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We compare the predictions of the single-particle Dirac equation with quantum field theory for an electron subjected to a space and time dependent field. We demonstrate analytically and numerically that a transition into the negative-energy subspace predicted by the single-particle Dirac equation is directly associated with the degree of suppression of pair-production as described by quantum field theory. We show that the portion of the mathematical wave function that populates the negative-energy states corresponds to the difference between the positron spatial density for systems with and without an electron initially present.

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The Dirac equation is the theoretical foundation for the relativistic interactions between atoms and intense laser fields. Its numerical and analytical solutions [1–5] permitted the discovery of a wide variety of relativistic phenomena. With the exception of numerical studies of the electron-positron pair production [6] in heavy-ion collisions, most investigations used the Dirac equation in its single-particle framework. In other words, this equation was solved for a specific single-particle initial state for which the Dirac equation [7] predicted its unitary (norm conserving) evolution. The single-particle approach applies to only those processes for which the fields are either short, weak, or slowly varying enough such that the production of pairs can be neglected.

In order to extend these studies to novel phenomena for which the number of particles is not conserved, such as the case of pair production processes, quantum field theory must be applied. The conceptual problem which we will address in this work is whether one can find any physical process that can be described by a transition from a positive to a negative energy state obtained from the mathematical solution of the (not second quantized) single-particle Dirac equation, or should one simply discard these mathematical solutions as unphysical? In the early days of relativistic quantum mechanics it was believed that these possible transitions were unphysical. But because they nevertheless occurred mathematically, one tried to introduce additional constraints to prohibit these transitions. One should mention that there have been some attempts to redefine the position operator in order to avoid conceptual problems associated with negative energy states. However, the corresponding Newton-Wigner position operator [8] predicts superluminal spreading behavior and therefore violates causality [7].

Another clever postulate assumed that all states with negative energies are "occupied" from the very beginning and that the Pauli principle would forbid the unexplainable downward transitions. This *ad hoc* fix to what was regarded as a major challenge at that time led to the introduction of the hole theory. An upward transition was interpreted as the creation of a hole in the negative continuum which was associated with the occurrence of a positively charged particle.

Only years later quantum field theory reexamined the hole theory by providing the appropriate interpretation of the negative Dirac continuum as the charge conjugated states of positrons with positive energy [9]. This interpretation could lead to the (incorrect) conjecture that the amount of downward transition in the single-particle framework is proportional to the amount of positrons created. To the best of our knowledge, despite the progress made in removing misconceptions about the hole theory, the question about any physical significance of the permitted downward transition has remained up to today. It is the purpose of this Brief Report to note that there is in fact a physical process that may be described quantitatively by these downward transitions.

The understanding of how quantum field theory can be used to predict the space-time evolution of particles has also led recently to the resolution of the Klein paradox [10]. It has also helped to remove the conceptual problem of the Schrödinger's *Zitterbewegung* [11] which is merely a mathematical signature of the single-particle Dirac equation and does not correspond to any real physical motion. Also in direct contrast to claims in many textbooks, there is no limitation in principle to the localization length of an electron [11].

In order to better understand the significance of the downward transitions, let us first briefly review its formulation. The Dirac equation that governs the evolution of the single-particle (four-component) wave function $\phi(x,t)$ is given by [7]

$$i\partial_t\phi(x,t) = \{c\boldsymbol{\alpha}\cdot[\mathbf{p} - e\mathbf{A}(x,t)] + \beta c^2 + eV(x,t)\}\phi(x,t). \tag{1}$$

Here c is the speed of light, and $\boldsymbol{\alpha}$ and β denote the 4×4 Dirac matrices (in atomic units). This equation permits us to compute the wave function uniquely from any arbitrary initial state $\phi(x,t=0)$. Let us assume that at the initial time, both external fields described by $\mathbf{A}$ and V are not strong enough to create pairs. We can define a complete basis in terms of the energy eigenstates that fulfill

$$\{c\boldsymbol{\alpha}\cdot[\mathbf{p} - e\mathbf{A}(x,t=0)] + \beta c^2 + eV(x,t=0)\}\mathbf{W}_{p,(n)}(x) = E_{p,(n)}\mathbf{W}_{p,(n)}(x), \tag{2}$$

where the subscript $p(n)$ denotes whether the energy is positive or negative. For the special case $A(x,t=0)=0$ and $V(x,t=0)=0$ we have the field-free spectrum $E_p \geqslant c^2$ and $E_n \leqslant -c^2$. This restriction, however, is not necessary in our discussion. As a side remark we might note that the charge

conjugated negative-energy eigenstates $CW_n^*(x)$ are (positive energy) solutions of the Dirac Hamiltonian for which the charge e is replaced by $-e$ corresponding to a positron [9].

Let us assume that our initial state is a superposition of states with positive energy, $|\phi(t=0)\rangle=\Sigma_p C_p|p\rangle$. As this state consists of positive energies only, one could interpret this as the state of an electron. If we evolve this state in time as $V(x,t)$ and $\mathbf{A}(x,t)$ are switched on, it is unavoidable that in addition to transitions between positive-energy states negative-energy states may also become populated. According to the single-particle Dirac equation (1), its norm-conserving time evolution is described by

$$|\phi(t)\rangle = \Sigma_p C_p \Sigma_n \langle n|U(t)|p\rangle|n\rangle + \Sigma_p C_p \Sigma_{p_1}\langle p_1|U(t)|p\rangle|p_1\rangle \equiv |\phi_-(t)\rangle + |\phi_+(t)\rangle, \tag{3}$$

where $\Sigma_{p(n)}$ denotes the summation (integration) over all states with positive (negative) energy. In general, each matrix element needs to be evaluated numerically by applying the time-ordered unitary propagator $U(t) \equiv T[\exp(-i\int_0^t dt'\{c\boldsymbol{\alpha}\cdot[\mathbf{p}-e\mathbf{A}(x,t')]+\beta c^2+eV(x,t')\})]$ to each possible state. Note that the single-particle scalar product $\langle\cdots\rangle$ contains the summation over the four spinor components as well as the integration over the spatial coordinate. Initially we have $\langle p|U(t=0)|p'\rangle=\delta_{pp'}$ and $\langle n|U(t=0)|p\rangle=0$, but as time evolves transitions into lower energy states are unavoidable as $\langle n|U(t)|p\rangle$ becomes nonzero and $|\phi_-(t)\rangle$ is populated. Its corresponding norm is given by $\langle\phi_-(t)|\phi_-(t)\rangle=\Sigma_n|\Sigma_p C_p\langle n|U(t)|p\rangle|^2$, whereas the norm of $|\phi(t)\rangle$ is always conserved, $\langle\phi(t)|\phi(t)\rangle=1$ according to the unitary character of $U(t)$.

Let us now illustrate the downward transition numerically and assume that the coefficients C_p are such that the initial state is spatially a Gaussian with width σ. To keep the discussion simple, we evolve the initial state $|\phi(t=0)\rangle$ under a static electric field given by the potential $V(x,t)=V_0 x\theta(W+x)\theta(W-x)\theta(t)$, where $\theta(\cdots)$ denotes the Heaviside unit-step function and $2W$ is the spatial width of the region in which the field is nonzero. For simplicity we choose $W\gg\sigma$ such that the electron experiences a spatially constant electric field.

In Fig. 1 we show the spatial density of the positive energy part, defined as $|\phi_+(x,t)|^2\equiv\phi_+^\dagger(x,t)\phi_+(x,t)=\Sigma_i|\phi_+^{(i)}(x,t)|^2$ after an interaction time of $t=1/(100c^2)$ ($\approx 5\times10^{-7}$ a.u.). Here Σ_i denotes the summation over the four spinor components. Its norm is given by $\int dx|\phi_+(x,t)|^2=0.999\,83$. As the time evolution is unitary, the missing part occupies the lower energy states and we show their spatial representation as well, which is given by $|\phi_-(x,t)|^2$ with a norm of 0.000 17.

Quantum field theory will show us that there is a physical process that can be described by the mathematical solution $\phi_-(x,t)$. To make contact with the above discussion, let us now study the interaction of an electron, initially given by the state $|\phi(t=0)\rangle=\Sigma_p C_p|p\rangle$, with a combination of external fields $\mathbf{A}(x,t)$ and $V(x,t)$ that are strong enough to create pairs from the vacuum. In quantum field theory the following

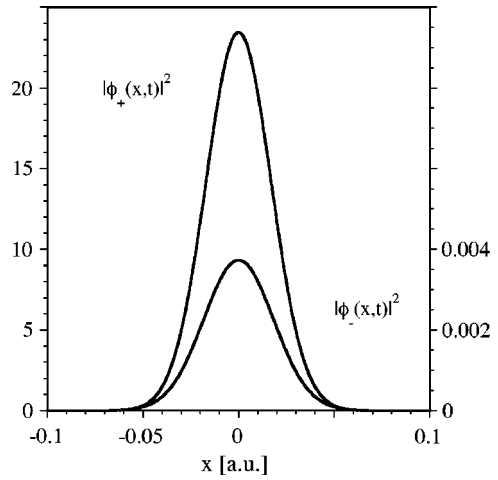

FIG. 1. Positive and negative energy parts of the solution of the single-particle Dirac equation at time $t=5\times10^{-7}$ a.u. for a static electric field given by the potential $V(x,t)=V_0 x\theta(W+x)\theta(W-x)\theta(t)$. ($V_0=5000c^2, W=0.166$ a.u.)

Dirac equation has to be solved for the electron-positron field $\hat{\Psi}$:

$$i\partial_t\hat{\Psi}(x,t) = \{c\boldsymbol{\alpha}\cdot[\mathbf{p}-e\mathbf{A}(x,t)]+\beta c^2+eV(x,t)\}\hat{\Psi}(x,t), \tag{4}$$

which is different from Eq. (1) due to the *operator* character. This equation is solved for the initial field,

$$\hat{\Psi}(x,t=0) = \Sigma_p\hat{b}_p(t=0)W_p(x) + \Sigma_n\hat{d}_n^\dagger(t=0)W_n(x), \tag{5}$$

where $\hat{b}_p$ and $\hat{d}_n^\dagger$ are the usual electron annihilation and positron creation operators, respectively. When inserted into the operator Dirac equation we obtain the solution

$$\hat{\Psi}(x,t) = \Sigma_p\hat{b}_p(t)W_p(x) + \Sigma_n\hat{d}_n^\dagger(t)W_n(x), \tag{6a}$$

where

$$\hat{b}_p(t) = \Sigma_{p'}\hat{b}_{p'}(t=0)\langle p|U(t)|p'\rangle + \Sigma_{n'}\hat{d}_{n'}^\dagger(t=0)\langle p|U(t)|n'\rangle, \tag{6b}$$

$$\hat{d}_n^\dagger(t) = \Sigma_{p'}\hat{b}_{p'}(t=0)\langle n|U(t)|p'\rangle + \Sigma_{n'}\hat{d}_{n'}^\dagger(t=0)\langle n|U(t)|n'\rangle. \tag{6c}$$

The full set of time-dependent expansion coefficients $\langle p_1|U(t)|p\rangle$ and $\langle n|U(t)|p\rangle$ is the building block for quantum field theory. Using the operator solution (6) we can now construct the electron's spatial probability density according to $\rho(x,t)=\langle\Psi(t=0)\|\hat{\Psi}^{\dagger(+)}(x,t)\hat{\Psi}^{(+)}(x,t)\|\Psi(t=0)\rangle$, where the superscript $(+)$ denotes the positive frequency part. The corresponding positron density as a function of its coordinate y is obtained via $\rho(y,t)=\langle\Psi(t=0)\|\hat{\Psi}_c^{\dagger(+)}(y,t)\hat{\Psi}_c^{(+)}(y,t)\|\Psi(t=0)\rangle$, where the subscript c denotes the charge conjugated field.

We compute the positron density for two different initial conditions, the pair-creation process from vacuum, for which $\|\Psi(t=0)\rangle=\|0\rangle$ denotes the vacuum state and the same pro-

cess in which an electron is initially present. In the latter case, $\|\Psi(t=0)\rangle$ corresponds to a state in which a electron occupies initially the single-particle states $|\phi(t=0)\rangle = \Sigma_p C_p|p\rangle$. Inserting the general quantum field theoretical solution in the expectation values, we obtain for the positron densities in these two cases

$$\rho(y,t;\mathrm{vac}) \equiv \langle 0\|\hat{\Psi}_c^{\dagger(+)}(y,t)\hat{\Psi}_c^{(+)}(y,t)\|0\rangle = \Sigma_p\Sigma_n|\langle n|U(t)|p\rangle W_n(y)|^2, \tag{7}$$

$$\rho(y,t;e^-) \equiv \langle \phi\|\hat{\Psi}_c^{\dagger(+)}(y,t)\hat{\Psi}_c^{(+)}(y,t)\|\phi\rangle = \Sigma_p\Sigma_n|\langle n|U(t)|p\rangle W_n(y)|^2 - |\Sigma_p C_p\Sigma_n\langle n|U(t)|p\rangle W_n(y)|^2. \tag{8}$$

The spatial integral over the two densities is the total probability to find a positron. For the system initially in vacuum, it amounts to $\int dy\rho(y,t;\mathrm{vac}) = \Sigma_p\Sigma_n|\langle n|U(t)|p\rangle|^2$, which is the same as the sum over all occupation numbers according to $\Sigma_n\langle 0\|\hat{d}_n^\dagger(t)\hat{d}_n(t)\|0\rangle$.

Comparing the two expressions (7) and (8) with Eq. (3) we find that they differ precisely by the density associated with the mathematical wave function ϕ_- obtained from the single-particle Dirac equation

$$\rho(y,t;e^-) = \rho(y,t;\mathrm{vac}) - \phi_-^\dagger(y,t)\phi_-(y,t). \tag{9}$$

This equation proves the main message of this paper. The creation of a positron is only possible if it is created with its twin partner, the electron. The initial electron, however, has occupied already some positive energy states $[\Sigma_p C_p|p\rangle]$ which the newly created electron would like to populate. The Pauli principle which is built into quantum field theory due to the anticommutation relationships between the fermionic operators, $[\hat{b}_{p_1},\hat{b}_{p_2}]_+=0$ and $[\hat{b}_{p_1},\hat{b}_{p_2}^\dagger]_+=\delta_{p_1p_2}$, restricts the occupation numbers to be at most 1.

In addition to the Pauli principle, Eq. (9) shows that the single-particle solution associated with the downward transition into the lower energy state has a direct and quantitative physical interpretation. The spatial distribution of $|\phi_-(x,t)|^2$ (displayed in Fig. 1) is a quantitative measure for the impact of the initial electron on the pair production process. At each time and for each location y it corresponds precisely to the amount of pair-production suppression due to the initial electron. In other words, as the initial electron evolves it blocks out the generation of the positron at spatial locations y according to $|\phi_-(y,t)|^2$.

To illustrate our analytical conclusion, we display the corresponding densities in Fig. 2. These densities were obtained via a large scale numerical simulation of the quantum field theoretical operator equation on a space-time grid to compute all possible matrix elements of $U(t)$. In Fig. 2(a) we show a snap shot of the positron's spatial density $\rho(y,t;\mathrm{vac})$ together with the potential $V(x)$ responsible for creating the particle. In Fig. 2(b) we display the positron's density $\rho(y,t;e^-)$ for the case with an initial electron. This distribution grows in time but it has a spatial hole close to $y=0$ indicating the suppression of pair production in this region where the electron was initially located. Outside this region

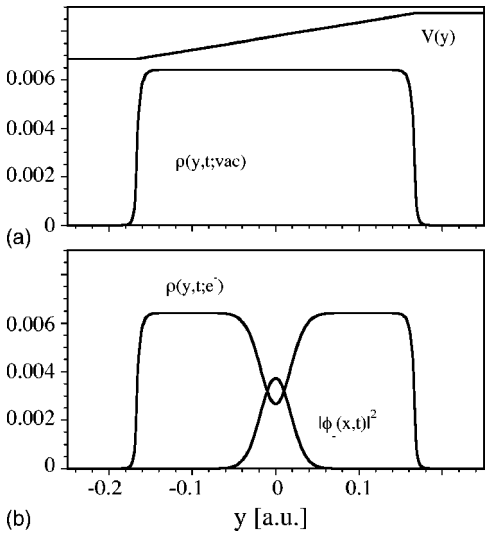

FIG. 2. (a) The spatial density for the positrons $\rho(y,t;\mathrm{vac})$ created by the supercritical field at time $t=5\times10^{-7}$ a.u. The second line is the supercritical potential $V(y,t)=V_0 y\theta(W+y)\theta(W-y)$. (b) The spatial density of the positron $\rho(y,t;e^-)$ that was created by the same potential, however with an initial electron present. The other curve is the spatial density associated with the negative energy solution $|\phi_-(y,t)|^2$ providing the missing portion. ($V_0=5000c^2, W=0.166$ a.u.)

the two densities are identical, $\rho(y,t;\mathrm{vac})=\rho(y,t;e^-)$. For comparison we graph on the same scale the density associated with the negative energy portion of the mathematical wave function solution $|\phi_-(x,t)|^2$. As can be seen from the two graphs, this "mathematical" density is precisely the missing part in the density $\rho(y,t;e^-)$ compared to the density without any initial electron $\rho(y,t;\mathrm{vac})$.

As a final point we should mention that in the regime of short times for which the probability of creation of more than one pair is negligible one can even compute the corresponding two-particle 4×4 and three-particle $4\times4\times4$ wave functions for the pair-production process for the two initial conditions. In contrast to the effective densities ρ that describe all pairs, these wave functions contain all information about the phases, spins as well as entanglement [12] between the particles. The 16 (64) spin component two (three) –particle wave functions are obtained via

$$\Phi_3(x_1,x_2,y,t;e^-) = \langle 0\|\hat{\Psi}^{(+)}(x_1,t)\hat{\Psi}^{(+)}(x_2,t)\hat{\Psi}_c^{(+)}(y,t)\|\phi\rangle/\sqrt{2} = \Sigma_p\Sigma_{p_2}\Sigma_n\Sigma_{p_1}\Sigma_{p_3}\langle p|U(t)|p_1\rangle\langle p_2|U(t)|p_3\rangle \times[C_{p_1}\langle n|U(t)|p_3\rangle^* - C_{p_3}\langle n|U(t)|p_1\rangle^*]W_p(x_1)\otimes W_{p_2}(x_2)\otimes CW_n^*(y)/\sqrt{2}, \tag{10}$$

$$\Phi_2(x,y,t;\mathrm{vac}) = \langle 0\|\hat{\Psi}^{(+)}(x,t)\hat{\Psi}_c^{(+)}(y,t)\|0\rangle = -\Sigma_p\Sigma_{n_1}\{\Sigma_{n_2}\langle n_1|U(t)|n_2\rangle^*\langle p|U(t)|n_2\rangle\}W_p(x)\otimes CW_{n_1}^*(y). \tag{11}$$

In the short-time limit, we can expand the time evolution matrix elements to $U(t)=1-iH(t/2)t$ leading to the simplifications $\langle p_1|U(t)|p_2\rangle=\delta_{p_1p_2}-i\langle p_1|H(t/2)|p_2\rangle t$, $\langle n_1|U(t)|n_2\rangle=\delta_{n_1n_2}-i\langle n_1|H(t/2)|n_2\rangle t$ and $\langle p|U(t)|n\rangle=-i\langle p|H(t/2)|n\rangle t$. In this short-time limit the two solutions simplify and fulfill for each positron coordinate y,

$$\int\int dx_1dx_2|\Phi_3(x_1,x_2,y,t)|^2 = \int dx|\Phi_2(x,y,t)|^2-\phi_-^\dagger(y,t)\phi_-(y,t) \tag{12}$$

which is the direct analog of Eq. (9), but phrased in the context of two and three particle wave functions and therefore valid only for short times. Integrating Eq. (12) over the y coordinate we obtain $\langle\Phi_3(t)|\Phi_3(t)\rangle=\langle\Phi_2(t)|\Phi_2(t)\rangle-\langle\phi_-(t)|\phi_-(t)\rangle$.

In closing, we should mention that the quantum field theory presented here relies on the strong field approximation [13] and does not include any fermionic interaction such as the Coulombic attraction between the electron and the positron. To include the photons as quantized particle to model all interactions, however, is presently far beyond the range of computational feasibility.

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