Photon quantum mechanics in real Hilbert space

Margaret Hawton
Department of Physics, Lakehead University, Thunder Bay, ON, Canada, P7B 5E1

Classically, electromagnetic pulses are described by real fields that couple to charged matter and propagate causally. We will show here that real fields of the form used in standard classical electromagnetic theory have a quantum mechanical interpretation in which the probability density for a photon to be at \( x \) is positive definite and operators representing all of the standard physical observables exist. A covariant alternative to the \( \omega^2 \) dependence that appears in most (but not all) presentations of quantum optics and quantum field theory is presented and real Lorentz scalar one photon advanced and retarded potentials are derived.

I. INTRODUCTION

This work was originally motivated by mathematical proofs that a positive frequency field cannot be confined to a finite region of space. According to the Hegerfeldt theorem a positive frequency field localized in a finite region for an instant spreads immediately throughout space [1]. It has been shown explicitly in the case of one dimensional square wells [2] and for three dimensional position eigenvectors [3, 4] that this instantaneous localization is only apparent since it is due to destructive interference of intrinsically nonlocal counterpropagating waves. In algebraic quantum field theory (QFT), the Reeh-Schleider theorem states that there are no local annihilation or creation operators [5]. However, confinement of real fields to a finite region is not a problem in classical electromagnetism (EM). It will be proved here that this use of real fields can be extended to photon quantum mechanics (QM).

The QM of electrons and other fermions is well understood but a consistent first quantized theory of the photon has been elusive. Photons have two properties not shared with electrons that have made derivation of photon QM difficult - they are neutral and massless. While fields describing charged particles are intrinsically complex, neutral particles should be described by real fields. Reality of the photon wave function ensures that photons and antiphotons, being indistinguishable, are equally probable and that, after second quantization, their field operators become Hermitian. This property is problematic in a first quantized theory since the standard relativistic scalar product is zero for neutral particles. Also, while the Wigner little group describing massive particles is the set of spatial rotations, the Wigner little group for massless particles is cylindrically symmetrical. In their seminal paper titled "Localized states of elementary systems", Newton and Wigner assumed invariance under spherically symmetrical rotations and concluded that "for equations with zero mass ... with spin 1 (i.e. Maxwell’s equations) we found that no localized states in the above sense exist. This is an unsatisfactory .. feature of our work" [6]. Both of these difficulties have been overcome [3, 4, 7–10] but here we will extend this work by formulating photon QM in terms of physically correct real fields.

In field theory, particles that transform into themselves are represented by real fields and Hermitian field operators [11]. These real fields can be written as linear combinations of the positive frequency particle terms, \( A^+ \), and negative frequency antiparticle terms, \( A^- \). The real fields \( A_c = (A^+_c + A^-_c)/\sqrt{2} \) and \( A_s = (A^+_s - A^-_s)/\sqrt{2i} \) are even and odd respectively under particle/antiparticle exchange (charge conjugation) where the subscripts \( c \) and \( s \) denote Fourier cosine and sine series respectively. The complex function defined as \( A = A_c + iA_s \) describes both of these potentials, so it will be used here to simplify the mathematics.

In Section II the photon equations of motion will be derived from the standard Lagrangian. The fields will be assumed to be real but for mathematical convenience these real fields will be identified with the real and imaginary parts of a complex field. The zeroth component of the modified standard relativistic four-current will be interpreted as a positive definite photon number density and used to define a scalar product. Interaction with polarized matter will be included so that these equations can be applied to photon propagation in a nonabsorptive medium and emission and absorption of photons by localized sources and sinks. In Section III the real Hilbert space will be defined and operators for all the usual physical observables, including position, will be reviewed to provide a complete first quantized description of single-photon states. In Section IV the fields will be second quantized and in the final Section we will summarize and conclude.

II. REAL AND COMPLEX FIELDS, LAGRANGIAN AND SCALAR PRODUCT

In this Section four-vector notation and complex fields whose real and imaginary parts are even and odd under QFT charge conjugation will be defined. The photon equations of motion, four-current and positive definite number density will be derived from the real standard Lagrangian written in terms of complex fields. A scalar product will be defined in position space and Fourier transformed to momentum space to complete the Hilbert space.

Relativistic notation and SI units will be used. The
contravariant space-time, wave vector and momentum four-vectors are \( x = x^\mu = (ct, x) \), \( k = (\omega_k/c, \mathbf{k}) \) and \( p = ik \) where \( kx = \omega_k t - \mathbf{k} \cdot \mathbf{x} \), the four-gradient is \( \partial = (\partial_{ct}, -\nabla) \), the four-potential is \( A(t, x) = A^\mu = \begin{pmatrix} \phi \cr \mathbf{A} \end{pmatrix} \) or \( a(t, k) = (a_0, \mathbf{a}) \) and \( a_\lambda(k) \) will denote a Lorentz invariant scalar describing a state with definite helicity, \( \lambda \). The covariant four-vector corresponding to \( U^\mu = (U_0, \mathbf{U}) \) is \( U_\mu = g_{\mu\nu} U^\nu = (U_0, -\mathbf{U}) \) where \( g_{\mu\nu} = g^{\mu\nu} \) is a 4 \times 4 diagonal matrix with diagonal \((-1, -1, -1, -1)\).

Positive and negative four-potentials describing photons and antiphotons respectively will be defined as

\[
A_+^0(x) = \sqrt{\frac{\hbar}{\epsilon_0}} \int \frac{dk}{(2\pi)^3} a_{r+}(k) e^{-ikx}, \quad (1)
\]

\[
A_-^0(x) = A_+^0(x), \quad (2)
\]

\[
a_{r+}(k) = a_r(k) e^{ikx}, \quad (3)
\]

for \( r = c \) and \( s \) where \( a_c(k) \) and \( a_s(k) \) are real, \( x' \) is a shift in the origin of the space-time coordinates, the superscript \( * \) denotes complex conjugation, the subscript \( t \) on the integral denotes evaluation at a fixed time \( t \) and \( dk = d^4k \) is an infinitesimal volume in \( k \)-space. The above form was selected because \( \lim_{\nu \to \infty} \Delta n/V = dk/(2\pi)^3 \) where \( \Delta n \) is the number of states and \( \int d^4k \left( \omega_k^2/c^2 - k^2 \right) = \int d^3k \frac{d\nu}{(2\pi)^2} 2\pi c/\nu \). Since \( kx \) and \( \int d^3k \frac{d\nu}{(2\pi)^2} \) are invariants, if \( A_r(x) \) is a four-vector, then \( a_r(k) \) are four-vectors. The real potentials

\[
A_c(x) = A_+^0(x) + A_-^0(x) = \sqrt{2} \text{Re}(A_+^0) \quad (4)
\]

\[
A_s(x) = A_+^0(x) - A_-^0(x) = \sqrt{2} \text{Im}(A_+^0) \quad (5)
\]

\[
= -\sqrt{2} \int \frac{dk}{(2\pi^3)} a_s(k) \sin |k(x-x')|, \quad (7)
\]

are even and odd respectively under spacetime reflection. The factor \( \sqrt{2} \) normalizes the cosine and sine functions squared whose average over a period is \( \frac{1}{2} \). For CPT symmetric particles this is equivalent to QFT charge conjugation. The functions \( A_c(x) \) and \( A_s(x) \) are real by definition. The complex four-potential will be defined as

\[
A(x) = A_c(x) + i A_s(x). \quad (8)
\]

Substitution of \((5)\) and \((7)\) in \((8)\) gives

\[
A(x) = \sqrt{\frac{\hbar}{2\epsilon_0}} \int \frac{dk}{(2\pi)^3} \left[ a_c(k) - a_s(k) \right] e^{ik(x-x')} + \left[ a_c(k) + a_s(k) \right] e^{-ik(x-x')} \quad (9)
\]

which shows that \( A \) is positive frequency only if \( a_c = a_s \). The sines and cosines of the positive and negative frequency plane waves \( e^{-ikx} \) and \( e^{ikx} \) form a basis, but here we start from the premise that only real fields are physically correct and only odd real fields couple correctly to charged matter. The positive and negative frequency fields are introduced to simplify the mathematics. The complex electric and magnetic fields are \( \mathbf{E} = -\partial_t \mathbf{A} - \nabla \phi \) and \( \mathbf{B} = \nabla \times \mathbf{A} \) and the antisymmetric Faraday tensor is

\[
F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \quad (10)
\]

where \( F_{00} = F_{ii} = 0 \) and \( F_{0i} = -F_{i0} = E_i/c \), \( F_{ij} = -F_{ji} = -\epsilon_{ijk} B_k \) and \( \epsilon_{ijk} \) is the Levi-Civita symbol.

The Lagrangian describing two real fields can be written in complex form provided this field and its complex conjugate are treated as formally independent \[12\]. In the presence of a matter four-current density \( J^\mu + c.c. \), the real Lagrangian density will be written as

\[
\mathcal{L} = \mathcal{L}_{std} + \mathcal{L}_{int} \quad (11)
\]

\[
\mathcal{L}_{std} = 0 \mathbf{E} \cdot \mathbf{E}^* - \frac{c^2}{2} \mathbf{B} \cdot \mathbf{B}^* \quad (12)
\]

\[
= \frac{1}{2} \epsilon_0 c^2 F_{\mu\nu} F^{\mu\nu} \quad (13)
\]

where \( c \) is the speed of light, \( \epsilon_0 \) is the dielectric permittivity, \( J^\mu_m = J^\mu_{cm} + i J^\mu_{sm} \) and \( J^\mu_m = (\rho_m c, \mathbf{J}_m) \). The Lagrange equations of motion are then

\[
\partial_{\mu} \left( \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} A_\nu)} \right) = \frac{\partial \mathcal{L}}{\partial A_\nu} \quad (14)
\]

where the momentum conjugate to \( A_\nu \) is

\[
\Pi^{\mu\nu} = \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} A_\nu)} = -\epsilon_0 c^2 \mathcal{F}^{\mu\nu} \quad (15)
\]

Eq. \[12\] then gives

\[
\epsilon_0 c^2 \partial_{\mu} \mathcal{F}^{\mu\nu} = J^\nu_m, \quad (16)
\]

that can be written as the Maxwell equations (ME)

\[
\nabla \cdot \mathbf{D} = \rho_m, \quad \nabla \times \mathbf{H} - \partial_t \mathbf{D} = \mathbf{J}_m \quad (17)
\]

where \( \mathbf{D} = \epsilon_0 \mathbf{E}, \mathbf{B} = \mu_0 \mathbf{H} \) and \( \mu_0 \epsilon_0 = 1/e^2 \). Substitution of \((10)\) in \((16)\) gives the wave equation

\[
\partial_{\mu} \partial^\mu A^\nu = \partial^\nu \Lambda + \mu_0 J^\nu_m \quad (18)
\]

where

\[
\partial_{\mu} \partial^\mu = \partial^2_\nu - \nabla^2 = \nabla^2. \quad (19)
\]

The gauge is determined by

\[
\Lambda = \partial_{\mu} A^\mu. \quad (20)
\]

In the Coulomb gauge \( \nabla \cdot \mathbf{A} = 0 \), so there are no longitudinal modes and the scalar field satisfying \( \nabla^2 \phi = -\rho/\epsilon_0 \) responds instantaneously to changes in charge density. Only the transverse modes propagate at the speed of
light and are second quantized in quantum electrodynamics (QED) to allow creation and annihilation of physical photons. In the Lorenz gauge $\Lambda = 0$ inserted into $\Box \bar{\alpha}$ gives $\partial_{\mu} \partial^\mu A^\nu = \mu_0 J^\mu_m$. In this gauge all four components of $A$ describing the scalar, longitudinal and transverse photon modes propagate at the speed of light and are second quantized in QED. Each complex equation in this paragraph is equivalent to two real equations; one for the even potentials and one for the odd potentials.

Using these complex fields a positive definite photon number density and a scalar product can be derived starting with the global phase change $A \rightarrow e^{i\alpha} A$, $A^* \rightarrow e^{-i\alpha} A^*$ that is a symmetry of the free space Lagrangian $L_{str}$. For an infinitesimal change in $A$, $\delta A \approx i \alpha A$ and $\delta A^* \approx -i \alpha A^*$ so, using $\Pi^{\mu\nu} = -\epsilon_0 c^2 F^{\mu\nu}$, the Noether four-current density becomes $J^\mu (x) \propto \bar{\varphi} F^{\mu\nu} A^\nu - F^{\mu\nu} A^\nu_{\ast}$. The four-current density $J^\mu (x) \propto \bar{\varphi} F^{\mu\nu} (x) A^\nu_{\ast} (x)$ was first obtained in [13] where it was used to derive a Hermitian number density operator.

Based on this expression negative frequency waves make a negative contribution to the number density $J^0 (x)$. To solve this problem Mostafazadeh and coworkers defined the sign of frequency operator $\tilde{\epsilon}$ as [2, 3]

$$\tilde{\epsilon} = i (-\nabla^2)^{-1/2} \partial_{ct}. \quad (21)$$

such that, if $A$ satisfies the photon wave equation, then $\tilde{\epsilon} A$ also satisfies the photon wave equation. With

$$\tilde{F}^{\mu\nu} = \epsilon F^{\mu\nu} \quad (22)$$

it can be verified by substitution that

$$J^\mu (x) = \frac{\epsilon_0 c^2}{2\hbar} \bar{\varphi} F^{\mu\nu} A^\nu + \text{c.c.} \quad (23)$$

satisfies a continuity equation in the homogenous case $J^m_m = 0$ and that $J^0 (x)$ is positive definite for both positive and negative frequency fields. The mathematical expression of the operator $\tilde{\epsilon}$ is discussed in [2, 3]. The operator $\left(-\nabla^2\right)^{-1/2}$ just extracts a factor $|k|^{-1/2}$ from the plane wave $e^{-ikx}$, while $i\partial^\mu e^{-ikx^\mu} = ek e^{-ikx^\mu}$ so that the operator $\tilde{\epsilon}$ extracts the sign of frequency, $\epsilon$. Thus $\tilde{\epsilon} \partial^\mu \cos (kx) = k^\mu \cos (kx)$ and $\tilde{\epsilon} \partial^\mu \sin (kx) = k^\mu \sin (kx)$ gives

$$J^\mu (x) = \frac{\epsilon_0 c^2}{\hbar} \left( \bar{\varphi} F^\mu_c A^\nu + \bar{\varphi} F^\mu_{\ast} A^\nu_{\ast} \right) \quad (24)$$

where $\bar{\varphi} F^\mu_c$ and $\bar{\varphi} F^\mu_{\ast}$ are, respectively, cosine and sine series. If $J^m_m = 0$, $J$ satisfies a continuity equation and the spatial integral of the number density $J^0 (x)$ is conserved.

The four-current [23] or [24] is not gauge invariant due to its dependence on $A$. In the Coulomb gauge only transverse waves propagate, while in the Lorenz gauge longitudinal and transverse photons exist, but their contributions to the scalar product cancel in free space [3]. With the mutually orthogonal polarization unit vectors $e^\mu$ defined such that 0 is time-like, 1 and 2 are transverse and 3 is longitudinal, $\epsilon_0 = n^\mu = (1, 0, 0, 0)$, $e_3 (k) = e_k = k / |k|$ and the definite helicity transverse unit vectors are

$$e_\lambda = \frac{1}{\sqrt{2}} (e_\theta + i \lambda e_\phi) \quad (25)$$

for $\lambda = \pm 1$ where $e_\theta$, $e_\phi$ and $e_k$ are $k$-space spherical polar unit vectors on the $t$-hyperplane. Since $e^\mu$ is a four-vector its coefficient in any expression for $a^\mu$ should be a Lorentz invariant scalar. Writing $\bar{\varphi} F^{\mu\nu}$ as an electric field divided by $c$ and including only transverse photons with helicity $\lambda = \pm 1$, the scalar product at a fixed time $t$ will be defined as

$$(A_1, A_2)_t = \frac{\epsilon_0}{\hbar} \sum_{\lambda = \pm 1} \int_{t} dx \bar{E}_{1\lambda} (x) \cdot A_{2\lambda} (x) \quad (26)$$

where the transverse $\lambda = \pm 1$ components of the potentials [3, 5] and [7] and their dual fields are

$$A_{\lambda} (x) = A_{c\lambda} (x) + i A_{s\lambda} (x), \quad (27)$$

$$A_{c\lambda} (x) = \sqrt{\frac{2\hbar}{\epsilon_0}} \int_{t} \frac{dk}{(2\pi)^3/2} a_{c\lambda} (k) \cos [k (x - x')], \quad (28)$$

$$A_{s\lambda} (x) = -\sqrt{\frac{2\hbar}{\epsilon_0}} \int_{t} \frac{dk}{(2\pi)^3/2} a_{s\lambda} (k) \sin [k (x - x')], \quad (29)$$

$$\bar{E}_{r\lambda} (x) = \bar{E}_{r\lambda} (x) = -\tilde{\epsilon} \partial_k A_{r\lambda} (x). \quad (30)$$

In these expressions

$$a_{r\lambda} (k) \equiv a_{r\lambda} (k) e_{\lambda}, \quad a_{r\lambda} (k) = a_{r\lambda} (k) e^{ikx}, \quad (31)$$

where $a_{r\lambda} (k)$ is a Lorentz invariant scalar. Differentiation of

$$A_{r\lambda} (x) = \sqrt{\frac{\hbar}{\epsilon_0}} \int_{t} \frac{dk}{(2\pi)^3/2} a_{r\lambda} (k) e^{-ikx} \quad (32)$$

gives the positive frequency dual electric fields

$$\bar{E}^{\lambda}_{r\lambda} (x) = \sqrt{\frac{\hbar}{\epsilon_0}} \int_{t} \frac{dk}{(2\pi)^3/2} a_{r\lambda} (k) e^{-ikx}. \quad (33)$$

As in [10] to [17] $A_{\lambda} = \sqrt{2} \text{Re} A^+_{\lambda}$, $A_{s\lambda} = \sqrt{2} \text{Im} A^+_{\lambda}$, $E_{\lambda} = \sqrt{2} \text{Re} \bar{E}^+_{\lambda}$ and $E_{s\lambda} = \sqrt{2} \text{Im} \bar{E}^+_{\lambda}$. Substitution of (27) gives the scalar product (26) in terms of its real even and odd components as

$$(A_1, A_2)_t = \frac{\epsilon_0}{\hbar} \sum_{\lambda = \pm 1} \int_{t} dx \left[ \bar{E}_{1\lambda} (x) \cdot A_{2\lambda} (x) + \bar{E}_{1\lambda} (x) \cdot A_{2\lambda} (x) \right]. \quad (34)$$

Bra-ket notation will be defined as in Schrödinger QM so that (34) can be written as

$$(A_1, A_2)_t = \frac{\epsilon_0}{\hbar} \sum_{\lambda = \pm 1} \left[ \langle \bar{E}_{1\lambda} \cdot A_{2\lambda} \rangle + \langle \bar{E}_{1\lambda} \cdot A_{2\lambda} \rangle \right]. \quad (35)$$
where

\[
\langle \tilde{E}_{1r\lambda} \cdot A_{2r\lambda} \rangle = \sum_{j=1}^{3} \langle \tilde{E}_{1r\lambda_j} | A_{2c\lambda_j} \rangle = \int d\mathbf{x} \tilde{E}_{1r\lambda}(x) \cdot A_{2r\lambda}(x)
\]

\[
= \int \frac{d\mathbf{k}}{(2\pi)^3} a_{1r\lambda}(\mathbf{k}) a_{2r\lambda}(\mathbf{k}) \frac{\omega_k}{\omega_k} e^{i\mathbf{k} \cdot (x_1 - x_2)}.
\]

Equality of these last two expressions is an expression of the Parseval-Plancherel identity. By inspection of \([33]\) and \([32]\), \(a_{r'x'\lambda}(\mathbf{k})\) are Fourier transforms of \(\frac{\sqrt{\pi}}{c} \tilde{E}_{1x\lambda}(x)\) while \(a_{r'x'\lambda}(\mathbf{k})/\omega_k\) are Fourier transforms of \(\frac{\sqrt{\pi}}{c} A_{1x\lambda}^\dagger(x)\). Explicitly, in \(\mathbf{k}\)-space, the scalar product is

\[
(A_1, A_2)_t = \sum_{\lambda = \pm 1} \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\omega_k}{\omega_k} (a_{1\lambda\lambda}(\mathbf{k}) a_{2\lambda\lambda}(\mathbf{k})
+ a_{1s\lambda}(\mathbf{k}) a_{2s\lambda}(\mathbf{k})) e^{i\mathbf{k} \cdot (x_1 - x_2)}.
\]

If \(A_2 = A_1\), the scalar product \((A_1, A_2)_t\) reduces to the spatial integral of number density \(J^0(t, \mathbf{x})\). Only free transverse photons are counted. In the presence of sources and sinks this photon number is not conserved. The sine and cosine series are orthogonal.

Inspection of \([35]\) and \([39]\) shows that these expressions for the scalar product involve both the potential and the electric field rather than a single function. QM based on scalar products of this form can be described and the electric field rather than a single function. QM versions for the scalar product involve both the potential and position eigenvectors are bases that allow for both possibilities.

The real Hilbert space is the vector space of all \(A_c\) and \(A_s\) and their derivatives with the scalar product \([36]\). Momentum is an observable. It can be verified by substitution in \([37]\) that the plane waves with definite momentum \(\hbar \mathbf{k}'\) defined covariantly as

\[
a_{r'x'\lambda}(\mathbf{k}) = (2\pi)^3 \omega_k \delta(\mathbf{k} - \mathbf{k}') e_{\lambda'}(\mathbf{k}')
\]

with \(\omega_k = c |\mathbf{k}|\) and \(r = c \) and \(s\) are biorthogonal in the sense that

\[
\langle A_{k\lambda}, A_{k'\lambda'} \rangle = \delta_{\lambda\lambda'} (2\pi)^3 \omega_k \delta(\mathbf{k} - \mathbf{k}').
\]

This normalization of the plane wave basis is invariant as can be seen from \(\int \frac{d\mathbf{k}}{\omega_k} \omega_k \delta(\mathbf{k} - \mathbf{k}') = 1\). In position space in the Heisenberg picture (HP)

\[
A_{k\lambda}(\mathbf{x}, t) = \sqrt{\frac{\pi}{\epsilon_0}} e^{-i\mathbf{k} \cdot \mathbf{x}} e_{\lambda}(\mathbf{k})
\]

where \(a_c = a_s\) so its real and imaginary parts are cosine and sine plane waves. This contrasts with \(A\) describing a physical state in which the cosine and sine terms should be independent real solutions to the wave equation. In a general physical state \(A\) the probability amplitude for wave vector \(\mathbf{k}\) is

\[
(A_{k\lambda}, A_r) = a_{r\lambda}(\mathbf{k})
\]

If \(\omega_k\) is replaced with \(\omega_k^{1/2}\) in [38] the noncovariant Newton-Wigner \([6]\) normalization, \(\langle A_{k\lambda}, A_{k'\lambda'} \rangle_{NW} = \delta_{\lambda\lambda'} (2\pi)^3 \delta(\mathbf{k} - \mathbf{k}')\), is obtained. The position space plane waves \([40]\) are eigenvectors of the four-momentum operator

\[
\hat{P} = (\hat{p}_0, \hat{\mathbf{p}}) = \hbar \left( \sqrt{-\nabla^2} - i\mathbf{e} \nabla \right)
\]

In \(\mathbf{k}\)-space the four momentum operator is \(\hat{P} = \hbar (\omega_k/c, \mathbf{k})\). In either case the four-momentum eigenvalues are

\[
P = \hbar (\omega_k/c, \mathbf{k}).
\]

The Hamiltonian operator

\[
\hat{H} = \hbar c \sqrt{-\mathbf{\nabla}^2}
\]

generates unitary transformations according to the Schrödinger equation

\[
i\hbar \partial_t A(t) = \hat{H} A(t).
\]

Position is also an observable. The Fourier transform of the localized state \(\delta(\mathbf{x} - \mathbf{x}')\) is the plane wave \(\exp(i\mathbf{k} \cdot \mathbf{x}')\) so the photon position eigenvectors in the HP should be of the form

\[
a_{r'x'\lambda}(\mathbf{k}) = \omega_k^c e_{\lambda}(\mathbf{k}) e^{ikx'}
\]

for \(r = c\) and \(s\) where \(kx' = \omega_k t' - \mathbf{k} \cdot \mathbf{x}'\) and \(\alpha = 0\) in the covariant formulation and \(\alpha = \frac{1}{2}\) for Newton Wigner position eigenvectors. Here the covariance is emphasized, so in the rest of this Section \(\alpha\) will be set equal to 0. In position space

\[
A_{\lambda}(\mathbf{x}) = -\frac{\hbar}{2\epsilon_0} \int \frac{d\mathbf{k}}{(2\pi)^3} e_{\lambda}(\mathbf{k}) e^{-i\mathbf{k} \cdot (x - x')}.
\]
where

\[ \hat{a} \]

states and position and angular momentum operators are reviewed for position eigenvectors proportional to \( \omega \) compensates for differentiation of \( \hat{a} \) in (37) the projection of an arbitrary physical state described by \( A \) and \( A_s \) onto the \( A_\lambda \) basis,

\[ \phi_{\lambda}(x) = (A_{\lambda}, A_r)_t = \frac{dE}{2\pi} \int_0^1 a_{\lambda}(k) e^{-ikx}, \quad (48) \]

has the mathematical form of a Lorentz invariant scalar potential that satisfies the zero mass Klein-Gordon (KG) equation.

The Schrödinger picture (SP) photon position operator with commuting components and eigenvectors

\[ \hat{R}(\theta) \]

can be derived by rotating \( \hat{e}_1 + i\hat{e}_2 \) about \( \hat{e}_2 \) by \( \theta \) then about \( \hat{e}_3 \) by \( \phi \) to give \( \hat{e}_3 + i\hat{e}_2 \) using the operator \( \hat{R} \) so that \( \hat{e}_\theta + i\lambda\hat{e}_\phi = \hat{R}(\hat{e}_1 + i\lambda\hat{e}_2) \) and \( i\hat{\theta}_k \) transforms to \( \hat{x} = \hat{R}i\hat{\theta}_k\hat{R}^{-1} \). Alternatively it can be obtained by brute force subtraction of the \( k \)-space gradient of \( e_{\lambda}(k) \) and \( |k|^2 \) to give

\[ \hat{x} = i\hat{\partial}_k - ia \frac{k}{|k|^2} + \frac{1}{|k|^2} k \cdot \hat{S} - \hat{\lambda} \frac{\cos \theta}{k \sin \theta} e_\phi \quad (49) \]

for position eigenvectors proportional to \( \omega_k^2 \) where \( \omega_k = c |k| \), the helicity operators is \( \hat{\lambda} = \hat{e}_\lambda \hat{S} \) for spin operator \( \hat{S} \) and the term \(-i\hat{\partial}_k |k| = \hat{\lambda} \frac{\cos \theta}{k \sin \theta} e_\phi \) compensates for differentiation of \( \omega_k^2 \) in (49). The HP photon position operator is given by \( \hat{x} \). The helicity \( \lambda \) photon position eigenvectors have a definite component of total angular momentum in the fixed but arbitrary direction \( \hat{e}_3 \) with indefinite spin and orbital contributions

\[ \hat{J} = \hat{x} \times \hat{P} + \hat{J}_{int}, \quad (50) \]

\[ \hat{J}_{int} = \hbar \lambda \left( \frac{\cos \theta}{\sin \theta} \hat{e}_\phi + \hat{e}_k \right). \quad (51) \]

where \( \hat{J}_{int} \) is the internal angular momentum operator and \( \hat{x} \times \hat{P} \) describes external angular momentum. The position and angular momentum operators are reviewed in more detail in [1, 15] where rotation about \( k \) through an Euler angle that gives a more general expression for \( \hat{J} \) is included.

Setting \( a_{\lambda}(k) \) in [18] equal to the \( \alpha = 0 \) physical states \( a_{\alpha=\lambda}(k) \) given by

\[ a_{\alpha=\lambda}(k) = \frac{1}{4\pi^2} \frac{1}{\omega_k} \sum_{\gamma=\pm} [\gamma \pi \delta (r - \gamma c \Delta t)] \]

\[ + P \left( \frac{1}{r - \gamma c \Delta t} \right) \]

\[ (52) \]

to give

\[ \phi_{c\lambda}(x) = (A_{c\lambda}, A_{c\alpha}) = \frac{1}{4\pi^2} \left[ P \left( \frac{1}{r - c \Delta t} \right) + P \left( \frac{1}{r + c \Delta t} \right) \right], \quad (53) \]

\[ \phi_{s\lambda}(x) = (A_{s\lambda}, A_{s\alpha}) = \frac{1}{4\pi^2} \left[ \delta (r + c \Delta t) - \delta (r - c \Delta t) \right], \quad (54) \]

for \( \lambda = \pm 1 \). Here \( P \) denotes the principal value integral that excludes the singularity in the integrand used to evaluate (52). Both (53) and (54) satisfy the homogeneous photon wave equation \( \Delta \phi_{\lambda}(x) = 0 \), but only \( \phi_{c\lambda}(x) \) is odd under QFT charge conjugation and couples to charged matter. Schwinger [17] inverted \( \Delta \) and found that the unique Green’s function solving \( \Delta \phi_{\lambda}(x) = \delta(x - x’) \delta(t - t’) \) is

\[ \frac{1}{4\pi^2} \left[ \delta (r + c \Delta t) + \delta (r - c \Delta t) \right] \]

where \( t’ = t - r/c < t \) is the retarded time and \( t’ = t + r/c > t \) is the advanced time. He concluded that the retarded potential is determined by boundary conditions and equals the sum of his unique contour integral independent Green function and a solution to a homogeneous wave equation. This retarded potential is important in classical EM and, according to [54], it can be applied to photon QM with the significant advantage that \( \phi_{c\lambda}(x) \) is a Lorentz scalar.

The scalar potential \( \phi_{s\lambda}(x) \) is generally known as the commutator or causal Green function since it has support only within the light cone [3, 18]. Its time derivative

\[ \psi_{s\lambda}(t, x) = \int \frac{dE}{2\pi^3} e^{-ik(x - x’)} \]

\[ (55) \]

forms a localized basis. The Born rule gives a probability interpretation of the state vector. It states that if an observable corresponds to a self-adjoint operator and the state vector describing a physical system is normalized, the sum of the absolute squares of the probability amplitudes of its eigenvalues is unity. For continuous observables such as position the sum becomes an integral. Here as in the Schrödinger description of the electron the localized functions \( \delta(x - x’) \) are not technically in the Hilbert space since they are not square integrable but they satisfy a completeness relation and form a very convenient basis [19], so the \( \delta \)-localized basis [55] will be used here. Expanding \( \psi_{s\lambda} \) in the \( \delta \)-basis at time \( t \) as

\[ \psi_{s\lambda}(t, x) = \int d\Delta t \delta(x - x’) \psi_{s\lambda}(t, x’), \quad (56) \]

it can be seen that \( \psi_{s\lambda}(x) \) is the probability amplitude for a photon to be in the state \( \delta(x - x’) \) on the \( t \)-hyperplane. The \( \lambda \)-helicity \( x \)-space probability density is

\[ \rho_{s\lambda}(t, x) = [\psi_{s\lambda}(t, x)]^2. \quad (57) \]
If \((A, A)\) is finite, \(A\) is normalizable as \((A, A) = 1\). The \(k\)-space probability density is
\[
\rho_{x\lambda}(k) = [a_{x\lambda}(k)]^2. \tag{58}
\]
Quantum mechanics requires state vectors to describe physical systems and operators representing observables such that the only possible result of a measurement is one of their eigenvalues \([k] \). Eqs. \((59)\) to \((68)\) provide a scalar Schrödinger-like description of a photon with helicity \(\lambda\) in which \(\psi_{x\lambda}(t, x)\) is the probability amplitude for a photon to be at \(x\) on the \(t\)-hyperplane and its Fourier transform \(a_{x\lambda}(k)\) is the probability amplitude for it to have momentum \(\hbar k\).

IV. SECOND QUANTIZATION

A first quantized photon cannot be created or destroyed - creation and annihilation of photons and the description of \(n\)-photon states requires second quantization. In QFT, QED and Quantum Optics fields are second quantized by raising them to the status of operators. The position eigenvectors \([24]\) are positive frequency so these functions plus their complex conjugates are real and become Hermitian operators when second quantized. For an arbitrary first quantized state generalized to include a factor \(\omega_k^0\) to accommodate the factor \(\omega_k^{1/2}\) commonly used,
\[
\hat{A}(x) = \sqrt{\frac{\hbar}{\epsilon_0}} \sum_{x=\pm 1} \int \frac{dk}{(2\pi)^3} (2\omega_k)^{\alpha-1} \left[ \hat{a}_{\lambda}(k) e^{i\omega_k x} + \hat{a}^\dagger_{\lambda}(k) e^{-i\omega_k x} \right] e^{ikx}, \tag{59}
\]
where the operator \(\hat{a}_{\lambda}(k)\) annihilates a photon with wave vector \(k\) and helicity \(\lambda\) and \(\hat{a}^\dagger_{\lambda}(k)\) creates one. The plane waves will be assumed to satisfy the commutation relations
\[
\left[ \hat{a}_{\lambda}(k), \hat{a}_{\lambda'}(k') \right] = 0, \quad \left[ \hat{a}^\dagger_{\lambda'}(k), \hat{a}^\dagger_{\lambda'}(k') \right] = 0,
\]
\[
\left[ \hat{a}_{\lambda}(k), \hat{a}^\dagger_{\lambda'}(k') \right] = \delta_{\lambda,\lambda'} (2\pi)^3 (2\omega_k)^{-2\alpha} \delta(k-k'). \tag{60}
\]
The usual text book choice is \(\alpha = \frac{1}{2}\) but \(\alpha = 0\) for which \([59]\) and \([60]\) are covariant is used here and in \([20, 21]\).

The field operator \([59]\) creates and annihilates photons at \(x\). The commutator
\[
\hat{C}_{\lambda}(x, x') \equiv i\frac{\epsilon_0}{\hbar} \left[ \hat{A}_{\lambda}(t, x) \cdot \hat{E}_{\lambda}(t', x') - \hat{E}_{\lambda}(t', x') \cdot \hat{A}_{\lambda}(t, x) \right] \tag{61}
\]
with \(\hat{E}_{\lambda}(x) = -\partial_t \hat{A}_{\lambda}(x)\) describes creation of a photon with helicity \(\lambda\) at \((t', x')\) followed by its annihilation at \((t, x)\) and creation at \((t, x)\) followed by annihilation at \((t', x')\). It can be verified by substitution at \(t = t'\) that
\[
\hat{C}_{\lambda}(t, x; t, x') = \delta(x-x'). \tag{62}
\]
Eq. \((61)\) leads to a physical interpretation of the potential \([24]\). Defining the vacuum state as \([0]\) and the one photon position eigenvectors
\[
|A_{x\lambda}\rangle = \hat{A}_{\lambda}(x) |0\rangle, \quad |E_{x\lambda}\rangle = \hat{E}_{\lambda}(x) |0\rangle \tag{63}
\]
and using the standard bra-ket notation, the vacuum expectation value of \((61)\) gives
\[
\langle 0 | \hat{C}_{\lambda}(x, x') | 0 \rangle = \phi_{x\lambda}(x) \tag{64}
\]
that propagates causally.

V. SUMMARY AND CONCLUSION

In its covariant \(\alpha = 0\) version, photon quantum mechanics as described here preserves the classical form of the EM potential and fields when first and second quantized. Only the interpretation need be changed - from real observable classical fields, to probability amplitudes, and then to operators that create and annihilate photons. The real potentials are even and odd under QFT charge conjugation, but only those that are odd can be localized in a finite region and coupled to charged matter. These even and odd fields are real and imaginary parts of a complex field whose use simplifies the mathematics and facilitates use of the standard Lagrangian and relativistic scalar product. Propagation of finite pulses is as in classical EM and mathematical techniques such as finite difference time domain (FDTD) \([22]\) developed to handle problems in classical EM theory can be applied directly to single photons. Projection onto momentum and position bases gives a covariant Schrödinger-like description of photon QM. Eqs. \([48]\) and \([59]\) to \([65]\) provide a scalar description of single photon states with a well defined physical interpretation that may prove to be useful in applications.

The need for a single photon wave function consistent with classical EM theory is illustrated by the interpretation of a recent experiment. Propagating light pulses were split by a Fresnel biprism and coincidence incidences were ten times more coincidence counts. This is a clear demonstration that a one-photon state exhibits quantum mechanical particle-like behavior. In analysis of their data the authors use the well-known result from Quantum Optics that phenomena like interference, diffraction, propagation, can be computed with the classical theory of light even in the single-photon regime.”
[1] G.C. Hegerfeldt, "Remark on causality and particle localization," *Phys. Rev. D* 10, 3320-3321 (1974)
[2] E. Karpov, G. Ordonez, T. Petrosky, I. Prigogine and G. Pronko, "Causality, delocalization, and positivity of energy," *Phys. Rev. A* 62, 012103 (2000)
[3] M. Hawton and V. Debierre, "Maxwell meets Reeh-Schlieder: the quantum mechanics of neutral bosons," *Phys. Lett. A* 381, 1926 (2017)
[4] M. Hawton, "Maxwell quantum mechanics," *Phys. Rev. A* 100, 012102 (2019)
[5] H. Reeh and S. Schlieder, "Bemerkungen zur unitaraquivalenz von Lorentzinvvarianten Feldern," *Nuovo Cimento* 22, 1051 (1961)
[6] T. D. Newton and E. P. Wigner, "Localized States for Elementary systems," *Rev. Mod. Phys.* 21, 400 (1949)
[7] M. Hawton, "Photon position operator with commuting components," *Phys. Rev. A* 59, 954-959 (1999); "Photon wave functions in a localized coordinate space basis," *Phys. Rev. A* 59, 3223-3227 (1999)
[8] A. Mostafazadeh and F. Zamani, "Quantum Mechanics of Klein-Gordon Fields I: Hilbert Space, Localized States, and Chiral Symmetry," *Ann. Phys.* 321, 2183 (2006)
[9] H. Babaei and A. Mostafazadeh, "Quantum Mechanics of a Photon," *J. Math. Phys.* 58, 082302 (2017)
[10] M. Hawton and V. Debierre, "Photon position eigenvectors, Wigner’s little group and Berry’s phase", *J. Math. Phys.* 60, 052104 (2019)
[11] M. Gell-Mann and A. Pais, "Behavior of Neutral Particles under Charge Conjugation," *Phys. Rev.* 97, 1387-1389 (1958)
[12] C. Cohen-Tannoudji, J. Dupont-Roc and G. Grynberg, *Photons and Atoms: Introduction to Quantum Electrodynamics*, Wiley-VCH (1997)
[13] M. Hawton and T. Melde, "Photon number density operator iE.Â," *Phys. Rev. A* 51, 4186 (1995)
[14] D. C. Brody, "Biorthogonal Quantum Mechanics," *J. Math. Phys. A: Math. Theor.* 47, 035305 (2014)
[15] M. Hawton and W. E. Baylis, "Photon position operators and localized bases," *Phys. Rev. A* 64, 012101 (2001); "Angular momentum and the geometrical gauge of localized photon states," 71, 033816 (2005)
[16] M. Dobrski, M. Przanowski, J. Tosiek and F. J. Turrubiates, "The geometrical interpretation of the photon position operator," *arXiv:2104.04351* (2021)
[17] S. L. Schweber, "Advanced and retarded solutions in field theory," *Int. J. of Theor. Physics* 3, 347-353 (1970)
[18] J. J. Halliwell and M. E. Ortiz, "Sum-over histories origin of the composition laws of relativistic quantum mechanics and quantum cosmology," *Phys. Rev. D* 48, 748-768 (1993)
[19] C. Cohen-Tannoudji, B. Diu and F. Laloë, *Quantum Mechanics Volume one*, Wiley (1977)
[20] C. Itzykson and J. B. Zuber, *Quantum Field Theory 1st ed.* McGraw-Hill, (1980)
[21] V. Debierre, The Photon Wave Function in Theory and in Practice, PhD thesis École Centrale de Marseille (2015)
[22] Dong-Yeop Na and Weng Cho Chew, "Quantum Electromagnetic Finite-Difference Time-Domain Solver," *Quantum Rep.* 2, 253-265 (2020)
[23] V. Jacques, E Wu, T. Toury, F. Treussart, A Aspect, P. Grangier and J.-F. Roch, "Single photon wave-front interference: and illustration of the light quantum in action, *arXiv:2011.12664 [quant-ph]*"