Angular momentum and the geometrical gauge of localized photon states

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Localized photon states have non-zero angular momentum that varies with the non-unique choice of a transverse basis and is changed by gauge transformations of the geometric vector potential **a**. The position operator must depend on the choice of gauge, but a complete gauge transformation of a physically distinct state has no observable effects. The potential **a** has a Dirac string singularity that is related to an optical vortex of the electric field.

The orbital angular momentum of optical beams has recently received considerable attention [1, 2]. The spin and orbital angular momentum of a photon, as traditionally defined, cannot be cleanly separated, although states can be constructed that have well defined total angular momentum per photon in any specified direction. Without loss of generality we choose this to be the z-direction, and describe the total, spin and orbital angular momentum along this direction with quantum numbers j_z, s_z and l_z respectively. For example, polarized paraxial Bessel beams for which $j_z = 0$ are superpositions of two beams: one with $l_z = 1$ and $s_z = -1$, and one with $l_z = -1$ and $s_z = 1$ [3]. In this letter we discuss the angular momentum of photons localized in all three spatial dimensions. We show that while geometric gauge transformations can change the angular momenta of the basis states and rotate and rescale associated singularities and optical vortices, these features can never be completely eliminated.

In spite of an extensive literature on nonlocalizability of photons, photon states with arbitrarily fast asymptotic power-law [4] or exponential [5] falloff of energy density have recently been constructed. What has not been analyzed in the past is the deviation of these localized states from spherical symmetry and their consequent angular momentum content. It has been argued that a converging or diverging one-photon state can never be localized exactly because of mathematical limitations imposed by quantum field theory and, for example, the Paley-Wiener theorem [5]. However, a momentum-space basis of exactly localized states such as

$$\underline{\Psi}_{\mathbf{r}',\lambda}(\mathbf{p}) = N p^{\alpha} e^{-i\mathbf{r}'\cdot\mathbf{p}} \underline{e}_{\mathbf{p}\lambda} \ . \tag{1}$$

can be constructed [6] with contributions from all $\mathbf{p}$, describing a photon that may be incoming or outgoing relative to the spacetime point of localization. This orthogonal basis, while probably not realizable as physical photon states, is convenient for calculation of the probability amplitude for photon position and, as we shall show here, for the specification of transverse bases in general.

The basis states are eigenstates of a photon position operator with commuting components. In spite of a long history arguing against the existence of such an operator, we found not one, but a whole family of such position operators related by geometric gauge transformations, with the gauge potential defining the rotation of the transverse basis about $\mathbf{p}$. Details, together with explanations where arguments against their existence fail, are given in Ref. [6]. We show here that the gauge choice determines the angular momenta of the basis.

Massless particles possess only two spin states, which can be taken as eigenstates of the helicity operator $\underline{\mathbf{S}}\cdot\hat{\mathbf{p}}$. The resulting coupling of spin and momentum means that the position operator, which generates translations in momentum space, generally does not commute with $\underline{\mathbf{S}}$. For particles of spin 1, the components of $\underline{\mathbf{S}}$ are 3×3 matrices that generate rotations of the field vectors, and the position operator is therefore not simply $i\hbar\nabla$, where ∇ is the gradient operator in $\mathbf{p}$-space, but rather a 3×3 matrix. One such operator is the Pryce photon position operator [6, 7], known since 1948,

$$\underline{\mathbf{r}}_P = \hbar\left(i\underline{I}p^{\alpha}\nabla p^{-\alpha} + \frac{1}{p^2}\mathbf{p}\times\underline{\mathbf{S}}\right), \tag{2}$$

where $\alpha = \frac{1}{2}$ for fields and $-\frac{1}{2}$ for the vector potential, $\underline{\mathbf{S}}$ is the dimensionless spin-1 operator, and $\underline{I}$ is the unit matrix. In our notation, underscore denotes a matrix and bold denotes a 3-component vector. Thus, the bold face signifies that $\underline{\mathbf{r}}_P$ has x, y and z components, while its underscore means that each of these components is a 3×3 array that operates on the vector field of a first-quantized photon state, expressed as a 3×1 array. This notation is carefully maintained to prevent confusion between these two vector roles.

The Cartesian components of $\underline{\mathbf{r}}_P$ do not commute and thus cannot define a basis of localized states. A family of position operators that do have commuting components is

$$\underline{\mathbf{r}}^{(\chi)} = i\hbar\underline{D}p^{\alpha}\nabla p^{-\alpha}\underline{D}^{-1} \tag{3}$$

where $\underline{D} = e^{-i\underline{S_3}\phi}e^{-i\underline{S_2}\theta}e^{-i\underline{S_3}\chi}$ is the rotation matrix with Euler angles ϕ, θ, χ that rotates the lab z axis into $\hat{\mathbf{p}}$. The role of the matrices $\underline{D}$ and $\underline{D}^{-1}$ is to decouple the spin and momentum, allowing the gradient operator to operate on the momentum dependence of the field while maintaining the transversality condition. A straightforward calculation gives [6]

$$\underline{\mathbf{r}}^{(\chi)} = \underline{\mathbf{r}}_P - \hbar\mathbf{a}^{(\chi)}\ \widehat{\mathbf{p}} \cdot \underline{\mathbf{S}} \tag{4}$$

with

$$\mathbf{a}^{(\chi)}(\theta, \phi) = \frac{\cos\theta}{p\sin\theta}\widehat{\boldsymbol{\phi}} + \nabla\chi(\theta, \phi). \tag{5}$$

The polar and azimuthal angles are denoted θ and ϕ in momentum space and ϑ and φ in position space.

As the basis vectors for the field and hence for the first-quantized photon wave function, we use complex vectors $\underline{e}_\lambda$ of definite helicity $\lambda = \pm 1$, with components

$$e^{(\chi)}_{\lambda,\mu}(\theta, \phi) = e^{(0)}_{\lambda,\mu}(\theta, \phi)\exp(-i\lambda\chi). \tag{6}$$

where

$$e^{(0)}_{\lambda,\mu}(\theta, \phi) = \left(\widehat{\boldsymbol{\theta}}_\mu + i\lambda\widehat{\boldsymbol{\phi}}_\mu\right)/\sqrt{2} \tag{7}$$

and we add $\underline{e}_0 = \widehat{\underline{\mathbf{p}}}$ to complete the triad. The "hat" denotes a unit vector, and $\mu = -1, 0$ and 1, label rows of the column vector, $\underline{e}_\lambda$, and denote components on the complex vectors $\left(\widehat{\underline{x}} - i\widehat{\underline{y}}\right)/\sqrt{2}$, $\widehat{\underline{z}}$ and $\left(\widehat{\underline{x}} + i\widehat{\underline{y}}\right)/\sqrt{2}$, respectively, which are eigenvectors of $\underline{S}_z$ with eigenvalue μ. Here we express the rotation matrix $\underline{D}$ in terms of the same components [8] and note that $e^{(\chi)}_{\lambda,\mu}(\theta, \phi) = D_{\mu\lambda} = D^*_{-\mu,-\lambda}$. The general transverse basis vector $\underline{e}^{(\chi)}_\lambda$ is rotated relative to $\underline{e}^{(0)}_\lambda$ by the Euler angle χ about $\mathbf{p}$, giving just a phase difference in the helicity basis.

While the phase of the basis vectors depends on the choice of χ, the physical fields are obviously independent of how we choose to orient the basis vectors around $\mathbf{p}$. Indeed, we can rotate the basis vectors around $\mathbf{p}$ by a different angle at different momentum-space positions (θ, ϕ), and this cannot change the physical field. In this sense, a reorientation transformation $\chi(\theta, \phi) \to \chi'(\theta, \phi)$ is a true local gauge transformation. It is a basic requirement of the covariance of the geometric representation. The invariance of the physical field and hence the photon wave function means that the coefficients of the field when expanded in the basis receive compensating phase factors [9].

The term $\mathbf{a}^{(\chi)}$ may be considered an abelian momentum-space vector potential, analogous to the vector potential $\mathbf{A}$ of electromagnetic theory [6]. The position operator $\underline{\mathbf{r}}^{(\chi)}$ in Eq.(4) depends on the gauge of $\mathbf{a}^{(\chi)}$ through $\nabla\chi(\theta, \phi)$, similar to the way the kinetic momentum $\mathbf{P}$ of a massive charged particle depends on the gauge of the vector potential $\mathbf{A}$. The role of the charge of the massive particle is seen to be taken in momentum space by the helicity of the photon, and it is relevant to recall here the well-known result that the helicity defines an invariant subspace of the Poincaré group. The basis vectors are taken as eigenstates of the position operator, and a gauge transformation cannot change their eigenvalues. Thus, a gauge transformation in the basis states $\underline{e}^{(\chi)}_\lambda$ of the helicity subspace λ, say $\underline{e}^{(\chi)}_\lambda \to \underline{e}^{(\chi')}_\lambda = T\underline{e}^{(\chi)}_\lambda$ must change the position operator according to the usual gauge rule

$$\mathbf{r}\underline{e}^{(\chi)}_\lambda \to \mathbf{r}'\underline{e}^{(\chi')}_\lambda = T\mathbf{r}\underline{e}^{(\chi)}_\lambda$$

and this gives the transformation $\mathbf{r}' = T\mathbf{r}T^{-1}$. In our case, T is the phase factor $T = e^{-i\lambda(\chi'-\chi)}$ and $\underline{\mathbf{r}} = i\hbar\underline{D}p^\alpha\nabla p^{-\alpha}\underline{D}^{-1}$ so that $\underline{\mathbf{r}}' = \underline{\mathbf{r}} - \lambda\nabla(\chi' - \chi)$, which is exactly the dependence we find for $\underline{\mathbf{r}}$ on the gauge transformation.

The field $\nabla \times \mathbf{a}^{(\chi)}$ in momentum space corresponds to that of a magnetic monopole at the origin. The potential $\mathbf{a}^{(0)}$ has singular "Dirac" strings of flux lines on the $\pm z$ axis that supply the flux emanating from the monopole. This is most easily seen by integrating $\mathbf{a}^{(0)}$ along a path encircling the z axis and equating this to the flux passing through the area bounded by the path. The singular strings in $\mathbf{a}^{(\chi)}$ represent an essential nonintegrability or path dependence that is responsible for the physical manifestation of the gauge potential [10]. As illustrated below, gauge transformations induced by changes in $\chi(\theta, \phi)$ can change the strings, but they do not alter the physical results. As shown in Ref. [6], the abelian potential $\mathbf{a}^{(\chi)}$ is part of a more general nonabelian gauge potential for SO(3).

The basis states (6) can be used to express either the ideally localized states (1) or more readily realizable states. Adlard, Pike and Sarkar [4], for example, constructed single-photon states with arbitrarily fast asymptotic power-law falloff of energy density and photodetection rate and Bialynicki-Birula [5] obtained converging or diverging localized states with an arbitrarily fast exponential falloff. An advantage of these states is that the falloff rate for the vector potential, the fields, and the Landau-Peierls photon wave function [11] are asymptotically all determined by the same exponential factor, and this avoids the problem that the fields themselves associated with exactly localized states are not localized [12]. As we show now, the gauge choice $\chi(\theta,\phi)$ affects the angular momenta of the basis states, whether applied to these asymptotically localized states or to the exactly localized states of Ref. [6].

The basis defined by

$$\chi(\theta,\phi) = -m\phi \tag{8}$$

has total z-angular momentum quantum number $j_z = m$ with the single-valued gauge potential

$$\mathbf{a}^{(\chi)} = \hat{\phi}\frac{\cos\theta - m}{p\sin\theta}. \tag{9}$$

The singularities in $\mathbf{a}^{(0)}$ along the $\pm z$ axis ($\theta = 0, \pi$) are thus changed in strength by the factors $1 \mp m$. For example, for $m = 1$, the singularity along the positive z axis is missing in $\mathbf{a}^{(\chi)}$ whereas that along the negative z axis carries twice the flux. Other choices of $\chi(\theta,\phi)$ can reorient the singularity along some other direction or replace it by a nonintegrable (multivalued) $\mathbf{a}^{(\chi)}$. A reorientation of the singularity does not produce any new physics, and as discussed above, for simplicity we choose a geometric gauge with the singularity on the $\pm z$-axis. (The most general choice of χ can give a singularity that is not straight as discussed in the literature on magnetic monopoles [13], perhaps with interesting consequences.) Restricting the Euler angle χ to functions given by Eq.(8), the basis vectors can be expanded in eigenvectors of the usual spin-1 matrix $\underline{S}_z$ and $L_z = -i\partial/\partial\phi$ as

$$\underline{e}_1^{(-m\phi)} = \frac{1}{2}\begin{pmatrix} (\cos\theta - 1)\exp\left[i(m+1)\phi\right] \\ -\sqrt{2}\sin\theta\exp(im\phi) \\ (\cos\theta + 1)\exp\left[i(m-1)\phi\right] \end{pmatrix} \tag{10}$$

The top row ($\mu = -1$) gives the projection of the basis state $\underline{e}_1^{(-m\phi)}$ onto a state with $\underline{S}_z$-eigenvalue -1 and L_z eigenvalue $m+1$ with probability $\frac{1}{4}(\cos\theta - 1)^2$; the second row ($\mu = 0$), has the corresponding eigenvalues 0 and m with probability $\frac{1}{2}(\sin\theta_{\mathbf{p}})^2$, while the third row ($\mu = 1$), has eigenvalues 1 and $m-1$ with probability $\frac{1}{4}(\cos\theta + 1)^2$. Thus, by inspection, it is confirmed that the total angular-momentum eigenvalue of $\underline{J}_z$ of the basis state is m. The expectation values of S_z and L_z for the basis state, obtained from the weighted sum, are then $\cos\theta$ and $-\cos\theta + m$, respectively, showing that its cosine terms exactly cancel, leaving the eigenvalue m of $\underline{J}_z$

Restrictions on the uncertainty of the angular momentum of a localized state are imposed by the commutation relations between the components of $\underline{\mathbf{r}}^{(\chi)}$ and $\underline{\mathbf{J}}$, which were found in Ref.[6] to be

$$\left[\underline{J}_j, \underline{r}_k\right] = i\epsilon_{jkl}\underline{r}_k - i\lambda\left(\partial\underline{S}_j^{(\chi)}/\partial p_k\right). \tag{11}$$

Note that the position operator does not transform as a simple vector because, through its coupling to the spin, a rotation induces a gauge change. For a photon at the origin for which $\langle\underline{r}_k\rangle = 0$, the usual relationship between uncertainty and the commutator gives

$$\Delta\underline{J}_j\Delta\underline{r}_k \geq \frac{1}{2}\left\langle\left|\partial\underline{S}_j^{(\chi)}/\partial p_k\right|\right\rangle \tag{12}$$

and

$$\Delta\underline{J}^2\Delta\underline{r}_k \geq \sum_j\left\langle\left|\underline{J}_j\partial\underline{S}_j^{(\chi)}/\partial p_k\right|\right\rangle. \tag{13}$$

When χ is given by Eq.(8) the z-component of $\underline{\mathbf{S}}^{(\chi)}$ reduces to $\underline{S}_z^{(-m\phi)} = m\underline{\mathbf{S}}\cdot\hat{\mathbf{p}}$ and within a state space of helicity λ, $\partial\underline{S}_z^{(-m\phi)}/\partial p_k = 0$. Thus the photon can simultaneously have a definite position and z-component of the total angular momentum. However, it does not have definite x or y-components of $\mathbf{J}$, and there is no definite value for the total angular momentum. Nothing can be known definitely about the values of $\underline{\mathbf{S}}$ or $\underline{\mathbf{L}}$ separately. This is consistent with the expansion (10).

In coordinate space the electric field describing the localized states discussed here can be written as

$$E_\mu(\mathbf{r},t) = \sum_{\lambda=\pm1}\int\frac{d^3p}{(2\pi\hbar)^3}f(p)\,g(\theta)\,e_{\lambda,\mu}^{(\chi)}(\theta,\phi) \times\exp\left[i(\mathbf{p}\cdot\mathbf{r} - pct)/\hbar\right] \tag{14}$$

where $g(\theta) = \sin\theta$ for the localized states considered in [5], while $g(\theta) = 1$ in [4] and [6] and, with the gauge choice (8),

$$e^{(\chi)}_{\lambda,\mu}(\theta,\phi) = e^{(\chi)}_{\lambda,\mu}(\theta,0)\, e^{i(m-\mu)\lambda\phi}. \tag{15}$$

To transform to coordinate space we use the expansion in spherical harmonics

$$\exp(i\mathbf{p}\cdot\mathbf{r}/\hbar) = 4\pi \sum_{l=0}^{\infty}\sum_{n=-l}^{l} i^l Y_l^n(\vartheta,\varphi)\, Y_l^{n*}(\theta,\phi)\, j_l(pr/\hbar)$$

and integrate over ϕ to obtain

$$E_\mu(\mathbf{r},t) = \frac{1}{\pi\hbar^3}\sum_{l=|m-\mu|}^{\infty} i^l Y_l^{m-\mu}(\vartheta,\varphi) \tag{16}$$

$$\times \int d(\cos\theta)\, Y_l^{m-\mu *}(\theta,0)\, g(\theta)\, e^{(\chi)}_{\lambda,\mu}(\theta,0) \tag{17}$$

$$\times \int dp p^2 f(p)\, j_l\left(\frac{pr}{\hbar}\right)\exp(-ipct/\hbar)$$

where the subscript μ implies the corresponding component in the expansion (10). The position space field components vary as $\exp[i(m-\mu)\varphi]$, indicating a z-component of orbital angular momentum equal to $\hbar l_z = \hbar(m-\mu)$. Thus the position space z-components of spin, orbital and total angular momentum are exactly the same as those in momentum space, and all of the specific results discussed above regarding the angular momentum apply in position space.

The ϑ dependence can be obtained by expanding the integrand as

$$\sqrt{2\pi}g(\theta)\, e^{(\chi)}_{\lambda,\mu}(\theta,0) = \sum_{l=|m-\mu|}^{\infty} c_{\mu,l} Y_l^{m-\mu}(\theta,0) \tag{18}$$

and using the orthogonality of the spherical harmonics with the same $|s_z|$ value. We consider a few examples. If $m = 1$ and $g = 1$ then $c_{0,l} = 4/\sqrt{6}Y_1^1\delta_{l,1}$ so that the z-component of the field, $\sim \sin\vartheta$. For the counterclockwise rotating component of the field, $c_{1,l} = 4/\sqrt{3}Y_0^0\delta_{l,0} + 2/\sqrt{6}Y_1^0\delta_{l,1}$ which gives a ϑ- independent term and a $\cos\vartheta$ term. The basis in Ref. [5] implies $m = 0$ and $g = \sin\theta$ and gives $c_{0,l} = 4/\sqrt{3}Y_0^0\delta_{l,0} - 10/\sqrt{8}Y_2^0\delta_{l,2}$. In all cases the field component vanishes along any axis for which the corresponding component of $\mathbf{L}$ has a nonzero value.

In place of the common orbital angular momentum operator $\mathbf{L} = -\,\mathbf{p}\times i\nabla$ in momentum space, we should for consistency with our position operator use

$$\underline{\mathbf{L}}^{(\chi)} = \underline{\mathbf{r}}^{(\chi)}\times\mathbf{p} = \underline{D}\mathbf{L}\underline{D}^{-1}\ . \tag{19}$$

The corresponding spin operator is

$$\underline{\mathbf{S}}^{(\chi)} \equiv \mathbf{J} - \mathbf{L}^{(\chi)} = \left(\mathbf{a}^{(\chi)}\times\mathbf{p} + \widehat{\mathbf{p}}\right)\underline{\mathbf{S}}\cdot\underline{\widehat{\mathbf{p}}} \tag{20}$$

where $\underline{\mathbf{J}} = -i\hbar\underline{I}\mathbf{p}\times\nabla + \underline{\mathbf{S}}$. The basis vectors are eigenvectors of $\underline{\mathbf{S}}\cdot\underline{\widehat{\mathbf{p}}}$ with eigenvalue λ, that is $\underline{\mathbf{S}}\cdot\underline{\widehat{\mathbf{p}}}\underline{e}_\lambda = \lambda\underline{e}_\lambda^{(\chi)}$. They are also eigenvectors of the position operator with eigenvalue 0, giving $\underline{\mathbf{r}}^{(\chi)}\underline{e}_\lambda^{(\chi)} = 0$ and thus $\underline{\mathbf{L}}^{(\chi)}\underline{e}_\lambda^{(\chi)} = 0$. Thus in a basis expansion, $\underline{\mathbf{L}}^{(\chi)}$ just differentiates the coefficient of $\underline{e}_\lambda^{(\chi)}$, giving no contribution due to the basis. The operator $\underline{\mathbf{S}}^{(\chi)}$ alone extracts the total angular momentum of the basis vector $\underline{e}_\lambda^{(\chi)}$. Thus use of the position operator, (4) separates the angular momentum of the basis from that in its coefficient. The gauge-dependent term $\mathbf{a}^{(\chi)}\ \widehat{\mathbf{p}}\cdot\underline{\mathbf{S}}$ in the position operator (4) can best be understood in terms of its relationship to the angular momentum of the basis. In position space, orbital angular momentum is associated with a component of the Poynting vector in the $\widehat{\boldsymbol{\varphi}}$ direction such that it spirals along the direction of propagation [1]. In momentum space the functional forms of the position and momentum operators are exchanged, and an analogous term appears in the position operator, representing a spiraling of the field about $\mathbf{p}$.

The singular string of $\mathbf{a}^{(\chi)}$ discussed above is the axis of a vortex. Expression (10) makes explicit the angular momenta of the basis vectors along the string, and associated clockwise and counterclockwise rotation about it. The polar angle $\theta = 0$ identifies the positive z-axis and the paraxial limit when describing a beam, while $\theta = \pi$ identifies the negative z-axis. If $m = 0$, the whole z-axis is singular, while if $m = 1$, there is no singularity associated with the positive z-axis ($l_z = 0$), but the negative z-axis has $l_z = 2$, that is it has twice the strength or topological charge. The singularity has just been moved from the positive to the negative z-axis. The center of the vortex has zero intensity due to the $\sin\theta$ dependence discussed above. The orbital angular momentum arises from a bright annular ring about the axis, as witnessed in the $j_l\,(pr/\hbar)\sin\vartheta$ dependence of the field (16), and the radius of this ring goes to zero with the parameter describing the spatial extent of the localized photon state.

In summary, each member of a family of position operators with commuting components defines a corresponding basis of transverse unit vectors. The choice of basis contributes a term $\lambda\mathbf{a}^{(\chi)} \times \mathbf{p}$ to the total angular momentum of the basis states and affects the associated optical vortex. However, a complete geometric gauge transformation does not change the total field describing a physically distinct photon state. The fact that the position operator given by Eq.(4) is not unique is a consequence of unavoidable ambiguity in the selection of a transverse basis, implicit in the description of any exactly or partially localized state.

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