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Wave and particle limit for multiple barrier tunneling

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Abstract
The particle approach to one-dimensional potential scattering is applied to non-relativistic tunneling between two, three and four identical barriers. We demonstrate as expected that the infinite sum of particle contributions yields the plane wave results. In particular, the existence of resonance/transparency for twin tunneling in the wave limit is immediately obvious. The known resonances for three and four barriers are also derived. The transition from the wave limit to the particle limit is exhibited numerically.

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1. Introduction

The particle approach to piece-wise potential scattering is characterized by considering the reflection and transmission amplitudes, successively, at each potential discontinuity. This method, applied also in optics [1], can be used as an alternative to plane wave continuity equations for the derivation of the transmission and reflection amplitudes, and find application in approximate solutions to one-dimensional potential problems [2, 3]. Several interesting papers have analyzed tunneling with this method [4–6]. However, in certain situations, this approach is the natural physical choice in the 'particle limit' in which the incoming wave packets are small compared to the potentials extension. However, it must be emphasized that the approach itself does not require the use of wave packets. It predicts multiple reflections and even for a single incoming wave it generally results in infinite reflected and transmitted waves. An example of this approach is the diffusion above a single potential barrier, from which one significant consequence, otherwise mysterious, is the step limit for large barriers [7]. The first barrier reflection coefficient reproduces the step result.

The alternative and standard approach to potential scattering is with a single wave analysis [8]. We refer to this as the 'wave limit'. It is characterized by continuity equations often best described by the use of matrices and yields a *single* reflected and transmitted amplitude. Due to the fact that the algebraic sum of the infinite contributions in the particle approach yields the wave result, the two methods are mathematically equivalent. However, they are not equivalent

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in practice because a sum of calculated terms, if finite, is an unambiguous process, but the decomposition of an expression as an infinite sum, on the other hand, is highly ambiguous, even if only one decomposition can lead to probability conservation and to the correct exit times of the separate wave packets. In the wave limit, probabilities are calculated by first summing the particle terms and then squaring the modulus. In the particle limit, the probabilities are calculated by first squaring the modulus of each term and then summing.

Resonance phenomena, within the Schrödinger equation, are well known for a single barrier when considering plane waves with energy above the potential value, i.e. $E > V_0$. It results in unit transmission probabilities. For a given plane wave energy there are unlimited such resonances as the barrier length increases. More realistically, for an incoming wave packet it can be shown that resonance occurs only if the barrier length is much smaller than the wave packet dimensions [9]. Resonance is a property of the wave nature of particles while, in the other limit in which the wave packet is small compared to the barrier length, the transmission amplitude *breaks up* into infinite transmitted (and consequently reflected) wave packets, the so-called 'particle limit'. There is no particle limit for tunneling, $E < V_0$, through a single barrier [10–12]. However, for more than one barrier there exists another coherence effect, tunneling resonances [13–18]. For particular values of the momentum and of the inter-barrier distance, identical barriers become *transparent*, i.e. the tunneling transmission probability equals unity.

In the following section, we recall the single barrier tunneling results and define the amplitudes relevant to the particle approach. We then consider the case of twin barriers. We illustrate our procedure for calculating the individual particle contributions and then sum them to obtain the wave limit result. This sum can also be viewed as a compact expression for the particle series. The resonance condition will be obvious in this expression. We will also prove probability conservation in both the wave and particle limit. Conservation of probability must also be valid for all intermediate (partial wave packet overlap) cases; however, no simple analytic calculation of these probabilities is known. In section 3, we describe some numerical calculations in which an incoming Gaussian wave packet is used. The existence, albeit degraded, of resonances is indicated by oscillations as a function of inter-barrier distance d. For large d, the particle picture sets in and the oscillatory behavior is *damped out*. In section 4, we consider the three identical barrier case and derive the, non-obvious, resonance conditions. To proceed to higher numbers of barriers it is more practical to change the method of calculation. In section 5, we derive a matrix expression for the wave limit and then describe how this can be rewritten in a form from which the individual particle series can be extracted. This is applied, as an example, to the case of four identical barriers and the first transmitted particle terms confirm the direct particle procedure. We draw our conclusions in section 6.

2. Twin barrier tunneling

To perform our calculation, we need the reflection and transmission amplitudes for a single barrier. The single barrier reflection amplitude depends not only upon the barrier height and length but also on the barrier position and consequently upon whether the barrier is encountered coming from the left or from the right. Nevertheless, the explicit rules are quite simple.

Let R be the reflection amplitude for a plane wave of unit amplitude with energy $E < V_0$ impinging on a barrier of length L from the left at $x = 0$, see figure 1(a). Let T be the transmission amplitude for the same wave. Note that the reflection and transmission probabilities, also known as the reflection and transmission coefficients, are consequently $|R|^2$

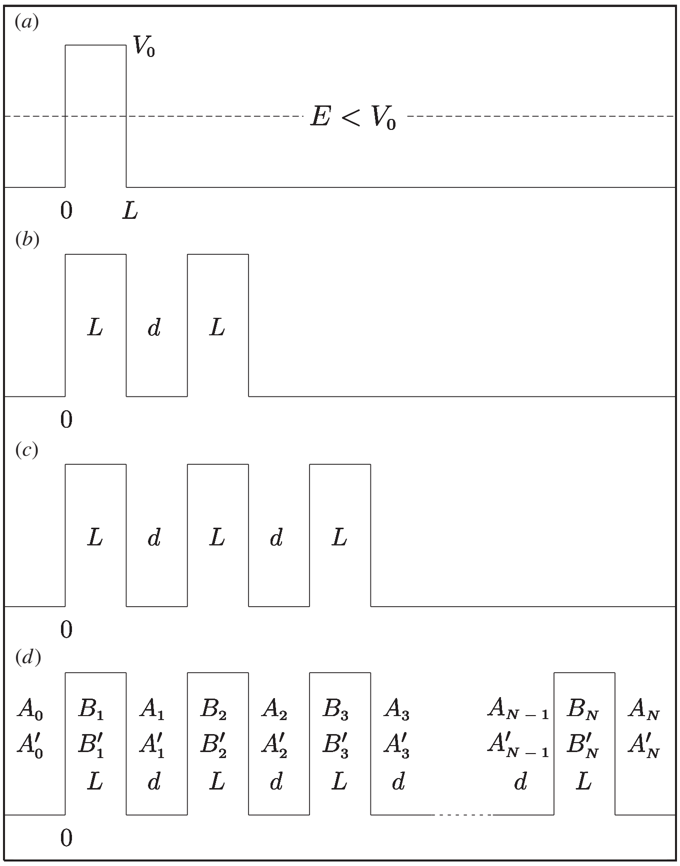

Figure 1. Potential shapes: (*a*) single barrier, (*b*) twin barriers, (*c*) triple identical barrier and (*d*) general structure for matrix calculation. In (*d*) the A/A' and B/B' terms indicate the amplitudes in the free and potential regions.

and $|T|^2$, respectively. Now, a standard plane wave calculation gives the results

$$R = -\,\mathrm{i}\,\frac{k^2+\rho^2}{2k\rho}\,\cos\phi\,\tanh(\rho L)\,\exp(\mathrm{i}\phi) = -\mathrm{i}\,|R|\,\exp(\mathrm{i}\phi), \tag{1}$$

$$T = \frac{\cos\phi}{\cosh(\rho L)}\,\exp[\mathrm{i}(\phi - kL)] = |T|\,\exp[\mathrm{i}(\phi - kL)], \tag{2}$$

with

$k = \sqrt{2mE}/\hbar, \quad \rho = \sqrt{2m(V_0 - E)}/\hbar$ and $\tan\phi = (k^2-\rho^2)\tanh(\rho L)/2k\rho,$

where by convention,

$$-\pi/2 < \phi < \pi/2.$$

Conservation of probability results from the fact that $|R|^2 + |T|^2 = 1$. Now, shift the front of the barrier from the origin to the position $x = a$. The reflection amplitude acquires an additional phase becoming

$$R\,\exp(2\,\mathrm{i}k\,a). \tag{3}$$

If the wave impinges the barrier from the right (momentum $-k$), we obtain instead

$$R\ \exp(-2\,\mathrm{i}k\,b), \tag{4}$$

where $b = a + L$. In both cases, the transmission amplitude remains *unchanged*. It does not depend upon the position of the barrier, but only upon its width (L) and height (V_0), apart, of course, upon the value of the energy E.

Now consider the twin barrier problem, the shape of the potential is drawn in figure 1(*b*). The particle approach stems from considering the hypothetical case of wave packets such that their spatial dimensions are small compared to d.

Consider an incoming wave packet from the left. When it reaches the first barrier at $x = 0$, it will produce a first reflected wave in the region $x < 0$ and a first transmitted wave into the inter-barrier separation. For *each* momentum component k, these are given by the

$$R \qquad \text{and} \qquad T$$

of the single barrier given above, with consequent conservation of probability. Now the wave packet in the inter-barrier region will travel to the second barrier and then be partially reflected by and partially transmitted through the second barrier. These amplitudes will be, respectively,

$$T \times R\,\mathrm{e}^{2\mathrm{i}k(L+d)} \qquad \text{and} \qquad T \times T.$$

The latter amplitude is the first contribution to the total transmission amplitude. Again probability is clearly conserved at this step. The reflected wave from the second barrier now traveling to the left impinges upon the first barrier at $x = L$ and, after its transmission through the first barrier, creates the second contribution to the total reflection amplitude,

$$TR\,\mathrm{e}^{2\mathrm{i}k(L+d)} \times T.$$

The reflected amplitude (at $x = L$) which moves back from the first to second barrier is

$$TR\,\mathrm{e}^{2\mathrm{i}k(L+d)} \times R\,\mathrm{e}^{-2\mathrm{i}kL}.$$

Again probability is conserved. Consequently, the second contribution to the total transmission amplitude is then given by

$$TR^2\,\mathrm{e}^{2\mathrm{i}kd} \times T.$$

The procedure repeats continuously and the sum of these contributions gives

$$R_S^{(2)} = R + RT^2\,\mathrm{e}^{2\mathrm{i}k(L+d)}\sum_{n=0}^{\infty}(R^2\,\mathrm{e}^{2\mathrm{i}kd})^n = R + RT^2\,\mathrm{e}^{2\mathrm{i}k(L+d)}/(1 - R^2\,\mathrm{e}^{2\mathrm{i}kd}), \tag{5}$$

$$T_S^{(2)} = T^2\sum_{n=0}^{\infty}(R^2\,\mathrm{e}^{2\mathrm{i}kd})^n = T^2/(1 - R^2\,\mathrm{e}^{2\mathrm{i}kd}), \tag{6}$$

where the bracketed upper script (2) on the lhs indicates the number of identical barriers and the subscript S refers to an infinite sum. The second equality in each of the above equations is legitimate because $|R^2\,\mathrm{e}^{2\mathrm{i}kd}| < 1$.

For an incoming wave packet which is small in spatial dimensions compared to the inter-barrier potential distance, the individual contributions used in the sums above should not be added because they are incoherent. Each will correspond to a separate outgoing (transmitted or reflected) wave packet,

$$\mathcal{R}_{\text{particle}}^{(2)} = |R|^2 + |R|^2|T|^4\sum_{n=0}^{\infty}|R|^{4n} = 2\,|R|^2/(1 + |R|^2), \tag{7}$$

$$\mathcal{T}^{(2)}_{\text{particle}} = |T|^4 \sum_{n=0}^{\infty} |R|^{4n} = |T|^2/(1+|R|^2). \tag{8}$$

This is what we call the *particle limit*. Since probability is conserved at each step of the above calculation, probability is conserved overall,

$$\mathcal{R}^{(2)}_{\text{particle}} + \mathcal{T}^{(2)}_{\text{particle}} = 1,$$

but the transmission and reflection probabilities in the *particle limit* are not those of the *wave limit* when each individual particle contribution is completely coherent [15, 17, 18]. In this case,

$$\mathcal{R}^{(2)}_{\text{wave}} = 2|R|^2[1+\cos(2\alpha)]/[1+|R|^4+2|R|^2\cos(2\alpha)], \tag{9}$$

$$\mathcal{T}^{(2)}_{\text{wave}} = |T|^4/[1+|R|^4+2|R|^2\cos(2\alpha)], \tag{10}$$

with

$$\alpha = \phi + kd,$$

and, as expected,

$$\mathcal{R}^{(2)}_{\text{wave}} + \mathcal{T}^{(2)}_{\text{wave}} = 1.$$

This result must not be misinterpreted as a proof of a single outgoing transmission/reflection amplitude. The transition between the wave and the particle limit will be discussed in more detail in the following section.

Now let us return to the transmission amplitude given in equation (6), seen in the wave limit,

$$T^{(2)}_S = T^2/D, \tag{11}$$

with

$$D = 1 - R^2\,\mathrm{e}^{2ikd} = 1 + |R|^2\,\mathrm{e}^{2\mathrm{i}\alpha}.$$

From this form, one immediately derives the condition for resonance tunneling for which the barriers become 'transparent'. The *maximum* of the above expression occurs when the modulus of the denominator is a minimum, i.e. when

$$\cos(2\alpha) = -1 \quad\Leftrightarrow\quad \cos(\alpha) = 0. \tag{12}$$

For these values of α:

$$T^{(2)}_S\,[\cos\alpha = 0] = T^2/|T|^2 \Rightarrow \mathcal{T}^{(2)}_{\text{wave}}\,[\cos\alpha = 0] = 1. \tag{13}$$

Observe that the transmission probability in the particle limit, equation (8), can *never* be unity, since $|T| < 1$. We may also determine the *minimum* value of $P^{(2)}_{\text{T,wave}}$ which occurs when

$$\cos(2\alpha) = +1 \Leftrightarrow \cos(\alpha) = \pm 1. \tag{14}$$

For these values of α:

$$T^{(2)}_S[\cos\alpha = \pm 1] = T^2/(1+|R|^2) \Rightarrow \mathcal{T}^{(2)}_{\text{wave}}[\cos\alpha = \pm 1] = 1/(1+2|R|^2/|T|^2)^2. \tag{15}$$

3. Transition between wave and particle limit

In this section, we intend to study numerically the behavior of a particular incident wave packet impinging on a double identical barrier potential (figure 1(*b*)) from the left. The results will graphically exhibit the transition from the wave to particle limits and also verify the validity of some of the expressions derived in the previous section. For the following numerical calculation, we will express all quantities in terms of the barrier height V_0 and/or mV_0. For our purposes, these values need not be explicitly fixed. We will consider below a set of barrier widths, the incoming wave packet's mean momentum (k_0)/energy (E_0) and a set of its momentum spread. The inter-barrier distance will be left as a continuous variable in our calculations. The incident wave packet is obtained by superposing the plane waves

$$\exp\left[\mathrm{i}\left(kx - \frac{Et}{\hbar}\right)\right]$$

with the coefficient

$$\frac{\sqrt{a}}{(2\pi)^{3/4}}\exp\left[-\frac{a^2}{4}(k-k_0)^2\right],$$

which correspond to a Gaussian function centered at $k_0 = \sqrt{2mE_0}/\hbar$ multiplied by a numerical factor which normalizes the wavefunction [8]. The transmitted wave packet can be written as

$$\Psi_{\mathrm{tra}}(x,t) = \frac{\sqrt{a}}{(2\pi)^{3/4}}\int_0^w \mathrm{d}k T_S^{(2)} \exp\left[-\frac{a^2}{4}(k-k_0)^2 + \mathrm{i}\left(kx - \frac{Et}{\hbar}\right)\right], \tag{16}$$

where $w = \sqrt{2mV_0}/\hbar$. Consequently, the probability of transmission is given by

$$\int_{2L+d}^{+\infty}\mathrm{d}x\ |\Psi_{\mathrm{tra}}(x,t)|^2 . \tag{17}$$

Now, we are interested in the *total* transmission probability. This is formally the limit of the above for $t\to\infty$. However, there is an alternative procedure to obtain the same result. We send the lower x limit to $-\infty$. This picks up all the future (at time t) probability contributions, i.e. *phantom* wave packets. An example of this phenomena is seen in numerical calculations with, say, the step potential for times before total ($E < V_0$) wave packet reflection. If one plots the reflected wave amplitude, it does not appear yet in the free potential region where destructive interference occurs but a wave does appear for x values in the *forbidden* region. Of course, the reflection coefficient does not apply there, and this traveling wave packet is only virtual or phantom. However, it eventually emerges as a physical wave packet in the free region at the appropriate reflection time. The above extension of the lower x integration limit is useful for Gaussian convolution because it yields a Dirac delta function. This allows us to immediately perform one of the momentum integrals. It in turn eliminates the time dependence as it must and yields the following expression for the total transmission probability,

$$\begin{aligned}\mathcal{P}_T^{(2)} &= \frac{\sqrt{2mV_0}\,a/\hbar}{\sqrt{2\pi}}\int_0^1 \mathrm{d}\left(\frac{\hbar k}{\sqrt{2mV_0}}\right)\ \left|T_S^{(2)}\right|^2 \exp\left[-\frac{(\sqrt{2mV_0}\,a/\hbar)^2}{2}\left(\frac{\hbar k - \hbar k_0}{\sqrt{2mV_0}}\right)^2\right]\\ &= \frac{\sqrt{2mV_0}\,a/\hbar}{\sqrt{2\pi}}\int_0^1 \mathrm{d}\sqrt{\frac{E}{V_0}}\left|T_S^{(2)}\right|^2 \exp\left[-\frac{(\sqrt{2mV_0}\,a/\hbar)^2}{2}\left(\sqrt{\frac{E}{V_0}} - \sqrt{\frac{E_0}{V_0}}\right)^2\right].\end{aligned} \tag{18}$$

From the previous equation, observing that $T_S^{(2)}$ is a function of E/V_0, $\sqrt{2mV_0}\,d/\hbar$ and $\sqrt{2mV_0}\,L/\hbar$, we immediately see that $\mathcal{P}_T^{(2)}$ is completely determined oncethe following four adimensional quantities are fixed:

$$\frac{E_0}{V_0},\quad \frac{\sqrt{2mV_0}a}{\hbar},\quad \frac{\sqrt{2mV_0}d}{\hbar}\quad \text{and}\quad \frac{\sqrt{2mV_0}L}{\hbar}.$$

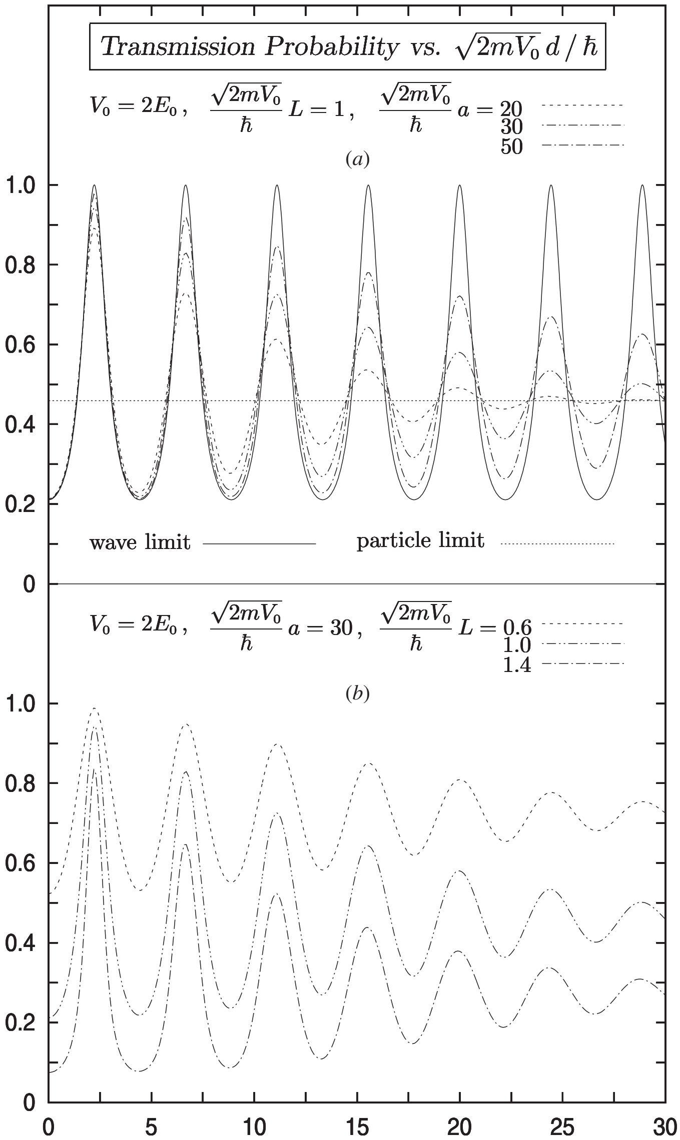

Figure 2. Transmission probability versus the inter-barrier distance. Upper curves are for a fixed barrier width (L) and various wave packet widths (a). Lower curves are for a fixed wave packet width and various barrier widths. The curves show the gradual transition from the wave limit (continuous line) to the particle limit (dotted line) exhibited by the damping of the oscillations. Observe that the particle limit is the same for all the curves plotted in figure 2(a) whereas each particle limit is different in figure 2(b). This is due to the fact that $\mathcal{T}^{(2)}_{\text{particle}}$ depends on the barrier width.

$\mathcal{P}^{(2)}_T$ is calculated numerically and plotted in figure 2, where we have chosen the ratio E_0/V_0 equals to $1/2$. In the upper part of figure 2(a), we set the barrier width,

$$\sqrt{2mV_0}L/\hbar = 1,$$

and display the total transmission probability versus the inter-barrier distance, $\sqrt{2mV_0}\,d/\hbar$, for various wave packet widths. The wave limit is obtained when each individual contribution to $|T_S^{(2)}|$ is completely coherent. This occurs when the inter-barrier potential distance (d) is small if compared to the wave packet spatial dimension (a),

$$\mathcal{P}_T^{(2)}[a \gg d] \rightarrow \left[\mathcal{T}_{\text{wave}}^{(2)}\right]_0,$$

where the subscript 0 indicates that $\mathcal{T}_{\text{wave}}^{(2)}$ at $E = E_0$. For plane waves, we would have a periodic resonance structure with maxima at

$$\sqrt{2mV_0}d/\hbar = (2n+1)\pi/\sqrt{2}.$$

As shown in figure 2(a), the only close approximation to a resonance/transparency occurs for the first maximum and for the largest spreads of the wave packet plotted. As $\sqrt{2mV_0}\,d/\hbar$ increases in our plot, for each choice of wave packet width the probability tends to a constant value. This constant value is equal to 0.46 and is in agreement with the particle limit given in equation (8). This is due to the fact that for an incoming wave packet which is small in spatial dimensions (a) compared to the inter-barrier potential distance (d) the contributions to $\left|T_S^{(2)}\right|$ are incoherent,

$$\mathcal{P}_T^{(2)}[a \ll d] \rightarrow \left[\mathcal{T}_{\text{particle}}^{(2)}\right]_0.$$

In figure 2(b), we set the wave packet width,

$$\sqrt{2mV_0}a/\hbar = 30,$$

and display the total transmission probability versus the inter-barrier distance, $\sqrt{2mV_0}\,d/\hbar$, for various barrier widths. Again the gradual transition from wave to particle limit is exhibited by the damping of the oscillations. Each particle limit is different because the values of R and T depend upon the barrier width. Also it is to be noted that the maxima and minima of each curve occur at the same values of $\sqrt{2mV_0}\,d/\hbar$. This is *not* true in general. It occurs here because of our choice of $E_0 = V_0/2$. This particular ratio results in $\phi = 0$. In general ϕ is dependent upon the barrier width and this would separate somewhat the maxima/minima.

The curves, plotted in figure 2, clearly show the transition from the wave to the particle limit. However, another even more direct way to show the particle limit is to display the probability density as a function of x for the transmitted wave. In figure 3, this is shown for a case in which multiple wave packets exist and for a time at which two have emerged. These are numerical calculations and we take the opportunity to compare the position of these first two maxima with that predicted by the stationary phase method, SPM, approximation [19] applied to the particle expression of equation (6),

$$T_S^{(2)} = T^2 + T^2R^2\,\mathrm{e}^{2ikd} + \cdots.$$

This method gives us the times of exit of the maxima and, knowing the group velocity $\hbar k_0/m$, we can calculate their later positions. The phase of the first transmitted wave packet is extracted from

$$T^2\,\mathrm{e}^{\mathrm{i}(kx-Et/\hbar)}.$$

The SPM then gives the position of the first maximum at time t,

$$x_1 = 2L - 2\,\frac{\partial\phi}{\partial k}\bigg|_0 + \frac{\hbar k_0}{m}t,$$

with the derivative calculated at the maximum of the Gaussian distribution, k_0. In this step, we have neglected the shift in this maximum produced by the transmission amplitude. The derivative term is proportional to twice the transition time through a single barrier. It is thus proportional to the time needed to tunnel through the twin barriers. Note that this contribution

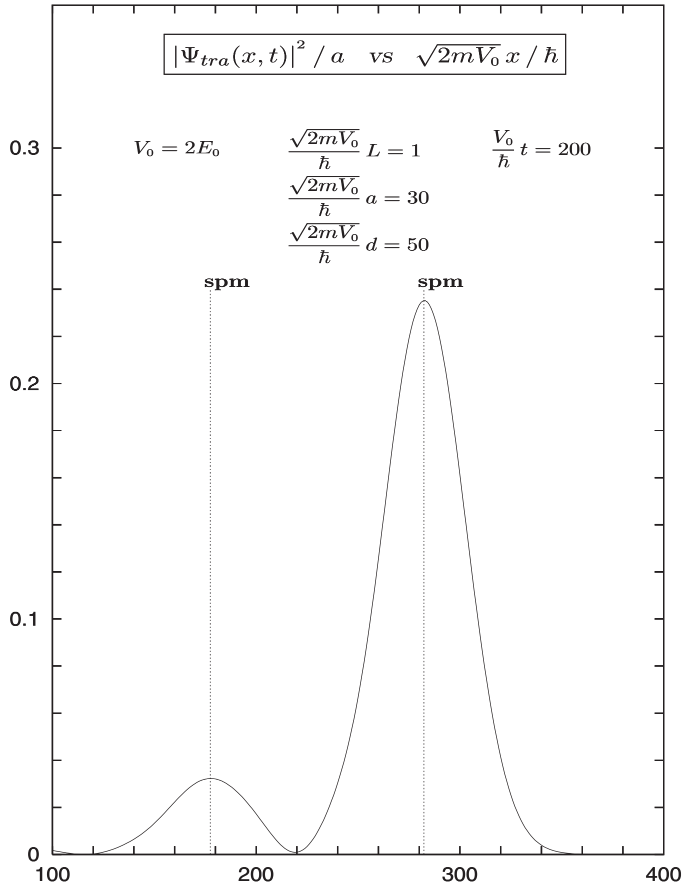

Figure 3. The density probability for the transmitted wave is plotted as a function of x for a fixed time. This time is such that two outgoing waves are seen. The SPM estimates (vertical lines) are in excellent agreement with the numerical calculation.

exists even if, as in our case, $\phi = 0$. The SPM transition time for a single barrier is surprising because for very large L it becomes independent of the barrier width. This is the Hartman effect [10], which has become of renewed interest in recent years [11, 12].

The phase of the second transmitted wave packet is obtained from

$$T^2\, e^{i(kx - Et/\hbar)} \times R^2\, e^{2ikd},$$

whence

$$x_2 = x_1 - 2\, \frac{\partial \phi}{\partial k}\bigg|_0 - 2d.$$

The derivative terms here are related to the reflection *delay* times and, as is well known, are seen to be equal to the tunneling times. These SPM positions of the maxima, for the case plotted in figure 3, are indicated by the vertical lines. Agreement with the numerical calculation is excellent.

However, note that if the SPM is applied to the summed (wave limit) expression it will yield a single maximum which does *not* coincide with any of the physical particle maxima.

The use of the SPM must be augmented with, at the very least, a knowledge of the number of maxima involved.

4. Three barrier analysis

The three identical barrier problem, figure 1(*c*), is somewhat more complicated than the twin barrier case, particularly in the extraction of the conditions for resonance/transparency. Now we have two identical inter-barrier regions and hence different processes or paths can contribute to coherent outgoing 'particles', i.e. with the same exit times. These terms must be summed before squaring the amplitudes. For brevity, we derive only the transmission amplitudes.

We proceed as follows. The leading transmission term is that without any internal reflection, i.e. T^3. After including all internal reflections, we find

$$T^3\{1 + 2R^2\,\mathrm{e}^{2\mathrm{i}kd} + 3R^4\,\mathrm{e}^{4\mathrm{i}kd} + \cdots\}. \tag{19}$$

The factor 2 before the $T^3R^2\,\mathrm{e}^{2\mathrm{i}kd}$ term allows for a double reflection, R^2, in each of the inter-barrier regions. The coefficient (three) in the third term allows for a four-fold reflection, R^4, in each of the inter-barrier regions plus a double reflection, $R^2 \times R^2$, in both regions. Using $R = -\mathrm{i}\,|R|\,\mathrm{e}^{\mathrm{i}\phi}$, equation (19) can be rewritten as follows:

$$T^3/(1 + |R|^2\,\mathrm{e}^{2\mathrm{i}\alpha})^2 = T^3/D^2. \tag{20}$$

However, this is by no means all; we can also have reflection from the third barrier, backward tunneling through the second barrier and reflection from the first barrier and again tunneling through the second barrier before exiting the structure. This contribution (to leading order) yields $T^5R^2\,\mathrm{e}^{2\mathrm{i}k(L+2d)}$. When all additional internal reflections are allowed for, we obtain the partial sum of

$$T^5R^2\,\mathrm{e}^{2\mathrm{i}k(L+2d)}\{1 + 4R^2\,\mathrm{e}^{2\mathrm{i}kd} + 10R^4\,\mathrm{e}^{4\mathrm{i}kd} + \cdots\}, \tag{21}$$

which leads to

$$T^5R^2\,\mathrm{e}^{2\mathrm{i}k(L+2d)}/D^4 = -T^3|R|^2|T|^2\,\mathrm{e}^{4\mathrm{i}\alpha}/D^4. \tag{22}$$

The higher denominator power (D^4) follows from the fact that each inter-barrier region is crossed twice in the leading $T^5R^2\,\mathrm{e}^{2\mathrm{i}k(L+2d)}$ path. This process continues for the $T^7R^4\,\mathrm{e}^{4\mathrm{i}k(L+2d)}$ term,

$$T^7R^4\,\mathrm{e}^{4\mathrm{i}k(L+2d)}/D^6 = T^3|R|^4|T|^4\,\mathrm{e}^{8\mathrm{i}\alpha}/D^6, \tag{23}$$

and so forth. The final result summing equations (20), (22) and (23) is

$$\begin{aligned} T_S^{(3)} &= \frac{T^3}{D^2}\left\{1 - \frac{|R|^2|T|^2}{D^2}\,\mathrm{e}^{4\mathrm{i}\alpha} + \frac{|R|^4|T|^4}{D^4}\,\mathrm{e}^{8\mathrm{i}\alpha} - \cdots\right\} \\ &= T^3\Bigg/\left[D^2\left(1 + \frac{|R|^2|T|^2}{D^2}\mathrm{e}^{4\mathrm{i}\alpha}\right)\right]. \end{aligned} \tag{24}$$

To determinate the resonances, in the wave limit, we first take the modulus squared of the denominator

$$|D^2 + |R|^2|T|^2\,\mathrm{e}^{4\mathrm{i}\alpha}|^2 = 1 + 5|R|^4 + 4|R|^2(1 + |R|^2)\cos(2\alpha) + 2|R|^2\cos(4\alpha)$$

and then differentiate with respect to α, equating to zero,

$$\sin(2\alpha)[1 + |R|^2 + 2\cos(2\alpha)] = 0.$$

This results in

- minimum values of the transmission probability when $\sin(2\alpha) = 0$, which yields

$$T_S^{(3)}[\cos\alpha = 0] = T^3/|T|^2, \qquad \mathcal{T}_{\text{wave}}^{(3)}[\cos\alpha = 0] = |T|^2, \tag{25}$$

$$T_S^{(3)}[\cos\alpha = \pm 1] = T^3/(1+3|R|^2), \qquad \mathcal{T}_{\text{wave}}^{(3)}[\cos\alpha = \pm 1] = |T|^2/(1+4|R|^2/|T|^2)^2, \tag{26}$$

- maximum values of the transmission probability when $\cos(2\alpha) = -(1+|R|^2)/2$, which yields the resonances

$$\mathcal{T}_{\text{wave}}^{(3)}\,[\cos\alpha = \pm|T|/2] = 1. \tag{27}$$

5. Continuity equations and matrix method

The procedure for calculating the particle terms for the case of more than three identical barriers becomes very difficult. Not only must we be careful of coherence but also calculate enough terms to extrapolate the total series. So, in this section we provide an alternative procedure based on the matrix method [1, 8]. We derive the expression for the *wave* transmission and reflection amplitudes for N identical barriers, figure 1(d), and then, based upon our results in the previous sections, we devise a procedure for deriving the *particle* sums. We will then apply this method to the $N = 4$ transmission amplitude.

We first define two 2×2 matrices: $W[\delta, x]$ and the diagonal $\Delta[\delta x]$,

$$W[\delta, x] = \begin{pmatrix} e^{\delta x} & e^{-\delta x} \\ \delta e^{\delta x} & -\delta\, e^{-\delta x} \end{pmatrix} = W[\delta, 0] \begin{pmatrix} e^{\delta x} & 0 \\ 0 & e^{-\delta x} \end{pmatrix} = W[\delta, 0]\Delta[\delta x].$$

Let the plane wave solutions in the free region to the left of the s-barrier be

$$A_s\, e^{ikx} + A'_s\, e^{-ikx},$$

and that within the barrier

$$B_s\, e^{\rho x} + B'_s\, e^{-\rho x}.$$

Thus, the plane waves in the extreme left region will be given in terms of A_0 (incoming) and A'_0 (reflected). The final factors on the extreme right of an N-barrier system will be A_N (transmitted) and A'_N (to be set to zero below).

The continuity equations at the two edges of the s-barrier read

$$W[ik, (s-1)(L+d)][A_{s-1} \quad A'_{s-1}]^t = W[\rho, (s-1)(L+d)][B_s \quad B'_s]^t,$$

$$W[\rho, sL+(s-1)d][B_s \quad B'_s]^t = W[ik, sL+(s-1)d][A_s \quad A'_s]^t, \qquad s = 1, 2, \ldots, N.$$

Applying successively these matrix equations, we can express the matrix equation between (A_0, A'_0) and (A_N, A'_N),

$$\begin{aligned} \begin{bmatrix} A_0 \\ A'_0 \end{bmatrix} &= \prod_{s=1}^{N} W^{-1}[ik, (s-1)(L+d)]W[\rho, (s-1)(L+d)]W^{-1} \\ &\quad \times [\rho, sL+(s-1)d]W[ik, sL+(s-1)d] \begin{bmatrix} A_N \\ A'_N \end{bmatrix} \\ &= \Delta[ikd]\{\Delta[-ikd]W^{-1}[ik, 0]W[\rho, 0]\Delta[-\rho L]W^{-1}[\rho, 0]W[ik, 0]\}^N \\ &\quad \times \Delta[ikNL + ik(N-1)d] \begin{bmatrix} A_N \\ A'_N \end{bmatrix}. \end{aligned}$$

Introducing the matrix M:

$$M = \Delta[-\mathrm{i}kd]W^{-1}[\mathrm{i}k,0]W[\rho,0]\Delta[-\rho L]W^{-1}[\rho,0]W[\mathrm{i}k,0],$$

the previous matrix equation can be rewritten as follows:

$$\begin{bmatrix} A_0 \\ A_0' \end{bmatrix} = \Delta[\mathrm{i}kd]\, M^N\, \Delta[\mathrm{i}kNL + \mathrm{i}k(N-1)d]\, \begin{bmatrix} A_N \\ A_N' \end{bmatrix}. \tag{28}$$

A straightforward calculation shows that

$$M = \begin{pmatrix} F & G^* \\ G & F^* \end{pmatrix}$$

with

$$F = \frac{1}{T\,\mathrm{e}^{\mathrm{i}k(L+d)}} = \frac{1}{|T|\,\mathrm{e}^{\mathrm{i}\alpha}} \qquad \text{and} \qquad G = \frac{R\,\mathrm{e}^{\mathrm{i}kd}}{T\,\mathrm{e}^{\mathrm{i}kL}} = -\mathrm{i}\frac{|R|}{|T|}\,\mathrm{e}^{\mathrm{i}kd}.$$

Observe that M has unit determinant, $|F|^2 - |G|^2 = 1$. For an incoming wave from the left, $A_N' = 0$, equation (28) gives

$$\begin{aligned} A_0 &= (M^N)_{11}\,\mathrm{e}^{\mathrm{i}kN(L+d)}\,A_N, \\ A_0' &= (M^N)_{21}\,\mathrm{e}^{\mathrm{i}k[NL+(N-2)d]}\,A_N, \end{aligned} \tag{29}$$

where the sub-indices specify the matrix element. Thus, the reflection and transmission amplitudes are given by

$$\begin{aligned} R_S^{(N)} &= \mathrm{e}^{-2\mathrm{i}kd}(M^N)_{21}/(M^N)_{11}, \\ T_S^{(N)} &= \mathrm{e}^{-\mathrm{i}kN(L+d)}/(M^N)_{11}. \end{aligned} \tag{30}$$

For two and three barriers, we have respectively

$$(M^2)_{11} = F^2 + |G|^2 \qquad \text{and} \qquad (M^3)_{11} = F(F^2+|G|^2) + |G|^2(F+F^*).$$

Consequently, in agreement with our previous results,

$$T_S^{(2)} = 1\bigg/\left[F^2\mathrm{e}^{2\mathrm{i}k(L+d)}\left(1+\frac{|G|^2}{F^2}\right)\right] = T^2/D$$

and

$$T_S^{(3)} = 1\bigg/\left\{F^3\mathrm{e}^{3\mathrm{i}k(L+d)}\left[\left(1+\frac{|G|^2}{F^2}\right)^2 + \frac{|G|^2}{F^4}\right]\right\} = T^3\bigg/\left[D^2\left(1+\frac{|R|^2|T|^2}{D^2}\mathrm{e}^{4\mathrm{i}\alpha}\right)\right].$$

These results are easy to find since we already knew the particle expressions. We now derive the $N = 4$ transmission amplitude. By using

$$(M^4)_{11} = (F^2+|G|^2)^2 + |G|^2(F+F^*)^2,$$

from equation (30), we obtain

$$T_S^{(4)} = 1\bigg/\left\{F^4\mathrm{e}^{4\mathrm{i}k(L+d)}\left[D^2 + \frac{|G|^2}{F^2}\left(1+\frac{|F|^2}{F^2}\right)^2\right]\right\}. \tag{31}$$

The leading term will be T^4/D^3. *This term must be factorized*. The remaining expression can and must be expressed in terms of $|R|^2$, $|T|^2$ and $\mathrm{e}^{2\mathrm{i}\alpha}$. By adding and subtracting, in the square bracket of the denominator of equation (31) a D^3 term, and by recalling that $|F|^2 = 1 + |G|^2$, we can rewrite the transmission amplitude as follows:

$$\begin{aligned} T_S^{(4)} &= 1\bigg/\left\{F^4\mathrm{e}^{4\mathrm{i}k(L+d)}\left[D^3 - \frac{|G|^2}{F^2}D^2 + \frac{|G|^2}{F^2}\left(D+\frac{1}{F^2}\right)^2\right]\right\} \\ &= 1\bigg/\left[F^4\mathrm{e}^{4\mathrm{i}k(L+d)}\left(D^3 + 2\frac{|G|^2}{F^4}D + \frac{|G|^2}{F^6}\right)\right] \\ &= T^4\bigg/\left[D^3\left(1+2\frac{|R|^2|T|^2}{D^2}\mathrm{e}^{4\mathrm{i}\alpha} + \frac{|R|^2|T|^4}{D^3}\mathrm{e}^{6\mathrm{i}\alpha}\right)\right]. \end{aligned} \tag{32}$$

To obtain the particle sum, we must define the denominator as a series in the numerator. For $N = 4$, we find up order $|T|^8$,

$$\frac{T^4}{D^3}\left\{1 - 2\,|R|^2\,\mathrm{e}^{4\mathrm{i}\alpha}\,\frac{|T|^2}{D^2} + \left(3\,|R|^4\,\mathrm{e}^{8\mathrm{i}\alpha} - |R|^2\,\mathrm{e}^{6\mathrm{i}\alpha}\right)\,\frac{|T|^4}{D^4} + \cdots\right\}. \tag{33}$$

For the individual particle contributions, we must expand the D terms in the numerator. The above result agrees with a direct, but more tedious, particle calculation to this order. The maximum and minimum values of the transmission probability are obtained by following the procedure of the previous section. This results in

- minimum values of the transmission probability

$$\mathcal{T}^{(4)}_{\text{wave}}[\cos\alpha = \pm|T|/\sqrt{6}] = |T|^2/(1 + 5|R|^2/27), \tag{34}$$

$$\mathcal{T}^{(4)}_{\text{wave}}[\cos\alpha = \pm 1] = 1/(1 + 8|R|^2/|T|^4)^2, \tag{35}$$

- maximum values of the transmission probability

$$\mathcal{T}^{(4)}_{\text{wave}}[\cos\alpha = 0] = \mathcal{T}^{(4)}_{\text{wave}}[\cos\alpha = \pm|T|/\sqrt{2}] = 1. \tag{36}$$

6. Conclusions

In this paper we have considered tunneling through two, three and four identical barriers. Our approach is that of considering the reflection and transmission amplitudes successively for each barrier, the so-called *particle approach*. This is directly relevant to situations in which the incoming (single) wave packet is small compared to the inter-barrier distance d. However, it also yields the wave limit if all particle contributions are summed and considered as a single outgoing reflected and transmitted wave. In this wave limit, one encounters resonance phenomena. We have re-derived the condition for resonances and expressed them in terms of $\cos\alpha$. Resonances do not occur in the particle limit. We have exhibited numerically the transition from the wave to particle limit for the case of twin tunneling by plotting the transmission probability as a function of the inter-barrier distance d. In the particle limit, oscillations die out.

The calculation of the individual particle terms becomes cumbersome for four barriers and higher. Care must be taken to sum coherent contributions which are produced from different paths within the potential structure. For these cases it is simpler to invert our procedure and first calculate the wave limit amplitude. This has been done, as an example, for the four barrier case in the previous section with the help of a matrix method and the rules given for its representation in 'particle' form, i.e. in terms of R and T and powers of $\mathrm{e}^{2\mathrm{i}\alpha}$. A series expansion of the denominators completes the procedure.

There are a number of consequences of our analysis which merit a mention.

(1) The resonance conditions for multiple identical barrier tunneling will automatically extrapolate into the case of $E > V_0$, i.e. for the above barrier diffusion. Thus, there are two classes of above barrier resonances.
   (a) When the above barrier resonance occurs for a single barrier, $|T| = 1$, independently of the value of d we have $T^{(2)}_S = T^2$, where T is now the above barrier expression, i.e. $\rho \to \mathrm{i}\,q$ with $q = \sqrt{2m(E - V_0)}/\hbar$ in equation (2).
   (b) When $|T| \neq 1$ but $\phi + kd = (n + 1/2)\,\pi$ as in the tunneling case. These are additional resonances corresponding to constructive interference effects of the twin barriers possible in the wave limit even if each single barrier is not resonant.

(2) For twin barriers, the conditions for tunnel resonance require *identical* barriers. For two different barriers, either in width or height or both, the formula for the transmission amplitude becomes

$$T_S^{(1+1)} = T_1 T_2 / \left(1 - R_1 R_2 \, \mathrm{e}^{2ikd}\right),$$

with the indices indicating the individual barrier amplitudes. Now, for no value of kd will this be of unit modulus. We expect the same to occur also for higher numbers of barriers.

(3) Consider twin tunneling at resonance. The phase of $T_S^{(2)}$ is totally given by the phase of T^2. The time calculated at $x = 2L + d$, the exit point for transmission, is

$$t = \left[\frac{\partial k}{\partial E}(x - 2L) + 2\frac{\partial \phi}{\partial E}\right]_{x=2L+d,k=k_0} = \frac{d}{v_g} + 2\left[\frac{\partial \phi}{\partial E}\right]_{k=k_0},$$

where v_g is the group velocity in the free space. Thus, due to the linear term in d, there is no generalized Hartman effect [15] at resonance.

Finally, we wish to place our results in a broader context. The existence of wave and particle limits is related to the relative sizes of the incoming wave packet and the size of the potential structure. The results of this paper are an example of the physical relevance of wave packet dimensions. Interesting applications occur in particle oscillation phenomena [20–23], relativistic tunneling [24–26], laser interaction with dielectric blocks [27, 28], and, generally speaking, in all interference based results. These features are generally neglected in the literature where only single plane waves are used. Plane waves are a legitimate operational tool, but working *only* with single plane waves (infinite wave packet size) may obfuscate significant physical insight.

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