

## Pair creation rates for one-dimensional fermionic and bosonic vacua

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We compare the creation rates for particle-antiparticle pairs produced by a supercritical force field for fermionic and bosonic model systems. The rates obtained from the Dirac and Klein-Gordon equations can be computed directly from the quantum-mechanical transmission coefficients describing the scattering of an incoming particle with the supercritical potential barrier. We provide a unified framework that shows that the bosonic rates can exceed the fermionic ones, as one could expect from the Pauli-exclusion principle for the fermion system. This imbalance for small but supercritical forces is associated with the occurrence of negative bosonic transmission coefficients of arbitrary size for the Klein-Gordon system, while the Dirac coefficient is positive and bound by unity. We confirm the transmission coefficients with time-dependent scattering simulations. For large forces, however, the fermionic and bosonic pair-creation rates are surprisingly close to each other. The predicted pair creation rates also match the slopes of the time-dependent particle probabilities obtained from large-scale *ab initio* numerical simulations based on quantum field theory.

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### I. INTRODUCTION

The creation of electron-positron pairs from the vacuum under a supercritical field is one of the most striking predictions of quantum electrodynamics [1]. This so-called spontaneous breakdown process of the vacuum, however, has not been observed directly. There were exciting experimental attempts in the 1980s to create these supercritical fields by colliding two highly charged relativistic ions onto each other [2,3]. While the first experimental data confirmed the predicted creation of positrons [4], it was later believed that the particles originated from the unavoidable nuclear processes [5] and not necessarily from the field induced breakdown of the vacuum. One can expect that very high laser fields (when focused) might exceed the predicted threshold for this process [6,7] in the next decade. A purely electromagnetically based observation would certainly open up new areas of study to better understand how energy can be converted into matter.

Numerous theoretical works have been devoted to obtain more accurate quantitative predictions for realistic and specific laboratory conditions while minimizing any simplifying assumptions [8–12]. Other works have focused more on examining the underlying mechanisms and on general fundamental questions concerning the pair creation processes, and also on the appropriate quantum field theoretical framework [13,14]. Our work belongs to the second category and we try to obtain a better understanding of the importance of the fermionic Pauli-exclusion principle for the pair creation process. Space-time resolved model calculation based on quantum field theory have shown that an incoming electron can suppress the pair creation process due to the Pauli blocking associated with occupied states [15,16]. To examine the relevance of the Pauli blocking for the breakdown of the vacuum we need to compare the predictions with an equivalent system that obeys a different particle statistics. To make a fair and transparent comparison, we require an analysis based on a universal approach and need a bosonic system that has the same nonrelativistic limit as the fermion system.

We chose a supercritical barrier and solve the quantum field theory based on the Dirac equation for fermions and on the Klein-Gordon equation for bosons. The quantum-mechanical aspects of each system have been discussed in the literature separately and with different frameworks, so direct comparisons are difficult. Some of these works predict quantitatively different quantum-mechanical data and interpretations [1,17–19]. Direct verification of the predictions are possible with *ab initio* quantum field theoretical calculations to clarify these issues.

The purpose of this work is fourfold. We want to provide a universal theoretical approach and apply it to a direct fermion to boson comparison for a specific force field. We point out the importance of the sign and magnitude of the transmission coefficient associated with the quantum-mechanical system and its relationship to the pair creation process. We also provide time-dependent particle probabilities from an *ab initio* quantum field theoretical simulation for the Klein-Gordon system. We show that the Pauli suppression reduces the pair creation rate for a fermionic system (relative to the bosonic system) only for a limited range of force fields. In fact, in the early transient regime more bosons can be created. Furthermore, in the limit of extremely large forces, both rates are essentially identical.

The paper is organized as follows. In Sec. II we review the framework of calculating bosonic and fermionic pair-creation rates from the vacuum expectation value of the electric current. In Sec. III we compute transmission coefficients for a specific external force. In Sec. IV the transmission coefficients are confirmed by time-dependent quantum-mechanical wave-packet calculations. In Sec. V the fermionic and bosonic pair creation rates are compared. In Sec. VI an *ab initio* quantum field theoretical numerical calculation based on the Dirac and Klein-Gordon (KG) equation is introduced to simulate the decay of the vacuum with time resolution. The resulting time-dependent probabilities for the particles grow in the steady-state regime linearly as a function of time and the corresponding slope matches the rates predicted from the quantum-mechanical transmission coefficient perfectly. In the last section we give a brief summary

and an outlook on the implications of the results for the bosonic Klein paradox. In our four appendices we discuss technical details such as the unusual boundary conditions for the Dirac and KG equations, and compare our approach with the data and conclusions obtained in previous works.

## II. BOSONIC AND FERMIONIC PAIR-CREATION RATES FROM THE CURRENT OPERATOR

The time evolution of the systems are described by the Dirac equation for the fermions and Klein-Gordon equation for the bosons,  $i\partial\phi(z,t)/\partial t = h\phi(z,t)$ . The two Hamiltonians take the form (in atomic units)

$$h_D = c\sigma_1 p_z + \sigma_3 c^2 + V(z) \quad (2.1a)$$

$$h_{KG} = p_z^2/2N + \sigma_3 c^2 + V(z) \quad (2.1b)$$

Here  $V(z)$  denotes the external electrostatic potential. For our numerical examples, we use the potential barrier studied by Sauter [20],  $V(z) = V[1 + \tanh(z/W)]/2$ , where  $W$  is the spatial extend of the corresponding force. For a better comparison, we assume that the fermion and boson masses as well as the amounts of the charges are identical,  $m=1$  a.u. and  $q=1$  a.u.

We focus our analysis on the direction of the force field ( $z$  axis) and redefine  $p_z = p$ . We can reduce the usual four-component spinor wave functions (for the Dirac case) to only two, and describe the fermionic as well as bosonic states with two-component vectors  $\phi(z,t) = \begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix}$ . This dimensional reduction is possible as the interaction with the time-independent external force field is modeled by an electric potential  $V(z)$  that is proportional to the unit operator in spinor space and the dynamics of the spin is not affected. For example, if we choose the spin to be along the  $z$  direction then only the first and third components of each of the free-energy eigenstates are nonzero. As a result, any general state for the Dirac system can be reduced to only two components. If we choose the Dirac representation for the  $\alpha$  matrices, the kinetic term  $c\alpha_z p_z + c^2\beta$  in the Dirac Hamiltonian becomes simply  $c\sigma_1 p_z + c^2\sigma_3$ , where  $\sigma_i$  are usual the  $2 \times 2$  Pauli matrices denoted by  $\sigma_1 \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ ,  $\sigma_2 \equiv \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$ ,  $\sigma_3 \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ . The nilpotent matrix  $N$  used in the Klein-Gordon equation (2.1b) is denoted by  $N \equiv \sigma_3 + i\sigma_2 \equiv \begin{bmatrix} 1 & 1 \\ -1 & -1 \end{bmatrix}$ . Had we chosen the  $x$  direction for the force, the first and forth spinor component were nonzero but the Hamiltonian would take the same form. The corresponding wave function for the Klein-Gordon system represents a spin-zero particle and therefore has only two components from the beginning. Such a simplified model has been used for fermions to study several aspects of the quantum relativistic dynamics including positive and negative-energy spectra [21–23].

While the Dirac Hamiltonian  $h_D$  is Hermitian, the Klein-Gordon Hamiltonian  $h_{KG}$  is not and thus leads to special properties concerning the inner product and conserved quantities. As the Feshbach-Villars form [19,24–28] of the Klein-Gordon equation (2.1b) is not as commonly used as its usual second-order differential equation in time, we should add a few comments here.

Due to its nonhermiticity, only the combined set of left-hand side (lhs) and right-hand side (rhs) eigenvectors of  $h_{KG}$  [29] leads to a biorthogonal basis system. However,  $h_{KG}$  has a special symmetry property. As its Hermitian conjugate form can be related to the original operator via  $h_{KG}^\dagger = \sigma_3 h_{KG} \sigma_3$ , the required lhs eigenvectors can be obtained directly from the right-hand side quantities via  $|\bar{E}\rangle \equiv (\sigma_3 |E\rangle)^\dagger$ . It follows also that the operator  $\sigma_3 h_{KG}$  is Hermitian, a property sometimes referred to as pseudohermiticity [25,26]. To accommodate for this symmetry and to stay within the manifold of rhs eigenvectors, one can equivalently introduce a generalized scalar product [27]  $\langle \phi_a | \phi_b \rangle_g \equiv \langle \phi_a | \sigma_3 \phi_b \rangle$ .

Alternatively, using this generalized scalar product, one can define the adjoint of an operator  $A$  as  $\bar{A} \equiv \sigma_3 A^\dagger \sigma_3$ , where the dagger denotes the usual transposition and complex conjugation. We note that  $h_{KG}$  is (generalized) Hermitian with regard to the generalized scalar product, i.e.,  $\langle \phi_a | h_{KG} \phi_b \rangle_g = \langle h_{KG} \phi_a | \phi_b \rangle_g$ , or  $h_{KG} = \bar{h}_{KG}$ , while the Dirac Hamiltonian is Hermitian, i.e.,  $\langle \phi_a | h_D \phi_b \rangle = \langle h_D \phi_a | \phi_b \rangle$ .

As we will see in Sec. IV below, this property has also consequences for the time-evolution operators  $\exp(-iHt)$ . While the Dirac propagator preserves the usual norm  $\langle \phi | \phi \rangle = \int dz \{ |\phi_1(z,t)|^2 + |\phi_2(z,t)|^2 \}$  of the two-component wave function, the Klein-Gordon propagator is only “generalized” unitary and preserves  $\langle \phi | \phi \rangle_g = \int dz \{ |\phi_1(z,t)|^2 - |\phi_2(z,t)|^2 \}$ .

The central quantities in quantum field theory are the two fermionic and bosonic field operators  $\hat{\Psi}_D$  and  $\hat{\Psi}_{KG}$ . The time evolution of both of these operators [30,31] can be obtained from either the Schrödinger-like equation,  $i\partial\hat{\Psi}(t)/\partial t = h\hat{\Psi}(t)$ , or the Heisenberg equation,  $i\partial\hat{\Psi}(t)/\partial t = [\hat{\Psi}, \hat{H}]$ . The corresponding quantum field theoretical Hamiltonians  $\hat{H}$  can be obtained from their quantum-mechanical limiting case via  $\hat{H}_D = \hat{\Psi}_D^\dagger h_D \hat{\Psi}_D$  and  $\hat{H}_{KG} = \hat{\Psi}_{KG}^\dagger \sigma_3 h_{KG} \hat{\Psi}_{KG}$ . Each of these operators can be expanded in terms of creation and annihilation operators. As the energy of the created particle is expected to be in the range  $c^2 < E < V - c^2$  for long times we omit other expansion terms outside this energy range,

$$\hat{\Psi}_D = \int dE \hat{f}_1(E) |F_1\rangle + \int dE \hat{f}_2^\dagger(E) |F_2\rangle, \quad (2.2a)$$

$$\hat{\Psi}_{KG} = \int dE \hat{b}_1(E) |B_1\rangle + \int dE \hat{b}_2^\dagger(E) |B_2\rangle. \quad (2.2b)$$

Here the states  $|F\rangle$  and  $|B\rangle$  can be chosen as the quantum-mechanical energy eigenstates of  $h_D$  and  $h_{KG}$ . The fermionic operators fulfill the commutator relation  $[\hat{f}_1(E), \hat{f}_1^\dagger(E')]_- = [\hat{f}_2(E), \hat{f}_2^\dagger(E')]_- = \delta(E - E')$ , while the bosonic operators anticommute,  $[\hat{b}_1(E), \hat{b}_1^\dagger(E')]_+ = [\hat{b}_2(E), \hat{b}_2^\dagger(E')]_+ = \delta(E - E')$ .

Even though the expansion of the field operators is chosen here in the dressed basis, it could have been expressed equivalently with respect to the force-free basis states and the corresponding field-free particle creation and annihilation operators (see Sec. VI). In fact, the identity of these two

expansions in this Schrödinger picture can be used to relate the dressed and undressed operators to each other via the resulting Bogoliubov Eqs [1,4,32].

For simplicity let us take a supercritical step potential ( $W \rightarrow 0$ ) as a special case,  $V(z) = V\theta(z)$ . Here  $\theta(z)$  denotes the Heaviside unit step function, defined as  $\theta(z) \equiv 0.5(|z| + z)/|z|$ . The corresponding energy eigenfunctions are doubly degenerate for each energy  $E$ . For the Dirac system the relevant subset of states can be chosen as

$$|F_1\rangle \equiv |p, -p:q\rangle_D = [W_{D+}(p) + r_D W_{D+}(-p)]\theta(-z) + t_D \mathcal{I} W_{D-}(q)\theta(z) \quad (2.3a)$$

$$|F_2\rangle \equiv |-p:-q,q\rangle_D = [t_D \mathcal{I} W_{D+}(-p)]\theta(-z) + [W_{D-}(-q) + r_D W_{D-}(q)]\theta(z) \quad (2.3b)$$

and for the Klein-Gordon system as

$$|B_1\rangle = |p, -p:q\rangle_{KG} = [W_{KG+}(p) + r_{KG} W_{KG+}(-p)]\theta(-z) + t_{KG} \mathcal{I} W_{KG-}(q)\theta(z), \quad (2.4a)$$

$$|B_2\rangle = |-p:-q,q\rangle_{KG} = [t_{KG} \mathcal{I} W_{KG+}(-p)]\theta(-z) + [W_{KG-}(-q) + r_{KG} W_{KG-}(q)]\theta(z) \quad (2.4b)$$

with the positive momenta  $p \equiv \sqrt{(E^2 - c^4)}/c$  and  $q \equiv \sqrt{[(E - V)^2 - c^4]}/c$ . The specific form of the two-component spinor states  $W(p, z)$  and their interpretation can be found in Appendixes A–D. There we will also derive the specific form of the coefficients  $r$ ,  $t$ , and  $\mathcal{I}$  and  $\mathcal{I}$  in terms of the energy of the incoming waves. Here it is only important to note that the scattering state  $|p, -p:q\rangle$  corresponds to an incoming particle from the left with momentum  $p$ , while the corresponding orthogonal scattering state with the same energy,  $|-p:-q,q\rangle$ , describes an incoming particle with momentum  $-q$  entering the force region (around  $z=0$ ) from the right side.

We will show how these quantum-mechanical states can contribute to finding the pair creation rates. If we assume that the supercritical barrier has been turned on slowly in time, then the initial force-free vacuum evolves adiabatically into the corresponding “dressed” state for the system with the potential. We denote this dressed state by  $|\text{vac}\rangle$ . To be consistent, this vacuum state has a vanishing excitation of the corresponding “dressed” energy eigenmodes,  $|F\rangle$  and  $|B\rangle$ . In operator language, this corresponds to  $\hat{f}_1(E)|\text{vac}\rangle = \hat{f}_2(E)|\text{vac}\rangle = 0$  as well as  $\hat{b}_1(E)|\text{vac}\rangle = \hat{b}_2(E)|\text{vac}\rangle = 0$ . The second condition can be expressed equivalently as  $\hat{b}_2(E)\hat{b}_2^\dagger(E')|\text{vac}\rangle = \delta(E - E')|\text{vac}\rangle$  and  $\hat{f}_2(E)\hat{f}_2^\dagger(E')|\text{vac}\rangle = \delta(E - E')|\text{vac}\rangle$ .

It is important, that in Eq. (2.2) we have assigned the creation (and not annihilation) operator  $\hat{f}_2^\dagger(E)$  and  $\hat{b}_2^\dagger(E)$ , to the states  $|F_2\rangle$  and  $|B_2\rangle$ . For the case of the fermions, this choice is arbitrary [33], however, for the expansion of the bosonic operator the above choice is essential. Had we assigned the annihilation operators  $\hat{f}_2(E)$  and  $\hat{b}_2(E)$ , respectively, to the states  $|F_2\rangle$  and  $|B_2\rangle$  in the fields  $\hat{\Psi}$ , the first

identity above, as  $\hat{f}_2^\dagger(E)\hat{f}_2(E')|\text{vac}\rangle = \delta(E - E')|\text{vac}\rangle$  would still hold for fermions, while the required equality for the bosons  $\hat{b}_2^\dagger(E)\hat{b}_2(E')|\text{vac}\rangle = \delta(E - E')|\text{vac}\rangle$  cannot be derived, as  $\hat{b}_2(E)|\text{vac}\rangle$  and  $\hat{b}_2^\dagger(E')|\text{vac}\rangle$  can be both non-zero. We thus find that the correct approach of Ref. [34] for fermions cannot be easily generalized for bosons. We will confirm these important choices with *ab initio* simulations below in Sec. V.

While viewed from a dressed particle picture, the state  $|\text{vac}\rangle$  is “empty,” from a force-free environment, however, the dressed vacuum is characterized by a constant flow of fermions or bosons to the left, and a flow of their corresponding antiparticles to the right (under the barrier). To evaluate this amount (pair creation rate), we have to calculate the quantum field theoretical expectation value of the current operator [35] in the fermionic or bosonic state  $|\text{vac}\rangle$ .

$$j = \langle\langle \text{vac} | \hat{j} | \text{vac} \rangle\rangle. \quad (2.5)$$

In order to have a consistent comparison between the fermions and bosons, we define  $j$  to represent the electrical current and associate the energy states of positive energy with positive charges for the Dirac as well as for the Klein-Gordon system. Correspondingly, for a given wave function  $\phi$  the quantum-mechanical charge density has to be defined as  $\rho_D \equiv \phi_D^\dagger \phi_D$  and  $\rho_{KG} \equiv \phi_{KG}^\dagger \sigma_3 \phi_{KG}$ . In order to fulfill the continuity equation ( $\partial\rho/\partial t + \partial j/\partial z = 0$ ) and the conservation law ( $\int dz \rho(z, t) = \text{const.}$ ) for both Hamiltonians, the two quantum-mechanical electric currents have to take the form  $j_D = c \phi_D^\dagger \sigma_1 \phi_D$  and  $j_{KG} = [\phi_{KG}^\dagger \sigma_3 N p \phi_{KG} - (p \phi_{KG}^\dagger) \sigma_3 N \phi_{KG}]/2$ . The corresponding quantum field operator versions of the currents are obtained by replacing the states  $\phi$  with the field operators  $\hat{\Psi}$  from Eq. (2.2). In order to predict consistently a total charge of zero for their respective vacuum states, the expressions also need to be antisymmetrized and symmetrized [36,37],

$$\hat{j}_D = c [\hat{\Psi}_D^\dagger \sigma_1 \hat{\Psi}_D - \hat{\Psi}_D \sigma_1 \hat{\Psi}_D^\dagger]/2 \quad (2.6a)$$

$$\hat{j}_{KG} = [\hat{\Psi}_{KG}^\dagger \sigma_3 N p \hat{\Psi}_{KG} - (p \hat{\Psi}_{KG}^\dagger) \sigma_3 N \hat{\Psi}_{KG} + \hat{\Psi}_{KG} \sigma_3 N p \hat{\Psi}_{KG}^\dagger - (p \hat{\Psi}_{KG}) \sigma_3 N \hat{\Psi}_{KG}^\dagger]/4. \quad (2.6b)$$

We can insert the field operators from Eq. (2.2) into Eq. (2.6) and insert the current operators into Eq. (2.5) to obtain the pair creation rates

$$j_D = c \int dE \langle\langle F_2 | \sigma_1 F_2 \rangle\rangle - \langle\langle F_1 | \sigma_1 F_1 \rangle\rangle, \quad (2.7a)$$

$$j_{KG} = \int dE \{ \langle\langle \bar{B}_2 | N p B_2 \rangle\rangle - \langle\langle p \bar{B}_2 | N B_2 \rangle\rangle + \langle\langle \bar{B}_1 | N p B_1 \rangle\rangle - \langle\langle p \bar{B}_1 | N B_1 \rangle\rangle \}/4. \quad (2.7b)$$

If we insert the special solutions for  $|F\rangle$  and  $|B\rangle$  of Eqs. (2.3) and (2.4) and their adjoints into these expressions, we obtain the final results

$$j_D = - \int_{c^2}^{V-c^2} dE T_D(E)/(2\pi), \quad (2.8a)$$

$$j_{KG} = \int_{c^2}^{V-c^2} dE T_{KG}(E)/(2\pi). \quad (2.8b)$$

Here we used the abbreviations  $T_D(E) = |t_D|^2 \mathcal{J}$  and  $T_{KG}(E) = -|t_{KG}|^2 \mathcal{J}$ . Even though the operator algebra for both systems is entirely different, we obtain (except the minus sign) in both cases the functionally identical dependence of the pair creation current on the transmission coefficient associated with the corresponding quantum-mechanical scattering system. Even though the current could depend on the position  $z$ , it is constant and therefore consistent with our steady-state assumption. We also note that Eq. (2.8) holds independently of the choice of charge of the incoming particle used to compute  $T(E)$ . In fact, the direction (sign) of the created current is determined uniquely by the sign of the potential  $V(z)$ . In our case  $V(z)$  was chosen repulsive with regard to an (hypothetically) incoming (from  $z = -\infty$ ) positive charge. In this case the supercritical potential would create positive charges that are ejected into the negative  $z$  direction and negative charges into the  $+z$  direction. In this situation the created current is negative for all values of  $z$ . We will see below that this sign is fully consistent with our expression of Eqs. (2.8), as  $T_D(E)$  is always positive, while  $T_{KG}(E)$  is always negative.

Had we computed the vacuum expectation value of the momentum (instead of the electric current) we would have obtained a negative value for  $z < 0$  and a positive value for  $0 < z$ . This shows that indeed positive (ejected to the left) and negative charges (ejected to the right) are created at the barrier.

To avoid any misconception from the very beginning for  $T_D(E)$  and  $T_{KG}(E)$ , it is crucial to point out that because of the supercriticality of the potential, neither of these mathematical functions describes a physical-scattering situation. If a real particle were injected into a supercritical force region, it would get reflected with 100% probability [15,16]. However, this incoming particle would modify the supercriticality induced pair creation process at the barrier that occurs due to the supercriticality. To describe this more complicated process accurately requires a quantum field theory, which is also related to the so-called Klein paradox [15,16,18,38,39].

### III. TRANSMISSION COEFFICIENTS FOR A SPECIFIC EXTERNAL FORCE

Even though the functional relationship between the pair creation probability and the quantum-mechanical transmission coefficient  $T$  is surprisingly identical for the bosons and fermions, the actual rates can be substantially different. To have a consistent framework it is essential to have a universal definition for  $T$ . Based on the continuity equation above, both the Dirac and the Klein-Gordon system have the property that at the potential step the (vectorial) sum of the incoming current density  $j_{inc}$  (which is positive in our case as we assume the incoming particle has a positive charge)

and the reflected current  $j_{refl}$  should be identical to the transmitted current density, i.e.,  $j_{inc} + j_{refl} = j_{trans}$ . To be general, a transmission coefficient should be defined by the ratio of the transmitted current density to the incoming density,  $T \equiv j_{trans}/j_{inc}$  and the reflection coefficient as  $R \equiv -j_{refl}/j_{inc}$ . We have introduced the minus sign to guarantee a positive coefficient  $R$ , as the reflected current always points in the opposite direction of the incoming current. As a result we *always* have  $R + T = 1$ , independent of the direction or charge of the incoming particle and independent of whether the system is fermionic or bosonic, or whether the potential is sub- or supercritical. This conclusion is different from previous findings, for a discussion see [1,17–19] and Appendix D.

To be quantitative, we analyze the special case of the Sauter potential [20]  $V(z) = V[1 + \tanh(z/W)]/2$ , for which the transmission coefficients can be obtained analytically in the subcritical ( $V < E - c^2$ ) and supercritical ( $E + c^2 < V$ ) scattering regime. In Appendixes B and C we derive explicitly the functional form of these coefficients for the special case  $W = 0$  and show the unique boundary conditions for the fermion and bosonic Hamiltonians. The functional dependence on the energy of the transmission coefficients depends on the regime.

For completeness, we begin here with the over-the-barrier regime for which the incoming energy  $E$  is larger than the potential height  $V$ ,

$$T_D = - \frac{\sinh[\pi p W] \sinh[\pi q W]}{\sinh[\pi(V/c + p)W/2] \sinh[\pi(V/c - p - q)W/2]}, \quad (3.1a)$$

$$T_{KG} = \frac{\cosh[\pi(p + q)W] - \cosh[\pi(p - q)W]}{\cosh[\pi[(WV/c)^2 - 1]^{1/2}] + \cosh[\pi(p + q)W]}. \quad (3.1b)$$

Here  $p$  is again the momentum of the incoming particle,  $p \equiv \sqrt{(E^2 - c^4)}/c$  and  $q$  is the smaller momentum the particle takes over the barrier  $q \equiv \sqrt{[(E - V)^2 - c^4]}/c$ . In the nonrelativistic limit ( $E \rightarrow c^2$ ) and ( $V \rightarrow 0$ ) both equations predict the identical transmission strength, so any difference between both expressions is a purely relativistic effect. For  $W \rightarrow 0$ , both expressions simplify significantly to

$$T_D = 1 - \frac{[(p - q)(E + c^2) - pV]^2}{[(p + q)(E + c^2) - pV]^2} \quad (3.2a)$$

$$T_{KG} = 4pq/(p + q)^2. \quad (3.2b)$$

In the next regime  $E - c^2 < V < E + c^2$  the incoming energy is less than the barrier, but the potential is not yet strong enough. As a result we have, except a finite tunneling (exponential damping), no transmission under the barrier,  $T_D = T_{KG} = 0$ . In this context we also point out that the literature [22,34] uses sometimes the term ‘‘Klein tunneling’’ for the supercritical case of nonzero transmission under the barrier. This term is a little bit misleading as quantum-mechanical tunneling by its very nature always involves exponential attenuation.

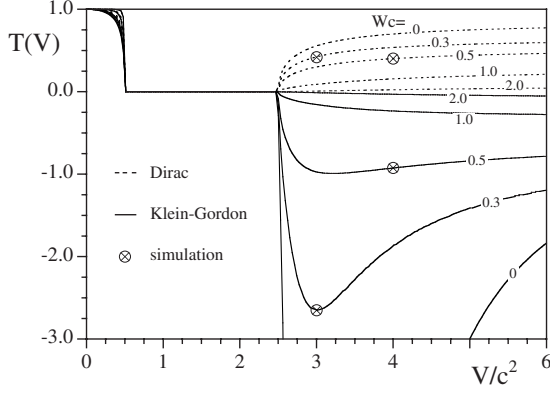


FIG. 1. The transmission coefficient  $T_D$  and  $T_{KG}$  for the Dirac and Klein-Gordon equation as a function of the potential strength  $V$  for a fixed energy  $E(=1.5 c^2)$ . The four circles are obtained from the area of the transmitted wave-function solution obtained from a time-dependent scattering simulation.

For the decay of the vacuum and the pair creation rates of Eq. (2.8), the supercritical limit is most important; here, the potential height  $V$  is extremely high,  $E+c^2 < V$ . The corresponding transmission coefficients are given by

$$T_D = - \frac{\sinh[\pi p W] \sinh[\pi q W]}{\sinh[\pi(V/c + p - q)W/2] \sinh[\pi(V/c - p + q)W/2]} \quad (3.3a)$$

$$T_{KG} = \frac{\cosh[\pi(p - q)W] - \cosh[\pi(p + q)W]}{\cosh\{\pi[(WV/c)^2 - 1]^{1/2}\} + \cosh[\pi(p - q)W]}. \quad (3.3b)$$

For  $W \rightarrow 0$ , both expressions simplify to

$$T_D = 1 - \frac{[(p + q)(E + c^2) - pV]^2}{[(p - q)(E + c^2) - pV]^2}, \quad (3.4a)$$

$$T_{KG} = -4pq/(p - q)^2. \quad (3.4b)$$

The interesting negative sign of the KG transmission coefficient is related to a sign change of the local Klein-Gordon charge density  $\phi_{KG}(z, t)^\dagger \sigma_3 \phi_{KG}(z, t)$  under the barrier. In contrast, the sign of the charge density  $\phi_D(z, t)^\dagger \phi_D(z, t)$  remains positive. We return to this important sign change in more detail and confirm it in Sec. IV. We note that also in the supercritical regime, we still have a positive momentum,  $q \equiv \sqrt{[(E - V)^2 - c^4]}/c$ .

In Fig. 1 we show  $T_D$  (dashed lines) and  $T_{KG}$  as a function of the height of the potential  $V$  for five widths  $W$  of the potential for an energy  $E = 1.5 c^2$ . For comparison, in the over-the-barrier transmission regime ( $V < E - c^2$ ) the classical transmission coefficient is always 1. In fact, a transmission that is less than unity is only caused by the steepness of the barrier and is therefore a purely quantum-mechanical effect. For the slowest ramp-up potential (with  $W = 2/c$ ) the Dirac and Klein-Gordon coefficients predict nearly the same transmission, while in the limit of  $W = 0$ , the transmission  $T_{KG}$  is less than  $T_D$  showing that the Klein-Gordon system is more sensitive to this quantum-mechanical effect.

There are several striking differences between both coefficients in the important supercritical regime ( $E + c^2 < V$ ). While the transmission coefficient  $T_D$  for the fermionic system remains positive and less than 1,  $T_{KG}$  is negative and can approach even minus infinity in the limit of the step potential. This singularity is located at the potential height  $V = 2E$ . However, this singularity occurs only for the special case  $W = 0$  and the minimum for  $T_{KG}$  shifts to higher values of  $V$  for increasing  $W$ .

It is important to note that a negative coefficient does not mean that any transmitted particles evolve to the left under the barrier. It simply reflects the sign change of the bosonic charge density under the barrier as we will show in Sec. IV. At the same time, the corresponding reflection coefficient  $R(=1 - T)$  can exceed 1. A reflection coefficient larger than unity suggests that the reflected current is larger than the incoming current. This bosonic phenomenon is reminiscent of super-radiance [35]. However, one has to be very careful with such an interpretation and the association of this mathematical observation with a (real) physical effect. It is important to keep in mind that we discuss only mathematical properties here using a (purely) quantum-mechanical description beyond its real range of validity. As in a supercritical system the number of particles changes, a physically correct description requires quantum field theory.

We also note that while the Dirac transmission depends only weakly on  $W$ , the Klein-Gordon transmission is quite sensitive. Also the superstrong field limit ( $V \rightarrow \infty$ ) is entirely different for bosons and fermions. For example, for  $W = 0$ ,  $T_D$  approaches the nonzero value  $2\sqrt{(E^2 - c^4)}/[E + \sqrt{(E^2 - c^4)}]$ , while  $T_{KG}$  predicts a vanishing transmission  $T_{KG} = 0$ . For  $W \neq 0$  and large energies, however,  $T_D$  approaches 1 and  $T_{KG}$  approaches  $-1$ . The graphs for  $T_{KG}(V)$  for different widths  $W$  can even cross as a function of  $V$ , while those for  $T_D(V)$  do not.

#### IV. TIME-DEPENDENT QUANTUM-MECHANICAL WAVE-PACKET CALCULATIONS

As the choice of the momentum  $q$  under the barrier is presented differently in some of the literature (see Appendix D), we have to confirm our choice with a time-dependent calculation. Time-dependent calculations are unambiguous yardsticks as they predict the evolution independent of any prior choices of boundary or continuity conditions or signs for the momentum of the final state. We have prepared an initial wave packet  $\phi(z, t=0) = \int dE C(E) W_+(p, z)$  as a superposition of free-energy eigenstates  $W_+(p, z)$  with a Gaussian amplitude that is centered around energy  $E = 1.5 c^2$ . We display in the Appendix A the special form of these two-component free-energy eigenstates  $W_+(p, z)$ . The complex amplitudes  $\{C(E) \sim \exp[-(p - p_0)^2] \exp[-ipz_0]\} dp/dE$  were chosen such that the wave packet is initially localized at  $z = z_0 (= -4 \text{ a.u.})$ , to the left of the potential barrier and has an initial spatial width of 1 a.u. The initial densities  $\rho_D(z) = \phi(z, t=0)^\dagger \phi(z, t=0)$  and  $\rho_{KG}(z) = \phi(z, t=0)^\dagger \sigma_3 \phi(z, t=0)$  are identical and shown by the dashed lines in Fig. 2 (note the different vertical scales).

In order to evolve these two-component initial states in time, we use the split-operator technique [40–43] in which

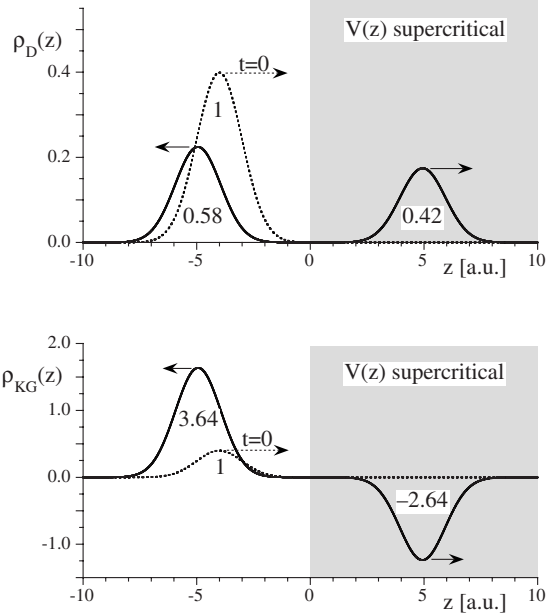


FIG. 2. The final charge density for the Dirac equation (top) and for the Klein-Gordon equation (bottom) for the quantum-mechanical scattering off a supercritical potential  $V(z)$ . The incoming density is identical in both cases and indicated by the dashed lines (note the different vertical scales). The incoming energy  $E = 1.5 c^2$  corresponds to a central momentum of  $p = \sqrt{5/4}c$  and an incoming velocity of  $0.745 c$ . The numbers under the densities are the corresponding areas. [ $V(z) = V[1 + \tanh(z/W)]/2$  with strength  $V = 3c^2$  and width  $W = 0.3/c$ , the final time is  $0.1$  a.u., the spatial axis was discretized into  $32\,768$  points and we used  $40\,000$  temporal steps.]

the time-evolution operator  $\exp[-iht]$  is decomposed into the consecutive actions of the operators  $\exp[-ih\Delta t]$ . Each of these  $N_t$  subinterval operators can be approximated [with a local error  $O(\Delta t^3)$ ] by  $\exp[-iht] \approx \exp[-iV\Delta t/2] \exp[-ih_0\Delta t] \exp[-iV\Delta t/2]$ , where  $h_0$  denotes the free kinetic Hamiltonian and  $\exp[-iV\Delta t/2]$  is the action due to the potential only. While the action of  $\exp[-iV\Delta t/2]$  can be performed conveniently in discretized coordinate space with  $N_z$  grid points, the action of the kinetic term can be calculated in momentum space for the Fourier-transformed state.

The kinetic operator  $\exp[-ih_0\Delta t]$  can be brought into its diagonal form and the diagonal matrix can be exponentiated. For the Dirac system, the kinetic  $2 \times 2$  matrix operator  $U_D = \exp[-ih_D\Delta t] = \exp[-i(c\sigma_1 p + \sigma_3 c^2)\Delta t]$  takes the following form with the four matrix elements:

$$(U_D)_{1,1} = \cos(E\Delta t) - ic^2 \sin(E\Delta t)/E, \quad (4.1a)$$

$$(U_D)_{1,2} = -icp \sin(E\Delta t)/E, \quad (4.1b)$$

$$(U_D)_{2,1} = (U_D)_{1,2}, \quad (4.1c)$$

$$(U_D)_{2,2} = \cos(E\Delta t) + ic^2 \sin(E\Delta t)/E, \quad (4.1d)$$

where  $E = \sqrt{c^4 + c^2 p^2}$  denotes the energy. For the Klein-Gordon system, the kinetic  $2 \times 2$  matrix operator  $U_{KG}$

$= \exp[-ih_{KG}\Delta t] = \exp[-i(p^2/2N + \sigma_3 c^2)\Delta t]$  has the matrix elements

$$(U_{KG})_{1,1} = \cos(E\Delta t) - i(p^2/2 + c^2)\sin(E\Delta t)/E, \quad (4.2a)$$

$$(U_{KG})_{1,2} = -i(p^2/2)\sin(E\Delta t)/E, \quad (4.2b)$$

$$(U_{KG})_{2,1} = i(p^2/2)\sin(E\Delta t)/E, \quad (4.2c)$$

$$(U_{KG})_{2,2} = \cos(E\Delta t) + i(p^2/2 + c^2)\sin(E\Delta t)/E. \quad (4.2d)$$

As a consequence of the different symmetry properties of the Hamiltonians, the operator  $U_D$  is unitary and conserves the “norm”  $\langle \phi | \phi \rangle$  of the states, while the operator  $U_{KG}$  is unitary only with respect to the generalized scalar product  $\langle \phi | \phi \rangle_g$  and therefore fulfills only  $U^{-1} = \bar{U} = \sigma_3 U^\dagger \sigma_3$ .

The final charge distribution at time  $t = 0.1$  a.u. is shown by the continuous line. As expected, the total area in both cases is conserved and equal to 1, corresponding to the conserved total charge. While the Dirac case the positive density remains positive, the Klein-Gordon case predicts a negative transmitted charge density. More quantitatively, for a simulation with  $N_z = 32\,768$  (corresponding to a grid spacing of  $\Delta z = 9.15 \times 10^{-4}$  a.u.  $\approx 0.12/c$ ) and  $N_t = 40\,000$  (corresponding to a temporal step size  $\Delta t = 2.5 \times 10^{-6}$  a.u.  $\approx 0.047/c^2$ ) we find areas of  $0.575\,59$  and  $0.424\,41$  under the reflected and transmitted Dirac density, whereas the Klein-Gordon case predicts an area of  $3.6449$  for the reflected and  $-2.6449$  for the transmitted charge density. The predicted transmission coefficients for the monochromatic incoming particles (with energy  $E = 1.5 c^2$ ,  $V = 3c^2$ , and  $W = 0.3/c$ ) from Eq. (3.3) amount to  $T_D = 0.424\,35$  and  $T_{KG} = -2.6452$ , respectively. Thus the areas under the transmitted densities differ by less than  $0.02\%$  from the predicted values confirming our sign choice for the momentum  $q$  and also the validity the assumptions leading to Eq. (3.3). A similarly excellent agreement was also obtained for other parameters and is indicated by the circles in Fig. 1.

The small remaining discrepancies between the areas and  $T(E)$  are due to the fact that an initially spatially localized wave packet is not fully monoenergetic and contains also other energy eigenstates. If the transmission coefficient  $T(E)$  is averaged over the corresponding energy range of the quantum state with the appropriate weighting factors, an even better agreement can be obtained.

We also observe that the numerical rate of convergence with respect to the number of temporal and spatial grid points is less for the KG system than for the more robust Dirac system. This is consistent with our discussion in the previous section, where the KG system was found to be more sensitive to quantum effects.

## V. COMPARISON OF THE PAIR CREATION RATES

By using the expressions for transmission coefficients in the supercritical regime of Eq. (3.3), we can now analyze the fermionic and bosonic pair creation rates for identical parameters. In Fig. 3 we show  $j_D$  and  $j_{KG}$  as a function of the potential strength  $V$  for  $W = 0.3/c$ . We see that for any

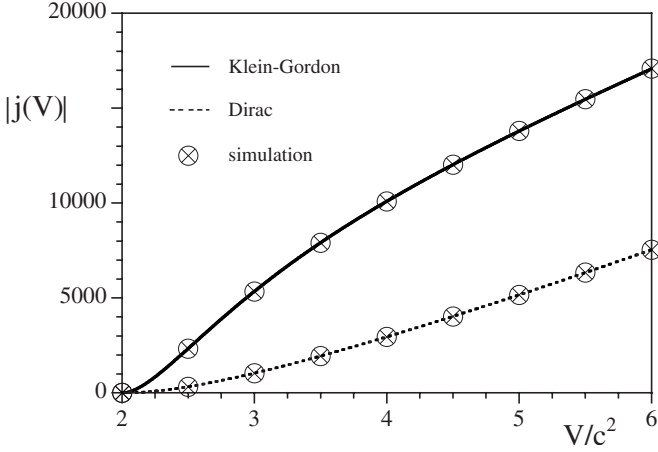


FIG. 3. The pair creation rates for a supercritical force field for the fermionic (dashed line) and bosonic (continuous line) systems as predicted by Eq. (2.8). The width of the potential was  $W=0.3/c$ . The circles are the corresponding rates obtained from the long-time behavior of the large-scale time-dependent *ab initio* simulations (see Sec. VI and Fig. 5).

strength of the potential  $V$ , the rate of boson-antiboson pair creation exceeds the Dirac rate. This imbalance is expected as the simultaneous generation of identical fermions should be suppressed due to the Pauli blocking (exclusion principle) whereas each boson mode can be occupied with an arbitrarily high number.

Even though limit of extremely large forces ( $V \rightarrow \infty$ ) is presently beyond experimental range, it is nevertheless interesting to point out a universal behavior. It turns out, that both rates scale linearly with  $V$ ,  $j(W, V) = \alpha(W)V$ . As in this limit both transmission coefficients approach  $\pm 1$  (for large energy  $E$  and independent of the width  $W$ ) the energy integrals for  $j$  become trivial and the constant  $\alpha(W)$  becomes identical for  $j_D$  and  $j_{KG}$ , i.e.,  $j(W, V) = -1/(2\pi)V$ . In other words, in the extreme force limit, the different fermion and bosonic commutator relationships (including the Pauli suppression) seem to become irrelevant. We are not able to give any intuitive explanation for this surprisingly universal and particle-type independent scaling behavior. However, if we perform the limit ( $W \rightarrow 0$ ) first, then the transmission  $T_{KG}$  becomes singular at  $E=V/2$  (see Fig. 1) and the energy integral diverges ( $j_{KG} = -\infty$ ), while  $T_D$  remains 1.

In Fig. 4 we also show the different kinetic-energy spectra of the created particles. This quantity is directly proportional to the energy dependence of the transmission coefficient  $|T(E)|$  for a given potential  $V (> 2c^2)$ . Both spectra reach their maximum at  $E=V/2$ . However, the energy distribution for the created fermions is much more flat than the one for the bosons, suggesting a relative suppression of bosons with very small and very large energies relative to those with  $E=V/2$ , or a bosonic enhancement.

## VI. RATES FROM TIME-DEPENDENT QUANTUM FIELD THEORETICAL SOLUTIONS

The derivation of the expressions of the rates [Eq. (2.8)] was based on several simplifying assumptions, such as a

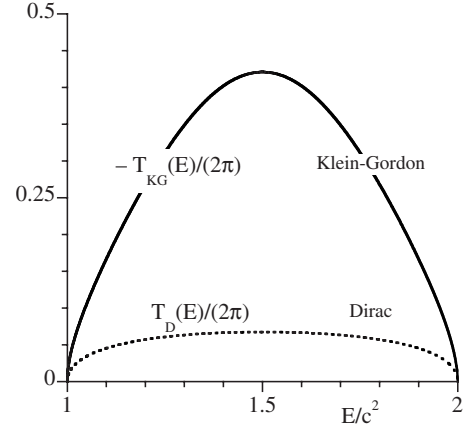


FIG. 4. The energy spectrum of the ejected particles in the long-time limit for the supercritical decay. The potential strength is  $V = 3c^2$  and the width is  $W=0.3/c$ .

vanishing width of the force field, asymptotically large times and that particles are only created in the energy range  $c^2 < E < V - c^2$ . To establish the validity of these assumptions, a full time-dependent quantum field theoretical simulation of the evolution of an initial (force-free) vacuum state must be performed. Numerical details of the procedure for the Dirac case can be found in the literature [14, 15, 43, 44]. With some modifications, this approach can be also applied to obtain the time evolution of the bosonic field operator. Differences are based on the different commutator relationships and the fact the underlying Hamiltonian for the KG system is Hermitian only for the generalized scalar product.

The field operator for both systems may be expanded in terms of positive and negative eigenstates of the force-free Hamiltonians  $|p\rangle$  and  $|n\rangle$ , respectively,

$$\hat{\Psi}(t) = \int_{c^2}^{\infty} dE_p \hat{b}_p(t) |E_p\rangle + \int_{-\infty}^{-c^2} dE_n \hat{d}_n^\dagger(t) |E_n\rangle. \quad (6.1)$$

These states are normalized for Dirac Hamiltonian according to  $\langle E_p | E_{p'} \rangle = \delta(E_p - E_{p'})$  and  $\langle E_n | E_{n'} \rangle = \delta(E_n - E_{n'})$ , and for Klein-Gordon Hamiltonian according to  $\langle E_p | \sigma_3 E_{p'} \rangle = \delta(E_p - E_{p'})$  and  $\langle E_n | \sigma_3 E_{n'} \rangle = -\delta(E_n - E_{n'})$ . As we noted, the field operator satisfies both the Heisenberg and Schrödinger equations  $i\partial/\partial t \hat{\Psi} = [\hat{\Psi}, H]$  and  $i\partial/\partial t \hat{\Psi} = h\hat{\Psi}$ , with  $H_D = \hat{\Psi}^\dagger h_D \hat{\Psi}$  and  $H_{KG} = \hat{\Psi}^\dagger \sigma_3 h_{KG} \hat{\Psi}$ . Thus it may also be expanded in terms of

$$\hat{\Psi}(t) = \int_{c^2}^{\infty} dE_p \hat{b}_p U(t) |E_p\rangle + \int_{-\infty}^{-c^2} dE_n \hat{d}_n^\dagger U(t) |E_n\rangle. \quad (6.2)$$

The solution to the time-dependent particle annihilation operator can be obtained as

$$\hat{b}_p(t) = \int_{c^2}^{\infty} dE_{p'} \hat{b}_{p'} U_{p,p'}(t) + \int_{-\infty}^{-c^2} dE_n \hat{d}_n^\dagger U_{p,n}(t) \quad (6.3)$$

Here we denote for Dirac system,  $U_{p,p'}(t) = \langle E_p | U_D(t) | E_{p'} \rangle$  and  $U_{p,n}(t) = \langle E_p | U_D(t) | E_n \rangle$  and for Klein-Gordon system,  $U_{p,p'}(t) = \langle E_p | \sigma_3 U_{KG}(t) | E_{p'} \rangle$  and  $U_{p,n}(t) = \langle E_p | \sigma_3 U_{KG}(t) | E_n \rangle$ . The part of the field operator associated with positive energy

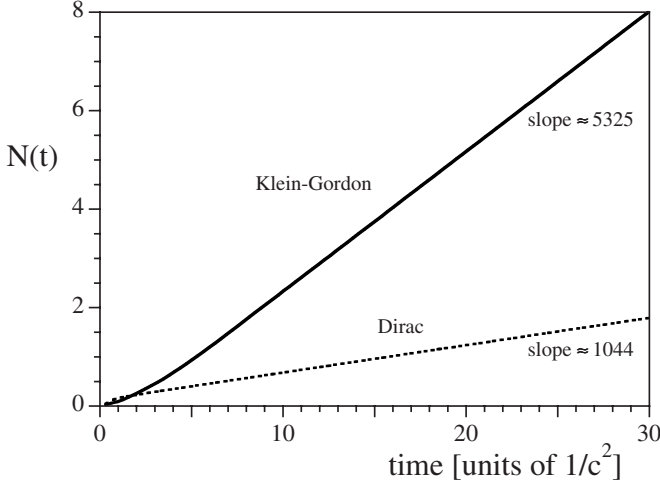


FIG. 5. The time dependence of the total number of created pairs during the supercritical decay. The slopes in the long-time regime are the circles shown in Fig. 3. The potential strength is  $V = 3c^2$  and the width is  $W = 0.3/c$ . [ $N_z = 512$  spatial grid points]

states is  $\hat{\Phi} = \int_{-\infty}^{\infty} dE_p \hat{b}_p(t) |E_p\rangle$  and the total number of particle pairs can be calculated as  $N_D(t) = \langle\langle \text{vac} | \hat{\Phi}^\dagger(t) \hat{\Phi}(t) | \text{vac} \rangle\rangle$  and  $N_{\text{KG}}(t) = \langle\langle \text{vac} | \hat{\Phi}^\dagger(t) \sigma_3 \hat{\Phi}(t) | \text{vac} \rangle\rangle$ . If we calculate the time evolution of these quantities, we obtain

$$N(t) = \int dE_p \int dE_n U_{p,n}(t) U_{p,n}(t)^*. \quad (6.4)$$

Computationally, the matrix elements  $U_{p,n}$  may be obtained by evolving  $|E_n\rangle$  in time to get  $U(t)|E_n\rangle$ . This state is then projected onto the state  $|E_p\rangle$  to determine  $U_{p,n}$ . This computation requires large amount of CPU time since the time evolution has to be accomplished numerically based on the split-operator method discussed in Sec. IV. Since  $N(t)$  requires the summation over all states  $|E_n\rangle$ , the simulations require  $N_t N_z \log(N_z)$  computer operations. In practice, we use  $N_z = 512$ ,  $N_t = 10\,000$  and a typical quantum field simulation takes about 10 hours on a Macintosh with Intel processors. We will refer the reader to numerical details of these large-scale simulations to a future work and just state here the main results. In Fig. 5 we show the time evolution of the expectation value of the total number of particles  $N(t)$ . In a time-dependent simulation, the supercritical force field  $V(z)$  must be turned on first. For simplicity, we have chosen a sudden turn on.

We see that after an initial transient period of a duration proportional to  $2/c^2$  ( $10^{-4}$  a.u.), the number of generated particle pairs increases linearly with time. The slope in this steady-state regime should be compared to the rates as predicted in Fig. 3. For example, for the simulation data in Fig. 3, the numerical values of the slopes can be read of as  $\approx 1044$  and  $\approx 5325$ . This compares very well with the corresponding rates 1040.64 and 5349.23 from Fig. 3 for  $V = 3c^2$ . We have repeated the simulation for nine different strengths of the potential  $V$  (from  $V = 2c^2$  to  $6c^2$ ) and included the numerically determined slopes as circles in Fig. 3. The agreement is obvious and gives clear credence to the analyti-

cal derivations of Sec. II and III above. We also note that during the transient part the number of created bosons  $N(t)$  can be less than those for the fermions. We presently do not have an intuitive explanation for this observation.

## VII. SUMMARY AND SHORT DISCUSSION

The purpose of this work has been, first, to provide a consistent and universal approach to study the supercritical decay of the bosonic and fermionic vacua. Second, using this framework we compared the pair creation rates for a bosonic and fermionic system under identical conditions for a specific supercritical force. We found that the bosonic pair creation rate exceeds the fermionic one for intermediate force strengths. For very large  $V$ , however, the rates are identical suggesting that the pair creation process is rather independent of other pairs and independent of the particle statistics. Third, our views are in contrast with some of the literature about the signs and magnitudes of the quantum-mechanical transmission coefficients in the supercritical force region. Some of these are not just a matter of interpretation, but could lead to quantitative different predictions concerning the Klein paradox. Fourth, we provided a simulation of the time-dependent particle probabilities  $N(t)$  from an *ab initio* quantum field theoretical simulation for the Klein-Gordon system. The obtained data show the transition from a transient regime (whose characteristics depend on the way the force is temporally turned on) to the universal steady-state regime in which the probability grows linearly with time. In this regime the numerically obtained slopes  $dN(t)/dt$  confirm quite accurately the predictions of approximate but analytical predictions for the pair creation rates.

An important future question is the impact on this finding for the bosonic Klein paradox that has been recently resolved for the fermionic system [15,16]. For the Klein-paradox situation the pair creation process at the supercritical potential step is being accompanied by an (additional) incoming fermion. As the fermion is reflected (with  $R=1$  and no transmission under the barrier), it suppresses the pair creation process due to Pauli blocking. A new fermion-antifermion pair cannot be created during those times when the incoming fermion occupies the space close to the force region. Only once the incoming fermion is completely scattered and has left the force region, the usual pair creation process sets in again. The obvious question is how the Klein paradox can be resolved also for a bosonic system. As this resolution requires a full time-dependent simulation that incorporates the dynamics of the incoming boson as well as the pair creation process, we will devote a future project to this task.

In the Dirac system, the quantum-mechanical transmission coefficient plays a fascinating dual role. Its energy integral is the main contributor to the steady-state pair creation rate at the supercritical barrier (without any incoming particle) while at the same time the transmitted wave-function portion [whose size is directly proportional to  $T(E)$ ] represents the amount of pair-creation suppression for the case an incoming particle (of energy  $E$ ) is injected into the spatial pair creation regime. It might be interesting to examine whether in the corresponding Klein-Gordon system, the cor-



responding negative and arbitrarily large transmission coefficient can play a similar role to describe the effect of an incoming boson on the pair creation process. The pair creation could be enhanced associated with the magnitude of the bosonic transmission coefficient. This can be shown by using a full quantum field theoretical simulation, similarly as the one reported for the fermion system [15,16].

Ultimately and most importantly, of course, these rates should be tested with experimental data and we can hope that one day an experimental confirmation of an observed spontaneous decay of the vacuum due to an external force can be made. To examine the predictions of quantum electrodynamics for the interaction of ultrarelativistic laser fields with various systems is certainly a topic of wide interest. For a few works that were published very recently, see, e.g., [45–51].

### ACKNOWLEDGMENTS

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### APPENDIX A: EIGENSTATES FOR DIRAC AND KLEIN-GORDON HAMILTONIANS FOR THE STEP POTENTIAL

The energy eigenspectra of the force-free Hamiltonians  $h_D = c\sigma_1 p + \sigma_3 c^2$  and  $h_{KG} = p^2/2 + \sigma_3 c^2$  are identical with a negative-energy continuum from  $-\infty$  to  $-c^2$ , and positive energies from  $c^2$  to  $\infty$ . The eigenvectors for the Dirac equation ( $h_D|W\rangle = E|W\rangle$ ) for the positive and negative energies  $E \equiv \pm \sqrt{c^4 + c^2 p^2}$  are given by

$$W_{D+}(p, z) = \frac{\begin{bmatrix} \sqrt{E+c} \\ \text{sgn}(p)\sqrt{E-c^2} \end{bmatrix}}{\sqrt{2E}} \frac{e^{ipz}}{\sqrt{2\pi}} \quad (\text{for } E \geq c^2), \quad (\text{A1})$$

$$W_{D-}(p, z) = \frac{\begin{bmatrix} \text{sgn}(p)\sqrt{-E-c^2} \\ \sqrt{-E+c^2} \end{bmatrix}}{\sqrt{-2E}} \frac{e^{-ipz}}{\sqrt{2\pi}} \quad (\text{for } E \leq -c^2), \quad (\text{A2})$$

and are normalized according to  $\langle W_{D\pm}(p) | W_{D\pm}(p') \rangle = \delta(E_p - E_{p'})$ . Each state is doubly degenerate and  $\text{sgn}(p)$  denotes the sign of the momentum  $p$ . The Klein-Gordon states ( $h_{KG}|W_{KG}\rangle = E|W_{KG}\rangle$ ) are normalized according to the sign of their energy,  $\langle W_{KG\pm}(p) | \sigma_3 W_{KG\pm}(p) \rangle = \pm \delta(E_p - E_{p'})$  and take the form

$$W_{KG+}(p) = \frac{\begin{bmatrix} c^2 + E \\ c^2 - E \end{bmatrix}}{\sqrt{4c^2 E}} \frac{e^{ipz}}{\sqrt{2\pi}} \quad (\text{for } E \geq c^2), \quad (\text{A3})$$

$$W_{KG-}(p) = \frac{\begin{bmatrix} c^2 + E \\ c^2 - E \end{bmatrix}}{\sqrt{-4c^2 E}} \frac{e^{-ipz}}{\sqrt{2\pi}} \quad (\text{for } E \leq -c^2). \quad (\text{A4})$$

We should stress that for a positive momentum  $p$ , all of the four states above have a positive phase velocity. In other words, the center of mass of a coherent superposition of these states centered around a positive  $p$  would move to the right, independent of whether we assign a certain charge to the underlying particle.

### APPENDIX B: THE DIRAC BOUNDARY CONDITIONS

For the case of a step potential  $V(z, t) = V\theta(z)$  the states of Eqs. (A1)–(A4) serve as the basic building blocks for the dressed eigenstates. For a given positive energy  $E$  and a supercritical potential ( $2c^2 < V$ ) we assume that for  $z < 0$  the eigenstate is a superposition of  $W_+(p, z)$  and  $W_+(-p, z)$  with  $p \equiv \sqrt{[E^2 - c^4]}/c$ , while for  $0 < z$  it is a superposition of the states  $W_-(q, z)$  and  $W_-(-q, z)$ , where  $q$  denotes the positive momentum  $q \equiv \sqrt{[(E-V)^2 - c^4]}/c$  and where we have to replace the parameter  $E$  in Eqs. (A2) and (A4) with  $E-V$ ,

$$|p, -p; q\rangle_D = [W_{D+}(p) + r_D W_{D+}(-p)]\theta(-z) + [t_D \mathcal{I} W_{D-}(q)]\theta(z), \quad (\text{B1})$$

$$|-p; -q, q\rangle_D = [t_D \mathcal{I} W_{D+}(-p)]\theta(-z) + [W_{D-}(-q) + r_D W_{D-}(q)]\theta(z). \quad (\text{B2})$$

We abbreviate the Jacobian  $\mathcal{J} = -(pE_q)/(qE)$  and  $\mathcal{I} = 1/\mathcal{J}$ . These states are normalized to  ${}_D\langle p, -p; q | p', -p'; q' \rangle_D = \delta(E_p - E_{p'})$  and  ${}_D\langle -p; -q, q | -p'; -q', q' \rangle_D = \delta(E_q - E_{q'})$ . One can also show that these two states are orthogonal to each other,  ${}_D\langle p, -p; q | -p'; -q, q \rangle_D = 0$ .

In order to find the correct expansion coefficients  $r_D$  and  $t_D$ , the states on both sides of the step barrier have to fulfill the appropriate matching condition. For the Dirac case,  $E\phi(z) = [-ic\sigma_1 \partial/\partial z + \sigma_3 c^2 + V\theta(z)]\phi(z)$ , we integrate both sides from  $z = -\varepsilon$  to  $z = +\varepsilon$  and obtain  $E[\phi(+\varepsilon) + \phi(-\varepsilon)] = -ic\sigma_1 \phi(+\varepsilon) + ic\sigma_1 \phi(-\varepsilon) + \sigma_3 c^2 \varepsilon [\phi(+\varepsilon) + \phi(-\varepsilon)] + V\varepsilon \phi(+\varepsilon)$ . Perform the limit  $\varepsilon \rightarrow 0$  and since  $\phi$  is finite, we obtain  $-ic\sigma_1 \phi(+\varepsilon) + ic\sigma_1 \phi(-\varepsilon) = 0$ . This reduces to the requirement that the each component of the state  $\phi = [\phi_1, \phi_2]$  matches with its partner, i.e.,  $\phi_1(-\varepsilon) = \phi_1(+\varepsilon)$  and  $\phi_2(-\varepsilon) = \phi_2(+\varepsilon)$ . The resulting two equations for two unknowns  $r_D$  and  $t_D$  can be solved and we obtain finally

$$r_D = \frac{-(cq)(cp) - (E_q + c^2)(E + c^2)}{-(cq)(cp) + (E_q + c^2)(E + c^2)},$$

$$t_D \mathcal{J} = (1 - r_D) \sqrt{\{E_q(E - c^2)/[E(E_q + c^2)]\}}. \quad (\text{B3})$$

If re-evaluate the current according to  $j_D = \phi^\dagger c\sigma_1 \phi$  we obtain

$$j_D(z) = [c^2 p / (2\pi E_p)] \{ (1 - |r_D|^2) \theta(-z) + \text{sgn}(q) |t_D|^2 \mathcal{J} \theta(z) \}, \quad (\text{B4})$$

where the continuity of current at  $z=0$ ,  $j_D(-\varepsilon) = j_D(+\varepsilon)$ , follows automatically. But the continuity of  $j$  by itself would not be a sufficient condition to obtain  $r_D$  and  $t_D$  as two conditions are required. The continuity results in  $1 - |r_D|^2 = \text{sgn}(q) |t_D|^2 \mathcal{J}$ .

### APPENDIX C: KLEIN-GORDON BOUNDARY CONDITIONS

Let us consider the corresponding superposition for the KG system

$$|p, -p: q\rangle_{\text{KG}} = [W_{\text{KG}^+}(p) + r_{\text{KG}}W_{\text{KG}^+}(-p)]\theta(-z) + [t_{\text{KG}}\mathcal{J}W_{\text{KG}^-}(q)]\theta(z), \quad (\text{C1})$$

$$|-p: -q, q\rangle_{\text{KG}} = [t_{\text{KG}}\mathcal{I}W_{\text{KG}^+}(-p)]\theta(-z) + [W_{\text{KG}^-}(-q) + r_{\text{KG}}W_{\text{KG}^-}(q)]\theta(z). \quad (\text{C2})$$

We assume again  $p > 0$  and also  $\mathcal{J} = (pE_q)/(|q|E)$  with  $E_q = E - V$ . These states are normalized to  ${}_{\text{KG}}\langle p, -p: q | \sigma_3 | p', -p': q' \rangle_{\text{KG}} = \delta(E_p - E'_p)$  and  ${}_{\text{KG}}\langle -p: -q, q | \sigma_3 | -p': -q', q' \rangle_{\text{KG}} = -\delta(E_q - E'_q)$ . Note the negative sign despite the fact that the state has positive energy. One can also show that these two states are orthogonal to each other.  ${}_{\text{KG}}\langle p, -p: q | \sigma_3 | -p: -q, q \rangle_{\text{KG}} = 0$ .

In case of the Klein-Gordon system, the boundary conditions are more complicated than for the Dirac case. The starting point is again the corresponding stationary equation,  $E\phi(z) = [-\partial^2/\partial z^2/2N + \sigma_3 c^2 + V\theta(z)]\phi(z)$ . If we integrate both sides of this equation from  $z = -\varepsilon$  to  $z = +\varepsilon$ , we obtain  $E\varepsilon[\phi(+\varepsilon) + \phi(-\varepsilon)] = -N\phi'(+\varepsilon)/2 + N\phi'(-\varepsilon)/2 + \sigma_3 c^2 \varepsilon[\phi(+\varepsilon) + \phi(-\varepsilon)] + V\varepsilon\phi(+\varepsilon)$ , where the prime denotes the spatial derivative. We can perform the limit  $\varepsilon \rightarrow 0$  and since  $\phi$  is finite, we obtain  $-N\phi'(+\varepsilon) + N\phi'(-\varepsilon) = 0$ . Using the explicit form of the matrix  $N$ , this reduces to the first boundary condition  $\phi'_1(-\varepsilon) + \phi'_2(-\varepsilon) = \phi'_1(+\varepsilon) + \phi'_2(+\varepsilon)$ . If we integrate the original energy eigenvalue equation via  $\int_{-\varepsilon}^{\varepsilon} dz \int_{-z}^z dz'$ , and follow similar arguments as above, we obtain the second boundary condition:  $\phi_1(-\varepsilon) + \phi_2(-\varepsilon) = \phi_1(+\varepsilon) + \phi_2(+\varepsilon)$ . In other words, in contrast to the Dirac equation, the state by itself can be *discontinuous* for a step potential. A similar conclusion was obtained in Ref. [19] where the boundary conditions were derived from the exact solution for the Sauter potential with finite  $W$  and then its limit  $W \rightarrow 0$  as taken. If apply these two boundary conditions to Eqs. (C1) and (C2), we can again eliminate  $t_{\text{KG}}$  and solve for  $r_{\text{KG}}$  to obtain

$$r_{\text{KG}} = (p + q)/(p - q),$$

$$t_{\text{KG}}\mathcal{J} = (2p)/(p - q)\sqrt{-E_q/E}. \quad (\text{C3})$$

If we calculate the current density according to  $j_{\text{KG}} = [\phi^\dagger \sigma_3 N p \phi - (p \phi^\dagger) \sigma_3 N \phi]/2$  we obtain

$$j_{\text{KG}}(z) = [c^2 p / (2\pi E)] \{ (1 - |r_{\text{KG}}|^2) \theta(-z) - \text{sgn}(q) |t_{\text{KG}}|^2 \mathcal{J} \theta(z) \}. \quad (\text{C4})$$

The continuity of current at  $z = 0$  leads to  $1 - |r_{\text{KG}}|^2 = -\text{sgn}(q) |t_{\text{KG}}|^2 \mathcal{J}$ .

### APPENDIX D: THE SIGN OF THE MOMENTUM $q$ UNDER THE BARRIER

Let us first comment on the Dirac case. Here the spatial density  $\phi^\dagger \phi$  remains positive under the unitary time evolu-

tion and the total area is conserved. For a traditional scattering situation (characterized by an incoming particle) it is therefore clear that any transmitted or reflected portion cannot exceed the area of the incoming state. Correspondingly, any reasonable reflection or transmission coefficient has to be less than 1. This requirement excludes also automatically any negative coefficients.

In our analysis above we chose the traditional scattering state  $|p, -p: q\rangle$  and (its orthogonal partner)  $|-p: -q, q\rangle$  as the two degenerate energy states. One could have equivalently chosen another pair to span the same Hilbert space, the state  $|p, -p: -q\rangle$  and its corresponding orthogonal partner  $|p: -q, q\rangle$ . Here it is important to note that the state with the negative momentum  $-q$ ,  $|p, -p: -q\rangle$  describes a wave function that approaches the barrier from the left *and* from the right side. In order to fulfill the required boundary conditions (Appendix B), the state  $|p, -p: -q\rangle$  would lead to two expansion coefficients for the corresponding free states for  $z > 0$  and  $z < 0$  where one exceeds unity and the other is negative. However, due to the ambiguity of which side of the barrier corresponds to the incoming portion one should not use the language of negative transmission coefficients or of reflection coefficients that exceed unity. In several standard textbooks [1,17] the coefficients for a negative momentum  $-q$  were then justified in terms of quantum field theoretical processes (pair creation at the barrier). It was argued that a reflection larger than unity corresponds to the combination of the reflected electron and the created electron due to the pair creation process. The negative transmission coefficient was interpreted as describing the flux of particles of opposite charge (positrons) evolving under the barrier. In our opinion, it is not satisfactory to try to interpret purely quantum-mechanical data in terms of a quantum field theoretical language; in the same sense as explaining data obtained from a nonrelativistic theory in terms of relativistic phenomena is inconsistent. We should also point out that in these calculations the important partner state  $|p: -q, q\rangle$  was neglected. To be more specific, for energy  $E = 1.5 c^2$  and width  $W = 0.3/c$  we have obtained (and confirmed with independent numerical simulations) the transmission coefficients  $T_{\text{D}} = 0.42435$  and  $T_{\text{KG}} = -2.6452$ , whereas for the opposite sign of the momentum  $q$ , one would obtain  $T_{\text{D}} = -0.737158$  and  $T_{\text{KG}} = 0.725667$ .

In case of the Klein-Gordon equation, the situation is (almost ironically) reversed. Here the (only generalized unitary) time evolution keeps the total charge density  $\int dz \phi^\dagger \sigma_3 \phi$  conserved and the integrand can be simultaneously positive and negative as a function of the position  $z$ . In the over-barrier scattering situation we have shown that the density does not change its sign. However, in the important case of a supercritical barrier, the charge density changes its sign under the barrier. Following consistently a universal definition for the transmission coefficient, defined in terms of the ratio of the electric current densities  $T = j_{\text{trans}}/j_{\text{inc}}$ , we obtain a negative value. This one can even exceed  $-1$  and approach  $-\infty$  in this case. However, it is important to note, that despite a negative sign of the current density the center of a spatially localized wave packet travels into the positive  $z$ -direction. Only a few works have studied the KG system in its two-spinor formulation. Ref. [19] defines both  $T$  and  $R$  as intrinsically positive

quantities to study quantum-mechanical scattering. As a result in this work it depends on the size of the potential  $V$ , whether  $R+T=1$  or  $R-T=1$  is the appropriate conservation law, another not very satisfactory conclusion. A conservation

law is more general if it does not depend on the choice of specific numerical parameters. In fact it produces the numerical values that disagree with our simulations.

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