Photon wave mechanics and position eigenvectors

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(Received 11 September 2006; revised manuscript received 9 March 2007; published 15 June 2007)

One and two photon wave functions are derived by projecting the quantum state vector onto simultaneous eigenvectors of the number operator and a recently constructed photon position operator [Phys. Rev. A **59**, 954 (1999)] that couples spin and orbital angular momentum. While only the Landau-Peierls wave function defines a positive definite photon density, a similarity transformation to a biorthogonal field-potential pair of positive frequency solutions of Maxwell's equations preserves eigenvalues and expectation values. We show that this real space description of photons is compatible with all of the usual rules of quantum mechanics and provides a framework for understanding the relationships amongst different forms of the photon wave function in the literature. It also gives a quantum picture of the optical angular momentum of beams that applies to both one photon and coherent states. According to the rules of quantum mechanics, this wave function gives the probability to count a photon at any position in space.

DOI: 10.1103/PhysRevA.75.062107 PACS number(s): 03.65.Ta, 42.50.Dv

I. INTRODUCTION

The current interest in entanglement and its application to quantum information has rekindled the controversy surrounding the photon wave function [1–6]. It is still unclear what form a real space photon wave function should take, or if one exists. In the standard formulation of quantum mechanics, the coordinate space wave function is the projection of the state vector onto an orthonormal basis of eigenvectors of a Hermitian position operator. It has been claimed since the early days of quantum mechanics that there is no position operator for the photon that allows the introduction of a wave function in this way. Contrary to these claims, we have recently constructed a photon position operator whose transverse eigenvectors form a real space basis. Here we will use this basis to obtain a photon wave function that is compatible with the usual rules of quantum mechanics. We will show that this clarifies a number of previously unresolved issues regarding the real space description of one photon and multiphoton states.

In 1933 Pauli [7] stated that the nonexistence of a density for the photon corresponds to the fact that the position of a photon cannot be associated with an operator in the usual sense. Based on definitions of center of mass, Pryce found the **k**-space photon position operator $\hat{\mathbf{r}}_P = i\nabla - i\hat{\mathbf{k}}/2k + \hat{\mathbf{k}} \times \mathbf{S}/k$ where S_j are the 3×3 spin 1 matrices, $\hat{\mathbf{k}}$ is a unit wave vector, and $\nabla_j = \partial/\partial k_j$ [8]. This operator does not have commuting components which suggests that three spatial coordinates cannot simultaneously have a definite value. In 1949 Newton and Wigner sought rotationally invariant localized states and the corresponding position operators. They were successful for massive particles and zero mass particles with spin 0 and 1/2, but found for photons "no localized states in the above sense exist" [9]. This result is widely quoted as a proof of the nonexistence of a photon position operator. It has been proved that there is no photon position operator with commuting components that transforms as a vector [10].

Our position operator [11] has commuting components but is not rotationally invariant and does not transform as a vector [12], and thus it is consistent with the previous work. Description of a localized state requires a sum over all **k**, and a localized photon can have definite spin in the **k** direction, that is it can have definite helicity, but it cannot have definite spin along any fixed axis. It is the total angular momentum (AM) that can have a definite value along some specified direction in space [13]. The position eigenvectors are not spherically symmetric, instead they have a vortex structure as is observed for twisted light [14]. Compared to the Newton Wigner position operators for which transformation of a particle's spin and position are separable, the photon position operator must incorporate an additional unitary transformation that reorients this vortex.

Valid position eigenvectors cannot violate the Hegerfeldt [15] and Paley-Wiener [16] theorems based on Fourier transform theory. Hegerfeldt proved that a positive frequency wave function can be exactly localized at only one instant in time and interpreted this to imply a violation of causality. Bialynicki-Birula [17] noted that the Paley-Wiener theorem limits $g(x) = \int_0^\infty dk\, h(k)\exp(-ikx)$ of the form $\exp(-Ax^\gamma)$ to $\gamma < 1$. He then applied this to separate outgoing and incoming exponentially localized spherical pulses in three dimensions. However, their sum is not subject to the exponential localization limit, as can be seen from the form of the k integral. Position eigenvectors require a sum over all wave vectors, and thus must be a sum of outgoing and incoming waves that interfere to give exact localization at a single instant in time, consistent with the Hegerfeldt theorem.

Maxwell's equations (MEs) are analogous to the Dirac equation when written in terms of the Riemann-Silberstein (RS) field vector, proportional to $\mathbf{E} \pm ic\mathbf{B}$ where c is the speed of light in vacuum, **E** is the electric field, and **B** is the magnetic induction. This suggests that the photon is an elementary particle like any other, and that MEs provide a first quantized description of the photon. Use of the positive frequency RS vector as a photon wave function in vacuum and in a medium has been thoroughly studied [1,18–20]. If a field $\boldsymbol{\Psi}^{(1/2)}$ with quantum electrodynamic weighting, $k^{1/2}$, is used

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as wave function, a metric factor k^{-1} is required in the scalar product. The real space squared norm then goes as $\int d^3r \int d^3r' \boldsymbol{\Psi}^{(1/2)*}(\mathbf{r}) \cdot \boldsymbol{\Psi}^{(1/2)}(\mathbf{r}')/|\mathbf{r}-\mathbf{r}'|^2$ and thus its integrand cannot be interpreted as a local number density [18,21]. Since the photon has no mass, it has been suggested that there is no photon number density, only energy density [20]. Photon number density based on the Landau-Peierls (LP) wave function $\boldsymbol{\Psi}^{(0)}$ (without the factor $k^{1/2}$) was investigated as early as 1930 [22,23]. Its absolute value squared is positive definite but it has the disadvantage that its relationship to electric current density and the electromagnetic fields is nonlocal in real space [18,22–24].

Returning to fieldlike $\boldsymbol{\Psi}^{(1/2)}$ functions, we will show here that it is possible to define a biorthonormal basis that gives a local density by combining the eigenvectors of an operator with those of its adjoint. This formalism has recently been applied to pseudo-Hermitian Hamiltonians that possess real spectra [25]. Such a basis provides an interesting alternative to explicit inclusion of a metric operator when working with electromagnetic fields. The density $\boldsymbol{\Psi}^{(1/2)*}(\mathbf{r}) \cdot \boldsymbol{\Psi}^{(-1/2)}(\mathbf{r})$ is local, but it not positive definite since it is not an absolute value squared. Only the LP wave function defines a positive definite photon density, equal to $|\boldsymbol{\Psi}^{(0)}(\mathbf{r})|^2$. However, we will show that the biorthogonal field-potential pair gives the same results in most calculations.

In the present paper one and two photon wave functions and photon density will be obtained by projection onto a basis of position eigenvectors. In Sec. II the photon position operator will be reviewed and the scalar product and hermiticity will be discussed. In Sec. III the orthonormal and biorthonormal eigenkets of the position operator will be obtained in the Heisenberg picture (HP). We will then derive photon wave functions from quantum electrodynamics (QED) in Sec. IV by projecting the state vector onto simultaneous eigenvectors of the photon position, helicity, and number operators. We will discuss MEs, photon wave mechanics, and angular momentum and beams in Secs. V–VII, respectively, and then conclude.

II. POSITION OPERATOR

We start with a discussion of the photon position operator. The procedure used in [11] was to construct an operator with transverse eigenvectors of definite helicity, $\sigma=\pm 1$. In $\mathbf{k}$ space, it is reasonable to expect that the transverse function

$$\psi^{(\alpha)}_{\mathbf{r},\sigma,j}(\mathbf{k}) = (\omega_k)^{\alpha} e^{(\chi)}_{\mathbf{k},\sigma,j} \exp(-i\mathbf{k}\cdot\mathbf{r})/\sqrt{V} \tag{1}$$

describes a photon located at position $\mathbf{r}$, where $\omega_k=kc$ in vacuum and the parameter χ will be discussed later in this section. Subscripts denote eigenvalues and Cartesian components of the vectors $\boldsymbol{\psi}$ and $\mathbf{e}$. Cartesian components are used where it is necessary to avoid confusing vector notation. The parameter α allows for both LP and field based wave functions. The position eigenvectors are electric and/or magnetic fields if $\alpha=1/2$, the vector potential if $\alpha=-1/2$, or LP wave functions if $\alpha=0$. This is consistent with the QED based interpretation that a mode with frequency ω_k has energy $\hbar\omega_k$ so that the square of the fields gives energy density while the wave function gives number density. The spherical polar definite helicity unit vectors are

$$\mathbf{e}^{(0)}_{\mathbf{k},\sigma} = (\hat{\boldsymbol{\theta}} + i\sigma\hat{\boldsymbol{\phi}})/\sqrt{2}, \tag{2}$$

where $\hat{\boldsymbol{\theta}}$ and $\hat{\boldsymbol{\phi}}$ are unit vectors in the increasing θ and ϕ directions. Periodic boundary conditions in a finite volume are used here to simplify the notation, and the limit as $V \to \infty$ can be taken to calculate derivatives and perform sums. If the wave function (1) is a position eigenvector it should satisfy the eigenvector equation

$$\hat{\mathbf{r}}^{(\alpha)} \psi^{(\alpha)}_{\mathbf{r},\sigma,j}(\mathbf{k}) = \mathbf{r}\, \psi^{(\alpha)}_{\mathbf{r},\sigma,j}(\mathbf{k}), \tag{3}$$

where $\hat{\mathbf{r}}^{(\alpha)}$ is the $\mathbf{k}$-space representation of the position operator and its eigenvalues, $\mathbf{r}$, can be interpreted as photon position.

The operator arrived at in [11] using the condition (3) is

$$\hat{\mathbf{r}}^{(\alpha)} = \hat{\mathbf{r}}^{(\alpha)}_P + S_{\mathbf{k}}\hat{\boldsymbol{\phi}} \cot\theta/k, \tag{4}$$

where

$$\hat{\mathbf{r}}^{(\alpha)}_P = iI\nabla - iI\alpha\hat{\mathbf{k}}/k + \hat{\mathbf{k}} \times \mathbf{S}/k \tag{5}$$

is a generalization of the Pryce operator, I is a 3×3 unit matrix, $(S_i)_{jk}=-i\epsilon_{ijk}$, and the component of spin parallel to $\mathbf{k}$, $S_{\mathbf{k}}=\hat{\mathbf{k}}\cdot\mathbf{S}$, extracts the helicity σ. The operator $\hat{\mathbf{r}}^{(\alpha)}$ is essentially the usual $\mathbf{k}$-space position operator, $i\nabla$, with terms added to compensate for differentiation of the unit vectors and k^{α} by ∇. The term $\hat{\mathbf{k}}\times\mathbf{S}/\mathbf{k}$ gives a transverse vector, while $S_{\mathbf{k}}\hat{\boldsymbol{\phi}}\cot\theta/k$ rotates $\hat{\boldsymbol{\theta}}$ and $\hat{\boldsymbol{\phi}}$ back to their original orientations, and $-iI\alpha\hat{\mathbf{k}}/k$ corrects for differentiation of k^{α}. It was proved in [11] that $\hat{\mathbf{r}}^{(\alpha)}$ has commuting components and satisfies the other expected commutation relations.

The photon's position coordinates must be real, and this normally implies that the position operator must be Hermitian. In the LP case the $\mathbf{k}$-space inner product is

$$\langle \boldsymbol{\Psi}^{(0)} | \tilde{\boldsymbol{\Psi}}^{(0)} \rangle = \sum_{\mathbf{k},j} \Psi^{(0)*}_j(\mathbf{k}) \tilde{\Psi}^{(0)}_j(\mathbf{k}),$$

where $\boldsymbol{\Psi}^{(\alpha)}(\mathbf{k})$ and $\tilde{\boldsymbol{\Psi}}^{(\alpha)}(\mathbf{k})$ are any two state vectors. It can be proved by converting the sum to an integral and integrating by parts that $\langle \boldsymbol{\Psi}^{(0)} | \hat{\mathbf{r}}^{(0)} \tilde{\boldsymbol{\Psi}}^{(0)} \rangle = \langle \hat{\mathbf{r}}^{(0)} \boldsymbol{\Psi}^{(0)} | \tilde{\boldsymbol{\Psi}}^{(0)} \rangle$ which implies that $\hat{\mathbf{r}}^{(0)}$ is Hermitian. The case $\alpha=1/2$ with inner product

$$\langle \boldsymbol{\Psi}^{(1/2)} | \tilde{\boldsymbol{\Psi}}^{(1/2)} \rangle = \sum_{\mathbf{k},j} k^{-1} \Psi^{(1/2)*}_j(\mathbf{k}) \tilde{\Psi}^{(1/2)}_j(\mathbf{k}) \tag{6}$$

was considered in [21] and [11]. Integration by parts in this case requires differentiation of k^{-1}, which again gives $\langle \boldsymbol{\Psi}^{(1/2)} | \hat{\mathbf{r}}^{(1/2)} \tilde{\boldsymbol{\Psi}}^{(1/2)} \rangle = \langle \hat{\mathbf{r}}^{(1/2)} \boldsymbol{\Psi}^{(1/2)} | \tilde{\boldsymbol{\Psi}}^{(1/2)} \rangle$, proving that $\hat{\mathbf{r}}^{(1/2)}$ is Hermitian based on the inner product (6). This leads to the nonlocal real space density discussed in the Introduction. Alternatively the inner product can be written as

$$\langle \boldsymbol{\Psi}^{(1/2)} | \tilde{\boldsymbol{\Psi}}^{(-1/2)} \rangle = \sum_{\mathbf{k},j} \Psi_j^{(1/2)*}(\mathbf{k}) \tilde{\Psi}_j^{(-1/2)}(\mathbf{k})$$

by defining $\tilde{\boldsymbol{\Psi}}^{(-1/2)} = \tilde{\boldsymbol{\Psi}}^{(1/2)}/k$, thus avoiding explicit inclusion of the factor k^{-1} and the consequent nonlocal real space density. The expectation value of the position operator then satisfies $\langle \boldsymbol{\Psi}^{(1/2)} | \hat{\mathbf{r}}^{(-1/2)} \tilde{\boldsymbol{\Psi}}^{(-1/2)} \rangle = \langle \hat{\mathbf{r}}^{(1/2)} \boldsymbol{\Psi}^{(1/2)} | \tilde{\boldsymbol{\Psi}}^{(-1/2)} \rangle$. If we apply this to the localized state $\boldsymbol{\Psi}^{(\alpha)} = \tilde{\boldsymbol{\Psi}}^{(\alpha)} = \boldsymbol{\psi}^{(\alpha)}_{\mathbf{r}',\sigma}$ this proves that the eigenvalue $\mathbf{r}'$ is still real. However, the position operators $\hat{\mathbf{r}}^{(1/2)}$ and $\hat{\mathbf{r}}^{(-1/2)} = \hat{\mathbf{r}}^{(1/2)\dagger}$ are not self-adjoint. Operators such are these are referred to a pseudo-Hermitian by Mostafazadeh [25]. Use of pseudo-Hermitian operators and a biorthonormal basis is discussed in more detail in the next section.

In [12] the position operator was generalized to allow for rotation about $\mathbf{k}$ through the Euler angle $\chi(\theta,\phi)$ to give the most general transverse basis,

$$\mathbf{e}^{(\chi)}_{\mathbf{k},\sigma} = e^{-i\sigma\chi} \mathbf{e}^{(0)}_{\mathbf{k},\sigma}. \tag{7}$$

It was found that the position operator can be written as

$$\hat{\mathbf{r}}^{(\alpha)} = D(k^{\alpha} i \nabla k^{-\alpha}) D^{-1}, \tag{8}$$

where $D = \exp(-iS_{\mathbf{k}}\chi)\exp(-iS_3\phi)\exp(-iS_2\theta)$. Starting from a wave vector parallel to $\hat{\mathbf{z}}$ and transverse unit vectors $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$, D rotates $\mathbf{k}$ from the z axis to an orientation described by the angles θ and ϕ, while at the same time rotating the transverse vectors first to $\hat{\boldsymbol{\theta}}$ and $\hat{\boldsymbol{\phi}}$ and then about $\mathbf{k}$ through χ. For example, when $\hat{\mathbf{r}}^{(1/2)}$ acts on a transverse field parallel to $\hat{\boldsymbol{\phi}}$ it rotates it to $\hat{\mathbf{y}}$ and divides it by $\sqrt{\omega_k}$, then operates on it with the usual $\mathbf{k}$-space position operator $i\nabla$. It then reverses the process by multiplying it by $\sqrt{\omega_k}$ and rotates it back to its original transverse orientation. This allows $\hat{\mathbf{r}}^{(1/2)}$ to extract the position of the photon from the phase of the coefficient of the transverse unit vector.

The quantum numbers $\{\mathbf{r},\sigma\}$ index the basis states for a given $\chi(\theta,\phi)$. The z axis can be selected for convenience and the choice $\chi = -m\phi$ gives [13]

$$\mathbf{e}^{(-m\phi)}_{\mathbf{k},\sigma} = \frac{\hat{\mathbf{x}} - i\hat{\mathbf{y}}}{2\sqrt{2}} (\cos\theta - \sigma) e^{i(m\sigma+1)\phi} - \frac{\hat{\mathbf{z}}}{\sqrt{2}} \sin\theta e^{im\sigma\phi} + \frac{\hat{\mathbf{x}} + i\hat{\mathbf{y}}}{2\sqrt{2}} (\cos\theta + \sigma) e^{i(m\sigma-1)\phi}. \tag{9}$$

For example, $\chi = -\phi$ $(m=1)$ rotates $\hat{\boldsymbol{\theta}}$ and $\hat{\boldsymbol{\phi}}$ back to the x and y axes to give unit vectors that approach $(\hat{\mathbf{x}} + i\sigma\hat{\mathbf{y}})/\sqrt{2}$ in the $\theta \to 0$ limit. This is useful in the description of paraxial beams since the unit vectors describe spin alone. Their coefficients then describe all of the orbital angular momentum so that a factor $\exp(il_z\phi)$ implies a z component of orbital angular momentum equal to $\hbar l_z$.

The spin and orbital AM of a photon are not separable beyond the paraxial approximation. For unit vectors of the form (9) the z component of total angular momentum and photon position operators satisfy [13]

$$[\hat{J}_z, \hat{r}_k] = i\hbar \epsilon_{zkl} \hat{r}_l. \tag{10}$$

This is just the usual commutation relation satisfied by a vector operator and an angular momentum component. Here it implies that photon position transforms as a vector under rotations about the axis of symmetry of the localized states. A photon on the z axis satisfies the uncertainty relation $\Delta J_z \Delta r_k \geqslant 0$. Unit vectors of the form (9) contribute a definite z component of the total AM, consistent with $\{s_z, l_z\}$ equal to $\{-1, m\sigma+1\}$, $\{0, m\sigma\}$, or $\{1, m\sigma-1\}$, with $j_z = m\sigma$, that is total AM has a definite value, but spin and orbital AM do not.

III. POSITION EIGENVECTORS

Here we will obtain the eigenvectors of the position operators discussed in Sec. II. The LP form of the position operator, $\hat{\mathbf{r}}^{(0)}$, is self-adjoint, has real eigenvalues, and defines an orthonormal basis as is usual in quantum mechanics. To obtain QED-like fields as eigenvectors, the choice $\alpha = 1/2$ is required. In this section we will use the mathematical properties of pseudo-Hermitian operators to obtained a completeness relation for the field like photon wave function and investigate how it is related to the LP wave function. The operators will be obtained in the HP picture, so time dependence as determined by the Hamiltonian must also be considered.

We will start with an examination of the expectation values to motivate the use of the biorthonormal formalism. Any Hermitian operator $\hat{o}$ satisfies the eigenvector equation $\hat{o}|f_n\rangle = o_n|f_n\rangle$ and its eigenvalues, o_n, are real. To transform from LP position eigenvectors to fields, multiplication by $\sqrt{\omega_k}$ is required. Assume that η is an operator with positive square root $\rho = \sqrt{\eta}$ which will equal $\sqrt{\omega_k}$ in the present application. We can write

$$\langle f_n|\hat{o}|f_m\rangle = \langle f_n|\rho(\rho^{-1}\hat{o}\rho)\rho^{-1}|f_m\rangle = \langle \phi_n|\hat{O}|\psi_m\rangle,$$

where $\hat{O} = \rho^{-1}\hat{o}\rho$ is a similarity transformation, $|\psi_m\rangle = \rho^{-1}|f_m\rangle$ and $|\phi_n\rangle = (\langle f_n|\rho)^{\dagger} = \rho^{\dagger}\rho|\psi_n\rangle$. The eigenvector equation becomes $\hat{O}|\psi_n\rangle = o_n|\psi_n\rangle$ and the eigenvalues and inner-products are preserved. If ρ is a unitary operator, that is if $\rho^{-1} = \rho^{\dagger}$, then $\hat{O}^{\dagger} = \hat{O}$ is Hermitian and $|\phi_n\rangle = |\psi_n\rangle$. The $|\psi_n\rangle$ and $|\phi_n\rangle$ eigenvectors are the same, and the usual quantum mechanical formalism is obtained. On the other hand, if ρ is a Hermitian operator satisfying $\rho^{\dagger} = \rho$ then $|\phi_n\rangle \neq |\psi_n\rangle$ and there are two distinct sets of eigenvectors. We can deal with this is one of two ways: (1) The metric operator $\eta = \rho^2$ can be introduced to give the new inner product $\langle \phi_n|\eta^{-1}\phi_m\rangle$ and work only with the $|\phi_n\rangle$ basis. (2) We can use the eigenvectors of $\hat{O}$ *and* the eigenvectors of $\hat{O}^{\dagger} = \eta\hat{O}\eta^{-1}$ which are $|\psi_n\rangle$and $|\phi_n\rangle$, respectively. Since $\langle f_n|f_m\rangle = \langle f_n|\rho\rho^{-1}|f_m\rangle$ transforms to $\langle \phi_n|\psi_m\rangle$, the eigenvectors $|\psi_m\rangle$ and $|\phi_n\rangle$ are biorthonormal [26]. If there is degeneracy, a biorthonormal basis can be obtained by defining a complete set of commuting operators (CSCO).

The properties of pseudo-Hermitian operators and biorthonormal bases have recently been investigated by Mostafazadeh and can be summarized as [25]

$$\hat{O}|\psi_n\rangle = O_n|\psi_n\rangle, \quad \hat{O}^\dagger|\phi_n\rangle = O_n^*|\phi_n\rangle,$$

$$\hat{O}^\dagger = \eta\hat{O}\eta^{-1}, \quad \langle\phi_n|\psi_m\rangle = \delta_{n,m},$$

with the completeness relation

$$\sum_n |\psi_n\rangle\langle\phi_n| = \sum_n |\phi_n\rangle\langle\psi_n| = \hat{1},$$

where η is a metric operator and $\hat{1}$ is the unit operator. If $\rho=\sqrt{\eta}$ exists,

$$\hat{o} = \rho\hat{O}\rho^{-1} = \rho^{-1}\hat{O}^\dagger\rho \tag{11}$$

is self-adjoint and the eigenvectors O_n are real. Expectation values are preserved by the similarity transformation, η.

To apply this formalism to the photon we take $\eta=\omega_k$ and work in $\mathbf{k}$ space. Then $\hat{o}=\hat{\mathbf{r}}^{(0)}$ is self-adjoint and the operators $\hat{O}^\dagger=\hat{\mathbf{r}}^{(1/2)}$ and $\hat{O}=\hat{\mathbf{r}}^{(-1/2)}$ have the biorthonormal eigenvectors $\boldsymbol{\psi}_{\mathbf{r},\sigma}^{(1/2)}(\mathbf{k})$ and $\boldsymbol{\psi}_{\mathbf{r},\sigma}^{(-1/2)}(\mathbf{k})$ given by Eq. (1) that go as $\sqrt{\omega_k}$ and $1/\sqrt{\omega_k}$, respectively, as required by QED for the electromagnetic fields and the vector potential. The position operators and their eigenvectors satisfy

$$\hat{\mathbf{r}}^{(-\alpha)\dagger} = \hat{\mathbf{r}}^{(\alpha)}, \tag{12}$$

$$\boldsymbol{\psi}_{\mathbf{r},\sigma}^{(-1/2)}(\mathbf{k}) = \omega_k^{-1/2}\boldsymbol{\psi}_{\mathbf{r},\sigma}^{(0)}(\mathbf{k}), \tag{13}$$

$$\boldsymbol{\psi}_{\mathbf{r},\sigma}^{(1/2)}(\mathbf{k}) = \omega_k^{1/2}\boldsymbol{\psi}_{\mathbf{r},\sigma}^{(0)}(\mathbf{k}), \tag{14}$$

the biorthonormality condition

$$\sum_j \langle\psi_{\mathbf{r}',\sigma',j}^{(-\alpha)}|\psi_{\mathbf{r},\sigma,\mathbf{j}}^{(\alpha)}\rangle = \delta^3(\mathbf{r}-\mathbf{r}')\delta_{\sigma,\sigma'}, \tag{15}$$

and the completeness relation

$$\sum_{\sigma,j}\int d^3r|\psi_{\mathbf{r},\sigma,j}^{(\alpha)}\rangle\langle\psi_{\mathbf{r},\sigma,j}^{(-\alpha)}| = \hat{1}. \tag{16}$$

Here δ^3 is the three-dimensional Dirac δ function and we can interchange α and $-\alpha$. The field and the LP operators, $\hat{o}$, are related as

$$\hat{O}^\dagger = \omega_k^{1/2}\hat{o}\omega_k^{-1/2}, \tag{17}$$

consistent with Eq. (8). This transforms the LP position operator $\hat{\mathbf{r}}^{(0)}$ to $\hat{\mathbf{r}}^{(1/2)}$, introducing an addition term $-i\hat{\mathbf{l}}/2k$. The momentum and angular momentum operators $\hbar\mathbf{k}$ and $\hbar(-\mathbf{k}\times i\nabla+\mathbf{S})$ are unaffected by the similarity transformation (17). In the angular momentum case this is because $\hat{\mathbf{k}}\times\mathbf{k}=0$.

Time dependence is determined by the Hamiltonian $\hat{H}+\hat{H}_0$ with

$$\hat{H} = \sum_{\mathbf{k},\sigma}\hbar\omega_k a_{\mathbf{k},\sigma}^\dagger a_{\mathbf{k},\sigma}, \tag{18}$$

where the zero point terms $\hat{H}_0=\Sigma_{\mathbf{k},\sigma}\hbar\omega_k/2$ which are unaffected by the photon state will be omitted here. The operator $a_{\mathbf{k},\sigma}$ annihilates a photon with wave vector $\mathbf{k}$ and helicity σ and satisfies the commutation relations $[a_{\mathbf{k},\sigma},a_{\mathbf{k}',\sigma'}^\dagger]=\delta_{\sigma,\sigma'}\delta_{\mathbf{k},\mathbf{k}'}$. The operators and their eigenkets are time dependent in the HP [27]. Using the unitary time evolution operator

$$U(t) = \exp(-i\hat{H}t), \tag{19}$$

the HP position operator becomes

$$\hat{\mathbf{r}}_{\mathrm{HP}}^{(\alpha)} = U^\dagger(t)\hat{\mathbf{r}}^{(\alpha)}U(t) = \hat{\mathbf{r}}^{(\alpha)} + \nabla\omega_k t \tag{20}$$

with eigenvectors $U^\dagger(t)|\boldsymbol{\psi}_{\mathbf{r},\sigma}^{(\alpha)}\rangle$ with $|\boldsymbol{\psi}_{\mathbf{r},\sigma}^{(\alpha)}\rangle$ given by Eq. (1) in $\mathbf{k}$ space. The coefficient of t in the last term of Eq. (20) is the photon group velocity.

We can define one-photon HP annihilation and creation operators for a photon with helicity σ at position $\mathbf{r}$ and time t as

$$\hat{\psi}_{\mathbf{r},\sigma,\mathbf{j}}^{(\alpha)}(t) \equiv \sum_{\mathbf{k}} (\omega_k)^\alpha e_{\mathbf{k},\sigma,\mathbf{j}}^{(\chi)} a_{\mathbf{k},\sigma}\frac{e^{i\mathbf{k}\cdot\mathbf{r}-i\omega_k t}}{\sqrt{V}}, \tag{21}$$

$$\hat{\psi}_{\mathbf{r},\sigma,j}^{(\alpha)\dagger}(t) \equiv \sum_{\mathbf{k}} (\omega_k)^\alpha e_{\mathbf{k},\sigma,j}^{(\chi)*} a_{\mathbf{k},\sigma}^\dagger\frac{e^{-i\mathbf{k}\cdot\mathbf{r}+i\omega_k t}}{\sqrt{V}}. \tag{22}$$

For $\alpha=1/2$, Eq. (21) implies that the biorthonormal pairs are related through

$$\hat{\boldsymbol{\psi}}_{\mathbf{r},\sigma}^{(1/2)}(t) = i\frac{\partial\hat{\boldsymbol{\psi}}_{\mathbf{r},\sigma}^{(-1/2)}(t)}{\partial t} \tag{23}$$

analogous to the relationship between the vector potential and the electric field in the Coulomb gauge. The one-photon position eigenkets normalized according to Eq. (15) are

$$|\boldsymbol{\psi}_{\mathbf{r},\sigma}^{(\alpha)}(t)\rangle = \hat{\boldsymbol{\psi}}_{\mathbf{r},\sigma}^{(\alpha)\dagger}(t)|0\rangle, \tag{24}$$

where $|0\rangle$ is the electromagnetic vacuum state. The projection of Eq. (24) onto the momentum-helicity basis, $\{|\mathbf{k},\sigma\rangle\}$, gives back Eq. (1) in the Schrödinger picture. The free space operators for a photon with helicity σ satisfy the $\mathbf{r}$-space dynamical equation

$$i\frac{\partial\hat{\boldsymbol{\psi}}_{\mathbf{r},\sigma}^{(\alpha)}(t)}{\partial t} = \sigma c\,\nabla\times\hat{\boldsymbol{\psi}}_{\mathbf{r},\sigma}^{(\alpha)}(t). \tag{25}$$

The annihilation and creation operators satisfy the equal time commutation relations

$$\sum_j [\hat{\psi}_{\mathbf{r},\sigma,j}^{(-\alpha)}(t),\hat{\psi}_{\mathbf{r}',\sigma',j}^{(\alpha)\dagger}(t)] = \delta_{\sigma,\sigma'}\delta^3(\mathbf{r}-\mathbf{r}'). \tag{26}$$

The Hermitian operator describing the density of photons with helicity σ, obtained by averaging over the α and $-\alpha$ forms, is

$$\hat{n}_\sigma^{(\alpha)}(\mathbf{r},t) = \frac{1}{2}\hat{\boldsymbol{\psi}}_{\mathbf{r},\sigma}^{(\alpha)\dagger}(t)\cdot\hat{\boldsymbol{\psi}}_{\mathbf{r},\sigma}^{(-\alpha)}(t) + \mathrm{H.c.} \tag{27}$$

The total number operator is

$$\hat{N} = \int d^3r\,\hat{n}^{(\alpha)}(\mathbf{r},t) = \sum_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma}^\dagger a_{\mathbf{k},\sigma}. \tag{28}$$

An alternative linear polarization basis can be obtained if we define operators that annihilate a photon state with polarization in the $\hat{\boldsymbol{\theta}}$ and $\hat{\boldsymbol{\phi}}$ directions as

$$\hat{\boldsymbol{\psi}}^{(\alpha)}_{\mathbf{r}}(t) = [\hat{\boldsymbol{\psi}}^{(\alpha)}_{\mathbf{r},1}(t) + \hat{\boldsymbol{\psi}}^{(\alpha)}_{\mathbf{r},-1}(t)]/\sqrt{2},$$

$$\hat{\boldsymbol{\phi}}^{(\alpha)}_{\mathbf{r}}(t) = -i[\hat{\boldsymbol{\psi}}^{(\alpha)}_{\mathbf{r},1}(t) - \hat{\boldsymbol{\psi}}^{(\alpha)}_{\mathbf{r},-1}(t)]/\sqrt{2}, \tag{29}$$

respectively. While the direction of these eigenvectors depends on $\mathbf{k}$, they do not rotate in space and time, and in that sense they are linearly polarized. The inverse transformation is

$$\hat{\boldsymbol{\psi}}^{(\alpha)}_{\mathbf{r},\sigma}(t) = [\hat{\boldsymbol{\psi}}^{(\alpha)}_{\mathbf{r}}(t) + i\sigma\hat{\boldsymbol{\phi}}^{(\alpha)}_{\mathbf{r}}(t)]/\sqrt{2}. \tag{30}$$

In free space

$$\frac{\partial\hat{\boldsymbol{\psi}}^{(\alpha)}_{\mathbf{r}}(t)}{\partial t} = c\,\nabla\times\hat{\boldsymbol{\phi}}^{(\alpha)}_{\mathbf{r}}(t), \tag{31}$$

$$\frac{\partial\hat{\boldsymbol{\phi}}^{(\alpha)}_{\mathbf{r}}(t)}{\partial t} = -c\,\nabla\times\hat{\boldsymbol{\psi}}^{(\alpha)}_{\mathbf{r}}(t).$$

If $\alpha=0$ these are the operators introduced by Cook [24], while if $\alpha=1/2$ their dynamics is ME-like.

The localized definite helicity basis states are eigenvectors of a CSCO, so it is the helicity basis that will be used here. Linearly polarized fields can be found by taking the sum and difference as in Eq. (29).

IV. WAVE FUNCTION

In this section we will obtain one and two photon wave functions and photon density by projection onto the basis of position eigenvectors found in Sec. III. This density is a two-point correlation function that is based on the LP or biorthonormal basis, rather than electric fields alone as in Glauber photodetection theory [28].

The QED state vector describing a pure state in which the number of photons and their wave vectors are uncertain can be expanded as

$$|\Psi\rangle = c_0|0\rangle + \sum_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}a^{\dagger}_{\mathbf{k},\sigma}|0\rangle + \frac{1}{2!}\sum_{\mathbf{k},\sigma;\mathbf{k}',\sigma'}\sqrt{\mathcal{N}_{\mathbf{k},\sigma;\mathbf{k}',\sigma'}}c_{\mathbf{k},\sigma;\mathbf{k}',\sigma'}a^{\dagger}_{\mathbf{k},\sigma}a^{\dagger}_{\mathbf{k}',\sigma'}|0\rangle + \cdots, \tag{32}$$

where $c_0=\langle 0|\Psi\rangle$, $c_{\mathbf{k},\sigma}\equiv\langle 0|a_{\mathbf{k},\sigma}|\Psi\rangle$, $c_{\mathbf{k},\sigma;\mathbf{k}',\sigma'}\equiv c_{\mathbf{k}',\sigma';\mathbf{k},\sigma}=\langle 0|a_{\mathbf{k},\sigma}a_{\mathbf{k}',\sigma'}|\Psi\rangle$, and $\mathcal{N}_{\mathbf{k},\sigma;\mathbf{k}',\sigma'}=1+\delta_{\mathbf{k},\mathbf{k}'}\delta_{\sigma,\sigma'}$. Division by 2! corrects for identical states obtained when the $\{\mathbf{k},\sigma\}$ subscripts are permuted while $\sqrt{\mathcal{N}}/2$ normalizes doubly occupied states. A more general state requires a formulation in terms of density matrices that will not be attempted here.

The one-photon real space wave function in the helicity basis, equal to the projection of this state vector onto eigenvectors of $\hat{\mathbf{r}}^{(\alpha)}_{\mathrm{HP}}$ as $\langle\psi^{(\alpha)}_{\mathbf{r},\sigma,j}|\Psi\rangle$, is

$$\boldsymbol{\Psi}^{(\alpha)}_{\sigma}(\mathbf{r},t) = \sum_{\mathbf{k}} c_{\mathbf{k},\sigma}\mathbf{e}^{(\chi)}_{\mathbf{k},\sigma}(\omega_k)^{\alpha}\frac{e^{i\mathbf{k}\cdot\mathbf{r}-i\omega_k t}}{\sqrt{V}}, \tag{33}$$

where we have used Eqs. (22), (24), and (32). The expansion coefficients depend on the choice of basis, for example when $\chi\rightarrow\chi+\Delta\chi$ the coefficients $c_{\mathbf{k},\sigma}\rightarrow c_{\mathbf{k},\sigma}\exp(-i\sigma\Delta\chi)$ analogous to gauge changes of the vector potential describing a magnetic monopole in real space [12]. In any basis the inner product $\langle\Psi|\Psi\rangle=\Sigma_{\mathbf{k},\sigma}|c_{\mathbf{k},\sigma}|^2\equiv|c_1|^2$ where $|c_1|^2$ is the net probability for one-photon in state $|\Psi\rangle$. The free space one-photon dynamical equations mirror the operator Eqs. (23) and (25). They are

$$i\frac{\partial\boldsymbol{\Psi}^{(-1/2)}_{\sigma}(\mathbf{r},t)}{\partial t} = \boldsymbol{\Psi}^{(1/2)}_{\sigma}(\mathbf{r},t),$$

$$i\frac{\partial\boldsymbol{\Psi}^{(\alpha)}_{\sigma}(\mathbf{r},t)}{\partial t} = \sigma c\,\nabla\times\boldsymbol{\Psi}^{(\alpha)}_{\sigma}(\mathbf{r},t). \tag{34}$$

To obtain the two-photon wave function we can project $|\Psi\rangle$ onto the two-photon real space basis

$$|\psi_{\mathbf{r},\sigma,j}(t),\psi_{\mathbf{r}',\sigma',j'}(t')\rangle = \hat{\psi}^{(\alpha)\dagger}_{\mathbf{r},\sigma,j}(t)\hat{\psi}^{(\alpha)\dagger}_{\mathbf{r}',\sigma',j'}(t')|0\rangle$$

giving

$$\Psi^{(\alpha)}_{\sigma,\sigma';j,j'}(\mathbf{r},\mathbf{r}';t,t') = \langle 0|\hat{\psi}^{(\alpha)}_{\mathbf{r},\sigma,j}(t)\hat{\psi}^{(\alpha)}_{\mathbf{r}',\sigma',j'}(t')|\Psi\rangle. \tag{35}$$

Use of Eq. (22) and $[a_{\mathbf{k},\sigma},a^{\dagger}_{\mathbf{k}',\sigma'}]=\delta_{\mathbf{k},\mathbf{k}'}\delta_{\sigma,\sigma'}$ to evaluate $\langle 0|\hat{\psi}^{(\alpha)}_{\mathbf{r},\sigma,j}(t)\hat{\psi}^{(\alpha)}_{\mathbf{r}',\sigma',j'}(t')a^{\dagger}_{\mathbf{k},\sigma''}a^{\dagger}_{\mathbf{k}',\sigma'''}|0\rangle$ then gives

$$\Psi^{(\alpha)}_{\sigma,\sigma';j,j'}(\mathbf{r},\mathbf{r}';t,t') = \frac{1}{2!\,V}\sum_{\mathbf{k},\sigma;\mathbf{k}',\sigma'}\sqrt{\mathcal{N}_{\mathbf{k},\sigma;\mathbf{k}',\sigma'}} \times c_{\mathbf{k},\sigma;\mathbf{k}',\sigma'}(\omega_k\omega_{k'})^{\alpha} \times [e^{(\chi)}_{\mathbf{k},\sigma,j}e^{(\chi)}_{\mathbf{k}',\sigma',j'}e^{i\mathbf{k}\cdot\mathbf{r}-i\omega_k t}e^{i\mathbf{k}'\cdot\mathbf{r}'-i\omega_{k'}t'} + e^{(\chi)}_{\mathbf{k}',\sigma',j}e^{(\chi)}_{\mathbf{k},\sigma,j'}e^{i\mathbf{k}\cdot\mathbf{r}'-i\omega_k t'}e^{i\mathbf{k}'\cdot\mathbf{r}-i\omega_{k'}t}] \tag{36}$$

which becomes a two-photon wave function if we set $t'=t$. A separate symmetrization step is not required since its symmetric form is a direct consequence of the commutation relations satisfied by the photon annihilation and creation operators.

To obtain an n-photon basis the creation operator can be applied to the vacuum n times with each occurrence having different parameters $\mathbf{r}$, σ, and j. The state vector can then be projected onto this basis to give the n-photon term. The result is the symmetric n-photon real space function

$$\Psi^{(\alpha)}_{\{m\}}(\mathbf{r},\ldots,\mathbf{r}^{[n-1]};t,\ldots,t^{[n-1]}) = \prod_{m=0}^{n-1}\langle\psi^{(\alpha)}_{m}||\Psi\rangle \tag{37}$$

where $|\psi^{(\alpha)}_{m}\rangle$ is a short hand for $|\psi^{(\alpha)}_{\mathbf{r}^{[m]},\sigma^{[m]},j^{[m]}}(t^{[m]})\rangle$ and m represents the mth set of variables, quantum numbers and components $\{\mathbf{r}^{[m]},t^{[m]},\sigma^{[m]},j^{[m]}\}$. Generally the n-photon states provide more information than can be measured. Instead the real space helicity σ photon density, equal to the

expectation value of the number density operator, Eq. (27), can be defined as

$$n_\sigma^{(\alpha)}(\mathbf{r},t)=\langle\Psi|\hat{n}_\sigma(\mathbf{r},t)|\Psi\rangle=\frac{1}{2}\sum_j\langle\Psi|\hat{\psi}_{\mathbf{r},\sigma,j}^{(\alpha)\dagger}(t)\hat{\psi}_{\mathbf{r},\sigma,j}^{(-\alpha)}(t)|\Psi\rangle+\text{c.c.} \tag{38}$$

The zero-photon contribution to n is 0, while the one-photon contribution is

$$n_\sigma^{(\alpha)}(\mathbf{r},t)=\frac{1}{2}\boldsymbol{\Psi}_\sigma^{(\alpha)*}(\mathbf{r},t)\cdot\boldsymbol{\Psi}_\sigma^{(-\alpha)}(\mathbf{r},t)+\text{c.c.} \tag{39}$$

For the two-photon state (35), substitution of Eq. (26) gives

$$n_\sigma^{(\alpha)}(\mathbf{r},t)=\frac{1}{2}\sum_{\sigma';j,j'}\int d^3r'\Psi_{\sigma,\sigma';j,j'}^{(\alpha)*}(\mathbf{r},\mathbf{r}';t,t)\times\Psi_{\sigma,\sigma';j,j'}^{(-\alpha)}(\mathbf{r},\mathbf{r}';t,t)+\text{c.c.},$$

implying that unobserved photons are summed over. A similar argument can be applied to each n-photon term. Photons are noninteracting particles and the existence of a photon density is consistent with Feynman's conclusion the photon probability density can be interpreted as particle density [29,30].

The bases obtained here provide a real space description of the multiphoton state that "encodes the maximum total knowledge describing the system" as discussed in Ref. [3]. The electric field wave function used in [2,5] or RS vectors in [1,18] by themselves do not provide a basis, and this is the root of the criticism of [2] made in [3]. The two-photon wave function (36) is symmetric in agreement with [1,2].

V. MAXWELL'S EQUATIONS

In this section we will show that MEs can be obtained from QED in two distinct ways. The first is the conventional approach of calculating the expectation value of operators with all modes populated as coherent states. The fields obtained in this way are real and they cannot be interpreted as wave functions. The second approach is to project the state vector onto the position eigenvectors obtained when a field operator acts on the vacuum state to give fields proportional to the one-photon wave function components in Sec. V.

If the multipolar Hamiltonian is used, the displacement is purely photonic, while the vector potential will include photon and matter contributions [31]. The vector potential operator is a sum over positive and negative frequencies, photon and matter parts, and both helicities. We can define

$$\hat{\mathbf{A}}(\mathbf{r},t)=\hat{\mathbf{A}}^{(+)}(\mathbf{r},t)+\hat{\mathbf{A}}^{(-)}(\mathbf{r},t),$$

$$\hat{\mathbf{A}}^{(+)}(\mathbf{r},t)=\hat{\mathbf{A}}_p^{(+)}(\mathbf{r},t)+\hat{\mathbf{A}}_m^{(+)}(\mathbf{r},t),$$

$$\hat{\mathbf{A}}_p^{(+)}(\mathbf{r},t)=\hat{\mathbf{A}}_1^{(+)}(\mathbf{r},t)+\hat{\mathbf{A}}_{-1}^{(+)}(\mathbf{r},t), \tag{40}$$

where $\hat{\mathbf{A}}^{(-)}=\hat{\mathbf{A}}^{(+)\dagger}$ and the subscripts m and p denote matter and photon parts, respectively. The electric field and magnetic induction are then given by

$$\hat{\mathbf{E}}=-\partial\hat{\mathbf{A}}/\partial t-\nabla\phi,$$

$$\hat{\mathbf{B}}=\nabla\times\hat{\mathbf{A}}. \tag{41}$$

In the presence matter of with polarization operator $\hat{\mathcal{P}}$ and magnetization $\hat{\mathcal{M}}$ the displacement and magnetic field operators are

$$\hat{\mathbf{D}}=\epsilon_0\hat{\mathbf{E}}+\hat{\mathcal{P}},$$

$$\hat{\mathbf{H}}=\hat{\mathbf{B}}/\mu_0-\hat{\mathcal{M}}, \tag{42}$$

where SI units are used, ϵ_0 is the permittivity and μ_0 the permeability of vacuum, and $c=1/\sqrt{\epsilon_0\mu_0}$.

The momentum conjugate to the vector potential is $-\hat{\mathbf{D}}_\perp$ where $\hat{\mathbf{D}}_\perp$ is the transverse part of the displacement operator [20,31]. These operators satisfy canonical commutation relations. Since $\hat{\boldsymbol{\psi}}_{\mathbf{r},\sigma}^{(-\alpha)}$ and $\hat{\boldsymbol{\psi}}_{\mathbf{r},\sigma}^{(\alpha)\dagger}$ satisfy Eq. (26) we can choose

$$\hat{\mathbf{A}}_\sigma^{(+)}(\mathbf{r},t)=\sqrt{\frac{\hbar}{2\epsilon_0}}\hat{\boldsymbol{\psi}}_{\mathbf{r},\sigma}^{(-1/2)}(t),$$

$$\hat{\mathbf{D}}_{\perp,\sigma}^{(+)}(\mathbf{r},t)=i\sqrt{\frac{\hbar\epsilon_0}{2}}\hat{\boldsymbol{\psi}}_{\mathbf{r},\sigma}^{(1/2)}(t). \tag{43}$$

This is equivalent to the usual QED expansion of $\hat{\mathbf{A}}$ and $\hat{\mathbf{D}}$ and thus is consistent with the operator MEs

$$\nabla\cdot\hat{\mathbf{B}}=0,\quad \nabla\times\hat{\mathbf{E}}=-\frac{\partial\hat{\mathbf{B}}}{\partial t},$$

$$\nabla\cdot\hat{\mathbf{D}}=\rho,\quad \nabla\times\hat{\mathbf{H}}=\mathbf{j}+\frac{\partial\hat{\mathbf{D}}}{\partial t}, \tag{44}$$

where ρ and $\mathbf{j}$ are the free charge and current densities. In free space $\hat{\mathbf{D}}_{\perp,\sigma}^{(+)}/\sqrt{\epsilon_0}=i\sigma\hat{\mathbf{B}}_\sigma^{(+)}/\sqrt{\mu_0}=\hat{\mathbf{F}}_\sigma^{(+)}/\sqrt{2}=i\sqrt{\hbar/2}\hat{\boldsymbol{\psi}}_{\mathbf{r},\sigma}^{(1/2)}$ where the RS operator is $\hat{\mathbf{F}}_\sigma^{(+)}=\hat{\mathbf{D}}_\sigma^{(+)}/\sqrt{2\epsilon_0}+\hat{\mathbf{B}}_\sigma^{(+)}/\sqrt{2\mu_0}$ as defined in [18].

Coherent states are the most classical, and they can be used to establish a connection between QED and the real Maxwell fields. Following Cohen-Tannoudji *et al.* [31] the complex Fourier transforms of the classical field vectors,

$$\mathcal{V}_\mathbf{k}(t)=\int d^3r\,\mathbf{V}(\mathbf{r},t)\frac{\exp(-i\mathbf{k}\cdot\mathbf{r})}{\sqrt{V}},$$

and the normal variables,

$$\boldsymbol{\gamma}_\mathbf{k}(t)=-i\sqrt{\frac{\epsilon_0}{2\hbar\omega_k}}[\mathcal{E}_\mathbf{k}^\perp(t)-c\hat{\mathbf{k}}\times\mathcal{B}_\mathbf{k}(t)],$$

can be defined. For a coherent state with the photon occupancy of mode $\{\mathbf{k},\sigma\}$ described by the complex parameter $\gamma_{\mathbf{k},\sigma}$, the average photon number is $n_{\mathbf{k},\sigma}=|\gamma_{\mathbf{k},\sigma}|^2$ and the probability amplitude for n photons is $\exp(-|\gamma_{\mathbf{k},\sigma}|^2/2)\gamma_{\mathbf{k},\sigma}^n/\sqrt{n!}$. The quasiclassical coherent state is a Gaussian wave packet that oscillates without deformation and with relative number

uncertainty $\Delta n_{\mathbf{k},\sigma}/n_{\mathbf{k},\sigma}=1/|\gamma_{\mathbf{k},\sigma}|$. In the limit of infinite photon number the electric and magnetic fields oscillate in a well defined way as do the solutions to the classical MEs. Thus

$$\mathbf{A}_{\mathrm{coh}}^{\perp(+)}(\mathbf{r},t)=\langle\{\gamma_{\mathbf{k},\sigma}\}|\hat{\mathbf{A}}_{p}^{\perp(+)}(\mathbf{r},t)|\{\gamma_{\mathbf{k},\sigma}\}\rangle = \sum_{\mathbf{k},\sigma}\sqrt{\frac{\hbar}{2\epsilon_0\omega_k}}\gamma_{\mathbf{k},\sigma}\mathbf{e}_{\mathbf{k},\sigma}^{(\chi)}\frac{e^{i\mathbf{k}\cdot\mathbf{r}}-i\omega_k t}{\sqrt{V}}, \tag{45}$$

$$\mathbf{A}_{\mathrm{coh}}^{\perp}(\mathbf{r},t)=\mathbf{A}_{\mathrm{coh}}^{\perp(+)}(\mathbf{r},t)+\mathrm{c}\cdot\mathrm{c}. \tag{46}$$

and the fields derived from it behave classically in the large photon number limit.

It is also possible to derive one photon positive frequency MEs from QED. We can define the one-particle states $|\mathbf{V}_{\mathbf{r},\sigma}\rangle=\hat{\mathbf{V}}_{\mathbf{r},\sigma}^{(-)}|g,0\rangle$ with $\hat{\mathbf{V}}^{(-)}=\hat{\mathbf{V}}^{(+)\dagger}$ and $\mathbf{V}^{(+)}=\Sigma_\sigma\mathbf{V}_\sigma^{(+)}$ for any field operator $\hat{\mathbf{V}}$ such that

$$\mathbf{V}_{\sigma}^{(+)}(\mathbf{r},t)=\langle g,0|\hat{\mathbf{V}}_{\mathbf{r},\sigma}^{(+)}|\Psi\rangle. \tag{47}$$

This can be viewed as the projection of the photon-matter state vector state onto the $n=1$ term of number-position-helicity basis. In the ground state $|0\rangle$ both the EM field and any matter present are in their lowest energy configurations. The operator $\hat{\mathbf{V}}^{(-)}$ creates one-particle that can be a photon or a material excitation. Since the space and time dependence originates entirely in the field operators, these functions satisfy ME dynamics. The one-photon MEs are, using Eq. (44),

$$\nabla\cdot\mathbf{B}^{(+)}=0,\quad \nabla\times\mathbf{E}^{(+)}=-\frac{\partial\mathbf{B}^{(+)}}{\partial t},$$

$$\nabla\cdot\mathbf{D}^{(+)}=\rho^{(+)},\quad \nabla\times\mathbf{H}^{(+)}=\mathbf{j}^{(+)}+\frac{\partial\mathbf{D}^{(+)}}{\partial t}. \tag{48}$$

Projection of the state vector onto a basis of one-photon position eigenvectors results in intrinsically positive frequency electric and magnetic fields defined by Eq. (47) that satisfy MEs. They can be manipulated to give any of the commonly used forms of MEs.

A wave equation can be obtained from Eq. (48) in the usual way to give

$$\frac{1}{c^2}\frac{\partial^2\mathbf{E}^{(+)}}{\partial t^2}+\nabla\times\nabla\times\mathbf{E}^{(+)}=-\mu_0\frac{\partial}{\partial t}\left(\frac{\partial\mathcal{P}^{(+)}}{\partial t}+\boldsymbol{\nabla}\times\mathcal{M}^{(+)}+\mathbf{j}^{(+)}\right). \tag{49}$$

The terms on the right-hand side are the polarization, magnetic, and external contributions to the time derivative of the current density [31]. If there is no magnetization or external current and the polarization is linear and isotropic we can write $\mathcal{P}=\epsilon_0\chi(k)\mathbf{E}$ which can be combined with the $\partial^2\mathbf{E}^{(+)}/\partial t^2$ term. Writing $\epsilon(k)=\epsilon_0[1+\chi(k)]$ the angular frequency in (18) is $\omega_k=kc\sqrt{1+\chi(k)}$. Analogous to the creation of an excitation of the electromagnetic field (a photon) by $\hat{\mathbf{D}}^{(-)}$, the polarization operator $\hat{\mathcal{P}}^{(-)}$ creates a matter excitation. Energy can be transferred between matter and the electromagnetic fields, so the matter and EM modes are coupled. Self-consistent solution of the matter-photon dynamical equations gives the polariton frequencies ω_k that determine time dependence.

The energy, linear momentum, and angular momentum of the free electromagnetic field are conserved. Their densities and associated currents satisfy continuity equations of the form $\partial\rho/\partial t+\nabla\cdot\mathbf{j}=0$. This can be verified using MEs, and the steps in this derivation are still valid if we replace the products of classical real fields with Hermitian linear combinations of products of operators. For example, the current describing the flow of energy density $\langle\hat{\mathbf{D}}^{(-)}\cdot\hat{\mathbf{D}}^{(+)}/2\epsilon_0+\hat{\mathbf{B}}^{(-)}\cdot\hat{\mathbf{B}}^{(+)}/2\mu_0\rangle$ is c^2 times the linear momentum density

$$\mathbf{P}(\mathbf{r},t)=\tfrac{1}{2}\langle\Psi|\hat{\mathbf{D}}^{(-)}\times\hat{\mathbf{B}}^{(+)}-\hat{\mathbf{B}}^{(-)}\times\hat{\mathbf{D}}^{(+)}|\Psi\rangle. \tag{50}$$

Together with their associated current densities the components of $\mathbf{P}$ also satisfy continuity equations which implies that $\int d^3r\,\mathbf{P}(\mathbf{r},t)$ is a constant of the motion. If $|\Psi\rangle$ is a one-photon state $\langle\Psi|\hat{\mathbf{D}}^{(-)}\times\hat{\mathbf{B}}^{(+)}|\Psi\rangle=\langle\Psi|\hat{\mathbf{D}}^{(-)}|0\rangle\times\langle 0|\hat{\mathbf{B}}^{(+)}|\Psi\rangle$ so that

$$\mathbf{P}(\mathbf{r},t)=\tfrac{1}{2}[\mathbf{D}^{(-)}(\mathbf{r},t)\times\mathbf{B}^{(+)}(\mathbf{r},t)+\mathrm{c.c.}] \tag{51}$$

with the fields derived using Eqs. (41), (42), and (47). For a coherent state, the quasiclassical expectation value $\langle\{\gamma_{\mathbf{k},\sigma}\}|\hat{\mathbf{D}}\times\hat{\mathbf{B}}|\{\gamma_{\mathbf{k},\sigma}\}\rangle\neq\mathbf{D}_{\mathrm{coh}}\times\mathbf{B}_{\mathrm{coh}}$ for small $|\gamma_{\mathbf{k},\sigma}|$. However, Eq. (50) can be evaluated exactly using $a_{\mathbf{k},\sigma}|\gamma_{\mathbf{k},\sigma}\rangle$ to give

$$\mathbf{P}(\mathbf{r},t)=\tfrac{1}{2}[\mathbf{D}_{\mathrm{coh}}^{(-)}(\mathbf{r},t)\times\mathbf{B}_{\mathrm{coh}}^{(+)}(\mathbf{r},t)+\mathrm{c.c.}] \tag{52}$$

with $\mathbf{A}_{\mathrm{coh}}^{\perp(+)}$ given by Eq. (45). In either case the angular momentum density is

$$\mathbf{J}(\mathbf{r},t)=\mathbf{r}\times\mathbf{P}(\mathbf{r},t). \tag{53}$$

We are now in a position to compare the classical and quantum fields and densities. Equation (46) describes real fields that are the expectation values for coherent quantum states. Expectation values do not describe one-photon states since in this case the expectation values of the field operators are zero. Instead, it is projection onto a basis of position eigenvectors that gives one-photon positive frequency fields, proportional to components of the wave function. For one-photon and coherent states momentum density can be written as a cross product of fields as in Eqs. (51) and (52). Equation (50) can be used to interpolate between these two extreme cases.

The density $\mathbf{D}^{(-)}\times\mathbf{B}^{(+)}$ can be rewritten as [31]

$$\mathbf{D}^{(-)}\times\mathbf{B}^{(+)}=\mathbf{D}^{(-)}\times(\nabla\times\mathbf{A}^{(+)}) =\sum_{j=1}^{3}D_j^{(-)}\nabla A_j^{(+)}-(\mathbf{D}^{(-)}\cdot\nabla)\mathbf{A}^{(+)}.$$

Its first term, equal to

$$\sum_{j=1}^{3}D_j^{(-)}\nabla A_j^{(+)}=\frac{1}{2}\sum_{j=1}^{3}\Psi_j^{(1/2)^*}(i\hbar\nabla)\Psi_j^{(-1/2)},$$

is the integrand in the expectation value of the real space momentum operator $-i\hbar\nabla$. The last term, $(\mathbf{D}^{(-)}\cdot\nabla)\mathbf{A}^{(+)}$, also contributes to the flow of energy density and has important

consequences. It is responsible for the spin term in the AM (53). This can be seen by writing

$$-\mathbf{r}\times(\mathbf{D}^{(-)}\cdot\nabla)\mathbf{A}^{(+)}=\mathbf{D}^{(-)}\times\mathbf{A}^{(+)}-(\mathbf{D}^{(-)}\cdot\nabla)(\mathbf{r}\times\mathbf{A}^{(+)}),$$

where $\mathbf{a}\times\mathbf{b}=-i(\mathbf{a}\cdot\mathbf{S})\mathbf{b}$ gives

$$\mathbf{D}^{(-)}\times\mathbf{A}^{(+)}=\frac{1}{2}\sum_{j=1}^{3}\Psi_j^{(1/2)^*}\hbar\mathbf{S}\Psi_j^{(-1/2)}.$$

Since $\nabla\cdot\mathbf{D}^{(-)}=\rho^{(-)}$, the last term contributes $\int d^3r\,\mathbf{r}\times\rho\mathbf{A}^{(+)}$ to $\int d^3r\,\mathbf{J}(\mathbf{r},t)$ after integration by parts which is zero in the absence of free charge.

VI. PHOTON WAVE MECHANICS

In this section we will discuss first quantized photon quantum mechanics. For definiteness we will refer to the Barut-Marlin rules for Schrödinger and Dirac particles stated in [32] as follows. (a) A basis for the space of wave functions, which describe all the possible states of a particle, is defined by a wave equation. (b) An inner product is defined in the space of the wave functions. (c) Expressions for the probability density and probability current are found. They should form a four-vector whose divergence vanishes. The expression for the probability density should be positive definite. (d) Operators which correspond to measurements are defined, in particular, momentum and position operators. (e) The eigenfunction of the operators, normalized to 1 (in the case of discrete spectrum) or a δ function (in the case of a continuous function), are found. (f) The position operator, defined in (d), and the inner product, defined in (b), uniquely determine an expression for the probability density. The theory is consistent only if this uniquely determined expression is identical with the one defined in (c) to satisfy a continuity equation. This is a consistency test.

In brief, these rules apply to the **r**-space wave mechanics of a single free photon in free space in the following sense: (a) Solutions to Eq. (34),

$$i\,\partial\boldsymbol{\Psi}_\sigma^{(\alpha)}(\mathbf{r},t)/\partial t=\sigma c\,\nabla\times\boldsymbol{\Psi}_\sigma^{(\alpha)}(\mathbf{r},t),\tag{54}$$

include positive and negative frequencies. The negative frequency solution can be eliminated on physical grounds [19,29], thus cutting the Hilbert space in half as is done for solutions to the Dirac equation [32]. (b) The inner product of the wave functions describing states $|\tilde{\Psi}\rangle$ and $|\Psi\rangle$,

$$\langle\tilde{\Psi}^{(\alpha)}|\Psi^{(-\alpha)}\rangle=\sum_\sigma\int d^3r\,\tilde{\boldsymbol{\Psi}}_\sigma^{(\alpha)\dagger}(\mathbf{r},t)\cdot\boldsymbol{\Psi}_\sigma^{(-\alpha)}(\mathbf{r},t),\tag{55}$$

exists and is invariant under similarity transformations between $\alpha=1/2$ and $\alpha=0$. (c) The real number and current densities obtained by averaging the α and $-\alpha$ densities

$$n^{(\alpha)}(\mathbf{r},t)=\frac{1}{2}\sum_\sigma\boldsymbol{\Psi}_\sigma^{(\alpha)^*}\cdot\boldsymbol{\Psi}_\sigma^{(-\alpha)}+\text{c.c.},$$

$$\mathbf{j}^{(\alpha)}(\mathbf{r},t)=-\frac{i\sigma c}{2}\sum_\sigma\boldsymbol{\Psi}_\sigma^{(\alpha)^*}\times\boldsymbol{\Psi}_\sigma^{(-\alpha)}+\text{c.c.},\tag{56}$$

satisfy the continuity equation

$$\frac{\partial n^{(\alpha)}(\mathbf{r},t)}{\partial t}+\nabla\cdot\mathbf{j}^{(\alpha)}(\mathbf{r},t)=0.\tag{57}$$

This can be verified using the wave equation. The density $n^{(0)}=\Sigma_\sigma|\Psi_\sigma^{(0)}|^2$ is positive definite, while $[n^{(1/2)},\mathbf{j}^{(1/2)}]$ is a four-vector that can be written as the contraction of second rank EM field tensors with four-potentials. (d) The momentum operator is $\hbar\mathbf{k}$ and the position operator is given by Eq. (4). (e) The eigenvectors of these operators are δ function normalized according to Eq. (15). (f) The position operator and inner product give the density $\frac{1}{2}\langle\boldsymbol{\psi}_{\mathbf{r},\sigma}^{(\alpha)}|\Psi\rangle^*\langle\boldsymbol{\psi}_{\mathbf{r},\sigma}^{(-\alpha)}|\Psi\rangle$ +c.c.. Some of these points will now be discussed in more detail.

Both positive and negative frequency solutions of the wave equation are mathematically allowed. The classical solutions are real, and real waves do not satisfy a continuity equation or allow a probability interpretation [33]. It has been argued by Inagaki for LP wave functions that the negative frequency solutions with momentum in opposite direction to the wave propagation should be discarded from the physical photon state [29]. A similar case is made by Bialynicki-Birula for elimination of the negative frequency fields in fieldlike wave functions [18,19].

As with MEs the photon wave equations can be written in a number of equivalent ways, and this will be considered next to allow comparison with the existing photon wave function literature. The six component wave function

$$\Psi_{\text{hel}}^{(\alpha)}=\begin{pmatrix}\boldsymbol{\Psi}_1^{(\alpha)}\\ \boldsymbol{\Psi}_{-1}^{(\alpha)}\end{pmatrix}\tag{58}$$

in the helicity basis and

$$\Psi_{\text{lin}}^{(\alpha)}=\begin{pmatrix}\boldsymbol{\Psi}^{(\alpha)}\\ \boldsymbol{\Phi}^{(\alpha)}\end{pmatrix}\tag{59}$$

in the linear polarization basis can be defined. The Schrödinger equation is then, using Eqs. (54) and (31) with $\nabla\times\mathbf{a}=-i(\mathbf{S}\cdot\boldsymbol{\nabla})\mathbf{a}$,

$$i\frac{\partial}{\partial t}\begin{pmatrix}\boldsymbol{\Psi}_1^{(\alpha)}\\ \boldsymbol{\Psi}_{-1}^{(\alpha)}\end{pmatrix}=c\begin{pmatrix}-i\mathbf{S}\cdot\boldsymbol{\nabla} & 0\\ 0 & i\mathbf{S}\cdot\boldsymbol{\nabla}\end{pmatrix}\begin{pmatrix}\boldsymbol{\Psi}_1^{(\alpha)}\\ \boldsymbol{\Psi}_{-1}^{(\alpha)}\end{pmatrix}\tag{60}$$

in the helicity basis and

$$i\frac{\partial}{\partial t}\begin{pmatrix}\boldsymbol{\Psi}^{(\alpha)}\\ \Phi^{(\alpha)}\end{pmatrix}=c\begin{pmatrix}0 & \mathbf{S}\cdot\boldsymbol{\nabla}\\ -\mathbf{S}\cdot\boldsymbol{\nabla} & 0\end{pmatrix}\begin{pmatrix}\boldsymbol{\Psi}^{(\alpha)}\\ \boldsymbol{\Phi}^{(\alpha)}\end{pmatrix}\tag{61}$$

in the linear polarization basis. If $\alpha=1/2$, Eq. (60) is of the form considered by Bialynicki-Birula and Sipe [18,20], while if $\alpha=0$ Eq. (61) is the form used by Inagaki [29]. However, Eqs. (60) and (61) themselves imply that either the helicity or the linear polarization basis can be used in combination with fieldlike $\alpha=1/2$ wave functions *or* LP $\alpha=0$ wave functions. The operator on the right-hand sides of Eqs. (60) and (61) is the real space one-photon Hamiltonian.

The density $i\epsilon_0\mathbf{E}\cdot\mathbf{A}/\hbar$ has appeared before in the classical context and in applications to beams. Cohen-Tannoudji *et al.* [31] transform the classical electromagnetic angular momentum as

$$\mathbf{J} = \epsilon_0 \int d^3r\, \mathbf{r} \times (\mathbf{E} \times \mathbf{B})$$

$$= \epsilon_0 \int d^3r \left[\sum_{i=1}^{3} E_i (\mathbf{r} \times \nabla) A_i + \mathbf{E} \times \mathbf{A} \right] \tag{62}$$

by requiring that the fields go to zero sufficiently quickly at infinity. Although this looks like an expectation value, the fields are classical. In a discussion of optical beams, van Enk and Nienhuis [34] separate monochromatic fields into their positive and negative frequency parts using

$$\mathbf{V} = [\mathbf{V}^{(+)} \exp(-i\omega t) + \mathbf{V}^{(-)} \exp(i\omega t)]/\sqrt{2}$$

and obtain for total field linear momentum and AM

$$\mathbf{P} = -i \int d^3r \left[\sum_{i=1}^{3} D_i^{(+)*} (i\nabla) A_i^{(+)} \right], \tag{63}$$

$$\mathbf{J} = -i \int d^3r \left[\sum_{i=1}^{3} D_i^{(+)^*} (-\mathbf{r} \times i\nabla + S) A_i^{(+)} \right]. \tag{64}$$

Here we have assumed the absence of matter in writing $\mathbf{D} = \epsilon_0 \mathbf{E}$, substituted $\mathbf{A}^{(+)} = i\omega \mathbf{D}^{(+)}$, and changed the notation a bit for consistency with the present work. These are classical expressions, but terms at frequency 2ω do not contribute to the total momentum and angular momentum, $\mathbf{P}$ and $\mathbf{J}$ [35]. They look like the expectations values of the linear and angular momentum operators that would be obtained using the biorthonormal wave function pair $\sqrt{\epsilon_0/\hbar}\mathbf{A}^{(+)\perp}_{\text{photon}}$ and $-i\mathbf{D}^{(+)}/\sqrt{\epsilon_0 \hbar}$. The number operator $i\hat{\mathbf{D}}^{(-)} \cdot \hat{\mathbf{A}}^{(+)}/2\hbar + \text{H.c.}$ was shown previously to be the zeroth component of a four-vector obtained by contraction of the second rank EM field tensor with the four-potential $(\phi, \mathbf{A})$ [36]. This demonstrates that the biorthonormal basis is of value for comparison with the existing literature.

It was noted in Sec. III that the biorthonormal inner product is equivalent to the use of a metric operator. Using Eq. (23) and $\hat{H} = \hbar kc$ in $\mathbf{k}$ space and substituting $\hat{H}$ for $i\partial/\partial t$ the inner product (55) can be written as

$$\langle \tilde{\Psi} | \Psi \rangle = \sum_{\sigma,j} \int \frac{d^3k}{kc} \tilde{\Psi}^{(1/2)^*}_{\sigma,j}(\mathbf{k},t) \Psi^{(1/2)}_{\sigma,j}(\mathbf{k},t)$$

$$= \sum_{\sigma,j} \int d^3r\, \tilde{\Psi}^{(1/2)^*}_{\sigma,j}(\mathbf{r},t) \hat{H}^{-1} \Psi^{(1/2)}_{\sigma,j}(\mathbf{r},t)$$

as in [21,38].

The number density is the expectation value of the number density operator (27) as discussed in Sec. IV. The $\alpha = \pm 1/2$ wave function pair gives a real local one-photon density $n^{(1/2)}$, but this density is not positive definite. This can be seen from the following example: If $|\Psi\rangle$ is a one-photon state that includes only wave vectors $\mathbf{k}_1$ and $\mathbf{k}_2 = \mathbf{k}_1 + \Delta\mathbf{k}$ both with helicity σ where $c_{\mathbf{k}_1,\sigma} = c_{\mathbf{k}_2,\sigma} = 1/\sqrt{2}$ then

$$n^{(1/2)} = \{1 + \tfrac{1}{2}(\sqrt{k_1/k_2} + \sqrt{k_2/k_1}) \cos[\Delta\mathbf{k} \cdot \mathbf{r} - ((k_1 - k_2)ct)]\}/V.$$

The cosine term can exceed the spatially uniform time independent term due to the $\sqrt{k}$ factors, leading to negative values. If $k_2 \approx k_1$, $n^{(1/2)}$ is approximately equal to the positive definite density, $n^{(0)}$, however only the LP wave function satisfies the positive definite requirement exactly.

It thus appears that LP wave functions are essential to a probability interpretation. Fieldlike wave functions can be obtained from the LP wave function by a similarity transformation, and thus are equivalent to it for the calculation of expectation values. The operators given by Eq. (29) in the $\alpha = 0$ case are identical to the operators examined by Cook. The equations that they satisfy differ from those for $\mathbf{D}$ and $\mathbf{B}$ only in that their relationship to charge and current sources is nonlocal. The LP number density has been criticized [18,20,23], but its scalar analog, obtained by taking Fourier transforms of the Schmidt modes, has recently been applied to spontaneous emission of a photon by an atom and spontaneous parametric down-conversion [6,37]. For narrowband superpositions of plane wave states the distinction between the LP and fieldlike form of the wave function has no observable consequences [6].

The operator (21) creates basis states that lead to the orthogonal transverse one-photon wave function $\Psi^{(\alpha)}_{\text{hel}}(\mathbf{r},t) = [\Psi^{(\alpha)}_1, \Psi^{(\alpha)}_{-1}]$ in the helicity basis. The wave function components $\Psi^{(-1/2)}$ are proportional to the vector potential, while $\Psi^{(1/2)}$ is related to EM fields. Contraction of the second rank field tensor $F^{\mu\nu} = \partial^\nu A^\mu - \partial^\mu A^\nu$ with the four-potential as $F^{\mu\nu^*} A_\nu$ gives a four-vector [36]. Thus $[n^{(1/2)}, \mathbf{j}^{(1/2)}]$ is a four-vector and photon density is its zeroth component.

In the linear polarization basis the density operators are

$$\hat{n}^{(\alpha)}(\mathbf{r},t) = \tfrac{1}{2}[\hat{\boldsymbol{\psi}}^{(\alpha)\dagger}_{\mathbf{r}} \cdot \hat{\boldsymbol{\psi}}^{(-\alpha)}_{\mathbf{r}} + \hat{\boldsymbol{\phi}}^{(\alpha)\dagger}_{\mathbf{r}} \cdot \hat{\boldsymbol{\phi}}^{(-\alpha)}_{\mathbf{r}} + \text{H.c.}],$$

$$\hat{\mathbf{j}}^{(\alpha)}(\mathbf{r},t) = \tfrac{1}{2}[\hat{\boldsymbol{\psi}}^{(\alpha)\dagger}_{\mathbf{r}} \times \hat{\boldsymbol{\phi}}^{(-\alpha)}_{\mathbf{r}} - \hat{\boldsymbol{\phi}}^{(-\alpha)\dagger}_{\mathbf{r}} \times \hat{\boldsymbol{\psi}}^{(\alpha)}_{\mathbf{r}} + \text{H.c.}], \tag{65}$$

with $\hat{\boldsymbol{\psi}}^{(\alpha)}_{\mathbf{r}}$ and $\hat{\boldsymbol{\phi}}^{(\alpha)}_{\mathbf{r}}$ given by Eq. (29). Mandel and Wolf noted the convenience of a photon number operator, equal to $\hat{\boldsymbol{\psi}}^{(0)\dagger}_{\mathbf{r}} \cdot \hat{\boldsymbol{\psi}}^{(0)}_{\mathbf{r}}$ in the present notation, to the theory of photon counting for an arbitrary quantum state [39]. Cook sought detector independent photon density and current operators that satisfy a continuity equation. His operators are just Eq. (65) if we take $\alpha = 0$. Inagaki reformulated Cook's theory in terms of conventional quantum mechanics [29]. These authors discuss the restrictions imposed by photon nonlocalizability, but the existence of a basis of position eigenvectors makes this unnecessary here. Our operators describe microscopic densities, and there is no restriction based on wave length.

The Lorentz transformation properties of the $\alpha = 0$ photon annihilation operators in the linear polarization basis were also considered by Cook [41]. He concluded that their continuity equation is covariant in the sense that it is related to the field vectors in the same way in all reference frames. The Hamiltonian, momentum, angular momentum, and Lorentz transformation operators must conform to the Poincaré algebra. Since the position operator generates a change in particle momentum, the boost operator is closely related to the position operator. For a free photon in $\mathbf{k}$-space the Lorentz operator corresponding to the $\alpha = 1/2$ case is [38]

$$\hat{\mathbf{K}}^{(1/2)} = k(i\nabla) + \hat{\mathbf{k}} \times \mathbf{S},$$

where $\hat{\mathbf{K}}^{(-1/2)} = \hat{\mathbf{K}}^{(1/2)\dagger}$. Using Eq. (17) this gives

$$\hat{\mathbf{K}}^{(0)} = k^{-1/2}\hat{\mathbf{K}}^{(1/2)}k^{1/2}$$

for the LP boost operator which incorporates the similarity transformation. In $\mathbf{k}$ space this is simple, but in $\mathbf{r}$ space it is nonlocal as discussed by Cook [41].

It is stated, in [42] for example, that "the non-Hermitian formulation is in most cases a mere change of metric of a well posed Hermitian problem. Nonetheless, it has been successfully argued that the non-Hermitian formalism is often more natural and simplifies calculations." These comments apply here. The choice of α does not affect expectation values, the inner product, and the existence of a wave equation and a continuity equation. Only the number and current densities themselves are affected. The field and LP bases can be viewed as alternative descriptions of the photon state. For most purposes fields are more closely related to the physics, but the LP basis is needed if the band width is large and photon number density is required.

According to the general rules of quantum mechanics, for a one-photon state the probability that a photon with helicity σ will be found at position $\mathbf{r}$ at time t is $|\Psi_\sigma^{(0)}(\mathbf{r},t)|^2$. More generally the photon number density is the expectation value of the number density operator, $n_\sigma^{(0)}(\mathbf{r},t) \approx n_\sigma^{(1/2)}(\mathbf{r},t)$, given by Eq. (38). Glauber [28] defined an ideal photodetector to be of negligible size with a frequency-independent photoabsorption probability. An ideal photon counting detector also has a quantum efficiency of $\eta=1$, that is any photon reaching the detector is counted. A detector with all of these characteristics measures photon position. Consider a one-photon pulse traveling in the z direction that is normally incident on a detector of thickness Δz and area ΔA. The probability that a photon is present in this detector, and hence that it is counted, is $n_\sigma^{(\alpha)}(\mathbf{r},t)\Delta A \Delta z$. In Glauber theory the count rate is $dn_G/dt \propto \langle \Psi | \hat{\mathbf{E}}^{(-)}(\mathbf{r},t) \cdot \hat{\mathbf{E}}^{(+)}(\mathbf{r},t) | \Psi \rangle$ where $(dn_G/dt)\Delta z/c$ is the probability the photon is counted during the time that it takes to traverse the detector. Since $n_\sigma^{(1/2)} = i\epsilon_0 \mathbf{E}_\sigma^{(-)} \cdot \mathbf{A}_\sigma^{(+)}/\hbar$ +c.c., where $A_\sigma^{(+)} \approx -iE_\sigma^{(+)}/\bar{\omega}$ for most beams available in the laboratory, the predictions of the present photon number based theory and Glauber photodetection theory are usually indistinguishable.

The number based theory has the advantage that the probability is normalizable, for example the probability to count one photon in a one-photon state in the whole of space using an array of detectors with $\eta=1$ is unity. The Glauber form of the count rate is based on the transition probability, however there are advocates for a photon number density approach, even within conventional photon counting theory. Mandel noted that "there are many problems in quantum optics, particularly those concerned with photoelectric measurements of the field, which are most conveniently treated with the help of an operator representing the number of photons" [39]. Mandel and Wolf based their general photon counting theory on a photon number operator [40]. Cook observed that there is no universal proportionality constant that relates photon flux to p^G, and thus the prevailing theory of photoelectron counting fails to provide a complete description of photon transport [24]. He proposed a modified photodetection theory based on photon number. A photon density $n_\sigma^{(0)} \times(\mathbf{r},t)$, equal to the probability density to count a photon at $\mathbf{r}$ at time t, is consistent with Cook's arguments *and* with the rules of quantum mechanics.

VII. ANGULAR MOMENTUM AND BEAMS

The physical interpretation of the position eigenvectors in [13] involving AM was motivated by the recent experimental and theoretical work on optical vortices. These vortices are spiral phase ramps described by fields that go as $\exp(il_z\varphi)$ and in experiments appear as annular rings around a dark center. It can be seen by inspection of Eq. (9) that the localized states must have orbital AM, and this implies a vortex structure that is affected by the choice of χ. Taking helicity $\sigma=1$ to give a concrete example, we can first take $m=0$ in Eq. (9) to give the spherical polar vectors $(\hat{\boldsymbol{\theta}}+i\sigma\hat{\boldsymbol{\phi}})/\sqrt{2}$ with total AM 0. At $\theta=0$ there is spin AM $\hbar$ and the orbital AM is $-\hbar$, while at $\theta=\pi$ the spin and orbital AM are $-\hbar$ and $\hbar$, respectively. If instead we choose $m=1$, the $\theta=0$ orbital AM is 0, but at $\theta=\pi$ it is $2\hbar$. For a localized state the vortex has not been eliminated, it has just been moved. Thus an understanding of optical AM is essential to the physical picture of the localized basis states that are used here to obtain the photon wave function.

Theoretically, the simplest beams with orbital AM are the nondiffracting Bessel beams (BBs), and these beams are closely related to our localized states. They satisfy MEs and have definite frequency, ck_0, and a definite wave vector, k_z, along the propagation direction. It then follows that the $\mathbf{k}$-space transverse wave vector magnitude $k_\perp = \sqrt{k_0^2 - k_z^2}$, and the angle $\theta = \tan^{-1}(k_\perp/k_z)$ also have definite values for BBs. Cylindrical symmetry is achieved by weighting all ϕ equally with a phase factor $\exp(im\phi)$. When Fourier transformed to $\mathbf{r}$ space the modes go as $\exp(-ik_0ct + il_z\varphi + ik_zz)J_{l_z}(k_\perp r)$ where $l_z=m$ and $m\pm1$ in Eq. (9), J_{l_z} are Bessel functions, φ the real space azimuthal angle, and r is the perpendicular distance from the beam axis [43]. If we select $\chi=0$ so that the $\mathbf{k}$-space unit vectors are $\hat{\boldsymbol{\phi}}$ and $\hat{\boldsymbol{\theta}}$ in the linear polarization basis, $\mathbf{B}$ is transverse to $\hat{\mathbf{z}}$ for the $\hat{\boldsymbol{\theta}}$ mode, and $\mathbf{E}$ is transverse for the $\hat{\phi}$ mode and the linearly polarized modes can be called transverse magnetic (TM) and transverse electric (TE), respectively.

The Bessel functions have a sinusoidal dependence on $k_\perp r$, and this implies that the BBs are standing waves that are a sum of incoming and outgoing waves. If integrated over $k_\perp$ the resulting wave is localized on the z axis at some instant in time that can be defined as $t=0$. Localization of beams in this way is discussed in [44,45]. If the BBs are then integrated over k_z, the result is equivalent to a sum over all wave vectors, and states localized in three dimensions are obtained. But note that this k_z sum includes waves traveling in the positive and negative $\hat{\mathbf{z}}$ directions. According to the Paley-Weiner theorem, $\int_0^\infty dk_z$ does not allow exact localization, but this restriction does not apply to an integral over all

positive and negative values. Position is not a constant of the motion, and localized states can exist only for an instant in time. Exactly localized states in free space are not physically possible because they require infinite energy. However, our primary concern here is with the use of localized basis states for calculation of the photon wave function, and we do not require that these basis states have a physical realization.

The real space mathematical description of beams used to interpret the AM experiments is usually based on the classical energy, linear momentum, and angular momentum densities. Here, with a basis of position eigenvectors in hand that leads to a wave function for a photon in an arbitrary state, we are in a position to consider the real space description of the AM of beams from a quantum mechanical perspective. The $\alpha=1/2$ wave function is a solution to MEs, and any derivation based on MEs can be adapted to the one-photon case. The expansion of vector potential in [44] that leads to paraxial fields to a first approximation can be applied to allow application of our formalism to the paraxial beams that are used in most optical experiments. Localized states do not exist within the paraxial approximation, and the paraxial approximation cannot be applied to the position eigenvectors.

A paraxial beam propagating in the $\hat{\mathbf{z}}$ direction with frequency ω, helicity σ, and z component of orbital AM $\hbar l_z$ can be described in cylindrical polar coordinates by the vector potential [46]

$$\mathbf{A}^{(+)}(\mathbf{r},t)=\tfrac{1}{2}(\hat{\mathbf{x}}+i\sigma\hat{\mathbf{y}})u(r)\exp[il_z\varphi+ik_z(z-ct)]. \quad (66)$$

This vector potential is equivalent to the wave function $\boldsymbol{\Psi}_{\sigma'}(\mathbf{r},t)=\delta_{\sigma,\sigma'}\sqrt{2\epsilon_0/\hbar}\mathbf{A}^{(+)}(\mathbf{r},t)$. The z component of the time average of the classical AM density, equal to $\frac{1}{2}\mathbf{r}\times(\mathbf{D}^*\times\mathbf{B}+\mathbf{D}\times\mathbf{B}^*)$, is then found to be

$$J_z(r)=\epsilon_0\left[\omega l_z|u(r)|^2-\frac{1}{2}\omega\sigma r\frac{\partial|u^2(r)|}{\partial r}\right]. \quad (67)$$

It equals the z component of the AM density (53) with momentum density given in Eq. (51) or (52) without the need for time averaging. Thus Eq. (67) can be interpreted as a quantum mechanical AM density that is valid for coherent and one-photon states, while Eq. (50) interpolates between these two cases.

The first term of Eq. (67) is consistent with orbital AM $\hbar l_z$ per photon since the photon density given by Eq. (39) reduces to $n^{(1/2)}(\mathbf{r},t)=\epsilon_0\omega|u(r)|^2/\hbar$. The last term of Eq. (67) does not look like photon spin density. The most paradoxical case is a plane wave, as discussed in [47]. For example a wave function proportional to $(\hat{\mathbf{x}}+i\sigma\hat{\mathbf{y}})\exp(ikz-i\omega t)$ implies linear momentum $\hbar k\hat{\mathbf{z}}$ per photon and hence no z component of AM. But we know that such a beam describes a stream of photons each with spin AM $\hbar\sigma$. It was observed in 1936 by Beth [48] that a circularly polarized beam can cause a disk to rotate, so the beam really does carry AM that it can transfer to the disk. The AM of this beam resides in its edges, as can be seen from Eq. (67). A new edge is created if the disk intercepts part of the beam and this reduces the AM of the beam, allowing the conservation of total AM [35]. This is analogous to the continuum description of a dielectric where it is know that the medium is composed of atoms, but a continuum description of a uniformly polarized dielectric results only is a surface charge. An even closer analogy exists between spin AM and a continuous magnetic medium where a current in individual molecules reduces to a macroscopic current at the edges of the medium.

In quantum mechanics operators describe observables and their eigenvalues are the possible results of a measurement. While spin and orbital AM are in general not separable, the choice $\chi=-\phi$ in Eq. (7) gives unit vectors $(\hat{\mathbf{x}}+i\sigma\hat{\mathbf{y}})/\sqrt{2}$ in the paraxial limit which implies spin quantum number $s_z=\pm1$. The wave function (66) is an eigenvector of $\hat{S}_z$ with eigenvalue s_z and of $\hat{L}_z=-i\hbar\partial/\partial\varphi$ with eigenvalue $\hbar l_z$ where φ the real space azimuthal angle. The latter orbital AM is equivalent to linear momentum $\hbar l_z/r$. For this definite helicity state only one term in the photon density (56) contributes. The probability density to detect this photon is $n^{(0)}(\mathbf{r},t)\cong n^{(1/2)}\times(\mathbf{r},t)$, where these field potential and LP densities are essentially equal for a paraxial beam. For a coherent state the expansion coefficients $c_{\mathbf{k},\sigma}$ in the one-photon wave function (33) are replaced with the amplitudes $\gamma_{\mathbf{k},\sigma}$. Small absorbing particles placed in these beams are essentially photodetectors that conserve AM by spinning about their centers of mass and rotating around the beam axis while they absorb photons [49]. The photon number density gives the probability to absorb a photon which carries with it spin AM $\hbar s_z$ and orbital AM $\hbar l_z$. For transparent particles the situation is more complicated, since reemission should also be considered.

VIII. CONCLUSION

We have derived one and two photon wave functions from QED by projecting the state vector onto the eigenvectors of a photon position operator. Largely because it is still widely believed that there is no position operator, this is the first time that a photon wave function has been obtained in this way. The two photon wave function is symmetric, in agreement with [1,2]. While only the LP wave function gives a positive definite photon density, fieldlike wave functions are widely used and are more convenient in many applications. Also, they given energy momentum and angular momentum density as in Eq. (51) for example. In the fieldlike helicity basis the wave function pair is

$$\boldsymbol{\Psi}_\sigma^{(-1/2)}(\mathbf{r},t)=\sqrt{\frac{2\epsilon_0}{\hbar}}\mathbf{A}_\sigma^{(+)}(\mathbf{r},t),$$

$$\boldsymbol{\Psi}_\sigma^{(1/2)}(\mathbf{r},t)=-i\sqrt{\frac{2}{\hbar\epsilon_0}}\mathbf{D}_\sigma^{(+)}(\mathbf{r},t). \quad (68)$$

The wave function components $\boldsymbol{\Psi}_\sigma^{(\alpha)}$ are given by Eq. (33). For definite helicity fields in free space, $\mathbf{B}^{(+)}$ and the Reimann-Silberstein field vector are just proportional to $\mathbf{D}^{(+)}$, and thus are equivalent to it. The linear polarization basis of TM and TE fields can be obtained by taking the sum and difference of the definite helicity modes as in Eq. (29). The photon density is Eq. (56)

$$n_{\sigma}^{(\alpha)}(\mathbf{r},t) = \tfrac{1}{2}\boldsymbol{\Psi}_{\sigma}^{(\alpha)^*} \cdot \boldsymbol{\Psi}_{\sigma}^{(-\alpha)} + \text{c.c.}, \tag{69}$$

where $n_{\sigma}^{(1/2)}$ is essentially equal to $n_{\sigma}^{(0)}$ except for very broad band signals. The one-photon density can be generalized to describe the photon density in an arbitrary pure state using the expectation value of the number operator, Eq. (38).

Systematic investigation of photon position operators and their eigenvectors clarifies the role of the photon wave function in classical and quantum optics. The LP wave function defines a positive definite photon number density and results in photon wave mechanics equivalent to Inagaki's single photon wave mechanics [29]. It is related to field based wave functions through a similarity transformation that preserves eigenvalues and scalar products. In free space the field (68) is proportional to the RS wave function investigated in [1,18–20]. The field $\mathbf{D}^{(+)}(\mathbf{r},t)$ is proportional to the Glauber wave function [2,5,28] which gives the photodetection amplitude for a detector that responds to the electric field [1]. While only fields and potentials are locally related to charge and current sources, Fourier transformation of $\mathbf{k}$-space probability amplitudes naturally leads to the LP form [6,37]. The similarity transformation between the field-potential and LP wave functions makes the choice a matter of convenience for most purposes.

By the general rules of quantum mechanics the LP wave function is the probability amplitude to detect a photon at a point in space. It and the closely related field-potential wave function pair obtained by solution of MEs are ideally suited to the interpretation of photon counting experiments using a detector that is small in comparison with the spatial variations of photon density. It is not subject to limitations based on nonlocalizability, and coarse graining or restriction to length scales smaller than a wave length is not required. Exact localization in vacuum requires infinite energy and is not physically possible, but position eigenvectors provide a useful mathematical description of photon density. Photon number density is equivalent to integration over undetected photons in a multiphoton beam. In an experiment where absorbing particles are placed in a beam, the particles act as photodetectors which can sense the spin and orbital angular momentum of the photons. Our formalism justifies the use of positive frequency Laguerre-Gaussian fields as photon wave functions and gives a rigorous theoretical basis for extrapolation of their range of applicability from the many photon to the one-photon regime.

ACKNOWLEDGMENT

The author acknowledges the financial support of the Natural Science and Engineering Research Council of Canada.

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