Positron Tunnelling through the Coulomb Barrier of Superheavy Nuclei

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We study beams of medium-energy electrons and positrons which obey the Dirac equation and scatter from nuclei with \(Z > 100\). At small distances the potential is modelled to be that of a charged sphere. A large peak is found in the probability of positron penetration to the origin for \(Z \approx 184\). This may be understood as an example of Klein tunnelling through the Coulomb barrier: it is the analogue of the Klein Paradox for the Coulomb potential.

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I. QUANTUM TUNNELLING AND KLEIN TUNNELLING

One of the principal characteristics of quantum mechanics as opposed to classical mechanics is that particles of energy \(E\) can pass through regions of a potential \(V(r)\) in which their kinetic energy \(T = E - V\) is negative, albeit with amplitudes which are exponentially suppressed. In two pioneering papers 70 years ago which demonstrated the importance of quantum tunnelling in the understanding of nuclear decays, the probability of an \(\alpha\)-particle to tunnel from the potential well of the nucleus through the Coulomb barrier was calculated \([2]\). The calculation in the quasi-classical case is straightforward \([2]\): the transition probability for decay \(w\) is given by

\[
\begin{align*}
\ln w = 2 \int_0^{r_c} \sqrt{2m} |V(r) - E| \\
&= \exp \left\{ -2\pi Z\alpha m/p \right\}
\end{align*}
\]

for \(V(r) = Z\alpha/r\) where \(r_c = Z\alpha/E\) is the classical turning point, and \(m\) and \(p\) are the mass and momentum of the \(\alpha\)-particle. The integral in the exponent is over the classically forbidden region in which \(T < 0\). Similarly a positron of energy \(E\), momentum \(p\), and mass \(m\) incident on a nucleus of charge \(Z\) can reach distances smaller than \(r_c\). If \(\rho = |\psi(0)|^2_{\text{pos}}/|\psi(0)|^2_{\text{id}}\) is the ratio of the probability of a positron penetrating a Coulomb barrier to reach the origin compared with the probability of an electron of the same energy, then essentially the same calculation gives non-relativistically

\[
\rho = e^{-2\pi y}
\]

where \(y = Z\alpha m/p\) so that \(\rho\) decreases exponentially with \(Z\) for fixed \(p\). If the particles are relativistic and satisfy the Dirac equation then Eq.\,(2) \(\text{is still obtained provided now } y = Z\alpha E/p\) \([1]\). For relativistic problems the kinetic energy \(T = E - V - m = \sqrt{m^2 + p^2} - V - m\) so that, classically, \(T\) is still positive definite but now \(r_c = Z\alpha/(E - m)\).

At the same time as the papers showing the effect of quantum tunnelling in \(\alpha\)-decay, Klein \([5]\) showed that electrons in the Dirac equation could in principle tunnel through a high repulsive barrier. This is the famous Klein Paradox. Calogeros and one of us (ND) have recently reassessed this phenomenon \([6]\) and call such quantum tunnelling without the expected exponential suppression \textit{Klein tunnelling}. To obtain Klein tunnelling it is essential that hole states (corresponding to negative energy states for free particles) as well as particle states are considered and allowed to propagate. For a particle of momentum \(p\) and energy \(E\) incident on a Klein step of height \(V\), a hole state of momentum \(-q\) will propagate under the barrier provided

\[
V = \sqrt{m^2 + p^2} - \sqrt{m^2 + q^2},
\]

which is possible for \(V > 2m\). In terms of the particle kinetic energy under the barrier

\[
T = E - V - m = -m - \sqrt{m^2 + q^2} \leq -2m,
\]

and where \(T \leq -2m\) hole states can propagate without exponential suppression. \(T \leq -2m\) for a Coulomb potential corresponds to penetrating under the barrier to distances \(r < r_K\), where \(r_K = Z\alpha/(E + m) < r_c\) is the Klein distance. While tunnelling from \(r_c\) to \(r_K\) is exponentially suppressed, tunnelling from \(r_K\) to \(r = 0\) is not; indeed the amplitude may even be enhanced. This is because the effective potential in a relativistic theory with a potential \(V\) which is the time component of a four-vector is given by

\[
2mV_{\text{eff}}(r) = 2EV(r) - V^2(r).
\]

In the region \(0 < r < r_K\), \(V(r) > E + m > E\) and so the effective Coulomb force is attractive \([3]\) when \(r\) is small enough \(\text{note that the force becomes attractive}\),
when dVEff/dr changes sign, not when Veff(r) changes sign.

When the Coulomb potential is investigated in the Dirac equation, the ground state energy E1 = 0 at Zα = 1 and becomes complex for Zα > 1 \[7\]. This is a consequence of the V^2(r) term in Eq. \[3\] which leads to the “collapse” of the particle to the origin, and hence to a problem which is not well-defined \[7\]. So the theory breaks down at Z_{\text{max}} = 1/\alpha \simeq 137. Since superheavy nuclei can be constructed in heavy ion collisions with values of Z larger than 137, this limitation on Z cannot be physical. A modified Coulomb potential which takes account of the finite size of the nucleus must therefore be used so that the singularity at small r is smoothed out. When this is done there seems to be no restriction on Z; furthermore bound state energies become negative for sufficiently large Z. These are interpreted as bound positron states \[8\], \[9\]. For Klein tunnelling through the (modified) Coulomb potential it was conjectured \[1\] that it might occur at values of Z large enough to obtain negative energy bound states. For the simplest such potential, due to Pieper and Greiner \[8\], the first negative energy bound state occurs at Z = 147. Hence the prediction of Calogeracos and Domby \[9\] that Klein tunnelling may occur for nuclei with Z \approx 150 or above. If it occurs, Klein tunnelling would lead to a breakdown of the exponential suppression given by Eq.\[4\].

In the Dirac equation in one-dimension, transmission resonances (with zero reflection coefficient) \[10\] have been demonstrated for electron scattering off square barriers \[11\] and off smooth potential barriers of Woods-Saxon \[12\] or Gaussian \[13\] form. These provide examples of Klein tunnelling. In each case, the transmission resonances occur when the corresponding attractive potential becomes supercritical (see next paragraph).

Since it is unlikely that superheavy nuclei with Z > 150 can be prepared and stay around for long enough for positrons to be scattered off them, we study positron scattering off nuclei with Z > 150 numerically by solving the Dirac equation for a modified Coulomb potential. We thus attempt to repeat Klein’s analysis for a modified Coulomb potential in place of a potential step. We do indeed find that positrons scattering off nuclei with Z > 150 and especially with Z > 170 no longer satisfy Eq.\[4\]. We find, in addition, an extremely sharp peak in ρ near Z = 184. We now outline the calculation.

II. MODIFIED COULOMB POTENTIAL:
BOUND AND CONTINUUM STATES

Following Pieper and Greiner \[8\], the modified Coulomb potential experienced by an electron or positron beam is taken to be the potential arising from a homogeneously charged sphere of radius b. More explicitly, the time component V(r) of the 4-vector potential is given by

\[ V(r) = \pm \frac{Z\alpha}{b} f(r/b), \]

where the dimensionless potential shape function f is defined as

\[ f(r/b) = \begin{cases} \frac{3}{2} + \frac{1}{2} \left( \frac{r}{b} \right)^2 & r \leq b \\ \frac{b}{r} & r > b \end{cases} \]

and b = (1.2)A^{1/3} fermi. We let ψ1 and ψ2 be the ‘large and small’ radial wave functions used to construct the Dirac spinor corresponding to a total angular momentum of j. We employ the variables τ = ±1, and k = j + \frac{1}{2}, so that the parity P of the spinor is given by P = (−1)^{j+1} = ±1. In the notation of Rose \[4\], with κ = τk, the coupled radial equations may be written

\[ \psi_2' - \frac{\tau k}{r} \psi_2 = (m + V - E)\psi_1 \]

\[ \psi_1' + \frac{\tau k}{r} \psi_1 = (m - V + E)\psi_2. \]

There are two distinct problems to be considered: (a) bound states; and (b) continuum states. For the bound states, we adopt the boundary conditions and normalization given by

\[ \psi_1(0) = \psi_2(0) = 0, \quad \int_0^\infty (\psi_1^2(r) + \psi_2^2(r))dr = 1. \]

We now choose j and τ, integrate out from the origin, and search for those energies which lead to spinors that have the desired number n1 of nodes in the ‘large’ radial component ψ1, and vanish at large distances. If the quantity ℓ = j + \frac{3}{2}τ represents the orbital angular-momentum quantum number in the first two components of the Dirac spinor, and ν = (n1 + 1 + ℓ), then the usual spectroscopic designation is written νℓj, where ℓ = \{0, 1, 2, \ldots\} \sim \{s, p, d, \ldots\}. The j = \frac{1}{2}, ℓ = 0 states, for example, correspond to τ = −1. We calculate the first few energy eigenvalues as a function of Z and our results agree with those given by Pieper and Greiner in their Table 3. In particular, we have found the critical values of the atomic number Z that yield the energies E = 0 (the threshold for bound positrons) and the supercritical values of Z corresponding to energy E = −m (corresponding to spontaneous positron production); some results are presented in Table 1.

| Z | E = 0 | E = −m |
|---|---|---|
| 1s1/2 | 146.7 | 170.4 |
| 2s1/2 | 195.7 | 237.0 |
| 2p1/2 | 188.1 | 185.8 |
| 3s1/2 | 290.1 | 316.5 |

Table 1: Values of Z for which E = 0 and E = −m
In the case of the continuum states, we adopt the following method. At very small distances \( r << b \), we assume that the large and small radial functions have the asymptotic pure-power forms \( C r^2 \) and the ratios given (after some elementary corrections) by Rose\(^4\). In this region there is then only one free parameter, which we take to be the amplitude \( C_{1e} \), or, for positrons, \( C_{1p} \), of the large component \( \psi_1(r) \); the small component is smaller here by the factor \( r^2 \). We fix \( j, \tau, \) and the incident momentum \( p \), and we integrate outwards, to a point \( r_b \) well beyond the classical turning point \( r_c \). At these distances the radial components have the large-\( r \) Coulombic asymptotic form, which is approximately sinusoidal with \( \psi_1 \)-amplitude, say \( A_1 \); in this region, the components are also (almost) exactly out of phase, so that when \( \psi_1 = A_1 \), we have \( \psi_2 = 0 \).

We now search, in each case, for the value of \( C_1 \) so that this asymptotic amplitude has the value \( A_1 = 1 \). Since the numerical process is, in principle, direction invariant, this corresponds to an ‘experiment’ in which the final amplitude of an incoming beam with unit amplitude is determined near the origin. Since we are calculating wave functions at the origin, only \( l = 0 \) states contribute and thus we restrict the analysis to \( \tau = -1 \) and \( k = 1 \). For a given \( Z \) we can express the positron-electron ratio in the form \( \rho = [C_{1p}/C_{1e}]^2 \).

### III. THE PEAK

As we are not interested in the detailed behaviour of the nuclear charge distribution we require \( b << r_K \). We also require \( r_c >> r_K \) so that the normal exponential suppression will be obtained for \( Z \) not too large. We ensure that this is so by choosing the momentum \( p \) in the range \( 0.1 m - 0.4 m \). For this momentum range and with \( Z < 150 \) we expect normal exponential suppression of the positrons by the modified Coulomb potential according to Fig.\(^3\): this is demonstrated in Fig. 1 where our calculation of \( \rho \) for \( Z = 100 \) is close to \( e^{-2 \pi y} \) asymptotically, showing that our method of calculation is satisfactory.

We now look at \( C_{1p}/C_{1e} \) for values of \( Z > 140 \). The principal discovery we report here is the existence of a pronounced peak in \( \rho = [C_{1p}/C_{1e}]^2 \) very near \( Z = 184 \). This peak is exhibited in Fig. 2 for the case \( p = (0.4) m \). At the peak maximum \( \rho \approx 2 \). The peak is so sharp that it seems to correspond to a singularity of some sort. It is convenient to look at the deviation from exponential suppression by introducing a Klein ”logarithmic form factor” \( R \) so that \( [C_{1p}/C_{1e}] = e^R e^{-\pi y} \), where \( R \) is given explicitly by

\[
R(Z, p) = \ln [C_{1p}/C_{1e}] + \pi y = \frac{1}{2} \ln(\rho) + \pi y. \tag{6}
\]

Thus \( R \) constant corresponds to normal exponential suppression. In Fig. 3 we exhibit more detail near the peak by plotting \( R \) in terms of \( Z \) for the two cases \( p = 0.1 m \) and \( 0.4 m \). The peak shifts slightly with momentum, with a limit, for \( p \rightarrow 0 \), very close to the \( p = 0.1 \) position shown. More specifically, we find peaks in \( \rho(Z, p) \) at positions \( Z_p \) given by \( Z_{0.4} = 184.8 \) and \( Z_{0.1} = Z_{0.02} = 183.8 \). This is fully consistent with a peak in \( \rho(Z, p = 0) \) at \( Z_0 = 183.8 \).

### IV. DISCUSSION

The enormous peak near \( Z = 184 \) in the scattering of positrons by superheavy nuclei was unexpected: it involves an enhancement in \( \rho \) by a factor \( 10^8 \) between \( Z = 179 \) and \( Z = 184 \). While a demonstration of a deviation from the pure exponential suppression of Eq.\(^3\) resulting from Klein tunnelling was the purpose of this calculation, we initially expected it to be a simple max-
cient is unity and the reflection coefficient is zero \cite{16}. It a transmission resonance where the transmission coefficient coincide. While the peak that we have found does not correspond to the first 1\textit{s}_1/2 supercritical state, it does correspond to the second 2\textit{p}_1/2 supercritical state (see Table 1). We show in a forthcoming paper \cite{14} that this correspondence exists independently of the exact form of the potential. This is also in agreement with the result of Müller, Rafelski and Greiner \cite{15} who predicted a resonance in the negative energy continuum in the \textit{s}_1/2 state at \( Z = 184 \).

To explain why the peak occurs in the state which corresponds to the 2\textit{p}_1/2 bound state of the electron is an exercise in Dirac’s hole theory. The vacuum state for our modified Coulomb potential at supercriticality contains a vacant 2\textit{p}_1/2 bound state of an electron of energy \( E = -\hbar^2/2m \); this in hole theory represents a positron state of zero kinetic energy. But to compare the original electron state with a positron state requires charge conjugation: equations (4,5) are invariant under the combined operation \( E \rightarrow -E; V \rightarrow -V; \tau \rightarrow -\tau; \psi_1 \leftrightarrow \psi_2 \). So the vacant electron 2\textit{p}_1/2 bound state corresponds to a resonant \textit{s}_1/2 positron scattering state since \( j = \frac{1}{2} \) for both states but \( \tau \) changes sign.

The (vacant) electron 2\textit{p}_1/2 bound state of zero kinetic energy at supercriticality can thus be considered as a positron resonance of zero kinetic energy. In one dimension non-relativistically a zero energy resonance is a transmission resonance where the transmission coefficient is unity and the reflection coefficient is zero \cite{16}. It seems likely that we have found a similar effect here in three dimensions since our peak occurs as close to zero kinetic energy (corresponding to the supercritical energy) as we can calculate. We should emphasise that we calculate the quantity \( p \) which is not a scattering cross section. Neither is it strictly a transmission coefficient. Nevertheless our peak is more like a transmission resonance than a resonant cross section. We will examine this point in more detail in a forthcoming paper.

We note finally that our example here of positron scattering by a modified Coulomb potential shows that the phenomenon discovered by Klein of Dirac particles tunnelling through repulsive potentials is a general characteristic of the Dirac equation in the presence of strong fields.

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\begin{figure}
\centering
\includegraphics[width=\textwidth]{fig3}
\caption{\( R \) as a function of \( Z \) for \( p = 0.4m \) (dashed) and \( p = 0.1m \) (solid)}
\end{figure}

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\footnote{We thank Dr. X. Artru for pointing this out.}