

Above barrier Dirac multiple scattering and resonances

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Abstract. We extend an above barrier analysis made with the Schrödinger equation to the Dirac equation. We demonstrate the perfect agreement between the barrier results and back to back steps. This implies the existence of multiple (indeed infinite) reflected and transmitted wave packets. These packets may be well separated in space or partially overlap. In the latter case interference effects can occur. For the extreme case of total overlap we encounter resonances. The conditions under which resonance phenomena can be observed is discussed and illustrated by numerical calculations.

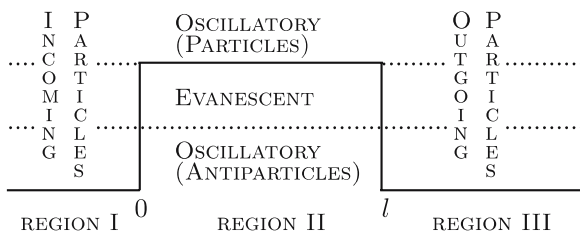
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1 Introduction

This paper considers the *above barrier* solutions of the Dirac equation for an electrostatic one-dimensional (z axis) potential,

$$V(z) = \begin{cases} 0, & z < 0 \quad (\text{region I}), \\ V_0, & 0 < z < l \quad (\text{region II}), \\ 0, & z > l \quad (\text{region III}). \end{cases}$$

It is very difficult and probably even confusing to treat, in a single article, all interactions of plane waves or wave packets with a barrier potential using the Dirac equation. This is because the physical content depends upon the energy of the incoming (particle) wave. In the figure below we depict the three potential regions. Also shown is the energy divided into three zones.



The upper energy zone, $E > V_0 - m$, is the one of interest to this work and involves diffusion phenomena. In the so called Klein zone [1], $E < V_0 - m$, oscillatory solutions exist in the barrier region. These are antiparticles [2–6]. Indeed, antiparticles see an opposite electrostatic potential to that seen by the particles and hence they will see a well potential where the particles see a barrier. The antiparticles thus live above the well potential and are legitimately oscillatory in form. In the tunnelling zone only evanescent waves exist in the barrier region [7, 8]. Of particular interest here is the possibility of an Hartman-like effect [9–11].

No barrier analysis can be interpreted without an understanding of the step potential results. In a latter section, we shall argue, for the step, that while pair production is innate in the Klein zone there is no pair production for above barrier diffusion where the non-relativistic limit reproduces the standard Schrödinger solutions. There is of course no Schrödinger limit for the Klein zone. The Klein zone of the step is characterized by the Klein paradox in which a reflection probability greater than the incoming probability occurs. The excess particle number (or charge) implies pair production. For above step diffusion this paradox does not exist and hence pair production is absent.

For the case of above barrier diffusion, we shall demonstrate in detail the equivalence of a two-step calculation and the barrier results. Such an equivalence has previously

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been demonstrated for the Schrödinger equation [12]. This method of calculation which employs the simple step results is not new. Multiple-step calculations have, for example, been used in the WKB applications to various potentials [13] and for the barrier potential in the Dirac equation in the Klein zone [14]. However, these authors employ the method only as a convenient mathematical tool. We, on the contrary, emphasize its physical significance in terms of multiple reflected and transmitted peaks (when the barrier width is much greater than the wave packets widths). The exit times for each can be calculated using the stationary phase method (SPM) [15, 16]. They occur with time intervals equal to twice the barrier width divided by the group velocity over the barrier.

The combined summed expressions for the reflection and transmission coefficients contain the well known resonance phenomena. We shall discuss under which conditions this resonance effect occurs and when the effect “breaks up” and the multiple peaks appear. Some numerical calculations will help us to illustrate this transition from an effective single outgoing wave packet (coherence) to essentially independent multiple wave packets (de-coherence).

In the next section we will give the necessary formulas and conditions assumed for our calculations. In Sect. 3, we consider the plane wave solutions for a step potential and more specifically for three related but distinct steps. One upward step at $z = 0$ and two downward steps at $z = 0$ and $z = l$. The extra phases that appear in the last case are essential for the calculation of the times of the outgoing peaks. We will then calculate the back to back step potential obtaining the individual amplitudes for the (infinite) reflected and transmitted terms. Each can be associated with a wave packet after integrating with a suitable convolution function. In Sect. 4, we calculate directly the plane wave solutions for the reflection and transmission coefficients for a barrier and make evident their equivalence to the sum of the results from the previous section. Section 5 discusses the question of resonance and points out that this phenomenon requires specific conditions to occur. We conclude in Sect. 6 with a resumé of our results.

2 Dirac solutions in a constant potential

The free Dirac equation reads

$$(i\gamma^\mu\partial_\mu - m)\Psi(\mathbf{r}, t) = 0, \quad (1)$$

with the gamma matrices satisfying $\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}$. It has four well known independent plane wave solutions

$$u^{(1,2)}(\mathbf{p}) \exp[i\mathbf{p}\cdot\mathbf{r} - iEt], \quad (E = |E|),$$

$$\text{and } u^{(3,4)}(\mathbf{p}) \exp[i\mathbf{p}\cdot\mathbf{r} - iEt] \quad (E = -|E|),$$

where $|E| = \sqrt{\mathbf{p}^2 + m^2}$. Using the Pauli-Dirac set of gamma matrices

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{and} \quad \boldsymbol{\gamma} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ -\boldsymbol{\sigma} & 0 \end{pmatrix},$$

the spinorial solutions are (for polarized states in the z -direction)

$$u^{(s)}(\mathbf{p}) = N \begin{pmatrix} \boldsymbol{\sigma}\cdot\hat{\mathbf{p}}\chi^{(s)} \\ E+m\chi^{(s)} \end{pmatrix}$$

$$\text{and } u^{(s+2)}(\mathbf{p}) = N \begin{pmatrix} -\frac{\boldsymbol{\sigma}\cdot\hat{\mathbf{p}}}{|E|+m}\chi^{(s)} \\ \chi^{(s)} \end{pmatrix}, \quad (2)$$

where $s = 1, 2$ and

$$\chi^{(1)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \chi^{(2)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

with $N = \sqrt{(|E| + m)}$: the covariant normalization choice such that $u^{(s)\dagger}u^{(s)} = u^{(s+2)\dagger}u^{(s+2)} = 2|E|$. We recall that the free Dirac Hamiltonian is

$$H_0 = \boldsymbol{\alpha}\cdot\hat{\mathbf{p}} + \beta m = \begin{pmatrix} m & \boldsymbol{\sigma}\cdot\hat{\mathbf{p}} \\ \boldsymbol{\sigma}\cdot\hat{\mathbf{p}} & -m \end{pmatrix}. \quad (3)$$

The different signatures of the energies between s and $s+2$ spinors follow readily from the alternative non-covariant form of the Dirac equation

$$i\partial_t\Psi(\mathbf{r}, t) = H_0\Psi(\mathbf{r}, t), \quad (4)$$

and the left hand side yields $E\Psi(\mathbf{r}, t)$ in all four cases while the right hand side yields $\pm|E|$ as the case may be. Actually, for $\Psi^{(s)}(\mathbf{r}, t)$ we appear to get a simple identity because we have conventionally used E rather than $|E|$ in its spinor representation. However, when $\mathbf{p} \equiv \mathbf{0}$ (the rest frame case) the Hamiltonian reduces to $m\gamma^0$ and the above equation yields $E = +m$ for $s = 1, 2$ and $E = -m$ for $s + 2 = 3, 4$. These solutions are oscillating solutions, valid when $E \geq m$ or $E \leq -m$. There are also evanescent solutions obtained from the above with the substitution $\mathbf{p} \rightarrow i\mathbf{p}$ for which the spatial dependence becomes $\exp[\mp\mathbf{p}\cdot\mathbf{r}]$ and occurs when $-m < E < m$.

Since we shall need the solutions for step and barrier potentials, we rewrite the above solutions in the presence of a constant potential V_0 . Consider an *electrostatic potential* $A_\mu = (A_0, \mathbf{0})$ included (via minimal coupling) in the Dirac equation

$$(i\gamma^\mu\partial_\mu - e\gamma^0A_0 - m)\Psi(\mathbf{r}, t) = 0 \quad (5)$$

or

$$i\partial_t\Psi(\mathbf{r}, t) = (H_0 + V_0)\Psi(\mathbf{r}, t), \quad (6)$$

where $V_0 = -eA_0$ (charge $-e$). For a stationary solution $\Psi(\mathbf{r}, t) \propto \exp[-iEt]$, we obtain

$$H_0\Psi(\mathbf{r}, t) = (E - V_0)\Psi(\mathbf{r}, t). \quad (7)$$

The spinorial solutions are now

$$u^{(s)}(\mathbf{q}; V_0) = \tilde{N} \begin{pmatrix} \boldsymbol{\sigma}\cdot\hat{\mathbf{q}}\chi^{(s)} \\ E - V_0 + m\chi^{(s)} \end{pmatrix}, \quad (8)$$

for $E - V_0 > m$, and

$$u^{(s+2)}(\mathbf{q}; V_0) = \tilde{N} \begin{pmatrix} -\frac{\boldsymbol{\sigma} \cdot \mathbf{q}}{|E - V_0| + m} \chi^{(s)} \\ \chi^{(s)} \end{pmatrix}, \quad (9)$$

for $E - V_0 < -m$, where $(E - V_0)^2 - \mathbf{q}^2 = m^2$ and $\tilde{N} = \sqrt{(|E - V_0| + m)}$. This shows that the two sets of solutions $u^{(s)}$ and $u^{(s+2)}$ are not determined by the sign of E but by whether $E > V_0 + m$ or $E < V_0 - m$, the latter being the defining condition for the Klein zone. Hence, E may be fixed but the solutions depend upon whether in any given region the energy is above or below the potential.

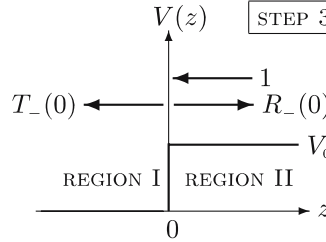
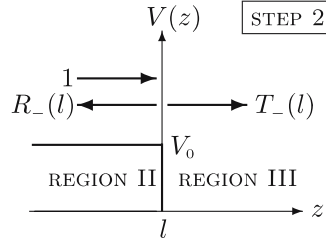
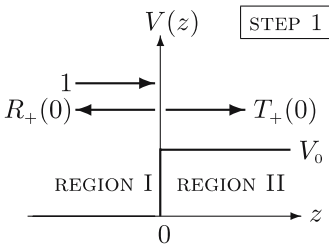
In any constant potential region *only two* solutions exist for a given E (be they oscillatory or evanescent). This fact is essential for a standard plane wave analysis. Because the Dirac equation is a first order equation in the spatial derivatives, for a step-wise continuous potential only continuity of the wave function exists. There is no loss of information with respect to the Schrödinger continuity (wave function and its spatial derivative) since continuity of the “small” component of the Dirac spinor yields in the non-relativistic limit the continuity of the Schrödinger wave function’s spatial derivative. Thus, continuity of the Dirac wave function implies four conditions at each interface, one for each spinor component. However, since the *signs* of the momenta are a priori arbitrary, we have two conditions which determine the spinor. Hence, for consistency, there can be *only two independent spinors* in each region and these must correspond to different helicity states or orthogonal combinations of them.

3 The two-step approach

Let us treat the barrier diffusions as an application of a two-step process. We have one upward step at $z = 0$ and one downward step at $z = l$. We assume an incoming above potential, positive helicity, plane wave state given by (the normalization of the spinor is inessential here)

$$\begin{pmatrix} 1 \\ 0 \\ p \\ E + m \\ 0 \end{pmatrix} \exp[i(pz - Et)],$$

with $E = \sqrt{p^2 + m^2}$. We shall need three step diffusions, the first at $z = 0$ both for incoming waves from the left and from the right. The second one is at $z = l$ only for incoming waves from the left. For reflection and transmission from an upward/downward potential we shall use the suffixes $+/-$.



For the first step, the solutions in region I and II are respectively given by

$$\begin{aligned} \Psi_I(z, t) = & \left\{ \begin{pmatrix} 1 \\ 0 \\ p \\ E + m \\ 0 \end{pmatrix} \exp[ipz] \right. \\ & \left. + R_+(0) \begin{pmatrix} 1 \\ 0 \\ -p \\ E + m \\ 0 \end{pmatrix} \exp[-ipz] \right\} \\ & \times \exp[-iEt], \\ \Psi_{II}(z, t) = & T_+(0) \begin{pmatrix} 1 \\ 0 \\ q \\ E - V_0 + m \\ 0 \end{pmatrix} \exp[iqz] \exp[-iEt], \end{aligned} \quad (10)$$

with $q = \sqrt{(E - V_0)^2 - m^2}$. All helicity (spin) flip terms (the other independent spinor solutions) here and elsewhere turn out to be absent, so we exclude them a priori for simplicity. Continuity at $z = 0$ yields

$$1 + R_+(0) = T_+(0)$$

$$\text{and } 1 - R_+(0) = T_+(0) \frac{q(E + m)}{p(E - V_0 + m)} = T_+(0) \frac{b}{a},$$

where $a = \sqrt{(E - V_0 + m)(E - m)}$ and $b = \sqrt{(E - V_0 - m)(E + m)}$ ($a > b$). Thus, we obtain

$$\text{Step 1: } \begin{cases} R_+(0) = (a - b) / (a + b), \\ T_+(0) = 2a / (a + b), \end{cases} \quad (11)$$

from which it follows that

$$1 - |R_+(0)|^2 = \frac{b}{a} |T_+(0)|^2.$$

While $|R_+(0)|^2$ is obviously the reflection probability, the “transmission” probability must therefore be (b/a)

$|T_+(0)|^2$. A demonstration of this for wave packets (albeit with the aid of some approximations) is given in the appendix. Since $|R_+(0)| < 1$, we do not have a Klein paradox here so no pair production is involved.

To understand physically the significance of single reflection and/or transmission coefficients one needs to use the stationary phase method for wave packets (normalized convolution integral of plane waves). This method, introduced by Stokes and Kelvin [1], estimates the position of the maximum of the wave packet by using the simple concept that, far from the vanishing derivative of the phase, the argument of the convolution integral oscillates many times and produces destructive interference. Consequently, the maximum of the wave packet occurs where the derivative of the phase vanishes [16]. For example, consider an amplitude

$$\Phi(z, t) = \int dk g(k) \exp[i\theta(k)] \exp[i(kz - Et)]$$

modulated by a real function $g(k)$, with a single steep maximum at k_0 . The time-space relationship for the maximum (maxima if Φ has spinor components) is given by

$$t = \left(\frac{dk}{dE} \right)_0 z + \left(\frac{d\theta}{dE} \right)_0,$$

and the zero suffix means that the term in parentheses is calculated at $k = k_0$. The delay factor is $(d\theta/dE)_0$. The group velocity is $v_g = (dE/dk)_0$. In our analysis the *primary* modulation function, $g(p)$, is that of the incoming wave packet

$$\Phi_{I,\text{inc}}(z, t) = \int_{p_{\min}}^{+\infty} dp g(p) \begin{pmatrix} 1 \\ 0 \\ p \\ E+m \\ 0 \end{pmatrix} \exp[i(pz - Et)]. \quad (12)$$

The “effective” modulation function in any given region is then given by $g A u_i$ where A is the plane wave amplitude (e.g. $R_+(0)$ or $T_+(0)$), and u_i stands for the spinor element considered. For each separate spinor component one must calculate the group velocity and eventual delay times. However, with our choice, all non-zero spinor components are real, so that there is no contribution to θ from them. Thus, with real $R_+(0)$ and $T_+(0)$ we have no time delay. It is true that the group velocities depend upon the spinor components momentum dependence (which shifts the value of k_0). However, this should be negligible for a very sharply peaked modulation function. It is demonstrably negligible in the two limits: the non-relativistic (NR) one where one can simply ignore the small components, and in the ultra-relativistic (UR) one when the (“small”) component $q/(E - V_0 + m)$ tends to one.

Returning to our calculations, we give without details the results for the other two steps. For step 2, we find

$$\text{Step 2: } \begin{cases} R_-(l) = [(b-a)/(a+b)] \exp[2iq l], \\ T_-(l) = [2b/(a+b)] \exp[i(q-p)l], \end{cases} \quad (13)$$

and for step 3,

$$\text{Step 3: } \begin{cases} R_-(0) = (b-a)/(a+b), \\ T_-(0) = 2b/(a+b). \end{cases} \quad (14)$$

The first of the barrier transmitted amplitudes is thus obtained by multiplying the “transmitted” amplitude of step 1, $T_+(0)$, by the transmission amplitude of step 2, $T_-(l)$,

$$[4ab/(a+b)^2] \exp[i(q-p)l].$$

The exit time is calculated after including the plane wave phase in region III,

$$t = \left(\frac{dp}{dE} \right)_0 z + \left(\frac{d\theta}{dE} \right)_0,$$

where $\theta = (q-p)l$. Thus, at $z = l$ we find

$$t = \left[\left(\frac{dp}{dE} \right)_0 + \left(\frac{dq}{dE} \right)_0 - \left(\frac{dp}{dE} \right)_0 \right] l = \left(\frac{dq}{dE} \right)_0 l.$$

This is just the time for a wave packet in region II with group velocity $(dE/dq)_0$ to travel a distance l (barrier width). At step 2 there is also a reflected amplitude given by $T_+(0)R_-(l)$. The corresponding wave packet travels back towards $z = 0$ and the second reflected wave exits into the left region I, with amplitude (unmodulated) $T_+(0)R_-(l)T_-(0)$ at the expected time

$$t = 2(dq/dE)_0 l.$$

The whole procedure may then be repeated ad infinitum.

Below, we list the first few individual reflected and transmitted waves together with the expressions for the general n th wave:

$$\begin{aligned} R_1 &= R_+(0) = \frac{a-b}{a+b}, \\ R_2 &= T_+(0) R_-(l) T_-(0) = \frac{4ab(b-a)}{(a+b)^3} \exp[2iq l], \\ R_3 &= T_+(0) R_-(l) R_-(0) R_-(l) T_-(0) \\ &= \frac{4ab(b-a)}{(a+b)^3} \exp[2iq l] \left(\frac{b-a}{a+b} \exp[iql] \right)^2, \\ &\vdots \\ R_n &= T_+(0) R_-(l) [R_-(0) R_-(l)]^{n-2} T_-(0) \\ &= \frac{4ab(b-a)}{(a+b)^3} \exp[2iq l] \left(\frac{b-a}{a+b} \exp[iql] \right)^{2n-4}. \end{aligned} \quad (15)$$

For the transmitted amplitude, we have

$$\begin{aligned}
 T_1 &= T_+(0) T_-(l) = \frac{4ab}{(a+b)^2} \exp[i(q-p)l], \\
 T_2 &= T_+(0) R_-(l) R_-(0) T_-(l) \\
 &= \frac{4ab}{(a+b)^2} \exp[i(q-p)l] \left(\frac{b-a}{a+b} \exp[iql] \right)^2, \\
 T_3 &= T_+(0) [R_-(l) R_-(0)]^2 T_-(l) \\
 &= \frac{4ab}{(a+b)^2} \exp[i(q-p)l] \left(\frac{b-a}{a+b} \exp[iql] \right)^4, \\
 &\vdots \\
 T_n &= T_+(0) [R_-(l) R_-(0)]^{n-1} T_-(l) \\
 &= \frac{4ab}{(a+b)^2} \exp[i(q-p)l] \left(\frac{b-a}{a+b} \exp[iql] \right)^{2n-2}.
 \end{aligned} \tag{16}$$

At each step one can check (in accordance with our previous discussion) that probability is conserved. If the individual wave packets are well separated (see the following section) the probability of, say, the n th transmitted wave will be just $|T_n|^2$ since it travels in a potential free region. A straightforward calculation then shows that the total transmission probability is,

$$\sum_{n=1}^{\infty} |T_n|^2 = \frac{16a^2b^2}{(a+b)^4} \left[1 - \left(\frac{b-a}{a+b} \right)^4 \right]^{-1} = \frac{2ab}{a^2+b^2}. \tag{17}$$

It is to be noted that this sum is independent of the barrier width l . A similar calculation can be performed for the region I reflected probabilities. This yields

$$\begin{aligned}
 \sum_{n=1}^{\infty} |R_n|^2 &= \left(\frac{a-b}{a+b} \right)^2 \\
 &+ \frac{16a^2b^2(b-a)^2}{(a+b)^6} / \left[1 - \left(\frac{b-a}{a+b} \right)^4 \right] \\
 &= \frac{(a-b)^2}{a^2+b^2}.
 \end{aligned} \tag{18}$$

Consequently, as expected

$$\sum_{n=1}^{\infty} \left\{ |R_n|^2 + |T_n|^2 \right\} = 1. \tag{19}$$

Our multiple peak interpretation is thus consistent with overall probability conservation. Finally, we observe that the time interval Δt between two successive outgoing peaks, in either of the potential free regions is

$$\Delta t = 2 \left(\frac{dq}{dE} \right)_0 l = 2 \left(\frac{E-V_0}{q} \right)_0 l.$$

4 The barrier analysis

Let us now perform the standard stationary plane wave analysis for the barrier – again neglecting a priori (for simplicity) spin flip. We have

$$\begin{aligned}
 \text{Region I: } z < 0, & \left(\begin{array}{c} 1 \\ 0 \\ p \\ E+m \\ 0 \end{array} \right) \exp[ipz] + R \left(\begin{array}{c} 1 \\ 0 \\ p \\ E+m \\ 0 \end{array} \right) \\
 & \times \exp[-ipz], \\
 \text{Region II: } 0 < z < l, & A \left(\begin{array}{c} 1 \\ 0 \\ q \\ E-V_0+m \\ 0 \end{array} \right) \exp[iqz] \\
 & + B \left(\begin{array}{c} 1 \\ 0 \\ q \\ E-V_0+m \\ 0 \end{array} \right) \exp[-iqz], \\
 \text{Region III: } l < z, & T \left(\begin{array}{c} 1 \\ 0 \\ p \\ E+m \\ 0 \end{array} \right) \exp[ipz].
 \end{aligned}$$

Continuity at $z = 0$ yields

$$\left(\begin{array}{c} 1 \\ R \end{array} \right) = \frac{1}{2a} \left(\begin{array}{cc} a+b & a-b \\ a-b & a+b \end{array} \right) \left(\begin{array}{c} A \\ B \end{array} \right).$$

From continuity at $z = l$,

$$\left(\begin{array}{cc} 1 & 1 \\ 1 & -1 \end{array} \right) \left(\begin{array}{c} A \exp[iql] \\ B \exp[-iql] \end{array} \right) = \left(\begin{array}{c} 1 \\ a/b \end{array} \right) T \exp[ipl].$$

Consequently,

$$\begin{aligned}
 \left(\begin{array}{c} A \\ B \end{array} \right) &= \frac{1}{2} \left(\begin{array}{cc} \exp[-iql] & 0 \\ 0 & \exp[iql] \end{array} \right) \left(\begin{array}{cc} 1 & 1 \\ 1 & -1 \end{array} \right) \\
 & \times \left(\begin{array}{c} 1 \\ a/b \end{array} \right) T \exp[ipl] \\
 &= \frac{\exp[ipl]}{2b} \left[\begin{array}{c} (b+a) \exp[-iql] \\ (b-a) \exp[iql] \end{array} \right] T.
 \end{aligned}$$

Using this equation to eliminate A and B from the continuity equation at $z = 0$ gives

$$\begin{aligned}
 \left(\begin{array}{c} 1 \\ R \end{array} \right) &= \frac{\exp[ipl]}{4ab} \\
 & \times \left[\begin{array}{c} (a+b)^2 \exp[-iql] - (a-b)^2 \exp[iql] \\ (a^2-b^2) \exp[-iql] - (a^2-b^2) \exp[iql] \end{array} \right] T,
 \end{aligned}$$

whence

$$R = i(b^2 - a^2) \sin[ql] / [2ab \cos[ql] - i(a^2 + b^2) \sin[ql]]. \tag{20}$$

and

$$T = 2ab \exp[-ip l] / [2ab \cos[ql] - i(a^2 + b^2) \sin[ql]] . \quad (21)$$

These amplitudes satisfy,

$$|R|^2 + |T|^2 = 1 . \quad (22)$$

If treated as single wave packets (one for R and one for T) the peaks emerge at a *common* time determined by their common denominators

$$t_R = t_T = \left(\frac{d\theta}{dE} \right)_0 , \quad \text{with } \tan \theta = \frac{a^2 + b^2}{2ab} \tan[ql] .$$

Note that the phase factor $\exp[-ip l]$ in T has been cancelled by the plane wave factor $\exp[ip z]$ calculated at $z = l$. The i factor in R is momentum independent so it does not contribute to the time equation. Also for completeness, we recall that a and b are real.

It is always a little surprising that the two exit times coincide. It also seems a little strange that the reflection time delay (t_R), compared to instantaneous reflection, depends upon the barrier width l . Is the assumption of single reflection and transmission peaks correct? This depends critically upon the size/width of the incoming wave packet. Before discussing further what seems a result contrary to the infinite multiple waves described in the previous section, we must make the following important observation:

$$T = \sum_{n=1}^{\infty} T_n \quad \text{and} \quad R = \sum_{n=1}^{\infty} R_n . \quad (23)$$

Indeed while we have begun our analysis from the two-step calculation we could have arrived at exactly the same result by expanding the denominators of R and T in an infinite series. The treatment of R and T as single wave packets represents the limit situation in which all the infinite reflected wave packets overlap and similarly for the transmitted wave packets. Plane waves can in this sense be considered as infinitely extended wave packets and they thus satisfy automatically this coherence condition. The two approaches are perfectly equivalent. A single peak may break up under suitable conditions into multiple peaks, or equivalently, multiple peaks may coalesce under suitable conditions into a single peak.

5 Resonance phenomena

One of the characteristics of the single wave packet situation is manifest in the expressions for R and T . The reflection coefficient R vanishes when $\sin[ql] = 0$. It follows that for values of l such that

$$l = n\pi / q \quad (n = 0, 1, \dots) ,$$

we obtain complete transmission. In Fig. 1, we show, for different values of V_0 , E_0 and m , the typical resonance

curves for $|T|$ (dotted lines). In principle it extends to infinite values of l . Any normalizing convolution integral will modify this. First, an integration over p , unless very “tight” about any p_0 value, will imply some averaging of this curve. For a spread in momentum Δp such that $\Delta q \geq \pi q_0$ the resonance effect will be completely averaged out. Secondly, for an incoming wave packet with finite spatial spread, say $\Delta z \sim 1/\Delta p$, we can ask when the multiple peaks, described in the previous section, are well separated. This occurs when the distance between two peaks is much greater than Δz . Thus, for complete decoherence

$$v_{g,III} \Delta t \gg \Delta z \sim \frac{1}{\Delta p} ,$$

where $v_{g,III}$ is the group velocity in region III and Δt the time interval between successive peaks. Now $\Delta t = 2l/v_{g,II}$,

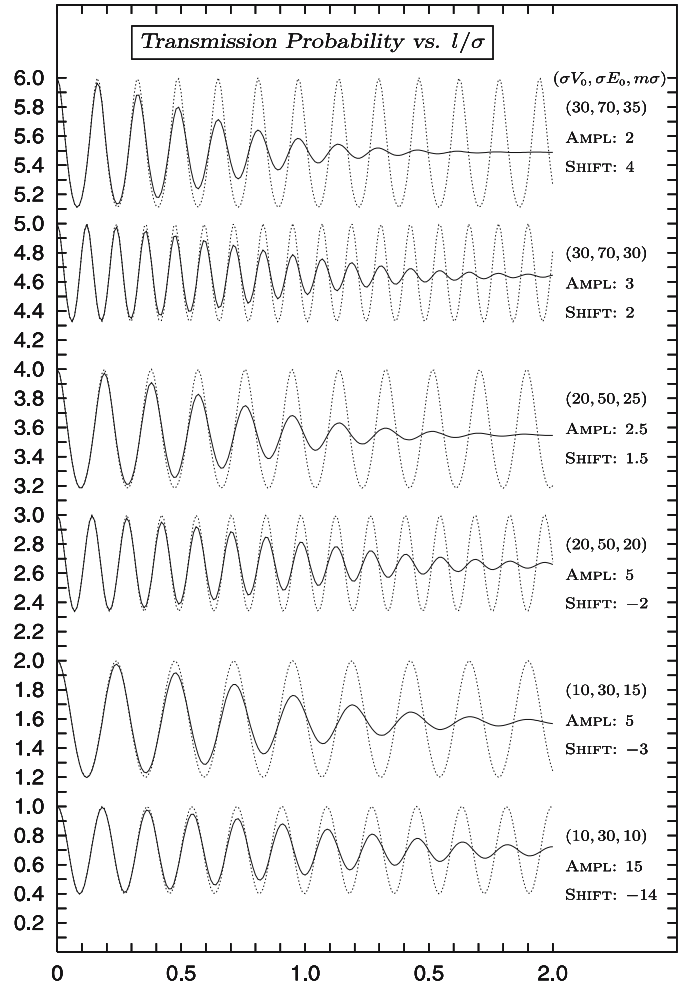


Fig. 1. Barrier width dependence of the transmission probability for different values of σV_0 , σE_0 and $m\sigma$ ($\hbar = c = 1$). The transmission probability $|T(p_0)|^2$ (see dotted lines) shows the typical resonance curves for plane waves. In our numerical calculations, performed for asymptotic times, we have used a gaussian incoming wave packet of width σ . The transmission probability $\sqrt{2/\pi} \sigma \int dp \exp[-\sigma^2(p - p_0)^2] |T(p)|^2$ (see solid lines) exhibits the tendency to the constant value $2a_0 b_0 / (a_0^2 + b_0^2)$ as predicted by the multiple scattering analysis

hence multiple peaks will be clearly separated when

$$2l \frac{v_{g,III}}{v_{g,II}} \gg \Delta z \quad \text{or} \quad \frac{2l}{\Delta z} \gg \frac{v_{g,II}}{v_{g,III}} = \frac{q_0}{p_0}.$$

For a plane wave $\Delta z = \infty$. Hence, for plane waves we have maximum coherence always. For any finite Δz , we see that coherence is lost as l increases. Decoherence implies (as proven in the previous section) that the total transmission probability becomes independent of l and is given by (17),

$$\sum_{n=1}^{\infty} |T_n|^2 = \frac{2ab}{a^2 + b^2}.$$

This value happens to coincide with $|T|$ (but not $|T|^2$) at the mid resonance values where $\cos[ql] = 0$. All of this is exhibited in our numerical calculations, in Fig. 1, where the exact value of the transmission probability is plotted against l . The tendency to a constant value as decoherence sets in is apparent.

The condition for decoherence is obviously achieved as $l \rightarrow \infty$. It is also obtained if $\Delta z \rightarrow 0$. However, $\Delta z \rightarrow 0$ implies $\Delta q \rightarrow \infty$ and we must be careful not to drop below the A (above barrier) zone. There is also a third limit in which it occurs: when $\frac{v_{g,II}}{v_{g,III}} \rightarrow 0$. Let us now consider this last limit in more detail. It can be achieved in two different ways. The first is by sending $q_0 \rightarrow 0$ with V_0 fixed, whence $p_0 \rightarrow \sqrt{V_0(V_0 + m)}$. The second is by keeping q_0 fixed and sending $p_0(E_0)$ and V_0 simultaneously to infinity so that $E_0 - V_0$ remains constant. The first choice is again difficult to realize because of the Heisenberg uncertainty principle. To see this concretely, consider a *symmetric* convolution function about $q_0(p_0)$. As $q_0 \rightarrow 0$ so too must $\Delta q \rightarrow 0$, since we must stay above the tunnelling zone. This means that automatically we must have $\Delta z \rightarrow \infty$. So contrary to our expectations we end up in the coherent state. The second choice however does indeed lead to complete decoherence, since it can be achieved while keeping the widths of the wave packets fixed.

6 Conclusions

In this paper we have considered diffusion of an incoming wave (or wave packet) with $E > V_0 + m$ by a one-dimensional potential barrier of height V_0 and width l . In front of and beyond the barrier, the potential is assumed to be zero (free space). In this study, we have employed the SPM. There is an inherent ambiguity in this method. Given a sum of terms, it may be applied individually to each or to the sum. In the former case a series of wave packet peaks are determined while in the latter case only one peak is predicted. It is easy to use the SPM in both the limit of complete coherence and complete decoherence. It is difficult to see how to use it for intermediate situations. In these cases we can fall back upon pure numerical calculations or possibly use cluster decompositions in which the wave packets are summed in finite numbers before applying the SPM. However, this possibility and its viability has still to be explored.

The overall reflection and transmission amplitudes (R and T) are characterized by resonance oscillations and by the feature that the reflection delay time is equal to the transmission time; at least when (or to the extent) that we can consider each a single wave packet. What we have shown in this paper is that, even with the Dirac equation, the barrier results can be obtained by treating the barrier as a two-step process. This procedure involves multiple reflections at each “step” and when $l \rightarrow \infty$ predicts the existence of multiple (infinite) outgoing peaks. However, by simply summing the individual amplitudes, one obtains exactly the standard barrier results. This has led us to postulate and then confirm numerically that with increasing l the resonance curves will lose coherence and tend to predicted constant values.

From an alternative, but equivalent viewpoint, it has also been noted that, whereas one cannot perform the limit $l \rightarrow \infty$ in the R and T amplitudes, one can expand the denominators, in a natural way, into an infinite series which reproduces exactly the two-step results. For any finite but sufficiently large l we predict the appearance of multiple peaks of which the first reflected term is simply the single-step result characterized by “instantaneous” reflection. As l increases the exit times of the other peaks grow. This suggests that for *finite times* (or simply ignoring secondary peaks) the single step is equivalent to a barrier with a *sufficiently* large width. So not only can we claim to have shown that a barrier is equivalent to two steps but, at least for the first reflected wave, that a wide barrier is in its turn an approximation of a single step.

We shall call upon these results in subsequent work in which we consider the tunnelling energy zones and the Klein zone. We consider these energy zones separately because they are characterized by different physical phenomena (resonance, tunnelling, pair production). For tunnelling, we shall be particularly interested in the extension of the Hartman effect [9–11] from the Schrödinger equation to the Dirac equation [7, 8]. This would justify the renaming of the effect to the Hartman paradox since it implies the existence of super-luminal velocities. Within the Klein zone we will again use the two-step method described in this paper.

Appendix

In order to obtain the expression of the transmitted probability for the step potential case, we consider the following incident wave packet:

$$\Phi_{I,inc}(z, t) = \int_{p_{\min}}^{+\infty} dp \, g(p) \begin{pmatrix} 1 \\ 0 \\ p \\ E + m \\ 0 \end{pmatrix} \exp[i(pz - Et)], \quad (\text{A.1})$$

where $p_{\min} = \sqrt{V_0(V_0 + 2m)}$ and $g(p)$ is a real function with a pronounced peak about the value $p = p_0$ chosen by

construction such that

$$\int_{-\infty}^{+\infty} dz |\Phi_{I,\text{inc}}(z, t)|^2 = \int_{p_{\min}}^{+\infty} dp g^2(p) \left[1 + \left(\frac{p}{E+m} \right)^2 \right] = 1. \quad (\text{A.2})$$

The transmitted wave packet can then be written as

$$\begin{aligned} \Phi_{II}(z, t) &= \int_{p_{\min}}^{+\infty} dp g(p) T_{+}(0) \begin{pmatrix} 1 \\ 0 \\ q \\ E - V_0 + m \end{pmatrix} \\ &\times \exp[i(qz - Et)] \\ &\simeq \left[T_{+}(0) \begin{pmatrix} 1 \\ 0 \\ q \\ E - V_0 + m \end{pmatrix} \right]_{p=p_0} \exp[iq_0 z] \\ &\times \int_{p_{\min}}^{+\infty} dp g(p) \exp \left[i(p - p_0) \frac{p_0(E_0 - V_0)}{q_0 E_0} z - Et \right]. \end{aligned} \quad (\text{A.3})$$

Consequently,

$$\begin{aligned} \int_{-\infty}^{+\infty} dz |\Phi_{II}(z, t)|^2 &\simeq \left[|T_{+}(0)|^2 \right]_0 \frac{E_0 - V_0}{E_0 - V_0 + m} \frac{q_0 E_0}{p_0(E_0 - V_0)} \\ &\times \int_{p_{\min}}^{+\infty} dp g^2(p) \end{aligned}$$

$$\begin{aligned} &\simeq \left[|T_{+}(0)|^2 \right]_0 \frac{2(E_0 - V_0)}{E_0 - V_0 + m} \frac{q_0 E_0}{p_0(E_0 - V_0)} \\ &\times \frac{E_0 + m}{2E_0} \\ &= \left[|T_{+}(0)|^2 \frac{b}{a} \right]_0. \end{aligned} \quad (\text{A.4})$$

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