Covariant photon quantum mechanics

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Recently a photon position operator with commuting components and a particle density that is positive definite for both positive and negative frequency states has led to a first quantized theory of the photon. Here we extend this theory to a manifestly covariant form and show for the first time that, with invariant plane wave normalization, the position operator is Hermitian with real instantaneously localized eigenvectors. Reality of the field and wave function ensure causal propagation and zero net absorption of energy in the absence of charged matter. The position space wave function is the real part of the projection of the photon’s state vector onto a basis of position eigenvectors. Manifest covariance and consistency with quantum field theory is maintained through use of the electromagnetic four-potential and the Gupta-Bleuler gauge condition.

I. INTRODUCTION

Up to the turn of this century there was no photon number density and no true photon quantum mechanics. This is a consequence of several obstacles to its development: Newton and Wigner \[1\] derived position operators for electrons and for spin 0 Klein-Gordon particles but found that, if invariance under rotations is assumed, no photon position operator exists. Even these Klein-Gordon position eigenvectors are problematic since they are not Lorentz covariant and they are nonlocal in configuration space. Pryce \[2\] derived a photon position operator but its components do not commute, so it does not define a basis of position eigenvectors. The standard density is positive definite only if the fields are restricted to positive frequencies, however positive frequency fields alone do not propagate causally \[3\] and in quantum field theory (QFT) \[4\] the fields describing neutral bosons are real. Some form of a photon wave function is thought to be useful in quantum optics but, as a consequence of the above mentioned obstacles, the usual rules of quantum mechanics were not followed. Instead the Reimann-Silberstein-Bialynicki-Birula \[5\] and Sipe \[6\] photon wave functions are based on energy density \[7\].

Recently, derivation of a photon position operator with commuting components \[8,9\] and a particle density that is positive definite for both positive and negative frequency waves \[10,11\] have led to photon quantum mechanics \[12,13\] with a Hilbert space consisting of solutions to Maxwell’s equations and an invariant inner product. However, this is not an entirely satisfactory first quantized theory since in \[12\] the position operator and its eigenvectors are of the Newton-Wigner form, while in \[13\] the position operator is not Hermitian and biorthogonality is derived from QFT. Here we transform to a new Hilbert space based on invariant plane wave normalization in which the position operator is Hermitian with covariant instantaneously localized eigenvectors. Consistent with \[delta\]-function normalization, the new inner product is a density.

At a fundamental level our world is described by QFT which is compatible with special relativity and quantum mechanics. The question of localizability is fundamental to QFT where particles interact locally at a common space-time coordinate. Particle position, while essential to this picture, is especially problematic in the case of photons that have no rest frame. We review and extend some recent literature that puts photon quantum mechanics on the same footing as the quantum mechanics of massive particles. The position eigenvalues are the spatial coordinate in the fields and QFT operators so they provide an interpretation of photon position. Since Klein-Gordon quantum mechanics illustrates most of the salient points, it will serve as an introduction to photon quantum mechanics.

Our goal is to provide a clear and physically intuitive description of Klein-Gordon and photon quantum mechanics and their relationship to QFT. The Klein-Gordon equation is the simplest relativistic wave equation so it will be discussed first, in Section II. In Section III, Maxwell quantum mechanics based on the 4-potential and the Gupta-Bleuler indefinite metric will be presented. In Section IV we conclude. Solutions to the Klein-Gordon and Maxwell equations will be referred to as the scalar potential and the 4-potential respectively and their time derivatives will be called fields. The term wave function will be reserved for the projection of a particle’s state vector onto a momentum basis or a basis of position eigenvectors. Since relativistic quantum mechanics is covariant, we will maintain manifest Lorentz covariance throughout.

II. KLEIN-GORDON QUANTUM MECHANICS

A. Klein-Gordon Hilbert space

After a brief summary of relativistic notation, positive and negative frequency solutions (\[epsilon = \pm\]) to the Klein-Gordon equation will be reviewed. Since the Mostafazadeh conjugate field \[11\] satisfies the Klein-Gordon equation, it will also be discussed. A general

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form of the Klein-Gordon continuity equation will be derived that includes the standard Klein-Gordon inner product and Mostafazadeh’s inner product. A Hilbert space based on $\epsilon = \pm$ solutions to the Klein-Gordon equation will then be defined and used in subsection B to calculate real fields and probability amplitudes.

In relativity the space-time coordinates are incorporated into the 4-vector $x = x^\mu = (ct, \mathbf{x})$ with Lorentz invariant length squared $x^2 = x_\mu x^\mu$ where $x_\mu = y_{\mu\nu}x^\nu$ and $y_{\mu\nu} = g^{\mu\nu}$ is a $4 \times 4$ matrix with diagonal $(-1, -1, -1, -1)$. The classical (in the non-quantum sense) energy-momentum 4-vector is $p^\mu = (E_p/c, \mathbf{p}) = \hbar (\omega_k/c, \mathbf{k})$ and the 4-potential is $A^\mu = (\phi/c, \mathbf{A})$ where $\phi$ and $\mathbf{A}$ are the scalar and vector potential respectively.

In first quantization energy and momentum are replaced with operators, that is $E_p \to -i\hbar \partial_t$ and $\mathbf{p} \to \hat{\mathbf{p}} = -i\hbar \partial_{\mathbf{x}}$. Here $E_p$ is the energy of a particle with momentum $\mathbf{p}$ and mass $m$, $c$ is the speed of light, $\hbar = 2\pi\hbar$ is Planck’s constant, $\partial_t = \partial/\partial t$ and $\partial_x = \nabla$. Some additional invariants that will be used here are $p_\mu p^{\mu} = E_p^2/c^2 - \mathbf{p}^2c^2 = m^2c^4$,

$$\Box \equiv \partial_\mu \partial^\mu = \partial^2_{tt} - \nabla^2,$$  \tag{1}

$kx = \omega_k t - \mathbf{k} \cdot \mathbf{x}$ and $\exp(-ikx)$. The $k$-space Lorentz gauge condition, $k \cdot A = 0$, is Lorentz invariant while the Coulomb gauge condition, $\mathbf{k} \cdot \mathbf{A} = 0$, is not so, in keeping with our theme of maintaining manifest covariance, we will use the Lorenz gauge in Section III.

Operation with $\hat{E}_p^2 = \mathbf{p}^2c^2 - m^2c^4$ on the potential $\phi(x) = \phi(t, \mathbf{x})$ gives the Klein-Gordon wave equation

$$\Box \phi(x) + \frac{m^2c^2}{\hbar^2} \phi(x) = 0.$$  \tag{2}

with solution $\phi(t, \mathbf{x}) = \sum_{\epsilon = \pm} \phi^\epsilon(t, \mathbf{x})$ where

$$\phi^\epsilon(t, \mathbf{x}) = i\sqrt{\hbar} \int \frac{dk}{(2\pi)^{3/2}\omega_k} \beta^\epsilon(k) e^{ik \cdot x - i\epsilon\omega_k t}.$$  \tag{3}

The unit imaginary $i$ was introduced for later convenience to give the odd integrand $\sin(kx + \arg \beta^+)$.

The Klein-Gordon equation is derived from the Lagrangian density $L = c^2 (\partial_\mu \phi)^2 - m^2c^4 \phi^2$ where the momentum conjugate to $\phi(x)$ is $\pi(x) = \partial L/\partial (\partial \phi/\partial t)$ so

$$\pi(x) = \partial_t \phi(x).$$  \tag{4}

The Euler-Lagrange equation of motion $\partial_\mu ((L/\partial (\partial_\mu \phi)) - \partial_t L/\partial \phi) = 0$ is \cite{12}.

The Mostafazadeh-Zamani \cite{11} conjugate field

$$\phi_c(x) = i\hat{D}^{-1/2}\partial_{ct} \phi(x)$$  \tag{5}

that leads to a positive define inner product also satisfies the Klein-Gordon equation. Their operator $\hat{D}$ is defined as

$$\hat{D} \equiv -\nabla^2 + m^2c^2/\hbar^2,$$  \tag{6}

so that the sign of the absorbed energy, $\epsilon$, is given by

$$i\hat{D}^{-1/2}\partial_{ct} \phi^\epsilon(x) = \epsilon \phi^\epsilon(x),$$  \tag{7}

that is $\phi^\epsilon_c(x) = \epsilon \phi^\epsilon(x)$. In terms of \cite{10} the Klein-Gordon equation reduces to

$$\left(\partial^2_{tt} + \hat{D}\right) \phi(x) = 0.$$  \tag{8}

In the $\epsilon = \pm$ basis time evolution is determined by $i\partial_t \phi^\epsilon(x) = c\epsilon\hat{D}^{1/2} \phi^\epsilon(x)$ that can be integrated from 0 to $t$ to give

$$\phi^\epsilon(t, \mathbf{x}) = \tilde{U}^\epsilon(t) \phi^\epsilon(0, \mathbf{x}),$$  \tag{9}

$$\tilde{U}^\epsilon(t) = e^{-i\epsilon\hat{D}^{1/2}t},$$  \tag{10}

$$\tilde{H}_{\epsilon\epsilon'} = i\delta_{\epsilon, \epsilon'}\hbar c\hat{D}^{1/2}$$  \tag{11}

where $\tilde{U}^\epsilon$ is a unitary operator, $\tilde{H}_{\epsilon\epsilon'}$ is the $2 \times 2$ Hamiltonian matrix \cite{12}, and the hyperplane on which $\phi^\epsilon(x)$ is given is defined here as $t = 0$.

The inner product at time $t$ is the spatial integral of the zeroth component of a conserved 4-current, so the Klein-Gordon continuity equation will be considered next. For any $\phi$ and $\tilde{\phi}$ that satisfy \cite{2}, a continuity equation can be obtained by subtracting $\tilde{\phi}$ multiplied by the Klein-Gordon equation for $\phi^\epsilon$ from $\phi^\epsilon$ times the Klein-Gordon equation for $\tilde{\phi}$. This is the method used to derive the Schrödinger continuity equation in undergraduate quantum mechanics. After cancellation of the $\partial_\mu \phi \partial^\mu \tilde{\phi}$ terms, substitution of the Klein-Gordon equation and multiplication by the constant $ig$,

$$ig\partial_\mu \phi^\epsilon(x) \to \hat{\theta}^\epsilon_t \tilde{\phi}(x) = 0$$  \tag{12}

where

$$f \to \hat{\theta}^\epsilon_f g = f (\partial_\mu g) - g (\partial_\mu f).$$  \tag{13}

Eq. \cite{12} is of the form

$$\partial_\mu \rho + \partial_\mathbf{x} \cdot \mathbf{j} = \partial_\mu J^\mu = 0$$  \tag{14}

where $\rho$ is density, $\mathbf{j}$ is current density and $J^\mu$ is 4-current density. If $\tilde{\phi} = \phi$ and $g = ec/\hbar$ where $e$ is the magnitude of the charge on the electron then $\rho$ is electric charge density and $\mathbf{j}$ is electric current density. If $\tilde{\phi} = \phi_c$ \cite{12} is the Mostafazadeh-Zamani continuity equation for particle density. For this case the constant $g$ will be determined in the next paragraph. Since the fields are real, $\phi^- = (\phi^+)^*$, $\tilde{\phi}^- = (\tilde{\phi}^+)^*$ and $\pi^- (\mathbf{k}) = (\pi^+ (\mathbf{k}))^*$ in \cite{4} and \cite{4}.

To maintain consistency with QFT the constant $g$ describing number density will be determined from the Klein-Gordon commutation relations. In QFT the expansion coefficients in \cite{4} are promoted to operators to give

$$\tilde{\phi}(t, \mathbf{x}) = \sqrt{\hbar} \int \frac{dk}{(2\pi)^3 2\omega_k} e^{i\mathbf{k} \cdot \mathbf{x}} \left[ a(\mathbf{k}) e^{-i\omega_k t} + a^d(\mathbf{k}) e^{i\omega_k t}\right]$$  \tag{15}
in which \( \hat{a}(k) \) annihilates a particle with wave vector \( k \) and \( \hat{a}^\dagger(k) \) creates one. The expression (15) assumes the Lorentz invariant commutation relation

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

(16)

but this choice is not universal. In (15, 16) for example \([\hat{a}(k), \hat{a}^\dagger(q)] = (2\pi)^3 \delta(k - q) \) leads to an additional factor \((2\omega_k)^{1/2}\) in the numerator of (14). States with wave vectors \( k \neq q \) are orthogonal, that is with

\[
|1_k\rangle = \hat{a}^\dagger(k)|0\rangle,
\]

(17)

\[
(1_k|1_q\rangle = (2\pi)^3 2\omega_k \delta(k - q).
\]

(18)

If the first term of (15) is called \( \hat{\phi}^+ \) and the second \( \hat{\phi}^- (t, x) \) annihilates a particle at \( x \), while \( \hat{\phi}^- (t, x) \) creates one. The field operator is \( \pi = \partial_t \hat{\phi} \). An annihilation operator acting on the vacuum state gives zero, that is \( \hat{a}(k)|0\rangle = 0 \) and \( \hat{\phi}^+(x)|0\rangle = 0 \). The x-space Klein-Gordon commutation relations at time \( t \) are

\[
[\hat{\phi}(t, x), \hat{\phi}(t, y)] = 0, \quad [\pi(t, x), \pi(t, y)] = 0
\]

and

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

(19)

Here we have referred to position or configuration space as x-space and momentum or reciprocal space as k-space. A creation operator acting on the vacuum state gives a 1-particle state. Using (4) and (17) and Dirac notation and defining the one Klein-Gordon particle state at \( x \) on the t-hyperplane as

\[
|\phi_x\rangle = \hat{\phi}^-(t, x)|0\rangle
\]

(20)

the vacuum expectation value of (19) can be written as

\[
\langle \phi_x|c\hat{D}^{1/2}|\phi_y\rangle = h\delta(x - y).
\]

Integration of \( \hat{\phi}^- (t_x, x) \pi^- (t_y, y)|0\rangle \) with \( r = x - y \) and \( t = t_x - t_y \) gives

\[
\langle \phi_x^c|c\hat{D}^{1/2}\phi_y^c\rangle = h \int \frac{d|k|e^{-i\omega_k t_x}e^{ikr}}{(2\pi)^3 2}\]

\[
= h \int \frac{\partial}{\partial r} \sum_{\gamma = \pm} \left[ \pi\delta(r - \gamma cct) + i\gamma PV \left( \frac{1}{r - \gamma cct} \right) \right].
\]

(21)

At \( t = 0 \) the principal value \( (PV) \) terms cancel while the \( \delta \)-functions add to give a factor 2. The 1/r tails of the \( PV \) terms are instantaneously masked by destructive interference [17], only their sum is localized. Eq. (21) was included to illustrate the nonlocality of the \( PV \) terms but at \( t = 0 \) the simpler expression

\[
\int \frac{d|k|}{(2\pi)^3} e^{ik(x - y)} = \delta(x - y),
\]

(22)

gives on the t-hyperplane

\[
\langle \phi_x^c|c\hat{D}^{1/2}|\phi_y^c\rangle = \frac{\hbar}{2} \delta(x - y).
\]

(23)

Eqs. (12) and (14) are consistent with the QFT commutation relations if \( g = c/\hbar \). This gives the number density

\[
\rho(x) = \frac{i}{\hbar} \phi^\ast(x) \leftrightarrow \partial_t \phi(x).
\]

(24)

On a hyperplane of simultaneity at instant \( t \) the conserved inner product is then

\[
\int d\sigma \rho(x) = \frac{i}{\hbar} \int d\sigma \phi^\ast(x) \leftrightarrow \partial_t \phi(x).
\]

(25)

Eq. (25) can be generalized to the covariant form

\[
\int d\sigma \rho_{\mu
u}(x) = \frac{i}{\hbar} \int d\sigma \phi^\ast_{\mu}(x) \leftrightarrow \partial_{\nu} \phi_{\nu}(x)
\]

(26)

on an arbitrary spacelike hyperplane with normal \( n_{\mu} \). The choice \( n = (1, 0, 0, 0) \) gives (25).

In the \( \epsilon = \pm \) basis with \( \phi = \phi_1 \), \( \phi = \phi_2 \) the inner product (25) can be written as

\[
\langle \phi_1, \phi_2\rangle = \frac{2c}{\hbar} \int d\sigma \phi_1^\ast(x) \hat{D}^{1/2}\phi_2(x) \delta_{\epsilon, \epsilon'}
\]

\[
= \frac{2c}{\hbar} \langle \phi_1^\ast|\hat{D}^{1/2}|\phi_2\rangle \delta_{\epsilon, \epsilon'}
\]

(27)

where \( \langle \chi_1|\chi_2\rangle = \int d\sigma \chi_1^\ast(x) \chi_2(x) \) is the usual Dirac bracket notation and we have made use of the fact that the two terms in (24) are equal if \( \epsilon' = \epsilon \) and cancel if \( \epsilon' = -\epsilon \).

The x-space function (3) can be generalized to a state vector in an arbitrary basis in a manner analogous to the vector notation used in three dimensions. Eq. (4) is isomorphic to the state vector

\[
|\phi^c\rangle = i\sqrt{\hbar} \int \frac{d|k|}{(2\pi)^3 2\omega_k} c^c(k)|1_k\rangle.
\]

(28)

The definition (28) was motivated by derivation of the QFT commutation relations (14) from (15) and (13) but invariant normalization of the plane wave basis is applicable to both first and second quantization. Substitution of (28) in the Klein-Gordon inner product (27) where \( c\hat{D}^{1/2} \rightarrow \omega_k \) gives its k-space form,

\[
\langle \phi_1, \phi_2\rangle = \int \frac{d|k|}{(2\pi)^3} c^c_1(k) c_2^\ast(k) \delta_{\epsilon, \epsilon'}.
\]

(29)

With the Newton-Wigner normalization

\[
(1_k|1_q)_{NW} = (2\pi)^3 \delta(k - q)
\]

(30)

the k-space inner product that replaces (29) is

\[
\langle \phi_1, \phi_2\rangle_{NW} = \delta_{\epsilon, \epsilon'} \int \frac{d|k|}{(2\pi)^3 2\omega_k} c^c_1(k) c_2^\ast(k).
\]

(31)
On the t-hyperplane the Hilbert space can be defined as \( \phi^\epsilon (x) \) with inner product \( (27) \) or \( c^\epsilon (k) \) with inner product \( (24) \). A mathematically rigorous treatment of the general case is presented by Mostafazadeh and Zamani \[11\]. Here we use Dirac notation except to call the inner product \( (\phi^\epsilon, \phi^\epsilon ') \) for conciseness and to emphasize that it can be evaluated in \( x \)-space or \( k \)-space. We follow the covariant notation in Itzykson and Zuber \[4\] except in discussion of the Newton-Wigner case.

### B. Klein-Gordon observables

An alternative to specifying the \( t \)-hyperplane is to work in the Schrödinger picture where operators and their eigenvectors are time independent and the time dependence is contained in the state vector. The inner product can then be transformed to the manifestly covariant Heisenberg picture using \( (10) \) to give

\[
(\phi^\epsilon_x, \phi) = (\phi^\epsilon_x, \tilde{\mathbf{U}}^\epsilon (t) \phi (0)) = (\tilde{\mathbf{U}}^{\epsilon \dagger} (t) \phi^\epsilon_x, \phi)
\]

where the subscript \( x = (t, \mathbf{x}) \) denotes the position eigenvector at \( \mathbf{x} \) on the \( t \)-hyperplane.

In \( k \)-space the momentum operator is \( \hat{\mathbf{P}} = \hbar \mathbf{q} \) and its eigenvector with momentum \( \hbar \mathbf{q} \) satisfies

\[
\hat{\mathbf{P}} |\mathbf{q}\rangle = \hbar \mathbf{q} |\mathbf{q}\rangle.
\]

These states will be normalized according to \( (18) \). The basis of momentum eigenvectors is orthogonal, Dirac \( \delta \)-function normalized, and complete \( (13) \). Thus any state \( |\phi\rangle \) can be described by an integral over these plane waves.

The configuration space wave function is the projection of a particle’s state vector onto a basis of position eigenvectors. In the Schrödinger picture the \( k \)-space eigenvector equation, position operator and position eigenvector at \( y \) are

\[
\hat{\mathbf{x}}^{(\alpha)} |\mathbf{y}\rangle = \mathbf{y} c^{(\alpha)}_\mathbf{y},
\]

\[
\hat{\mathbf{p}}^{(\alpha)} \mathbf{y} = \mathbf{i} \partial_k - \mathbf{i} \mathbf{k} |\mathbf{y}|,\]

\[
c^{(\alpha)}_\mathbf{y} (\mathbf{k}) = [\mathbf{k}^\alpha \mathbf{e}^{-\mathbf{i} \mathbf{k} \mathbf{y}}].\]

The choice \( \alpha = 0 \) corresponds to the invariant normalization \( (13) \) with inner product \( (29) \), while the Newton-Wigner choice \( \alpha = 1/2 \) requires \( (30) \) and \( (31) \). In either case

\[
(\phi^\epsilon_x, \phi^\epsilon_y') = \delta (\mathbf{x} - \mathbf{y}) \delta_{\epsilon, \epsilon'}
\]

which is clearly not an invariant, rather it is a density as it must be for \( \delta \)-function normalization. The form of \( (29) \) is due to the substitution \( \pi^\epsilon (\mathbf{k}) \rightarrow c^\epsilon (\mathbf{k}) |\mathbf{k}\rangle \) so that a factor \( \omega_k \) is introduced into the inner product \( (27) \) and the new \( k \)-space wave function is the coefficient of \( |\mathbf{k}\rangle \).

Since the covariant case \( \alpha = 0 \) is the focus of this paper, we will define \( c_y = \mathbf{y}^{(0)} \). The state vector isomorphic to \( (36) \), will be called \( (1 x) \). In the Heisenberg picture the \( k \)-space position eigenvectors are

\[
c^\epsilon_x (k) = \langle 1_k | 1_x \rangle = e^{i \omega_k t} e^{-i \mathbf{k} \mathbf{x}}.
\]

The eigenvectors are the possible observed values, so they must be real. Since \( c^{(\alpha)}_x \) and \( c^{(\alpha)}_y \) are eigenvectors of \( \hat{\mathbf{x}}^{(\alpha)} \) and \( \hat{\mathbf{y}}^{(\alpha)} \) is Hermitian, the expectation value of the position operator gives

\[
\left( \hat{\mathbf{x}}^{(\alpha)} x^{(\alpha)} \phi^\epsilon_y \right) = \mathbf{y} (\phi^\epsilon_x, \phi^\epsilon_y), \]

\[
\left( \hat{\mathbf{y}}^{(\alpha)} x^{(\alpha)} \phi^\epsilon_y \right)^* = \left( \hat{\mathbf{x}}^{(\alpha)} y^{(\alpha)} \phi^\epsilon_x \phi^\epsilon_y \right)^*.
\]

If \( \alpha = 1/2 \), \( x^{(1/2)} \mapsto \mathbf{x}^{(1/2)} = \mathbf{x}^{(1/2)} \) is the well known Newton-Wigner result. If \( \alpha = 0 \) the inner product is \( (29) \) and \( \hat{\mathbf{x}}^{(0)} \mapsto \hat{\mathbf{x}}^{(0)} \). In either case it is Hermitian. Since according to \( (29) \) and \( (37) \), \( \phi^\epsilon_x, \phi^\epsilon_y \) is \( \delta (\mathbf{x} - \mathbf{y}) \), it follows that

\[
(\mathbf{y} - \mathbf{x}^\epsilon) \delta (\mathbf{x} - \mathbf{y}) = 0,
\]

that is the eigenvalues of \( \hat{\mathbf{x}}^{(\alpha)} \) are real as expected for Hermitian operators.

The state vector \( (28) \) can be projected onto the \( k \)-space or the \( x \)-space basis. Defining \( (1_k | \phi^\epsilon \rangle = \phi^\epsilon (k) \) with \( k = (\epsilon \omega_k/c, \mathbf{k}) \) projection of \( (28) \) onto \( k \)-space using \( (18) \) gives

\[
\phi^\epsilon (k) = i \sqrt{\hbar} c^\epsilon (k).
\]

Eq. \( (37) \) is the closure relation for the basis of position eigenvectors so any potential and field can also be expanded in this basis \( (10) \). Projection of \( (28) \) onto the position basis with substitution of the complex conjugate of \( \phi^\epsilon (k) \) and \( \phi^\epsilon (x) = \langle 1_x | \phi^\epsilon \rangle \) gives the coordinate space potential and field

\[
\phi^\epsilon (x) = i \sqrt{\hbar} \int_{t}^{t+\Delta t} \frac{dk}{(2 \pi)^3} e^{-i \omega_k t} e^{i \mathbf{k} \cdot \mathbf{x}} c^\epsilon (k),
\]

\[
\pi^\epsilon (x) = \epsilon \sqrt{\hbar} \int_{t}^{t+\Delta t} \frac{dk}{(2 \pi)^3} e^{-i \omega_k t} e^{i \mathbf{k} \cdot \mathbf{x}} c^\epsilon (k).
\]

Substitution of \( (13) \) in \( (29) \) then gives the \( x \)-space inner product

\[
(\phi^\epsilon_1, \phi^\epsilon_2) = \frac{1}{\hbar} \int_{t}^{t+\Delta t} \int_{t}^{t+\Delta t} \delta_{\epsilon, \epsilon'} d\mathbf{x} \pi^\epsilon_1 (x) \pi^\epsilon_2 (x).
\]

The new Hilbert space is \( c^\epsilon (k) \) with inner product \( (29) \) or \( \pi^\epsilon (x) \) with inner product \( (14) \). The HP wave function which equals the probability amplitude for space-time coordinate \( x \) and sign of absorbed energy \( \epsilon \) is given by \( (29) \) with \( c^\epsilon (k) = e^{i \mathbf{k} \cdot \mathbf{x}} \) as

\[
\psi^\epsilon (x) = (\phi^\epsilon_1, \phi^\epsilon_2)
\]

\[
= \int \frac{dk}{(2 \pi)^3} e^{i \mathbf{k} \cdot \mathbf{x}} c^\epsilon (k).
\]
At $t = 0$ the configuration space position eigenvector at $y$ is $\pi_y(x) = \sqrt{\delta(x - y)}$, the wave function is $(\phi_x, \phi_y) = \delta(x - y)$, the position operator is $\hat{x} = x$, and the position eigenvector equation is

$$\hat{x} \delta(x - y) = y \delta(x - y).$$

(47)

In phasor notation the real potential, field and wave function $\phi(x)$, $\pi(x)$ and $\psi(x)$ are given by

$$\phi(x) = \text{Re} \phi^+(x),$$

$$\pi(x) = \text{Re} \pi^+(x),$$

$$\psi(x) = \text{Re} \psi^+(x).$$

(48), (49), (50)

The solutions to (21) are subject to conditions $\phi(0, x)$ and $\partial_t \phi(t, x) |_{t=0} = \pi(0, x)$ on $t = 0$. The choice $e^+(k) = \exp(-ik \cdot y)$ gives $\phi(0, x) = 0$, $\pi(0, x) = \sqrt{\delta(x - y)}$ and $\psi(x) = \delta(x - y)$. The corresponding field and wave function are instantaneously localized at $t = 0$ and propagate on a spherical shell, inward converging on $y$ at earlier times ($t < 0$) and outward at later times ($t > 0$) as described by the real $\delta$-function term in (21). On the $t = 0$ hyperplane this is the position eigenvector at $y$. The photon is absorbed and reemitted so there is no net absorption of energy and $(\hat{x}, \hat{H}\hat{y}) = 0$.

The orbital angular momentum (AM) operator is

$$\hat{L} = \hat{x} \times \hat{P} = -\hat{P} \times \hat{x}.$$  

(51)

A Klein-Gordon particle has zero spin so it has no intrinsic AM.

### III. MAXWELL QUANTUM MECHANICS

In this Section we will extend the results of II to four dimensions using the Lorenz gauge and the photon position operator with commuting components $\hat{L}$ and $\hat{P}$.

#### A. Photon Hilbert space

Because QFT is based on local interactions it is common in QFT to use the Lorenz gauge and the Gupta-Bleuler indefinite metric $[13, 19, 20]$. This approach is covariant and based on four essentially identical copies of the solution to the $m = 0$ Klein-Gordon equation discussed in the last Section. The Lagrangian is the usual one plus a term proportional to the square of the Lorenz gauge condition, $L = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} - \frac{1}{2}m^2(\partial_{\mu}A^{\mu})^2$. Here $F^{\mu\nu}$ is the usual electromagnetic tensor whose first row is $F^{\mu0} = (0, E)/c$ and the field conjugate to $A_\nu$ is $\partial L/\partial (\partial_\nu A_\nu) = F^{\mu0} - g^{0\nu}(\partial_\mu A^\nu) = \pi^\nu$ with

$$\pi^\nu = -\epsilon_{0}\partial_\nu A^\nu.$$  

(52)

The Lagrange equations of motion are

$$\square A^\nu = 0.$$  

(53)

Since this equation is second order in both space and time and $m = 0$, it has the remarkable property that it is unchanged by multiplication by $\hbar^2$ so it can be interpreted as a classical or a quantum wave equation. The covariant 4-potential operator is $\hat{A}^\mu (x) = \sqrt{\frac{n}{\epsilon_0}} \sum_{\lambda=0,3} \int \frac{dk}{(2\pi)^3 2\omega_k} \left[ \hat{a}_\lambda (k) e_k^\mu e^{-ikx} + \hat{a}_\lambda^\dagger (k) e_{\lambda^*}^\mu e^{ikx} \right].$  

(54)

With the polarization unit vectors defined such that 0 is time-like, 1 and 2 are transverse and 3 is longitudinal,

$$e_0 = n^\mu = (1, 0, 0, 0), \ e_3 (k) = e_k = k/k,$$

(55)

$$e_1^\lambda (k) \cdot e_{\lambda'}(k) = \delta_{\lambda \lambda'}$$

(56)

Defining

$$\zeta = (-1, 1, 1, 1)$$

(57)

this can be written as

$$e_{\lambda^*}^\mu (k) = e_0^0 e_{\lambda^*}^\lambda - e_1^\lambda(\lambda') \delta_{\lambda \lambda'}.$$  

(58)

The operator version of the Lorenz gauge condition is then

$$\left[ \hat{a}_0 (k) - \hat{a}_3 (k) \right] |0\rangle = 0.$$  

(59)

In the absence of an electric 4-current density the number of longitudinal photons must equal the number of scalar photons.

The one photon states will be defined as

$$|1_{k\lambda}\rangle = \hat{a}_{1\lambda} (k) |0\rangle,$$

$$|A_{k\lambda}^\mu\rangle = \hat{A}_{1\lambda}^\mu (x) |0\rangle,$$

(60), (61)

with plane wave normalization

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

(62)

Following (28) a general photon state vector can be expanded in the plane wave basis as

$$|A_{k\lambda}^\mu\rangle = -\sqrt{\frac{n}{\epsilon_0}} \int \frac{dk}{(2\pi)^3 2\omega_k} e_\lambda^\mu (k) e_{\lambda^*}^\lambda (k) |1_{k\lambda}\rangle.$$  

(63)

The inner product on a $t$-hyperplane should equal the spatial integral of the $0^{th}$ component of a 4-current. By analogy with (12) and (13) and using the usual convention that repeated indices are to be summed over, the covariant photon 4-current will be defined as

$$J^\mu (x) = -\frac{ie_0 c}{\hbar} A^\mu_v (x) \tilde{\nabla}^\nu \hat{A}^\nu (x)$$

(64)

where $A$ and $\hat{A}$ satisfy (53) and $m = 0$ so $\hat{D} = -\nabla^2$. Following the arguments in Section II it can be verified
that this \( J^\mu(x) \) satisfies a continuity equation. The positive definite number density is \( J^0(x) \). The minus sign in ensures that its space-like terms are positive while its time-like term is negative, making \( J^0(x) \) positive definite. The conjugate field and sign of the energy are given by

\[
A_\epsilon \equiv i\widehat{D}^{-1/2}\partial_t A, \\
i\widehat{D}^{-1/2}\partial_t A^\epsilon = eA^\epsilon
\]

where \( \epsilon = + \) describes absorption and \( \epsilon = - \) denotes emission. The photon inner product that replaces (27) is

\[
\left( A_{\epsilon}^{\ast\lambda}, A_{2\lambda}^\nu \right) = \frac{2\epsilon_0c}{\hbar} \int_t dx A_{\epsilon\lambda}^\ast(x) \widehat{D}^{1/2} A_{2\lambda}^\nu(x) \delta_{\epsilon,\epsilon'}
\]

(67)

where in the second line the sum over \( \nu \) has been evaluated to give the factor \( \delta_{\lambda,\lambda'}\zeta_\lambda \) that follows from (58). Substitution of (63) in (68) with \( \epsilon\omega D/\hbar \rightarrow \omega_k \) gives

\[
\left( A_{\epsilon}^{\ast\lambda}, A_{2\lambda}^\nu \right) = \frac{\epsilon_0c}{\hbar} \int_t \frac{dk}{(2\pi)^3} \epsilon_k^\ast \zeta^\lambda_\nu (k) \epsilon_k^\nu (k) \delta_{\epsilon,\epsilon'}\delta_{\lambda,\lambda'}\zeta_\lambda.
\]

(69)

All modes of the 4-potential can be treated exactly as in Section II except that \( A^0 \) makes a negative contribution to the inner product, while its spatial components make positive contributions. Since \( |\epsilon\rangle \) implies an equal number of scalar and longitudinal photons, their contributions cancel. States \( |n\rangle \) containing no transverse modes but only \( n \) scalar/longitudinal pairs are equivalent to the vacuum so their contribution to the Fock space inner product is \( (n|n) = \langle 0|0 \rangle \).

The one-photon inner product \( \left( A_{1\lambda}', A_{2\lambda}^\nu \right) \) does not count these scalar/longitudinal pairs and contains no vacuum contribution so only transverse photons are counted.

### B. Photon observables

In \( k \)-space \( \hat{P} = \hbar k \) and the photon position operator with commuting components, \( \hat{x} \), is related to the position operator \( i\hbar \partial_k \) as \( \hat{x} = \hat{R} k \partial k - \hbar \hat{R}^{-1} \) where (6)

\[
\hat{R} = \exp(-i\hat{S}_2\phi) \exp(-i\hat{S}_3\theta).
\]

(70)

The operator \( \hat{R} \) rotates \( \epsilon_1 + i\sigma \epsilon_2 \) about \( \theta \), then about \( \epsilon_3 \) by \( \phi \) to give \( \epsilon_0 + i\sigma \epsilon_2 \), and finally about \( \epsilon_k \) by \( \chi \). Here \( \partial_k \) is the \( k \)-space gradient, \( \hat{S}_i \) are the Cartesian components of the spin operator \( \hat{S} \),

\[
\hat{\sigma} = \epsilon_k \cdot \hat{S}.
\]

(71)

is the helicity operator, \( \theta \) and \( \phi \) are the \( k \)-space spherical polar angles, \( \chi(\theta, \phi) \) is the Euler angle and the \( k \)-space spherical polar unit vectors are \( \epsilon_\theta, \epsilon_\phi \) and \( \epsilon_k \). The transverse unit vectors \( \hat{R} (\epsilon_1 + i\lambda\epsilon_2)/\sqrt{2} \) with helicity \( \lambda = \pm 1 \) are

\[
e^{(\lambda)}_\chi = \frac{1}{\sqrt{2}} (\epsilon_\theta + i\lambda \epsilon_\phi) e^{-i\chi}.
\]

(72)

The longitudinal unit vector is \( \hat{R} \epsilon_3 = \epsilon_k \) and the scalar unit vector is unrotated by \( \hat{R} \), that is \( \epsilon_0 = n \).

Following Newton-Wigner, in \( \hat{P} \) the photon position operator was constructed to extract the coordinate \( y \) from its eigenvectors

\[
e^{(\lambda)}_\chi = \omega_\nu^\lambda e^{-ik\cdot y} e^{\mu} (k).
\]

This gives

\[
\hat{x}^{(\lambda)} = i\partial_\nu - \alpha \frac{k}{|k|^2} + \frac{1}{k^2} k \cdot \hat{S} - \partial_\lambda (\theta, \phi)
\]

(75)

equals the Pryce position operator plus a term proportional to

\[
a = \frac{\cos \theta}{k \sin \theta} \epsilon_\phi + \partial_\lambda (\theta, \phi).
\]

(76)

It is this additional term that gives \( \hat{x}^{(\lambda)} \) commuting components. The Euler angle \( \chi(\theta, \phi) \) is defined as a general rotation about \( k \). Any possible transverse basis is the set of eigenvectors of \( \hat{S}_3 \) for some \( \chi(\theta, \phi) \). Since experiments are often performed on optical beams with definite angular momentum, the case \( \chi = -m \phi \) for which the position eigenvectors have intrinsic angular momentum \( l \mu \sigma \) in some arbitrary but fixed direction is of special interest. For this choice of \( \chi \)

\[
a^{(m)} = \frac{\cos \theta - m}{k \sin \theta} \epsilon_\phi
\]

(77)

With \( \epsilon_0 = (1,0,0,0) \), \( \epsilon_1 = \epsilon^{(x)}_1 \), \( \epsilon_2 = \epsilon^{(x)}_2 \) and \( \epsilon_3 = \epsilon_k \) in (68) the Schrödinger picture position eigenvector at \( y \) is \( \hat{P} \).

In the Heisenberg picture

\[
e^{(\lambda)}_\chi = \epsilon^{(\lambda)}_\chi(k) = \epsilon^{(\lambda)}_\chi(k)
\]

(78)

where \( \epsilon^{(\lambda)}_\chi(k) \equiv \epsilon^{(\lambda)}_\chi(k) \) as in Section II. The \( k \)-space velocity operator is

\[
v = \frac{1}{\hbar} [\hat{x}, \hat{H}] = \epsilon \epsilon_k.
\]

(79)
By substitution of (78) in (69) it can be verified that the position eigenvectors satisfy
\[ (A'^{\mu}_{x\mu}, A'^{\mu}_{y\mu}) = \delta (x - y) \delta_{\epsilon,\epsilon'} \delta_{\lambda,\lambda'} \zeta_{\lambda}. \] (80)
As in Section II, (80) is a density. This is a feature of the \( \delta \)-function normalization of a continuous basis.

The position eigenvectors form a basis where (80) is their closure relation. The 4-potential and 4-field analogous to (48), (49) and (50) are obtained by projection of (63) onto the \( |I'_{\lambda} \rangle \) basis is
\[ A'^{\mu}_{\lambda} (x) = -i \sqrt{\frac{\hbar}{\epsilon_0}} \int \frac{dk}{(2\pi)^3} e^{-i\omega_k t} e^{ik \cdot x} \pi^{\mu}_{\lambda} (k), \] (81)
\[ \pi^{\mu}_{\lambda} (x) = \epsilon \sqrt{\frac{\hbar}{\epsilon_0}} \int \frac{dk}{(2\pi)^3} e^{-i\omega_k t} e^{ik \cdot x} \epsilon^{\mu}_{\lambda} (k). \] (82)
Due to their \( e^{-i\omega_k t} e^{ik \cdot x} \pi^{\mu}_{\lambda} (k) \) dependence these 4-vectors satisfy Maxwell’s equations. Substitution of (82) in (79) gives the \( x \)-space inner product
\[ (A'^{1}_{\lambda}, A'^{1}_{2\lambda}) = -\frac{1}{\epsilon_0 \hbar} \int d x \pi^{1\mu}_{\lambda} (x) \pi^{1\mu}_{\lambda} (x). \] (83)

With the 4-potential written as \( A^{\mu} = (\phi (x) / c, A (x)) \) the electric field \( E = -\partial A - \nabla \phi \) equals the field \( \bar{A} \) for its transverse components \( i = 1, 2 \) but for its \( i = 3 \) component.

For any 4-potential, \( A \), satisfying Maxwell’s equations the \( \mu \)-independent Heisenberg picture \( x \)-space photon wave function is, using (82),
\[ \psi_{\lambda} (x) = (A'^{1\mu}_{\lambda}, A) = \int \frac{dk}{(2\pi)^3} e^{-i\omega_k t} e^{ik \cdot x} \pi^{1\mu}_{\lambda} (k). \] (84)

Here \( x = (t, x) \) denotes the position eigenvector at \( x \) on the \( t \)-hyperplane.

In the phasor notation used in classical electromagnetic theory the real potential, field and wave function analogous to (48), (49) and (50) are
\[ A^{\mu}_{\lambda} (x) = \text{Re} A'^{\mu}_{\lambda} (x), \] (85)
\[ \pi^{\mu}_{\lambda} (x) = \text{Re} \pi^{\mu}_{\lambda} (x), \] (86)
\[ \psi_{\lambda} (x) = \text{Re} \psi_{\lambda} (x) \] (87)
and the \( x \)-space probability density is
\[ \rho_{\lambda} (x) = |\psi_{\lambda} (x)|^2. \] (88)

The choice \( C^{t\mu}_{\lambda} (k) = e^{-ik \cdot x} \) gives, at \( t = 0 \), a position eigenvector at \( y \) whose properties are discussed in the next paragraph. The wave function \( \psi_{\lambda} (x) \) describes in-out propagation of a \( \lambda \)-polarized photon localized at \( y \) at time \( t = 0 \). It propagates inwards on a spherical shell if \( t < 0 \) and outwards if \( t > 0 \).

The transverse photon position eigenvectors have a definite 3-component of total angular momentum with indefinite spin and orbital contributions. Writing the total angular momentum as the sum of its extrinsic and intrinsic parts,
\[ J = \hbar x \times k + J_{int}, \] (89)
\[ J_{int} = \hbar \lambda \left( \frac{\cos \theta - m}{\sin \theta} e^{i \phi} \right). \] (90)
Using \( e_{\theta} \cdot e_{3} = -\sin \theta \) and \( e_{k} \cdot e_{3} = \cos \theta \),
\[ J_{int,3} = \hbar m \lambda. \] (91)

In Cartesian components
\[ e_{\lambda} = \frac{1}{\sqrt{2}} \left[ (\cos \theta - \lambda) e^{i(m \lambda + 1) \phi} (e_{1} - i e_{2}) \right. \] (92)
\[ - \sqrt{2} \sin \theta e^{i(m \lambda + 1) \phi} (e_{1} + i e_{2}) \].

With \( J_{3} = L_{3} + S_{3} \) where \( L_{3} \) and \( S_{3} \) are spin and intrinsic orbital angular momentum parallel to the 3-axis, in the first term of (92) \( L_{3} = \hbar (m \lambda + 1) \) and \( S_{3} = -\hbar \lambda \), in the second \( L_{3} = \hbar m \lambda \) and \( S_{3} = 0 \), while in the third term \( L_{3} = \hbar (m \lambda - 1) \) and \( S_{3} = \hbar \lambda \). In all terms their sum is \( \hbar m \lambda \).

IV. CONCLUSION

In this paper we have derived a manifestly covariant quantum mechanical theory of Klein-Gordon neutral bosons and photons. The solutions to their equations of motion are real but, as in classical electromagnetic theory, we found it convenient to define the Hilbert space as a basis of positive and negative frequency waves with a positive definite norm. The positive (or negative) frequency solution can then be used to calculate real fields and wave functions as a final step. We extended the previous work by emphasizing manifest covariance, consistency with QFT and real potentials, fields and wave functions. By incorporating invariant plane wave normalization in the inner product we transformed it to a form in which the position operator is Hermitian and orthogonality of its covariant eigenvectors can be verified directly without recourse to the similarity transformation to the Newton-Wigner basis. The guiding principles of manifest covariance and consistency with QFT led to use of the 4-potential subject to the Gupta-Bleuler gauge constraint. The photon inner product is the sum over definite helicity transverse modes and a longitudinal-scalar mode equivalent to the vacuum. All observables are described by Hermitian operators and the position space wave function is the projection of the photon’s state onto a basis of position eigenvectors.

According to the Reeh-Schlieder theorem there are no local annihilation or creation operators, so a photon cannot be destroyed locally. In a source free region reality of the field and wave function implies no
net absorption. The real photon wave function $\psi_y(x) = \frac{1}{\sqrt{2}} \left( (A^+_x, A_y) + (A^+_y, A_x) \right)$ is an entangled sum of the probability amplitudes for a photon emitted at $y$ and absorbed at $x$ or emitted at $x$ and absorbed at $y$. This is of the form \[21\] where $x$ and $y$ are on a space-like hyperplane. Individually these terms are nonlocal, only their real sum propagates causally. With the addition of photon probability density, Maxwell’s theory based on Faraday experiments \[21\] can be thought of as the first excursion into quantum mechanics. Maxwell’s equations are the original field theory, so it should perhaps not come as a surprise that they have a first quantized interpretation. Since our formalism is consistent with the quantum electrodynamic creation and annihilation operators, it can be extended to coherent and Fock states. In the absence of sources and sinks there is no net photon absorption since the field is real and positive energy absorption is cancelled out by negative energy emission. If the electric 4-current density $J_e$ is nonzero, Maxwell’s wave equation is no longer source free and \[21\] is replaced with \[\Box A^e(x) = -\mu_0 J_e(x)\] so nonzero net absorption is possible and the spatial integral of the inner product \[69\] is not conserved.

Acknowledgement: I thank Juan Leon for valuable discussion and for convincing us to take Reeh-Schlieder seriously.

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