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Causality and relativistic localization in one-dimensional Hamiltonians

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We compare the relativistic time evolution of an initially localized quantum particle obtained from the relativistic Schrödinger, the Klein-Gordon and the Dirac equations. By computing the amount of the spatial probability density that evolves outside the light cone we quantify the amount of causality violation for the relativistic Schrödinger Hamiltonian. We comment on the relationship between quantum field theoretical transition amplitudes, commutators of the fields and their bilinear combinations outside the light cone as indicators of a possible causality violation. We point out the relevance of the relativistic localization problem to this discussion and comment on ideas about the supposed role of quantum field theory as a vehicle of making a theory causal by introducing antiparticles.

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I. INTRODUCTION

In classical mechanics two physical events occurring at (z_1, t_1) and (z_2, t_2) can be causal if the interval $c^2(t_1 - t_2)^2 - (z_1 - z_2)^2$ is positive. In this case a light signal would have enough time to travel from one event to the other. The Lorentz transformation $[\begin{smallmatrix} z' \\ t' \end{smallmatrix}] = \Lambda[\begin{smallmatrix} z \\ t \end{smallmatrix}]$ preserves this distance. If the system is relativistically invariant then the cause (z'_1, t'_1) precedes the effect (z'_2, t'_2) in any frame. For a single-particle system, the Hamiltonian $h(p) = [m^2c^4 + c^2p^2]^{1/2}$ is relativistically invariant such that $[\begin{smallmatrix} p' \\ h' \end{smallmatrix}] = \Lambda[\begin{smallmatrix} p \\ h \end{smallmatrix}]$ simplifies to $h' = h(p')$. In this case the corresponding velocity $dz/dt = dh/dp = c^2p/[m^2c^4 + c^2p^2]^{1/2}$ is always less than c and causality is guaranteed.

In quantum mechanics and quantum field theory, however, the nature of causality is not so clear. In fact, while the quantum expectation value of the velocity $\langle c^2p/[m^2c^4 + c^2p^2]^{1/2} \rangle$ is also less than c , certain portions of the wave function can actually evolve faster than the speed of light, despite the Lorentz invariance of $h(p)$. We are not aware of any studies that have examined quantitatively the amount of this causality violation and how it depends on the properties of the initial quantum state.

One can find statements in the literature that the causality violation can be solved in a “miraculous way” [1] by quantum field theory by introducing antiparticles. In this work we discuss three Lorentz invariant Hamiltonians, associated with the relativistic Schrödinger (rS), the Dirac (D), and the Klein-Gordon (KG) equations as examples for causality preserving and non-preserving quantum mechanical systems. We then use the usual framework based on canonical second-quantization of the fields to construct the three corresponding quantum field theoretical descriptions. This allows us to compare the properties of a noncausal but Lorentz invariant quantum field theory (rS) with two well-known causal theories (D and KG). In other words, for these free-particle systems the predictions with regard to causality of the field theoretical version are identical to the quantum mechanical formulations and antiparticles are simply redefinitions of the quantum mechanical negative energy solutions and cannot be arbitrarily introduced to cure the causality violation of the rS system.

We also point out the special role of a possible lack of particle localization in coordinate space for single particles and provide a quantum mechanical interpretation of nonvanishing quantum field transition amplitudes between two states outside the light cone. It has been argued that whether particles can propagate over spacelike intervals does not indicate any causality violation and that only commutator relationships among the fields should be considered [1,2]. In quantum field theory, the action of the Dirac and Klein-Gordon field operator on the vacuum generates a particle whose (field theoretical) charge density and associated quantum mechanical charge density for the same state are *not* localized (by which we mean that it has an infinite spatial support). The quantum field theoretical transition amplitude between two different states can be equivalently expressed as an overlap integral over the two associated quantum mechanical wave functions. As a result one could take the point of view that transition amplitudes would provide information about the lack or presence of causality only if the quantum mechanical wave functions of the particles were localized.

The paper is organized as follows: In the second section we introduce the three quantum Hamiltonians, evolve an initially localized probability density in time and measure the amount that has moved outside the light cone as a function of time. We also show that this amount is transient and that the largest amount of causality violation can be achieved for a spatially infinitely narrow state. We provide the formulas for the associated propagators and show that parts of the corresponding Green’s function for the positive energy states are nonzero outside the light cone for each of the three systems. However, it corresponds to a causality violation only for the rS system, whereas the D and KG systems are nevertheless causal. In the third section we second-quantize the system consistent with the spin-statistics theorem, and compute the quantum field theoretical transition amplitudes and study the commutation properties of quantum field theoretical observables. We show that for the rS system, it is not possible to introduce antiparticles to cure its causality violation despite its Lorentz invariance.

II. QUANTUM MECHANICAL CONSIDERATIONS

To keep our analysis simple, we permit only one spatial dimension [3,4]. In atomic units ($m = 1$, $\hbar = 1$, and the speed of light $c = 137.036$), the three Hamiltonians take the form

$$h_{rS} = [c^4 + p^2 c^2]^{1/2}, \quad (2.1a)$$

$$h_D = c\sigma_1 p + \sigma_3 c^2, \quad (2.1b)$$

$$h_{KG} = (\sigma_3 + i\sigma_2)p^2/2 + \sigma_3 c^2, \quad (2.1c)$$

where $p \equiv -i\partial/\partial z$ is the momentum operator along the z direction and the usual 2×2 Pauli matrices are denoted by $\sigma_1 \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, $\sigma_2 \equiv \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$, and $\sigma_3 \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$. While the relativistic Schrödinger (rS) operator describes the time evolution of a single wave function, the Dirac (D) and Klein-Gordon (KG) equations evolve a two-component spinor $\phi(z,t) = \begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix}$. The Dirac spinor has been reduced from four to only two components, as we focus on only one spin direction. We prefer the Feshbach-Villars [5] representation over the usual second order in time Klein-Gordon equation, $[c^{-2}\partial^2/\partial t^2 - \partial^2/\partial z^2 + c^2]f(z,t) = 0$, as it allows us to compare all three systems within an identical theoretical framework based on Hamiltonians. We also note that each of the three Hamiltonians is form invariant under the corresponding Lorentz transformation.

The total ‘‘charge’’ defined here as $\int dz \rho(z,t) = 1$ is conserved for all three Hamiltonians. For the relativistic Schrödinger Hamiltonian h_{rS} we have $\rho_{rS}(z,t) \equiv |\phi(z,t)|^2$, for the Dirac system with h_D we have $\rho_D(z,t) \equiv \phi^\dagger \phi = |\phi_1(z,t)|^2 + |\phi_2(z,t)|^2$, and as the corresponding Klein-Gordon Hamiltonian h_{KG} [5–7] is pseudo-Hermitian ($h_{KG}^\dagger = \sigma_3 h_{KG} \sigma_3$), we find $\rho_{KG}(z,t) \equiv \phi^\dagger \sigma_3 \phi = |\phi_1(z,t)|^2 - |\phi_2(z,t)|^2$. All three Hamiltonians have been used in the past to study several aspects of the quantum relativistic dynamics including positive and negative energy states [8–11].

A. Space-time evolution of the wave functions

Let us first compute the quantum mechanical time evolution of a localized state $\rho(z,t=0) = \theta(\delta-z)\theta(z+\delta)/(2\delta)$ with an initial spatial width 2δ . More specifically, we choose the states $\phi_{rS}(z,t=0) = \rho(z)^{1/2}$, $\phi_D(z,t=0) = \phi_{KG}(z,t=0) = [\rho(z)^{1/2}, 0]$. In contrast to various other definitions of localization (‘‘ δ -like’’ densities or L^2 -integrable), here and below we call a state ‘‘localized’’ if it has a finite support in space. We should mention that the ϕ_{rS} state is unique, in the sense that if we had transformed it to any Lorentz boosted frame, it would be no longer localized but require an infinite spatial support. In contrast, the states ϕ_D and ϕ_{KG} remain localized in any frame.

We also point out that for the D and KG systems these localized states require contributions from energy eigenstates with positive as well as negative energy. In contrast to the rS system, for the D and KG systems it is not possible to construct a spatially localized state based on positive energy states alone. This relativistic localization problem [12,13] is a consequence of the incompleteness of the Hilbert space for positive energy states. Several textbooks have concluded that therefore the physical electron can no longer be considered as a point particle as it is spread out over a distance given

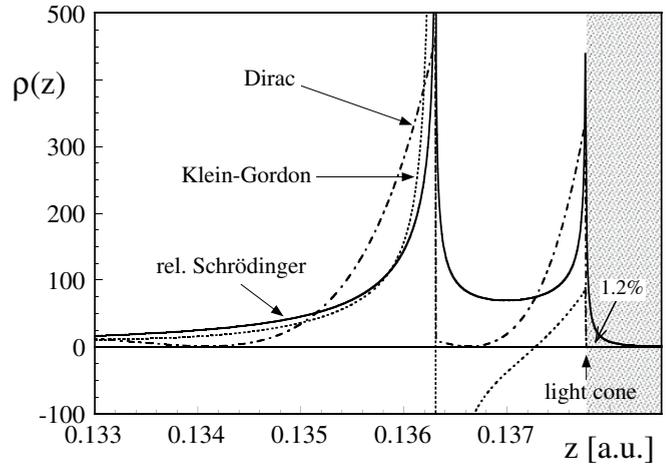


FIG. 1. The final charge densities for Dirac (dot-dash), Klein-Gordon (dot), and relativistic Schrödinger Hamiltonians. While the Dirac and Klein-Gordon densities stay within the light cone, the relativistic Schrödinger density has a portion of weight 1.2% outside of the light cone. ($\delta = 0.1/c$, $T = 0.001$ a.u., numerical box length $L = 0.4$ a.u. with NDIM = 200 000 grid points.)

by the Compton wavelength [14–17]. This observation will be relevant for the discussion of causality violation in the quantum field theoretical description in Sec. III.

In Fig. 1 we show the resulting three densities $\rho(z,t)$ at time $t = T$ and near one edge of the light cone. We note that while the Dirac and Klein-Gordon densities maintain the sharp wave front, the relativistic Schrödinger density has removed the sharp corner and the density has become delocalized in the sense that the spatial support domain has become the entire z axis. In other words, there is some nonzero probability density that has evolved faster than the speed of light, located in the spacelike regions $z < -\delta - ct$ and $\delta + ct < z$.

The two peaks at each side of the rapidly spreading distribution are separated by 2δ , which is the spatial width of the initial density. As the small length scales that characterize the sharp corners in the initial density can be loosely associated with large momenta, one could interpret these peaks as the result of spatially localized high momentum regions that evolve mainly with the speed of light c .

As a side remark, we note that if we had analyzed the real and imaginary parts of the time evolved wave function for h_{rS} instead of the density, we would have found that the violation of causality is exclusively associated with the imaginary part of $\phi_{rS}(z,t)$. The real part maintains its sharp edge and no portion leaks outside the light cone. This is related to the initial state chosen real and this property will be confirmed by our analytical analysis in Sec II B.

In order to determine the time dependence of the total probability of the particle to be detected outside this light cone, we have graphed in Fig. 2 the ‘‘outside probability,’’ defined as $N(t,\delta) = \int dz \rho(z,t)$, where the integration ranges from $z = \delta + ct$ to $z = \infty$. We show the time dependence of this causality violating portion for various initial widths δ . The probability $N(t)$ grows from zero to a maximum value and then decreases back to zero suggesting that the causality violation is a transient effect. While at earlier times some fraction of

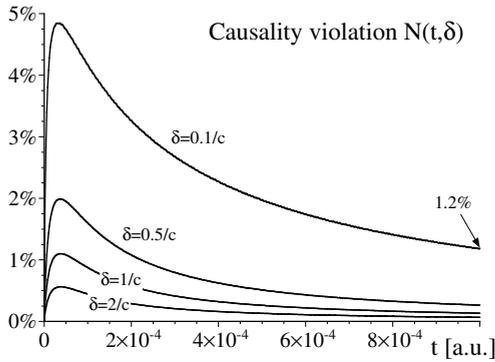


FIG. 2. The amount of probability outside of the light cone ($\delta + ct < z$) as a function of time for various initial wave function widths δ for the relativistic Schrödinger Hamiltonian. ($L = 0.4$ a.u., NDIM = 800 000.)

the total probability manages to propagate faster than c , after a longer time the front of the light cone $z = \delta + ct$ “catches up” with this portion and even passes it. In other words, this transient causality violation portion is not able to maintain its (initially) faster speed and somehow “slows down.”

We have also studied the maximum amount of causality violation for various widths δ , and found that there is a maximum at 8.2% in the limit of $\delta \rightarrow 0$. For comparison, we should mention that under a completely nonrelativistic time evolution ($h = p^2/2$) and for the state for $\delta = 0.1/c$ we would find that 46% of the wave packet evolves (irreversibly) to the right of the light cone. The same amount can be obtained if we integrate the corresponding momentum density from $p = c$ to ∞ .

The (initially) sharp edges of $\phi_{rS}(z, t=0)$ at $z = \pm \delta$ have permitted a rather straightforward determination of the amount of causality violation for h_{rS} . In order to examine whether the causality violation could be caused by the sharp edges, we have also analyzed smooth wave functions. For example, calculations for an initial Gaussian wave packet (initially centered at $z = 0$) have indicated as well that the probability density between the moving light front $z(t) = d + ct$ and $z = \infty$ can also temporarily increase as a function of time for any parameter d that exceeds the Gaussian’s initial width. Furthermore, this portion associated with the causality violation is again imaginary. So these findings are general and the causality violation is not a special property restricted to only sharply localized initial states. This finding is also consistent with work by Hegerfeldt [18,19] who showed analytically that states with exponentially bounded tails violate causality.

B. Analysis of the quantum mechanical propagators

More general information about the time evolution of arbitrary initial states for the three Hamiltonians can be obtained from the corresponding Green’s function G in the spatial representation [2].

$$\begin{aligned} \phi(z, t) &= \int dz' G(t, z - z') \phi(z', t=0) \\ &= (2\pi)^{-1/2} \int dp \exp[-ih(p)t] \exp[ipz] \phi(p). \end{aligned} \quad (2.2)$$

Here $\phi(p) \equiv (2\pi)^{-1/2} \int dz' \exp[-ipz'] \phi(z', t=0)$ is the momentum representation of the initial state and $h(p)$ is the Hamiltonian where the momentum operator $-i\partial/\partial z$ is replaced with the variable p . As the three Hamiltonians of Eq. (2.1) have identical positive energy spectra, $E = (c^4 + c^2 p^2)^{1/2}$, the derivations for the corresponding propagator are very similar. The action of the time evolution operator $\exp[-ih(p)t]$ can be simplified if we introduce the energy subspace projectors P^+ and P^- . For a given momentum p , they can be expressed as $P^+ = [1 + h(p)/E]/2$ and $P^- = [1 - h(p)/E]/2$. Note that for h_{rS} the second projector P^- is zero and $P^+ = 1$. If we insert the unit operator $P^+ + P^-$ after $\exp[-ih(p)t]$, the action of this propagator can be performed in each energy subspace, using $\exp[-ih(p)t] P^\pm = \exp[\mp iEt] P^\pm$. Furthermore, we can introduce the time-derivative operator, $P^\pm \exp[\mp iEt] = [\pm i\partial/\partial t \pm h(p)] \exp[\mp iEt]/[2E]$. As an intermediate result we obtain

$$\begin{aligned} \phi(z, t) &= (2\pi)^{-1/2} \int dp [i\partial/\partial t + h(p)] \\ &\quad \times \exp[ipz] \{ \exp[-iEt] - \exp[iEt] \} / [2E] \phi(p). \end{aligned} \quad (2.3)$$

If we factor the operator $[i\partial/\partial t + h(-i\partial/\partial z)]$ out of the integral and replace the momentum wave function by its Fourier integral, we obtain the desired form $\phi(z, t) = \int dz' G(t, z - z') \phi(z', t=0)$, where the function g is related to G through $G(t, z - z') = [i\partial/\partial t + h(-i\partial/\partial z)] g(t, z - z')$. Here the universal function $g(t, y)$ is defined as $g(t, y) \equiv (4\pi)^{-1} \int dp \exp[ipy] \{ \exp[-iEt] - \exp[iEt] \} / E$. Note that this function is identical for h_D and h_{KG} , while for h_{rS} the second exponential (associated with negative energy $-E$) is zero. As in the special case of the rS system, the actions of $i\partial/\partial t$ and $h_{rS}(-i\partial/\partial z)$ on $g(t, z - z')$ are identical to each other, and the Green’s function can be also expressed as $G_{rS}(t, y) = (2\pi)^{-1} \int dp \exp[ipy] \exp[-iEt]$. By substituting $E = (c^4 + c^2 p^2)^{1/2}$ into Eq. (2.3), we can solve the two integrals for g^+ and g^- analytically [2,20,21] (with $g^+ + g^- = g$) and obtain for the function that determines the evolution of states with positive energy:

$$\begin{aligned} g^+(t, y) &= (4\pi)^{-1} \int dp \exp[ipy] \exp[-iEt] / E \\ &= \begin{cases} \{-N_0[c^2 t^2 - y^2]^{1/2} - i J_0[c^2 t^2 - y^2]^{1/2}\} / (4c) & \text{if } (y^2 < c^2 t^2), \text{ inside the light cone,} \\ K_0[c^2(y^2 - c^2 t^2)^{1/2}] / (2\pi c) & \text{if } (c^2 t^2 < y^2), \text{ outside the light cone,} \end{cases} \end{aligned} \quad (2.4a)$$

and for the negative-energy subspace:

$$g^-(t, y) = -(4\pi)^{-1} \int dp \exp[ipy] \exp[iEt]/E$$

$$= \begin{cases} \{N_0[c(c^2t^2 - y^2)^{1/2}] - iJ_0[c(c^2t^2 - y^2)^{1/2}]\}/(4c) & \text{if } (y^2 < c^2t^2), \text{ inside the light cone,} \\ -K_0[c(y^2 - c^2t^2)^{1/2}]/(2\pi c) & \text{if } (c^2t^2 < y^2), \text{ outside the light cone.} \end{cases} \quad (2.4b)$$

Here we use three types of zeroth-order Bessel functions: $J_0(x)$ is the usual Bessel function of the first kind, the Bessel function of the second kind (Neumann function) is denoted by $N_0(x)$ [= $Y_0(x)$], and $K_0(x)$ is the modified Bessel function of the second kind.

Neither g^+ nor g^- vanish outside the light cone. However, this does not necessarily lead to a causality violation. For example, even for the positive energy portion of the state only, $\phi^+(z) \equiv P^+ \phi(z)$, the evolution $\phi^+(z, t) = [i\partial/\partial t + h] \int dz' g^+(t, z - z') \phi^+(z')$ is fully causal for the D and KG systems, [i.e., $\phi^+(z, t) = 0$ outside the light cone], even though the function $g^+(t, y)$ does not vanish for $c^2t^2 < y^2$.

Also, it is obvious that the function $g(t, y) = g^+(t, y) + g^-(t, y)$ vanishes for $c^2t^2 < y^2$ and therefore preserves causality for h_D and h_{KG} . This is consistent with the conservation of the sharp wave fronts shown in Fig. 1. We also see that $g^+(t, y)$ for timelike events is complex, while for noncausal (spacelike) events it is real, again consistent with the graphs in Fig. 1.

It is sometimes argued that the causality violation for the specific functional form given by h_{rS} is related to the fact that this operator is nonlocal and that the Taylor series of the square root of the momentum operator contains derivatives of all orders. However, in our opinion, this is not necessarily a reason for the causality violation. One can show [21–23] that the time evolution for *any* Hamiltonian $h(p)$ that is a continuous and positive function of the momentum operator will distribute the support of an initially localized state to any region in space. Therefore an infinite propagation speed is actually rather universal and not unique to the specific square root functional form of h_{rS} .

III. QUANTUM FIELD THEORETICAL CONSIDERATIONS

A. Second-quantization of the three Hamiltonians and locality

Quantum field theory permits us to examine causality from the perspective of using “local” operators. In order to construct the corresponding field theories for the three quantum Hamiltonians h of Eqs. (2.1), we first have to find the corresponding classical mechanical Lagrange density $L(\phi, \dot{\phi})$, such that the corresponding Euler-Lagrange equations $[d/dt(\partial/\partial\dot{\phi}) - (\partial/\partial\phi)]L(\phi, \dot{\phi}) = 0$ are identical to the required equations $i\dot{\phi}(z, t) = h\phi(z, t)$ for each Hamiltonian h . We obtain

$$L = \Pi\dot{\phi} + i\Pi h\phi, \quad (3.1)$$

where we have defined the adjoint (dual) field Π to be consistent with the requirement that $\Pi = \partial L/\partial\dot{\phi}$. The specific form of this canonical conjugate field follows from the requirement that the total action $\iint dz dt L$ has to be real. In other words, we require $i\Pi h\phi = (i\Pi h\phi)^\dagger$ to be valid for each of the three Hamiltonians. More specifically, for h_{rS} and h_D we have

the symmetry $h_{rS}^\dagger = h_{rS}$ and $h_D^\dagger = h_D$ leading to $\Pi_{rS} = i\phi_{rS}^\dagger$ and $\Pi_D = i\phi_D^\dagger$. The Klein-Gordon Hamiltonian, however, is only generalized Hermitian, $h_{KG}^\dagger = \sigma_3 h_{KG} \sigma_3$, such that the KG-adjoint operator must take the form $\Pi_{KG} = i\phi_{KG}^\dagger \sigma_3$.

In order to second-quantize the Lagrange densities, we replace the classical fields ϕ and Π by quantum field operators, denoted by $\hat{\Psi}$ and $\hat{\Pi}$, and require them to satisfy either the equal-time commutators $[\hat{\Psi}_a(z), \hat{\Pi}_b(z')]_- = i\delta(z - z')\delta_{a,b}$ or the anticommutators $[\hat{\Psi}_a(z), \hat{\Pi}_b(z')]_+ = i\delta(z - z')\delta_{a,b}$ (for the two spinor components $a, b = 1, 2$). As the quantum fields have to also satisfy the corresponding equations $i\partial\hat{\Psi}(z, t)/\partial t = h\hat{\Psi}(z, t)$, we can expand the field operators as

$$\hat{\Psi}_{rS}(z, t) \equiv (2\pi)^{-1/2} \int dp \hat{b}(p) \exp(ipz - iEt), \quad (3.2a)$$

$$\hat{\Psi}_D(z, t) \equiv (2\pi)^{-1/2} \int dp [\hat{b}(p) u(p) \exp(ipz - iEt) + \hat{d}^\dagger(p) v(-p) \exp(-ipz + iEt)], \quad (3.2b)$$

$$\hat{\Psi}_{KG}(z, t) \equiv (2\pi)^{-1/2} \int dp [\hat{a}(p) r(p) \exp(ipz - iEt) + \hat{c}^\dagger(p) w(-p) \exp(-ipz + iEt)]. \quad (3.2c)$$

where we have introduced the fermionic and bosonic creation and annihilation operators. The functions that follow the raising and lowering operators in Eqs. (3.2) have to satisfy the corresponding equations $i\partial f/\partial t = hf$.

Furthermore, we also require the total quantum field theoretical Hamiltonian, defined from the usual Legendre transformation as $\hat{H} = \int dz (\Pi\dot{\phi} - L) = -i \int dz \hat{\Pi} h \hat{\Psi}$ to be bounded from below.

For the Hamiltonian h_{rS} and the corresponding field $\hat{\Psi}_{rS}(z, t)$ given by Eq. (3.2a), the creation and annihilation operators can be chosen to fulfill either the anticommutator and commutator relationships, $[\hat{b}(p), \hat{b}^\dagger(p')]_+ = \delta(p - p')$ or $[\hat{b}(p), \hat{b}^\dagger(p')]_- = \delta(p - p')$. The spectrum of \hat{H}_{rS} would be positive in any case, $\hat{H}_{rS} = \int dp E(p) \hat{b}^\dagger(p) \hat{b}(p)$, so there are two equivalent second-quantization schemes.

Due to the existence of negative energies, however, only one of the two schemes is appropriate for h_D and h_{KG} . The spectrum of the Hamiltonian $\hat{H}_D = \int dz \hat{\Psi}_D^\dagger h_D \hat{\Psi}_D$ is only positive if we choose the operators to fulfill the anticommutation rules, $[\hat{d}(p), \hat{d}^\dagger(p')]_+ = [\hat{b}(p), \hat{b}^\dagger(p')]_+ = \delta(p - p')$, while the energies of the corresponding Hamiltonian $\hat{H}_{KG} = \int dz \hat{\Psi}_{KG}^\dagger \sigma_3 h_{KG} \hat{\Psi}_{KG}$ are only positive if we choose the operators to fulfill the commutation rules $[\hat{a}(p), \hat{a}^\dagger(p')]_- = [\hat{c}(p), \hat{c}^\dagger(p')]_- = \delta(p - p')$. This connection between the symmetry of the Hamiltonian h and the relationship for the

operator products is an equivalent view of the spin-statistics theorem [24], according to which bosons (fermions) require commutators (anticommutators). Note that in our case the information about the spin has not been explicitly used.

The corresponding two-component spinor coefficients in Eq. (3.2b) for the Dirac system can be chosen as $u(p) \equiv N_u \{1, pc/[c^2 + E(p)]\}$ and $v(p) \equiv N_v \{1, pc/[c^2 - E(p)]\}$, where the real normalization constant can be found to guarantee that $\Sigma_a u_a(p)u_a(p) = \Sigma_a v_a(p)v_a(p) = 1$ and $\Sigma_a v_a(p)u_a(p) = 0$. Using the expansion of the 2×2 unit operator $\mathbf{1} = u(p) \otimes u^\dagger(p) + v(p) \otimes v^\dagger(p)$ and the Hamiltonian $h(p) = E u(p) \otimes u^\dagger(p) - E v(p) \otimes v^\dagger(p)$, it also follows that the spinor projectors simplify to $u(p) \otimes u^\dagger(p) = (\mathbf{1} + h_D/E)/2$ and $v(p) \otimes v^\dagger(p) = (\mathbf{1} - h_D/E)/2$, which is helpful for some of the algebra following.

For the KG system the Hamiltonian h_{KG} is not Hermitian. As a result we have to distinguish between left- and right-hand-side eigenvectors of h_{KG} [25]. The right-hand-side column eigenvectors are $r(p) \equiv N_r [1, -p^2/(2c^2 + p^2 + 2E)]$ and $w(p) \equiv N_w [1, -p^2/(2c^2 + p^2 - 2E)]$, where the two normalization constants N can be found from the orthonormality condition with the corresponding left-hand-side column eigenvectors, $r_L(p) \equiv N_r^* [1, p^2/(2c^2 + p^2 + 2E)]$ and $w_L(p) \equiv N_w^* [1, p^2/(2c^2 + p^2 - 2E)]$. As for a given momentum p the unit operator can be decomposed as $\mathbf{1} = r(p) \otimes r_L^\dagger(p) + w(p) \otimes w_L^\dagger(p)$ and the Hamiltonian as $h = E r(p) \otimes r_L^\dagger(p) - E w(p) \otimes w_L^\dagger(p)$, it also follows that the spinor projectors simplify again to $r(p) \otimes r_L^\dagger(p) = (1 + h_{KG}/E)/2$ and $w(p) \otimes w_L^\dagger(p) = (1 - h_{KG}/E)/2$. Note that because of the symmetry $h_{KG}^\dagger = \sigma_3 h_{KG} \sigma_3$ the pairs in this particular dual set are related by $r_L = r \sigma_3$ and $w_L = -w \sigma_3$.

For the special case of neutral bosons, the particles are identical to their antiparticles and $\hat{\Psi}_{KG}$ can be simplified by replacing \hat{c}^\dagger in the second term in Eq. (3.2c) with $-i\hat{a}^\dagger$. This simplification leads to the symmetry between the two spinor components $\hat{\Psi}_1^\dagger = \hat{\Psi}_2$, which is also fully consistent with the reality of the solution of the (original) Klein-Gordon wave equation, which is second order in time.

When expressed as a function of the lowering and raising operators in momentum space and after omitting the infinite constant term, we obtain

$$\hat{H}_{rS} \equiv \int dp E(p) \hat{b}^\dagger(p) \hat{b}(p), \quad (3.3a)$$

$$\hat{H}_D \equiv \int dp E(p) [\hat{b}^\dagger(p) \hat{b}(p) + \hat{d}^\dagger(p) \hat{d}(p)], \quad (3.3b)$$

$$\hat{H}_{KG} \equiv \int dp E(p) [\hat{a}^\dagger(p) \hat{a}(p) + \hat{c}^\dagger(p) \hat{c}(p)]. \quad (3.3c)$$

Before we continue with our discussion on causality, we should mention that in deriving Eqs. (3.3b) and (3.3c) we had to use $\hat{d}\hat{d}^\dagger = \delta(0) - \hat{d}^\dagger\hat{d}$ and $\hat{c}\hat{c}^\dagger = \delta(0) + \hat{c}^\dagger\hat{c}$ for equal momenta. In each case we omitted the resulting infinite energy term in \hat{H} . In the older literature one sometimes finds an attempt to associate the infinity in \hat{H}_D with a filled negative energy Dirac sea, but the same infinity occurs also for a bosonic system \hat{H}_{KG} for which one can hardly invoke any Pauli exclusion principle or any concepts of negative energy seas.

B. Quantum field theoretical transition amplitudes and localization

Let us now use the fields in Eqs. (3.2) to calculate the usual (2×2) transition amplitudes $A(z,t)$ for a particle to move from location $z = 0$ to location z within time t :

$$\begin{aligned} A_{rS}(z,t) &\equiv \langle \text{vac} | \hat{\Psi}_{rS}(z,t) \otimes \hat{\Psi}_{rS}^\dagger(z=0,t=0) | \text{vac} \rangle \\ &= (i\partial/\partial t + h_{rS})g^+(t,z), \end{aligned} \quad (3.4a)$$

$$\begin{aligned} A_D(z,t) &\equiv \langle \text{vac} | \hat{\Psi}_D(z,t) \otimes \hat{\Psi}_D^\dagger(z=0,t=0) | \text{vac} \rangle \\ &= (i\partial/\partial t + h_D)g^+(t,z), \end{aligned} \quad (3.4b)$$

$$\begin{aligned} A_{KG}(z,t) &\equiv \langle \text{vac} | \hat{\Psi}_{KG}(z,t) \otimes \hat{\Psi}_{KG}^\dagger(z=0,t=0)\sigma_3 | \text{vac} \rangle \\ &= (i\partial/\partial t + h_{KG})g^+(t,z). \end{aligned} \quad (3.4c)$$

In evaluating these scalar products we have used $\langle \text{vac} | \text{vac} \rangle = 1$. If we insert the solutions for the field operators into the scalar products, we find again the same function $g^+(t,z)$ that is related to the quantum mechanical function defined in terms of the Bessel functions in Eq. (2.4). We note that none of the three transition amplitudes vanishes outside the light cone, $z > ct$. It has been argued [1] that the fact that particles can propagate over spacelike intervals should not be used to discuss causality.

One could propose an alternative interpretation and argue that any nonvanishing transition amplitude $A_{a,a}(z,t=0)$ would indeed indicate a causality violation if the states defined as $|a,z\rangle \equiv \hat{\Psi}_a^\dagger(z,t=0)|\text{vac}\rangle$ were actually truly localized at z . It turns out that the reason for the nonvanishing amplitude for the rS system is actually quite different than that for the D and KG systems. For example, in this view only the nonvanishing probability $A_{rS}(z,t)$ indicates an actual causality violation. For $t = 0$ we obtain $A_{rS}(z,t=0) = \delta(z)$, in other words, the two states for $z = 0$ and $z \neq 0$ do not have any overlap and are therefore orthogonal to each other. However, within an infinitesimal amount of time $t \neq 0$, we have $A_{rS}(z,t) \neq 0$ for any z . This nonvanishing overlap with an, in principle, infinitely distant state is a clear indication of an ‘‘instant’’ spreading and therefore a signature of causality violation for \hat{H}_{rS} .

On the other hand, the corresponding two transition amplitudes $A_D(z,t=0)$ and $A_{KG}(z,t=0)$ are nonzero already for $t = 0$ and $z \neq 0$. In a quantum mechanical interpretation, this would reflect the (simultaneous) overlap of two *spatially extended* quantum mechanical states, and not necessarily any causality violation, as the corresponding states for $z = 0$ and $z \neq 0$ overlap already for $t = 0$. It is not surprising that the two states continue to overlap also for later times $t \neq 0$, and therefore $A_{rS}(z,t) \neq 0$ for any z cannot be used as a criterion to judge whether causality is violated or not.

However, the spatial extension of the particle associated with state $|a,z=0\rangle$ is a nontrivial topic by itself. If we calculate the spatial density for this state from the expectation value of the quantum field theoretical charge density operator $\hat{Q}(z) \equiv \Sigma_b [\hat{\Psi}_b^\dagger(z)\hat{\Psi}_b(z) - \hat{\Psi}_b(z)\hat{\Psi}_b^\dagger(z)]/2$, defined as $\langle a,z=0 | \hat{Q}(z) | a,z=0 \rangle$ we would find (see the Appendix) that this density is also not localized. This lack of localization is consistent with the observation that the scalar product $A_{a,b}(z,t=0) \equiv \langle a,z | a,z=0 \rangle$ does not vanish for $z \neq 0$. This suggests that the two nonorthogonal states $|a,z=0\rangle$ and $|a,z\rangle$ must have some ‘‘overlap’’ as their corresponding (field

theoretical) charge densities are not localized in two disjoint regions.

This quantum mechanical perspective is discussed in more detail in the Appendix. If we compute the corresponding quantum mechanical wave functions associated with the states $|a, z=0\rangle$ and $|a, z\rangle$ one can show that the quantum field theoretical scalar product is identical to the quantum mechanical scalar product, which can be expressed as a spatial integral over the two wave functions. Due to the relativistic localization problem discussed in Sec. II, these quantum wave functions are centered *around* z and have a spatial width proportional to the inverse Compton wavelength $1/c$. As a result, any two delocalized states overlap, which is then consistent with the nonvanishing scalar product for $\langle a, z|a, z=0\rangle$.

It is interesting to note that while the wave functions of the states $\hat{\Psi}_D^\dagger(z, t=0)|\text{vac}\rangle$ and $\hat{\Psi}_{KG}^\dagger(z=0, t=0)\sigma_3|\text{vac}\rangle$ are extended in coordinate space, the corresponding states $\hat{b}^\dagger(p)u^\dagger(p)|\text{vac}\rangle$ and $\hat{a}^\dagger(p)r_L^\dagger(p)|\text{vac}\rangle$ are sharply localized in momentum space, i.e., $\langle p|p'\rangle = \delta(p-p')$ and suggest a vanishing overlap.

We might note that the nonvanishing width of the wave function for the electronic state $\hat{\Psi}_a^\dagger(z, t=0)|\text{vac}\rangle$ is associated with the relativistic localization problem according to which positive as well as negative energy eigenstates are required to form a state with an infinitely narrow density. It turns out that the peculiar field theoretical state defined as $|a, Z\rangle \equiv [\hat{\Psi}_a^\dagger(Z) + \hat{\Psi}_a(Z)]|\text{vac}\rangle$ would have the required “localization” property $\langle b, Z|a, Z=0\rangle = \delta(Z)\delta_{a,b}$. As the transition amplitude vanishes outside the light cone it could be used to measure causality at later times. We point out that this is a very peculiar superposition state of an electron with a positron where both particles share the same coordinate. As for each of the three Hamiltonians the overlap integral $\langle b, Z|a, Z=0\rangle = \delta(Z)\delta_{a,b}$ vanishes for $t=0$, one could argue that the transition matrix elements $\langle a, Z, \lambda a, Z=0, t=0\rangle$ can actually be used to characterize causality. In fact, if the states are evolved under \hat{H}_{rS} , this transition amplitude becomes nonzero outside the light cone, whereas for \hat{H}_D and \hat{H}_{KG} it remains zero.

In the literature [1] one finds statements such as “to really discuss causality, however, we should ask not whether particles can propagate over spacelike intervals, but whether a measurement performed at one point can affect a measurement at another spacelike point.” A possible causality violation can then be discussed in terms of the commutativity of the observables. For example, causality should hold if any measurement of observable A at location $z=0$ should not affect any measurement of observable B at location z . We therefore require that the expectation value $\langle A B\rangle$ factors into products of single expectation values for any state, $\langle A B\rangle = \langle A\rangle \langle B\rangle$. Any two measurements are independent of each other if the operators commute, $[A, B]_- = 0$.

We would have to test this equality for any pairs of quantum field theoretical observables. For the rS system, any observable is represented by a Hermitian operator and therefore has to be at least a bilinear combination of the field operator $\hat{\Psi}_{rS}$ and its Hermitian conjugate form $\hat{\Psi}_{rS}^\dagger$. In other words, examining just the simple commutators of the form $[\hat{\Psi}_{rS}(z, t), \hat{\Psi}_{rS}(z=0, t=0)]_-$ or $[\hat{\Psi}_{rS}^\dagger(z, t), \hat{\Psi}_{rS}(z=0, t=0)]_-$, or the relationship between the

field and its conjugate at equal times, $[\hat{\Psi}_{rS}(0), \hat{\Psi}_{rS}^\dagger(0)]_-$, would not be helpful.

The test whether the quantum field theoretical observables for (z, t) and $(z=0, t=0)$ commute with each other outside the light cone is rather straightforward [2] as any commutator of the general form $[AB, CD]_-$ can be rewritten in terms of anticommutators as $A[B, C]_+D - [A, C]_+BD + CA[B, D]_+ - C[A, D]_+B$ or in terms of commutators as $AC[B, D]_- + A[B, C]_-D + C[A, D]_-B + [A, C]_-DB$. The first expression is obviously useful for the fermionic D system, whereas the second expression can be used for the bosonic rS and KG systems. For simplicity we can assume that the operators A, B, C, and D represent the field operators and their adjoints. For the relativistic Schrödinger system we obtain $[\hat{\Psi}_{rS}(z, t), \hat{\Psi}_{rS}^\dagger(z=0, t=0)]_- = G_{rS}(t, z)$. This shows that the rS system is also quantum field theoretically noncausal. It is consistent with the nonvanishing $A_{rS}(z, t)$ for $z > ct$. For the Dirac system, we obtain $[\hat{\Psi}_b(z, t), \hat{\Psi}_a^\dagger(z=0, t=0)]_+ = (i\partial/\partial t + h_D)_{a,b}g(t, z)$ and similarly for the KG system, $[\hat{\Psi}_b(z, t), (\hat{\Psi}_a^\dagger(z=0, t=0)\sigma_3)_a]_- = (i\partial/\partial t + h_{KG})_{a,b}g(t, z)$. Both propagators $g(z, t)$ vanish outside the light cone and therefore suggest that the D and KG systems are causal.

IV. SUMMARY AND DISCUSSION

The main purpose of the present work was twofold. First, it quantified the amount of causality violation for the rS system and showed that it is just a transient effect. Secondly, it pointed out that the discussions of the relativistic localization problem of quantum mechanics and causality need to be considered together.

By comparing causal and noncausal quantum field theories we critically examined various claims about causality. Using the rS system as an example, we have shown that contrary to statements in the literature, quantum field theory cannot be used to “repair” a theory that is already noncausal in quantum mechanics [26]. We also provide an alternative view and argue that the quantum field theoretical transition amplitude between two states at different times can be used to distinguish between causal and noncausal systems. For this amplitude to serve as a useful measure, however, it is necessary that the two states have a vanishing scalar product initially. By defining a quantum field theoretical state as a superposition of a particle and its antiparticle, we have shown that this can be accomplished, permitting us to distinguish consistently between causality violating and preserving Hamiltonians based on transition amplitude outside the light cone.

In this context it is important to point out that from a quantum mechanical perspective, it seems not possible that the action of the quantum field operator at z on the vacuum state can generate a particle whose charge, energy and momentum densities are sharply localized at z , while at the same time any two states that are localized in two disjoint regions ($z \neq z'$) are not orthogonal to each other. In fact, the corresponding wave functions are spatially extended while at the same time they contain a δ -function-like singularity that makes these states non-normalizable. The nonvanishing scalar products are directly related to the overlap of the corresponding quantum mechanical wave functions, which have an infinite extension.

In this context, both the quantum field theoretical and the associated quantum mechanical charge densities for identical states (with positive energy) are not localized. A possible difference between them could be an argument for considering the Dirac and the Klein-Gordon equations entirely in a quantum field theoretical context and not as relativistic extensions of the Schrödinger equation in quantum mechanics.

The usual resolutions to conceptual problems of relativistic quantum mechanics such as the Zitterbewegung or the Klein paradox are based on the fact that quantum field theory can provide the correct interpretation of negative energy states. In this work, however, the states $\hat{\Psi}^\dagger|\text{vac}\rangle$ considered here do not describe any antiparticles and their wave functions contain no negative energy states.

We also note that it is nontrivial to discuss cause and effect in the context of an isolated single particle system. Studies based on these systems can only be used to address the question whether a particle can evolve faster than the speed of light. It has been argued that the independence of two quantum mechanical measurements of spacelike detectors could be used to analyze causality. This sequence of arguments requires the corresponding commutators of the fields or bilinear combinations of them to vanish outside the light cone. In our view, to study cause and effect, truly interacting particle systems should be studied. However, these are very difficult if carried out on a quantum field theoretical level. For a recent attempt to explore the quantum field theoretical interaction between two electrons via force intermediating virtual bosons with temporal resolution see Ref. [27].

In contrast to many physical properties whose invariance under time evolution follows directly from underlying symmetry properties of the Hamiltonian, it seems to us that causality cannot be directly associated with such a fundamental symmetry. As the example studied in this work (and tachyons [28–30] are just another example), Lorentz invariance by itself is not the fundamental reason that leads to causality. It is not clear to us which fundamental property makes some Hamiltonians causal and others non-causal. In fact, while a classical particle speed under h_{SR} is less than c , the quantum mechanical wave packet spreading can exceed c . In this context we would like to point out again the result derived by Hegerfeldt [22] about the universality of noncausal Hamiltonians.

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APPENDIX

We focus our discussion here on the Dirac case. All conclusions are similar for the KG system, even though the derivations are slightly different due to the different commutators. Any quantum field theoretical state $|\Phi\rangle$ that describes an electron can be mapped onto a corresponding quantum mechanical two-component wave function [31], defined as $\varphi_a(z) \equiv \langle \text{vac} | \hat{\Psi}_a(z) | \Phi \rangle$ for $a = 1, 2$. In fact, all field theoretical

scalar products between two states $\langle \Phi' | \Phi \rangle$ can be computed as ordinary scalar products between the corresponding wave functions:

$$\langle \Phi' | \Phi \rangle = \sum_a \int dz \varphi'_a(z)^* \varphi_a(z). \quad (\text{A1})$$

This equality can be easily proven if we use that in the single-electron subspace only the positive energy part of $\hat{\Psi}$, defined as $\hat{\Psi}^{(+)}$ [and proportional to $\hat{b}(p)$], is relevant for the scalar product $\langle \text{vac} | \hat{\Psi}_a(z) | \Phi \rangle$. We therefore have $\langle \Phi' | \hat{\Psi}_a^\dagger(z) | \text{vac} \rangle \langle \text{vac} | \hat{\Psi}_a(z) | \Phi \rangle = \langle \Phi' | \hat{\Psi}_a^{(+)\dagger}(z) \hat{\Psi}_a^{(+)}(z) | \Phi \rangle$ and the identity operator can be expressed as $\sum_a \int dz \hat{\Psi}_a^{(+)\dagger}(z) \hat{\Psi}_a^{(+)}(z) = 1$ in this single-electron space.

As a side issue, we remark that therefore field theoretical observables $\langle \Phi | \hat{O} | \Phi \rangle$ can be computed as ordinary scalar products from the corresponding wave function, $\langle \Phi | \hat{O} | \Phi \rangle = \sum_a \int dz \varphi_a^*(z) o_{qm} \varphi_a(z)$, if a corresponding quantum mechanical operator acting in coordinate space can be found that fulfills $\hat{O} = \sum_a \int dz [\hat{\Psi}_a^{(+)\dagger}(z) o_{qm} \hat{\Psi}_a^{(+)}(z)]$. Furthermore, one can show that if the time dependence of the field theoretical state is given by $i\partial|\Phi\rangle/\partial t = \hat{H}|\Phi\rangle$, then the corresponding quantum wave function fulfills $i\partial\varphi(z,t)/\partial t = h\varphi(z,t)$, where $\hat{H} = \sum_a \int dz [\hat{\Psi}_a^\dagger(z) h \hat{\Psi}_a(z)]$.

Let us now return to the specific quantum field theoretical state

$$|a, z\rangle \equiv \hat{\Psi}_a^\dagger(z, t=0) |\text{vac}\rangle, \quad (\text{A2})$$

which can be written as $(2\pi)^{-1/2} \int dp \hat{b}^\dagger(p) u_a(p) \exp(-ipz) |\text{vac}\rangle$. We show first that its quantum field theoretical charge density defined as

$$\rho_{qf}(z') \equiv \sum_b \frac{1}{2} \langle a, z | [\hat{\Psi}_b^\dagger(z') \hat{\Psi}_b(z') - \hat{\Psi}_b(z') \hat{\Psi}_b^\dagger(z')] | a, z \rangle \quad (\text{A3})$$

is not localized at z , in other words we have to show $\rho_{qf}(z') \neq 0$ if $z' \neq z$. This can be easily proven:

$$\rho_{qf}(z') \equiv \sum_b \frac{1}{2} \langle \text{vac} | \hat{\Psi}_a(z) [\hat{\Psi}_b^\dagger(z') \hat{\Psi}_b(z') - \hat{\Psi}_b(z') \hat{\Psi}_b^\dagger(z')] \hat{\Psi}_a^\dagger(z) | \text{vac} \rangle. \quad (\text{A4})$$

If we use the equal time anticommutator relationships $[\hat{\Psi}_b(z'), \hat{\Psi}_a^\dagger(z)]_+ = 0$ for $z' \neq z$ and $[\hat{\Psi}_b(z), \hat{\Psi}_a(z')]_+ = 0$, we can exchange some of the operators and obtain

$$\rho_{qf}(z') \equiv \sum_b \frac{1}{2} \langle \text{vac} | \hat{\Psi}_a(z) \hat{\Psi}_a^\dagger(z) [\hat{\Psi}_b^\dagger(z') \hat{\Psi}_b(z') - \hat{\Psi}_b(z') \hat{\Psi}_b^\dagger(z')] | \text{vac} \rangle. \quad (\text{A5})$$

As $|\text{vac}\rangle$ is not an eigenstate of the charge operator with eigenvalue zero, we obtain $\rho_{qf}(z') \neq 0$ for $z \neq z'$. We mention that in quantum field theory the state $|a, z\rangle$ is also not localized with respect to its energy and momentum densities, defined as $\sum_b \frac{1}{2} \langle a, z | \{\hat{\Psi}_b^\dagger(z') [h_D \hat{\Psi}(z')]_b - [h_D \hat{\Psi}(z')]_b \hat{\Psi}_b^\dagger(z')\} | a, z \rangle$ and $\sum_b \frac{1}{2} \langle a, z | \{\hat{\Psi}_b^\dagger(z') p \hat{\Psi}_b(z') - [p \hat{\Psi}_b(z') \hat{\Psi}_b^\dagger(z')]\} | a, z \rangle$, respectively.

Let us now discuss the quantum mechanical wave function associated with the state $|a, z\rangle$. We obtain $\varphi_b(z'; a, z) \equiv \langle \text{vac} | \hat{\Psi}_b(z') | a, z \rangle = (2\pi)^{-1} \int dp u_b(p) \exp[ip(z' - z)] u_a(p)$

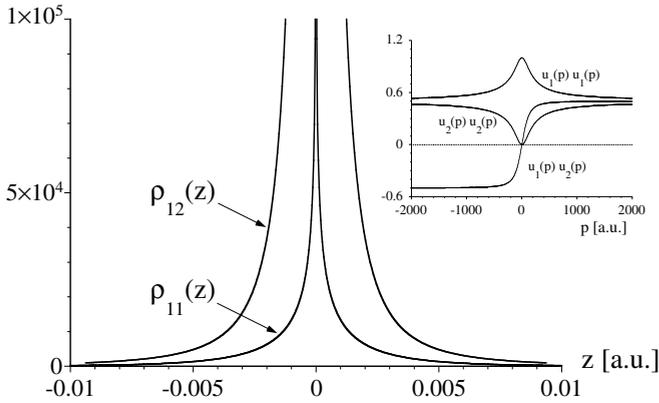


FIG. 3. The quantum mechanical charge densities associated with the quantum field theoretical state $|a,0\rangle \equiv \hat{\Psi}_a^\dagger(0,t=0)|\text{vac}\rangle$ for the Dirac theory.

$\langle \text{vac}|\text{vac}\rangle$. If we use the form of the Dirac spinors $u_a(p)$, we find that $\varphi_b(z';a,z)$ is spatially extended as well as highly singular for $z=z'$.

In the inset in Fig. 3 we have graphed the momentum dependence of the relevant part of the three integrands $u_1(p)u_1(p)$,

$u_2(p)u_2(p)$, and $u_1(p)u_2(p)$. As for large momentum p each of the two spinor components of $u(p)$ approaches $\frac{1}{2}$, the resulting wave function is proportional to the δ function $\sim\delta(z-z')$ for z close to z' . In other words, this peculiar wave function is *not* square-integrable, as $\int dz' [|\varphi_1(z';a,z)|^2 + |\varphi_2(z';a,z)|^2] = \infty$ for $a=1,2$. We also note that the corresponding quantum mechanical charge densities associated with this state for $a=1$ and $a=2$ are identical:

$$\rho_{\text{qm}}(z') = |\varphi_1(z';a,z)|^2 + |\varphi_2(z';a,z)|^2. \quad (\text{A6})$$

Moreover, the graph of each individual contribution (shown in the figure) is clearly *not* spatially localized. In fact, it has a spatial extension of approximately the electron's Compton wavelength $1/c = 0.0073$ a.u..

We have discussed in Sec. II that in quantum mechanics it is not possible for *any* state with positive-only energy contributions to be perfectly localized. As a result, the overlap integral between the wave function for the states $\varphi_b(z';a,z)$ and $\varphi_b(z';a,z=0)$ can be nonzero, which is then fully consistent with the nonvanishing quantum field theoretical amplitude $\langle a,z_1|a,z_2\rangle$ for $z_1 \neq z_2$ at time $t=0$.

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