# Topological Aberration of Optical Vortex Beams: Determining Dielectric Interfaces by Optical Singularity Shifts

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We predict the splitting of a high-order optical vortex into a constellation of unit vortices, upon total internal reflection of the carrier beam, and analyze the splitting. The reflected vortex constellation generalizes, in a local sense, the familiar longitudinal Goos-Hänchen and transverse Imbert-Fedorov shifts of the centroid of a reflected optical beam. The centroid shift is related to the center of the constellation, whose geometry otherwise depends on higher-order terms in an expansion of the reflection matrix. We derive an approximation of the amplitude around the constellation as a complex analytic polynomial, whose roots are the vortices. Increasing the order of the initial vortex gives an Appell sequence of complex polynomials, which we explain by an analogy with the theory of optical aberration.

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Understanding and manipulating the spatial structure of light beams is a fundamental theme of modern optics. Beyond the simple structure of plane waves, beams with inhomogeneous complex amplitude can carry quantized orbital angular momentum (OAM) [1], which has many applications, including free-space classical and quantum communication [2–4], superresolved microscopy [5] and extrasolar planet detection [6,7].

Free space optical modes carrying quantized OAM have optical vortices (phase singularities) on their axes [8,9]: they have the amplitude structure $r^{|\ell|}\exp(i\ell\phi)$ close to the beam axis, for $\ell$ an integer. Around the axis, as the intensity becomes zero, the phase gradient becomes infinitely large. The core region close to the axis of such beams is therefore exceptionally sensitive to any imperfections in the transmission along the path of the beam. Any disruption to the pure azimuthal phase structure around the axis of the beam breaks the axial, strength-$\ell$ vortex into a constellation of $|\ell|$ unit strength zeros [10]. We call this effect *topological aberration*, as the effect of aberration disrupts the topology of the simple optical mode.

Here, we describe in detail the topological aberration which an OAM-carrying beam experiences under dielectric reflection by an oblique angle. We will see that the resulting constellation of zeros from the original strength-$\ell$ vortex depends on an aberrationlike analysis of the complex reflection coefficient in Fourier space, which is sensitive to terms up to order $|\ell|$ in its Taylor expansion. It is therefore possible, using the spatial distribution of phase singularities, to determine higher orders of the effective reflection-induced aberration of the beam. Furthermore, this phenomenon will affect any vortex beam reflected by a mirror, prism or beam splitter. As measurement techniques become more sophisticated, appreciation of this universal azimuthal symmetry breaking will become increasingly important. Although the fact that a high-order vortex breaks apart upon perturbation has been long understood, our main result here is a formula for an aberrated constellation of vortices. This comes from a local approximation, treating the neighbourhood of the aberrated vortex as a complex analytic function, determined completely by the zeros.

Tracking the change of position of optical vortices on reflection echoes the study of optical beam shifts, where the centroid of a homogeneously polarized beam is shifted by an amount proportional to the optical wavelength, either in the plane of incidence (Goos-Hänchen shift [11]), transverse to it (Imbert-Fedorov shift [12,13]), or some combination of the two. The net shift requires the initial transverse polarization to be homogeneous, and that the beam be narrow and axisymmetric in intensity, but is otherwise independent of the original amplitude profile. In recent years, there has been an explosion of interest in various types of beam shift, including both fundamental insight and possible applications [14].

It is simple to see the connection between beam shifts and aberration: for total reflection in the plane of incidence ($p$ polarization) or perpendicular to it ($s$ polarization), the reflection coefficient [15] is a simple "tilt" [16] to first order; as the reflection coefficient acts on direction, in real space the reflected beam is translated. In partial reflection when the modulus of the reflection coefficients vary, there are also angular shifts of the beam's propagation direction [17].

The notion of using the displacement of an on-axis zero to study beam shifts goes back to Hans Wolter in 1949 [18], who observed that the position of a zero is a precise marker depending on local information, rather than the beam centroid, which depends on the global distribution of intensity. Our approach may be thought of as generalizing Wolter's approach to any incident polarization and vortex order, all of which may be further extended to other aberrations of vortex beams, including refraction.

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Optical vortices are objects of scalar optics, and hence it is natural in our framework to consider a *polarized component* of the reflected beam; beam shifts for polarized components are analogous to quantum "weak values" of the reflection operator [19], which have shifts in both real and Fourier space. The spatial shift to the centroid of vortex-carrying beams involves both "spatial" and "angular" parts of phase-flat beams [20–22]; we will see that this general shift is simply the first term, analogous to tilt, in an aberration expansion of the polarized component's reflection matrix. In our calculation, higher aberration orders of the reflection matrix are realized as coefficients of a complex polynomial approximating the low amplitude in the core of the reflected beam: the vortex positions are related to these aberration terms by the fundamental theorem of algebra.

The basic beam geometry is demonstrated in Fig. 1, choosing a natural coordinate system based on the construct of a virtual reflected beam [23], which is obtained by

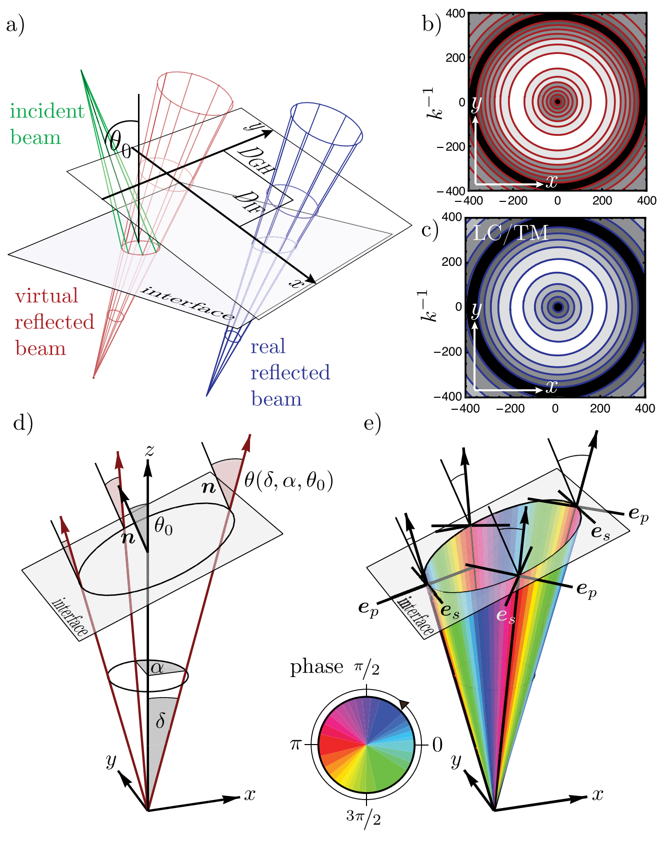


FIG. 1 (color online). Incident and reflected beam geometry. (a) Schematic of the relation between the interface plane and our coordinate frame, showing the incident, virtual and real reflected beam. For each beam the cone depicts a section of constant $\delta$. (b) Intensity profile of an incident Bessel beam. (c) Shifted intensity profile of the real reflected beam for $\theta_0 = 44°$ and $n = 2/3$. (d) Schematic of the beam coordinates. The local plane and angle of incidence depend both on $\delta$ and $\alpha$. (e) Beam coordinates for a $\ell = -4$ vortex beam (phase indicated by color wheel) and local resolution into $\mathbf{e}_s$ and $\mathbf{e}_p$.

specular reflection of every plane wave in the incident beam. The central propagation direction is (0, 0, 1), and we will make much use of spherical angles about this direction: azimuth $\alpha$ and polar angle $\delta$. Since reflection flips the sign of $\ell$, the reflected beam is $\sigma(\delta)\exp(-i\ell\alpha)$, with real $\sigma(\delta)$ tightly centered around $\delta = 0$, such that the second moment $\sigma_2 = \int_0 d\delta|\sigma(\delta)|^2\delta^3 \ll 1$ (where the extra $\delta \approx \sin\delta$ is the Jacobian in spherical polars). The upper limit of this integral is larger than the width of the spectrum. In these coordinates, the normal to the incidence plane has direction $(-\sin\theta_0, 0, \cos\theta_0)$, so, for each component of the spectrum labeled by $\delta$, $\alpha$, the incidence angle $\theta$ is given by $\cos\theta = \cos\delta\cos\theta_0 - \cos\alpha\sin\delta\sin\theta_0$. This angular dependence appears in the reflection coefficients $r_s(\theta)$ and $r_p(\theta)$ [16], which are defined with respect to the local plane of incidence for every plane wave within the spectrum [see Fig. 1(d)]. The indices $s$ and $p$ thereby refer to the directions orthogonal ($s$) and parallel ($p$) to the local plane of incidence [see Fig. 1(e)] and the general reflection matrix $\mathbf{R} = r_s\mathbf{P}_s - r_p\mathbf{P}_p$ consists of the projectors $\mathbf{P}_j = \boldsymbol{e}_j \otimes \boldsymbol{e}_j$, $j = s, p$ of the incident field onto the local $\boldsymbol{e}_s$ and $\boldsymbol{e}_p$ direction [see Fig. 1(e)] multiplied by the appropriate reflection coefficient. $\mathbf{R}$ acts on an initial polarization $\boldsymbol{E}$, which for the central wave vector is a 2D constant Jones vector with components $E_x$ and $E_y$. This is the global polarization of the incident field which we distinguish from the local polarization in terms of $s$ and $p$ components. Because of transversality, however, the other plane waves in the spectrum have a small $z$ component such that $\boldsymbol{E} = (E_x, E_y, -(E_x\cos\alpha + E_y\sin\alpha)\tan\delta)$. As we only consider a polarized component of the beam, the reflected beam is filtered by a constant polarization analyzer $\boldsymbol{F}$ with components $(F_x, F_y, 0)$. All of the physics of beam reflections can be explained by a Taylor expansion about $\delta = 0$ of the scalar multiplication operator $\boldsymbol{F}^*\mathbf{R}\boldsymbol{E}$ in Fourier space as we briefly summarize in the following (also see Ref. [24]).

In the transverse plane the real-space scalar reflected beam is given by

$$\psi(\boldsymbol{r}) = \int_0 d\delta \int_{-\pi}^{\pi} d\alpha\,\sigma(\delta)\delta e^{ik\sin\delta\boldsymbol{r}\cdot(\cos\alpha,\sin\alpha)-i\ell\alpha}\boldsymbol{F}^*\mathbf{R}\boldsymbol{E}, \tag{1}$$

where $\boldsymbol{r} = (x, y)$ and $k$ is the wave number of the incident light. The formula for the beam shift follows from a first order Taylor expansion of the reflection matrix term,

$$\boldsymbol{F}^*\mathbf{R}\boldsymbol{E} \approx \bar{R}[1 + \delta\boldsymbol{\mathcal{D}}\cdot(\cos\alpha, \sin\alpha)] \approx \bar{R}e^{\delta\boldsymbol{\mathcal{D}}\cdot(\cos\alpha,\sin\alpha)}, \tag{2}$$

where $\boldsymbol{\mathcal{D}} = (\mathcal{D}_x, \mathcal{D}_y)$ is a complex 2-vector with components $\mathcal{D}_x = (F_x^*E_xr_p' - F_y^*E_yr_s')/(F_x^*E_xr_p - F_y^*E_yr_s)$ and $\mathcal{D}_y = (F_y^*E_x + F_x^*E_y)\cot\theta_0(r_p + r_s)/(F_x^*E_xr_p - F_y^*E_yr_s)$.

When $\ell = 0$, the spatial shift is given by $-\mathrm{Im}\boldsymbol{\mathcal{D}}/k$, which adds to the $(x, y)$-dependent term in the exponent in

(1) when identifying $\sin\delta$ with $\delta$. This is the well-known Artmann formula for spatial beam shifts [25]. The angular shift is the angular mean of the Fourier transform of $\psi$, which is given by $\boldsymbol{\sigma}_2\mathrm{Re}\boldsymbol{\mathcal{D}}$ [23,26]. For $\ell \neq 0$ the net vortex beam shift $\boldsymbol{D}_{\mathrm{centroid}}$ is given by

$$k\boldsymbol{D}_{\mathrm{centroid}} = -\mathrm{Im}\boldsymbol{\mathcal{D}} - i\ell\boldsymbol{\sigma}_2\mathrm{Re}\boldsymbol{\mathcal{D}}, \tag{3}$$

where $\boldsymbol{\sigma}_2$ is the second Pauli matrix [19,22]. The first term here is the usual Artmann translation; the second term, usually associated with the angular shift, comes from the azimuthal complex amplitude structure of the vortex beam.

The shift to the intensity centroid of a vortex-carrying beam is different from the shift of the vortex itself [21,27]. The translation $-\mathrm{Im}\boldsymbol{\mathcal{D}}$ affects the entire beam including a vortex and the centroid. However, $\mathrm{Re}\boldsymbol{\mathcal{D}}$, being associated with a change in the profile of the beam, affects them differently: for an asymmetric profile, a vortex, being an absence of intensity, repels the intensity centroid, and it follows from the more general argument below that the shift of a vortex in a $|\ell| = 1$ beam $\boldsymbol{D}_{\mathrm{vortex}}$ is

$$k\boldsymbol{D}_{\mathrm{vortex}} = -\mathrm{Im}\boldsymbol{\mathcal{D}} \pm i\boldsymbol{\sigma}_2\mathrm{Re}\boldsymbol{\mathcal{D}}, \tag{4}$$

where $\pm$ refers to $\ell \gtrless 0$.

When $|\ell| > 1$, topology preserves the overall vortex charge, but the symmetry is broken and typically there is a constellation of $|\ell|$ unit-charge vortices in the reflected beam, with separation comparable to the beam shift itself. An example of a numerical calculation of the reflection of an $\ell = -4$ Bessel beam [28], with several different incident and analyzer polarizations, is shown in Fig. 2. The constellation is not simply a regular polygon or "row" [29], but a more complicated function of incident and analyzer polarization, incidence angle $\theta_0$ and refractive index $n$. The centroid of the vortices, represented by the white circle, is the same as the position of the single shifted vortex $\boldsymbol{D}_{\mathrm{vortex}}$: the centroid of the $|\ell|$ vortex points is a discrete, topological counterpart to the shift of the intensity centroid, but without the $\ell$ weighting, anticipated in Ref. [21].

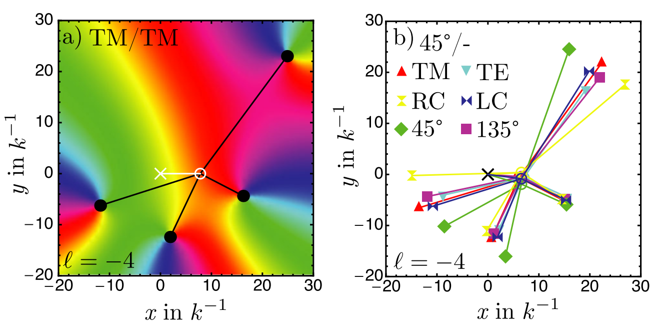


FIG. 2 (color online). (a) Plot comparing the constellation of vortices obtained from the roots of the local expansion in (8) with a numerical calculation of the phase of the field. The incident field is a Bessel beam with $\ell = -4$ incident at $\theta_0 = 46°$ and a fixed opening angle of $\delta = 0.01$. The incident polarization $\boldsymbol{E}$ and the analyzer $\boldsymbol{F}$ are both oriented in the $x$ direction (TM/TM). $\times$ marks the origin and $\bigcirc$ the centroid of the vortices. (b) Plot showing the variation of constellations for 45° diagonal incident polarization and different analyzer settings including linear in the $x$ (TM) and $y$ direction (TE), right (RC), and left (LC) circular polarization, as well as 45° and 135° diagonal polarization.

To analyze these constellations we now derive an analytic approximation for the reflected vortex beam close to the beam axis, as a complex polynomial in $x + iy$ or $x - iy$ depending on the sign of $\ell$ [29], by collecting all the terms of the lowest order in $\delta$ in the expansion of the reflection matrix (2). Up to order $|\ell|$, this can be written as

$$\boldsymbol{F}^*\mathbf{R}\boldsymbol{E} \approx \bar{R}\left(1 + \delta C_1 + \frac{1}{2}\delta^2 C_2 + \cdots \frac{1}{|\ell|!}\delta^{|\ell|}C_{|\ell|}\right), \tag{5}$$

where $\bar{R} = \boldsymbol{F}^*\mathbf{R}\boldsymbol{E}|_{\delta=0}$. The argument throughout assumes $\bar{R} \neq 0$, so it does not hold in exceptional circumstances, such as incident in-plane polarization at the Brewster angle. The original beam shift follows from $C_1 = \boldsymbol{\mathcal{D}} \cdot (\cos\alpha, \sin\alpha)$, which contains only single powers of $\sin\alpha$ and $\cos\alpha$ and depends on the first derivatives of the reflection coefficients. The higher coefficients $C_m$ contain combinations of $\sin^u\alpha\cos^v\alpha$ and $r_j^q = (d^q/d\delta^q)r_j|_{\delta=0}$ for $j = s, p$ with $u + v = m$ and $q \leq u, v$. Each $C_m$ may thus be written as a complex Fourier series

$$C_m = \frac{c_m^+ e^{im\alpha} + c_m^- e^{-im\alpha}}{2^m} + \cdots \tag{6}$$

This expansion of the reflection matrix is analogous to an aberration expansion in terms of complex Zernike modes [30], with $m$ giving the order of aberration: $c_1^\pm$ corresponds to tilt, $c_2^\pm$ to astigmatism, etc.

The core of the reflected vortex beam can be found by combining Eqs. (1) and (5); after integration over the azimuthal $\alpha$, each $e^{\pm iq\alpha}$ contributes a Bessel function $J_{\ell\mp q}$, which is Taylor approximated close to the axis. The lowest order term in the beam is $\delta^{|\ell|}$, which comes from each $c_m^\pm$ for $\ell \gtrless 0$; all other terms have higher order and therefore smaller contribution. The size of the $m$th contribution, corresponding to $c_m^\pm$ is

$$\frac{c_m^\pm \delta^m}{2^m m!}\int_{-\pi}^{\pi} d\alpha e^{ik\delta r\cos(\alpha-\phi)-i(\ell\mp m)\alpha} \approx \delta^{|\ell|}c_m^\pm 2\pi i^{|\ell|-m}[2^{|\ell|}m!(|\ell|-m)!]^{-1}[k(x\mp iy)]^{|\ell|-m}. \tag{7}$$

substituting $r\exp(\mp i\phi) = x \mp iy$.

On collecting common factors, the reflected field near the axis for a given $\ell$ is proportional to

$$\psi \propto \zeta^{|\ell|} - i|\ell|c_1^\pm\zeta^{|\ell|-1} - \frac{|\ell|^2 - |\ell|}{2}c_2^\pm\zeta^{|\ell|-2} + \ldots + (-i)^{|\ell|}c_{|\ell|}^\pm, \tag{8}$$

where we have used $\zeta = k(x \mp iy)$ with "$-$" for $\ell > 0$ and "$+$" for $\ell < 0$. Each root of this complex polynomial corresponds to a vortex, and the constellation depends on the roots of the polynomial with coefficients given by $(-i)^n c_m^{\pm}$ times a binomial coefficient as in (8). For increasing $|\ell|$ the polynomials in (8) form an Appell sequence [31], with coefficients generated by the sequence $c_m^{\pm}$ of coefficients from the Zernike expansion of the reflection matrix, for which there are many relations between the roots and the coefficients [32]. The integral over $\delta$ as in (1) does not affect Eq. (8), since these terms have the same, lowest-order contribution in $\delta$, and so the constellation is independent of the spectrum and hence the radial profile of the beam, as long as it is narrowly confined in Fourier space.

In the complex plane, the arithmetic mean (centroid) of the roots of a polynomial of the form (8) is given by $ic_1^{\pm}$ [32], which proves that the mean position of the vortices is always given by $ic_1^{\pm} = \boldsymbol{\mathcal{D}} \cdot (i, \pm 1)$. The vortex centroid shift is independent of $\ell$, and can be understood purely in terms of the representation of the beam as a polynomial in the complex $(x \mp iy)$ plane.

The vortex constellation for $|\ell| > 1$ is sensitive to terms beyond the first-order shift. The second order term $c_2^{\pm}$ is related to the complex astigmatism of $\boldsymbol{F}^* \mathbf{R} \boldsymbol{E}$, proportional to $e^{\pm 2i\alpha}$. When $|\ell| = 2$, Eq. (8) is a quadratic equation with $c_2^{\pm}$ the "constant"; $ic_1^{\pm}$ is the midpoint of the two roots, and their separation from the midpoint is $\pm\sqrt{c_2^{\pm} - (c_1^{\pm})^2}$ (where the complex argument represents the direction and the overall $\pm$ is independent of the sign of $\ell$). Measurement of the two singularity positions would therefore provide the two complex numbers $c_1^{\pm}$ and $c_2^{\pm}$, from the first two orders of the Zernike expansion of the reflection coefficient. The former contains zeroth and first derivatives of the reflection coefficients via the complex shift vector $\boldsymbol{\mathcal{D}}$ and the latter is given by $c_2^{\pm} = (F_x^*, F_y^*) \cdot \mathfrak{c}_2^{\pm} \cdot (E_x, E_y)/(F_x^* E_x r_p - F_y^* E_y r_s)$, where the $\mathfrak{c}_2^{\pm}$ matrix is given by

$$\mathfrak{c}_2^{\pm} = (r_s + r_p)\cot^2\theta_0 \begin{pmatrix} 1 & \pm i \\ \pm i \sec^2\theta_0 & -1 \end{pmatrix} + \frac{1}{2}\cot\theta_0 \begin{pmatrix} -r_p' & 0 \\ 0 & -r_s' \end{pmatrix} \mp i(r_s' + r_p')\cot\theta_0 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} r_p'' & 0 \\ 0 & -r_s'' \end{pmatrix}. \quad (9)$$

This complicated form of $\mathfrak{c}_2^{\pm}$ shows that for higher order shift effects, a separation in terms of diffractive corrections and optical spin-orbit interaction is no longer possible [14].

To give an estimate of the separation of two vortices we note that for total internal reflection in a glass prism with $n = 1.49$ and for a typical wavelength of $0.623\ \mu$m, and an incidence angle of $\theta_0 = 45°$, the distance between the two vortices varies in the range of $1\ \mu$m to $4\ \mu$m depending on the choice of incident and analyzer polarization. For the same parameters in partial reflection the range of separation is smaller and varies between $0.4\ \mu$m and $1.2\ \mu$m. In both cases the separation is roughly twice the spatial shift of the intensity centroid.

In Fig. 3 we illustrate how this "singularimetry" would give increasing information as positive $\ell$ increases (a) and as negative $\ell$ increases (b). As $|\ell|$ increases, the constellations increase in complexity, but maintain common features (such as their center), as their coefficients are algebraically related in Eq. (8). These complex coefficients are proportional to the $c_m^{\pm}$, which correspond to successive azimuthal aberration terms (tilt, astigmatism, etc.). This is shown in Figs. 3(c)–3(g), which illustrate how a fixed reflection matrix term $\boldsymbol{F}^* \mathbf{R} \boldsymbol{E}$ as a function of $\alpha$, $\delta$ (c) is decomposed into aberration terms of increasing order. In the sense of quantum weak values [33], we note that going beyond $|\ell| = 1$ accesses weak information beyond the first order.

Our argument extends beyond reflection, to any paraxial vortex beam experiencing an aberrationlike multiplication in Fourier space: rather than a single order $\ell$ on-axis vortex, the beam will have a constellation of $\ell$ vortices which can be represented by a polynomial with coefficients dependent on the azimuthal terms. This effect of

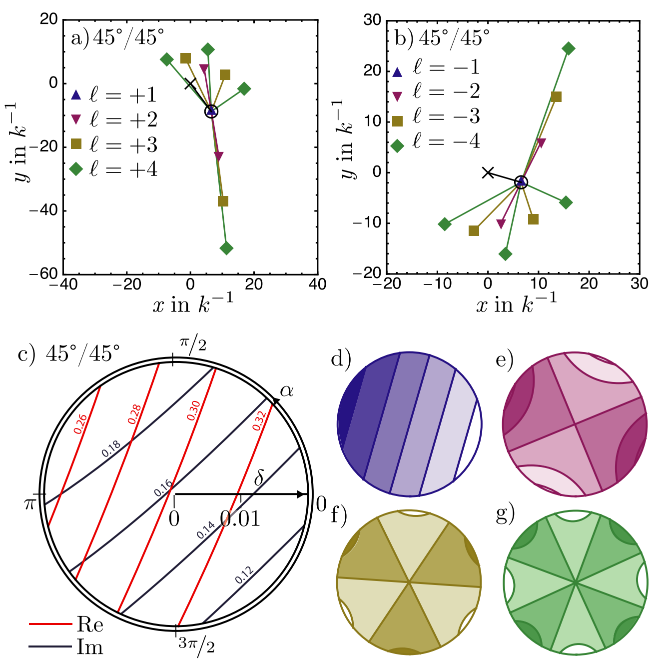


FIG. 3 (color online). Vortex constellations for increasing positive $\ell$ (a) and negative $\ell$ (b). (c) Contours in Fourier space (conical beam geometry) of the real and imaginary part of $\boldsymbol{F}^* \mathbf{R} \boldsymbol{E}$ for $\theta_0 = 46°$ and both $\boldsymbol{F}$ and $\boldsymbol{E}$ set to 45° diagonal polarization. (d)–(g) Contour plots for of the real parts of the coefficients in (8) multiplied by the appropriate Fourier factor $\exp(-im\alpha)$ for comparison with $\ell < 0$ in (b). (d) $m = 1$, (e) $m = 2$, (f) $m = 3$, (g) $m = 4$. [Scaling identical to figure (c)]. The gradient over the contours in (d) corresponds to the shift as indicated by the black line between $\times$ and $\bigcirc$ in (b).

topological aberration will affect any vortex beam undergoing oblique reflection or refraction in a real optical system, suggesting a fundamental limitation on the purity of quantized OAM modes in optical devices [34,35]. However, as the connection between vortex positions and the aberrations is so algebraically direct, any singularimetric device which measures the precise vortex distribution has direct access to the beam shift and later terms, without any further analysis of the overall beam.

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