# Unitarity and electron-positron pairs created by strong external fields

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Lowest-order perturbative calculations of the electron-positron production probability in relativistic heavy-ion collisions exceed unitarity bounds for the heaviest collision systems at extreme relativistic energies and sufficiently small impact parameters. Starting with the exponential representation of the time-evolution operator in the Furry picture, we derive manifestly unitary and gauge-invariant expressions for transition amplitudes and probabilities associated with the created electron-positron pairs by employing the Magnus expansion to first order. The time-evolved ground state of the electron-positron field around the heavy nuclei is expressed as a superposition of the unperturbed vacuum state and virtual excitation modes consisting of electron-positron pairs.

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# I. INTRODUCTION

In recent years the process of electromagnetic production of electron-positron pairs in fast peripheral collisions of heavy ions became a subject of considerable theoretical and experimental interest. The transverse components of the electromagnetic fields associated with the moving ions steadily increase with collision energy, giving rise to sizable pair-production cross sections. Lepton-pair production is a process of basic interest but one that also has important practical implications in the design and operation of heavy-ion colliders. For example, the case of pair production with the electron bound to one of the colliding ions is a major limitation of the beam lifetime.

Most of the theoretical approaches to the electromagnetic production of  $e^+e^-$  pairs are based on lowest-order time-dependent perturbation theory [1-4] or on the Fermi-Weizsäcker-Williams method of virtual photons [5-7]. For a review of the theoretical and experimental status in this field, see, e.g., [8]. An important point was recently addressed by Baur and Bertulani [3], namely, that in almost central heavy-ion collisions, lowest-order perturbative calculations violate unitarity bounds for sufficiently high collision energies  $(E_{lab} \ge 10^3 \text{ GeV/u})$ , i.e., the probability for single-pair creation exceeds unity. This indicates the breakdown of lowest-order perturbation theory and the possibility of multiple-pair production. It was demonstrated by Baur [9], by employing the sudden and quasiboson approximations and neglecting rescattering effects, that the probability distribution of creating N pairs in a single collision is described by a Poisson distribution and that the average number of created pairs is just equal to the value of the perturbative single-pair creation probability in lowest order. Essentially, the same result was independently derived by Rhoades-Brown and Weneser [10] and by Best, Greiner, and Soff [11].

The difficulties associated with the unitarity violation in lowest-order perturbative calculations clearly necessitate radically new theoretical treatments of this problem. At moderate relativistic energies, nonperturbative calculations based either on the direct solution of the timedependent Dirac equation on the lattice [12-14] or on the single-center coupled-channel formalism [15-17] indicate that higher-order effects are of major importance for the electromagnetic production of lepton pairs in relativistic heavy-ion collisions. While in the direct solution of the Dirac equation convergence problems arise due to the small lattice size [13], coupled-channel calculations have been recently criticized [18] as being extremely gauge dependent due to basis truncation. In spite of their power in the realistic treatment of the collision dynamics, these nonperturbative methods require extremely large computation times and, due to limited computer storage, at high energies one still has to rely on perturbative methods.

The purpose of this work is to show how unitarity can be restored by employing an alternative expansion of the time-evolution operator associated with the system under consideration, namely, the Magnus expansion [19]. The structure of the Magnus expansion has been studied by several authors [20-23], and in Refs. [24-30] various applications are presented. An application of the Magnus expansion in first order to the problem of pair creation with the electron bound to one of the colliding ions has been performed in [16], based on a single-particle formulation of the ionization process [30], in which only a single bound state below the Fermi level and the positiveenergy continuum are taken into account. Moreover, due to the use of distorted wave functions, such a treatment is not invariant under local gauge transformations.

In the present paper we present a systematic treatment of electron-positron pair production by external fields within the Magnus approach. In particular, we include the many-particle features of this process explicitly and maintain local gauge invariance of the theory. The major theoretical ingredients of our investigation are presented in Sec. II, where our approximations are specified and an analytic expression for the time-evolved ground state of the electron-positron field is derived. The application of this formula to the calculation of transition amplitudes is presented in Sec. III. Section IV contains a summarizing discussion and some concluding remarks.

## **II. FORMULATION OF THE PROBLEM**

The conventional perturbative series expansion obtained by iterating the integral equation for the timeevolution operator  $\hat{U}(t)$  (we use natural units  $\hbar = m = c = 1$ ),

$$\begin{aligned} \hat{U}(t) &= \hat{1} - i \int_{-\infty}^{t} d\tau \, \hat{H}_{I}(\tau) \hat{U}(\tau) \\ &= \hat{1} - i \int_{-\infty}^{t} d\tau \, \hat{H}_{I}(\tau) \\ &+ (-i)^{2} \int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\tau_{1} \hat{H}_{I}(\tau) \hat{H}_{I}(\tau_{1}) + \cdots, \quad (1) \end{aligned}$$

where  $\hat{H}_I(\tau)$  represents the interaction Hamiltonian in the interaction picture, has two practical disadvantages associated with the truncation after a finite number of terms. First, one obtains a manifestly nonunitary approximation for  $\hat{U}(t)$  and second, the interaction strength has to be small enough in order to obtain accurate results by taking into account only a few terms. While the last condition is well fulfilled in processes involving singly charged ions, the situation is fundamentally different in collisions with fully stripped heavy ions since, due to the presence of the large external charge -eZ, in such systems the effective coupling constant  $\alpha Z$  approaches unity (where  $\alpha = e^2$  is the fine-structure constant and we use e < 0).

By considering the differential equation for the timeevolution operator  $i\partial_t \hat{U}(t) = \hat{H}_I(t)\hat{U}(t)$ , with the initial condition  $\hat{U}(t_i) = \hat{1}$  for  $t_i \to -\infty$ , Magnus started with an exponential ansatz and obtained a representation of the solution in the form

$$\widehat{U}(t) = \exp\{\widehat{\Omega}(t)\} = \exp\left\{\sum_{n=1}^{\infty} \widehat{\Omega}_n(t)\right\}, \qquad (2)$$

where the operator  $\hat{\Omega}(t)$  is anti-Hermitian  $(\hat{\Omega}^{\dagger} = -\hat{\Omega})$ and each term  $\hat{\Omega}_n$  in the infinite sum can be expressed in terms of *n*-fold time integrals over (n-1)-fold nested commutators of the interaction Hamiltonian  $\hat{H}_I(\tau)$ :

(3)

$$\begin{split} \hat{\Omega}_{1}(t) &= -i \int_{-\infty}^{t} d\tau \hat{H}_{I}(\tau) ,\\ \hat{\Omega}_{2}(t) &= \frac{(-i)^{2}}{2} \int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\tau_{1} [\hat{H}_{I}(\tau), \hat{H}_{I}(\tau_{1})] ,\\ \hat{\Omega}_{3}(t) &= \frac{(-i)^{3}}{6} \int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\tau_{1} \int_{-\infty}^{\tau_{1}} d\tau_{2} \{ [[\hat{H}_{I}(\tau), \hat{H}_{I}(\tau_{1})], \hat{H}_{I}(\tau_{2})] + [[\hat{H}_{I}(\tau_{2}), \hat{H}_{I}(\tau_{1})], \hat{H}_{I}(\tau_{1})] \} . \end{split}$$

Terms of higher order can be generated recursively [21,31], but in some special cases the expansion actually terminates after a few terms. The series  $\widehat{\Omega}(t)$  can be regarded as the continuous analog to the Baker-Campbell-Hausdorff formula for discrete operators. An inspection of Eqs. (3) shows that terms with  $n \ge 2$  are sensitive to correlations between the strength of the interaction at different times, while in the term with n = 1 only the total time-integrated interaction strength enters. Clearly, for time-independent perturbations, expansion (2) ends after the first term, i.e.,  $\hat{\Omega}_1$  is the exact solution. Therefore, one can expect contributions from terms with  $n \ge 2$  to be of minor importance in the case that the interaction depends weakly on time. We also note that in the opposite limit of infinitely short interaction times, terms with  $n \ge 2$ vanish. A major advantage of the Magnus expansion (2) is that it guarantees unitarity, independently of where the series is truncated, and therefore conserves probability.

By employing the exponential representation (2) of the time-evolution operator  $\hat{U}(t)$ , we investigate the electromagnetic production of electron-positron pairs in collisions of fast and fully stripped heavy ions by making the usual assumptions of (i) a coordinate system fixed on the target nucleus (charge number  $Z_T$ ) which is at rest, (ii) an unperturbed motion of the projectile nucleus (charge number  $Z_P$ ) with constant velocity  $\mathbf{v} = (0,0,v)$  along a rectilinear trajectory parallel to the z axis at an impact parameter  $\mathbf{b} = (b_x, b_y, 0)$ , (iii) neglecting QED-radiative corrections, and (iv) neglecting the fermionic current contained in the Maxwell equations of motion, as it is much

smaller than the strong, external heavy-ion current, which is regarded as classical. These simplifying assumptions decouple the Maxwell-Dirac field equations of motion [13] and we have to deal with a classical, timedependent external source interacting with the electronpositron field  $\widehat{\psi}(x)$ . Here and in the following, the "hat" symbol indicates second-quantized fields, while the argument x denotes space-time coordinates. The timedependent electromagnetic field associated with the moving projectile creates  $e^+e^-$  pairs in the strong Coulomb field of the target nucleus by exciting electrons from the negative-energy states below the Fermi energy  $E_F = -m$ (this choice corresponds to a fully ionized atom) into empty states above -m. The Lorentz transformation of the Coulombic projectile potential from the projectile into the target frame yields the Liénard-Wiechert potential [we use the metric  $g_{\mu\nu} = \text{diag}(1, -1, -1, -1)$ ]

$$A_{\mu}^{(P)}(x) = -\frac{\gamma e Z_{P}}{r'}(1,0,0,-\beta) , \qquad (4)$$

where  $\beta = v$ ,  $\gamma = (1 - \beta^2)^{-1/2}$ , and the lepton-projectile distance, as seen in the projectile system, is denoted by

$$r' = \sqrt{(x - b_x)^2 + (y - b_y)^2 + \gamma^2 (z - vt)^2}$$

For a systematic iteration procedure it is convenient to perform the investigation in the Furry (bound-state interaction) picture with respect to the lepton-target interaction; this corresponds to an expansion in terms of the electric charge -e and not in the external charge  $-eZ_T$  [32]. In this representation, the second-quantized electron field operator  $\hat{\psi}(x)$  satisfies the time-dependent Dirac equation in the presence of the strong external Coulomb field of the target nucleus  $A_{\mu}^{(T)}(x) = -eZ_T(1,0)/r$ 

$$\{\gamma^{\mu}[i\partial_{\mu}-eA^{(T)}_{\mu}(x)]-m\}\widehat{\psi}(x)=0, \qquad (5)$$

and its evolution in the static field is solved by an eigenfunction expansion,

$$\hat{\psi}(\mathbf{x}) = \sum_{e>F} \hat{b}_e \varphi_e(\mathbf{r}) e^{-iE_e t} + \sum_{p$$

with the help of a complete set of solutions of timedependent single-particle solutions of the Dirac equation:

$$\{\gamma^{\mu}[i\partial_{\mu}-eA_{\mu}^{(T)}(x)]-m\}\varphi_{e,p}(x)=0.$$
(7)

In Eq. (6) the first summation comprises all states above the Fermi level (electron states) and the second incorporates all states below -m (positron states);  $E_e$  and  $E_p$  are the energy eigenvalues of  $\varphi_e(\mathbf{r})$  and  $\varphi_p(\mathbf{r})$ , respectively, while  $\hat{b}_e$  and  $\hat{d}_p^{\dagger}$  are single-electron and single-positron annihilation and creation operators, respectively, satisfying the same anticommutation relations for fermions as in the free-field case:

$$\{\hat{b}_i, \hat{b}_j^\dagger\} = \{\hat{d}_i, \hat{d}_j^\dagger\} = \delta_{ij} , \qquad (8)$$

while all other combinations anticommute. The interaction Hamiltonian  $\hat{H}_I(t)$  in Eqs. (1) and (3) is expressed in this specific approach as the space-integrated product of the fermion current in the Furry picture  $\hat{j}_F^{\mu}(x)$  and the projectile potential  $A_{\mu}^{(P)}(x)$  which is, as stated before, a *c* number:

$$\hat{H}_{I}(t) = \int d^{3}r : \hat{j}_{F}^{\mu}(x) : A_{\mu}^{(P)}(x)$$

$$= e \int d^{3}r : \hat{\overline{\psi}}(x) \gamma^{\mu} \hat{\psi}(x) : A_{\mu}^{(P)}(x) . \qquad (9)$$

The adjoint lepton field is defined by  $\widehat{\psi}(x) = \widehat{\psi}^{\dagger}(x)\gamma^{0}$  and the four-current operator is normal ordered as indicated by the colons (creation operators stand to the left of annihilation operators) such that the vacuum energy is substracted.

By inserting the eigenfunction expansion (6) in expression (9), one obtains an alternative representation for  $\hat{H}_I(t)$  in terms of the single-fermion creation and annihilation operators, i.e.,

$$\hat{H}_{I} = \sum_{i,j} \hat{b}_{i}^{\dagger} \hat{b}_{j} \tilde{\chi}_{ij}(t) + \sum_{i,\alpha} [\hat{b}_{i}^{\dagger} \hat{d}_{\alpha}^{\dagger} \tilde{\chi}_{i\alpha}(t) + \hat{d}_{\alpha} \hat{b}_{i} \tilde{\chi}_{\alpha i}(t)] - \sum_{\alpha,\beta} \hat{d}_{\beta}^{\dagger} \hat{d}_{\alpha} \tilde{\chi}_{\alpha\beta}(t) .$$
(10)

Here, the minus sign in front of the last term on the right-hand side stems from the normal-ordering procedure, and latin (greek) indices  $i, j, \ldots$  ( $\alpha, \beta, \ldots$ ) denote appropriate quantum numbers for electron (positron) states. In a spherically symmetric basis, we have to deal with a radial quantum number n, a total angular momentum quantum number J, a magnetic quantum number  $\mu$ , and parity [33]. The explicitly time-dependent functions  $\tilde{\chi}_{ab}(t)$  are transition-matrix elements between arbitrary

single-fermion states a and b in the external target potential

$$\widetilde{\chi}_{ab}(t) = e \int d^3 r \, \overline{\varphi}_a(\mathbf{r}, t) \gamma^{\mu} \varphi_b(\mathbf{r}, t) A_{\mu}^{(P)}(\mathbf{r}, t) = -\gamma e^2 Z_P \int d^3 r \, \varphi_a^{\dagger}(\mathbf{r}, t) \frac{1 - \beta \alpha_3}{r'} \varphi_b(\mathbf{r}, t) , \qquad (11)$$

where  $\alpha = \gamma^0 \gamma$ , and we introduced the explicit representation of the projectile potential (4), while the four spinors  $\varphi_a(x)$  and  $\varphi_b(x)$  are solutions of the time-dependent Dirac equation (7). We now introduce the vacuum state  $|0\rangle$  at  $t \to \infty$  as the state of lowest energy in the external field of the target nucleus such that the boundary between particle and antiparticle (hole) states is just the Fermi energy  $E_F = -m$  [34]. This definition of the vacuum state is consistent with the Dirac sea picture in the sense that the particle number operator has the eigenvalue 0 for states with energy  $E_n$  above the Fermi energy  $E_F$ , and the eigenvalue 1 for states with energy below  $E_F$ , i.e.,

$$\hat{b}_{n}^{\dagger}\hat{b}_{n}|0\rangle = 0 \quad \text{for } E_{n} > E_{F} ,$$

$$\hat{b}_{n}\hat{b}_{n}^{\dagger}|0\rangle = 0 \quad \text{for } E_{n} < E_{F} ,$$

$$\hat{d}_{n}^{\dagger}\hat{d}_{n}|0\rangle = 0 \quad \text{for } E_{n} > |E_{F}| ,$$
(12)

where we introduce positron (or "hole") creation operators  $\hat{d}_n^{\dagger}$  for the electron annihilation operators  $\hat{b}_n$  of negative-energy modes.

Under the action of the time-evolution operator  $\hat{U}(t)$  defined in Eq. (2), the free vacuum state  $|0\rangle$  evolves into the perturbed ground state  $|\tilde{0}\rangle$  at  $t \to \infty$  according to

$$|\tilde{0}\rangle = \lim_{t \to \infty} \hat{U}(t) |0\rangle = \lim_{t \to \infty} \left\{ \exp\left[\sum_{n=1}^{\infty} \hat{\Omega}_{n}(t)\right] |0\rangle \right\}, \quad (13)$$

such that the exact amplitude for the vacuum state at  $t \rightarrow -\infty$  to remain unchanged, i.e., the vacuum-to-vacuum amplitude, is expressed as

$$\langle \tilde{0} | 0 \rangle = \lim_{t \to \infty} \langle 0 | \hat{U}^{\dagger}(t) | 0 \rangle$$
  
= 
$$\lim_{t \to \infty} \left\langle 0 \left| \exp \left\{ -\sum_{n=1}^{\infty} \Omega_n(t) \right\} \right| 0 \right\rangle,$$
 (14)

where the minus sign in the exponent stems from the anti-Hermitian nature of the operators  $\hat{\Omega}_n(t)$  in the Magnus expansion (3). It is instructive to remember that the corresponding vacuum-to-vacuum amplitude, which is obtained in a first-order calculation by truncating the Dyson expansion (1) for  $\hat{U}(t)$  after the second term, is just unity independent of the interaction strength. This is easily verified by employing the representation (10) for  $\hat{H}_I(t)$  and making use of the action of the single-fermion operators on the free ground state (12), which is normalized to 1:

$$\langle \mathbf{0} | \tilde{\mathbf{0}} \rangle^{(1)} = \left\langle \mathbf{0} \left| \left[ \hat{\mathbf{1}} - i \int_{-\infty}^{\infty} d\tau \, \hat{H}_{I}(\tau) \right] \right| \mathbf{0} \right\rangle$$
  
=  $\langle \mathbf{0} | \mathbf{0} \rangle = 1 .$  (15)

In order to obtain an explicit representation of the

time-evolved state  $|\tilde{0}\rangle$  from Eq. (13), we make the following three approximations

(i) We consider only the first term  $\Omega_1(t)$  in the Magnus expansion (3), i.e., we neglect contributions from terms with  $n \ge 2$  which, as we argued before, are associated with the temporal extent of the interaction. This should be a fairly good approximation for highly relativistic energies and impact parameters of the order of the electron Compton wavelength, since in this case the duration of the external perturbation, which is estimated to be of the order  $t \simeq b/(\gamma\beta)$ , is much smaller than characteristic excitation times  $T=2\pi/(E_e+E_p)$  of the unperturbed system, such that time correlations are of minor importance.

(ii) We neglect rescattering effects, i.e., all terms proportional to  $\hat{b}_i^{\dagger} \hat{b}_j$  and  $\hat{d}_{\beta}^{\dagger} \hat{d}_{\alpha}$  contained in the first and last summations of the interaction Hamiltonian  $\hat{H}_I(t)$  from Eq. (10), respectively, will be ignored.

(iii) We allow for only one particle and one hole in the intermediate states, i.e., terms containing combinations of single-fermion operators describing the simultaneous creation or annihilation of more than one  $e^+e^-$  pair, such as  $(\hat{b}_i^{\dagger}\hat{a}_{\alpha}^{\dagger})(\hat{b}_j^{\dagger}\hat{a}_{\beta}^{\dagger})$  or  $(\hat{b}_i\hat{a}_{\alpha})(\hat{b}_j\hat{a}_{\beta})$ , will be set equal to zero. This leads to a selective summation of diagrams. In our case these are just electron-positron loops, or bubble diagrams i.e., this assumption has essentially the same physical content as the Tamm-Dancoff approximation [35].

With these assumptions it becomes possible to sum the interaction to all orders in the external charge  $-eZ_P$ . We first define an electron-positron state  $|e^+e^-\rangle$  by the action of the single-fermion operators on the Dirac vacuum:

$$|e^+e^-\rangle = \hat{b}_e^\dagger \hat{d}_p^\dagger |0\rangle , \qquad (16)$$

such that with assumptions (i) and (ii) the transition amplitude for the creation of one electron-positron pair is expressed by projecting the time-evolved ground state (1) on the  $|e^+e^-\rangle$  state (16) as

$$A_{ep} = \langle e^+ e^- | \tilde{0} \rangle$$
$$= \left\langle 0 \left| \hat{O}_{ep} \exp \left\{ \sum_{i,\alpha} [\hat{O}_{i\alpha}^\dagger \chi_{i\alpha} - \hat{O}_{i\alpha} \chi_{i\alpha}^\dagger] \right\} \right| 0 \right\rangle, \quad (17)$$

where we introduced the two-fermion operators  $\hat{O}_{i\alpha}^{\dagger} = \hat{b}_i^{\dagger} \hat{d}_{\alpha}^{\dagger}$  and  $\hat{O}_{i\alpha} = \hat{d}_{\alpha} \hat{b}_i$ , which create and annihilate electron-positron pairs, respectively. The transition amplitudes  $\chi_{i\alpha}$  are represented with definition (11) as

$$\chi_{i\alpha} = -i \int_{-\infty}^{\infty} dt \, \tilde{\chi}_{i\alpha}(t) , \qquad (18)$$

and if one regards the functions  $\varphi_i^{\dagger}(x)$ ,  $V_P(x) = e \gamma^0 \gamma^{\mu} A_{\mu}^{(P)}(x)$ , and  $\varphi_{\alpha}(x)$  in Eq. (11) as matrices

depending on the continuous space-time variables, one may write in a symbolic notation

$$\chi_{\alpha i} = -i\varphi_{\alpha}^{\dagger} V_{P} \varphi_{i} = (i\varphi_{\alpha}^{T} V_{P}^{*} \varphi_{i}^{*})^{*} = (i\varphi_{i}^{\dagger} V_{P} \varphi_{\alpha})^{\dagger} = -\chi_{i\alpha}^{\dagger},$$
(19)

which reflects just the fact that the interaction is Hermitian. This last relation also explains the presence of the minus sign in the exponent of Eq. (17) which constitutes the basic relation for the calculation of the single-pair excitation amplitude  $A_{ep}$ .

Now it is useful to analyze some properties of the pair operators  $\hat{O}_{i\alpha}^{\dagger}$  and  $\hat{O}_{i\alpha}$ . Due to their fermionic character, the single-lepton operators satisfy the obvious relations

$$\hat{b}_i^{\dagger 2} = \hat{b}_i^2 = \hat{d}_{\alpha}^{\dagger 2} = \hat{d}_{\alpha}^2 = 0$$
 for  $i > F$  and  $\alpha < F$ , (20)

which express the Pauli principle. As a consequence of these relations, the pair operators satisfy

$$\hat{O}_{i\alpha}^{\dagger}\hat{O}_{j\beta}^{\dagger} = \hat{O}_{i\alpha}\hat{O}_{j\beta} = 0 \quad \text{if } i = j \text{ or } \alpha = \beta .$$
(21)

At this point we implement the third approximation (iii) as stated earlier, namely, that only excitations consisting of one particle and one hole contribute to the creation of a single electron-positron pair. In other words, we assume that relation (21) holds for all pair indices. Making use of the anticommutation relations (8) and Eqs. (12), one easily finds

$$[\hat{O}_{j\beta},\hat{O}_{i\alpha}^{\dagger}] = \delta_{ij}\delta_{\alpha\beta} - \delta_{\alpha\beta}\hat{b}_{i}^{\dagger}\hat{b}_{j} - \delta_{ij}\hat{d}_{\alpha}^{\dagger}\hat{d}_{\beta}$$
(22)

and

$$\hat{O}_{i\alpha}|0\rangle = \langle 0|\hat{O}_{i\alpha}^{\dagger} = 0 \text{ for } i > F \text{ and } \alpha < F$$
. (23)

In order to simplify the notation, we denote in the following pairs of indices  $(i,\alpha), (j,\beta), \ldots$ , corresponding to different  $e^+e^-$  pairs by  $\sigma_1, \sigma_2, \ldots$ , such that the approximated time-evolution operator  $\hat{\mathcal{U}}$  which enters into the amplitude (17) can be expressed as

$$\widehat{\mathcal{U}} = \exp\left\{\sum_{\sigma} [\widehat{O}_{\sigma}^{\dagger} \chi_{\sigma} - \widehat{O}_{\sigma} \chi_{\sigma}^{\dagger}]\right\}$$
$$= \sum_{n=0}^{\infty} \frac{1}{n!} \left\{\sum_{\sigma} (\widehat{O}_{\sigma}^{\dagger} \chi_{\sigma} - \widehat{O}_{\sigma} \chi_{\sigma}^{\dagger})\right\}^{n}.$$
(24)

As a direct consequence of considering only 1p-1h excitations, i.e., Eq. (21) without restrictions, each term in expansion (24) contains solely combinations of the type  $(\hat{O}_{\sigma}^{\dagger}\hat{O}_{\sigma})$  and  $(\hat{O}_{\sigma}\hat{O}_{\sigma}^{\dagger})$ , such that each created pair is subsequently annihilated, etc. Consequently, different contributions contained in the expansion (24) are of the form

$$\hat{\mathcal{U}}^{(0)} = 1, 
\hat{\mathcal{U}}^{(1)} = \sum_{\sigma} (\hat{\mathcal{O}}_{\sigma}^{\dagger} \chi_{\sigma} - \hat{\mathcal{O}}_{\sigma} \chi_{\sigma}^{\dagger}), 
\hat{\mathcal{U}}^{(2)} = \frac{1}{2!} \sum_{\sigma_{1}\sigma_{2}} [-\hat{\mathcal{O}}_{\sigma_{1}}^{\dagger} \hat{\mathcal{O}}_{\sigma_{2}} (\chi_{\sigma_{1}} \chi_{\sigma_{2}}^{\dagger}) - \hat{\mathcal{O}}_{\sigma_{1}} \hat{\mathcal{O}}_{\sigma_{2}}^{\dagger} (\chi_{\sigma_{1}}^{\dagger} \chi_{\sigma_{2}})], 
\hat{\mathcal{U}}^{(3)} = \frac{1}{3!} \sum_{\sigma_{1}\sigma_{2}\sigma_{3}} [-\hat{\mathcal{O}}_{\sigma_{1}}^{\dagger} \hat{\mathcal{O}}_{\sigma_{2}} \hat{\mathcal{O}}_{\sigma_{3}}^{\dagger} (\chi_{\sigma_{1}} \chi_{\sigma_{2}}^{\dagger} \chi_{\sigma_{3}}) + \hat{\mathcal{O}}_{\sigma_{1}} \hat{\mathcal{O}}_{\sigma_{2}}^{\dagger} \hat{\mathcal{O}}_{\sigma_{3}} (\chi_{\sigma_{1}}^{\dagger} \chi_{\sigma_{2}} \chi_{\sigma_{3}})], 
\vdots$$
(25)

n even:

$$\widehat{\mathcal{U}}^{(n)} = \frac{1}{n!} \sum_{\sigma_1, \dots, \sigma_n} (-)^{n/2} [\widehat{\mathcal{O}}_{\sigma_1}^{\dagger} \cdots \widehat{\mathcal{O}}_{\sigma_n} (\chi_{\sigma_1} \cdots \chi_{\sigma_n}^{\dagger}) + \widehat{\mathcal{O}}_{\sigma_1} \cdots \widehat{\mathcal{O}}_{\sigma_n}^{\dagger} (\chi_{\sigma_1}^{\dagger} \cdots \chi_{\sigma_n})]$$

n odd:

$$\widehat{\mathcal{U}}^{(n)} = \frac{1}{n!} \sum_{\sigma_1, \ldots, \sigma_n} (-)^{(n-1)/2} [\widehat{\mathcal{O}}^{\dagger}_{\sigma_1} \cdots \widehat{\mathcal{O}}^{\dagger}_{\sigma_n} (\chi_{\sigma_1} \cdots \chi_{\sigma_n}) - \widehat{\mathcal{O}}_{\sigma_1} \cdots \widehat{\mathcal{O}}_{\sigma_n} (\chi^{\dagger}_{\sigma_1} \cdots \chi^{\dagger}_{\sigma_n})] .$$

Now we are in a position to evaluate the action of the operator  $\hat{\mathcal{U}}$  on the Dirac vacuum  $|0\rangle$ . It is convenient to consider terms with *n* even and *n* odd, separately. It follows with (24) and (25)

$$\widehat{\mathcal{U}}|0\rangle = \sum_{n=0}^{\infty} \widehat{\mathcal{U}}^{(n)}|0\rangle = \sum_{m=0}^{\infty} [\widehat{\mathcal{U}}^{(2m)} + \widehat{\mathcal{U}}^{(2m+1)}]|0\rangle ; \qquad (26)$$

for odd terms (n = 2m + 1)

$$\hat{\mathcal{U}}^{(2m+1)}|0\rangle = \frac{(-)^{m}}{(2m+1)!} \sum_{\sigma_{1},\dots,\sigma_{2m+1}} [\hat{O}_{\sigma_{1}}^{\dagger}\cdots\hat{O}_{\sigma_{2m+1}}^{\dagger}(\chi_{\sigma_{1}}^{\dagger}\cdots\chi_{\sigma_{2m+1}}^{\dagger}) \\ -\hat{O}_{\sigma_{1}}\cdots\hat{O}_{\sigma_{2m+1}}(\chi_{\sigma_{1}}^{\dagger}\cdots\chi_{\sigma_{2m+1}}^{\dagger})]|0\rangle ,$$

$$= \frac{(-)^{m}}{(2m+1)!} \sum_{\sigma_{1},\dots,\sigma_{2m+1}} \hat{O}_{\sigma_{1}}^{\dagger}\cdots\hat{O}_{\sigma_{2m+1}}\chi_{\sigma_{1}}\cdots\chi_{\sigma_{2m+1}})|0\rangle ,$$
(27)

since the term represented in the second line of these relations vanishes due to Eq. (23). Expression (27) can be reduced further if one employs the commutator relation (22) satisfied by the pair operators  $\hat{O}_{\sigma}^{\dagger}$  and  $\hat{O}_{\sigma}$ :

$$\hat{O}_{\sigma_{1}}^{\dagger} [\hat{O}_{\sigma_{2}} \hat{O}_{\sigma_{3}}^{\dagger}] \cdots [\hat{O}_{\sigma_{2m}} \hat{O}_{\sigma_{2m+1}}^{\dagger}] |0\rangle 
= \hat{O}_{\sigma_{1}}^{\dagger} [\hat{O}_{\sigma_{3}}^{\dagger} \hat{O}_{\sigma_{2}} + \delta_{\sigma_{2}\sigma_{3}} - \delta_{\alpha_{2}\alpha_{3}} \hat{b}_{i_{3}}^{\dagger} \hat{b}_{i_{2}} - \delta_{i_{2}i_{3}} \hat{d}_{\alpha_{3}}^{\dagger} \hat{d}_{\alpha_{2}}] 
\times \cdots [\hat{O}_{\sigma_{2m+1}}^{\dagger} \hat{O}_{\sigma_{2m}} + \delta_{\sigma_{2m}\sigma_{2m+1}} - \delta_{\alpha_{2m}\alpha_{2m+1}} \hat{b}_{i_{2m+1}}^{\dagger} \hat{b}_{i_{2m}} - \delta_{i_{2m}i_{2m+1}} \hat{d}_{\alpha_{2m+1}}^{\dagger} \hat{d}_{\alpha_{2m}}] |0\rangle 
= \hat{O}_{\sigma_{1}}^{\dagger} \delta_{\sigma_{2}\sigma_{3}} \cdots \delta_{\sigma_{2m}\sigma_{2m+1}} |0\rangle .$$
(28)

Here we used the action of the single-fermion operators on the ground state, Eq. (12), with the result that contributions from expressions contained in one of the *m* brackets are simply Kronecker symbols. This is, of course, a remarkable simplification of expression (27), since we obtain for odd terms in (26)

$$\widehat{\mathcal{U}}^{(2m+1)}|0\rangle = \frac{(-)^m}{(2m+1)!} \sum_{\sigma_1, \dots, \sigma_{2m+1}} \widehat{O}^{\dagger}_{\sigma_1} \delta_{\sigma_2 \sigma_3} \cdots \delta_{\sigma_{2m} \sigma_{2m+1}} (\chi_{\sigma_1} \cdots \chi_{\sigma_{2m+1}})|0\rangle$$

$$= \frac{(-)^m}{(2m+1)!} \left[ \sum_{\sigma} \widehat{O}^{\dagger}_{\sigma} \chi_{\sigma} |0\rangle \right] \left[ \sum_{\tau} |\chi_{\tau}|^2 \right]^m.$$
(29)

We emphasize that the summations over  $\sigma$  and  $\tau$  comprise all electron-positron states, respectively. For even contributions  $\hat{U}^{(n)}$  (n = 2m) we obtain with Eqs. (25) and (26)

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$$\begin{aligned} \widehat{\mathcal{U}}^{(2m)}|0\rangle &= \frac{(-)^{m}}{(2m)!} \sum_{\sigma_{1},\dots,\sigma_{2m}} [\widehat{\mathcal{O}}_{\sigma_{1}}^{\dagger}\cdots\widehat{\mathcal{O}}_{\sigma_{2m}}(\chi_{\sigma_{1}}\cdots\chi_{\sigma_{2m}}^{\dagger}) + \widehat{\mathcal{O}}_{\sigma_{1}}\cdots\widehat{\mathcal{O}}_{\sigma_{2m}}^{\dagger}(\chi_{\sigma_{1}}^{\dagger}\cdots\chi_{\sigma_{2m}})]|0\rangle \\ &= \frac{(-)^{m}}{(2m)!} \sum_{\sigma_{1},\dots,\sigma_{2m}} (\widehat{\mathcal{O}}_{\sigma_{1}}\widehat{\mathcal{O}}_{\sigma_{2}}^{\dagger})\cdots(\widehat{\mathcal{O}}_{\sigma_{2m-1}}\widehat{\mathcal{O}}_{\sigma_{2m}}^{\dagger})(\chi_{\sigma_{1}}^{\dagger}\cdots\chi_{\sigma_{2m}})|0\rangle \\ &= \frac{(-)^{m}}{(2m)!} \sum_{\sigma_{1},\dots,\sigma_{2m}} \delta_{\sigma_{1}\sigma_{2}}\cdots\delta_{\sigma_{2m-1}\sigma_{2m}}(\chi_{\sigma_{1}}^{\dagger}\chi_{\sigma_{2}}\cdots\chi_{\sigma_{2m-1}}^{\dagger}\chi_{\sigma_{2m}})|0\rangle \\ &= \frac{(-)^{m}}{(2m)!} \left[\sum_{\tau} |\chi_{\tau}|^{2}\right]^{m}|0\rangle , \end{aligned}$$
(30)

where we employed, as before, the relations (22), (23), and (28). By inserting results (29) and (30) into Eq. (26), the action of the time-evolution operator on the free vacuum state yields the final formula for the time-evolved ground state  $|\tilde{0}\rangle$ :

$$\begin{split} |\tilde{0}\rangle &= \sum_{m=0}^{\infty} \left[ \frac{(-)^m}{(2m)!} + \frac{(-)^m}{(2m+1)!} \sum_{\sigma} \hat{O}^{\dagger}_{\sigma} \chi_{\sigma} \right] \left[ \sum_{\tau} |\chi_{\tau}|^2 \right]^m |0\rangle \\ &= \left\{ u + v \sum_{\sigma} \hat{O}^{\dagger}_{\sigma} \chi_{\sigma} \right\} |0\rangle . \end{split}$$
(31)

In the last step we introduced the *c*-number quantities

$$u = \sum_{m=0}^{\infty} \frac{(-)^{m}}{(2m)!} \left[ \sum_{\tau} |\chi_{\tau}|^{2} \right]^{m} = \cos \sqrt{\sum_{e,p} |\chi_{ep}|^{2}} ,$$

$$v = \sum_{m=0}^{\infty} \frac{(-)^{m}}{(2m+1)!} \left[ \sum_{\tau} |\chi_{\tau}|^{2} \right]^{m} = \frac{\sin \sqrt{\sum_{e,p} |\chi_{ep}|^{2}}}{\sqrt{\sum_{e,p} |\chi_{ep}|^{2}}} .$$
(32)

Expression (31) reflects just the fact that the time-evolved vacuum state can be represented as a superposition of the free vacuum state and virtual excitations consisting of one electron and one positron.

#### **III. TRANSITION AMPLITUDES**

Returning to the problem of calculating transition amplitudes, this is now a rather simple task due to the compact structure (31) of the time-evolved ground state. First, we consider the vacuum-to-vacuum amplitude from Eq. (14), which in our approach can be expressed as

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$$A_{|0\rangle \to |0\rangle} = \left\langle 0 \left| \left[ u + v \sum_{e,p} \hat{O}_{ep}^{\dagger} \chi_{ep} \right] \right| 0 \right\rangle$$
$$= \cos \sqrt{\sum_{e,p} |\chi_{ep}|^2}, \qquad (33)$$

where the free ground state is assumed to be normalized to unity. Evidently, this result demonstrates that in our approach the vacuum state is not stable under external perturbations, in contrast to the perturbative evaluation from Eq. (15). In addition, it is clear from (33) that the probability for the ground state to remain unchanged cannot exceed unity. To be more precise, we notice that,

in a proper normalization, the quantity  $\sum_{e,p} |\chi_{ep}|^2$ represents just the total probability for the creation of a single electron-positron pair  $P^{(PT)}$  as calculated in firstorder perturbation theory with respect to the leptonprojectile interaction. Thus, the probability for the vacuum state to remain unchanged is just

$$P_{|0\rangle \to |0\rangle} = \cos^2 \sqrt{P^{(PT)}}$$
 (34)

Secondly, the amplitude  $A_{ep}$  (17) associated with the creation of a single electron-positron pair out of the vacuum is easily written with Eq. (31) and the commutation relation (22) as

$$A_{|0\rangle \rightarrow |e^{+}e^{-}\rangle} = \left\langle 0 \left| \hat{\partial}_{ep} \left[ u + v \sum_{e',p'} \hat{\partial}_{e'p'}^{\dagger} \chi_{e'p'} \right] \right| 0 \right\rangle$$
$$= v \sum_{e',p'} \delta_{ee'} \delta_{pp'} \chi_{e'p'} \langle 0 | 0 \rangle$$
$$= \chi_{ep} \frac{\sin \sqrt{\sum_{e,p} |\chi_{ep}|^2}}{\sqrt{\sum_{e,p} |\chi_{ep}|^2}} = \chi_{ep} \frac{\sin \sqrt{P^{(PT)}}}{\sqrt{P^{(PT)}}} . \tag{35}$$

By summing the expression for  $|A_{ep}|^2$  over all singlefermion states, one obtains the total probability for the creation of a single pair to be

$$P_{|0\rangle \to |e^{+}e^{-}\rangle} = \sin^2 \sqrt{\sum_{e,p} |\chi_{ep}|^2} = \sin^2 \sqrt{P^{(PT)}},$$
 (36)

which, obviously, cannot exceed unity. We would like to note that this expression is formally similar to results obtained in the treatment of ionization [30] and chargetransfer [36] processes, where the negative-energy continuum is not taken into account.

Third, the total probability for the special case of pair production with the electron bound to one of the colliding ions, i.e., the so-called process of bound-free pair creation, is obtained from (35) by summing the expression for  $|A_{ep}|^2$  over the positron states as

$$P^{\text{(bound free)}} = \sum_{p < F} |\chi_{ep}|^2 \frac{\sin^2 \sqrt{\sum_{e,p} |\chi_{ep}|^2}}{\sum_{e,p} |\chi_{ep}|^2} = \sum_{p < F} |\chi_{ep}|^2 \frac{\sin^2 \sqrt{P^{(PT)}}}{P^{(PT)}} .$$
(37)

Finally, we note that from the explicit representation of the single-fermion amplitudes, Eqs. (11) and (18),

$$\chi_{i\alpha} = -ie \int d^4x \,\overline{\varphi}_i(x) \gamma^{\mu} \varphi_{\alpha}(x) A^{(P)}_{\mu}(x) , \qquad (38)$$

which is invariant under local gauge transformations [15,18], the expressions (34), (36), and (37) for the total probability are also gauge invariant.

At this point we remark that our approach is not directly applicable to multiple electron-positron pair production, since all excitation amplitudes associated with the creation of more than one pair are just zero in the present formulation. This is, of course, the direct consequence of neglecting virtual excitation modes consisting of several electron-positron pairs. To be more precise, for multiple-pair creation one must go beyond the Tamm-Dancoff approximation by allowing for many electron-positron pairs to be simultaneously excited in intermediate states as is, for example, the case in the random-phase approximation to many-particle systems.

By assuming that the pair operators  $\hat{O}_{\sigma}$  and  $\hat{O}_{\sigma}^{\dagger}$  satisfy the commutation relation defining the quasiboson approximation employed in Ref. [9], i.e.,

$$[\hat{O}_{\sigma}, \hat{O}_{\sigma_1}^{\dagger}] = \delta_{\sigma\sigma_1}, \qquad (39)$$

the time-evolution operator  $\hat{\mathcal{U}}$  from Eq. (24) is factorized as

$$\hat{\mathcal{U}} = \exp\{\sum_{e,p} \hat{b}_e \hat{d}_p \chi_{ep}^{\dagger}\} \exp\{\sum_{e,p} \hat{b}_e^{\dagger} \hat{d}_p^{\dagger} \chi_{ep}\} \exp\{-\frac{1}{2} P^{(PT)}\} .$$
(40)

Since this formula is similar to the expression used in Eq. (8) of Ref. [9], it leads to the same expressions for creation probabilities as in Refs. [9–11]. Of course, the approximate equation (39) permits to allow for any number of pairs in intermediate states, which is reflected by the appearance of additional terms of the type  $(\prod_{i\geq 1} \hat{O}_{\sigma_i})(\prod_{j>1} \hat{O}_{\sigma_j}^{\dagger})$  in the expansion of the exponential functions from Eq. (40). However, the error introduced by neglecting interference effects between different real or virtual pairs, i.e., by disregarding the fermionic nature of the constituents, is difficult to estimate. We notice that contributions of the type  $(\prod_{i\geq 1} \hat{O}_{\sigma_i})(\prod_{j>1} \hat{O}_{\sigma_j}^{\dagger})$  describing the simultaneous excitation of several pairs can be represented with the exact commutation relation (22) as

$$\hat{O}_{\sigma_1}\hat{O}_{\sigma_2}^{\dagger}\hat{O}_{\sigma_3}^{\dagger} = \hat{O}_{\sigma_2}^{\dagger}\hat{O}_{\sigma_1}\hat{O}_{\sigma_3}^{\dagger} + [\delta_{\sigma_1\sigma_2} - \delta_{\alpha_1\alpha_2}\hat{b}_{i_2}^{\dagger}\hat{b}_{i_1} \\ - \delta_{i_1i_2}\hat{d}_{\alpha_2}^{\dagger}\hat{d}_{\alpha_1}]\hat{O}_{\sigma_3}^{\dagger}, \qquad (41)$$

where the term with i = 1 and j = 2 was considered for simplicity. The first contribution on the right-hand side of this equation represents just an excitation of the 1p-1htype, while the other terms are associated with the creation of a single pair. In particular, the last two terms with an extra minus sign describe the additional rescattering of created pairs and are neglected in an approximation of the quasiboson type. Since the total probability for the creation of any number of pairs is just unity, an overestimation of total probabilities corresponding to more than one pair leads to an underestimation of the total probability for the creation of a single pair. If one interprets the earlier result [9-11]

$$P(1 \text{ pair}) = \exp(-P^{(PT)})$$

as a lower limit of the total single-pair probability, the corresponding expression (36) obtained in this work is to be regarded as an upper limit of the probability, since our approach does not include the possibility of simultaneous creation of several electron-positron pairs.

Concerning the probability for the creation of a specific pair (e,p), i.e., the partial probability  $P_{ep}$ , we obtain from the amplitude (35)

$$P_{ep} = |\chi_{ep}|^2 \frac{\sin^2 \sqrt{P^{(PT)}}}{P^{(PT)}} , \qquad (42)$$

where  $|\chi_{ep}|^2$  represents the corresponding partial probability in first order. The factor  $\sin^2 \sqrt{P^{(PT)}}/P^{(PT)}$  takes into account all possible single-particle transitions from the negative-energy states below  $E_F = -m$  into empty levels above the Fermi level incorporating the many-particle features of the pair creation process. In particular, it includes the effect of the depopulation of the initial negative-energy state caused by transitions to all final states providing a renormalization of the lowest-order perturbative probability  $|\chi_{ep}|^2$ . We would like to note that the corresponding earlier formula [9–11] for the partial probability associated with a particular pair (e,p), i.e.,

$$P_{ep} = |\chi_{ep}|^2 \exp(-P^{(PT)})$$
,

yields a lower value of the probability as compared to our expression (42) for  $P^{(PT)} < \pi^2$ . This feature is consistent with the earlier interpretation of the single-pair probabilities derived in the present work as upper bounds of the exact probabilities.

The range of validity of the results obtained in the present investigation cannot be given rigorously. However, the presence of the factor  $\sin^2 \sqrt{P^{(PT)}}$  in the different expressions for single-pair probabilities (36), (37), and (42) indicates that for too large values of  $P^{(PT)}$  our approach gives unphysical results. To be more specific, we note that in the present investigation the single-pair probabilities are just zero in the case that  $\sin^2 \sqrt{P^{(PT)}} = 0$ , which is, of course, not realistic for  $P^{(PT)} \neq 0$ . Consequently, for  $P^{(PT)} \geq \pi^2$  the present approach definitely breaks down. In addition, due to the decrease of the total probability (36) in the region  $\pi^2/4 \le P^{(PT)} \le \pi^2$ , it is to be expected that for  $P^{(PT)} \ge \pi^2/4$  contributions associated with the simultaneous excitation of several pairs become of importance. In this case one should go beyond the 1p-1h excitations of the type included in the present investigation by incorporating excitation modes consisting of many particle-hole pairs in the formalism. In conclusion, we regard the value  $P^{(PT)} \simeq \pi^2/4$  as quantifying some limitations of the present investigation.

### **IV. SUMMARY**

We conclude the discussion by pointing out the main results we obtained and the approximations we made in this investigation. Starting with the Magnus exponential representation of the time-evolution operator in the Furry picture, we can sum up a restricted class of diagrams, namely, those associated with electron-positron loops, to infinite order in the external charge  $-eZ_P$  by making three basic assumptions: (a) We neglect correlations between the interaction strength at different times by taking into account only the total interaction associated with the first term of the Magnus expansion, (b) we neglect rescattering effects, and (c) our treatment incorporates solely virtual excitation modes of one particle and one hole of the type encountered in the Tamm-Dancoff approximation to many-particle systems. With these approximations, the time-evolved ground state of the electronpositron field around the nuclei is represented as a superposition of excitation modes consisting of one electron and one positron and the unperturbed vacuum state. We also find that in our approach the vacuum state is unstable against external perturbations, in contrast to perturbative calculations. Further, we derive expressions for electron-positron transition amplitudes and production probabilities, which are shown to be both manifestly unitary and gauge invariant.

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