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Relativistic considerations of quantum mechanical tunnel effect

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Abstract : On analyzing relativistic tunnel effect across a one dimensional potential step, one arrives at Klein's paradox which predicts a negative transmission coefficient and a reflection coefficient over unity for incident electrons Here, the tunnel effect produced by relativistic electrons impinging upon a one dimensional potential step and a rectangular potential barrier have been examined both on time-independent and time-dependent considerations. As a consequence of this, an interpretation of Klein's paradox apart from several interesting results follow.

Keywords : Relativistic effects, Dirac equation, Klein's paradox

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The relativistic energy-momentum relation of an electron is given by [1]

$$p_0^2 c^2 = \left(E - V_0\right)^2 - m^2 c^4 , \quad (1)$$

$$= \left(E + mc^2 - V_0\right)\left(E - mc^2 - V_0\right) . \quad (2)$$

Keeping the total energy E constant the variation of p_0^2 as a function of V_0 may be studied using (2): (i) If $(E - mc^2) > V_0$ both factors in (2) are positive. This implies that p_0^2 remains positive in this energy range, (ii) if $(E - mc^2) < V_0 < (E + mc^2)$ the first factor in (2) is positive while the second one is negative. Consequently, p_0^2 turns out to be negative in this case, (iii) lastly, if $(E + mc^2) < V_0$, both factors in (2) become negative. As such p_0^2 once again becomes positive. These variations of p_0^2 against V_0 has been depicted in Figure 1. These three energy ranges may now be identified. The first case when $(E - mc^2) > V_0$ the electrons can move over the barrier displaying their usual wave-particle characteristics. In the second case when $(E - mc^2) < V_0 < (E + mc^2)$, electrons do not find any negative energy state within the barrier to provide them a direct passage across it. Transmission of electrons

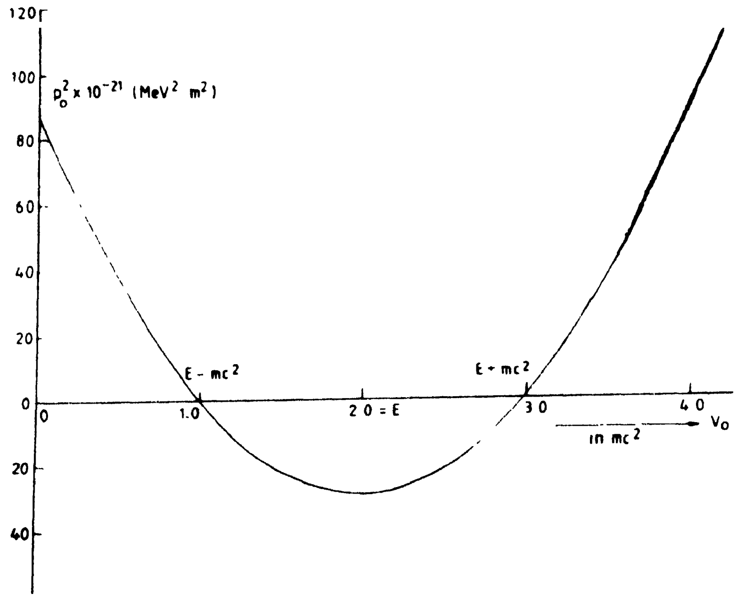

Figure 1. Variation of p_0^2 with V_0.

through the barrier by quantum mechanical tunnelling is then the only possibility. Finally, when $(E + mc^2) < V_0$, the incident electrons face a potential barrier of a height exceeding $2mc^2$. Therefore, when such electrons fall upon a barrier (formed of vacuum) pair production takes place inside it. Electrons are then transferred to their positive energy states existing on either side of the barrier leaving behind vacancies in their negative energy states inside. These vacant states are then capable of providing a direct passage to incident electrons to pass through the barrier.

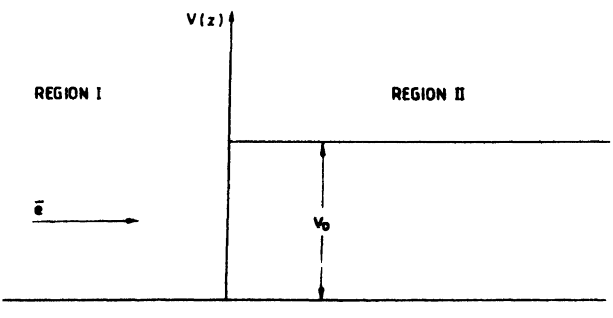

Figure 2. Electron scattering at a one dimensional potential step

Let a relativistic electron with its spin up be incident upon a rectangular potential step of a height V_0 as shown in Figure 2. The spin down possibility need not be considered here as there is no chance of any spin flip during tunnelling because the barrier is purely electrostatic in nature.

$(E - mc^2) < V_0 < (E + mc^2)$:

Eq. (1) may also be rewritten as,

$$\left(\pm\, ip_0 c\right)^2 = p'^2 c^2 = m^2 c^4 - \left(E - V_0\right)^2, \tag{3}$$

where $p' = ip_0$ represents the barrier momentum of the electron. The wave equation obtained by solving Dirac equation [1] in region I of Figure 2 may be written as,

$$\Psi_1(z) = \begin{matrix} 1 \\ 0 \\ cp/E + mc^2 \\ 0 \end{matrix} \qquad R \begin{matrix} \\ 0 \\ -cp/E + mc^2 \\ 0 \end{matrix} \qquad \backslash^e \tag{4}$$

where $p = p_0$ (see eq. 1) for region I as $V_0 = 0$. The wave function in region II may similarly be expressed as

$$\Psi_2(z) = T \begin{matrix} \\ 0 \\ icp'/E + mc^2 - V_0 \\ 0 \end{matrix} \qquad \backslash^e \tag{5}$$

where $\chi = p'/\hbar$. On matching ψ_1 with ψ_2 at $z = 0$, one finds

$$1 + R = T \tag{6}$$

and

$$1 - R = i\,\frac{cp'}{cp}\,\frac{\left(E + mc^2\right)}{\left(E + mc^2 - V_0\right)}\,T = i\,\gamma T, \tag{7}$$

where

$$\gamma = \left[\frac{\left(E + mc^2\right)\left(V_0 - E + mc^2\right)}{\left(E - mc^2\right)\left(E + mc^2 - V_0\right)}\right]^{1/2} \tag{8}$$

The variation of γ^2 as a function of V_0 has been plotted in Figure 3. Solving eqs. (6) and (7) simultaneously, one finds that

$$R = \frac{+\, i\gamma}{-\, i\gamma}, \tag{9}$$

and

$$T = \frac{2}{1 - i\gamma} \tag{10}$$

The incident, reflected and transmitted current densities may now be obtained by using [1]

$$J = c\,\Psi^+ \alpha\, \Psi,$$

where α is an appropriate Dirac Matrix. Since electrons move only along z-axis, eq. (11) modifies to

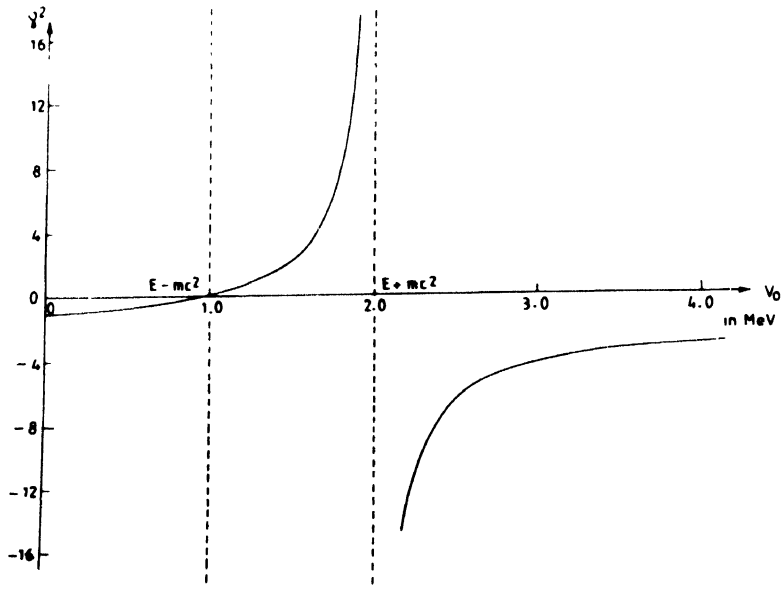

Figure 3. Variation of γ^2 with V_0.

$$J = C\Psi^{+} \alpha_3 \Psi, \tag{12}$$

because $\alpha_1 = 0 = \alpha_2$. Next, using eqs. (4) and (12), the incident current density is given by

$$J_i = c\, \Psi_i^{+} \alpha_3 \Psi_i = \frac{2c^2 p}{\left(E + mc^2\right)}. \tag{13}$$

Similarly, the reflected and the transmitted current densities work out to be

$$J_r = \frac{2c^2 p}{\left(E + mc^2\right)} |R|^2 \tag{14}$$

and

$$J_t = 0. \tag{15}$$

On dividing (14) by (13), one obtains

$$r \text{ (reflection coeff.)} = \frac{J_r}{J_i} = \left|\frac{1 + i\gamma}{1 - i\gamma}\right|^2 = 1. \tag{16}$$

Similarly dividing (15) by (13), one gets

$$t \text{ (transmission coeff.)} = \frac{J_t}{J_i} = 0. \tag{17}$$

The above set of expressions for r and t are identical to those obtained on non-relativistic considerations also [1].

$V_0 > (E + mc^2)$:

In this case, the barrier height ($V_0 - E_k$) (E_k = relativistic K.E. of electrons) exceeds $2mc^2$. The expression for γ (eq. 8) then modifies to

$$\gamma = \left[\frac{\left(E+mc^2\right)\left(V_0 - E + mc^2\right)}{(-1)\left(E - mc^2\right)\left(V_0 - E - mc^2\right)}\right]^{1/2} = -i\gamma', \tag{18}$$

where γ' is a positive quantity. Expressing (9) and (10) in terms of γ', one finds

$$R = \frac{1+\gamma'}{1-\gamma'} \quad \text{and} \quad T = \frac{2}{1-\gamma'}. \tag{19}$$

Thus,
$$r = |R|^2 = \left[\frac{1+\gamma'}{1-\gamma'}\right]^2 \tag{20}$$

turns out to be more than unity for $\gamma' \lesssim 1$. On using (12) one finds

$$J_t = c\,\Psi_2^+ \alpha_3 \Psi_2 = \frac{2c^2 p'' \, |T|^2}{\left(E + mc^2 - V_0\right)}, \tag{21}$$

where
$$c^2 (p'')^2 = \left[\left(V_0 - E\right)^2 - m^2 c^4\right]. \tag{22}$$

On dividing (21) by (13) one gets

$$t = \frac{J_t}{J_i} = -\frac{c^2 p''}{c^2 p} \frac{\left(E + mc^2\right)|T|^2}{\left(V_0 - E + mc^2\right)}. \tag{23}$$

On substitution for $p.p''$ and $|T|^2$ in (23) one gets

$$t = -\cdot \frac{4\gamma'}{(1-\gamma')^2}. \tag{24}$$

Thus, the transmission coefficient for this case turns out to be a negative quantity. On adding (20) and (24), one however, finds $r + t = 1$. This unusual set of results *viz.* $r > 1$ and $t < 0$ is well known as Klein's paradox [2].

This result may however, be explained on the basis of Dirac theory of electrons. As the barrier height ($V_0 - E_k$) exceeds $2mc^2$, the incident electrons initiate pair production. The generated electrons are then released at the incident end as unfilled states at lower energies are only available there. This augments the reflection. As the electrons move towards the incident end instead of tunnelling out, $t < 0$.

We next proceed to analyze quantum mechanical tunnelling of electrons on the basis of relativistic equations of Dirac. This problem would be analyzed both for time-dependent and time-independent cases.

Time-independent case :

A rectangular potential barrier of height V_0 and width W (Figure 4) will be considered for this analysis.

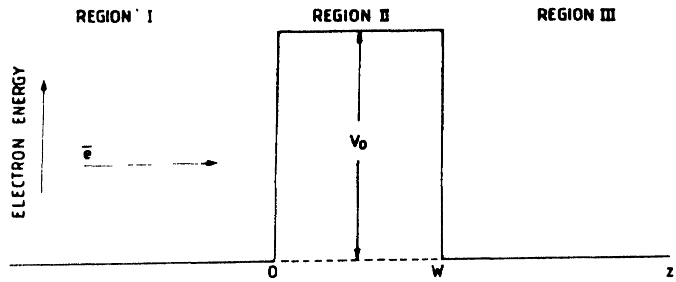

Figure 4. A rectangular potential barrier

$(E - mc^2) < V_0 < (E + mc^2)$:

The time-independent wave equations obtained by solving Dirac's relativistic equations in the three regions of the barrier may be expressed as

$$\Psi_1(z) = \begin{pmatrix} 1 \\ 0 \\ cp/E + mc^2 \\ 0 \end{pmatrix} e^{ipz/\hbar} + R \begin{pmatrix} 1 \\ 0 \\ -cp/E + mc^2 \\ 0 \end{pmatrix} e^{-ipz/\hbar}, \tag{25}$$

$$\Psi_2(z) = D \begin{pmatrix} 1 \\ 0 \\ icp'/E + mc^2 - V_0 \\ 0 \end{pmatrix} e^{p'z/\hbar} + F \begin{pmatrix} 1 \\ 0 \\ -icp'/E + mc^2 - V_0 \\ 0 \end{pmatrix} e^{p'z/\hbar} \tag{26}$$

and

$$\Psi_3(z) = T \begin{pmatrix} 1 \\ 0 \\ cp/E + mc^2 \\ 0 \end{pmatrix} e^{ipz/\hbar} \tag{27}$$

On matching Ψ_1, Ψ_2 and Ψ_3 at the respective barrier discontinuities, one gets after necessary simplifications

$$|T|^2 = \frac{1}{1 + 1/4\,(\gamma + 1/\gamma)^2 \sin h^2(p'W/\hbar)} \tag{28}$$

and

$$|R|^2 = \frac{1/4\,(\gamma + 1/\gamma)^2 \sin h^2(p'W/\hbar)}{1 + 1/4\,(\gamma + 1/\gamma)^2 \sin h^2(p'W/\hbar)}, \tag{29}$$

so that $|R|^2 + |T|^2 = 1$ as usual. On using (12), the tunnelling current density is obtained as

$$J_t = \frac{2c^2 p'}{\left(E + mc^2 - V_0\right)} \frac{|T|^2}{\gamma} \tag{30}$$

On dividing (30) by (13) one gets $t = |T|^2$. Similarly, on dividing (14) by (13) one obtains $r = |R|^2$.

$V_0 > (E + mc^2)$:

As the barrier height in this case exceeds $2mc^2$, the characteristic of the barrier is different from its classical counterpart in the sense that pair production may set in inside it. According to (22), the barrier electron momentum p'' now turns out to be positive and real. The time-dependent wavefunctions in different regions of Figure 4 are given exactly by similar set of equations as (25) to (27) with a difference that p' in (26) is to be replaced by $(-ip'')$. Ψ_2 in this case has a propagating character even inside the barrier. On matching these wavefunctions at respective boundaries one obtains after necessary simplifications

$$|R|^2 = \frac{1/4\ (\gamma' + 1/\gamma')^2 \sin^2(p''W/\hbar)}{1 + 1/4\ (\gamma' + 1/\gamma')^2 \sin^2(p''W/\hbar)}, \tag{31}$$

and

$$|T|^2 = \frac{1}{1 + 1/4\ (\gamma' + 1/\gamma')^2 \sin^2(p''W/\hbar)}, \tag{32}$$

γ' has already been related to γ (see eq. 18). (32) predicts that if $p''W = n\hbar$ (where n is any integer), the barrier becomes completely transparent to incident electrons.

Time-dependent case :

In this formalism, the potential barrier would be treated to provide a non-conservative field of force. As such the electron energy inside the barrier unlike the conventional cases (discussed above) cannot be defined. During tunnelling the potential barrier would be regarded to induce a fluctuation in the original electron energy value to an extent equal to the barrier height [3].

$(E - mc^2) < V_0 < (E + mc^2)$:

If the barrier height and width are respectively V_0 and W, the Dirac Hamiltonian in this time-dependent case may be written as

$$H = c\,\alpha . p + \beta mc^2 + V_0 \pm \Delta E, \tag{33}$$

where α and β are appropriate Dirac matrices. ΔE is the energy fluctuation induced by the barrier [3]. This is given by

$$\Delta E \simeq \left(V_0 - E + mc^2\right), \tag{34}$$

and it is the energy uncertainty introduced as a result of quantum measurement. As such the tunnelling time τ can be expressed as [3]

$$\tau \simeq h \Big/ \left(V_0 - E + mc^2\right). \tag{35}$$

For electron tunnelling along z-axis, the time-dependent Schrödinger's equation may be written as

$$i\hbar \frac{\partial}{\partial t} \Psi(z,t) = H\,\Psi(z,t). \tag{36}$$

Presuming $\Psi = x(z)T(t)$ and upon combining (33) and (36) we find,

$$\frac{i\hbar}{T(t)} \frac{dT(t)}{dt} \pm \Delta E = \frac{\hbar c}{i} \frac{\alpha_3}{X(z)} \frac{dX(z)}{dz} + \left(\beta mc^2 + V_0\right) = E, \tag{37}$$

where the separation constant E turns out to be the electron energy before incidence. On solving the time part of (37) one finds [3]

$$T(\tau) = T(0)\,\exp\left[-\frac{i\tau}{\hbar}\left(E \pm \hbar/\tau\right)\right]. \tag{38}$$

Eq. (38) clearly predicts that as a result of quantum measurement carried out by the potential barrier, the transmitted electrons have an energy spread ΔE $(= \pm \frac{\hbar}{\tau})$ about E. Next, the space part of (37) may be identified as,

$$\gamma_3' \frac{dX(z)}{dz} + \left(k_c - \gamma_4 Q\right) X(z) = 0, \tag{39}$$

where

$$\left.\begin{aligned} k_c &= mc^2/c\hbar \\ Q &= \left(E - V_0\right)/c\hbar \end{aligned}\right\}. \tag{40}$$

Next presuming $X = \begin{pmatrix} X_A \\ X_B \end{pmatrix}$, eq. (39) reduces to

$$\frac{d^2X(z)}{dz^2} - \chi^2 X(z) = 0, \tag{41}$$

where

$$\chi^2 = \left(K_c^2 - Q^2\right). \tag{42}$$

The solution of (41) yields

$$X(z) = \begin{pmatrix} X_{A0} \\ X_{B0} \end{pmatrix} \exp(\pm\chi z). \tag{43}$$

The evolving barrier wavefunction may now be written down by appropriately combining (38) and (43) as

$$\Psi(z,t) = Aa_l(t)\,X_l(z)\,\exp\left(-iE_l t/\hbar\right) + Ba_r(t)\,X_r(z)\,\exp\left(-iE_r t/\hbar\right), \tag{44}$$

where $(E_l - E_r) \simeq \Delta E$. A, B, $a_l(t)$ and $a_r(t)$ are appropriate constants. Let us assume

$$z_l = AX_l(z) = A \begin{pmatrix} 1 \\ 0 \\ i\,\hbar\,\chi c/E + mc^2 - V_0 \\ 0 \end{pmatrix} e^{-xz} \tag{45}$$

and

$$z_r = BX_r(z) = B \begin{pmatrix} 1 \\ 0 \\ -i\,\hbar\,\chi c/E + mc^2 - V_0 \\ 0 \end{pmatrix} e^{xz}. \tag{46}$$

On combining (44) and (36) and presuming that $a_r(t) << a_l(t) \sim 1$, one gets

$$\dot{a}_r(t) = \frac{T_{lr}\delta}{i\hbar S} \exp\left(-i\omega_{lr}t\right), \tag{47}$$

where $\omega_{lr} = \left(E_l - E_r\right)/\hbar$ and

$$T_{lr} = \int_0^W z_r^+(\pm\Delta E)\, z_l dz = \frac{2AB^*\left(E - V_0\right) W(\pm\Delta E)}{\left(E + mc^2 - V_0\right)}, \tag{48}$$

$$S = \int_0^W \left|z_r\right|^2 dz = \frac{|B|^2(2mc^2)\exp(2\chi W)}{(2x)\,(E - V_0 + mc^2)}, \tag{49}$$

and

$$\delta = \exp(-i\theta). \tag{50}$$

Integration of (47) now yields,

$$a_r(t) = (-i\delta)\frac{T_{lr}}{\hbar S} \exp\left(-i\omega_{lr}t/2\right) \frac{\sin\left(\omega_{lr}t/2\right)}{\left(\omega_{lr}t/2\right)}. \tag{51}$$

The tunnelling probability at $t = \tau$ may now be obtained as [3]

$$\left[\Psi^+\Psi\right]_{t=\tau} = \frac{8}{(1+\gamma^2)\left(E + mc^2 - V_0\right)} \Bigg[mc^2 \exp(-2xz) + \frac{2\left(E - V_0\right)^2 \exp(2xW)}{mc^2} \sin\left(\frac{\omega_{lr}\tau}{2} - \theta\right) \frac{\sin\left(\omega_{lr}\tau/2\right)}{\left(\omega_{lr}\tau/2\right)} + \frac{\left(E - V_0\right)^2 \exp(2xz)}{mc^2 \exp(4xW)} \cdot \frac{\sin^2\left(\omega_{lr}\tau/2\right)}{\left(\omega_{lr}\tau/2\right)^2}\Bigg]. \tag{52}$$

The evolved form of one electron tunnelling current density [3] is also obtainable by solving the equation of continuity and is given by

$$J = J_{01} \frac{\sin(\omega_{lr}\tau)}{(\omega_{lr}\tau)} + J_{02} \sin(\omega_{lr}\tau - \theta), \tag{53}$$

where

$$J_{01} = J_{02} = \frac{32qW(E-V_0)^2 \exp(-2xW)}{\tau mc^2 (1+\gamma^2)(E+mc^2-V_0)}. \tag{54}$$

The quantum mechanical tunnel effect has been reviewed here for relativistic electrons. Since negative energy states cannot exist inside the barrier for electrons in the energy range $(V_0 - E_k) < 2mc^2$ electrons can negotiate the barrier only by quantum mechanical tunnelling. However, for $(V_0 - E_k) > 2mc^2$ the negative energy states inside the barrier finds themselves situated above the positive energy states of incident electrons. They may then propagate freely through the barrier negative energy states as they do over the barrier.

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