Removal of self-interactions in the Dirac-Maxwell equations in one spatial dimension

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We propose a theoretical framework that permits us to eliminate the unphysical self-repulsion that occurs if a spatially localized charged particle interacts with its own electric field. As an example of this framework, we study the time-resolved interaction between an electronic and positronic wave packet by solving the coupled set of two-particle Dirac-Maxwell equations. The restriction of the dynamics to only one spatial dimension permits us to neglect the magnetic field and therefore any effects due to retardation are absent. Here the unwanted self-repulsion can be removed by separating the total electric field into two portions, each of which is generated by only one particle and is evolved independently of the other. For example, the Maxwell equation for the electronic field has only the electronic charge density as a source term and only this field is coupled to the positron in the two-particle Dirac equation.

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I. INTRODUCTION

In the fundamental electromagnetic force between two charged particles, the charge plays a dual role when this interaction is implemented in the QED Lagrangian via the minimum coupling principle. On one hand, the charge and current density associated with the particle act as the source terms in the set of the Maxwell equations that determine the dynamics of the electromagnetic field operators. On the other hand, the same electromagnetic field is then coupled back as an effective force field in the Dirac equation for the electron-positron field operator where the charge is the coupling strength [1,2]. In the classical mechanical limit of a point charge, this description is not problematic, as the total energy of the electromagnetic field generated by a point particle (obtained as an integral over space) does not depend on the location of the particle. As a result, the force this charge would experience due to its own field (the spatial derivative of the total energy) is zero.

It is nearly impossible to find analytical solutions for the fully coupled QED dynamics of particles and photons for general situations. It is also extremely difficult to simulate the dynamics numerically if the electromagnetic field is described by a second-quantized bosonic field operator. However, one can obtain some first insight into the dynamics if one studies an approximate theoretical framework, where the source terms in the Maxwell equations, which are quadratic functions of the electron-positron field operator, are replaced by their field theoretical expectation value. As the source terms become a classical function, the electromagnetic field no longer needs to be described by an operator and a numerical description becomes possible. In the literature this simplification is sometimes called the "classical field" approximation.

But this approximation has some unphysical consequences with regard to the dynamics of charged quantum particles, one of which is spatial self-repulsion. It turns out that a quantum particle can react to its own electromagnetic field leading to a significant enhancement of the spatial spreading of its wave packet as if portions within the same wave packet (representing a single particle) repel each other. Using a comparison with a relativistic ensemble of mutually interacting classical quasiparticles, it was suggested recently [3] that this quantum mechanical self-repulsion can be understood in terms of simple classical mechanics. The probability density associated with a quantum state represents a temporal average of infinitely many (repeated consecutive) measurements of the same (single) particle. However, under the classical field approximation this density is being treated by the Maxwell equation as a charge cloud associated with a distribution of many simultaneous equal charges. As the resulting effective repulsive field in the Dirac equation couples back to the entire wave packet, all parts within this wave packet repel each other.

A similar type of self-repulsion problem is also encountered in density functional theory [4,5]. However, the starting point for this theory is a description in which the effect of the total electromagnetic field as a fundamental provider for forces (with its own independent dynamics) has been approximated by the sum of two-body Coulombic interaction energies. Here the Coulombic direct interaction term in this theory has an electron-electron repulsion that does not distinguish between the electrons so that each electron, in addition to repelling other electrons, repels itself as well. In the Hartree-Fock theory [6], however, the self-repulsion of an electron is exactly canceled by the exchange interaction.

In this work we examine if it is possible to eliminate the self-repulsion within a field theoretical framework on the fundamental level where all interactions are provided by the total electromagnetic field and there are no direct pairwise interactions. The basic idea that we propose in this work is to distinguish between the fields generated by different particles and therefore we are able to couple each particle solely to the fields that were created by the other particles. In the usual quantum mechanical multiparticle wave function description based on pairwise interaction energies the dynamics cannot be separated into states for each particle (as the important correlation among particles would be lost). However, we show that within the framework of field theory this separation is possible, as long as the interaction is sufficiently weak such that the dynamics does not change the total number of particles. While this procedure of separation of the fields could be performed for a three-dimensional system including the magnetic field and retardation effects, we examine this idea

here for a more idealized system of an electron and positron where the dynamics has been restricted to only one spatial dimension.

The article is organized as follows. In the second section we first review the transition from a quantum field theoretical framework to a quantum mechanical description. We also describe the classical field approximation in the Maxwell equations and introduce a partitioning of the Dirac equation. In the third section we solve the coupled Dirac-Maxwell equation for electron-positron scattering with full space-time resolution following the usual approach of quantum field theory. In this case the expected attraction of two oppositely charged particles will be accompanied by the unphysical self-repulsion of each wave packet individually. In the fourth section we examine a proposal for an alternative description, where we no longer describe the dynamics by a single electromagnetic field, but we define individual fields that are associated with each particle. In this framework it is possible that each particle is only permitted to couple to the electromagnetic field associated with other particle. The corresponding numerical results will be compared directly in Sec. V with those of Sec. III. In Sec. VI we focus on the growth of the spatial width in these cases. In Sec. VII we summarize the results and point out important challenges, such as truly relativistic dynamics where the number of particles can change and we argue that the removal of the unphysical self-repulsion is necessary. A recent area of research where precisely this question is rather relevant is the breakdown process of the vacuum, where an external supercritical field can create electron-positron pairs from the vacuum [7–9].

II. CLASSICAL-FIELD APPROXIMATION IN QUANTUM FIELD THEORY

A. Connection between quantum field theory and quantum mechanics

Before we can begin our main discussion about the classical field approximation and the self-repulsion, we have to start with a brief excursion and review the relationship between field theory and quantum mechanics. In relativistic quantum field theory, the time evolution of electrons and positrons is described by the field operator $\Psi(x,t)$, which fulfills the equal-time anticommutator relationship $\{\Psi(x,t),\Psi^\dagger(x',t)\} = i\hbar\delta(x-x')$. Here t denotes time and x is the spatial coordinate, which we assume from now on to be just one coordinate direction. The time evolution of $\Psi(x,t)$ from the initial $\Psi(x,t=0)$ is given by both the Heisenberg equation of motion and the Dirac equation [10,11].

In quantum mechanics and the Schrödinger picture, a general system of N different particles is described by a wave function $\phi(x_1,x_2,\ldots,x_N,t)$, where x_i denotes the coordinate of each particle along the x axis. The time evolution of this wave function is obtained from the multiparticle Schrödinger or Dirac equation.

The key connection between the information contained in a quantum field theoretical description and a possible quantum mechanical description is given by the transition amplitude,

$$\phi(x_1,x_2,\ldots,x_N,t) = \langle\langle \text{vac} \parallel \Psi_1(x_1,t=0)\Psi_2(x_2,t=0)\cdots \times \Psi_N(x_N,t=0) \parallel \Phi(t)\rangle\rangle, \quad (2.1a)$$

where the double bars denote the field theoretical (not quantum mechanical) state $\|\Phi(t)\rangle\rangle$, the vacuum state is denoted by $\|\text{vac}\rangle\rangle$, and the subscript $i = 1, 2, \ldots, N$ in Ψ_i denotes the field operator associated with the ith particle species. For example, as we see below, for an electron (positron) one usually chooses the electronic (positronic) portion of the electron-positron field operator Ψ. If the coupling between the particles is sufficiently weak such that there are no direct transitions between the states of different particle manifolds (and therefore the total number of particles does not change as a function of time), then Eq. (2.1a) can also be written as [12,13]

$$\phi(x_1,x_2,\ldots,x_N,t) = \langle\langle \text{vac} \parallel \Psi_1(x_1,t)\Psi_2(x_2,t)\cdots \times \Psi_N(x_N,t) \parallel \Phi(t=0)\rangle\rangle, \quad (2.1b)$$

as the time evolution leaves the vacuum state invariant in this case. We should remark that it still can be very illustrative if one maps Ψ onto ϕ even for very strongly coupled systems where the dynamics does change the number of particles [14].

To return to the special case of an electron-positron system, here the electronic portion of Ψ can be obtained by introducing the subspace projector $P_+ \equiv \Sigma_{p(+)}|p(+)\rangle\langle p(+)|$, which is defined in terms of the sum (integral) over all (single-particle) energy eigenstates $|p(+)\rangle$ of the unperturbed Dirac Hamiltonian with positive energy $E(+) \equiv [m^2c^4 + c^2p^2]^{1/2}$, defined as $H_0|p(+)\rangle = E(+)|p(+)\rangle$. In one spatial dimension this unperturbed Dirac Hamiltonian can be represented by $H_0 \equiv c\sigma_1 p + \sigma_3 mc^2$, where σ_i denotes the usual 2×2 Pauli matrices.

Equivalently, the subspace projector can also be expressed in terms of the Dirac operator as $P_+ \equiv (1 + H_0/|H_0|)/2$ where $|H_0|$ denotes the Klein-Gordon–like [15,16] operator $|H_0| \equiv [m^2c^4 + c^2p^2]^{1/2}$. The corresponding positronic portion of Ψ requires the definition of the antilinear charge conjugation operator $Q \equiv i\sigma_1 K$, where K is the usual complex conjugation. This operator Q converts the usual fully coupled Dirac equation $i\hbar\partial_t\Psi(x,t) = H(q)\Psi(x,t)$, where $H(q) = c\sigma_1[p - qA(x,t)/c] + \sigma_3 mc^2 + qV(x,t)$, with q the (negative) charge of the electron, into the corresponding one for a positron $i\hbar\partial_t Q\Psi(x,t) = H(-q)Q\Psi(x,t)$, as we have $QH(q)Q^{-1} = -H(-q)$. Therefore the complete composition of the field operator is given by $\Psi = \Psi_{\text{elec}} + Q^{-1}\Psi_{\text{posi}}$, where $\Psi_{\text{elec}} \equiv P_+\Psi$ and $\Psi_{\text{posi}} \equiv Q(1-P_+)\Psi$.

If we introduce the fermionic annihilation operators b_p and d_p, the electron-positron field operator can be expanded in terms of the spatial representation of the time-evolved (single-particle) energy eigenstates $W_p(+,x,t)$ and $W_p(-,x,t)$ as

$$\Psi(x,t) = \Sigma_{p(+)}b_p W_p(+,x,t) + \Sigma_{p(-)}d_p{}^\dagger W_p(-,x,t) = \Sigma_{p(+)}b_p(t)W_p(+,x) + \Sigma_{p(-)}d_p{}^\dagger(t)W_p(-,x), \quad (2.2)$$

where the two-component $W_p(+,x)$ denotes the energy eigenstate of the force-free Hamiltonian operator $H_0 \equiv c\sigma_1 p + \sigma_3 mc^2$ with momentum p and positive energy $E(+)$ given in their spatial representation by

$$W_p(+,x) \equiv \chi\{1, cp/[mc^2 + E(+)]\}^T \exp(ipx/\hbar), \quad (2.3a)$$

$$W_p(-,x) \equiv \chi\{-cp/[mc^2 + E(+)], 1\}^T \exp(ipx/\hbar), \quad (2.3b)$$

where $\chi \equiv (2\pi)^{-1/2}\{1 + c^2p^2/[mc^2 + E(+)]^2\}^{-1/2}$ denotes the normalization factor.

B. The classical field approximation in the Maxwell operator equations

The most general and possibly fully correlated initial quantum field theoretical state for an electron and positron can be written as

$$\| \Phi(t=0)\rangle\rangle = \Sigma_{p1}\Sigma_{p2} C(p_1,p_2) b_{p1}{}^{\dagger} d_{p2}{}^{\dagger} \| \text{vac}\rangle\rangle, \quad (2.4)$$

where the expansion coefficients $C(p_1,p_2)$ fulfill the normalization $\Sigma_{p1}\Sigma_{p2}|C(p_1,p_2)|^2 = 1$. Using the prescription of Eq. (2.1) for mapping of the initial state $\| \Phi\rangle\rangle$ onto the corresponding quantum mechanical two-particle wave function, we obtain $\phi(x_e,x_p,t) = \Sigma_{p1}\Sigma_{p2} C(p_1,p_2) P_+ W_{p1}(+,x_e,t) Q(1-P_+) W_{p2}(-,x_p,t)$.

For the remainder of this article, we will assume that the coupling between the electron and positron is sufficiently weak such that at any time there are no significant transitions between states of the positive and negative energy subspaces, $\langle p(+)|p(-,t)\rangle = 0$. In this important special case we can neglect the action of the subspace projectors, $P_+ W_{p1}(+,x,t) = W_{p1}(+,x,t)$ and $(1-P_+)W_{p1}(-,x,t) = W_{p1}(-,x,t)$, and obtain

$$\phi(x_e,x_p,t) = \Sigma_{p1}\Sigma_{p2} C(p_1,p_2) W_{p1}(+,x_e,t) Q W_{p2}(-,x_p,t). \quad (2.5)$$

Next we describe how the time evolution of the two-particle state is obtained from quantum field theory. On a fundamental level, in the absence of any external force field, any interaction between two charged particles is facilitated by the exchange of photons, where the time evolution of the photonic field operators A and V is described by the Maxwell equations that have commutators of the electron-positron field operator and its adjoint as source terms. In one spatial dimension, the coupled Dirac-Maxwell equations of relativistic QED are given by

$$i\hbar\partial_t \Psi(x,t) = \{c\sigma_1[p - q_e A(x,t)/c] + \sigma_3 mc^2 + q_e V(x,t)\}\Psi(x,t), \quad (2.6a)$$

$$\partial_x(-\partial_x V - \partial_{ct} A) = \varepsilon_0{}^{-1} q_e [\Psi(x,t)^{\dagger}, \Psi(x,t)]/2, \quad (2.6b)$$

$$\partial_t(-\partial_x V - \partial_{ct} A) = -\varepsilon_0{}^{-1} c\, q_e [\Psi(x,t)^{\dagger}, \sigma_1 \Psi(x,t)]/2. \quad (2.6c)$$

We will use from now on the spatial gauge ($A = 0$) and atomic and cgs units, where the four fundamental constants [amount of the charge of the electron $|q_e|$, its mass m, and Coulomb's and Planck's constants $1/(4\pi\varepsilon_0)$ and $\hbar$] are all unity by definition. For better clarity, however, we will leave here the negative charge of the electron q_e as a parameter in our description and denote below with q_p the corresponding (positive) charge of the positron. Note that while the corresponding temporal gauge ($V = 0$) has its direct three-dimensional (3D) analog [2], the spatial gauge cannot be generalized and is intrinsic to systems in one spatial dimension without a magnetic field. While some of the expressions would be more complicated, all the conclusions of this work would be the same had we used the (more general) temporal gauge. The spatial gauge is obviously not suitable to describe electromagnetic radiation and retardation effects. In the spatial gauge the corresponding electric field operator is obtained from the photonic field operator as $E = -\partial_x V$.

Due to the operator character of the scalar potential V these coupled operator equations are very difficult to solve. However, if we *replace* the two source terms on the right-hand side of the Maxwell equations by their field theoretical expectation values with regard to the initial state $\| \Phi(t=0)\rangle\rangle$,

$$q(x,t) \equiv q_e \langle\langle \Phi(t=0) \| [\Psi^{\dagger}(x,t), \Psi(x,t)]/2 \| \Phi(t=0)\rangle\rangle, \quad (2.7a)$$

$$j(x,t) \equiv q_e c \langle\langle \Phi(t=0) \| [\Psi^{\dagger}(x,t), \sigma_1 \Psi(x,t)]/2 \| \Phi(t=0)\rangle\rangle, \quad (2.7b)$$

they become c numbers and also the potential $V(x,t)$ automatically becomes a classical field in the Dirac equation. This important step is the *classical field approximation*, sometimes also referred to as the mean field approximation. In our spatial gauge, the Maxwell equations (2.6b) and (2.6c) reduce to the usual Gauss's law $-\partial_x^2 V = 4\pi\, q(x,t)$ and Ampere's law $\partial_t\partial_x V = 4\pi\, j(x,t)$. Due to the continuity equation, $\partial_t q = -\partial_x j$, both laws are redundant as they can be derived from each other.

If we insert the formal solution of the field operator $\Psi(x,t)$ and $\| \Phi(t=0)\rangle\rangle$ in terms of Eqs. (2.2) and (2.4) into the expectation values for $q(x,t)$ and $j(x,t)$ of the approximation of Eqs. (2.7), we obtain

$$q(x,t) = q_{\text{vac}}(x,t) + q_{\text{elec}}(x,t) + q_{\text{posi}}(x,t), \quad (2.8a)$$

$$j(x,t) = j_{\text{vac}}(x,t) + j_{\text{elec}}(x,t) + j_{\text{posi}}(x,t). \quad (2.8b)$$

Each density consists of three parts. The first one is universal to any field theoretical state $\| \Phi\rangle\rangle$ and does not depend on the specific form of the electron-positron state $\| \Phi\rangle\rangle$. After the subtraction of a diverging term [17] it corresponds to the vacuum's charge and current density that has been induced by the electric field associated with the classical potential

$$\begin{aligned} q_{\text{vac}}(x,t) &\equiv \langle\langle \text{vac} \| q_e [\Psi(x,t)^{\dagger}, \Psi(x,t)]/2 \| \text{vac}\rangle\rangle \\ &= q_e [\Sigma_p |W_p(-,x,t)|^2 - \Sigma_p |W_p(+,x,t)|^2]/2, \end{aligned} \quad (2.9a)$$

$$\begin{aligned} j_{\text{vac}}(x,t) &\equiv \langle\langle \text{vac} \| q_e c [\Psi(x,t)^{\dagger}, \sigma_3 \Psi(x,t)]/2 \| \text{vac}\rangle\rangle \\ &= q_e c [\Sigma_p W_p^{\dagger}(-,x,t)\sigma_3 W_p(-,x,t) \\ &\quad - \Sigma_p W_p^{\dagger}(+,x,t)\sigma_3 W_p(+,x,t)]/2. \end{aligned} \quad (2.9b)$$

Here the absolute value signs include the summation over the spinor components. The second and third portions are associated with the charge (current) density of the electron and positron:

$$\begin{aligned} q_{\text{elec}}(x,t) &= q_e \Sigma_{p2} |\Sigma_p C(p,p_2) W_p(+,x,t)|^2 \\ &= q_e \int dx_2 |\phi(x,x_2,t)|^2, \end{aligned} \quad (2.10a)$$

$$\begin{aligned} j_{\text{elec}}(x,t) &= q_e c \Sigma_{p3}\Sigma_{p1}\Sigma_{p2} C^*(p_1,p_3) C(p_2,p_3) \\ &\quad \times W_{p1}^{\dagger}(+,x,t)\sigma_3 W_{p2}(+,x,t) \\ &= q_e c \int dx_2 \phi^{\dagger}(x,x_2,t)\sigma_3 \phi(x,x_2,t), \end{aligned} \quad (2.10b)$$

$$q_{\rm posi}(x,t) = q_p \Sigma_{p1} |\Sigma_p QC(p_1,p) W_p(-,x,t)|^2 = q_p \int dx_1 |\phi(x_1,x,t)|^2, \quad (2.10c)$$

$$j_{\rm posi}(x,t) = q_p \Sigma_{p1}\Sigma_{p3}\Sigma_{p4} C^*(p_1,p_3) C(p_1,p_4) \times [QW_{p3}(-,x,t)]^\dagger \sigma_3 QW_{p4}(-,x,t) = cq_p \int dx_1 \phi^\dagger(x_1,x,t)\sigma_3 \phi(x_1,x,t), \quad (2.10d)$$

where we have used Eq. (2.5). If we continue to assume that the contributions to the total charge and current density are mainly from the two charges, we can neglect $q_{\rm vac}(x,t)$ and $j_{\rm vac}(x,t)$ in the Maxwell equations. This means that we no longer have to solve the Dirac equation for each single-particle state $W_p(\pm,x,t)$ of the entire Hilbert space, but we can simply evolve the two-particle wave function $\phi(x_1,x_2,t)$ directly in time and use it to construct the source terms for the Maxwell equations.

However, before we show in Sec. III below that the classical field approximation leads unavoidably to the occurrence of the unphysical self-repulsion, we simplify first in the next subsection, Sec. II C, the formalism. We will then show in Sec. IV how this formalism can be applied to remove the self-repulsion from the dynamics.

C. The partitioning of the Dirac equation for the parts of the field operator

If the interaction between two particles is approximated by an effective pairwise (instantaneous) interaction energy of the form $W(x_1 - x_2)$, then it is not possible to split the two-particle Dirac or Schrödinger equation into two equations for each particle separately without losing relevant information about the correlation between both particles. In other words, if the initial two-particle state is a simple product of two one-particle states, then the time evolution usually correlates the two states such that the final state can no longer be expressed as a simple product of two single-particle states. In fact, the deviation from this product form has been used in the literature [18–20] to define a quantitative measure for the degree of correlation.

In Appendix A we show that the Dirac equation for field operator Ψ in Eq. (2.6a) can be split into two equations for the electronic and positronic portion of Ψ, if there is no supercritical external field and the internal potential $V(x,t)$ is sufficiently weak such that there are no transitions between the positive and negative energy manifold and the total number of particles remains invariant.

$$i\partial_t \Psi_{\rm elec}(x,t) = [c\sigma_1 p + \sigma_3 c^2 + q_e V(x,t)]\Psi_{\rm elec}(x,t), \quad (2.11a)$$

$$i\partial_t \Psi_{\rm posi}(x,t) = [c\sigma_1 p + \sigma_3 c^2 + q_p V(x,t)]\Psi_{\rm posi}(x,t). \quad (2.11b)$$

These two equations are still coupled with each other via the time-dependent internal potential $V(x,t)$, whose space-time evolution in the Maxwell equations (in the spatial gauge) is governed by the total charge density as a source term, which is a nonlinear function of $\Psi_{\rm elec}(x,t)$ and $\Psi_{\rm posi}(x,t)$.

$$-\partial_x^2 V(x,t) = 4\pi[q_{\rm elec}(x,t) + q_{\rm posi}(x,t)] = 4\pi\left[q_e \int dx_p |\phi(x,x_p,t)|^2 + q_p \int dx_e |\phi(x_e,x,t)|^2\right]. \quad (2.11c)$$

If we can separate the total field operator into electronic and positronic portions that are based on field-free states we show in Appendix B that the corresponding two-particle wave function $\phi(x_e,x_p,t)$ can be obtained from the solution to the two-center Dirac equation,

$$i\partial_t \phi(x_e,x_p,t) = \{[c\sigma_1 p_1 + \sigma_3 c^2 + q_e V(x_e,t)] \otimes \mathbf{1}_{\rm posi} + \mathbf{1}_{\rm elec} \otimes [c\sigma_1 p_2 + \sigma_3 c^2 + q_p V(x_p,t)]\} \times \phi(x_e,x_p,t). \quad (2.12)$$

Here $\mathbf{1}_{\rm elec}$ and $\mathbf{1}_{\rm posi}$ denote the unit operator for each particle space. Note that the two subspace Hamiltonians commute, but due to the time dependence in each potential the two particles are nevertheless directly coupled with each other. It is quite interesting that in the special case where the initial electron-positron state is simply a product, $\phi(x_e,x_p,t=0) = \phi_e(x_e)\phi_p(x_p)$, then Eq. (2.12) predicts that each orbital has to fulfill its own equation,

$$i\partial_t \phi_e(x,t) = [c\sigma_1 p + \sigma_3 c^2 + q_e V(x,t)]\phi_e(x,t), \quad (2.13a)$$

$$i\partial_t \phi_p(x,t) = [c\sigma_1 p + \sigma_3 c^2 + q_p V(x,t)]\phi_p(x,t). \quad (2.13b)$$

In this special case, the total charge density in the Maxwell equation also simplifies to $q_{\rm elec}(x,t) + q_{\rm posi}(x,t) = q_e|\phi_e(x,t)|^2 + q_p|\phi_p(x,t)|^2$. This means that due to the time dependence of the total classical potential $V(x,t)$ [and its highly nonlinear dependence on $\phi_e(x,t)$ and $\phi_p(x,t)$ in the corresponding Maxwell equation], we have the interesting and rather unusual situation here that also at later times the two-particle wave function remains a simple product, $\phi(x_e,x_p,t) = \phi_e(x_e,t)\phi_p(x_p,t)$, even though the associated two particles are directly coupled and mutually affect their time evolution. Therefore both particles are highly correlated with each other, despite the simple product form of their state, $\phi = \phi_e\phi_p$.

D. Interparticle coupling via a single field and via effective pairwise interaction energies

It is important to point out that our framework where the total potential $V(x,t)$ is coupled to each particle in the (time-dependent) Hamiltonian in general might not be equivalent to a description where the quantum interaction is given by an effective instantaneous Coulombic pairwise interaction energy $W(x_e - x_p)$. In fact, the main focus of this work is to examine the dynamics on a level, at which the electromagnetic field associated with both particles remains an independent dynamical degree of freedom (whose space-time evolution is determined by the Maxwell equations). This is especially crucial in three dimensions where due to the magnetic field retardation effects automatically play an important role and the interaction cannot simply be expressed without additional

approximations by an instantaneous Coulombic interaction energy of the form $W(\mathbf{r}_e - \mathbf{r}_p)$.

In contrast to the more complicated 3D situation, in our case of Eq. (2.12) there is no retardation and consequently each potential energy term $q_e V(x_e,t)$ and $q_p V(x_p,t)$ could be expressed as a nonlinear function of the wave functions. Using the general Green's function solution of $V(x) = (-2\pi)\int dx' f(x-x')|x'|$ as a solution to $-\partial_x^2 V = 4\pi f(x)$, Gauss's law (2.11c) can be solved for each potential leading to $V(x) = -2\pi \int dx'[q_{\rm elec}(x-x',t) + q_{\rm posi}(x-x',t)]|x'|$. This step would eliminate the Maxwell equations and would correspond to the total time-dependent interaction energies in Eq. (2.12),

$$q_e V(x_e,t) = -2\pi q_e \int dx|x|[q_{\rm elec}(x_e - x,t)+q_{\rm posi}(x_e - x,t)], \tag{2.14a}$$

$$q_p V(x_p,t) = -2\pi q_p \int dx|x|[q_{\rm elec}(x_p - x,t)+q_{\rm posi}(x_p - x,t)], \tag{2.14b}$$

which due to the nonlocal nature of the interaction cannot be reduced to an interaction energy that simply depends on $|x_p - x_e|$.

However, this situation is entirely different if either the individual charge densities are very narrow or they do not overlap. For instance, in the classical limit of two point charges, an interaction energy $W(x_e - x_p)$ can actually be constructed without approximation. Here the charge densities are infinitely narrow and localized around the position of the charges, $q_{\rm elec}(x,t) = q_e\delta[x - x_e(t)]$ and $q_{\rm posi}(x,t) = q_p\delta[x - x_p(t)]$, where $x_e(t)$ and $x_p(t)$ denote the electron's (positron's) classical trajectory. In this special case each interaction energy can be simplified to $q_e V(x_e,t) = q_p V(x_p,t) = -2\pi q_e q_p |x_e(t) - x_p(t)| \equiv W(x_e - x_p)$. In other words, we have here a simplified Hamilton function where it is possible to eliminate the original energies $q_e V(x_e,t)$ and $q_p V(x_p,t)$ as force intermediators (and correspondingly the Maxwell equations) entirely.

III. NUMERICAL ILLUSTRATION: ELECTRON-POSITRON SCATTERING

In order to represent two initially separated wave packets, we choose in this work the specific expansion coefficients

$$C(p_1,p_2) = \Xi \exp[i\,p_1 x_{\rm elec}]\exp[-(p_1 - p_{\rm elec})^2/\Delta p^2] \times \exp[i\,p_2 x_{\rm posi}]\exp\left[-\left(p_2 - p_{\rm posi}\right)^2/\Delta p\right], \tag{3.1}$$

where $x_{\rm elec}$, $x_{\rm posi}$, $p_{\rm elec}$, and $p_{\rm posi}$ denote the electron's and positron's most likely initial position and momentum and Δp is the momentum width, whose inverse is directly related to the initial spatial width of each wave packet Δx. Ξ denotes the normalization constant such that $\sum_{p1}\sum_{p2}|C(p_1,p_2)|^2 = 1$. In order to illustrate the effect of the spreading enhancement due to the self-repulsion, we have used in our numerical simulations below $x_{\rm elec} = -1.5$ a.u., $x_{\rm posi} = 1.5$ a.u., $p_{\rm elec} = 0$, $p_{\rm posi} = 0$, and $\Delta p = 2$, corresponding to two initially nonoverlapping wave packets where each particle is at rest. The scattering is therefore caused here entirely by the mutual attraction between both particles. The Gaussian superposition of plane-wave states can describe strictly a physical electron only in the absence of any forces. As in one spatial dimension the corresponding Coulomb force between two particles does not fall off as a function of the interparticle distance (as in the three-dimensional counterpart), it is very difficult to define the precise state of a "force-free" particle. This is also related to Eq. (2.1) above, for which it was implicitly assumed that any interparticle interaction can be turned off adiabatically.

To enhance this attractive force, we have assumed that each particle has a charge of ± 100 a.u. The resulting effective coupling strength of $q_e q_p = 100^2$ is still small enough to neglect pair creation. In order to see pair-creation effects in one spatial dimension a typical interaction energy has to be at least $2mc^2$. For example, only an infinitely steep potential step with height $2mc^2$ can provide a sufficiently large force density to trigger any pair creation and if the step is more slowly ramped up in space, even fewer particles are created. For our parameters the corresponding energies are much lower and also the relevant spatial scales are not of the order of the electron's Compton wavelength.

We note that the coefficient in Eq. (3.1) was of the product form $C(p_1,p_2) = C_1(p_1)C_2(p_2)$, such that we can use the partitioned set of Dirac-Maxwell equations (2.13). It turns out that the simplified set of equations (2.13) can be solved numerically on a space-time grid using a fast Fourier transform (FFT) based split-operator technique [21–25] for both the Dirac and the Maxwell equations. The algorithmic details are presented in Ref. [9].

In Fig. 1 we present some snapshots of the total charge density $q(x,t) = q_{\rm elec}\int dx_{\rm p}|\phi(x,x_p,t)|^2 + q_{\rm posi}\int dx_e|\phi(x_e,x,t)|^2$ for three moments in time. As the initial state for the electric potential we have chosen the solution to Gauss's law according to Eq. (2.13b). To obtain a very rough estimate of the involved time scales, two nonrelativistic point particles (of mass m_e

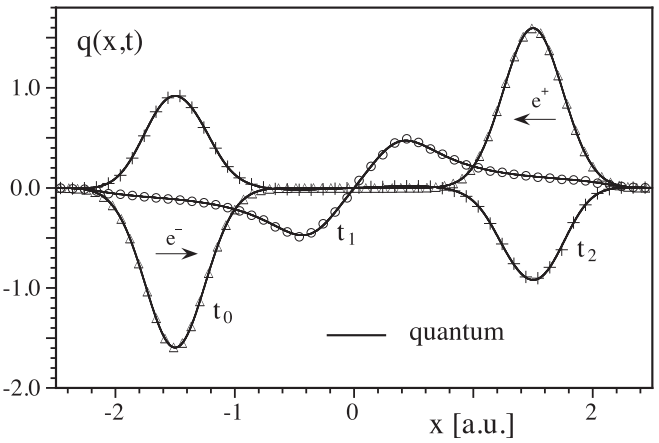

FIG. 1. Three snapshots of the total charge density for the scattering process of an electron (initially located at $x = -1.5$ a.u.) and positron (initially located at $x = 1.5$ a.u.). The times are $t_0 = 0$ a.u., $t_1 = 0.011$ a.u., and $t_2 = 0.022$ a.u. The triangles, circles, and crosses are the corresponding charge densities obtained from a time-evolved classical ensemble with 20 000 point particles to represent each quantum particle. (Parameters are $L = 6$ a.u., $N_x = 8192$ spatial grid points.)

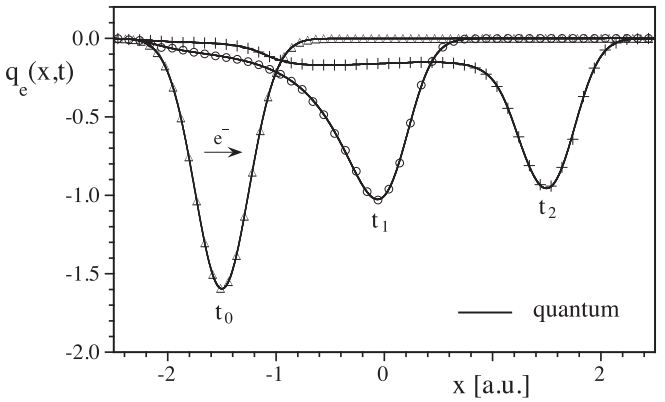

FIG. 2. Three snapshots of the electronic portion of charge density for the same scattering process as in Fig. 1.

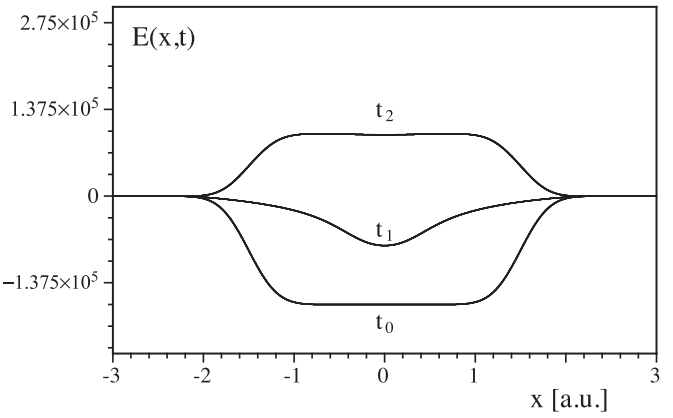

FIG. 3. Three snapshots of the total electric field during the same scattering process as in Figs. 1 and 2.

and m_p) would pass through each other after a time $T = [2\mu|x_{\rm posi}-x_{\rm elec}|/(2\pi|q_e|q_p)]^{1/2}$, where $m \equiv m_e m_p/(m_e+m_p)$ is the reduced mass. For our parameters, this would amount to a time of about $T = 7\times10^{-3}$ a.u., at which both particles would have accelerated to a speed of 434 a.u. ($= 3.17c$). The motion is therefore highly relativistic and the particles have maximal speeds close to c. As the two wave packets (particles) approach each other, their spatial width increases. In other words, in addition to the attractive force due to the other particle (of opposite charge), each wave packet itself seems to self-repel, leading to an enhanced spatial width.

During the intermediate time the two particles cross through each other, leading to an almost vanishing charge density. At the final time the total area under each particle seems to be much less than it was initially. This is related to the fact that major portions of each particle have spread out significantly. To illustrate that spatial regions with no major charge density are actually the result of two overlapping particles with opposite charge, we have shown in Fig. 2 the individual charge densities associated with the electron $q_{\rm elec}(x,t)$. The spreading is now much more obvious. Snapshots at longer times suggest that due to the self-repulsion, major portions of the two particles push themselves to $\pm\infty$.

To examine how quantum mechanical this scattering dynamics really is, we have accompanied the quantum mechanical densities with the corresponding charge densities obtained from a classical ensemble of 20 000 interacting point particles. We describe in Appendix C more details about this approach. The agreement is superb, which suggests that (in agreement with the predictions for self-repulsion for a single particle [3]), self-repulsion within the more complicated framework of electron-positron scattering can also be modeled in terms of a relativistic classical mechanical ensemble of mutually interacting particles. In the next section we propose how one could remove this unwanted and unphysical self-repulsion from the quantum dynamics without going to the less fundamental framework of a pairwise interaction energy.

In order to better understand the reason for the enhanced spreading, we show in Fig. 3 also the temporal snapshots of the corresponding total electric field at the same three moments in time. This field is obtained from the derivative of the total internal potential $E(x,t) \equiv -\partial_x V(x,t)$. Initially, $E(x,t)$ vanishes in the two semi-infinite regions outside the electron ($x < x_{\rm elec}-\Delta x/2$) and outside the positron ($x_{\rm posi}+\Delta x/2 < x$) as the two fields associated with each charge cancel out. In between the two charges the electric field is negative and constant $E(x,t) = 2\pi q_e q_p$. Since the spatial overlap of the two particles charge densities does not vanish even at longer times when major portions have separated from each other, the corresponding electric field close to $x = 0$ is much smaller than its initial value $2\pi q_e q_p$. Also due to both particles have partly switched their locations, the electric field has reversed its sign. As the two particles evolve under their mutual attraction the total electric field shrinks, but this is not in contradiction to the conservation of the total matter-field energy, as we discuss below.

IV. THE REMOVAL OF THE SELF-REPULSION BY PARTITIONING THE CLASSICAL POTENTIAL

The main idea here is to probe the predictions of a quantum mechanical (or field theoretical) system of two particles for an interaction where each particle is coupled exclusively to the electric field generated by the other particle. In this way, the unphysical self-repulsion should be eliminated from the description.

The starting point of our discussion is very similar to Eq. (2.9); however, we have split the internal electric field and correspondingly the total potential into two parts $V(x,t) = V_{\rm elec}(x,t) + V_{\rm posi}(x,t)$, where the subscript elec (posi) denotes the electric field generated exclusively by the electron (positron). In other words, instead of the usual Maxwell equation, Gauss's law, $-\partial_x^2 V(x,t) = 4\pi q(x,t)$, with the total charge density as its source, we have now a set of two separate equations:

$$-\partial_x^2 V_{\rm elec}(x,t) = 4\pi q_{\rm elec}(x,t), \tag{4.1a}$$

$$-\partial_x^2 V_{\rm posi}(x,t) = 4\pi q_{\rm posi}(x,t). \tag{4.1b}$$

While the usual Dirac equations for $\Psi_{\rm elec}$ and $\Psi_{\rm posi}$ contain the total potentials associated with the total field $V(x,t) = V_{\rm elec} + V_{\rm posi}$, we couple this time only the potentials created by the positron (electron) to $\Psi_{\rm elec}$ ($\Psi_{\rm posi}$). As a result,

the direct analog of Eq. (2.11) now reads

$$i\partial_t \Psi_{\rm elec}(x,t) = [c\sigma_1 p + \sigma_3 c^2 + q_e V_{\rm posi}(x,t)]\Psi_{\rm elec}(x,t), \tag{4.2a}$$

$$i\partial_t \Psi_{\rm posi}(x,t) = [c\sigma_1 p + \sigma_3 c^2 + q_p V_{\rm elec}(x,t)]\Psi_{\rm posi}(x,t). \tag{4.2b}$$

Following the same procedure as outlined in Sec. II C and Appendix A, we can introduce the corresponding two-particle wave function, which then has to satisfy the two-particle Dirac equation:

$$\begin{aligned} i\partial_t \phi(x_e,x_p,t) = \{&[c\sigma_1 p_e + \sigma_3 c^2 + q_e V_{\rm posi}(x_e,t)] \otimes \mathbf{1}_{\rm posi} \\ &+ \mathbf{1}_{\rm elec} \otimes [c\sigma_1 p_p + \sigma_3 c^2 + q_p V_{\rm elec}(x_p,t)]\} \\ &\times \phi(x_e,x_p,t). \end{aligned} \tag{4.3}$$

In order to justify that our new set of equations is physically meaningful, it is required to show that also in this dynamics the total energy is conserved. For easier readability we shift the discussion to Appendix D and prove that there is an $e_{\rm tot}$ that is indeed conserved in time; i.e., $de_{\rm tot}/dt = 0$, if $\phi(x_e,x_p,t)$ satisfies the corresponding Dirac equation with h_D given by Eq. (4.3) and the fields satisfy the Maxwell equation (4.1). We simply state here the result that the total energy takes the form

$$\begin{aligned} e_{\rm tot} = &\iint dx_1 dx_2 \phi^\dagger h_D(t)\phi - 1/(4\pi) \\ &\times \int dx \partial_x V_{\rm elec}(x,t)\partial_x V_{\rm posi}(x,t), \end{aligned} \tag{4.4}$$

where $h_D(t) = [c\sigma_1 p_1 + \sigma_3 c^2 + q_e V_{\rm posi}(x_e,t)] \otimes \mathbf{1}_{\rm posi} + \mathbf{1}_{\rm elec} \otimes [c\sigma_1 p_{2+}\sigma_3 c^2 + q_p V_{\rm elec}(x_p,t)]$. The term $1/(4\pi)\int dx \partial_x V_{\rm elec}\partial_x V_{\rm posi}$ corresponds to the cross term of the usual energy of the total field $1/(8\pi)\int dx[E_{\rm elec} + E_{\rm posi}]^2$. For classical point particles (Appendix C) the individual field energies $1/(8\pi)\int dx E^2_{\rm elec}$ and $1/(8\pi)\int dx E^2_{\rm posi}$ do not depend on time and can be discarded from the energy. Also note that the overall minus sign for the total field energy in Eq. (4.4) is characteristic of the spatial gauge ($A = 0$). In the temporal gauge, a similar term would occur but with the opposite sign.

Using the same Green's function technique in Sec. II D, Gauss's law (4.1a) and (4.1b) can be solved for the potentials leading to $V_{\rm posi}(x_e,t) = -2\pi\int dx q_{\rm posi}(x_e{-}x,t)|x|$ and $V_{\rm elec}(x_p,t) = -2\pi\int dx q_{\rm elec}(x_p{-}x,t)|x|$. If we assume again the classical limit as $q_{\rm elec}(x,t) = q_e\delta[x{-}x_e(t)]$ and $q_{\rm posi}(x,t) = q_p 0[x{-}x_p(t)]$, this would reduce again to $q_e V_{\rm posi}(x_e,t) = q_p V_{\rm elec}(x_p,t) = -2\pi q_e q_p|x_e(t){-}x_p(t)|$, reflecting again the attractive force field between both particles. In other words, from a classical mechanical perspective of point particles, both interactions of Secs. III and IV are identical. This makes sense as self-repulsion only occurs if a particle is quantum and therefore its density is spatially extended.

V. NUMERICAL ILLUSTRATION: ELECTRON-POSITRON INTERACTION WITHOUT SELF-REPULSION

In this section we will repeat the same simulation as displayed in Fig. 1, but this time we examine the interaction between the electron and positron wave packet for the proposed interaction introduced in the prior section where the self-repulsion was removed. Due to the product structure of the initial state, also here the equations for the wave functions can be separated into the coupled set

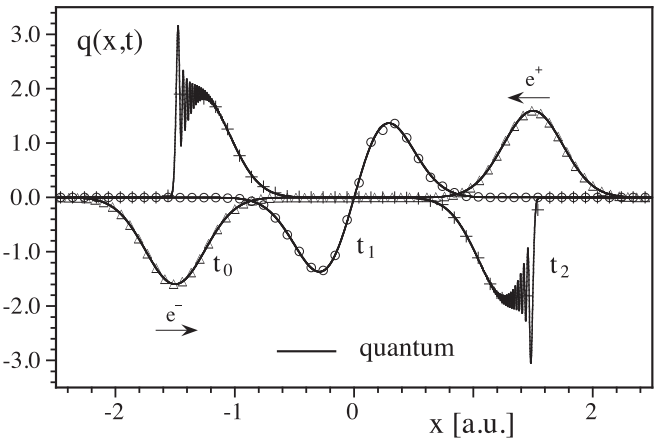

FIG. 4. Three snapshots of the total charge density for the same scattering process of an electron with a positron, but this time the unphysical self-repulsion mechanism has been removed from the dynamics. The triangles, circles, and crosses are again the corresponding charge densities obtained from a time-evolved classical ensemble with 20 000 point particles to represent each quantum particle. (All parameters the same as in Fig. 1.)

$$i\partial_t \phi_e(x,t) = [c\sigma_1 p + \sigma_3 c^2 + q_e V_{\rm posi}(x,t)]\phi_e(x,t), \tag{5.1a}$$

$$i\partial_t \phi_p(x,t) = [c\sigma_1 p + \sigma_3 c^2 + q_p V_{\rm elec}(x,t)]\phi_p(x,t). \tag{5.1b}$$

The corresponding Maxwell equation for the two potentials $V_{\rm elec}(x)$ and $V_{\rm posi}(x)$ is given by

$$-\partial_x^2 V_{\rm elec}(x,t) = 4\pi q_e|\phi_e(x,t)|^2, \tag{5.1c}$$

$$-\partial_x^2 V_{\rm posi}(x,t) = 4\pi q_p|\phi_p(x,t)|^2. \tag{5.1d}$$

In Fig. 4 we display the time evolution of the scattering event as predicted by Eq. (5.1).

We find that while the center of charge motion is similar to that of Fig. 1, this time the data do *not* contain the unphysical self-spreading. In other words, while the electron and the positron attract each other and therefore are accelerated to each other, each wave packet spreads only slightly due to the inherent (and physical) spreading mechanism that is associated with the nonvanishing momentum uncertainty in each packet. In contrast to the data of Fig. 1, this time both particles are truly bound. In other words, after a certain time both particles come to rest and are mutually accelerated towards each other. Due to the existence of a turning point we find the occurrence of rapid spatial oscillations associated with the expected interference of mutually oppositely propagating parts of the same wave function. Once again the comparison with the corresponding data obtained from the classical ensemble matches very well, but close to the turning points they can only reproduce the charge density on a spatially averaged scale. Once each particle has turned around the classical quantum agreement is again

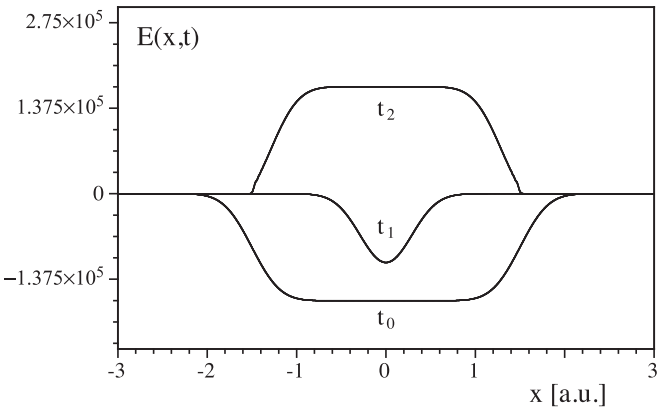

FIG. 5. Three snapshots of the total electric field during the same scattering event as depicted in Fig. 3. For a better comparison, we have placed the symbols for the times (t_0, t_1, and t_2) at the same coordinate location within the graph as in Fig. 3.

superb, showing that even in the absence of self-repulsion the dynamics is essentially classical mechanical.

The absence of the self-repulsion is also manifested in the corresponding evolution of the total electric field $E(x,t)$. As the initial field is solely determined by the initial charge density it is identical to the case studied in Sec. III above. However, as in this section the particles do not couple to the total electric field but only to its components separately, the particles' time evolution is different and therefore also the electric field evolves differently.

In Fig. 5 we show that there are two major differences compared to the electric field with self-repulsion. First, while at the intermediate time (when both particles cross) the electric field is more negative at $x = 0$ than in Fig. 3, at longer times the electric field is much higher at $x = 0$. Second, as the two opposite charges are confined to a certain spatial region (between the two turning points), the electric field is also more localized than in the case where the self-repulsion is present.

VI. COMPARISON OF THE SPATIAL WIDTH WITH AND WITHOUT SELF-REPULSION

In order to provide a direct comparison of the scattering event with and without self-repulsion for the entire scattering event as a function of time, we have graphed in Fig. 6 the spatial width of the electron's charge density, defined as

$$\Delta x(t) = \left\{ \int dx x^2 |q_{\rm elec}(x,t)|/q_e - \left[\int dx x q_{\rm elec}(x,t)/q_e \right]^2 \right\}^{1/2}. \tag{6.1}$$

For reasons of the symmetry of our specific initial conditions above, the positron's width is the same.

In principle there are three mechanisms that affect this spatial width. The most common one is due to the nonvanishing variance of the momentum Δp, where as a result different components of the wave packet evolve with different velocities, leading to the usual relativistic [26] and also nonrelativistic quantum mechanical spreading. The second mechanism is due to the self-repulsion where portions within the same charge density repel each other. The third mechanism is associated with the electron-positron scattering process, where different positions within each wave packet experience different forces that also depend on time.

For better clarity we have separated the data for $\Delta x(t)$ for the two cases with (6a) and without self-repulsion (6b). From the different vertical scales of the two figures it is obvious that the self-repulsion enhances the spatial spreading significantly in all cases as expected. Also, in each of the two figures we have superimposed the widths obtained from the quantum simulations based on the coupled Dirac-Maxwell equations that led to Figs. 1 and 4. They are marked by the open circles and show once again that, despite the inherent nonlinearity due to the relativistic dynamics and the scattering, they match perfectly with the corresponding ones obtained from the simulations (continuous lines) based on 20 000 classical particles (see Appendix C).

In order to judge the importance of relativistic effects, we have also included the corresponding widths from a

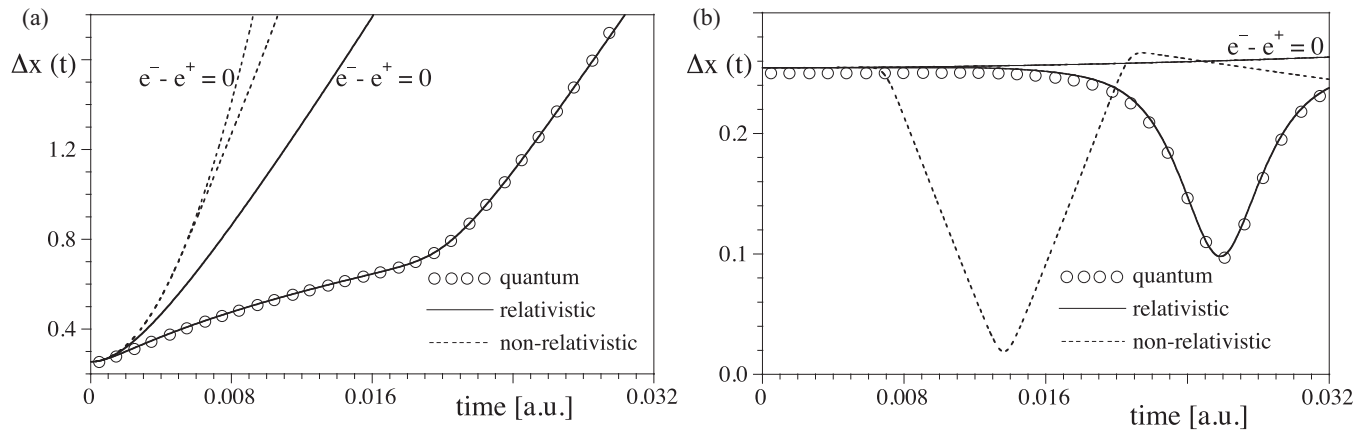

FIG. 6. The time dependence of the spatial width of the electron during the scattering event. The left panel (a) is for the case of self-repulsion (see Fig. 1) while the right one is for the case without self-repulsion (see Fig. 4). The open circles are the quantum data taken from the densities used in these two figures. The data labeled ($e^- - e^+ = 0$) show the electron's width in the absence of any interaction with the positron. The dashed lines are the nonrelativistic limit.

nonrelativistic simulation, obtained by setting the speed of light parameter c to infinity (instead of $c = 137.036$ a.u.) in the numerical code. Finally, in order to be able to judge the impact of the e^-–e^+ interaction we have computed also the corresponding widths for an electron that was entirely decoupled from the positron (labeled e^-–$e^+ = 0$ in the figure).

Let us first discuss the results of Fig. 6(a) (with self-repulsion). We observe that the two widths obtained from the nonrelativistic simulations lead to the largest width. In other words, relativity suppresses the growth of the width in this case. This finding will be in contrast to the data in the absence of self-repulsion. Finally, in order to be able to judge the impact of the e^-–e^+ interaction we have computed also the width for an electron that was entirely decoupled from the positron (labeled e^-–$e^+ = 0$ in the figure). We see that the growth of the width is much larger if there are no collisions (in both the nonrelativistic as well as relativistic case), suggesting that the collision suppresses the wave-packet spreading. We will see the same tendency also for the case of no self-repulsion.

Let us now analyze the data in Fig. 6(b), corresponding to the absence of self-repulsion. For comparison, the nearly straight line in Fig. 6(b) shows the width for the usual wave-packet spreading in the absence of any collision (e^-–$e^+ = 0$). Here due to the small speeds the relativistic and nonrelativistic cases are graphically indistinguishable.

We have already suggested above that the collision somehow suppresses the growth of the width. In fact, the data shown in Fig. 6(b) suggest that for the parameters presented here we observe an interesting *collision-induced spatial narrowing* of the state. This narrowing is even more pronounced in the nonrelativistic case, where the two charges accelerate themselves to much larger speeds such that the collision happens at much earlier times. This collisionally induced narrowing after the collision can be explain qualitatively in terms of nonrelativistic classical mechanics. Let us assume that the left- and rightmost edge of the electron wave packet (centered at $x = x_{\rm elec}$ and of initial spatial width Δx) can be represented by particles at rest with locations $x_L = -\Delta x/2 + x_{\rm elec}$ and $x_R = x_{\rm elec} + \Delta x/2$, with $|x_R| < |x_L|$. If we assume that the attractive positron is fixed at the origin $x = 0$, then both electrons reverse their acceleration direction when they pass the positron at $x = 0$. As the right electron was initially closer to the positron it arrives at $x = 0$ first, after a time $t_R = [-2x_R/a]^{1/2}$, where a denotes the acceleration. It is therefore slowed down while the left electron is still accelerated. In this way the left electron can catch up to the right electron, diminishing therefore the spatial width of the whole distribution they represent. Equivalently, as the total round-trip period $\{T_R = 4[-2x_R/a]^{1/2}\}$ for the right electron is less than that of the left electron, the two particles will actually pass through each other, again reducing the width. This is different than the situation where the relative coordinate would be described by a harmonic oscillator, where the period of oscillation would not depend on the initial elongation.

VII. SUMMARY AND OUTLOOK

In this work we have proposed a theoretical description of the interaction between two quantum particles, where the unphysical self-interaction and the resulting spatial self-repulsion mechanism can be removed. This interaction conserves the total energy and is based on partitioning the Dirac equation and solving the Maxwell equation for each field separately. In our discussions we have limited ourselves to a range of interaction for which the particles are permitted to move with relativistic motion but it is not strong enough to induce any pair creation.

This work also leads to several future challenges. The absence of the magnetic field in our reduced dimensional system leads to the absence of any retardation effect and as a result, the Maxwell equations for the electric field could be formally solved via simple spatial integrals over the expectation values of the functions of the electron-positron field operator. However, in our simulations, we have not made use of this possible simplification and viewed the fields as truly independent dynamical variables. We therefore believe that the main idea of removing self-repulsion by splitting the total electromagnetic field into components that are associated with each particle (and solving therefore several coupled Maxwell equations instead of one for the total field) should generalize also to a real 3D system, even though the actual extension may not be trivial.

The source of the self-repulsion is of course the classical field approximation, where an intrinsically second-quantized electric field operator turns automatically into a classical function of space and time. Alternatively, to avoid self-repulsion, one could also try to maintain the fully second-quantized theoretical framework but make different approximations that would make the dynamics numerically feasible. For recent work in that direction, see [27].

We have seen in Sec. IV that due to the instantaneous nature of the Maxwell equations in one dimension, the time-dependent effective internal energies $q_e V_{\rm posi}(x_e,t)$ and $q_p V_{\rm elec}(x_p,t)$ could be solved formally (as a function of $q_{\rm elec} = q_e \int dx_p |\phi(x,x_p,t)|^2$ and $q_{\rm posi} = q_p \int dx_e |\phi(x_e,x,t)|^2$). If we were to insert this expression back into the Dirac equation for the two-particle wave function $\phi(x_e,x_p,t)$, we would obtain a Hamiltonian that contains ϕ. This would therefore lead to an equation of motion for $\phi(x_e,x_p,t)$ that is highly nonlinear in ϕ. At the moment it is not clear how the solutions would compare to those of a much simpler system, where the (instantaneous) interaction potential was chosen from the very beginning to be equal to $-2\pi q_e q_p |x_e - x_p|$ in the Hamiltonian, as suggested by the corresponding classical Hamilton function for point particles. We view this question rather puzzling as, for instance, the 3D analog, $[1/|r_e - r_p|]$ for this instantaneous pointlike interaction potential is used routinely as a starting point to predict rather accurately the energy levels of multielectron atoms. These studies use then subsequently Hartree-Fock–like approximations where many-body wave functions are approximated by products of (appropriately antisymmetrized or symmetrized) single-particle orbitals.

In the same vein it is interesting to note that any interaction potential $W(x_e - x_p)$ would normally correlate the particles and therefore does not permit the total wave function to remain a simple product of an electron and positron state. However, in our situation (of the coupled Dirac-Maxwell equation), the corresponding total wave function maintains its simple product form, even though the dynamics of each particle is obviously caused directly by the other particle.

It might seem at first more complicated to include the total electric field as a dynamically coupled independent variable. However, quite to the contrary, it turns out that solving numerically two coupled Dirac-Maxwell equations for $\phi_e(x,t)$, $\phi_p(x,t)$, $V_e(x,t)$, and $V_p(x,t)$ requires much less computer memory and CPU time than computing $\phi(x_e,x_p,t)$ for a given (approximate) interaction energy $W(x_e–x_p)$. One could therefore suggest that for multiparticle simulations with more than two particles it might be actually rather advantageous to replace the usual pairwise Coulombic interaction energy $\sum_{i,j} W(\mathbf{r}_{e,i}–\mathbf{r}_{p,j})$ by individual potentials $V_{e,i}(x,t)$ and $V_{p,j}(x,t)$ whose dynamics is governed by the corresponding Maxwell equations.

As we have outlined in the Introduction, one of the main motivations for this preliminary work was to develop techniques that permit us to study the effect of the Coulombic electron-electron, positron-positron, and electron-positron forces on the strong-field-induced pair-creation process from the quantum vacuum. This process can presently only be treated in an intrinsic field theoretical framework that is based on the classical field approximation, and the removal of the unphysical self-repulsion mechanism is an essential challenge for further progress. By splitting the electronic and positronic portion of the total fermion operator and solving the corresponding coupled equations for each of them, it was possible to stay in this field theoretical framework. However, in the present work we have assumed that transitions between states of the positive and negative energy manifold could be neglected, and one could possibly include them in a perturbative way to account for pair creation. We will report on this exciting approach in a future work.

ACKNOWLEDGMENTS

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APPENDIX A: PARTITIONING OF THE DIRAC EQUATION FOR THE FIELD OPERATOR

Here we derive the equations of motion for the electronic and positronic part of the field operator from the Dirac equation $i\partial_t\Psi(x,t) = [c\sigma_1 p + \sigma_3 c^2 + q_e V(x,t)]\Psi(x,t)$. If we multiply both sides of this equation with the operator P_+ we obtain

$$i\partial_t P_+\Psi(x,t) = [c\sigma_1 p + \sigma_3 c^2 + q_e V(x,t)]P_+\Psi(x,t). \quad \text{(A1)}$$

Here we have used $[P_+, c\sigma_1 p + \sigma_3 c^2] = 0$, which follows directly from the definition of the projector $P_+ \equiv (1 + H_0/|H_0|)/2 \equiv \sum_{p_{(+)}} |p(+)\rangle\langle p(+)|$. More importantly, we have also assumed that the interaction part of the Hamiltonian, $H_{\rm int} \equiv q_e V(x,t)/2$, is sufficiently weak to couple the upper and lower energy states with each other; in other words, we assume $P_- H_{\rm int} P_+ = P_+ H_{\rm int} P_- = 0$, where P_- is the complementary operator ($P_- + P_+ = 1$). It follows then that $P_+ H_{\rm int} = H_{\rm int} P_+$, which we have used to derive Eq. (A1). The vanishing commutator can be easily proven as $P_+ H_{\rm int} = P_+ H_{\rm int}(P_- + P_+) = P_+ H_{\rm int} P_+ = (1–P_-)H_{\rm int} P_+ = H_{\rm int} P_+$. Using the definition of the electronic portion of the field operator $\Psi_{\rm elec} \equiv P_+\Psi$, we obtain the equation for the electronic field operator,

$$i\partial_t\Psi_{\rm elec}(x,t) = [c\sigma_1 p + \sigma_3 c^2 + q_e V(x,t)]\Psi_{\rm elec}(x,t). \quad \text{(A2)}$$

Very similarly, we can also multiply both sides of the Dirac equation with $Q(1–P_+)$, where Q is the charge conjugation operator.

$$-i\partial_t Q(1 - P_+)\Psi(x,t) = Q[c\sigma_1 p + \sigma_3 c^2 + q_e V(x,t)] \times (1 - P_+)\Psi(x,t). \quad \text{(A3)}$$

Here we used again the same assumption as above and the fact that the operator Q involves complex conjugation and is therefore antilinear. The action of the charge conjugation operator on the Hamilton is given by $Q[c\sigma_1 p + \sigma_3 c^2 + q_e V] = –[c\sigma_1 p + \sigma_3 c^2 – q_e V]Q$, such that we obtain after the cancellation of the overall minus sign,

$$i\partial_t Q(1 - P_+)\Psi(x,t) = [c\sigma_1 p + \sigma_3 c^2 – q_e V(x,t)]Q(1 - P_+)\Psi(x,t). \quad \text{(A4)}$$

In other words, using the definition of $\Psi_{\rm posi} \equiv Q(1–P_+)\Psi$ we obtain the second equation if we replace the electron's negative charge q_e with $–q_p$ corresponding to the positive charge q_p of the positron.

$$i\partial_t\Psi_{\rm posi}(x,t) = \left[c\sigma_1 p + \sigma_3 c^2 + q_p V(x,t)\right]\Psi_{\rm posi}(x,t). \quad \text{(A5)}$$

APPENDIX B: FROM THE FIELD-OPERATOR EQUATION TO THE EQUATION FOR THE WAVE FUNCTIONS

Here we show how the equation of motion for the electron-positron wave function $\phi(x_1,x_2,t)$ can be obtained from quantum field theory. Applying the general definition for the mapping of the field operator onto a multiparticle wave function of Eq. (2.1b) to the special case of the electron-positron system case we have

$$\phi(x_e,x_p,t) = \langle\langle \text{vac} \parallel \Psi_e(x_e,t)\Psi_p(x_p,t) \parallel \Phi(t=0)\rangle\rangle, \quad \text{(B1)}$$

where $\Psi_e(x,t) = P_+\Psi(x,t)$ denotes the electronic portion of the field operator and $\Psi_p(x,t) = Q(1–P_+)\Psi(x,t)$ is the corresponding positronic portion. If we take the time derivative of $\phi(x_e,x_p,t)$ and insert its definition in terms of the field operators we obtain, after applying the product rule,

$$\begin{aligned} i\partial_t\phi(x_e,x_p,t) &= i\partial/\partial t\langle\langle \text{vac} \parallel \Psi_e(x_e,t)\Psi_p(x_p,t) \parallel \Phi(t=0)\rangle\rangle \\ &= \langle\langle \text{vac} \parallel [i\partial/\partial t\Psi_e(x_e,t)]\Psi_p(x_p,t) \parallel \Phi(t=0)\rangle\rangle + \langle\langle \text{vac} \parallel \Psi_e(x_e,t)[i\partial/\partial t\Psi_p(x_p,t)] \parallel \Phi(t=0)\rangle\rangle. \end{aligned} \quad \text{(B2)}$$

Next, using the corresponding time evolution equation for the field operators we obtain

$$\begin{aligned} i\partial_t\phi(x_e,x_p,t) &= \langle\langle \text{vac} \parallel [H_e\Psi_e(x_e,t)]\Psi_p(x_p,t) \parallel \Phi(t=0)\rangle\rangle + \langle\langle \text{vac} \parallel \Psi_e(x_e,t)[H_p\Psi_p(x_p,t)] \parallel \Phi(t=0)\rangle\rangle \\ &= H_e\phi(x_e,x_p,t) + H_p\phi(x_e,x_p,t) \\ &= \{[c\sigma_1 p_e + \sigma_3 c^2 + q_e V(x_e,t)] \otimes \mathbf{1}_{\text{posi}} + \mathbf{1}_{\text{elec}} \otimes [c\sigma_1 p_p + \sigma_3 c^2 + q_p V(x_p,t)]\}\phi(x_e,x_p,t). \end{aligned} \tag{B3}$$

APPENDIX C: CLASSICAL SIMULATIONS BASED ON TWO ENSEMBLES OF POINT CHARGES

Here we just sketch briefly how the time evolution of the electron and positron wave packet can be simulated with two ensembles of N classical point charges each. The first ensemble approximates the electronic wave packet, where each point charge has an effective mass of $m_i \equiv m_e/N$ and a charge of $q_{e,i} \equiv q_e/N$, where m_e and q_e are the total mass and charge of the corresponding quantum particle. Similarly, the positron's wave packet is also simulated with N positively charged quasipoint particles with same mass but with positive charge $q_{p,i} \equiv q_p/N$ each. The trajectories of each quasiparticle are denoted by $x_{e,i}(t)$ and $x_{p,i}(t)$. In the case where the self-repulsion has not been removed, each particle's energy is coupled in the time-dependent Hamilton function $H(t)$ to the total potential $V(x,t)$. The space-time evolution of the total potential $V(x,t)$ is governed by the Maxwell equation with the total charge density acting as the source term.

$$H(t) = \sum_{i=1}^{N} \left\{ \left[{m_i}^2c^4 + c^2 p_{e,i}^2 \right]^{1/2} + q_{e,i} V(x_{e,i},t) + \left[{m_i}^2c^4 + c^2 p_{p,i}^2 \right]^{1/2} + q_{p,i} V(x_{p,i},t) \right\}, \tag{C1a}$$

$$-\partial_x^2 V(x,t) = 4\pi \sum_{i=1}^{N} \left[q_{e,i}\delta(x - x_{e,i}(t)) + q_{p,i}\delta(x - x_{p,i}(t)) \right]. \tag{C1b}$$

We assume that the initial positions and momenta are distributed in such a way that the corresponding distribution as a function of the position and momentum matches that of the corresponding quantum system. In order to quantitatively compare the dynamics of the total quantum charge density with that of the classical ensemble, we have solved the coupled Hamilton equations of motion,

$$dx_{e,i}(t)/dt = dH(t)/dp_{e,i} = c^2 p_{e,i}\left[{m_i}^2c^4 + c^2 p_{e,i}^2 \right]^{-1/2}, \tag{C2a}$$

$$dx_{p,i}(t)/dt = dH(t)/dp_{p,i} = c^2 p_{p,i}\left[{m_i}^2c^4 + c^2 p_{p,i}^2 \right]^{-1/2}, \tag{C2b}$$

$$dp_{e,i}(t)/dt = -q_{e,i} dV(x_{e,i},t)/dx_{e,i}, \tag{C2c}$$

$$dp_{p,i}(t)/dt = -q_{p,i} dV(x_{p,i},t)/dx_{p,i}, \tag{C2d}$$

together with the Maxwell equation (C1b). The sum of all individual particle trajectories was then used to compute the time evolution of the total charge density via

$$q_{\text{class}}(x,t) \equiv \sum_{i=1}^{N} \left[q_{e,i} G(x - x_{e,i}(t)) + q_{p,i} G(x - x_{p,i}(t)) \right]. \tag{C3}$$

Here we have defined for computational convenience a narrow Gaussian function $G(x) \equiv (2\pi)^{-1/2} w^{-1} \exp(-0.5x^2/w^2)$ instead of the infinitely narrow delta function used in the charge density of Eq. (C1b). Here the numerical parameter w has to be chosen sufficiently small not to affect the overall structure of $q_{\text{class}}(x,t)$ but large enough that the discreteness of the individual orbits does not become visible.

Similarly, the time dependence of the (squared) spatial width of the electron cloud was obtained as

$$\Delta x_{e,\text{class}}^2(t) \equiv (1/N) \sum_{i=1}^{N} x_{e,i}^2(t) - \left[(1/N) \sum_{i=1}^{N} x_{e,i}(t) \right]^2. \tag{C4}$$

In the case where the self-repulsion was removed (by dividing the total potential in electronic and positronic parts as outlined in Sec. IV) we have solved the corresponding equations of motion for the Hamilton function,

$$H(t) = \sum_{i=1}^{N} \left\{ \left[{m_i}^2c^4 + c^2 {p_{e,i}}^2 \right]^{1/2} + q_{e,i} V_{\text{posi}}(x_{e,i},t) + \left[m_i^2c^4 + c^2 p_{p,i}^2 \right]^{1/2} + q_{p,i} V_{\text{elec}}(x_{p,i},t) \right\}, \tag{C5a}$$

where the two potentials are given separately by

$$-\partial_x^2 V_{\rm elec}(x,t) = 4\pi \sum_{i=1}^{N} q_{e,i}\delta(x - x_{e,i}(t)), \tag{C5b}$$

$$-\partial_x^2 V_{\rm posi}(x,t) = 4\pi \sum_{i=1}^{N} q_{p,i}\delta(x - x_{p,i}(t)). \tag{C5c}$$

We should finish this Appendix by pointing out that once again, the Maxwell equations of motion can be eliminated effectively if we introduce effective interaction energies in the multiparticle Hamilton function

$$H_{\rm effective} = \sum_{i=1}^{N}\left[{m_i}^2c^4 + c^2p_{e,i}^2\right]^{1/2} + \sum_{i=1}^{N}\left[{m_i}^2c^4 + c^2p_{p,i}^2\right]^{1/2} + W_{\rm sr}(x_{e,i}) + W_{\rm sr}(x_{p,i}) + W_{\rm co}(x_{e,i},x_{p,j}), \tag{C6}$$

where the self-repulsion energies are defined as $W_{\rm sr}(x_{e,i}) = -\pi q_{e,i}^2\Sigma_i\Sigma_j|x_{e,i} - x_{e,j}|$ and $W_{\rm sr}(x_{p,i}) = -\pi q_{p,i}^2\Sigma_i\Sigma_j|x_{p,i} - x_{p,j}|$ and the collisional energy is $W_{\rm co}(x_{e,i},x_{p,j}) = -\pi q_{e,i}^2\Sigma_i\Sigma_j|x_{e,i} - x_{p,j}|$. One can easily see that the set of equations of motion (C2) are reproduced and those without the self-repulsion are reproduced if $W_{\rm sr} = 0$.

APPENDIX D: ENERGY CONSERVATION FOR THE TRUNCATED DYNAMICS

In this Appendix we will show that even the truncated dynamics for which the quantum mechanical self-repulsion has been removed is a conservative system such that the total energy is invariant. It turns out that the specific functional form of the conserved total energy can be determined, if it is possible to construct a Lagrangian, whose corresponding Euler-Lagrange (E-L) equations reproduce the given equations of motions. In the first part of this Appendix we present this Lagrangian and then show how the spatial integral over the Hamiltonian (obtained from a Legendre transformation) provides the desired conserved energy. In the second part of this Appendix we generalize this Lagrangian to the one for the two-particle-field system where self-repulsion was removed. We show that its E-L equations reproduce our original equations of motion and then prove the time independence of the corresponding energy, which was obtained again from a Legendre transformation.

1. Energy conservation for single-particle-field dynamics

Our method to construct the conserved energy for our system is based on finding the corresponding Lagrangian density $L(\phi,\partial_t\phi,\partial_x\phi)$ first [28]. We will show below that then the quantity $\int dx[\partial L/\partial(\partial_t\phi)\partial_t\phi - L]$ is always conserved in time, independent even on how $L(\phi,\partial_t\phi,\partial_x\phi)$ actually depends on its three arguments ϕ, $\partial_t\phi$, and $\partial_x\phi$.

The proof for this claim that $d/dt\int dx[\partial L/\partial(\partial_t\phi)\partial_t\phi - L] = 0$ is straightforward if we invoke the corresponding E-L equation whose solutions minimize the action $\iint dxdtL$. They are given by $d/dt[\partial L/\partial(\partial_t\phi)] + d/dx[\partial L/\partial(\partial_x\phi)] - \partial L/\partial\phi = 0$. If we introduce the canonical momentum $P \equiv \partial L/\partial(\partial_t\phi)$, then this E-L equation reduces to $dP/dt + d/dx[\partial L/\partial(\partial_x\phi)] - \partial L/\partial\phi = 0$. We can then simplify $d/dt\int dx[P\partial_t\phi - L] = \int dx[dP/dt\partial_t\phi + P\partial_t\partial_t\phi - dL/dt]$ by replacing the third term dL/dt by $P\partial_t\partial_t\phi + \partial L/\partial(\partial_x\phi)\partial_t\partial_x\phi + \partial L/\partial\phi\partial_t\phi$, and then also replace here $\partial L/\partial\phi$ by $dP/dt + d/dx[\partial L/\partial(\partial_x\phi)]$. The first two terms under the integral $dP/dt\partial_t\phi$ and $P\partial_t\partial_t\phi$ cancel out and we are left with $d/dt\int dxH = -\int dx\{\partial_t\partial_x\phi\partial L/\partial(\partial_x\phi) + \partial_t\phi d/dx\partial L/\partial(\partial_x\phi)\} = -\int dxd/dx\{\partial_t\phi\partial L/\partial(\partial_x\phi)\}$, which is zero, if the product $\partial_t\phi\partial L/\partial(\partial_x\phi)$ vanishes at the boundary $x = \pm\infty$. In other words, $\int dxH$ is the conserved energy.

As a concrete example, let us now construct the Lagrangian density for interaction of a single particle with its own field, such that its set of three E-L equations reproduce to the Dirac-Maxwell equations.

$$i\partial_t\phi(x,t) = [c\sigma_1 p + \sigma_3c^2 + qV(x,t)]\phi(x,t), \tag{D1a}$$

$$\partial_x E(x,t) = 4\pi q(x,t), \tag{D1b}$$

$$\partial_t E(x,t) = -4\pi j(x,t). \tag{D1c}$$

These three equations can be derived if we assume the Lagrangian $L = L[\phi^\dagger,\phi,\partial_t\phi,\partial_x\phi,V,\partial_xV]$ to take the form

$$L = \phi^\dagger[i\partial_t - c\sigma_1 p - \sigma_3c^2]\phi - q\phi^\dagger V\phi + 1/(8\pi)(\partial_xV)^2. \tag{D2}$$

We can therefore apply the Legendre transformation and construct the Hamiltonian energy density. This leads then to the expression for the conserved energy $e_{\rm tot}$,

$$e_{\rm tot} = \int dx\{\phi^\dagger[c\sigma_1 p + \sigma_3c^2 + qV]\phi - 1/(8\pi)(\partial_xV)^2\}. \tag{D3}$$

2. Energy conservation for two-particle-field dynamics without self-repulsion

In this section of Appendix D we will use the functional form of the energy of Eq. (D3) as a guidance to construct the corresponding energy for the two-particle dynamics given by the set of equations (3.1) for $\phi(x_1,x_2,t)$ and Gauss's law for the

two potentials $V_{\rm elec}$ and $V_{\rm posi}$ given by

$$-\partial_x^2 V_{\rm elec}(x,t) = 4\pi q_{\rm elec}(x,t), \tag{D4a}$$

$$-\partial_x^2 V_{\rm posi}(x,t) = 4\pi q_{\rm posi}(x,t), \tag{D4b}$$

$$i\partial_t \phi(x_1,x_2,t) = h_D \phi(x_1,x_2,t), \tag{D5}$$

with $h_D \equiv [c\sigma_1 p_1 + \sigma_3 c^2 + q_e V_{\rm posi}(x_e,t)] \otimes \mathbf{1}_{\rm posi} + \mathbf{1}_{\rm elec} \otimes [c\sigma_1 p_p + \sigma_3 c^2 + q_p V_{\rm elec}(x_p,t)]$. In the field-energy term $-1/(4\pi)(\partial_x V)^2$ in Eq. (D3)V represents the total potential $V_{\rm tot}$. In case of two potentials, this would generalize to $V_{\rm tot} = V_{\rm elec} + V_{\rm posi}$. If we neglect the two direct product terms $(\partial_x V_{\rm elec})^2$ and $(\partial_x V_{\rm posi})^2$ we obtain $-1/(4\pi)\partial_x V_{\rm posi}\partial_x V_{\rm elec}$. This suggests that a potential candidate for the conserved total energy could be of the form

$$e_{\rm tot} = \iint dx_1 dx_2 \phi^\dagger h_D \phi - 1/(4\pi) \int dx \partial_x V_{\rm elec}(x,t) \partial_x V_{\rm posi}(x,t). \tag{D6}$$

To prove this we have to show that the temporal derivative of this $e_{\rm tot}$ vanishes. The derivative of $e_{\rm tot}$ is

$$\begin{aligned} de_{\rm tot}/dt &= \iint dx_1 dx_2 \{(\partial_t \phi^\dagger) h_D \phi + \phi^\dagger h_D (\partial_t \phi) + \phi^\dagger (\partial_t h_D) \phi\} - 1/(4\pi) \int dx \{\partial_t \partial_x V_{\rm elec}(x,t) \partial_x V_{\rm posi}(x,t) \\ &\quad + \partial_x V_{\rm elec}(x,t) \partial_t \partial_x V_{\rm posi}(x,t)\} \\ &= \iint dx_1 dx_2 \{(\partial_t \phi^\dagger) h_D \phi + \phi^\dagger h_D (\partial_t \phi) + \phi^\dagger (\partial_t h_D) \phi\} - 1/(4\pi) \int dx \{-\partial_t V_{\rm elec}(x,t) \partial_x^2 V_{\rm posi}(x,t) - \partial_t V_{\rm posi}(x,t) \partial_x^2 V_{\rm elec}(x,t)\}. \end{aligned} \tag{D7}$$

If we replace $\partial_t \phi^\dagger$ with $i\phi^\dagger h_D$ and $\partial_t \phi$ with $-i h_D \phi$ then the first two terms (integrated over x_1 and x_2) cancel as h_D is Hermitian. In the field-energy term we can integrate by parts, and use Gauss's law to replace the factors $\partial_x^2 V_{\rm elec}(x,t)$ by $-4\pi q_{\rm elec}(x,t)$ and $\partial_x^2 V_{\rm posi}(x,t)$ by $-4\pi q_{\rm posi}(x,t)$. Finally if we use $\partial_t h_D = \partial_t [q_e V_{\rm posi}(x_e,t) + q_p V_{\rm elec}(x_p,t)]$ we obtain

$$de_{\rm tot}/dt = \iint dx_e dx_p \phi^\dagger \phi \{q_e \partial_t V_{\rm posi}(x_e,t) + q_p \partial_t V_{\rm elec}(x_p,t)\} - 1/(4\pi) \int dx \{\partial_t V_{\rm elec}(x,t) 4\pi q_{\rm posi}(x,t) + \partial_t V_{\rm posi}(x,t) 4\pi q_{\rm elec}(x,t)\}. \tag{D8}$$

As $\int dx_e \phi^\dagger(x_e,x_p,t)\phi(x_e,x_p,t) \equiv \rho_{\rm posi}(x_p,t)$ and similarly $\int dx_p \phi^\dagger \phi \equiv \rho_{\rm elec}(x_e,t)$, the first term in Eq. (D8) simplifies to

$$\iint dx_e dx_p \phi^\dagger \phi \{q_e \partial_t V_{\rm posi}(x_e,t) + q_p \partial_t V_{\rm elec}(x_p,t)\} = \int dx_e q_{\rm elec}(x_e,t) \partial_t V_{\rm posi}(x_e,t) + \int dx_p q_{\rm posi}(x_p,t) \partial_t V_{\rm elec}(x_p,t), \tag{D9}$$

where we have used $q_e \rho_{\rm elec}(x_e,t) = q_{\rm elec}(x_e,t)$ and $q_p \rho_{\rm posi}(x_p,t) = q_{\rm posi}(x_p,t)$. As a result, we have two pairwise cancellations with the second term in Eq. (D8) confirming $de_{\rm tot}/dt = 0$, which completes our proof.

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