Lorentz invariant photon number density

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A Lorentz invariant positive definite expression for photon number density is derived as the absolute square of the invariant scalar product of a polarization sensitive position eigenvector and the photon wave function. It is found that this scalar product is independent of the form chosen for the wave function and that the normalized positive frequency vector potential-electric field pair is a convenient choice of wave function in the presence of matter. The number amplitude describing a localized state is a δ-function at the instant at which localization and detection are seen as simultaneous.

I. INTRODUCTION

The concept of photon number density arises in the interpretation of experiments such as photon counting and the creation of correlated photon pairs in a nonlinear material. In spite of its relevance to experiment and the foundations of quantum mechanics, no relativistically invariant positive definite expression for photon number density exists at present. Mandel [1] defined a coarse-grained number operator to count photons in a region large in comparison with the wavelength of any occupied mode of the field. However photons can be counted, and hence localized, in a photodetector much smaller than this wave length. Here I will show that the absolute square of the Lorentz invariant scalar product of a localized state and the photon wave function is a local positive definite number density.

In nonrelativistic quantum mechanics the 1-particle number density is the absolute square of the real space wave function. The wave function can be obtained by projection of the state vector onto a basis of simultaneous eigenvectors of the position and spin operators. Although this was long thought to be impossible for the photon, we recently constructed a photon position operator with commuting components [2, 3] and derived a photon wave function [6] and the positive frequency vector potential-electric field (AE) wave function pair were considered and a scalar product was defined to complete the Hilbert space. It was proved that the scalar product is invariant under the similarity transformation relating the AE and LP forms of its integrand, implying that they are equivalent when used for calculation of transition amplitudes and expectation values.

Since position is an observable, the number amplitude to detect a particle at position \( \mathbf{r} \) with spin \( \sigma \) equals the scalar product of the corresponding position-spin eigenvector with the particle’s wave function. In real space this number amplitude, \( \langle \mathbf{r}, \sigma | \Psi (t) \rangle = \int d^3 \mathbf{r}' \psi^*_{\mathbf{r}, \sigma} (\mathbf{r}') \Psi_{\sigma} (\mathbf{r}', t) \), is equal to the wave function, \( \Psi_{\sigma} (\mathbf{r}, t) \), only if the position eigenvectors are localized states of the form \( \psi_{\mathbf{r}, \sigma} (\mathbf{r}') = \delta^3 (\mathbf{r}' - \mathbf{r}) \). While this is true for a nonrelativistic massive particle, it is not the case for the photon. A transverse vector is not of the simple δ-function form, and thus it is not the amplitude to detect a photon at \( \mathbf{r} \). In addition, photons are often most conveniently described in terms of potentials or fields because of their simple relationship to the matter current density. The Fourier components of the vector potential and electric field describing a localized state go as \( \omega_k^{3/2} \) where \( \mathbf{k} \) is the wave vector and \( \omega_k \) is the angular frequency. They are not δ-functions even if their vector properties are ignored.

In this paper, the relationship between the photon wave function and number density will be examined. In Section II, our previous work on the photon position operator and wave function will be summarized. In Section III a Lorentz invariant scalar product will be defined. The number amplitude for arbitrary polarization, equal to the scalar product of a position eigenvector and the wave function, will be found in Section IV. In Section V, interaction with matter will be considered, and photon number density will be discussed in relation to the recent and historical literature.

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II. POSITION OPERATOR AND WAVE FUNCTION

The photon position operator with commuting components and transverse eigenvectors can be written as [2]
\[
\hat{r}^{(\alpha, \chi)} = iD_{\chi}^{(\alpha)} \nabla (\omega_k)^{-\alpha} D^{-1}
\]
where \( \nabla \) is the \( k \)-space gradient and \( D = \exp (-iS_k) \exp (-iS_{\theta} \theta) \) is the rotation matrix with Euler angles \( \phi, \theta, \chi \). The operator \( \hat{D} \) rotates the unit vectors \( \hat{x}, \hat{y}, \hat{z} \) into the spherical polar unit vectors \( \hat{\theta}, \hat{\varphi}, \hat{\chi} \) and then rotates \( \hat{\theta} \) and \( \hat{\varphi} \) about \( \hat{k} \) by \( \chi(k) \). Thus \( \hat{r}^{(\alpha, \chi)} \) rotates the transverse and longitudinal unit vectors to the fixed directions \( \hat{x}, \hat{y}, \hat{z} \), eliminates the factor \( (\omega_k)^{\alpha} \), operates with \( i\nabla \) to extract the position information from the phase of the wave function, and then reinserts the factor \( (\omega_k)^{\alpha} \) and returns the unit vectors to their original orientations. The eigenvectors of \( \hat{D} \) form a basis for the LP wave function if \( \alpha = 0 \), and for a wave function proportional to the vector potential if \( \alpha = -1/2 \) and its conjugate momentum if \( \alpha = 1/2 \).

In the Schrödinger picture (SP) the simultaneous eigenvectors of the position and helicity operators,
\[
\hat{\psi}^{(\alpha, \chi)}(\chi)(k) = (\omega_k)^{\alpha} \exp(-i\hat{r} \cdot \hat{\chi}) \frac{e^{(\chi)}}{2\pi^{3/2}},
\]
form a basis for the Hilbert space, \( \mathcal{H} \). The transverse unit vectors are
\[
e^{(\chi)}_{\sigma}(k) = \frac{1}{\sqrt{2}} \left( \hat{\theta} + i\sigma \hat{\varphi} \right) \exp(-i\sigma \chi)
\]
for circular polarizations \( \sigma = \pm 1 \) and the longitudinal unit vector is \( e_0 = \hat{k} \). The real linear polarization unit vectors
\[
e^{(\chi)}_{r_1}(k) = \frac{1}{\sqrt{2}} \left( e^{(\chi)}_1 + e^{(\chi)}_{-1} \right),
\]
\[
e^{(\chi)}_{r_2}(k) = \frac{1}{\sqrt{2}} \left( e^{(\chi)}_1 - e^{(\chi)}_{-1} \right),
\]
give eigenvectors of \( \hat{r}^{(\alpha, \chi)} \) but not the helicity operator. While all \( \chi \) are needed to interpret an experiment that measures polarization, only one basis is needed to describe the photon state, and the \( \chi = 0 \) definite helicity basis will be used here for simplicity. In this basis, the probability amplitude for the state with polarization \( e^{(\chi)}_{\sigma}(k) \) incorporates the phase factor \( \exp(-i\sigma \chi) \).

The wave function was obtained in [4] as the projection of the quantum electrodynamics (QED) state vector onto a basis of position-helicity eigenvectors. If the operator \( a^\dagger_{\sigma}(k) \) creates a photon with wave vector \( k \) and circular polarization \( e^{(\sigma)}_{\sigma}(k) \), the 1-photon \( k \)-space basis states are \( |k, \sigma\rangle = a^\dagger_{\sigma}(k) |0\rangle \) where \( |0\rangle \) is the vacuum state. Creation operators for a photon at position \( r \) can be defined as
\[
\hat{\psi}^{(\alpha, \chi)}(r, \sigma) = (\omega_k)^{\alpha} \exp(-i\hat{r} \cdot \hat{k}) e^{(\sigma)}_{\sigma}(k) \frac{a^\dagger_{\sigma}(k)}{2\pi^{3/2}}.
\]

Any state vector can be expanded in Fock space as \( |\Psi(t)\rangle = \sum_{\alpha=0}^{\infty} c_{\alpha} |\psi_{\alpha}(t)\rangle \) where the 1-photon term \( |\psi_{\alpha}(t)\rangle = \sum_{\sigma=\pm 1} \int d^3k \langle k, \sigma | \Psi(t) \rangle |k, \sigma\rangle \) is completely described by the probability amplitude
\[
\langle k, \sigma | \Psi(t) \rangle = c_{\alpha} \exp(-i\omega_k t).
\]

The projection onto the definite helicity position eigenvectors, \( \Psi_{\sigma}(r, t) = \langle 0 | \psi^{(\sigma)}_{r, \sigma} | \Psi(t) \rangle \), is a six component wave function whose dynamics is described by a diagonal Hamiltonian \([4, 6]\). The expectation value can be evaluated using \([\alpha, \sigma, k'], \sigma, k]\rangle = \delta_{\alpha, \sigma} \delta^3(k - k') \). Here the focus is on the scalar product and polarization will be summed over to give the 3-vector wave function \( \Psi^{(\alpha)}(r, t) \) where
\[
\Psi^{(\alpha)}(r, t) = \int d^3k c_{\sigma}(k) e^{(\sigma)}_{\sigma}(k) \frac{\exp(i\hat{r} \cdot \hat{k} - i\omega_k t)}{2\pi^{3/2}},
\]
\[
\Psi^{(\alpha)}(k) = \sum_{\sigma=\pm 1} \Psi^{(\alpha)}_{\sigma}(k).
\]

III. INVARIANT SCALAR PRODUCT

To prove the invariance of the scalar product that completes \( \mathcal{H} \), 4-vector notation and the Lorentz gauge will be used. The contravariant energy-momentum 4-vector is \( mk \) where \( k = k^\mu = (\omega_k/c, k) \) and the covariant 4-vector is \( k_{\mu} = g_{\mu
u}k^\nu \) where \( g \) is a diagonal tensor with \( g_{00} = -1 \) and \( g_{ii} = 1 \) for \( i = 1 \) to 3. In addition to the transverse and longitudinal eigenvectors, scalar position eigenvectors can be defined \([10]\) and the 4-potential can be used as wave function \([11]\). In the Lorentz gauge the momentum conjugate to \( A^+(x) \) is \( \Pi^+(x) = \varepsilon_{\mu\nu} A^{(+)\mu}\partial A^{(+\nu)} / \partial t \) \([12]\) where the superscript \((+)\) denotes the positive frequency part. This is equivalent to \( \varepsilon^{(+\mu)} = i\partial \phi^{(+)\mu} / \partial t \) that follows from \([4]\). Since only positive frequencies arise in the wave function, the invariant volume integral can be written as
\[
\int d^4k \delta(k^\mu k_{\mu} + \kappa^2) \Theta(\omega_k) = c \int d^3k \frac{\delta^3(k - k_\kappa)}{2\omega_k}
\]
where the Heaviside step function \( \Theta(\omega_k) \) is invariant under proper Lorentz transformations and \( \kappa = mc / h = 0 \) for a free photon.
The real space wave function satisfying Ψ(−1/2) (x) = \sqrt{2\alpha/\hbar A^{(+)}(x)} is a 4-vector. Use of (8) in (7) for α = −1/2 gives

\[ Ψ^{(−1/2)}(x) = \int \frac{d^3k}{\omega_k} \exp (ikx) \Psi^{(1/2)}(k) \tag{10} \]

for physical states with exp(−iωkt) time dependence. This implies that Ψ(1/2) (k) must be a 4-vector. Thus the scalar product of |Φ1⟩ and |Ψ1⟩,

\[ ⟨Φ1|Ψ1⟩ = \int d^3k Φ^{(−1/2)*}(k) ω_1(k) Ψ^{(1/2)}(k), \tag{11} \]

is an invariant. This is the form normally used in field theory, incorporating the metric ω_1 = 1. Alternatively, the integrand \( ω_1 Ψ^{(1/2)}(k) / ω_k \) can be written as the product of LP wave functions, \( ω_1 Φ^{(0)}(k) Φ^{(0)}(k) \), or as the potential-conjugate momentum product, \( Φ^{(−1/2)*}(k) Ψ^{(1/2)}(k) \), to give the invariant scalar product (11) as

\[ ⟨Φ1|Ψ1⟩ = \int d^3k Φ^{(−α)*}(k) Ψ^{(α)}(k). \tag{12} \]

In the Lorentz gauge there are longitudinal and scalar photons in addition to the observable transverse photons. Scalar and longitudinal photons can be dealt with by introducing an indefinite metric (12). However the Lorentz gauge was only needed to prove invariance and its further use here is not required.

In any specific reference frame it is possible to make a gauge transformation to the transverse (Coulomb) gauge. Eq. (12) then reduces to

\[ ⟨Φ1|Ψ1⟩ = \int d^3k Φ^{(−α)*}(k) • Ψ^{(α)}(k). \tag{13} \]

The conjugate momentum is \( Π^{(+) = −e_0E^{(+)}} \) for the minimal coupling Hamiltonian (⊥ denotes the transverse part), so the α = ±1/2 conjugate pair are the vector potential and the electric field (AE). Since the \( (ω_1)±α \) factors cancel and the dot product of like unit vectors is unity, Eq. (13) can also be written as

\[ ⟨Φ1|Ψ1⟩ = \sum_{σ = ±1} \int d^3kdσ \langle k | c_σ(k) \rangle \tag{14} \]

where the d's are the coefficients in the expansion of |Φ1⟩. This is just the QED scalar product.

For any operator, \( O \), describing an observable, \( O Ψ^{(α)}(k) \) must be in \( H \) and the eigenvalues of \( O \) must be real. This is obviously the case for the momentum and energy operators, \( ℏk \) and \( ℏω_k \). For the position operator, using (5),

\[ Ψ^{(α)}^∗(k) = (ω_k)^α e^{(α)}_σ(k) iV [c_σ(k,t) \exp (iσχ)] \tag{15} \]

since \( (ω_k)^α \) is an eigenvector of \( \tilde{r}^{(α,χ)} \) with eigenvalue zero. Thus (16) is in \( H \). Using the scalar product (11) the wave function is just \( Ψ^{(1/2)*}(k) \) and it can be proved as in (13) that \( \tilde{r}^{(1/2,χ)} \) is Hermitian. If (13) is used, it can be proved using (15) that \( ⟨Φ1|Ψ1⟩ = \langle Φ1|\tilde{r}^{(α,χ)}Ψ1⟩ \) which implies that \( \tilde{r}^{(0,χ)} \) is Hermitian and must have real eigenvalues and orthonormal eigenvectors. This follows the usual rules of operator algebra since \( D \) is unitary and \( iV \) is Hermitian. The α = ±1/2 basis is related to the α = 0 basis by \( \tilde{r}^{(α,χ)} = (ω_k)^α \tilde{r}^{(0,χ)} (ω_k)^−α \). This similarity transformation preserves the scalar product and hence expectation values and the reality of the position eigenvectors (6, 14). The wave functions \( Ψ^{(−1/2)}_σ \) and \( Φ^{(1/2)}_σ \) form a biorthonormal pair and the position operator satisfies \( \tilde{r}^{(−1/2,χ)} = \tilde{r}^{(1/2,χ)} \), so it can be called pseudo-Hermitian (14).

In real space, the most convenient form for the scalar product is not obvious. If (11) is transformed directly, the metric factor \( ω_k^−1 \) must be replaced by the inverse of the Hamiltonian operator, implying a nonlocal integrand \( d^3r \). Eq. (13) transformed to real space is

\[ ⟨Φ1|Ψ1⟩ = \int d^3r Φ^{(−α)*}(r,t) • Ψ^{(α)}(r,t), \tag{16} \]

as can be verified by substitution of (7) and integration over \( d^3r \) to give \( δ^3(k − k′) \) and then (13). The integrand of (15) is local, making it a useful form of the scalar product.

It can be seen by inspection of Eqs. (11) to (10) that the scalar product is unaffected by the change of metric from (11) to (12), and is invariant under the similarity transformations between the AE and LP forms of the wave function and under the unitary transformation between r-space and k-space. It is also invariant under the unitary transformations \( \exp (−iS_k χ) \) to \( χ \neq 0 \) bases. The AE form of the wave function is preferable in most applications, since the relationship of the LP wave function to matter source terms is nonlocal (15), but the choice is a matter of convenience.

IV. PHOTON NUMBER AMPLITUDE

The probability amplitude for a measured result is the amplitude for a transition from the photon state described by \( c_σ(k) \) to a final state that is an eigenvector of the operators representing the experiment. For a measurement of momentum \( ℏk \) and polarization \( e^{(χ)}_σ \) this final state is described by \( d_σ(k′) = δ_σ,σ_′ \exp (−iσχ) δ^3(k′ − k) \). Substitution in (14) gives the probability amplitude \( c_σ(k) \exp (iσχ) \) where the factor \( \exp (iσχ) \) rotates the polarization about \( k \) by −χ. The helicity is an invariant and a Lorentz transformation just changes \( χ \), so the probability to detect a photon with definite helicity and wave vector is invariant. For a measurement of the linear polarization \( e^{(χ)}_{Rj} \), given by (14), the momentum eigenvectors
are $d_\sigma (k') = \exp \left(-i\sigma \chi \right) \delta^3 \left(k' - k \right) / \sqrt{2}$ and $d_\sigma (k') = i \left(-1\right)^{j} \exp \left(-i\sigma \chi \right) \delta^3 \left(k' - k \right) / \sqrt{2}$ for $j = 1$ and 2 respectively, so (14) gives the probability amplitude to detect a photon with wave vector $k$ and this polarization direction as

$$c_{R1} (k, \chi) = \frac{1}{\sqrt{2}} \left[ c_1 (k) \exp (i\chi) + c_{-1} (k) \exp (-i\chi) \right],$$

(17)

$$c_{R2} (k, \chi) = \frac{i}{\sqrt{2}} \left[ c_1 (k) \exp (i\chi) - c_{-1} (k) \exp (-i\chi) \right].$$

If $\chi = 0$ the measured polarization directions are $\hat{\theta}$ and $\hat{\phi}$, and $c_{R1}$ and $c_{R2}$ are the amplitudes for transverse magnetic and transverse electric modes respectively [16]. Probability density is the absolute valued squared, so the magnetic and transverse electric modes respectively, so (14) gives the probability amplitude to detect a photon with definite helicity is

$$\left| \hat{\chi} \right|^2 = \frac{1}{2} \left[ \left| c_1 \right|^2 + \left| c_{-1} \right|^2 \right],$$

(18)

This is the probability amplitude for a position eigenvector if the phase $\chi \rightarrow \chi - \sigma \omega_k t$ in (11). The amplitude for a photon in state $c_\sigma (k)$ to make a transition to this state is given by substitution of (18) into (14) as

$$c_\sigma (r, t) = \int d^3 k \exp \left(i\sigma \chi + i k \cdot r - i\omega_k t \right) c_\sigma (k).$$

(19)

It equals the inverse Fourier transform of $c_\sigma (k) \exp (i\sigma \chi - i\omega_k t)$.

As a consistency check, consider a photon with polarization $e_\sigma (x)$ localized at $r'$ at time $t'$. The probability amplitude for this state is $c_\sigma (k) = d_\sigma (k, r', t')$ and (19) can be integrated to give the number amplitude $c_\sigma (r, t) = \delta_{\sigma, \sigma'} \delta^3 (r - r')$ if $t = t'$, that is if localization and measurement are seen as simultaneous. All $k$'s are included with equal weight in (18) and exact localization, which is limited by the Hegerfeldt theorem [17], is only possible because of interference effects between the converging and the diverging wave. Eq. (18) describes a situation where there is no physical detector at $r$, so absorption is followed immediately by re-emission.

V. CONCLUSION

The most widely accepted photon wave function in the current literature is the Glauber photodetection amplitude (18), $E_0^{(+)} (r, t) = \left\langle 0 \left| \hat{\mathbf{E}} (r, t) \right| \Psi \right\rangle$, where $\hat{\mathbf{E}} (r, t)$ is the Heisenberg picture (HP) electric field operator and $E_0^{(+)}$ is proportional to $\Psi^{1/2}$ given by (7). This can be combined with $\Psi^{-1/2}$ to give a scalar product with a local integrand and a complete description of photon quantum mechanics. Since the scalar product is invariant under unitary and similarity transformations and the prediction of the experimental results requires only the scalar product, the choice of wave function can be based on convenience. If desired, the remaining fields $D_0^{(+)} = e_0 E_0^{(+)} + P^{(+)}$, $H^{(+)}$ and $B^{(+)} = \mu_0 H^{(+)} + M^{(+)}$ can defined similarly [4, 10] where $|0\rangle$ is the matter-field ground state and $P$ and $M$ create and destroy matter excitations. Since the HP field operators satisfy classical dynamical equations, the equations satisfied by these positive frequency fields are identical in form to Maxwell’s equations and describe the dynamics of the 1-polariton state.

Evaluation of the photon number amplitude (19) is straightforward since it just requires integration of the scalar QED probability amplitude. Polarization unit vectors as a function of $k$ can be selected for convenience, for example, $\chi = -\phi$ gives $e^{(-\phi)} (k \mathbf{z}) = (\hat{x} + i\sigma \hat{y}) / \sqrt{2}$ for a paraxial beam propagating parallel to $\hat{z}$. Number amplitude itself has intrinsic physical significance. It is number amplitude that, after Schmidt diagonalization, was used as a photon wave function by Chan, Law and Eberly [21]. Also, number amplitude is proportional to $E_0^{(+)}$ to a good approximation. The positive frequency electric field of a localized photon state drops off as $r^{-7/2}$ where $r$ is the distance from the point of photon localization [20]. Thus photon number density, equal to the absolute square of (19), is an excellent approximation to the Glauber photodetection probability, proportional to $\left| E_0^{(+)} \right|^2$.

Number density may prove to be of fundamental importance. Cook pointed out that photon current density cannot be made precise within the Glauber theory, so that it fails to provide a complete description of photon transport [15]. Calculation of the probability density to detect a photon as the absolute square of the scalar product of the 1-photon wave function and a position eigenvector using (19) follows the usual rules of quantum mechanics. There is no such connection between Glauber photodetection theory and the basic rules of quantum mechanics. It is an ongoing goal of this author to thoroughly understand the relationship of photon number density to photon fields, energy density, the interpretation of photon counting experiments, and fundamental issues relating to photon localizability.

In summary, photon number amplitude in real space was calculated as the invariant scalar product of a localized state with definite polarization and the 1-photon wave function. It gives an excellent approximation to the Glauber photodetection probability, with the advantage that the orthonormal position eigenvectors lead to mutually exclusive probability densities and an integrated
probability of unity. When described in terms of this number amplitude, the localized basis states combine the orthonormality of the NW states with the Lorentz invariance of Philips’ localized states [8, 9]. The positive frequency vector potential and electric field provide a complete description of photon quantum mechanics, including interaction with matter. This should make it possible to test the relevance of the photon number concept to experiment.

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