 = [\kappa(-a)]^{1/2} [\kappa(-a)]^{-1/2} = 1.$$

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