Maxwell meets Reeh-Schlieder: the quantum mechanics of neutral bosons

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We find that biorthogonal quantum mechanics with a scalar product that counts both absorbed and emitted particles leads to covariant position operators with localized eigenvectors. In this manifestly covariant formulation the probability for a transition from a one-photon state to a position eigenvector is the first order Glauber correlation function, bridging the gap between photon counting and the sensitivity of light detectors to electromagnetic energy density. The position eigenvalues are identified as the spatial parameters in the canonical quantum field operators and the position basis describes an array of localized devices that instantaneously absorb and re-emit bosons.

I. INTRODUCTION

In nonrelativistic quantum mechanics (QM) the wave function is the projection of a particle's state vector onto a basis of position eigenvectors and its absolute square is the positive definite probability density. However, many experimental tests of QM are performed on photons and there is currently no well-defined relativistic QM [1–5] of photons or the neutral Klein-Gordon (KG) bosons often considered in their place for simplicity [6, 7]. Recently it was claimed that the photon wave function [8] and Bohmian photon trajectories [9] were observed using weak measurements. This interpretation, justified by the analogy between the paraxial and Schrödinger equations, is disputed and an alternative interpretation based on the electromagnetic field has been presented [3–5]. In quantum optics most theorists deny the existence of number density and instead base calculations on energy density [3, 4], although QM based on number density has been proposed [10]. The photon wave function and its application to emission by an atom and Bohmian trajectories are reviewed in [11–13]. Two sources of nonlocality have contributed to the perception that there is no relativistic QM or number density: Wave functions are assumed to be of positive frequency while Hegerfeldt's theorem [10] tells us that this restriction leads to instantaneous spreading, and the Newton-Wigner (NW) position eigenvectors [14] are localized in the sense that they are orthogonal but their relationship to the physical fields and to current sources is nonlocal in configuration space. We will argue here that both of these sources of nonlocality are nonphysical: In biorthogonal QM [15] the nonlocal transformation to the NW basis is not required [12] and a scalar product exists [13] that does not require separation of the fields into their nonlocal [6] positive and negative frequency parts [2, 16]. As a consequence real fields are allowed and the paradoxical observer dependence of particle density on acceleration [7, 25] can be avoided. In the manifestly covariant formalism derived here we identify the position eigenvalues of relativistic QM with the spatial parameters in the canonical quantum field theory (QFT) operators and the localized states as derivatives of Green functions that describe an array of emitting and absorbing devices localized in spacetime. This unifies the physical interpretation of the position coordinate in classical electromagnetism, relativistic QM and QFT.

The conventional scalar product [7] is a difference of particle and antiparticle terms so it is indefinite unless the field is limited to positive frequencies. The scalar product derived in [23–25] is positive definite for both positive and negative frequency fields. If this scalar product is used, inclusion of negative frequency states becomes mathematically straightforward. First quantized fields describing neutral KG particles and photons are real so inclusion of negative frequency fields is not only reasonable, it is essential. For photons the first quantized theory derived in [23] restricted to real fields is essentially classical electrodynamics with a rule for calculating number density. However, QFT is required for description of multiphoton states and entanglement. It is a consequence of the Reeh-Schlieder (RS) theorem [26] of algebraic QFT (AQFT) [27] that there are no local creation or annihilation operators and the vacuum is entangled across spacelike separated regions [6, 12, 25]. Any number operator that counts a particle by annihilating it with the positive frequency part of a field operator and then recreating it is nonlocal. Localization is a finite region requires summation over positive and negative frequencies [30]. A particle’s energy must be bounded from below to prevent it from acting as an infinite energy source [4] so it is essential to make a distinction between energy and frequency. In AQFT, also called local QFT, causality is enforced by the microcausality assumption that field operators defined across space-like separated regions commute [2]. In Sections 3 and 4 both positive and negative frequency states will be defined and in Section 6 their interpretation in terms of absorbed and emitted positive energy particles will be elaborated on. We find no conflict of our localized bases with AQFT; rather the RS

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theorem and microcausality support our proposal that, in a covariant formulation, both absorbed and emitted neutral bosons should be counted.

The wave functions derived in [22, 26] are projections of the field onto NW position eigenvectors [21]. NW found a position operator for KG particles, but they concluded that the only photon position operator is the Pryce operator whose vector components do not commute [31], making the simultaneous determination of photon position in all three directions of space impossible. They had assumed symmetrically position eigenstates for photons, while photon position eigenvectors have an axis of symmetry like twisted light [32]. The photon Poincaré group is discussed in [23, 26]. Following the NW method with omission of the spherical symmetry axiom, a photon position operator with commuting components and cylindrically symmetrical eigenvectors can be constructed [33]. Since spin and orbital angular momentum are not separately observable [35], its eigenvectors have only definite total angular momentum along some fixed but arbitrary axis [34]. A generalization of this cylindrically symmetric NW position operator was derived independently in [23]. Here we retain this symmetry but omit the NW similarity transformation that leads to nonlocality in configuration space.

The similarity transformation to the NW basis preserves scalar products but its nonlocal relationship to the physical fields has been interpreted as a nonlocal relationship between number density and energy density [14]. The nontrivial metric factor in the NW basis is not physically observable [36], and this suggests that nonlocality of the NW position eigenvectors is also not physically observable. Here we will work in the formalism of biorthogonal QM [21] that does not require transformation to the NW basis. Biorthogonal QM in a finite dimensional Hilbert space is summarized here as follows: The eigenvectors of a quasi-Hermitian operator $\hat{O}$ and its adjoint $\hat{O}^\dagger$ are not orthogonal, as is the case for conventional Hermitian operators, but biorthogonal. This means that, given the eigenvector equations

$$\hat{O}|\omega_i\rangle = \omega_i|\omega_i\rangle,$$

(1)

$$\hat{O}^\dagger|\omega_j\rangle = \omega_j|\omega_j\rangle,$$

(2)

we have $\langle \omega_j|\omega_i\rangle = \delta_{ji} \langle \omega_i|\omega_i\rangle$ and the completeness relation $\hat{1} = \sum_i |\omega_i\rangle \langle \omega_i|$. An arbitrary state $|\psi\rangle$ has an associated state $|\tilde{\psi}\rangle$. If an arbitrary state vector is expanded as $|\psi\rangle = \sum_i c_i |\omega_i\rangle$ in the Hilbert space $\mathcal{H}$ then in biorthogonal QM its associated state is $|\tilde{\psi}\rangle = \sum_i c_i |\tilde{\omega}_i\rangle \in \mathcal{H}^*$ where $c_i = \langle \omega_i|\psi\rangle = \langle \tilde{\omega}_i|\tilde{\psi}\rangle$. Using these expansions it is straightforward to verify that $\langle \tilde{\psi}_1|\tilde{\psi}_2\rangle = \langle \psi_1|\psi_2\rangle$. The probability for a transition from a quantum state $|\psi\rangle$ to an eigenvector $|\omega_i\rangle$ of $\hat{O}^\dagger$ is

$$p_i = \frac{\langle \tilde{\omega}_i|\psi\rangle^2}{\langle \tilde{\psi}|\psi\rangle \langle \tilde{\omega}_i|\tilde{\omega}_i\rangle}.$$  

(3)

A generic operator can be written in the form

$$\hat{F} = \sum_{i,j} f_{ij} |\omega_i\rangle \langle \omega_j|$$

(4)

where $f_{ij} = \langle \omega_i|\hat{F}|\omega_j\rangle$ can be viewed as a matrix [21]. An equivalent bottom up approach is to start with a set of linearly independent not necessarily orthogonal vectors and obtain a biorthogonal basis and operators describing observables [36]. In Section 3 we will apply this formalism to the biorthogonal position eigenvectors $|\phi(x)\rangle = \tilde{\phi}(x)|0\rangle$ and $|\tilde{\phi}(x)\rangle = |\pi(x)\rangle \propto \tilde{\pi}(x)|0\rangle$ where $x^\mu = (ct, \mathbf{x})$, $\tilde{\phi}(x)$ is a field operator, $\tilde{\pi}(x)$ is its conjugate momentum operator, and $|0\rangle$ is the global vacuum state. Extension of biorthogonal QM to this infinite-dimensional Hilbert space is not rigorous; for example completeness could fail as discussed in [21].

The rest of this paper is organized as follows: In Section 2 KG wave mechanics, with the field rescaled here to facilitate application to particles with zero mass, is reviewed. In Section 3 the covariant position operator and positive definite probability density are derived. In Section 4 the KG position observable discussed in Sections 2 and 3 is extended to photons. In Section 5 the wave function of the photon emitted by an atom is discussed, in Section 6 inclusion of negative frequency states, causality and localized states are examined, and in Section 7 we conclude.

II. KLEIN-GORDON WAVE MECHANICS

We will start with a review of the KG position observable problem. The KG equation

$$\partial_\mu \partial^\mu \phi(x) + \frac{m^2 c^2}{\hbar^2} \phi(x) = 0$$

(5)

describes charged and neutral particles with zero spin (pions). Here covariant notation and the mostly minus convention are used in which $x^\mu = x = (ct, \mathbf{x})$, $\partial_\mu = (\partial_t, \nabla)$, $m$ is the mass of the KG particle, $c$ is the speed of light, $2\pi\hbar$ is Planck’s constant and $f_1 \partial_\mu f_2 \equiv f_1 (\partial_\mu f_2) - (\partial_\mu f_1) f_2$. The function $\phi(x)$ is any scalar field that satisfies the KG equation (5). The four-density satisfies a continuity equation. Plane wave normal mode solutions to (5) proportional to $\exp(-i\omega t)$ are referred to as positive frequency solutions, while those proportional to $\exp(i\omega t)$ are negative frequency. Completeness requires that both positive and negative frequency modes be included. Their contributions to $J^\mu_{KG}(x)$ are of opposite sign, so $J^\mu_{KG}(x)$ is interpreted as charge density and the quantity $g$ in (6) is set equal to $qc/\hbar$ for particles of charge $q$. 
If only particles, as opposed to both particles and antiparticles, are to be considered, then the KG field can be restricted to positive frequencies and the scalar product

\[
(\phi_1, \phi_2)^\text{KG} = \frac{1}{\hbar} \int dx \phi_1(x)^* \hat{\partial}_t \phi_2(x) \tag{7}
\]
is positive definite. Here \(t\) denotes a spacelike hyperplane of simultaneity at instant \(t\). The integrand of (7) looks like a particle density but this is misleading since \(J^\mu_{\text{KG}}(x)\) can still be negative if components with two or more different frequencies are added. Restriction to positive frequencies is especially problematic in the case of neutral particles that should be described by real fields.

The problem of a probability interpretation for KG particles has a long history. Lack of a probability interpretation led Dirac to derive his celebrated equation for spin half particles, but this does not solve the problem for KG fields. In a seminal paper intended to clarify the confusion about relativistic wave mechanics, Feshbach and Villars reviewed the two component formalism that separates the wave function into its particle and antiparticle parts for charged or for neutral particles. Their treatment of neutral particles was based on energy density. Since this work various strategies have been employed to derive a positive definite probability density. The four-current density can be redefined so that its zeroth component is positive definite, but this construction has no apparent physical basis and it fails if \(m = 0\). It has been proposed that for charged pions only positive definite eigenstates of the Hamiltonian are physical. A new \(J^\mu(x)\) was derived that does not require separation of the field into positive and negative frequency parts so it can be applied to the real fields that describe neutral pions. If \(\phi(x)\) is restricted to positive frequencies it reduces to (4) so this \(\phi(x)\) that describes an arbitrary linear combination of positive and negative frequency fields, including real fields, will be used here.

Working in the two component formalism with a pseudo-Hermitian Hamiltonian Mostafazadeh defined the positive-definite Hermitian operator

\[
\hat{D} \equiv -\nabla^2 + m^2 c^2 / \hbar^2 \tag{8}
\]
in terms of which the KG equation is \((\hat{D} + \hat{\partial}_ct^2) \psi = 0\). He derived the conjugate field

\[
\phi_c(x) = i \hat{D}^{-1/2} \hat{\partial}_ct \phi(x) \tag{9}
\]
such that if \(\phi = \phi^+ + \phi^-\) then \(\phi_c = \phi^+ - \phi^-\). This implies that \(\phi_c\) is a scalar. It is then straightforward to verify that \(\phi_c\) satisfies the KG equation and that

\[
J^\mu_c(x) = \frac{1}{\hbar} \phi(x)^* \hat{\partial}_t \phi_c(x) \tag{10}
\]
satisfies the continuity equation \(\partial_\mu J^\mu = 0\). Up to a constant that just scales \(J^\mu\), is the expression derived in [4, 44]. Like (11), \(J^\mu(x)\) is manifestly covariant. It was proved in [26, 14] that the scalar product

\[
(\phi_1, \phi_2) = \frac{1}{\hbar} \int dx \phi_1(x)^* \hat{\partial}_t \phi_2(x) \tag{11}
\]
is positive definite, time independent and can be written in covariant form as

\[
(\phi_1, \phi_2) = \frac{2e}{\hbar} \sum_{\epsilon = \pm} \langle \phi_1 | \hat{D}^{1/2} \phi_2 \rangle \tag{13}
\]

where

\[
\langle \chi_1 | \chi_2 \rangle = \int dx \chi_1^*(x) \chi_2(x). \tag{14}
\]

The non-relativistic Hilbert space is the vector space of square integrable continuous functions with the scalar product (11). In the relativistic Hilbert space the scalar product used here is (13). These scalar products can be evaluated in configuration space or in \(k\)-space. The covariant Fourier transform is

\[
\phi^\epsilon(x) = \int \frac{dk}{(2\pi)^3} \pi^\epsilon(k) e^{-i(\omega_k t - k \cdot x)}. \tag{15}
\]

Since \(\phi^\epsilon(x)\) is a scalar and \(dk / [(2\pi)^3 2\omega_k]\) is invariant, \(\pi^\epsilon(k) \in \mathcal{H}^*\) is a scalar, analogous to the transformation properties of photons. For \(\omega_k = \sqrt{k^2 c^2 + m^2 c^4 / \hbar^2}\) the function \(\phi^\epsilon(x)\) satisfies the KG equation and (13) can be written as

\[
(\phi_1, \phi_2) = \frac{1}{\hbar} \sum_{\epsilon = \pm} \int \frac{dk}{(2\pi)^3 2\omega_k} \pi^\epsilon_1(k) \pi^\epsilon_2(k). \tag{16}
\]

In the biorthogonal formalism the bases \(\{\phi^j_\chi, (k)\} = \{\pi^\chi_\chi, (k) / \omega_k\} \in \mathcal{H}\) and \(\{\pi^\chi_\chi, (k) \in \mathcal{H}^*\) are biorthogonal and complete and the Hermitian adjoint of an operator is its complex conjugate transpose. Since the scalar product (13) is positive definite, standard QM can be recovered if a nontrivial metric operator \(\langle \cdot | \Theta \cdot \rangle\) is introduced. In this metric formulation the basis \(\{\pi^\chi_\chi, (k) \) and operators are Hermitian. With the metric \(\langle \cdot | \cdot \rangle\) operators representing observables can be non-Hermitian with biorthogonal eigenvectors. The norm and orthogonality of the elements of the Hilbert space and the concept of Hermiticity are determined by the
definition of scalar product. Newton and Wigner defined the KG fields \( \tilde{\phi}_x (k) \propto e^{-i k \cdot x} \omega_k^{1/2} \) that satisfy \((\phi_1, \phi_2) \propto \delta (x_1 - x_2) \) and are eigenvectors of the position operator \( i \nabla_k - \frac{\omega_k^2}{2} \). Hermiticity of the NW position operator with eigenvectors of this form is discussed by Pike and Sarkar \(^17\). The NW position operator has played a central role in the discussion of relativistic particle position since its publication in 1949 \(^20\), but this operator is not covariant and its eigenvectors are not localized. We will show in the next section that the formalism of biorthogonal QM is to avoid falling into the trap of treating position operators that satisfy the completeness relation are consistent with \(^18\). If limited to the calculation of scalar products and expectation values the biorthogonal formalism is completely equivalent to the Hermitian formalism with a nontrivial metric, so the role biorthogonal QM is to avoid falling into the trap of treating NW nonlocality as a physically observable effect.

III. KG POSITION EIGENVECTORS

In this Section the second quantized formulation will be discussed first to motivate the definition of the biorthogonal basis. Positive and negative frequency basis states are then defined that provide a configuration space basis for first or second quantized states. A completeness relation, position operator and particle number density are derived within the framework of biorthogonal QM. The relationship of this covariant position operator to the Hermitian NW position operator is examined.

In QFT particles are created at a point in spacetime by a field operator or its canonical conjugate. The interaction picture (IP) scalar field operators \( \hat{\phi} (x) \) and \( \tilde{\pi} (x) = \partial_t \hat{\phi} (x) \) will be written as

\[
\hat{\phi} (x) = \sqrt{\hbar} \int \frac{dk}{(2\pi)^3 2\omega_k} e^{i (k \cdot x - \omega_k t)} \hat{a}^\dagger (k) + \text{H.c.},
\]

\[
\tilde{\pi} (x) = i \sqrt{\hbar} \int \frac{dk}{(2\pi)^3 2} e^{i (k \cdot x - \omega_k t)} \hat{a}^\dagger (k) + \text{H.c.}
\]

where H.c. is the Hermitian conjugate and the k-space covariant commutation relations are \(^4\)

\[
[\hat{a} (k), \hat{a}^\dagger (q)] = (2\pi)^3 2\omega_k \delta (k - q).
\]

On the t hyperplane the field operators satisfy the commutation relations

\[
[\hat{\phi} (x), \tilde{\pi} (y)] = i \hbar \delta (x - y).
\]

If the global vacuum state \( |0\rangle \) is defined by the condition \( \forall k \hat{a} (k) |0\rangle = 0 \) then, as we will show below, the field operators create biorthogonal states.

In the IP the basis vectors are time dependent \(^32\). To accommodate the possibility of including negative frequency wavefunctions, \( \epsilon = \pm \) states will be defined as

\[
|\phi^\epsilon (x)\rangle = \sqrt{\hbar} \int \frac{dk}{(2\pi)^3 2\omega_k} e^{i (\omega_k t - k \cdot x)} |1_k\rangle,
\]

\[
|\pi^\epsilon (x)\rangle = \sqrt{\hbar} \int \frac{dk}{(2\pi)^3 2} e^{i (\omega_k t - k \cdot x)} |1_k\rangle,
\]

where \( |\pi^\epsilon (x)\rangle \equiv e^{\tilde{D}^{1/2}} |\phi^\epsilon (x)\rangle \) so that the phase factor \( i \) has been absorbed into the bases and

\[
i \partial_t |\phi^\epsilon (x)\rangle = -\epsilon e^{\tilde{D}^{1/2}} |\phi^\epsilon (x)\rangle.
\]

With these definitions annihilation is described by projection onto \( |\pi^\epsilon (x)\rangle \) so that \( \langle \pi^\epsilon (x) | \psi^\pm \rangle \) is positive frequency while

\[
\langle \pi^- (x) | \psi^- \rangle = \langle \pi^+ (x) | \psi^+ \rangle^* = \langle \psi^+ | \pi^+ (x) \rangle
\]

is negative frequency where \( \epsilon = + \) refers to a particle arriving from the past and absorbed on \( n \), while \( \epsilon = - \) refers to a particle emitted on \( n \) and propagating into the future. These basis vectors are biorthogonal in the sense that

\[
\langle \pi^\epsilon (x) | \phi^{\epsilon'} (y) \rangle = \frac{\hbar}{2} \delta_n (x - y) \delta_{\epsilon \epsilon'}.
\]

Based on \(^12\) there are no \( \epsilon = + / \epsilon = - \) cross terms in the scalar product. The notation \( \delta_n (x - y) \) is defined to select \( x \) and \( y \) such that \( x^\mu = y^\mu \) on the hyperplane with normal \( n_\mu \). Since \( |\phi^\epsilon (x)\rangle \) and \( |\pi^\epsilon (x)\rangle \) are biorthogonal, they satisfy the completeness relation

\[
\hat{\mathfrak{T}} = \frac{2}{\hbar} \sum_{\epsilon = \pm} \int dx |\phi^\epsilon (x)\rangle \langle \pi^\epsilon (x) |
\]

where the factor \( 2/\hbar \) is due to normalization (see \(^25\)). The states \(^21\) can be interpreted as basis states for solutions to the first quantized KG wave equation or as one-particle states in QFT.

It can be verified by substitution that the basis states \(^21\) and \(^22\) are eigenvectors of a position operator of the form \(^14\),

\[
\hat{x} = \frac{2}{\hbar} \sum_{\epsilon = \pm} \int dx x |\phi^\epsilon (x)\rangle \langle \pi^\epsilon (x) |,
\]

and its adjoint, that is

\[
\hat{x} |\phi^\epsilon (x)\rangle = x |\phi^\epsilon (x)\rangle,
\]

\[
\hat{x}^\dagger |\pi^\epsilon (x)\rangle = x |\pi^\epsilon (x)\rangle,
\]

consistent with their biorthogonality. Any classical or one-particle state can therefore be projected onto the configuration space basis as

\[
|\psi (t)\rangle = \hat{x} |\psi (t)\rangle = \frac{2}{\hbar} \sum_{\epsilon = \pm} \int dx |\phi^\epsilon (x)\rangle \langle \pi^\epsilon (x) | \psi (t) \rangle,
\]

\[
|\tilde{\psi} (t)\rangle = \hat{x}^\dagger |\tilde{\psi} (t)\rangle = \frac{2}{\hbar} \sum_{\epsilon = \pm} \int dx |\pi^\epsilon (x)\rangle \langle \phi^\epsilon (x) | \tilde{\psi} (t) \rangle.
\]
The wave function
\[ \psi^\epsilon (x) = (\pi^\epsilon (x) | \phi^\epsilon (t)) \]
completely describes the state \(|\Psi(t)\rangle\) in the \(|\phi^\epsilon (x)\rangle\) basis of position eigenvectors. It may have positive frequency \((\epsilon = +)\) and negative frequency \((\epsilon = -)\) components.

According to the rules of biorthogonal QM outlined in Section 1 we have the equality
\[ \langle \phi^\epsilon (x) | \psi^\epsilon (t) \rangle = \langle \pi^\epsilon (x) | \psi^\epsilon (t) \rangle. \]
Using (25), (30) and (33) the squared norm of \(|\psi (t)\rangle\),
\[ \langle \psi | \psi \rangle = \frac{2}{\hbar} \sum_{\epsilon = \pm} \int dx |(\pi^\epsilon (x) | \psi^\epsilon (t))|^2, \]
and the probability density,
\[ p^\epsilon (x) = \frac{2}{\hbar} |(\pi^\epsilon (x) | \psi^\epsilon (t))|^2, \]
is positive definite where \(\langle \psi | \psi \rangle = 1\) for a one-particle state. The expectation value of the position operator [27] is \(\langle \psi | \hat{x} \psi \rangle = \frac{2}{\hbar} \sum_{\epsilon = \pm} \int dx \pi^\epsilon (x) x \psi^\epsilon (x)\).

Since this application of biorthogonal QM is based on an invariant scalar product, the QM that it describes is covariant. In particular, the wave function of a plane wave, \(|1_q\rangle\), is \((1_k | 1_q\rangle = (2\pi)^3 2\omega_\epsilon \delta (k - q)\) in Fourier space and \(|\phi^\epsilon (x) | 1_q\rangle = \sqrt{\hbar e^{-i(\omega_k - q \cdot x)}}\) in configuration space and a localized state, \(|\phi (y)\rangle\), is \((1_k | \phi (y)\rangle = \sqrt{\hbar e^{i(\omega_k t - k \cdot x)}}\) in Fourier space and \(|\pi^\epsilon (x) | \phi (y)\rangle = \frac{i}{\hbar} \delta_n (x - y)\) in configuration space. Eqs. (26) and (27) can be generalized to
\[
\hat{t} = \frac{2}{\hbar} \int d\sigma |\phi (x)\rangle \langle -i e_n \partial^\mu \phi (x)|, \quad (36)
\]
\[
\hat{x}_i = \frac{2}{\hbar} \int dx_i |\phi (x)\rangle \langle -i e_n \partial^\mu \phi (x)|, \quad (37)
\]
respectively where \(x_i n^\mu = ct_0\) on the hyperplane with normal \(n_i\) and \(t_0\) is the hyperplane of simultaneity [51, 59]. The matrix representing the position observable in configuration space is
\[ x_i (x, y) = \sum_{\epsilon = \pm} \langle \pi^\epsilon (x) | \hat{x}_i \pi^\epsilon (y) \rangle_n = x_i \delta_n (x - y) \quad (38)\]
where \(x_i\) is on the \(n\) hyperplane.

The relationship of the relativistic position operator to the nonrelativistic position operator \(i\nabla\) and the NW position operator can be seen by transforming to Fourier space. The position operator [27] is in the IP while the conventional position operator is time independent so it is in the Schrödinger picture (SP). For positive frequency fields the SP position operator [27] is
\[ \hat{x}^{SP} = \int \frac{dk}{2(2\pi)^3} \int \frac{dq}{2(2\pi)^3} \int dx \ exp(-i k \cdot x) \frac{1}{\omega_k} |1_k| e^{i q \cdot x}. \]
Since \(\int dx \exp(i q \cdot \nabla k) e^{-i k \cdot x} = (2\pi)^3 i \nabla k \delta (q - k)\),
\[ \hat{x}^{SP} (k) = i \nabla k, \quad (40)\]
so that \(i \nabla k\) is the position operator in the \(|1_k/k\rangle\langle 1_k|\) basis. When operating on \(e^{-i k \cdot x}\) it extracts the position \(x\) where the particle was created. With positive definite Hermitian metric \(\Theta\), the scalar product is \(|\Theta|\) and an operator \(\tilde{O}\) is quasi-Hermitian if \(\Theta \tilde{O} = \tilde{O} \Theta\) [16]. Since according to (27) \(\tilde{x} = D^{1/2} \tilde{D}^{-1/2}\), the position operator is quasi-Hermitian. Indeed defining \(S = \Theta^{1/2}\), the operator \(\tilde{\sigma} = \tilde{\sigma}^\dagger = S^{-1} \tilde{O}^\dagger \tilde{S}\) is Hermitian. In (10) the metric is \(\Theta = \omega_k^{-1}\) so \(S = \omega_k^{-1/2}\), the basis is \(|\omega_k^{-1/2} | 1_k\rangle\) and the matrix representing the NW position operator [20, 26, 44],
\[ \hat{x}^{NW} (k) = \omega_k^{1/2} \nabla k \omega_k^{-1/2}, \quad (42)\]
is of the form \(\tilde{\sigma} = S^{-1} \tilde{O}^\dagger S\) for \(\tilde{O} = \hat{x}^{SP} (k)\) where \(\omega_k^{1/2} \nabla k \omega_k^{-1/2} = i \nabla k - \frac{c}{\omega_k} k\). The factors \(\omega_k^{1/2}\) introduce nonlocality into the configuration space description of the position eigenvectors. This nonlocality is not physical since it does not appear in the manifestly covariant description of the position observable. This is consistent with the metric operator being not physically observable as discussed in [30].

IV. PHOTONS

For photons the scalar field \(\phi\) should be replaced with the four-vector potential \(A^\mu\). Both \(A_\mu \partial^\nu A^\mu = (A_{\nu} \partial_{\mu} A^\nu, A_\nu \nabla A^\nu)\) and \(A_\mu F^{\mu\nu} = (A \cdot E/c, A \times B)\) multiplied by \(i e_0 c / \hbar\) are candidates for the four-current density, \(F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu\) being the Faraday tensor. The properties of an operator of the form \(i A_{\mu} F^{\mu\nu}\) were investigated in [50]. The Coulomb gauge condition \(\nabla \cdot A = 0\) is not Lorentz invariant, but \(A_\mu\) can be chosen to transform as a Lorentz four-vector up to an extra term that maintains the Coulomb gauge in all frames of reference [18]. To avoid the complications associated with nonphysical longitudinal and scalar photons the Coulomb gauge will be used in this Section. In a source-free region in the Coulomb gauge both \(A_\mu \partial^\nu A^\mu\) and \(A_\mu F^{\mu\nu}\) reduce to \((A_\perp \cdot E/c, A_\perp \times B)\).

Following (10) we can define
\[ J^\mu (x) = \frac{i e_0 c}{\hbar} \sum_{\lambda, i} A_{\lambda i} (x) e^{i \xi_\perp A_{\lambda ci} (x)} \quad (43)\]
where \(A_\lambda\) is a transverse vector potential of helicity \(\lambda\) that satisfies the classical Maxwell wave equation \((\tilde{D} + \partial^2 c_t) A_\lambda = 0\) where \(m = 0\) so \(\tilde{D} = -\nabla^2\). The conjugate field is \(A_{\lambda c} \equiv i \tilde{D}^{-1/2} \partial_{ct} A_\lambda = A_\lambda^+ - A_\lambda^\perp\)
where $A_\lambda = A^\dagger_\lambda + A^-_\lambda$. It can then be verified by substitution that (53) satisfies the continuity equation $\partial_\mu J^\mu (x) = 0$. As a consequence the scalar product $\int d^3 x' n_\mu J^\mu (x')$ is Lorentz invariant up to a term that maintains the Coulomb gauge. The photon scalar product that replaces (53) is

$$\langle A_1, A_2 \rangle = \frac{2 \epsilon_0 c}{\hbar} \sum_{\lambda, \epsilon, i} \left\langle A^\epsilon_{1 \lambda} | \tilde{D}^{1/2} A^\epsilon_{2 \lambda} \right\rangle$$

(44)

where $A = A^\mu = (0, A_\perp)$.

For photons described in the Coulomb gauge, the field operator is $\tilde{A}_\perp(x,t)$ and its canonical conjugate is $-\epsilon_0 \tilde{E}_\perp(x,t)$ where $\tilde{E}_\perp$ is the electric field operator. The Fourier space spherical polar coordinates will be called $k, \theta_k$ and $\phi_k$ and their corresponding unit vectors $e_k, e_\theta$ and $e_\phi$. The definite helicity transverse unit vectors are $e_k(k) = (e_\theta + i \lambda e_\phi) / \sqrt{2}$ where $\lambda$ is helicity. The NW photon position operator with commuting components can be written in Fourier space as

$$\tilde{x} = \tilde{E} \left( \varpi_k^{-1/2} \nabla_k \omega_k \right) \tilde{E}^{-1}$$

where $\tilde{E}$ is a rotation through Euler angles to fixed reference axes. The basic idea is the same as was used in the derivation of the NW position operator in (26); the position information is contained in the factor $\exp(ik \cdot x)$ in the wave function but the factor $\omega_k^{1/2}$ must be eliminated before the nonrelativistic position operator $\nabla_k$ can be used to extract this information. For the transverse fields that describe photons an additional unitary transformation $\tilde{E}$ that rotates the field vectors to axes fixed in space is needed. A position eigenvector has a vortex structure like twisted light (32) in which the photon position eigenvalue $\mathbf{x}$ is the center of internal angular momentum (31). We have seen here that it is also the parameter $\mathbf{X}$ in the field operators. In the position operator derived in (32) the relevant case is $\alpha = 0$.

Following the derivation in Section 3, the IP photon position operator is

$$\hat{x} = \frac{2 \epsilon_0 c}{\hbar} \sum_{\epsilon, \lambda, \pm} \int dx \cdot \mathbf{x} | A^\epsilon_{\lambda} (x) \rangle \langle \mathbf{x} | A^\prime \lambda \rangle (x) \rangle,$$

(45)

the position eigenvector equations are

$$\hat{x} | A^\epsilon \lambda \rangle (x) \rangle = \mathbf{x} | A^\epsilon \lambda \rangle (x) \rangle,$$

(46)

$$\hat{x} | E^\epsilon \lambda \rangle (x) \rangle = \mathbf{x} | E^\epsilon \lambda \rangle (x) \rangle$$

(47)

and position basis states are

$$| A^\epsilon \lambda \rangle (x) \rangle \rangle \equiv \tilde{A}^- \lambda \rangle (x) \rangle,$$

(48)

$$| A^\epsilon \lambda \rangle (x) \rangle = \tilde{A}^\dagger \lambda \rangle (x) \rangle \rangle^\dagger$$

(49)

$$| E^\epsilon \lambda \rangle (x) \rangle = c \tilde{D}^{1/2} | A^\epsilon \lambda \rangle (x) \rangle,$$

(50)

Here the potential operator reads

$$\tilde{A}^- \lambda (x) = \sqrt{\frac{\hbar}{\epsilon_0}} \int \frac{dk}{(2\pi)^3 2\omega_k} e^{i(k \cdot \mathbf{x} - \omega_k t)} \tilde{a}^- \lambda (k).$$

(51)

The Fourier space canonical commutation relations and orthogonality relations are

$$\left[ \tilde{a}^\dagger \lambda (k), \tilde{a}^\dagger \lambda (q) \right] = (2\pi)^3 2\omega_k \delta (k - q) \delta_{\sigma \sigma'},$$

(52)

$$\langle 1_{\lambda, k} | 1_{\sigma, q} \rangle = (2\pi)^3 2\omega_k \delta (k - q) \delta_{\lambda \sigma},$$

(53)

where $| 1_{\lambda, k} \rangle \equiv a^\dagger \lambda (k) | 0 \rangle$. These photon position eigenvectors are biorthogonal that is

$$\sum_{i=1}^3 \left\langle E^\epsilon_{\lambda i} (x) | A^\sigma_{\epsilon i} (y) \right\rangle = \frac{\hbar}{2\epsilon_0} \delta_n (x - y) \delta_{\lambda \sigma} \delta_{\epsilon \epsilon'}$$

(54)

where the subscripts $i$ denote Cartesian components of the three-vectors, $\epsilon = +$ for absorption at $x$ while $\epsilon = -$ for emission at $x$, and the scalar product (51) is $(A^\epsilon \lambda \rangle (x), A^\sigma \lambda \rangle (y)) = \delta_n (x - y) \delta_{\lambda \sigma}$. For free photons described by transverse fields the completeness relation is

$$\tilde{E} = \frac{2 \epsilon_0 c}{\hbar} \sum_{\epsilon, \lambda, \pm} \int dx \left| A^\epsilon \lambda (x) \rangle \langle \mathbf{x} \right| \langle \mathbf{x} | E^\epsilon \lambda \rangle (x) \rangle,$$

(55)

where we have defined

$$| A^\epsilon \lambda \rangle (x) \rangle \rangle \equiv \sum_{i=1}^3 | A^\epsilon_{\lambda i} (x) \rangle \langle E^\epsilon_{\lambda i} (x) \rangle.$$

(56)

The identity operator $\tilde{E}$ on the space of transverse photons is closely connected to the so-called ‘transverse Dirac delta’ of QED (32). For any transverse state we can then write

$$| \psi \rangle (t) = \frac{2 \epsilon_0 c}{\hbar} \sum_{\epsilon, \lambda, \pm} \int dx | A^\epsilon \lambda \rangle (x) \rangle \langle \mathbf{x} | \psi (t) \rangle,$$

(57)

and the wave function

$$\psi^\epsilon \lambda (x) = \langle \mathbf{x} | \psi \rangle (t)$$

(58)

completely describes the state $| \psi \rangle (t)$ in either basis of position eigenvectors. The dual state vector is

$$\left| \psi \rangle (t) \right>= \frac{2 \epsilon_0 c}{\hbar} \sum_{\epsilon, \lambda, \pm} \int dx | E^\epsilon \lambda \rangle (x) \rangle \langle \mathbf{x} | A^\epsilon \lambda (x) \rangle \rangle,$$

(59)

the squared norm is

$$\langle \psi \langle \tilde{\psi} \rangle = \frac{2 \epsilon_0 c}{\hbar} \sum_{\epsilon, \lambda, \pm} \int dx | \psi^\epsilon \lambda (x) |^2$$

(60)

and the probability density for a transition from $| \psi \rangle (t)$ to the $\epsilon$-frequency position eigenvector with helicity $\lambda$

$$p^\epsilon \lambda (x) = \frac{2 \epsilon_0 c}{\hbar} | \psi^\epsilon \lambda (x) |^2$$

(61)

$$= \frac{\langle \psi \langle \tilde{\psi} \rangle | \psi^\epsilon \lambda (x) |^2}{\sum_{\epsilon, \lambda, \pm} \int dx | \psi^\epsilon \lambda (x) |^2}.$$
is positive definite with \( \langle \psi | \bar{\psi} \rangle = 1 \) for a one-photon state.

A state can be Fourier expanded as
\[
|\psi_\perp (t)\rangle = \sum_{\lambda, \epsilon = \pm} \frac{\dd k}{(2\pi)^{3/2}} c_\lambda (k, t) |1, \lambda, k\rangle. \tag{62}
\]

Eqs. 45 to 53 give \( (\mathbf{E}_\lambda (x) |1, \lambda, k\rangle / \omega_k = (\mathbf{A}_\lambda (x) |1, \lambda, k\rangle \) so that \( |1, \lambda, k\rangle / \omega_k \in \mathcal{H} \) and \( |1, \lambda, k\rangle \in \mathcal{H}^* \). Substitution in 55 then gives the dual state vector
\[
|\bar{\psi}_\perp (t)\rangle = \sum_{\lambda, \epsilon = \pm} \int \frac{\dd k}{(2\pi)^{3/2}} c_\lambda (k, t) |1, \lambda, k\rangle. \tag{63}
\]

The probability amplitude for a transition to a \( \epsilon \)-frequency plane wave state with wave vector \( \mathbf{k} \) and helicity \( \lambda \) is proportional to \( \langle 1, \lambda, k | \bar{\psi}_\perp (t) \rangle = c_\lambda (k, t) \). According to the rules of biorthogonal QM outlined in the Introduction the probability density for this transition is
\[
p_\lambda (k) = \frac{\langle 1, \lambda, k | \bar{\psi}_\perp (t) \rangle^2}{(2\pi)^3 2} = \frac{\langle \bar{\psi}_\perp (t) | \psi_\perp (t) \rangle}{\sum_{\lambda, \epsilon = \pm} \int \dd k |c_\lambda (k, t)|^2}. \tag{64}
\]

Time dependence of \( c_\lambda (k, t) \) indicates the presence of a source. When a photon is emitted by an atom, the expectation value of the photon number is smaller than one and approaches unity as \( t \to \infty \). If \( |\psi_\perp (t)\rangle \) is normalized so that \( n(t) = \langle \bar{\psi}_\perp (t) | \psi_\perp (t) \rangle \) is the number of photons, the probability density for \( k^\mu = (\epsilon \omega_k, \mathbf{k}) \) is \( \frac{1}{(2\pi)^{3/2}} |c_\lambda (k, t)|^2 \) while the probability density to find a photon at \( x \) on the hyperplane \( \sigma \) is \( \frac{2\pi|\psi_\perp (k, x)|^2}{\omega_k} \). In the SP the photon position operator 45 can be written as
\[
\hat{X}^{\text{SP}} (k) = \hat{E} \hat{\nabla} k \hat{E}^{-1} \tag{65}
\]

The scalar product \( \langle \mathbf{E}_\lambda (x) \psi (t) \rangle = \langle \mathbf{E}_\lambda (x) | \psi (t) \rangle \) that leads to an invariant probability to annihilate a photon is proportional to probability amplitude, not the electric field. Glauber defined an ideal photon detector as a system of negligible size with a frequency-independent photon absorption probability [52]. For the positive frequency one-photon state \( |\psi (t)\rangle \) he found that the probability to count a photon is proportional to \( \langle \mathbf{E}_\lambda (x) | \psi (t) \rangle^2 \). Glauber considered photodetection to be a square law process and interpreted it to be responsive to the density of electromagnetic energy, but number density gives an invariant probability to count a photon while energy density does not. Indeed, the biorthogonal completeness relation 45 implies that a basis of ideal Glauber detectors can be defined provided the state vector \( |\psi \rangle \in \mathcal{H} \) of the photon at hand has been created by the \( \mathbf{A} \cdot \mathbf{p} \) minimal coupling Hamiltonian. In that case, \( \langle \mathbf{E}_\lambda (x) | \psi (t) \rangle^2 \) is proportional to photon probability density.

Here a positive definite particle density is obtained in the physical Hilbert space according to the rules of biorthogonal QM summarized in the Introduction. An alternative approach is to transform the physical fields to the NW representation using the nonlocal operator \( \hat{D}^{-1/4} \) and its inverse [23, 26]. The disadvantage to this approach is that the relationship between the NW wave function and a current source is nonlocal. Here the field due to the local interaction Hamilton \( J_\mu (x) \mathcal{A}^\mu (x) \) is calculated first and the probability amplitude for a transition to a position eigenvector is then obtained using the invariant scalar product (44). These fields have well defined Lorentz and gauge transformation properties. The positive definiteness of the probability follows then directly from the mathematical rules of biorthogonal QM.

An advantage of the second quantized formalism included here is that multiphoton wave functions can be introduced as in [15, 16, 52]. For example, to the two photon state \( |\psi_2\rangle \) can be associated the wave function
\[
\psi_{\lambda_1, \lambda_2} (x_1, x_2, t) = \langle \mathbf{E}_{\lambda_1} (x_1) \mathbf{E}_{\lambda_2} (x_2) | \psi_2 (t) \rangle \tag{66}
\]

with \( \mathbf{E}_{\lambda_1} (x_1) \mathbf{E}_{\lambda_2} (x_2) = \hat{E}_{\lambda_1} (x_1) \hat{E}_{\lambda_2} (x_2) |0\rangle \). This wave function localizes the photons at spatial points \( x_1 \) and \( x_2 \) at time \( t \) and can describe entangled two-photon states.

V. WAVE FUNCTION OF A PHOTON EMITTED BY AN ATOM

The wave function [58] for a photon emitted by a two-level atom initially in its excited state was derived in [12] and [53], to first order in the IP minimal coupling interaction Hamiltonian \( \hat{H}_I = (e/m_e) \mathbf{A} (\hat{\mathbf{x}}, t) \cdot \hat{\mathbf{p}} (t) \). For a two-level atom initially in its excited state \( |e\rangle \) with no photons present, the positive frequency IP wave function describing decay to its ground state \( |g\rangle \) while emitting one photon is
\[
\psi (t) = c_e (t) |e, 0\rangle \tag{67}
\]

\[
+ \sum_{\lambda = \pm} \int \frac{\dd k}{(2\pi)^{3/2}} c_{\epsilon, \lambda} (k, t) |g, 1, \lambda, k\rangle
\]

where
\[
c_{\epsilon, \lambda} (k, t) = \frac{e}{m_e} \langle g, 1, \lambda, k | \mathbf{A} (\hat{\mathbf{x}}, t) \cdot \hat{\mathbf{p}} (t) | e, 0 \rangle \tag{68}
\]

Here \( \hbar \omega_0 \) is the level separation between the ground and excited states and \( \mathbf{x} \) and \( \mathbf{p} \) are the electron position and momentum operators. For \( \langle \bar{\psi}_\perp \rangle \) given by [63] the transverse single-photon state and its dual are thus given
by
\begin{align}
|\psi_\perp(t)\rangle &= \sum_{\lambda = \pm} \int \frac{dk}{(2\pi)^2} \frac{1}{2\omega_k} e_{g,\lambda}(k, t) |1_{\lambda, k}\rangle, \quad (69) \\
|\tilde{\psi}_\perp(t)\rangle &= \sum_{\lambda = \pm} \int \frac{dk}{(2\pi)^2} \frac{1}{2\omega_k} e_{g,\lambda}(k, t) |1_{\lambda, k}\rangle. \quad (70)
\end{align}

In [18, 53] the minimal coupling Hamiltonian created the photon state vector $|\psi_\perp\rangle$ in the $|A_{\lambda}(x)\rangle$ basis so the appropriate wave function is $\langle E_{\lambda}(x)|\psi_\perp\rangle$. Indeed we have from [58] and [57]
$$\psi_\perp(x) = \sqrt{\frac{\hbar}{\epsilon_0}} \frac{1}{2\pi} \int \frac{dk}{2\pi} e_{\lambda}(k) e^{-ik\cdot x} c_{g,\lambda}(k, t). \quad (71)$$

The positive frequency wave function of the emitted photon is calculated, but causal solutions that include negative frequencies are also considered. Taking into account a factor $-i$ in the electric field operator used in [18, 53], $e_{g,\lambda} = -ie_{\lambda}^+\| e_{\lambda}\|$ in [52]. Substitution of the wave function $\psi_\lambda(x) = \langle E_{\lambda}(x)|\psi_\perp(t)\rangle$ in [61] gives the probability density in space to count a photon at time $t$. Since in [18, 53] the wave function is normalized as $\langle \psi_\perp|\psi_\perp\rangle = 1$, the factor $\langle \psi_\perp|\psi_\perp\rangle$ in [61] and [64] approaches $1/\omega_0$ as $t \to \infty$.

If the standard (dipolar) $E \cdot x$ Hamiltonian were to be used instead, the photon would be created in the $|E_{\lambda}(x)\rangle$ basis and the appropriate wave function would be $\langle A_{\lambda}(x)|\psi_\perp(t)\rangle$.

VI. LOCALIZED STATES

In Sections 3 and 4, starting with biorthogonal bases motivated by the canonical commutation relations, a bottom-up version of the formalism of biorthogonal QM 21, 56 was used to derive relativistic QM for KG particles and photons. For generality, a scalar product that is positive definite for both positive and negative frequency fields 26 was selected. The positive and negative frequency components are separately biorthogonal, but they do not propagate causally. In this Section we will show that sums of positive and negative frequency position eigenvectors are covariant position eigenvectors that do propagate causally.

Nonlocality due to the similarity transformation to the NW basis is completely eliminated in the biorthogonal formalism. The Philips states 54 used by Marolf and Rovelli to model Lorentz invariant detectors 55 combined with their duals are biorthogonal. While the NW position operator is Hermitian and the NW basis is equivalent to the biorthogonal basis in the sense that scalar products are preserved, their eigenvectors are nonlocal in configuration space due to the Fourier space factor $\omega_k^{1/2}$. In addition, the NW representation requires redefinition of the field operators, while the biorthogonal representation is based on the canonical field operators so it can be compared directly to the standard localization scheme 3.

There is a source of nonlocality that is intrinsic to all one-particle positive frequency states. According to the Hegerfeldt theorem 19, positive frequency states initially localized in a finite region will spread instantaneously to fill all of space. Physically this is because localization of positive frequency waves is due to destructive interference between intrinsically nonlocal counterpropagating waves 50. If negative frequency states are excluded, there are no localized states that evolve causally 4, 3. According to the RS theorem the global vacuum is cyclic for every local algebra. As a consequence, every local event has a nonzero probability of occurring in the vacuum and local creation, annihilation and number operators do not exist. For example, $\hat{\phi}^-(x)|0\rangle$ is intrinsically nonlocal, so $\hat{\phi}^-(x)$ is not a local operator. As discussed in Halvorson’s critique of NW localization 3, 57, the use of positive frequency orthogonal (or biorthogonal) bases does not eliminate these consequences of the RS theorem, it merely masks them for an instant. True localization requires a sum over positive and negative frequencies 19.

The derivations in Sections 3 and 4 can be applied to a first or a second quantized theory, but we will start by discussing of the simpler case of first quantized fields which for photons are just "classical" solutions to Maxwell’s wave equation. For this case biorthogonality of the basis vectors can be verified directly without reference to the canonical commutation relations, annihilation and creation operators or the vacuum. Neutral KG particles and photons are described by real functions of $x$ that propagate causally. What is new here is that the configuration space bases 21 and 56 lead to the particle densities 58 and (61) where $\langle \psi_\perp|\psi_\perp\rangle$ is the total number of particles.

Annihilation and creation operators are intrinsic to any second quantized theory, and we have seen that these operators are nonlocal. To salvage the concept of local measurements Knight defined strict localization as indistinguishability from the vacuum in spacelike separated regions so that $\langle \psi_\perp|\hat{Q}|\psi_\perp\rangle = \langle 0|\hat{Q}|0\rangle$ 58. Here $\hat{Q}$ is some function of the field operators $\hat{\phi}(x_i)$ and $\hat{\pi}(x_i)$ and these operators commute at spacelike separated $x_i$. If $g(x)$ is a localized solution to the KG equation and
$$\tilde{R} = \int dx \left[ g(x) \partial_\alpha \hat{\phi}(x) - \hat{\phi}(x) \partial_\alpha g(x) \right], \quad (72)$$
then $|\psi_\perp\rangle = \exp(i\tilde{R})|0\rangle$ is strictly localized. This is an interesting state, since it is the coherent field operator radiated by a classical current distribution 12. However, all terms in $|\Psi\rangle$ are positive frequency and no such state containing a finite number of particles is strictly localized.

Energy must certainly be bounded from below 4, but we propose that positive and negative frequencies can...
be included if both absorbed and emitted particles are counted on a spacelike hyperplane. The motivation for this interpretation was the photon-matter interaction, \( \hat{j}(x) \cdot \hat{A}(x) \). Particle position is defined here as the space-time coordinate \( x \) appearing in the vector potential \( \hat{A}(x) \) and its derivatives, or in the field operators \( \hat{\phi}(x) \) and \( \hat{\pi}(x) \). In QFT these fields describe absorption and emission of photons by an atom or of neutral KG particles by an Unruh-Davies monopole detector \( \mathbb{H} \). The positive frequency parts of \( \hat{A}(x) \) and \( \hat{\phi}(x) \) describes absorption of positive energy particles, while their negative frequency parts describe emission of positive energy particles.

We will show next that this interpretation is consistent with microcausality which is the requirement that observables be described by field operators that commute for spacelike separated events: The relationship of microcausality to inclusion of negative frequencies in the scalar product \( \langle \psi(x) \mid \varepsilon(y) \rangle \) can be seen by substituting \ref{21} in the vacuum expectation value of \ref{20} to give

\[
\langle \phi(x) \mid \pi(y) \rangle = \left\langle 0 \right| \hat{\phi}^+(x) \hat{\pi}^-(y) \hat{\pi}^+(y) \hat{\phi}^-(x) \left| 0 \rightangle = \langle \hat{\phi}^+(x) \mid \hat{\pi}^+(y) \rangle + \langle \hat{\pi}^+(y) \mid \hat{\phi}^+(x) \rangle = \langle \hat{\phi}^+(x) \mid \hat{\pi}^+(y) \rangle + \langle \hat{\phi}^-(x) \mid \hat{\pi}^-(y) \rangle. \tag{73} \]

On the \( t_x = t_y \) hyperplane events \( x' = (ct_x, x) \) and \( y' = (ct_y, y) \) appear simultaneous but an inertial observer with velocity \( c/\beta \) will see these events as time ordered. Since the Fourier space integrand of \( \langle \hat{\phi}^+(x) \mid \hat{\pi}^+(y) \rangle \) is proportional to \( e^{-i k(x-t_y)} \) while that of \( \langle \hat{\pi}^+(y) \mid \hat{\phi}^+(x) \rangle \) will be seen as proportional to \( e^{i k(x-t_y)} \), if \( t_x > t_y \) the first term is positive frequency (\( \epsilon = + \)) while the second is negative frequency (\( \epsilon = - \)). This assignment is not unique, since an observer with velocity \( -c/\beta \) will see the opposite time order. Thus the manifestly covariant scalar product \ref{19} is a sum over absorbed and emitted particles as in \ref{21}.

The basis states \ref{21} and the scalar product \ref{19} are directly related to the QFT Green functions as defined in \ref{24}. These propagators satisfy the KG equation \ref{5} with a \( \delta^4(x-y) \) source and are of the form

\[
G(x-y) = \frac{1}{(2 \pi)^3} \int d^4k f(k^0) \delta(k^2 - m^2) e^{-ik(x-y)}.
\tag{74} \]

The choice \( f(k^0) = \Theta(k^0) \) gives the positive and negative frequency Wightman functions \( G^+(x-y) = G^+(y-x) \) and \( G^-(x-y) = G^+(y-x) \), \( f(k^0) = -ie(k^0) \) gives the causal or commutator function \( G(x-y) \) for which \( iG(x-y) = G^+(x-y) - G^-(x-y) \) and \( \partial_{ct_x} G(x-y) \mid_{ct_x} = -\delta(x-y) \), and \( f(k^0) = 1 \) gives the Hadamard/Schwinger Green function for which \( G^{(1)}(x-y) = G^+(x-y) + G^-(x-y) \). These propagators can be related to the functions defined in Sections 2 and 3 by identifying

\[
\psi_y^\epsilon(x) \equiv \langle \pi^\epsilon(x) \mid \phi^\epsilon(y) \rangle = i\frac{\hbar}{2} \partial_{ct_y} G^\epsilon(x-y) \tag{75} \]
as the probability amplitude for absorption at \( x \) of a particle emitted by a source at \( y \) (\( \epsilon = + \)), or absorption at \( y \) of a particle emitted at \( x \) (\( \epsilon = - \)). The \( \epsilon \)-frequency potential-like field at \( x \) due to a localized source at \( y \) is \( \phi_y^\epsilon(x) \equiv \langle \phi^\epsilon(x) \mid \phi^\epsilon(y) \rangle \) so \( G^{(1)}(x-y) = \phi_y^+(x) + \phi_y^-(x) \) and \( iG(x-y) = \phi_y^+(x) - \phi_y^-(x) \) are the field and its conjugate defined in Section 2. The position eigenvectors evolve in time like derivatives of the corresponding QFT propagators. With \( t \equiv t_x - t_y \) and \( r \equiv |x-y| \),

\[
\psi_y^\epsilon(x) = \int \frac{dk}{(2\pi)^3} e^{-i\epsilon |\omega_k(ct_x - ct_y) - k(x-y)|} \tag{76} \]

where \( k \) was replaced with \(-k\) in the \( \epsilon = - \) term. At \( t = 0 \) the delta functions add while the principal values terms cancel so \( \psi_y^\epsilon(x) \) is localized. However, for \( t_x \neq t_y \), \( \psi_y^\epsilon(x) \) has a nonlocal imaginary part that leads to instantaneous spreading. Any state vector can be expanded in the \( |\phi^\epsilon(x)\rangle \) basis with wave function components \( \psi^\epsilon(x) \) given by \ref{12} or in the \( |\phi_c(x)\rangle, |\phi(x)\rangle \) basis with wave function components \( \psi_c(x) = \langle \phi^+_c(x) + \phi_-(x) \rangle / \sqrt{2} \) and \( \psi(x) = \langle \phi^+(x) - \phi^-(x) \rangle / \sqrt{2} \). For the state \( \psi(x) = \phi_{ct_x} G(x-y) \) which equals \(-\frac{i\hbar}{2} \delta(x-y) \) at \( t_x = t_y \) is a position eigenvector. These basis states satisfy the boundary conditions \( \phi_{ct_x}(x) = 0 \) and \( \partial_{ct_x} \phi_{ct_y} = \delta(x-y) \) on the \( t_x \) hyperplane and provide a basis for the real fields that are consistent with microcausality. For \( t_x > t_y \) \( \phi_{ct_x} \) propagates outward on the spherical shell \( r = ct \), while for \( t_x < t_y \) it propagates inward on \( r = -ct \). The positive and negative frequency Wightman function are covariant in the senses that they can evaluated on an arbitrary spacelike hyperplane \ref{10}, but this does not take into account the observer dependence of time ordering that is reflected in the sign of the exponent in \ref{75}. A sum over positive and negative frequencies is required for causal time evolution and observer independence of the wave function with time order taken into account. According to \ref{73} the emission at \( y \) with absorption at \( x \) and emission at \( x \) with absorption at \( y \) are correlated in the \( \epsilon = \pm \) basis.

Time development is described by the operator \( \hat{U}(t) = \exp(-i\hat{H}t) \) where \( \hat{H}_{\epsilon\epsilon'} = \epsilon \hbar \hat{D}^{1/2} \delta_{\epsilon\epsilon'} \) are the elements of the \( 2 \times 2 \) matrix that generates infinitesimal displacements in time \( \ref{24} \). The symbol \( \hat{\omega} \) is used here to emphasize that it is a frequency, not an energy, operator. Its spectrum, \( \epsilon = |\hat{\omega}| \), is not bounded below. It is this property that allows the states \ref{70} to escape the nonexistence theorem proved in \ref{8} and consequences of the antilocal operator \( \hat{D}^{-1/2} \) discussed by Halvorson \ref{1}. The spectrum of the energy operator, \( \hat{H}_{\epsilon\epsilon'} = \hbar \epsilon \hat{D}^{1/2} \delta_{\epsilon\epsilon'} \), is bounded below. Hegerfeldt assumed positive energies which we identify here with positive frequencies, so the consequences of his theorem are avoided.

The field due to a distributed source is \( \phi(x) = \int dy G(x-y) j(y) \). The causal behavior of space-like
separated particle devices described by Eq. (25) of [62] is of this form. For photons interacting with charged matter J and \( \phi \) should be replaced with the four-vectors \( J^\mu \) and \( A^\mu \). If restricted to positive frequencies, the wave function \( \psi_\lambda (x) = (E_\lambda^+ (x) | \psi (t) \rangle \) emitted by an atom does not evolve causally due to the factor \( \Theta (k^0) \) of [53]. However the field due to the current \( J_k (y) = \langle \psi | \hat{\mathbf{p}} \delta (y - y') \psi \rangle \) with \( \hat{\mathbf{p}} = \frac{\hbar}{im} \mathbf{\nabla} \delta (y) \) and \( \psi (t) \) given by [67] can be written as an integral over the causal propagator \( G (x - y) \) which contains no factor \( \Theta (k^0) \). The atomic source current at time \( t_0 \) due to a dipole localized at \( y = 0 \) is \( J_k (y) = j_k \delta (y - y') \Theta (t_0) \exp (-i \Omega_0 t_0) \) where \( \Omega_0 = \omega_0 + \omega_{LS} - i \Gamma / 2 \), \( \Gamma \) is the decay rate and \( \omega_{LS} \) is the partial Lamb shift [53]. The wave function emitted by this current source observed at time \( t_2 \) is then proportional to \( j_k \Theta (t_2 - |x| / c) \exp [-i \Omega_0 (t_2 - |x| / c)] \) so it propagates causally [53]. Negative frequencies are allowed since there are local vacuum fluctuations correlated across space-like separated regions even in the global vacuum. In the covariant localized basis absorption and emission are equally likely, but the wave function of an atom known to be initially excited in the global vacuum is the sum of a large positive frequency emission term and a very small negative frequency absorption term [53] that here is attributed to local vacuum fluctuations. While absorption and emission are equally likely in the basis vectors, knowledge that the atom was initially in its excited state in the global vacuum leads a device dominated by emission.

Localization and causality is more complicated in the case of photons [18]. The completeness relation [55] can be used to expand the first quantized vector potential in the coordinate space basis as in [29] or to expand the state vector in the configuration space basis as in our Sections 4 and 5. In the former case the probability amplitude to find the photon at \( x \) is proportional to the scalar \( \sum_\lambda (E_\lambda^+ (x) | A_\lambda \rangle \). If \( A_\lambda \) is the position eigenvector \( \hat{\mathbf{a}}_\lambda \), this is given by [64] so it is localized at \( y \). This is consistent with the wave function defined in [29]. If the state vector is expanded, the wave function is a transverse vector and a covariant description requires the Lorenz gauge. In this gauge the causal photon Green function is \( g^{\mu \nu} G (x - y) \) where \( g^{\mu \nu} = \text{diag} (1, -1, -1, -1) \) and the source for \( A^\mu (x) \) is a conserved four-current [29, 63]. All components of \( A^\mu (x) \) propagate causally on the light cone. In a source free region where the photon is on its mass shell the longitudinal part of the electric field \( E (x) = -\partial_0 A (x) - \nabla \phi (x) \) is zero due to the Lorenz gauge condition so \( E (x) \) and \( B (x) = \nabla \times A (x) \) are transverse. Propagation is causal and the photon position eigenvectors are localized. As discussed in the Introduction, the photon position eigenvectors have defined total angular momentum along their axis of cylindrical symmetry. All of the commutation relations of the Poincaré group are satisfied as discussed in [16, 52], where the relevant case for the biorthogonal basis is \( \alpha = 0 \). The spacetime location of a position eigenvector is defined as the argument \( x \) in \( A^\mu (x) \), the internal angular momentum of a position eigenvector includes the orbital angular momentum relative to \( x \) and the external angular momentum operator is \( \hat{\mathbf{a}} \times \hat{\mathbf{p}} \).

The position eigenvectors describe a particle at position \( x \), but it is uncertain whether it was annihilated or created there. Only \( \mathbf{k} \)-space is a true Fock space so particles must be created and annihilated globally. The KG and photon position eigenvectors (including the negative frequency ones) are given in terms of this Fock basis in (21-22) and (48-51) respectively. This is consistent with the Reeh-Schlieder conclusion that there are no local creation or annihilation operators. For a detector array arranged to capture all photons of interest, locally there is only probability density for the presence of a photon at \( x \) on some hyperplane. The experimenter must examine the whole array to count photons. When applied globally, the number operator [50]

\[
\hat{N}_\lambda = \frac{\hbar \omega_0}{c} \int d\mathbf{x} E_\lambda^+ (x, t) \cdot A_\lambda^+ (x, t) + H.c.
\]

(77)
counts photons with helicity \( \lambda \) at time \( t \).

VII. CONCLUSION

The formalism of biorthogonal systems can be, as we saw, called in action in relativistic quantum mechanics. It is particularly well-matched to the relativistic scalar product. In the biorthogonal formalism, both the Wigner-Bargmann quantum field operator (for photons, the vector potential) and its canonically conjugate momentum (for photons, the electric field) are put on an equal footing, and they generate respectively the direct and the dual basis of position eigenvectors of two different position operators, which are the Hermitian conjugate of each other. Our formalism further clarifies the meaning of the free parameter \( \alpha \) [16, 18, 31] in the photon position operator.

The probability density [61] suggests a resolution of the apparent dichotomy between photon number counting and the sensitivity of a detector to energy density. The wave function \( \langle E_\lambda^+ (x) | \psi (t) \rangle \) together with the state vector [67] describes creation of a photon in the time interval \( 0 \leq t' \leq t \) followed by its detection at time \( t \). Since it is created in the \( | A_\lambda (x) \rangle \) basis and observed in the dual \( | E_\lambda^+ (x) \rangle \) basis, that wave function is proportional to a probability amplitude. The probability density for a transition from \( | \psi_\perp (t) \rangle \) to the position eigenvector at \( x \), given by \( \frac{\hbar}{\alpha} | \langle E_\lambda^+ (x) | \psi (t) \rangle |^2 \), is of the Glauber form [52]. However, in contrast to theories of photodetection based on energy density, we have proposed, through the position amplitude \( \langle E_\lambda^+ (x) | \psi (t) \rangle \) in the dual basis, a true position measurement that describes an array of ideal photon counting detectors.
For a state vector that is an arbitrary linear combination of positive and negative frequency terms the probability density for a transition to the position eigenvector at $x$ is positive definite. This probability density describes a particle at spatial location $x$ independent of whether it was absorbed or emitted. Thus (61) can be interpreted as probability density even if the wave function $\psi_k^\pm$ is real as in classical electromagnetism. This application of biorthogonal QM is based on an invariant positive definite scalar product so transition probabilities are invariant and positive definite, the position operator is covariant, and there is no NW $\omega_{k}^{1/2}$ nonlocality in the wave function. In any theory that combines relativity with QM the position coordinate is problematic. In QM a position measurement should be associated with a Hermitian position operator, but the only orthogonal position eigenvectors available in the published literature are nonlocal and noncovariant [20]. The NW construction can be extended to photons [34] but then coupling of photon number amplitude to current density is nonlocal [64]. In the biorthogonal formalism number density is derived from the canonical fields and it becomes clear that the relationships amongst number, energy and current density are all local. If the NW basis is restricted to the calculation of scalar products and expectation values there is no disagreement between the conventional treatment of particle position based on the NW position operator $|\psi\rangle$ and biorthogonal QM. However, one should not fall into the trap of believing that NW nonlocality is physically real and hence observable.

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