PHYSICAL REVIEW A **72**, 064103 (2005)

Klein paradox with spin-resolved electrons and positrons

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(Received 8 August 2005; published 30 December 2005)

Using numerical solutions to relativistic quantum field theory with space-time resolution, we illustrate how an incoming electron wave packet with a definite spin scatters off a supercritical potential step. We show that the production rate is reduced of only those electrons that have the same spin as the incoming electron is reduced. This spin-resolved result further clarifies the importance of the Pauli-exclusion principle for the Klein paradox.

DOI: 10.1103/PhysRevA.72.064103 PACS number(s): 03.65.Pm, 03.65.−w

I. INTRODUCTION

In 1929 the Swedish physicist Oskar Klein observed that the single-particle Dirac equation predicts a counterintuitive process for an incoming electron that is scattered off a repulsive potential step whose height exceeds twice the rest mass energy of the electron [1]. It was found that part of the mathematical wave-packet solution to the Dirac equation is permitted to transmit under the potential barrier even though its incoming kinetic energy is far less than the potential energy of the barrier. This nonvanishing penetration into an energetically forbidden area is called the "Klein paradox." There is a vast amount of literature devoted to this paradox and many textbooks on relativistic quantum mechanics discuss it to illuminate the importance of the negative energy states that are unavoidable for the Dirac equation without second quantization [2].

There have been many attempts to interpret this counterintuitive transmission behavior of the mathematical solutions to the single-particle Dirac equation. Some works based on a steady-state analysis predict transmission coefficients that are negative and reflection coefficients that exceed unity [3]. These unusual numerical values for the coefficients were explained in terms of positrons that were "knocked out" [2,4] from the lower energy continuum during the collision. A nice review about this effect has been written by Dombey and Calogeracos [5].

Several works [2,6,7] went beyond the simple framework of the single-particle Dirac equation and used quantum field theory to predict the pair production rate at the supercritical barrier, however, they did not take the effect of the incoming electron into account.

In 2003 the Klein paradox was revisited from a field-theoretical point of view leading to an alternative interpretation [8,9]. The time- and position-dependent electron-positron field operator was computed numerically for an electron injected into a supercritical potential barrier. In contrast to previous statements in the literature, these studies suggest that the electron does not "knock out" electron-positrons pairs [2] nor does it "stimulate" [4] the generation of the pairs. In fact, these quantum field-theoretical simulations accompanied by analytical estimates suggest that while the incoming electron is at the barrier, it actually suppresses the pair production. As the potential barrier is supercritical, it produces a constant rate of electron-positron pairs which is then inhibited temporarily by the scattering electron, suggesting a simple intuitive picture based on the Pauli-exclusion principle. This work [8] was based on the calculation of three-particle wave functions only and therefore did not take the generation of more than one electron-positron pair at the barrier into account. Furthermore, the study did not distinguish between ejected electrons with positive and negative spins.

In this work we will show that both a resolution for the spin as well as the inclusion of multiple pair creation are necessary for a *quantitative* interpretation of the Klein paradox. This will be accomplished by analyzing the particles with regard to their spins and by computing the total spatial probability density instead of wave functions.

II. KLEIN PARADOX WITHOUT SECOND QUANTIZATION

Let us briefly review the predictions of the Klein paradox in the nonsecond quantized framework. The single-particle Dirac equation [10] for the four-component wave function along the z axis takes the following form (in atomic units):

$$i\partial_t \phi(z,t) = [c\alpha_z p_z + \beta c^2 + V(z,t)]\phi(z,t), \qquad (2.1)$$

where α_z is the z component of the 4×4 Pauli matrix, β is the diagonal matrix, and c is the speed of light, $c=137.036$ a.u.. We have solved this equation numerically [11] for an incoming electron wave packet initially located at $z_0=-0.2$ a.u. far to the left of a potential barrier $V(z,t)$. This state is given by the Gaussian superposition of momentum eigenstates

$$\phi_\uparrow(z,t=0) = \mathcal{N}\Sigma_p \exp(ipz_0)\exp[-(p-p_0)^2\Delta z^2] w_{p\uparrow}(z) \qquad (2.2)$$

with the normalization constant $\mathcal{N}$, the initial spatial width $\Delta z=0.03$ a.u., and the central momentum $p_0=106.4$ a.u. associated with a speed of $0.62c$. The summation Σ_p in Eq. (2.2) is over all eigenstates with positive energy satisfying $(c\alpha_z p_z+\beta c^2)w_{p\uparrow}(z)=\sqrt{(c^4+c^2p^2)}w_{p\uparrow}(z)$. For the discussion in Sec. III below it is important to note that due to the conservation of helicity, the spin along the propagation direction can be chosen sharp and we have $\langle S_z\rangle=1/2$ for this particular state indicated by the direction of the arrow in the subscript.

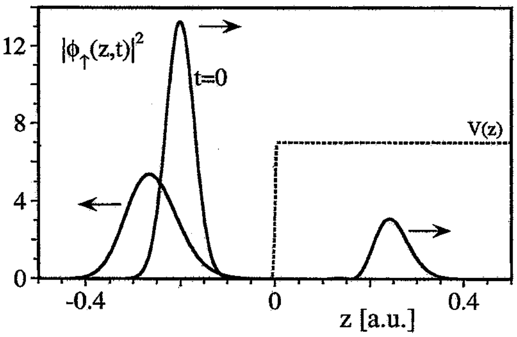

FIG. 1. The graph on the top shows the absolute value square of the wave function solution to the single-particle Dirac equation, $|\phi_\uparrow(z,t)|^2$ at time $t=5.47\times10^{-3}$ a.u. We also show the incoming wave packet at $t=0$. The incoming wave packet has split into two wave packets, a reflected one (with norm 0.7255) moving to the left and another one propagating under the barrier (with norm 0.2745). For reference, the dashed line indicates the shape of the supercritical potential barrier $[P_0=106.4$ a.u., $\Delta z=0.03$ a.u., $V_0=2c^2+10^4$ a.u., $W=0.3/c]$.

We choose a simple steplike potential of the form $V(z,t)=V_0[\tanh(z/W)+1]/2\theta(t)$, where $\theta(t)$ denotes the unit step function. The potential is characterized by the length scale W which is the width of the region where the corresponding force, proportional to the derivative $V'(z)$, is nonzero. We chose $W=0.3/c$ and $V_0=2c^2+c^2/2$, which is larger than the energy E of the incoming electron, therefore prohibiting any (nonrelativistic) transmission.

In Fig. 1 we show the initial wave packet $|\phi_\uparrow(z,t=0)|^2$ together with a snapshot of the final mathematical state $|\phi_\uparrow(z,t)|^2$ at time $t=5.5\times10^{-3}$ a.u. The reflected wave packet has a weight of only 0.7255, whereas there is also a transmitted portion under the barrier (with norm of 0.2745). Due to the norm conservation by the unitary time evolution, it should be clear that this theoretical framework without second quantization cannot predict any pair production and the reflection and transmission coefficients have to be positive and add to unity. Alternatively, using a standard steady-state analysis one can determine the transmission coefficient [12]

$$T(E)=-\sinh(\pi pW)\sinh(\pi\kappa W)/\{\sinh[\pi(V_0/c+p+\kappa)W/2]\sinh[\pi(V_0/c-p-\kappa)W/2]\} \tag{2.3}$$

which is nonzero for $V_0>2c^2$ even if $E<V_0$. Here $p\equiv\sqrt{[(E/c)^2-c^2]}$ and the *negative* momentum $\kappa\equiv-\sqrt{[(E-V_0)^2/c^2-c^2]}$. For our parameters $(E=V_0/2)$ we obtain $T(E)=0.272$ which matches the norm of the transmitted wave function solution with an error of less than 1%. A quantitative interpretation of this mysterious mathematical wave-function solution under the barrier is the subject of the next section.

To better connect these findings with the ones discussed below, it is important to point out that the (mathematical) transmission of 0.2745 does not mean that some of the electron gets lost or even transmitted. In fact, the entire incoming electron (100%) gets reflected. However, a portion of weight 0.2745 becomes "invisible" within this single-particle framework and can no longer be described by a simple wave function as the electron gets entangled with the environment.

III. KLEIN PARADOX WITH THE SECOND-QUANTIZED DIRAC EQUATION

In order to discuss the predictions by quantum field theory for the same physical process, we have to solve the Dirac equation for the electron-positron *operator* $\hat{\Psi}(z,t)$:

$$i\partial_t\hat{\Psi}(z,t)=[c\alpha_z p_z+\beta c^2+V(z,t)]\hat{\Psi}(z,t). \tag{3.1}$$

This operator equation can be solved numerically if the field operator $\hat{\Psi}$ is expanded in the Fermion creation and annihilation operators, $\hat{\Psi}(z,t)=\Sigma_p\hat{b}_p(t)w_p(z)+\Sigma_n\hat{d}_n^\dagger(t)w_n(z)$, where $w_p(z)$ and $w_n(z)$ are (four-component) free-particle basis states. The parameter p labels states with positive energy $c^2\leqslant e_p$ and n labels the negative energies $e_n\leqslant-c^2$. The operators evolve in time according to

$$\hat{b}_p(t)=\Sigma_{p'}\hat{b}_{p'}(t=0)\langle p|U(t)|p'\rangle+\Sigma_{n'}\hat{d}_{n'}^\dagger(t=0)\langle p|U(t)|n'\rangle \tag{3.2a}$$

$$\hat{d}_n^\dagger(t)=\Sigma_{p'}\hat{b}_{p'}(t=0)\langle n|U(t)|p'\rangle+\Sigma_{n'}\hat{d}_{n'}^\dagger(t=0)\langle n|U(t)|n'\rangle, \tag{3.2b}$$

where the coefficients are the matrix elements of the unitary propagator $U(t)\equiv\exp[-iHt]$ between the states. These matrix elements are the building blocks of quantum field theory for noninteracting Fermions. Each possible initial state of the entire Hilbert space needs to be evolved in time to compute all matrix elements and to obtain the field $\hat{\Psi}(z,t)$. [11].

In order to obtain spatially resolved probability densities for the electrons and the positrons, we have to compute the positive energy part of the field operator by projecting the field on the subspaces spanned by the electron (positron) states,

$$\hat{\Psi}^{(+)}(z,t)\equiv\Sigma_p\hat{b}_p(t)w_p(z), \tag{3.3a}$$

$$\hat{\Psi}_c^{(+)}(z,t)\equiv\Sigma_n\hat{d}_n(t)Cw^*{}_n(z), \tag{3.3b}$$

where the subscript c is associated with the charge conjugation operation. Correspondingly, $Cw_n^*(z)$ are positron states with positive energy $-e_n$ associated with the charge conjugated Hamilton operator.

In order to classify the electron and positron densities according to their spin, we have separated the corresponding components of the field operator into two parts, $\hat{\Psi}^{(+)}(z,t)=\hat{\Psi}_\uparrow^{(+)}(z,t)+\hat{\Psi}_\downarrow^{(+)}(z,t)$, where the first operator is obtained by projecting only on those states $w_{p\uparrow}(z)$ that have a positive spin along the z direction.

We can now define the total spatial density for the electrons, $\rho_{\uparrow\downarrow}^-(z,t)$, and the positrons, $\rho_{\uparrow\downarrow}^+(z,t)$, as

$$\rho_{\uparrow\downarrow}^-(z,t)\equiv\langle\varphi(t=0)\|\hat{\Psi}_{\uparrow\downarrow}^{\dagger(+)}(z,t)\hat{\Psi}_{\uparrow\downarrow}^{(+)}(z,t)\|\varphi(t=0)\rangle, \tag{3.4a}$$

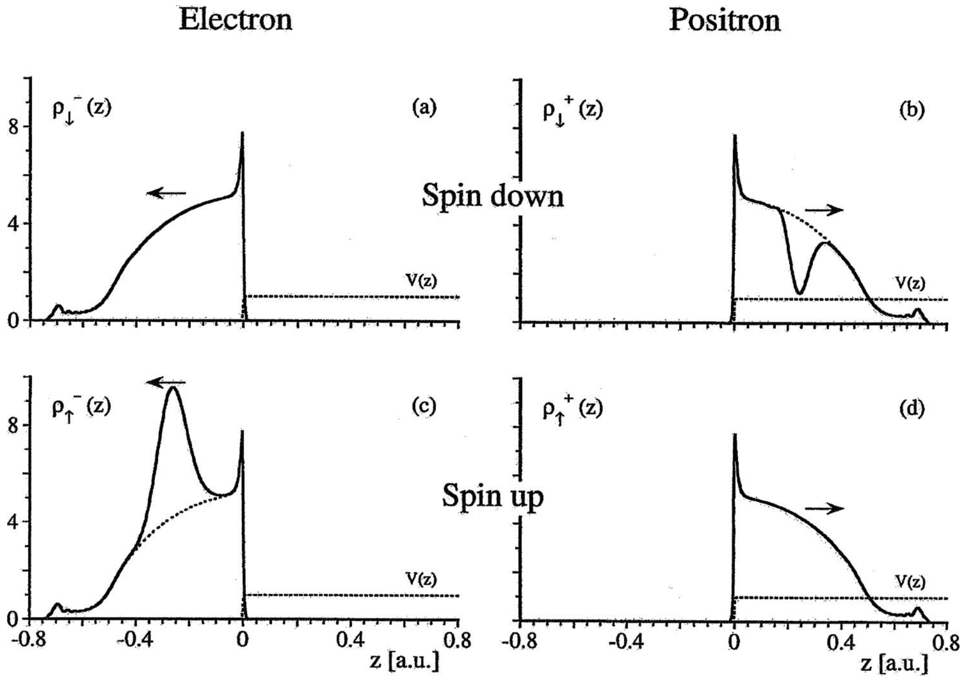

FIG. 2. The graphs on the top show snapshots of the electronic and positronic spatial probability density with negative spin, $\rho^{-}_{\downarrow}(z,t)$ and $\rho^{+}_{\downarrow}(z,t)$, as obtained by quantum field theory. The lower graphs show the corresponding spatial densities with positive spin. The dashed line in (b) was obtained by adding the transmitted solution of Fig. 1 to $\rho^{+}_{\downarrow}(z,t)$. The dashed line in (c) was obtained by subtracting the reflected solution of Fig. 1 from $\rho^{-}_{\uparrow}(z,t)$. Note the direct correspondence of the "hole" in the positron density $\rho^{-}_{\downarrow}(z,t)$ with the shape of the transmitted portion of Fig. 1 (identical parameters as in Fig. 1).

$$\rho^{+}_{\uparrow\downarrow}(z,t) \equiv \langle \varphi(t=0)\|\hat{\Psi}^{\dagger(+)}_{\uparrow\downarrow c}(z,t)\hat{\Psi}^{(+)}_{\uparrow\downarrow c}(z,t)\|\varphi(t=0)\rangle. \tag{3.4b}$$

The multiparticle initial state is denoted by $\|\varphi(t=0)\rangle$ and represents the Fock state for the incoming electron analogous to the single-particle state of Eq. (2.2). We should note that as we project the field operators on eigenstates of the force-free Hamiltonian, the corresponding spin-dependent density has a simple meaning only in those spatial regions, in which the force vanishes [13].

In Figs. 2(a) and 2(b) we show the snapshots, taken at the same time as Fig. 1, of the final electron (left) and positron (right) density with negative spin, $\rho^{-}_{\downarrow}(z,t)$ and $\rho^{+}_{\downarrow}(z,t)$. As our incoming electron has a positive spin and the potential barrier cannot couple electrons with different spins, the final electron density is entirely due to the pair-production process induced by the supercritical potential region [14,15] and therefore shows no resemblance to the data shown in Fig. 1. This (non-norm conserving) process cannot be described by the single-particle framework as outlined in Sec. II. The total area under the density (called weight) is 2.122, indicating the production of more than just a single electron-positron pair. This weight is identical to the sum of all occupation numbers, $\Sigma_{p}\langle\varphi(t=0)\|\hat{b}^{\dagger}_{p\downarrow}(t)\hat{b}_{p\downarrow}(t)\|\varphi(t=0)\rangle$.

The little maxima at $z=-0.7$ a.u. and $z=0.7$ a.u. are associated with very early electrons and positrons, respectively, that move with nearly the speed of light and were created when the supercritical barrier was turned on instantaneously at $t=0$.

The electron and positron distributions with the same spin, however, are not entirely symmetrical around $z=0$. The positron density $\rho^{+}_{\downarrow}(z,t)$ has a weight of only 1.848 due to a hole located at $z=0.25$ a.u. This hole is caused by the incoming electron of opposite spin. In the absence of any incoming electron, the positron density (with spin down) and the electron density (with spin up) would be completely symmetrical. The dashed line that is also displayed in the positron density was obtained by adding the transmitted portion of the single-particle wave function $|\phi_{\uparrow}(z,t)|^2$ from Fig. 1 (with weight 0.2745) to the density of the positron $\rho^{+}_{\downarrow}(z,t)$. We see that the hole associated with the reduction of positron generation is perfectly filled up by the (mathematical) transmitted portion shown in Fig. 1.

This hole is the key to the resolution of the Klein paradox. The incoming electron suppresses the pair-production process due to the Pauli principle. Electrons with specific energy and spin up can no longer be generated by the supercritical potential as the incoming electron already occupies these (Fermionic!) states. As a result, the production rate for the electron and correspondingly also for its partner, the positron with down spin, become suppressed. This effect is interesting as the suppression occurs only during those times when the incoming electron overlaps with the barrier. An argument based solely on occupation numbers could not predict this, as the corresponding states were already "occupied" at times when the incoming electron was far away from the barrier.

Alternatively, one could equally argue that the incoming electron has no impact on the creation process at first, and only after a pair has been created, would the incoming electron (with spin up) annihilate with the created positron (with spin down) and therefore effectively reduce the pair production. This view is suggested when the process is described in terms of the electronic wave function, $\Phi_{\uparrow}(z,t)\equiv\langle 0\|\hat{\Psi}^{(+)}_{\uparrow}(z,t)\|\varphi(t=0)\rangle$, where $\langle 0\|$ is the vacuum state. The mathematical wave function discussed in Sec. II, $\phi_{\uparrow}(z,t)$, can also be related to the quantum field operator; however, via the sum over positive *and* negative frequency parts,

$$\phi_\uparrow(z,t) \equiv \langle 0\|\hat{\Psi}_\uparrow^{(+)}(z,t)\|\varphi(t=0)\rangle + \langle 0\|\hat{\Psi}_\uparrow^{(-)}(z,t)\|\varphi(t=0)\rangle. \tag{3.5}$$

Only the first term corresponds to an electron, $\Phi_\uparrow(z,t)$, whereas the second term is the transmitted part of the mathematical wave function $\phi_\uparrow(z,t)$. While the norm of the electronic state $\Phi_\uparrow(z,t)$ reduces (from 1 to 0.7255) during the scattering process, the norm of the $e^- - e^- - e^+$ wave function, defined as [16]

$$\Phi_{\uparrow\uparrow\downarrow}(z_1,z_2,z_3,t) \equiv \langle 0\|\hat{\Psi}_\uparrow^{(+)}(z_1,t)\hat{\Psi}_\uparrow^{(+)}(z_2,t)\hat{\Psi}_{c\downarrow}^{(+)}(z_3,t)\|\varphi(t=0)\rangle/\sqrt{2} \tag{3.6}$$

grows from its initial value of zero to 1.12. As the norms of the one- and three-particle wave functions, $\Phi_\uparrow(z,t)$ and $\Phi_{\uparrow\uparrow\downarrow}(z_1,z_2,z_3,t)$, add up to only 1.84 (instead of 2.842), the creation of multiple pairs (that was neglected in Ref. [8]) is important for this parameter regime. This analysis in terms of wave functions also illustrates how part of the incoming electron (with weight 0.2745) gets strongly entangled with the created $e^- - e^+$ pair.

In the bottom graphs of Fig. 2 we show the spin-up component of the final electron and positron densities. The electron density contains a large "bump" at $z=-0.25$ a.u., which is identical to the location of the reflected electron from the single-particle theory outlined in Sec. II above. The dashed line corresponds to the electron density, however, with the reflected wave function solution of Fig. 1, $|\phi_\uparrow(z,t)|^2$, subtracted. Similar to $\rho_\downarrow^-(z,t)$, the spin-up component of the created positron, $\rho_\uparrow^+(z,t)$, is also unaffected by the scattering [Fig. 2(d)].

In summary, these spin-resolved densities suggest the following overall interpretation. An electron wave packet (with initial norm 1) enters the potential region, 0.7255 of it gets directly reflected without any impact on the pair-production process. This portion can be described by an (uncorrelated) single-particle wave function as discussed in Sec. II and displayed in Fig. 1. The remaining 0.2745 of the reflected electron gets strongly entangled with the pair-production process and reduces effectively the norm of the created electron and positron density from 2.122 to only 1.8478 leading to the holes. However, the electronic hole can be filled up by the reflected electron (with norm 1.0) such that we observe the bump that increases the total electron density (created in the absence of any incoming electron) to a total weight of 2.8478. The weight of the created positron with spin down (with the hole) is only 1.8478, whereas the positron with spin up has a weight of 2.122.

ACKNOWLEDGMENTS

This work has been supported by the NSF. We also acknowledge support from the Research Corporation and NCSA for supercomputing time.

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