Quantum theory of structured monochromatic light

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Abstract – Applications that envisage utilizing the orbital angular momentum (OAM) at the single photon level assume that the OAM degrees of freedom of the photons are orthogonal. To test this critical assumption, we quantize the beam-like solutions of the vector Helmholtz equation from first principles. We show that although the photon operators of a diffracting monochromatic beam do not in general satisfy the canonical commutation relations, implying that the photon states in Fock space are not orthogonal, the states are \textit{bona fide} eigenstates of the number and Hamiltonian operators. As a result, the representation for the photon operators presented in this work form a natural basis to study structured monochromatic light at the single photon level.

Introduction. – Electromagnetic beams are commonly used in atomic and condensed matter physics to probe the structure of matter by utilizing the polarization dependence of light-matter interactions. It is now well known that optical beams that are spatially structured in the transverse direction can carry a finite OAM along the direction of propagation of the beam in addition to the elementary polarization \cite{1,2}. It has been further demonstrated \cite{3,4} that the OAM is carried by the individual photons. This has fundamental implications, \textit{e.g.}, it was recently shown that a single photon can contribute additional quanta of angular momentum to a single trapped ion (on top of the spin angular momentum), thus resulting in a strong modification of the selection rules \cite{5}. Besides novel spectroscopic applications, the infinite dimensionality of the integer valued OAM degree of freedom can be exploited to increase the information coding density for quantum information applications as shown recently \cite{6}.

The control necessary for the implementation of various quantum protocols rely strongly on the ability to entangle the OAM of multiple photons \cite{7,8}. This requires a detailed enumeration of the \textit{orthogonal} degrees of freedom that the photons inherit from the additional spatial structure of the beam. In this paper, we derive from first principles the photon operators and the Fock states (defined as the eigenstates of both the number and the Hamiltonian operators) of the beam-like solutions of the Maxwell wave equation in free space. The states are conventionally labelled by a complete set of OAM (angular) and radial indices, and in our case also by the energy. We emphasize that the properties of the classical solutions carrying OAM are well known both in the paraxial and non-paraxial limit (see \cite{9,10}), in this paper we focus solely on the properties of the Fock states of these classical beam-like solutions.

To quantify the relationship between a classical beam of light and the photons corresponding to the beam modes (which we call the beam-photons), we draw on the general framework proposed by Titulaer and Glauber (TG) \cite{11} to describe photons in an arbitrary basis. They introduced a new set of photon operators, \(\hat{b}_j = \sum_k U_j(k)\hat{a}(k)\), in terms of the standard Dirac \cite{12,13} photon annihilation operators \(\hat{a}(k)\) in the plane-wave basis (the polarization index is suppressed for brevity); here, the information of the specific three-dimensional wave profile is arranged into the unitary transformation “matrix” \(U\) \cite{14}. When the transformation is applied on the positive-frequency part of the electric field operator, originally written in the plane-wave basis as \[ E^+(r,t) = i k \sum_k \mathcal{E}_k e^{i k \cdot r - i \omega_k t} \hat{a}(k), \] it reduces in the TG basis to \( E^+(r,t) = i \sum \mathcal{E}_j(r,t) \hat{b}_j, \) where \( \mathcal{E}_j(r,t) = \sum_k U_j^*(k) \mathcal{E}_k e^{i k \cdot r - i \omega_k t}. \) The key is that since \( \omega_k = c k \) and \( e_k \cdot k = 0, \) \( \mathcal{E}_j \) is guaranteed to solve Maxwell’s source free equations. Conversely, given a complete set of time-dependent classical solutions \( \mathcal{E}_j, \) the corresponding photon states in Fock space are fully specified by \( U_j \) and the photon number in each \( j \)-mode. Note that since \( U \) is unitary, the TG operators satisfy the canonical commutation relation \( \{ \hat{b}_j, \hat{b}_j^\dagger \} = \delta_{jj}. \) In this paper, we extend this analysis to the case of monochromatic beams.

Typical problems in optics utilize nearly monochromatic and strongly directional laser beams. In an ideal wave,
the spatial and temporal parts of the electric fields are separated as $E_j(r, t) = e^{-iωt}E_j(r, ω)$. Substituting this form into Maxwell’s wave equation gives the reduced vector Helmholtz equation [15] $(∇^2 + ω^2/c^2)E_j(r, ω) = 0$. Only solutions that simultaneously satisfy the transversality condition $∇·E_j(r, ω) = 0$ solve the free-field Maxwell’s equations. Hence the problem of identifying the photons of a monochromatic wave reduces to quantizing the transverse solutions of the vector Helmholtz equation.

A well-known family of solutions are the Gaussian beams, which includes the Hermite and the Laguerre-Gaussian (LG) beams. These solutions can be systematically obtained in a series expansion in powers of the diffraction angle; the lowest-order terms in the series were shown by Lax et al. [16] to correspond to the well-known paraxial approximation [15]. A quantum theory must take into account all the terms of the series. Previous works attempted to quantize the approximate solution found in the paraxial limit [17–19]. Exact wave-packet schemes; the wave-packets are, however, necessarily non-quantization [20] can avoid such incomplete quantization found in the paraxial limit [17–19]. Exact wave-packet evanescent modes are explicitly suppressed as follows:

$$d_{λs}(q, ω) = \Theta(ω - cq)\hat{a}_{λs}(q, ω), \quad (1a)$$
$$\hat{a}_{λs}(q, ω) = \int_0^{∞} dq_\zeta √J(q, \zeta)\hat{a}_{λ}(q, s\zeta)δ(ω - ω_k). \quad (1b)$$

The operators $\hat{a}_{λ}(q, s\zeta)$ are the standard photon operators in the plane-wave basis; they satisfy the canonical relation

$$[\hat{a}_{λ}(q, s\zeta), \hat{a}_{λ}^I(q', s'\zeta')] = δ_{λ, λ'}δ_{s, s'}δ(q - q')δ(ζ - ζ'). \quad (2)$$

Equation (1b) is an integral extension of the proposals put forward by Visser [22] and Aiello et al. [21]. The advantage of the extended representation is that the inverse of (1) can be used to express the plane-wave operators directly in terms of the monochromatic free-field operators as follows:

$$\hat{a}_{λ}(q, s\zeta) = √J(q, \zeta)\int_0^{∞} dω \hat{d}_{λs}(q, ω)δ(ω - ω_k). \quad (3)$$

Here, $J(q, \zeta) = dω/dζ = cζ/√ζ^2 + c^2q^2$ is the Jacobian of the transformation $ω = c√ζ^2 + c^2q^2$; it is essential to preserve the canonical commutation relations of the AS operators (see eq. (4) below). When $ω ≥ cq$, the argument of the $δ$-function in (1b) is real and can be rewritten using the identity $δ(ω - ω_k) = J^{−1}(q, \zeta)δ(ζ - √ω^2/c^2 - q^2)$, which is well defined on the real axis $ζ = [0, ∞)$; the presence of the $Θ$-function in (1a) gives $\hat{d}_{λs}(q, ω) = \hat{a}_{λs}(q, ω)$. On the other hand, when $ω < cq$, the actual values of $\hat{a}_{λs}(q, ω)$ are irrelevant since $\hat{d}_{λs}(q, ω)$ vanishes by construction. The evanescent regime $ω < cq$ is thereby explicitly suppressed.

Substituting the integral representation (1) into eq. (2) gives the new commutation relation

$$[\hat{d}_{λs}(q, ω), \hat{d}_{λ' s'}^I(q', ω')] = δ_{λ, λ'}δ_{s, s'}δ(q - q')δ(ω - ω')Θ(ω - cq). \quad (4)$$

Note that the $Θ$-factor appears explicitly above. Finally, the vacuum, defined in the plane-wave basis as $\hat{a}_{λ}(k_s)|0⟩ = 0, ∀k_s$, is consistently defined using
The total number, \( \hat{N} \) appropriately chosen unitary transformation matrix that a given family of beams can be characterized by an beam-like solutions of the vector Helmholtz equation. The transformation \( U \), independent. (The formalism may be extended with very little effort to include non-trivial vector beams that are formed by using non-separable combinations of the spatial and polarization modes [25].) Formally, eq. (12) is inverted using the completeness relation \( \sum_j U_j^*(q) U_j(q') = \delta(q - q') \), so that

\[
\hat{d}_{\lambda s,j}(q, \omega) = \sum_j U_j^*(q) \hat{b}_{\lambda s,j}(\omega).
\]

Unlike the TG operators of the time-dependent wave solutions of Maxwell’s equations, we show below that restricting the phase space to the homogenous solutions of the Helmholtz equation imposes non-trivial constraints on the commutation relations and the vacuum. The first requirement for the vacuum given in eq. (5a) is satisfied by (12) by simply setting

\[
b_{\lambda s,j}(0) = 0, \quad \forall \omega.
\]

Equation (13), on the other hand, leads to the following constraint on the vacuum when the second condition (5b) that annihilates the evanescent states is enforced

\[
\sum_j U_j(q) \hat{b}_{\lambda s,j}^\dagger(\omega) = 0, \quad \forall \omega < c q.
\]

This linear dependence is reflected in the non-canonical form of the commutation relation obtained by substituting (12) into the commutator (4); it reads as follows:

\[
[\hat{b}_{\lambda s,j}(\omega), \hat{b}_{\lambda s',j'}^\dagger(\omega')] = \delta_{\lambda \lambda'} \delta_{s s'} \delta(\omega - \omega') F_{j,j'}(\omega),
\]

where the elements

\[
F_{j,j'}(\omega) = \sum_q U_j(q) U_{j'}^*(q) \Theta(\omega - \omega).
\]

Note that \( F \) is an Hermitian projection matrix, i.e., \( F^\dagger(\omega) = F(\omega) \) and \( F^2(\omega) = F(\omega) \). It is therefore singular and non-invertible with eigenvalues 1 and 0 for any finite \( \omega \). The commutators therefore cannot be brought into the canonical form by simply rescaling the photon operators. Hence, although the beam-photon states \( \hat{b}_{\lambda s,j}^\dagger(0) \) are complete because \( U \) is unitary, they are not orthonormal. Nevertheless, we now demonstrate that the states formed by the action of \( \hat{b}_{\lambda s,j}^\dagger(0) \) on \( |0\rangle \) are bona fide eigenstates of the number operator \( \hat{N} \) and therefore from (8) have a well-defined energy equal to \( h\omega \) per photon.

To this end, we first substitute the photon operator (13) into eq. (9) for \( \hat{N}(\omega) \) and use the orthogonality relation \( \sum_q U_j(q) U_{j'}^*(q) = \delta_{j,j'} \) to get

\[
\hat{N}(\omega) = \sum_{\lambda s,j} \hat{b}_{\lambda s,j}^\dagger(\omega) \hat{b}_{\lambda s,j}(\omega).
\]

It follows from the commutation relation (16) that

\[
[\hat{N}, \hat{b}_{\lambda s,j}^\dagger(\omega)] = \delta(\omega - \omega') \sum_{j'} b_{\lambda s,j}^\dagger(\omega) F_{j,j'}(\omega),
\]

\[
[\hat{N}, \hat{b}_{\lambda s,j}(\omega)] = \sum_{j'} \hat{b}_{\lambda s,j}^\dagger(\omega) F_{j,j'}(\omega).
\]
Here, \( \hat{N} \) as in (11) is the total number operator. Next, we decompose \( F \), defined in (17), as

\[
\begin{align*}
F_{j',j}(\omega) &= \delta_{j',j} - \Delta F_{j',j}(\omega), \\
\Delta F_{j',j}(\omega) &= \sum_{q} U_{j'}(q)U_{j}(q)\Theta(\omega - cq),
\end{align*}
\]

which simply follows by writing \( \Theta(\omega - cq) = 1 - \Theta(cq - \omega) \). It is easily shown that the second term in the decomposition in eq. (15) annihilates the vacuum [26]

\[
\sum_{j'} \hat{b}_{l,s,j'}^{\dagger}(\omega)\Delta F_{j',j}(\omega)|0\rangle = 0
\]

by rewriting the left-hand side using eq. (21b) as

\[
\sum_{q} U_{j'}(q) \left[ \Theta(\omega - c) \sum_{j'} U_{j}(q)\hat{b}_{l,s,j'}^{\dagger}(\omega)|0\rangle \right]
\]

and noting that the sum in the brackets vanishes when the condition in eq. (15) on the vacuum is applied. It follows from eqs. (19)–(22) that

\[
\begin{align*}
\hat{N}(\omega')\hat{b}_{l,s,j}(\omega)|0\rangle &= \delta(\omega' - \omega)\hat{b}_{l,s,j}(\omega)|0\rangle, \\
\hat{N}\hat{b}_{l,s,j}^{\dagger}(\omega)|0\rangle &= \hat{b}_{l,s,j}(\omega)|0\rangle.
\end{align*}
\]

Equations (24) and (25) combined with the Hamiltonian (8) allows us to conclude that the state \( \hat{b}_{l,s,j}(\omega)|0\rangle \) corresponds to exactly one photon with energy \( h\omega \). Hence, all the physical photon states in Fock space are generated by the successive action of the \( \hat{b}_{l}^{\dagger} \) operators on the vacuum. Note that all information of the unphysical evanescent regime is contained in the definition of the \( \hat{b}_{l}^{\dagger} \) operators on the vacuum; they do not appear in the physical states in the Fock space. This is our main result in this work. (Recent works [27,28] have approached the problem of dealing with the unphysical evanescent states using a field theory formulation.)

We emphasize, however, that the photon states, which are bona fide eigenstates of the number and the Hamiltonian operators, do not in general form an orthonormal set in the mode indices \( j \); the overlap of the single photon states is obtained from the commutation relation (16) as

\[
(0|\hat{b}_{l,s,j}^{\dagger}(\omega)\hat{b}_{l',s',j'}^{\dagger}(\omega')|0\rangle = \delta_{l,l'}\delta_{s,s'}\delta(\omega - \omega')F_{j,j'}(\omega).
\]

It is our understanding that earlier works have forced canonical commutation relations on to the beam-photon operators in the paraxial limit [17–19]; this assumption is not strictly valid as shown in eq. (26).

**Beam-photon operators – Integer OAM case.** We now focus on the special case of Gaussian beams that carry a finite integer OAM. Since the frequency \( \omega = c\sqrt{q^{2} + \zeta_{j}^{2}} \) is independent of the polar angle, \( \theta_{q} \), a beam-like solution with a finite OAM can be constructed by summing coherently over the angle weighted by the element [20,29] \( U_{l}(\theta_{q}) = (2\pi)^{-\frac{1}{2}}e^{-i\theta_{q}} \). This generates a Bessel beam of integer order \( l \) when \( q \) is fixed. Note that Bessel beams are non-diffracting [30,31].

Diffracting monochromatic beams with a finite OAM that are confined in the transverse direction can be constructed by integrating over the magnitude \( q \) with an appropriately chosen weight function \( V(q) \). To this end, we choose the \( U \) matrix to have the general form:

\[
U_{ml}(q) = \frac{1}{\pi}e^{-il\theta_{q}}V_{ml}(q),
\]

where \( V \) is normalized to ensure unitarity as follows:

\[
\int_{-\infty}^{\infty} dq q^{2}V_{ml}(q)V_{m'l'}(q) = 2\pi\delta_{m,m'}.
\]

The mode indices \( m \) and \( l \), collectively referred to as \( j = \{ml\} \), denote the radial and azimuthal indices, respectively. The angular dependence appears as a phase factor, while the overlap of the single photon \( q \) satisfies \( q \ll \omega/c \). This relation introduces a single length scale, \( w_{0} \), commonly called the beam waist. We incorporate the waist size by writing \( V(q) \) in terms of dimensionless variables \( \hat{V} \) and \( w_{0}q \) as

\[
V_{ml}(q) = w_{0}V_{ml}(w_{0}q).
\]

In a typical example of a beam, e.g., the Gaussian beam, \( V_{ml}(w_{0}q) \) falls rapidly as \( q^{2}w_{0}^{-2} \) when \( w_{0}q \gg 1 \). Clearly, when \( \omega \gg c/w_{0} \), the relevant \( q \)’s satisfy \( q \ll \omega/c \).

To formalize these different regimes, it is convenient to define the dimensionless frequency parameter

\[
f_{\omega} = \frac{\omega}{w_{0}c}
\]

which is nothing but a measure of the diffraction angle. Physically, \( f_{\omega} \ll 1 \) corresponds to a weakly diffracting beam. Lax et al. [16] successfully developed a series solution of the vector Helmholtz equation in powers of \( f_{\omega} \); they showed that keeping only the lowest power in \( f_{\omega} \), valid when \( f_{\omega} \ll 1 \), reproduces the paraxial limit.

A similar analysis is carried out here for the dependence of \( F \) on \( f_{\omega} \). Substituting eqs. (27) and (28) into eq. (17), the overlap matrix reduces to

\[
F_{ml,m'l'}(f_{\omega}) = \delta_{l,l'}\int_{0}^{\infty} \frac{kdk}{2\pi} V_{m}(k)V_{m'}(k)\Theta(1/f_{\omega} - k).
\]

Here, \( \kappa = w_{0}q \) and the argument of the \( \Theta \)-function is made dimensionless by rewriting it as \( \Theta(\omega - c\kappa) = \Theta(w_{0}\omega/c - w_{0}q) \). Since \( F \) is diagonal in the \( l \) index, it is convenient to separate \( F \) into two parts as (cf. eq. (21))

\[
\begin{align*}
F_{ml,m'l'}(f_{\omega}) &= \delta_{l,l'}\int_{0}^{\infty} \frac{kdk}{2\pi} V_{m}(k)V_{m'}(k)\Theta(1/f_{\omega} - k). \\
\Delta F_{ml,m'l'}(f_{\omega}) &= \int_{1/f_{\omega}}^{\infty} \frac{kdk}{2\pi} V_{m}(k)V_{m'}(k).
\end{align*}
\]

Our key observation is that in the case of a Gaussian function that falls off as \( V(k) \sim e^{-\kappa^{2}} \) for \( \kappa \gg 1 \), \( \Delta F \)
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in (31b) vanishes faster than any power of $f_\omega$ in the
limit $f_\omega \ll 1$; this is readily seen by taking the deriva-
tive $\partial f_\omega \Delta F \sim |v(1/f_\omega)|^2 \sim e^{-1/f_\omega^2}$. The same is true
for all higher-order derivatives as well. Thus, for beams
with a Gaussian profile, the expansion takes the form
$F_{m,n,m'} = \delta_{m,n-m'} + O(e^{-1/f_\omega^2})$ in the limit $f_\omega \ll 1$.

The fact that the asymptotic series for $F(f_\omega)$ is not a
polynomial series is our main result in this section.

We caution here that since $F$ is singular and non-
invertible for any finite $\omega$, the $O(e^{-1/f_\omega^2})$ can never be
ignored even for arbitrarily small $f_\omega$ (paraxial limit), and
become increasingly more relevant when the beams are
tightly focussed. This is a rigorous result which neces-
sarily emerges when the evanescent regime is suppressed
in frequency space. We emphasize that it was already
pointed out by TG [11] that the classical solutions (the
mode functions) do not in general form an orthonormal
basis. However, for the purposes of the current study,
we are able to use the basis.

Quantizing the vector Helmholtz equation. – For
completeness, the relationship between the solutions of the
vector Helmholtz equation and the beam-photon operators
developed above are made explicit.

As is well known, Maxwell’s equations for the electric
and magnetic fields separate into independent longitudinal
and transverse components in the Coulomb gauge. In
vacuum, the true dynamical degrees of freedom are ex-
posed by expressing the fields in terms of the transverse
vector potential $A_\perp$, which satisfies the wave equation
$\Box A_\perp \equiv \left(\partial^2 - c^2 \nabla^2\right) A_\perp = 0$. The wave solutions are
quantized by raising $A_\perp$ to the operator level in the stan-
dard way [13]. The positive-frequency part takes the form

$$A_\perp^{(+)}(r,t) = \sum_{\lambda = 1,2} \int \frac{d^3 k}{2\pi} \sqrt{-\epsilon A_k} \hat{a}_\lambda(k) e^{ik \cdot r - i\omega t}.$$  \hspace{1cm} (32)

For dimensional reasons, we deviate from standard nota-
tion by not including the $\sqrt{\epsilon}/(2\pi)$ factor in the defini-
tion of $A_k$, which is defined here as
$A_{\lambda k} = \sqrt{\epsilon k} / \omega_k$ in cgs units.

In eq. (32), $\hat{a}_\lambda(k)$ is the photon annihilation oper-
ator; the labels $\lambda = 1,2$ and $2$ stand for the two stand
for the two photon polarizations. The Coulomb gauge is en-
forced by demanding
that the polarization vectors satisfy $k \cdot e_\lambda(k) = 0$. The
two orthogonal unit vectors may always be chosen to sat-
ify the standard conventions: $e_1(k) \times e_2(k) = \hat{k}$, with
$e_1(-k) = -e_1(k)$ and $e_2(-k) = e_2(k)$. An explicit rep-
resentation is given as

$$e_1(k) = \frac{\hat{n} \times k}{|\hat{n} \times k|} \quad \text{and} \quad e_2(k) = \hat{k} \times e_1(k).$$  \hspace{1cm} (33)

For now, $\hat{n}$ is an arbitrary fixed unit vector and $\hat{k}$ is the
unit vector in the direction of $k$.

Lax et al.’s analysis [16] of the wave equation for the
electric field is easily extended to the vector potential in
the Coulomb gauge to show that the transversality con-
dition prevents a plane-polarized field from being globally
defined in a beam. For this reason, one usually works,
following Davis [32], in the Lorentz gauge where $\nabla \cdot A_\perp$ is finite. Nevertheless, there are clear advantages to working
in the Coulomb gauge [13], e.g., although the equations in
the Coulomb gauge are not manifestly covariant, $A_\perp$
itself is gauge invariant.

The limitations of the Coulomb gauge are easily over-
come by introducing the Hertz magnetic potential $A_\perp$
$F = \nabla \times Z$. The more general Whittaker potentials,
including both the $E$- and $H$-type potentials, have been
realized to be an economical parameterization to analyze
both the classical [34] and the quantum [20] properties of
beams. For our purpose, it is sufficient to recognize that
it is the magnetic potential that best describes strongly
plane-polarized beams in the paraxial limit [34].

To see this, it is straightforward to verify by inspecting
eqs. (32) and (33) that the $Z_{\lambda}$’s satisfying $A_\perp^{(+)} = \nabla \times Z_{\lambda}^{(+)}$ can be written as (up to a gradient term)

$$Z_1^{(+)} = i \int \frac{d^3 k}{2\pi} \sqrt{-c A_k} \hat{a}_1(k) \frac{\hat{n}}{|\hat{n} \times k|} e^{i k \cdot r - i\omega t}, \hspace{1cm} (34a)$$

$$Z_2^{(+)} = i \int \frac{d^3 k}{2\pi} \sqrt{-c A_k} \hat{a}_2(k) \frac{\hat{n} \times k}{|\hat{n} \times k|} e^{i k \cdot r - i\omega t}. \hspace{1cm} (34b)$$

Note that both $Z_1$ and $Z_2$ satisfy the wave equation. $Z_1$
is special in that its polarization does not vary with $k$, i.e., it is globally plane-polarized along the constant vector
$\hat{n}$. Also note that the $Z_{\lambda}$’s are free from the auxiliary
transversality conditions; in particular, $\nabla \cdot Z_1 \neq 0$.

For concreteness, we fix $\hat{n}$ to say, $\hat{y}$ and analyze $e_1$
(see (33)) in the paraxial limit: $e_1(k) = (\hat{y} \times k) / |\hat{y} \times k| = (k_x, 0, -k_z) / \sqrt{k_x^2 + q_y^2} \approx \hat{x}$ in the limit $k_2 \gg q_y$. Hence, choosing $\hat{n} = \hat{y}$ describes a strongly polarized $A_{1,\perp}$ field
along $\hat{e}_1 \approx \hat{x}$. Note that although $Z_1$ is globally plane-
polarized, the Coulomb gauge condition $\nabla \cdot A_\perp = 0$ neces-
sarily generates a small longitudinal component [16] for
$A_\perp$ proportional to $(q_y/k_x) \hat{z} \sim f_\perp \hat{z}$. The potential $Z_1$
is therefore ideally suited to study plane-polarized beam
solutions, which is the only case that we analyze in this
work. Without loss of generality, we choose $\hat{n} = \hat{y}$ from
here on. It follows from eq. (34a) that $Z_1$ can be expressed
in terms of a scalar operator as

$$Z_1^{(+)}(r,t) = i \sum_s \hat{Z}_{1s}(r,t) \hat{y}, \hspace{1cm} (35)$$

$$\hat{Z}_{1s}(r,t) = \int \frac{d^3 k_s}{2\pi} \sqrt{-c A_k} \hat{a}_1(k_s) e^{i k_s \cdot r - i\omega t}, \hspace{1cm} (36)$$

where both the left and right moving ($s = \pm$) operators
$\hat{Z}_{1s}$ satisfy the scalar wave equation $\Box \hat{Z}_{1s} = 0$ with no
additional auxiliary conditions. This reduction to the un-
constrained scalar wave equation is the main advantage of
the magnetic Hertz potential representation.

To find an expression for $\hat{Z}_{1s}(r,t)$ in the AS represen-
tation, we first rewrite the photon operators $\hat{a}_1(k_s)$ in
$\hat{Z}_{1s}(r,t)$ in terms of the AS operators $\hat{d}_{1s}(q,\omega)$ (setting
\[ \hat{Z}_{1s}(r, t) = \sum_{m,l} \int_0^\infty \text{d}\omega \mathcal{A}_\omega e^{-i\omega(t - kz/c)} Z_{1s,ml}(r, \omega) \hat{b}_{1s,ml}(\omega), \]  
\[ Z_{1s,ml}(r, \omega) = f_\omega \int_0^{1/f_\omega} \frac{d^2\kappa}{(2\pi)^2} e^{ik\frac{\phi_0}{\omega}} \exp \left[ is\left(\frac{z}{z_R}\right)\frac{1}{2\kappa} \left(1 - f_\omega^2 \kappa^2\sin^2\theta_m\right)^{1/2} \right] e^{i\theta_m} \psi_{ml}(\kappa). \]  
\[ (37a) \]

\[ (37b) \]

\[ \lambda = 1 \) using the inverse relation (3); this is followed by rewriting \[ \hat{d}_{1s}(q, \omega) \) in terms of the beam-operators \[ \hat{b}_{1s,j}(\omega) \) using eq. (13). After a few elementary manipulations, we obtain for \[ \hat{Z}_{1s}(r, t) \) the expression derived in eqs. (37):

\[ \text{see eqs. (37a) and (37b) above} \]

The Rayleigh length, defined here as \[ z_R = w_0/f_\omega, \) corresponds to the length scale over which the beam stays well collimated along \( z \). The wave vector is specified as \( \kappa_\omega = \kappa \cos \theta_m, \) where the dimensionless integration variable \( \kappa = w_0 q. \) The prefactor \( \mathcal{A}_\omega = \sqrt{\hbar c/\omega}. \)

To appreciate the integral solution in eq. (37b), we substitute eq. (37a) in the wave equation \[ \square Z_{1s} = 0 \) and obtain the reduced scalar Helmholtz equation [16] written entirely in terms of the dimensionless variables, \( \tilde{\rho} = \rho/w_0 \) and \( \tilde{z} = z/z_R, \) as

\[ \left[ \nabla_{\tilde{\rho}}^2 + 2i\tilde{\rho}\partial_{\tilde{z}} + f_\omega^2 \partial_{\tilde{z}}^2 \right] Z_{1s,ml}(r, \omega) = 0. \]  
\[ (38) \]

The function \( Z_{1s,ml}(r, \omega) \) in (37b) is therefore the exact monochromatic beam solution of (38) for any \( f_\omega \) once the form of \( \tilde{V}_{ml} \) is specified. Note that the additional factor \( (1 - f_\omega^2 \kappa^2)^{1/4} \) in eq. (37b) is absent in the commonly proposed expressions for the non-paraxial extension of the classical modes (see, e.g., refs. [2,35] for the specific case of the LG beams) – since this factor originates from the Jacobian which was introduced to ensure the normalization of the photon number, it cannot be determined classically by solving the wave equation (38).

For completeness, we end by studying the inverse problem of determining \( \tilde{V}_{ml} \) corresponding to an arbitrary solution \( \hat{Z}_{1s,ml}(r, \omega) \) of the wave equation; this step is useful to delineate the quantum degrees of freedom of a given classically generated OAM beam. We show that due to the simplified dependence of the Hertz potential on the parameter \( f_\omega, \) the form of \( \tilde{V}_{ml} \) can be conveniently derived from the paraxial limit of \( Z_{1s,ml}. \) To this end, we observe that the leading behavior of \( Z_{1s,ml} \) in (37b) is of \( \mathcal{O}(f_\omega) \), which can be made explicit by writing

\[ Z_{1s,ml}(r, \omega) \equiv f_\omega \tilde{Z}_{1s,ml}(\tilde{\rho}, \tilde{z}, f_\omega), \]  
\[ (39) \]

where \( \tilde{Z}_{1s,ml} \) corresponds to the integral in (37b). (Note that the leading behavior of \( \mathcal{A}_\omega \sim \mathcal{O}(f_\omega^0) \).) Since the paraxial approximation corresponds to keeping terms [16] up to \( \mathcal{O}(f_\omega) \), the paraxial limit is straightforwardly obtained by setting \( f_\omega = 0 \) (keeping \( z_R \) fixed) in \( \tilde{Z}_{1s,ml}. \)

Denoting the limit as \( \tilde{Z}_{1s,ml}^{(0)}(\tilde{\rho}, \tilde{z}) \equiv \tilde{Z}_{1s,ml}(\tilde{\rho}, \tilde{z}, 0), \) we directly arrive at the minimal Fresnel representation

\[ \tilde{Z}_{1s,ml}^{(0)}(\tilde{\rho}, \tilde{z}) = \int \frac{d^2\kappa}{(2\pi)^2} e^{ik\tilde{\rho}} e^{i\theta_m} \psi_{ml}(\kappa) e^{-\frac{i}{2}\kappa^2 \tilde{z}^2}. \]  
\[ (40) \]

Following the standard interpretation, we see that \( \tilde{Z}_{1s,ml}^{(0)}(\tilde{\rho}, \tilde{z}) \) at a finite \( \tilde{z} \) is got by using the Fresnel propagator [15], \( e^{-\frac{i}{2}\kappa^2 \tilde{z}^2} \), to propagate the transverse two-dimensional Fourier transform, \( F.T.[\tilde{Z}_{1s,ml}^{(0)}(\tilde{\rho}, 0)] \), from the object plane located at \( \tilde{z} = 0 \) to the image plane located at \( \tilde{z} \). Hence, \( \tilde{V}_{ml} \) is the Fourier transform of the paraxial solution of the magnetic Hertz potential at the object plane

\[ e^{-i\theta_m} \tilde{V}_{ml}(\kappa) = F.T.[\tilde{Z}_{1s,ml}^{(0)}(\tilde{\rho}, 0)]^*. \]  
\[ (41) \]

This is a general result that can be used to determine \( \tilde{U}_{ml} \) given information on the object plane. The \( U \) thus obtained can be substituted in eq. (12) to derive the corresponding beam-photon operators.

As an example, we derive an explicit expression for the beam-operators of the LG beam below. LG beams are defined on the optical plane by the family of eigenstates of a two-dimensional simple harmonic oscillator. (We set \( h = 1 \), the mass to unity and the oscillator frequency as \( w_0^2. \) ) In cylindrical coordinates, the normalized eigenstates, \( \psi_{ml}(\tilde{\rho}) = e^{i\theta_m} \psi_{ml}(\tilde{\rho}), \) have well-defined angular momentum \( l \) with the radial function defined as \( \psi_{ml}(\rho) = C_{ml}^l|\tilde{\rho}|^l e^{-\frac{i}{2}\kappa^2 L_{ml}^l(\tilde{\rho}^2)}. \) Here, \( l = 0, \pm1, \ldots \) and the radial index \( m = 0, 1, \ldots \); the polar angle \( \theta \) in real space is defined as \( \tilde{\rho} = \rho(\cos \theta, \sin \theta); \) the special functions \( L_{ml}^l \) are the associated Laguerre polynomials; the normalization constant equals \( C_{ml}^l = \sqrt{\pi/(m + l)!}. \)

The Fourier transform \( \Phi_{ml}(\kappa) = \int d^2\tilde{\rho} e^{ik\tilde{\rho}} \tilde{\psi}_{ml}(\tilde{\rho}) \) is well known [36], it reads as

\[ \Phi_{ml}(\kappa) = 2\pi e^{i\phi_{ml}} e^{-i\kappa \phi_{ml}} \phi_{ml}^*(\kappa), \]  
\[ (42a) \]

\[ \phi_{ml}^*(\kappa) = C_{ml}^l|\kappa|^l e^{-\frac{i}{2}\kappa^2 L_{ml}^l(\kappa^2)}, \]  
\[ (42b) \]

where the additional phase \( e^{i\phi_{ml}} = |\text{sign}(l)| e^{-i\pi m/2}. \) Comparing the Fourier transform (42) with the definition of \( \tilde{V}_{ml} \) in eq. (41), we get for the LG beams

\[ \tilde{V}_{ml}^{\ell\ell}(k) = 2\pi e^{i\phi_{ml}} \phi_{ml}^*(\kappa). \]  
\[ (43) \]

It can be shown using standard integrals that when \( \tilde{V}_{ml}^{\ell\ell} \) is substituted back into eq. (40) it generates the LG beam solution in the paraxial limit [16].
The AS operators, $\hat{d}_{\lambda}(q,\omega)$, may be further expanded in the plane-wave basis using eq. (1). We emphasize that the form of $\hat{b}_{1,m}^{\text{LG}}(\omega)$ is valid to all orders in $f_\lambda$; no approximations were made at the operator level when going to the paraxial limit.

**Conclusion.** – In this work, we investigate how the conserved quantities of a classical monochromatic electromagnetic beam are distributed amongst the photons that make up the beam, which we call the beam-photons. We demonstrate rigorously to all orders beyond the paraxial limit that there exists beam-photon operators, $\hat{b}_\lambda^{\text{LG}}(\omega)$, that create single photons with well-defined energy $\hbar \omega$. In the special case of Gaussian beams with a finite orbital angular momentum, or OAM, the Fock states are shown to be orthogonal in the azimuthal (angular) index, $l$, but they are non-orthogonal in the radial index, $m$. Importantly, we show that they are not orthogonal even in the paraxial limit. (The general form of the overlap function $F_{\lambda j}(\omega)$ is derived in eq. (26); here $j \in \{m\}$.) The overlap of the single photon states, or in other words, the non-orthogonality of the various transverse channels clearly limits the density of information that can be coded using the integer valued OAM degree of freedom in quantum information processing applications. Furthermore, in spectroscopic applications involving absorption and emission of single photons in atomic and solid state systems the cross-section will be suppressed by the overlap function. The quantitative effect of the overlap on physical processes needs further study that is not pursued in this paper.

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