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Transmission coefficient for one-dimensional potential barriers using continued fractions

J P Vigneron and Ph Lambin

Institut de Physique, B5, Université de Liège, B-4000 Sart Tilman/Liège 1, Belgium

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Abstract. An explicit formula is given for evaluating the transmission coefficient of one-dimensional potential barriers corresponding to localised forces. The method is based on a simple discretisation of the Schrödinger equation leading to a three-term recursion relation. A continued fraction is then introduced in a quite natural way. Examples are provided to shed some light on the efficiency of the procedure, as compared to semiclassical approximations.

1. Introduction

In many instances the tunnelling of particles through a potential barrier has been invoked to reach some degree of understanding of the transport phenomena in heterogeneous systems. α-particle decay (Gamow 1928, Gurney and Condon 1929) and field emission from metal surfaces (Fowler and Nordheim 1928) are early examples of this effect. Later, the development of metal–insulator–metal junctions (Fisher and Giaever 1961, Nicol *et al* 1960, Giaever 1960) led to the realisation of tunnel-emission electronic devices (Mead 1961) which still keep on developing today. Point-contact diodes, used as infrared detectors, rectification or frequency mixing devices, have also been recently interpreted in terms of a barrier penetration (Lucas *et al* 1977).

In most of these cases, a calculation of the transmission coefficient for a one-dimensional model potential was necessary. Unless the model was simple enough to be exactly soluble (Duke 1969, especially chap 4), the most widely used method is certainly the semiclassical WKB approach (Wentzel 1926, Kramers 1926, Brillouin 1926a, b, Langer 1937, Furry 1947). The transmission factor is often very easily written in this approximation but, in many cases, the value obtained gives only a crude idea of the real penetration coefficient. By contrast, the expression considered here can, in principle, produce a value of the transmission coefficient arbitrarily accurate, very good accuracy often being obtained with very slight computation effort. In essence, the method consists in approximating the Schrödinger equation itself by using an appropriate discretisation scheme and solving exactly this approximate problem. This is, to some extent, an alternative to the semiclassical method where approximate (i.e. asymptotic) piece-wise solutions are connected to fit as well as possible the exact Schrödinger equation.

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2. Discretisation

A previously developed example (Vigneron and Lambin 1979) shows that the following discrete form of the one-dimensional Schrödinger equation:

$$\frac{\psi(x+h)-2\psi(x)+\psi(x-h)}{h^2}=[v(x)-\epsilon]\psi(x) \tag{2.1}$$

keeps most of the properties of the original continuous form:

$$\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2}=[v(x)-\epsilon]\psi(x) \tag{2.2}$$

in the case of a periodic potential $v(x)$. The advantage of the discrete formulation is that it can be solved efficiently in many cases by means of continued fractions. The same scheme will be used here to derive an expression of the transmission coefficient in a one-dimensional barrier. In this problem, the concept of current of probability density is of prime importance. It is crucial to realise that this concept can also arise from the discrete formulation (2.1).

Consider the grid points (x_p), where p is an integer in the range $-\infty<p<+\infty$, separated by a step size $h=x_{p+1}-x_p$. The discrete equation can be put into the form

$$R_{p-1}=b_p(\epsilon)-\frac{1}{R_p} \tag{2.3}$$

where

$$R_p=\frac{\psi(x_p)}{\psi(x_{p+1})} \tag{2.4}$$

and

$$b_p(\epsilon)=2+h^2[v(x_p)-\epsilon]. \tag{2.5}$$

The current of probability for the continuous case (2.2) is defined as

$$j(x)=-\mathrm{i}\left(\psi^*(x)\frac{\mathrm{d}\psi}{\mathrm{d}x}-\psi(x)\frac{\mathrm{d}\psi^*}{\mathrm{d}x}\right). \tag{2.6}$$

For any steady state, $j(x)$ is independent of the abscissa x. If this expression is discretised over the grid by using the approximations (correct to order h^2 like (2.1)):

$$\psi(x_{p+\frac{1}{2}})=\tfrac{1}{2}[\psi(x_{p+1})+\psi(x_p)] \tag{2.7a}$$

$$\frac{\mathrm{d}\psi(x_{p+\frac{1}{2}})}{\mathrm{d}x}=\frac{1}{h}[\psi(x_{p+1})-\psi(x_p)] \tag{2.7b}$$

it gives rise to the following corresponding value:

$$j(x_{p+\frac{1}{2}})=-2\frac{|\psi(x_{p+1})|^2}{h}\operatorname{Im} R_p. \tag{2.8}$$

This quantity can be regarded as a rigorous equivalent of the current of probability density for the discretised problem. Considering indeed relation (2.3), it is quite straightforward that, for any value of p:

$$j(x_{p-\frac{1}{2}})=j(x_{p+\frac{1}{2}}). \tag{2.9}$$

That property simply expresses the spatial uniformity of the current of probability as required for a steady state. In the next section, this concept of discrete current will be used for deriving an expression of the transmission coefficient of a potential barrier arising from a localised force.

3. Transmission coefficient for a localised force

The restriction to a localised force, which is considered in the present approach, simply means that one is considering potential functions similar to that shown in figure 1. The potential $v(x_p)$ varies only inside the interval $[x_0, x_{n+1}]$ and remains constant outside this interval:

$$\text{in region I } (x \leqslant x_0): \qquad v(x) = v_{\mathrm{I}} \tag{3.1}$$

$$\text{in region II } (x_0 < x < x_{n+1}): \qquad v(x) \text{ arbitrary} \tag{3.2}$$

$$\text{in region III } (x \geqslant x_{n+1}): \qquad v(x) = v_{\mathrm{III}}. \tag{3.3}$$

The step size h is related to the number n of points defined inside this interval (x_0 and x_{n+1} excluded):

$$h = \frac{x_{n+1} - x_0}{n+1}. \tag{3.4}$$

Outside region II, the discretised Schrödinger equation reduces to a linear finite-difference equation with constant coefficients:

$$\psi(x_{p+1}) - \beta\psi(x_p) + \psi(x_{p-1}) = 0 \tag{3.5}$$

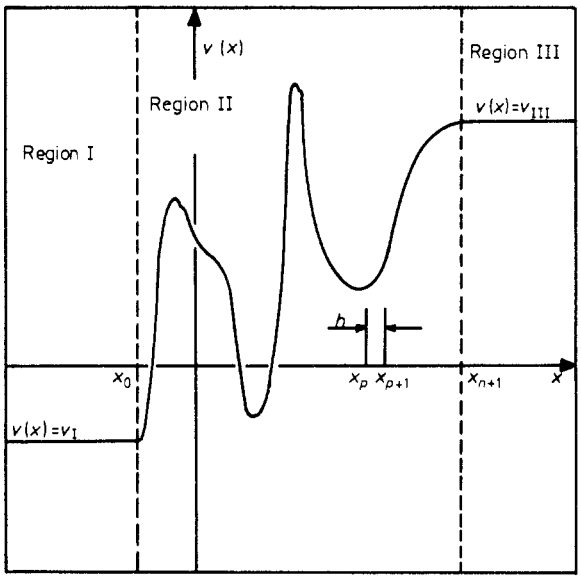

Figure 1. The kind of potential considered in this paper. This potential is constant outside region II.

with, in region I,

$$\beta = \beta_{\mathrm{I}} = 2 + h^2[v_{\mathrm{I}} - \epsilon] \tag{3.6}$$

and, in region III,

$$\beta = \beta_{\mathrm{III}} = 2 + h^2[v_{\mathrm{III}} - \epsilon]. \tag{3.7}$$

This equation can be solved exactly in both regions. In region I, from which one supposes the incidence of particles, the wavefunction is a linear superposition

$$\psi(x_p) = Au(x_p) + Bw(x_p) \tag{3.8}$$

of the following simple waves ($p \leqslant 0$):

$$u(x_p) = [R^-]^{|p|} \tag{3.9}$$

with

$$R^- = \frac{\beta_{\mathrm{I}}}{2} - \mathrm{i}\left[\left(1 - \left(\frac{\beta_{\mathrm{I}}}{2}\right)^2\right]^{1/2}\right. \tag{3.10}$$

corresponding to incident particles and carrying a positive current, given by

$$j_u = \frac{2}{h}\left[1 - \left(\frac{\beta_{\mathrm{I}}}{2}\right)^2\right]^{1/2}, \tag{3.11}$$

and

$$w(x_p) = [R^+]^{|p|} \tag{3.12}$$

with

$$R^+ = \frac{\beta_{\mathrm{I}}}{2} + \mathrm{i}\left[1 - \left(\frac{\beta_{\mathrm{I}}}{2}\right)^2\right]^{1/2} \tag{3.13}$$

which corresponds to reflected particles and carries a negative current

$$j_w = -\frac{2}{h}\left[1 - \left(\frac{\beta_{\mathrm{I}}}{2}\right)^2\right]^{1/2}. \tag{3.14}$$

The current supported by the wave (3.8) can be shown to be simply $|A|^2 j_u + |B|^2 j_w$. This assertion is also true in the continuous case for pure travelling waves in a region where the potential is constant. That property is not destroyed by the discretisation process considered here.

In region III, the escaping particles are described by the single term

$$\psi(x_{n+1+p}) = \left\{\frac{\beta_{\mathrm{III}}}{2} + \mathrm{i}\left[1 - \left(\frac{\beta_{\mathrm{III}}}{2}\right)^2\right]^{1/2}\right\}^p \tag{3.15}$$

for which the current of probability is simply

$$j_t = \frac{2}{h}\left[1 - \left(\frac{\beta_{\mathrm{III}}}{2}\right)^2\right]^{1/2}. \tag{3.16}$$

The reflection coefficient is defined, as in the continuous case, as the ratio of the reflected to the incident currents:

$$R = \left|\frac{|B|^2 j_w}{|A|^2 j_u}\right| = \frac{|B|^2}{|A|^2} \tag{3.17}$$

and the transmission coefficient as the ratio of the transmitted to the incident current:

$$T = \frac{j_t}{|A|^2 j_u}. \tag{3.18}$$

With these definitions, the spatial uniformity of the total current (which yields $j_t = |A|^2 j_u + |B|^2 j_w$) is simply expressed as

$$R + T = 1, \tag{3.19}$$

a result in agreement with what is obtained from the continuous equation. The reflection coefficient can then be evaluated as follows. From the recurrence relation (2.3), the quantity R_{-1} can readily be expressed as a terminating continued fraction

$$R_{-1} = b_0(\epsilon) - \cfrac{1}{b_1(\epsilon) - \cfrac{1}{b_2(\epsilon) - \cdots \cfrac{1}{b_n(\epsilon) - \cfrac{1}{\frac{\beta_{III}}{2} - i\left[1 - \left(\frac{\beta_{III}}{2}\right)^2\right]^{1/2}}}}}. \tag{3.20}$$

But, on the other hand, by using (2.4) and (3.8), the same quantity can be expressed as

$$R_{-1} = \frac{\psi(x_{-1})}{\psi(x_0)} = \frac{AR^- + BR^+}{A + B}. \tag{3.21}$$

From this, the reflection coefficient can be derived,

$$R = \frac{|B|^2}{|A|^2} = \left|\frac{R_{-1} - R^-}{R_{-1} - R^+}\right|^2, \tag{3.22}$$

and easily computed. Gautschi (1967) reviews some algorithms for the evaluation of continued fractions. The best suited here is certainly the forward recursion method, which has over the direct backward computation the advantage of avoiding much complex arithmetic. The procedure is described in detail by Wall (1967). It consists in evaluating the continued fraction as

$$R_{-1} = A_{n+2}/B_{n+1} \tag{3.23}$$

where the numerator and the denominator are obtained by means of the following recursion relations, which hold for $p = 2, 3, \ldots, n$,

$$A_{p+1} = A_p b_p(\epsilon) - A_{p-1} \tag{3.24}$$

$$B_p = B_{p-1} b_p(\epsilon) - B_{p-2}. \tag{3.25}$$

The starting values are, respectively,

$$A_1 = b_0(\epsilon) \qquad A_2 = b_0(\epsilon) b_1(\epsilon) - 1 \tag{3.26}$$

and

$$B_0 = 1 \qquad B_1 = b_1(\epsilon). \tag{3.27}$$

The last step, which is the only one requiring complex arithmetic, leads to evaluate the final approximant

$$A_{n+2} = A_{n+1} z - A_n \tag{3.28}$$

$$B_{n+1} = B_n z - B_{n-1} \tag{3.29}$$

where

$$z = \frac{\beta_{\mathrm{III}}}{2} - \mathrm{i}\left[1 - \left(\frac{\beta_{\mathrm{III}}}{2}\right)^2\right]^{1/2}. \tag{3.30}$$

Using this result, the reflection coefficient can be evaluated from

$$R = \frac{|A_{n+2} - R^- B_{n+1}|^2}{|A_{n+2} - R^+ B_{n+1}|^2} \tag{3.31}$$

and the transmission coefficient follows immediately from (3.19).

4. Examples

The transmission coefficient produced by the algorithm just described is now compared to some classical results. An interesting case that can possibly be considered refers to the well-known model

$$v(x) = \frac{1}{\cosh^2 x} \tag{4.1}$$

which can be treated exactly, at least for energies ϵ smaller than the maximum potential value: $\epsilon < 1$. The exact transmission coefficient is here given by the following formula (see, for example, Landau and Lifshitz 1967):

$$T = \frac{\sinh^2 \pi\sqrt{\epsilon}}{\sinh^2 \pi\sqrt{\epsilon} + \cosh^2 \pi\sqrt{3}/2}. \tag{4.2}$$

From another viewpoint, the WKB approximation is certainly the most usual method used for determining the penetration factor of such a smooth barrier. In this latter approach, the transmission coefficient is given by the following simple expression:

$$T_{\mathrm{WKB}} = \mathrm{e}^{-2K} \tag{4.3}$$

where

$$K = \int_a^b (v(x) - \epsilon)^{1/2}\, \mathrm{d}x \tag{4.4}$$

where a and b are the classical turning points corresponding to the actual value of the energy ϵ. This approximation is only justified if the transmission coefficient is small. This is normally not the case near the top of the potential barrier, where K tends to vanish. This reduces the validity of such an expression to a region of energy reasonably smaller than the maximum of the potential hill. This is certainly a serious drawback of the semiclassical method, which is not encountered in the direct numerical approach described in this paper. Kemble (1958) has proposed a modification of the expression (4.3), accounting for a quadratic behaviour of the potential near the top of the barrier.

The expression

$$T_K = \frac{1}{1+e^{2K}}, \tag{4.5}$$

being exact for a parabolic hill and identical to (4.3) for large K, is believed to provide a better value of the transmission factor for the whole range of energy.

The results provided by the different approaches are compared in table 1. The WKB expression can be obtained exactly for this case:

$$T_{WKB} = e^{-2\pi(1-\sqrt{\epsilon})}. \tag{4.6}$$

Table 1. Comparison between the exact, WKB and continued fraction approaches for the determination of the transmission coefficient. The potential barrier is described by $v(x) = 1/\cosh^2 x$.

	Transmission coefficient T				
				Continued fraction (3.31)	
Energy	Exact (4.2)	WKB (4.3)	Kemble (4.5)	$n = 50$	$n = 200$
0·2	0·059 2832	0·031	0·030	0·0594	0·059 275
0·4	0·180 3214	0·099	0·090	0·1805	0·180 35
0·6	0·354 6720	0·243	0·195	0·3546	0·354 70
0·8	0·540 5463	0·515	0·340	0·5400	0·540 49
1	0·696 2282	1·000	0·500	0·6955	0·696 13

Kemble's method does not produce a better result than the WKB method except perhaps near $\epsilon \approx 1$, where both give quite inaccurate results. In performing the numerical computation of equation (3.31), a potential value $v(x) = 0$ has been taken for $x \leqslant -5$ and $x \geqslant 5$, for both $n = 50$ and $n = 200$ in table 1. Taking $v(x) = 0$ only for $x \leqslant -10$ and $x \geqslant 10$ with the same discretising step did not change the transmission coefficient by more than 0·01% in any case. As expected, the direct numerical approach gives a far better result in the whole range of energy, even for a rather small number of points defining the discrete mesh. The convergence of the method when n is increased is not very fast (h^2 convergence). The produced transmission coefficient is however already pretty good for a reasonable step size ($n \approx 50$).

When the height of the barrier is made higher by multiplying the previous potential (4.1) by some large amplitude v_0, the WKB approximation is expected to provide a better result. Table 2 compares the semiclassical approximation with the continued fraction method in the case where v_0 equals 15. As in table 1, the potential is taken to be zero for $x \leqslant -5$ and $x \geqslant 5$. For small values of the transmission coefficient, the WKB approximation can be compared to the continued fraction method with 50 points. However, for energies lying near the top of the barrier, the semiclassical approach becomes less accurate. Another feature of the discretisation method is that a better precision can be reached if, as shown in table 2, one reduces the step size.

From the data provided in tables 1 and 2 it can be noticed that, for a given step size, the present method loses accuracy when the barrier height is increased (by contrast with WKB). This can be understood as follows: the local period (or decay length) of the wavefunction $\psi(x)$ at the point x is of the order of $(|v(x) - \epsilon|)^{1/2}$. In order to describe

Table 2. Comparison between the exact, WKB and continued fraction approaches for the determination of the transmission coefficient. The potential barrier is described by $v(x) = 15/\cosh^2 x$.

	Transmission coefficient T					
				Continued fraction (3.31)		
Energy	Exact	WKB (4.3)	Kemble (4.5)	$n = 50$	$n = 200$	$n = 400$
3	$0{\cdot}17634\times10^{-5}$	$0{\cdot}14\times10^{-5}$	$0{\cdot}14\times10^{-5}$	$0{\cdot}21\times10^{-5}$	$0{\cdot}178\times10^{-5}$	$0{\cdot}1770\times10^{-5}$
6	$0{\cdot}15996\times10^{-3}$	$0{\cdot}13\times10^{-3}$	$0{\cdot}13\times10^{-3}$	$0{\cdot}17\times10^{-3}$	$0{\cdot}161\times10^{-3}$	$0{\cdot}1602\times10^{-3}$
9	$0{\cdot}50592\times10^{-2}$	$0{\cdot}41\times10^{-2}$	$0{\cdot}41\times10^{-2}$	$0{\cdot}52\times10^{-2}$	$0{\cdot}507\times10^{-2}$	$0{\cdot}5063\times10^{-2}$
12	$0{\cdot}85846\times10^{-1}$	$0{\cdot}76\times10^{-1}$	$0{\cdot}71\times10^{-1}$	$0{\cdot}8579\times10^{-1}$	$0{\cdot}85840\times10^{-1}$	$0{\cdot}85843\times10^{-1}$
15	0·55074	1·00	0·50	0·547	0·5504	0·5506

correctly the variations of the wavefunction in a discrete scheme, this period should contain several step lengths. This restriction amounts to requiring that

$$h^2(v(x)-\epsilon) \ll 1. \tag{4.7}$$

If the energies ($v(x)$ and ϵ) are multiplied by v_0, the step size must be reduced by a factor

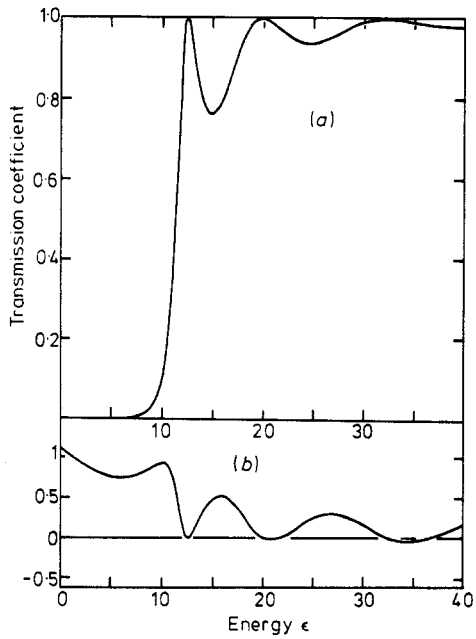

Figure 2. Transmission coefficient produced by the continued fraction approach for a square-top barrier of height 10 and width 2. The interval [0, 2] has been divided into 101 sub-intervals. The relative discrepancies between the approximate and exact values are given in units of 10^{-3}. (*a*) Transmission coefficient calculated from equation (3.31). (*b*) Relative deviation from the exact result (in units of 10^{-3}):

$$\frac{T - T\,(\text{exact})}{|T(\text{exact})|}.$$

$\sqrt{v_0}$ in order to expect to keep a constant accuracy. To impose the condition (4.7) is also important from a practical point of view. When (4.7) is satisfied, all coefficients $b_p(\epsilon)$ in the continued fraction (3.20) have a nearly constant value of the order of 2. The polynomials generated by equations (3.24) and (3.25) bear resemblance to Chebyshev polynomials (obtained for $b_p(\epsilon) = 2$). The local values of these polynomials remain reasonable: an overflow has never been encountered so far in computing (3.20) by the method suggested in § 3.

In the region $\epsilon < v_0$, the transmission factor increases monotonously. It should be interesting to know if the continued fraction approach is also successful in accounting for resonances at higher energies. A typical model for illustrating this situation is the square-top barrier, for which the penetration factor exhibits characteristic interference oscillations. The case where a potential discontinuity occurs can also be treated in the present approach. However, the quadratic convergence rate of the method is reduced to a linear rate, unless the discontinuity is one of the discretisation points and the potential is defined as the arithmetic mean of its left and right limits at that point. Figure 2 displays the result obtained in the case of the following potential:

$$\begin{aligned} v(x) &= 10 \qquad \text{for } 0 < x < 2 \\ v(x) &= 5 \qquad \text{for } x = 0 \text{ and } x = 2 \\ v(x) &= 0 \qquad \text{otherwise.} \end{aligned} \tag{4.8}$$

The transmission coefficient is plotted against the energy together with the relative difference between the numerical and the exact values. The agreement is found to be quite remarkable.

5. Conclusion

The numerical method proposed here to evaluate the transmission coefficient of a one-dimensional potential barrier is based on a simple discretisation of the kinetic energy operator. This scheme transforms the continuous Schrödinger equation into a three-term recursion relation, well suited to be handled by means of continued fractions. The discrete equation retains the most important features of the continuous original problem and the concepts developed in this latter case can be adapted to the discrete formulation. In this context, the current of probability density is redefined in a suitable form accounting for the discrete aspect of the Hamiltonian. Using this concept leads us to formulate an explicit expression for the transmission coefficient. Unlike analytic approximations (like that obtained from WKB formulae), the method can produce an arbitrarily accurate transmission factor by reducing the step size. Though the (quadratic) convergence is somewhat slow, a reasonable number of steps will often produce an accurate result. The algorithm is extremely easy to implement and does not require much memory allocation. It is expected to give a fast and accurate answer to most one-dimensional scattering problems, as soon as an effective potential can be assumed.

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