Klein Paradox in Spatial and Temporal Resolution

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Based on spatially and temporally resolved numerical solutions to the relativistic quantum field equations, we provide a resolution to the controversial issue of how an incoming electron scatters off a supercritical potential step and how the electron-positron pair production is affected by this collision. The treatment of the problem as a correlated three-particle problem suggests revealing insight into the process.

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Relativistic quantum field theory is regarded as one of the most accurate descriptions of nature. The prediction of the anomalous electron spin by this theory has, for instance, been experimentally confirmed with unprecedented accuracy. The Dirac equation without second quantization, in contrast, is known to lead to interpretational problems when applied to processes in which a single-particle interpretation is inadequate. The best-known example of a paradoxical outcome is the so-called "Klein paradox" [1] describing a nonvanishing transmission of an incoming electron as it scatters off an electrostatic potential step whose height is much larger than the electron's kinetic energy. The Schrödinger equation as well as classical mechanical theories for this scattering predicts a complete reflection for the electron. Since then many works have been published to "resolve" the Klein paradox. Some of these works are not fully consistent with each other. In this Letter, we analyze the Klein process in full time resolution based on the Dirac quantum field equation.

As the analysis in the field formulation of the problem is very challenging, several works have resorted to the single-particle Dirac wave function solutions without second quantization. In this restricted framework the time evolution operator of the single-particle wave function is unitary and as a result the reflection coefficient cannot be greater than 1, in contrast to some previous claims. This fact is also consistent with time-resolved wave-packet calculations [2]. What makes the matter more confusing is that the transmission coefficient calculated from the single-particle wave function turns out to match the steady state pair-production rate of the potential step in the absence of any incoming electron [3].

Most treatments of the Klein paradox within the framework of field theory omit the effect due to the incoming electron and focus on the steady state electron-positron pair-production rate from the supercritical potential. Several important questions concerning how the scattering of the incoming electron is affected by the pair production as well as how the pair-production rates are affected by the incoming electrons have, to the best of our knowledge, not been adequately addressed. A time-resolved analysis is thus the natural way to approach the problem.

In this Letter we comment on these challenges. Our results are derived from correlated three-particle wave functions that were constructed numerically from the corresponding time-dependent quantum field. We show analytically and confirm numerically how the pair-production rate gets modified during those times when the incoming electron wave packet overlaps spatially with the potential barrier.

The time evolution of the field can be expressed in terms of the electron annihilation and positron creation operators as $\hat{\Psi}(x,t) = \Sigma_p \hat{b}_p W_p(x,t) + \Sigma_n \hat{d}_n^\dagger W_n(x,t)$, where the term $\Sigma_{p(n)} \cdots$ denotes the summation (integration) over all states with positive (negative) energy. The functions $W_{p(n)}(x,t) \equiv \langle x \mid W_{p(n)}(t)\rangle$ denote the solutions to the time-dependent Dirac equation under the initial condition $W_{p(n)}(x, t=0) \equiv W_{p(n)}(x)$, where $W_{p(n)}(x)$ is an energy eigenfunction. In previous studies we have shown that the Dirac equation can be solved numerically for arbitrary initial states on a space-time grid using a third- or fifth-order FFT-based split operator algorithm [2]. Using the complete set of solutions $W_{p(n)}(x,t)$, the field operator can be constructed. The time dependence of the corresponding Fermion operators may be written as

$$\hat{b}_p(t) = \Sigma_{p'} \hat{b}_{p'} \langle W_p \mid W_{p'}(t)\rangle + \Sigma_{n'} \hat{d}_{n'}^\dagger \langle W_p \mid W_{n'}(t)\rangle, \quad (1a)$$

$$\hat{d}_n^\dagger(t) = \Sigma_{p'} \hat{b}_{p'} \langle W_n \mid W_{p'}(t)\rangle + \Sigma_{n'} \hat{d}_{n'}^\dagger \langle W_n \mid W_{n'}(t)\rangle. \quad (1b)$$

The only time dependence is contained in the matrix elements which are denoted by $\langle W_p \mid W_n(t)\rangle \equiv U_{pn}(t)$, etc., for convenience in the following discussion.

The Dirac-Hamiltonian for this problem is given (in atomic units) by $H(t) = c\boldsymbol{\alpha}\cdot\mathbf{p} + \beta mc^2 + V(x)\theta(t)$, where $\boldsymbol{\alpha}$ and β are the usual 4×4 Dirac matrices, and $\theta(t)$ denotes the Heaviside unit step function. As a potential of height V_0 and width W we choose $V(x) = 0.5V_0[1 + \tanh(x/w)]$. Using plane waves one can find [4] the transmission coefficient in the corresponding single-particle formalism as a function of the energy E:

$$T(E) = -\frac{\sinh(\pi k W)\sinh(\pi\kappa W)}{\sinh[\pi(V_0/c + k + \kappa)W/2]\sinh[\pi(V_0/c - k - \kappa)W/2]}, \tag{2}$$

where $k \equiv \sqrt{[(E - V_0)^2 - c^4]}/c$ and $\kappa \equiv -\sqrt{[E^2 - c^4]}/c$.

In order to better judge the impact of the incoming electron let us first comment on the pair-production process associated exclusively with a supercritical potential without the incoming electron. Using the operator solutions Eq. (1) we can compute numerically the total electron population $\Sigma_p\langle 0\|\hat{b}_p^\dagger(t)\hat{b}_p(t)\|0\rangle = \Sigma_p\Sigma_n|U_{pn}(t)|^2$ as a function of time. The results for three potential strengths V_0 are displayed in Fig. 1. The early time regime ($t \lesssim 1/c^2 \approx 0.5 \times 10^{-4}$ a.u.) is followed by a linear growth regime characterized by a constant rate. This rate becomes zero if the potential is subcritical, i.e., $V_0 \leq 2c^2$. Incidentally, for $V_0 > 2c^2$ the pair-production rate in the long-time limit is directly related to the transmission coefficient (2) via $\int dE\, T(E)/(2\pi)$. This relationship is remarkable as $T(E)$ was derived for a completely different physical situation and from a theory that was not even second quantized.

What is noteworthy from Fig. 1 is that for a subcritical potential the pair-production probability does not totally vanish. It is also interesting that after the transient time the probability can actually decrease for subcritical potentials, which can be interpreted as a temporary pair-annihilation process until the pair-production rate levels to zero. The probability grows initially quadratically in time.

The pair-production process can also be analyzed via the corresponding time-dependent energy spectrum of the emitted electron, defined as $P(E, t) = \langle 0\|\hat{b}_p^\dagger(t)\hat{b}_p(t)\|0\rangle = \Sigma_n|U_{pn}(t)|^2$. Figure 2 shows that at early stages $P(E, t)$ decreases monotonically as a function of energy. As time progresses, more energy close to $V_0/2$ is generated. In the steady state regime, the energy spectrum would grow linearly in time, in agreement with the analytical expression $P(E, t) = T(E)t/(2\pi)$ shown by the circles for $t = 53.2 \times 10^{-4}$ a.u. Here $T(E)$ is again identical to the transmission coefficient (2).

Let us now bring the incoming electron into the discussion. We assume that initially the electron is localized and described by a coherent superposition of energy eigenstates, $\Psi(x, t = 0) = \Sigma_p C_p W_p(x)$, such that its initial center is at position x_0 (<0). The corresponding electron and positron populations can be calculated:

$$\Sigma_p\langle\Psi(t = 0)\|\hat{b}_p^\dagger(t)\hat{b}_p(t)\|\Psi(t = 0)\rangle = 1 + \Sigma_n\Sigma_p|U_{pn}(t)|^2 - \Sigma_n|\Sigma_p C_p U_{np}(t)|^2, \tag{3a}$$

$$\Sigma_n\langle\Psi(t = 0)\|\hat{d}_n^\dagger(t)\hat{d}_n(t)\|\Psi(t = 0)\rangle = \Sigma_n\Sigma_p|U_{pn}(t)|^2 - \Sigma_n|\Sigma_p C_p U_{np}(t)|^2. \tag{3b}$$

Each term in Eq. (3) has an important interpretation. The number 1 in (3a) describes the incoming electron while the term $\Sigma_n\Sigma_p|U_{pn}(t)|^2$ is associated with the pair production in the absence of any incoming electron as we derived above. The last term is always negative and therefore decreases the pair production. We should point out that this finding contradicts the conclusions made in several works where the incoming electron was noted to "knock out" electrons from the barrier [5] or to "stimulate" [6] pair production. We have found a clear reduction instead of the suggested enhancement of the pair-production rate.

The suppression of pair production observed here, however, affects only a positron whose spin is antiparallel

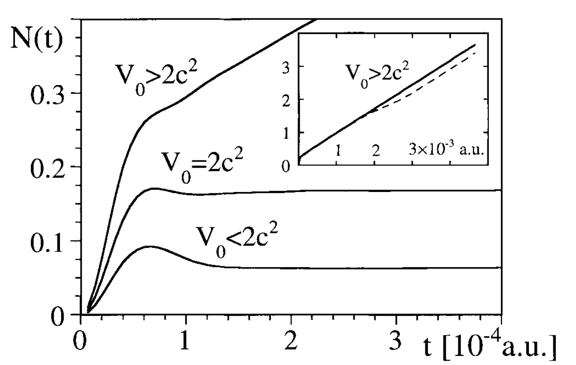

FIG. 1. The electron population $N(t) \equiv \Sigma_p\langle 0\|\hat{b}_p^\dagger(t)\hat{b}_p(t)\|0\rangle$ from potentials with three different heights V_0 as a function of time. ($V_0 = 2c^2 - 0.53c^2$, $2c^2$, $2c^2 + 0.53c^2$, $W = 0.3/c$). The dashed line of the inset (for $V_0 = 2c^2 + 0.53c^2$) shows the reduction of the pair production due to an incoming electron scattering off the potential at $t = 2 \times 10^{-3}$ a.u.

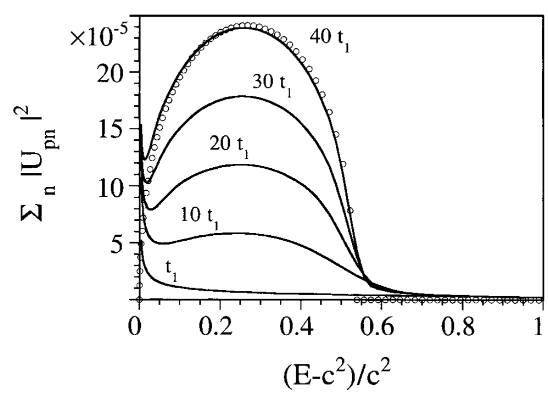

FIG. 2. The electron spectrum $P(E, t)$ generated by a supercritical potential at various times as a function of the energy E. The times are $t = 1.33$, 13.3, 26.6, 39.9, and 53.2×10^{-4} a.u. The long-time spectrum is compared with the analytical expression $T(E)t/(2\pi)$ as indicated by the circles for $t = 53.2 \times 10^{-4}$ a.u. ($V_0 = 2c^2 + 0.53c^2$, $W = 0.3/c$).

to that of the incoming electron. As the pair-production process preserves the total spin (=0) and the electron and positron created during the pair production have opposite spins, one could be tempted to associate this suppression in the pair production with the Pauli exclusion principle which restricts the generation of an electron into a state that is already occupied by the incoming electron [7]. However, as it turns out, the situation is much more complicated as the amount of the suppression does depend crucially on the precise phase relationship among the complex superposition amplitudes C_p and not simply on the state occupation probability $|C_p|^2$. In fact, the magnitude of the pair-production rate suppression depends on time. Analyzing the last term in Eq. (3b) for an incoming wave packet one can show that the rate is suppressed only at those times when the wave packet overlaps spatially with the potential barrier.

In order to simulate how the pair production is suppressed as a function of time, a large scale numerical simulation of the field equations is necessary which requires several CPU days on a supercomputer. Using the numerical solution of the field operator $\hat{\Psi}$ we have computed the three-particle wave function according to

$$\Phi(x_1, x_2, y, t) = \langle 0 \| \hat{\Psi}^{(+)}(x_1, t)\hat{\Psi}^{(+)}(x_2, t)\hat{\Psi}_c^{(+)}(y, t) \| \Psi(t = 0)\rangle/\sqrt{2}, \quad (4)$$

where the subscript c denotes the charge conjugation and the superscript $(+)$ denotes the positive frequency part [8]. This wave function is a $4 \times 4 \times 4$ spinor and describes in spatial and temporal resolution how the incoming Gaussian wave packet scatters off the potential which due to its supercriticality can also emit an electron-positron pair. With the exception of very early times, the emitted electron associated with the pair evolves to the left, whereas the positron created evolves to the right. Before the electron wave packet can reach the potential, the pair-production process is unaffected by the distant incoming electron. During the time interval when the electron wave packet overlaps with the potential, however, the pair-production process is suppressed. This was also indicated in the inset of Fig. 1.

This effect is shown in spatial resolution in Fig. 3. Graphed in the figure are the reflected electron density $\rho_e(x, t)$ and the positron density $\rho_p(y, t)$ at a given time, after the electron has completely scattered from the potential. The density $\rho_e(x, t)$ was obtained by integrating the absolute value square of the three-particle spinor state over all spatial as well as spin degrees of freedom except for the electron's coordinate x. The positron density $\rho_p(y, t)$ results from a similar integration over all electronic degrees of freedom.

For comparison we have included with the dashed line the corresponding positron density obtained from a calculation without any incoming electron. The comparison clearly shows the existence of a positron "hole" around $y = 0.15$ a.u. reflecting the lack of positron production at earlier times when the incoming electron wave packet scattered off the potential.

To connect these findings with previous calculations, we have indicated by the dotted line the transmitted part of the wave packet obtained from a solution of the non-quantized single-particle Dirac equation. Quite remarkably, this transmitted part presents exactly the missing portion of the positron density due to the incoming electron.

As the electron created during the pair-production process and the reflected electron are indistinguishable from each other, we believe an interpretation of the process based on electron labeling is not straightforward. We therefore cannot comment on whether 100% of the incoming electron is reflected or whether part of the incoming electron is used to annihilate a newly generated positron such that the remaining electron (created by the potential) would contribute to the outgoing electron flux.

We finish with another observation. If one computes the single-electron wave function from the quantum field operator according to $\psi(x, t) = \langle 0 \| \hat{\Psi}^{(+)}(x, t) \| \psi(t = 0)\rangle$, the time evolution operator for $\psi(x, t)$ is not unitary, in fact there is no electron transmission into the barrier and

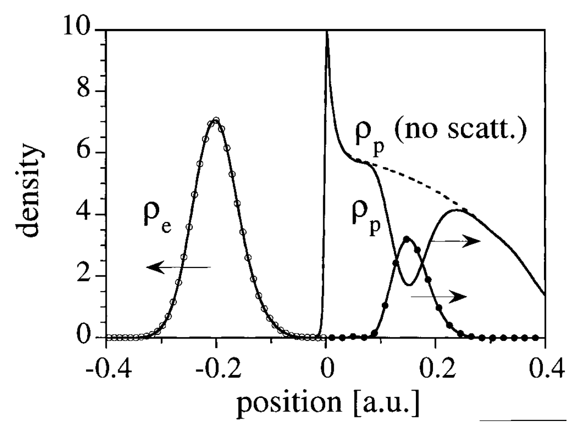

FIG. 3. Temporal snapshot of the positron's spatial probability distribution obtained from the three-particle wave function. The electron spatial distribution is left out for graphical clarity; for a complete animation, see [10]. The minimum at $x = 0.15$ a.u. is the result due to the pair-production suppression at earlier times when the incoming electron collided with the potential. For comparison we also show the density (open and closed circles) corresponding to the reflected and "transmitted" wave packet obtained from an independent single-particle calculation. The dashed line shows the corresponding positron density without any incoming electron. (The average kinetic energy of the incoming electron is 5000 a.u. and its width Δx is 0.03 a.u., $V_0 = 2c^2 + 0.53c^2$, $W = 0.3/c$, $x_0 = -0.2$ a.u., with a snapshot taken at time $t = 43.9 \times 10^{-4}$ a.u.)

the norm of the reflected electron is less than the incoming electron. In other words, the missing amount that has been associated with the ''Klein tunneling'' [9] is simply removed from the single-electron wave function if computed strictly from the quantum field.

In conclusion, we have reported for the first time on space-time resolved data for the Klein paradox as a three-particle problem. Analytical derivations suggest that the incoming electron suppresses the pair production. This finding contradicts previous studies noting a reflection coefficient larger than 1 and claiming that pair production is triggered by the incoming electron. In addition, our numerical time-resolved calculations [10] suggest that this suppression happens only when the incoming electron's spatial density overlaps with the potential region. Finally, the ''transmitted portion'' of the wave packet under the barrier obtained from a nonquantized single-particle treatment of the problem corresponds precisely to the amount by which the positron's spatial density is reduced by the incoming electron.

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[1] O. Klein, Z. Phys. **53**, 157 (1929); **41**, 407 (1927).
[2] J.W. Braun, Q. Su, and R. Grobe, Phys. Rev. A **59**, 604 (1999).
[3] A. Hansen and F. Ravndal, Phys. Scr. **23**, 1036 (1981).
[4] F. Sauter, Z. Phys. **69**, 742 (1931); **73**, 547 (1931).
[5] W. Greiner, B. Müller, and J. Rafelski, *Quantum Electrodynamics of Strong Fields* (Springer-Verlag, Berlin, 1985), p. 120.
[6] N. Nitta, T. Kudo, and H. Minowa, Am. J. Phys. **67**, 966 (1999).
[7] B. R. Holstein, Am. J. Phys. **66**, 507 (1998).
[8] S. S. Schweber, *An Introduction to Relavistic Quantum Field Theory* (Harper & Row, New York, 1962).
[9] N. Dombey and A. Calogeracos, Phys. Rep. **315**, 41 (1999).
[10] For a computer movie of the time evolution, see www.phy.ilstu.edu/ILP/movies