ANTIPARTICLES CREATION IN TUNNELLING

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Abstract
We study particle interaction with a Dirac step potential. In the standard Klein energy zone, the hypothesis of Klein pair production predicts the existence of free/oscillatory antiparticles. In this paper, we discuss the tunneling energy zone characterized by evanescent wave functions in the classically forbidden region. We ask the question of the nature, particle or antiparticle, of the densities within the classically forbidden region. The answer to this question is relevant to the correct form of the reflection coefficient.

I. INTRODUCTION

When considering the Dirac equation for a step potential,

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

three distinct energy zones are evident [1,2],

- zone 1 - \(E > V_0 + m\) (diffusion),
- zone 2 - \(V_0 - m < E < V_0 + m\) (tunneling),
- zone 3 - \(E < V_0 - m\) (Klein pair production [3]).

We are using here standard barrier language (tunneling) extended to the step potential. The argument for pair production [4–7] will be re-derived below. In a previous paper [7], we studied the Klein energy zone 3 in which it has been hypothesized that pair production occurs. The reflected beam is of the same nature (particle) as that of the incoming beam, while the created antiparticles see a well potential and consequently travel forward freely. Wave packets can be formed and group velocities defined. In this paper, we consider the tunneling energy zone characterized by evanescent (non free) solutions in the classical forbidden region. For these solutions currents (and consequently group velocities) do not exist. One of the conclusions of this work will be that the tunneling energy zone must be considered as two separate tunneling zones,

- zone 2a - \(V_0 < E < V_0 + m\),
- zone 2b - \(V_0 - m < E < V_0\).

The distinction will be the nature of the “particles” within the step. We shall argue that in zone 2a they are particles, while within 2b they are antiparticles. This will necessarily require a modification of the reflection coefficient \(R\) which will be discontinuous in phase at \(E = V_0\).

Since the Dirac equation is a spinor equation [1], let us simplify our language by referring to the particles as electrons and the antiparticles as positrons. We assume incoming electrons from the left. As is standard, we work analytically with plane waves, but at some point we will perform numerical calculations using gaussian wave packets.

In the next section, we recall the results for diffusion. Subsequently, in section III, we pass to what we wish to call the Dirac tunneling (zone 2a). We observe there the analytical connection between the diffusion and tunneling results. In section IV, we jump to the Klein energy zone where

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pair production is assumed and derive the reflection and transmission amplitudes. In analogy with the diffusion-Dirac tunneling relationship, we derive the Klein tunneling results in section IV. Our conclusions, in particular the nature of the “particles” in the classically forbidden region, are drawn in the final section.

Throughout the paper extensive use is made of charge density in the free region as a function of time. The increase or decrease during reflection (transition period) is an excellent indicator of the charge of particles under the step.

II. DIFFUSION $E > V_o + m$

Let the incoming electrons be spin up, this choice does not influence our results. Continuity at $z = 0$ reads

$$u(p, E) + R u(-p, E) = T u(q, E - V_o),$$

where $u(p, E) = |1, 0, p/(E + m), 0\rangle$, $p = \sqrt{E^2 - m^2}$ and $q = \sqrt{(E - V_o)^2 - m^2}$. We have, for simplicity, absorbed the spinor normalizations ratio within $T$. Solving for $R$ and $T$, we find

$$R = \frac{1 - \alpha}{1 + \alpha} \quad \text{and} \quad T = \frac{2}{1 + \alpha},$$

where $\alpha = q(E + m) / p(E - V_o + m) > 0$. There is no room for spin flip. Obviously the fermions in region II are electrons because flux conservation requires this. Indeed flux conservation with our choices for $R$ and $T$ implies

$$|R|^2 + \alpha |T|^2 = 1.$$ (3)

Observe that of course $R < 1$, with $R \to 0$ for $E \to \infty$, but $R \to 1$ for $E \to V_o + m$. In this limit ($\alpha \to 0$) there is no flux in region II, but that is because the electron velocity has gone to zero. We point out that there is nevertheless an electron density proportional to $|T|^2 (\to 4$ in this limit).

III. DIRAC TUNNELING $V_o < E < V_o + m$

The spatial dependence in region II is now $\exp[-\tilde{q} z]$ with $\tilde{q} = \sqrt{m^2 - (E - V_o)^2} > 0$. Thus, $\tilde{q}^2 = -q^2$. For diffusion it was of course $\exp[i q z]$. This readily suggests how we must modify our spinors in the continuity equations. Formally $q^2$ is now negative whence $q$ is now imaginary. To pass from the oscillatory behavior in diffusion to the evanescent behavior, we simply perform $q \to i \tilde{q}$. This must be done also within the spinor. Solving the continuity equations now yields

$$R = \frac{1 - i \tilde{\alpha}}{1 + i \tilde{\alpha}} \quad \text{and} \quad T = \frac{2}{1 + i \tilde{\alpha}},$$ (4)

where $\tilde{\alpha} = \tilde{q}(E + m) / p(E - V_o - m) > 0$.

The well known feature of this result is that $|R| = 1$, total reflection occurs consistent with the fact that while there are fermions within the step there is no flux since the spatial dependence is evanescent, more specifically exponentially decreasing with increasing $z$.

Now, we are tempted both by continuity of particle density in the transition from diffusion to/from tunneling to identify these fermions as electrons. However, there exists a consistency check involving wave packets in region I. With wave packets (we shall use gaussian momentum distributions) the solution of the Dirac equation is no longer stationary but represents an incident right moving wave packet for $t \ll 0$ and a reflected left moving wave packet for $t \gg 0$. This situation could have been "read" from our plane wave results. The important difference between plane waves vs. wave packets occurs when considering $t \approx 0$. This is a period of transition for wave packets during which fermion density in region II (under the step) first grows from zero ($t \ll 0$) and then returns to zero ($t \gg 0$). During this transition it is legitimate to ask how the total numbers of electrons in region I changes. We have discovered that this depends crucially upon the analytic expression for the reflection coefficient.
In Fig. 1b, we show the ratio of this density to the incoming density as a function of time. That is, we have plotted 

$$r(t) = \int_{-\infty}^{0} \text{d}z \left| \Psi_{I}(z, t) \right|^2 / \int_{-\infty}^{0} \text{d}z \left| \Psi_{I}(z, -\infty) \right|^2,$$

where 

$$\Psi_{I}(z, t) = \int_{0}^{w} \text{d}p \, g(p) \left[ u(p, E) e^{ipz} + R u(-p, E) e^{-ipz} \right] e^{-iEt},$$

with 

$$g(p) = \exp\left(\frac{p - p_0}{\sqrt{2}} \right)^2 \frac{\text{d}^2}{4}$$

and 

$$w$$

is the maximum value of 

$$p$$

compatible with the tunneling energy zone, i.e. 

$$w = \sqrt{V_0(V_0 + 2m)},$$

and 

$$p_0 < w$$

the chosen value of peak incoming momentum. As can be seen from the plot, the value of 

$$r(t)$$

is at all times \( \leq 1 \). During transition there is a loss of electrons in free space (region I) which necessarily implies that the fermions within region II must be dominantly electrons [10]. Invoking total normalization conservation implies they are all electrons. Charge conservation is hence conserved as it must be.

We would considered the non relativistic limit, 

$$m \gg V_0 > E_{\text{xR}} = E - m,$$

and consequently the Schrödinger equation approximation. With Schrödinger antiparticle production is ignored. Consequently, we would have automatically assumed that the objects within the classically forbidden region were electrons. However, this would not have been by itself a proof. Before considering the other tunneling energy zone, we jump to the Klein zone and its interpretation.

IV. KLEIN PAIR PRODUCTION \( E < V_0 - m \)

This energy zone is characterized by oscillatory solutions in region II as occurs for diffusion [3]. Indeed, 

$$E - V_0 < -m,$$

and even if 

$$E - V_0$$

is negative, this also implies a real 

$$q$$

as for diffusion. Again the continuity equation is given by Eq. (1) if the solution in region II is chosen to be the plane wave 

$$u(q, E - V_0) \exp[\alpha(qz - Et)].$$

The essential difference here compared to diffusion is that 

$$\alpha$$

is now negative, consequently \( |R| > 1 \). This fact implies that more electrons are reflected than those incident, see Fig. 1d.

Mathematically, this is in accord with the observation that the wave in region II has a negative group velocity, 

$$q/(E - V_0),$$

i.e. it represents “electrons” incident from the right. Where one to assume the alternative oscillatory behavior \( \exp[-iqz] \) one would have obtained \( |R| < 1 \) as in diffusion. However, Klein observed that the only physical interpretation for “free” fermions in region II is that they be positrons. Since the potential is subtracted from the energy, it is an electrostatic potential. Consequently, if an “electron” sees a potential \( V_a \), a positron sees a potential \(-V_a\). Its wave function is the complex conjugate of the “electron” wave function (charge conjugation), so the physical positron wave function will be proportional to \( \exp[-i(q_a z - E_a t)] \) where 

$$q_a = \sqrt[4]{E_a - (-V_0)}$$

with 

$$E_a$$

the positron energy. To have a common time dependence, \( \exp[-iEt] \) (essentially for the continuity equations), we must have 

$$E_a = -E,$$

which while negative is nevertheless above the potential \(-V_0\) seen by the positron. Indeed 

$$-E > -V_0 + m$$

so it represents free positrons. The group velocity, 

$$q_a/\sqrt[4]{(E_a - (-V_0))} = q/(V_0 - E),$$

is now positive and, consequently, the flux of positrons will be from left to right and charge conservation will hold although conserved fermion density will not. The excess of reflected electrons is equal to the positrons created at the potential discontinuity. We have pair production. This interpretation involving Klein pair production is quite conventional [4-6].

The alternative with \( |R| < 1 \) in the Klein zone would correspond to incoming antiparticle flux from the right and pair annihilation with some of the incident electrons. In either case, positrons are needed to explain the oscillatory behavior in region II.

We wish to recall a few facts about this particular form of pair production. Since the electrons/positrons live in separate regions with diverse potentials, the creation process is achieved with zero net energy cost, zero net current, and zero net helicity [7].

V. KLEIN TUNNELING \( V_0 - m < E < V_0 \)

Now, to analytically continue from the Klein zone into what we have labelled the Klein tunneling zone 2b, we make the hypothesis that the spatial wave function to consider in the Klein zone, 

$$E < V_0 - m,$$
is \( \exp[-iqz] = \exp[-iqz] \). As we argued above when passing from the diffusion zone to the tunneling zone, which we called the Dirac tunneling zone, we must have in region II the form \( \exp[-qz] \). This is now achieved by \( q \rightarrow -iq \). Whence

\[
R = \frac{1 + i\tilde{\alpha}}{1 - i\tilde{\alpha}} \quad \text{and} \quad T = \frac{2}{1 - i\tilde{\alpha}},
\]

with \( \tilde{\alpha} \) as defined above. Formally, this \( R \) is the complex conjugate of the previous Dirac tunneling expression. However, we must always remember that the two expressions are valid in different energy zones (2a and 2b). Again \( |R| = 1 \) implying total reflection also in this tunneling zone.

Now, we perform our wave packet analysis. In Fig.1c, we see that during transition there is an excess of electrons in region I. This implies, with the analogous argument to that for the Dirac tunneling zone, that the fermions in region II are positrons. This is in accordance with the feature that as we pass from Klein to tunneling, at the energy interface \( E = V_0 - m \), there will be a constant density of stationary positrons in region II. Here continuity is maintained again in perfect analogy with what happens for electrons when passing from diffusion to Dirac tunneling. Had we chosen to follow the alternative route, \( q \rightarrow iq \), we would have predicted below potential electrons in region II. In this case the reflection coefficient would have been the complex conjugate to that given above, and formally coincided with the \( R \) for Dirac tunneling.

In Fig.2, we plot the values of \( \text{Arg}[R] \) and \( |R| \) vs. \( E/m \) for the case \( V_0 = 3.5m \). The tunneling zone is clearly identified by \( |R| = 1 \) and consists of what we have labelled Klein tunneling (KT) and Dirac tunneling (DT). Note the discontinuity in phase at \( E = V_0 \). We also observe that there is a peak value to Klein pair production \( (|R| > 1) \) at \( E = V_0/2 \).

VI. CONCLUSIONS

For our step analysis, we have divided the incoming particle range \( E \) into four sub-ranges separated at the values \( V_0 + m, V_0, \) and \( V_0 - m \) (obviously the last interface requires \( V_0 > 2m \) since always \( E \geq m \)). In the higher band, \( E > V_0 + m \), we have diffusion characterized by a reflection coefficient \( |R| < 1 \). In the second, we encounter a tunneling zone although for a step (or in practice for a very large barrier) no tunneling actually occurs. In this energy zone \( |R| = 1 \), but nevertheless electrons exist within the classically forbidden region II. We then jumped to the Klein zone \( E < V_0 - m \) and recalled the interpretation of the “free” particles (oscillatory spatial wave function) with positrons travelling over a potential of \(-V_0\). Extrapolating \( E \) upwards \((E_0 \downarrow)\) into the \( 2b \) tunneling zone, we derived a new \( R \) still with \( |R| = 1 \) but consistent with positrons in region II.

Now, we wish to make two technical points.

1) In this paper, we have used exclusively the spinors \( u^{(1)} \). However, for \( E < V_0 \), we have \( E-V_0 < 0 \). Comparing with the study of free fermions when \( V_0 = 0 \), we are in the realm of “negative energy”. We have argued elsewhere [7] that it is thus more logical to use \( w^{(3)} \) for \( E < V_0 \). The fact is that, surprisingly, this would change none of our results. So, we stick to \( u^{(1)} \) for simplicity, in accordance with most literature including Klein himself [3,6]. Actually, within the Klein zone, we have above potential positrons so there the use of \( w^{(3)} \) is fully justified.

2) The creation of positrons implies that the two step approach to the analysis of say a barrier (or multiple step for a general potential structure) is not the same as the standard solution involving coupled matrix equations. For example, the positrons created alla Klein in a barrier (potential well for them) are permanently trapped therein [2]. This feature would not be evident in the standard procedure. Indeed, the standard solution for a barrier in the Klein energy zone gives \( |R| < 1 \). This fact has generated some doubts, even recently, with Klein’s interpretation. We are of the opinion that when the solutions differ the multiple step solution is the only consistent one. Other solutions can be traced to the summation of non convergent series.

The main conclusion of this paper is that the tunneling zone must be divided into two parts, 2a \((V_0 < E < V_0 + m)\) and 2b \((V_0 - m < E < V_0)\). In the former the fermions in region II are electrons, in the latter they are positrons. Pair creation is thus predicted even for below potential conditions. This extends the Klein pair production to this part of the tunneling energy zone. The appropriate \( R \) function in zone 2b has been found and it is formally the complex conjugate of that in zone 2a.
There is a consequent discontinuity at $E = V_0$ both for the phase of $R$ and for the nature of the fermions. Another byproduct of this phase change is that in DT the reflected wave packets are time delayed while in KT they are time advanced. Obviously, these conclusions are subject to eventual experimental verification, possibly by the measurement of the ratio of the reflected particles to the incoming particles in region I, defined by the observable $r(t)$ given in Eq.(5). To the best of our knowledge even the creation of Klein pairs has yet to be verified experimentally. Pair creation is of course basic to field theory [2], and that is why Klein’s hypothesis is considered a precursor to field theory.

Recent developments in graphene physics [11-13] have shown that a Dirac like excitation with a zero mass occurs. This opens up a very practice possibility of testing both Klein pair productions and tunneling aniparticles proposed in this paper.

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Figure 1: The ratio of particles in region I to those of an incident gaussian wave packet peaked at \( E_0 \) and with localization \( \Delta \) as a function of time. The value of \( V_0 \) has been set to 3.5 m. The four
Figure 2: The phase and modulus of $R$ as a function of $E/m$ for $V_0 = 3.5m$. The discontinuity in the phase is at $E = V_0$ and the peak value of the modulus in the Klein zone is at $E = V_0/2$. 

(a) $\text{Arg}[R]/\pi$ vs. $E/m$

(b) $\text{Mod}[R]$ vs. $E/m$