The paraxial approximation fails to describe the interaction of atoms with general vortex light fields

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Neglecting the electric field component along the light’s propagation direction is a common practice, known as paraxial approximation. However, experimental evidence and theory on the head-on excitation of atoms by Laguerre-Gaussian beams reveal that the full vector character of the light field has to be taken into account. Optical vortices are a large family of fields, being Laguerre-Gaussian only one particular case. Now we extend the study of the applicability of the paraxial approximation to a broader set of optical vortices by considering the interaction of atoms with generalized Laguerre-Gaussian and generalized Bessel beams. We demonstrate that all vortex beams here considered look the same close to the beam axis, where the atom is placed. From this, we conclude that the paraxial approximation fails for the large set of vortex beams, and that a full understanding of the interaction of optical vortices with atoms requires the inclusion of all vector components of the electric field.

INTRODUCTION

The paraxial approximation (PA) is the assumption that rays comprising a light beam are almost parallel to the optical axis. Mathematically, we characterize the beam parallelism by the paraxial ratio $q_r/q_z$ of radial to longitudinal wave number with $k^2 = q_r^2 + q_z^2$ and $q_r \propto w_0^{-1}$, or equivalently by the ratio $\lambda/w_0$ of wavelength ($\lambda$) to waist ($w_0$). The paraxial approximation can be derived from the wave equation or Maxwells equation. In the latter case, one expands the electromagnetic fields in terms of powers of $q_r/q_z$; each term in the series accounts for an increasing degree of non-paraxiality. To order zero in $q_r/q_z$, the beam is completely transverse, a common approximation in theory and experiments dealing with Transverse Electromagnetic Modes. A less stringent demand is to retain the first order in $q_r/q_z$, that leads to a non-zero component of the electric field in the direction of light’s propagation.

Optical vortices (OV) or twisted light are light beams with phase singularities, carrying spin and orbital angular momentum (OAM). Research in OV spans nowadays a diversity of physics areas with possible application. In addition to the phase singularity and OAM, OV have other surprising features defying our common sense built up on plane-wave models and Gaussian beams. In particular, OV having opposite (antiparallel) orbital and spin AM are most unusual.

In 2016, Schmiegelow et al\textsuperscript{27} experimentally probed quadrupole transitions between Zeeman split magnetic levels in a single $^{40}$Ca\textsuperscript{+} (Fig 1) used Gaussian and LG beams, with OAM per photon $\hbar \sigma = 0, \pm 1$, respectively. Circular polarization (polarization vector $e_\sigma = (\hat{x} + i \sigma \hat{y})/\sqrt{2}$) $\sigma = \pm 1$, and wavelength $\lambda = 0.729 \mu m$. Under these conditions, the paraxial ratio is $\lambda/w_0 = 0.27$. As discussed above, the PA dictates the neglect of the longitudinal component (here along the z axis) for modeling such a beam. Accordingly, the first theoretical model disregarded the electric field component $E_z$. This model was quite successful in reproducing the data for quadrupole transitions induced by Gaussian and parallel-momenta LG beams. However, data points for transitions induced by antiparallel-momenta LG beams could not be understood within the PA model. This motivated a reexamination of the model’s assumptions, that led to the understanding that $E_z$ might play an unexpected relevant role in the latter cases. To test whether or not this is the case, the first model (PA) was contrasted to a Vector Model (VM), as we briefly describe below –for more details see Refs.\textsuperscript{28} The field is given by $E(r,t) = E^{(+)}(r)e^{-i\omega t} + c.c.$
with

\[
E_{\perp}^{(+)}(r) = (\hat{x} + i\sigma \hat{y}) \frac{E_0}{\sqrt{\pi} |\ell|!w_0} \left( \frac{\sqrt{2}}{w_0} r \right)^{|\ell|} e^{i\ell\sigma_1 x_1} e^{ikz},
\]

\[
E_{z}^{(+)}(r) = -i (\ell\sigma - |\ell|) (1 - \delta_{\ell,0}) \frac{E_0}{\sqrt{\pi} |\ell|!w_0} \left( \frac{\sqrt{2}}{w_0} r \right)^{|\ell|-1} e^{i(\ell+\sigma)\sigma_1 x_1} \ e^{ikz},
\]

with separated transverse \(E_{\perp}^{(+)}(r)\) and longitudinal \(E_{z}^{(+)}(r)\) components. Note that the paraxial ratio appears only in \(E_z\) as \(1/(kw_0)\), with \(k = 2\pi/\lambda\).

One can compare experiments to theory thanks to the proportionality between Rabi frequency (measured in the \(^{40}\text{Ca}^+\) experiment) and light-matter interaction matrix element. We considered two different theoretical models: i) PA: the ion interacts solely with the transverse component of the electric field in all cases or ii) VM: the ion interacts with all three component of the electric field. Both models were compared to experimental data to draw conclusions on the validity of the PA for LG beams of the type used in Ref.27. More specifically, the theoretical procedure consisted of: i) writing down the light-matter Hamiltonian \(H_I = -q \int_0^1 \mathbf{r} \cdot \mathbf{E}(\mathbf{r}, t) d\mathbf{u}\); ii) separating longitudinal and transverse sections; iii) transforming from cylindrical to spherical coordinates; iv) rewriting in terms of spherical tensors; v) using Wigner-Eckard’s theorem to evaluate matrix elements between initial (S-) and final (D-) states of the atom; finally, (vi) comparing ratios of matrix elements to ratios of measured Rabi frequencies.

We tested the two different models mentioned above. Table 1 shows the results. For example, “c/a” is the ratio of transitions induced by an antiparallel (“c”) to a parallel (“a”) momenta LG beams, and the matrix element corresponding to c can be calculated either without (second row) or with (third row) \(E_z\). An excellent match between theory and experiment occurs for all cases when the longitudinal component of the electric field is included (third row). In contrast, when the PA is assumed, there is agreement for ratios of transitions induced solely by parallel OV and Gaussian beams. From this results we concluded that Laguerre-Gaussian beams of the type considered violate the PA approximation.

### TABLE I. Experimental data (ratios of Rabi frequencies) and theoretical predictions (ratios of matrix elements) of the ion-OV interaction. Two different models are considered: (i) PA, that assumes \(E_z = 0\) even for anti-parallel OV (ii) VM, that assumes \(E_z \neq 0\) for anti-parallel OV.

|                        | \(c/a\) | \(e/a\) | \(e/c\) | \(d/b\) |
|------------------------|---------|---------|---------|---------|
| Experimental data      | 0.95(6) | 0.43(2) | 0.45(2) | 0.61(3) |
| Paraxial Approximation | 0.32    | 0.45    | 1.41    | 0.71    |
| model \([E_z(r) = 0]\)|         |         |         |         |
| Vector Model \([E_z(r) \neq 0]\)| 0.95   | 0.45    | 0.47    | 0.71    |

The question arises, if this failure of PA is a general feature of vortex beams.

### GENERALIZED OPTICAL VORCICES

Optical vortices are a family of fields, characterized by phase singularities in one or more components. Instances of OV are: Laguerre-Gauss, Bessel, Mathieu, azimuthally polarized, etc.

Recently\(^{29}\) we identified the existence of a large group of OV containing fields with varying degrees of relative strengths of electric to magnetic fields, parametrized by a real number \(\gamma\). For example, a beam with \(\gamma = 1\) has a strong magnetic field at the phase singularity\(^{19}\). On the other side, one finds fields with strong electric components for \(\gamma = 0\). In between, a more common OV\(^{11,12}\) with features closer to non-vortex beams is found at \(\gamma = 1 + \omega/(cq_z)\)^{\(-1\). The general expression for the OV for all \(\gamma\) are derived in Ref.\(^{29}\) here we present the electric field

\[
\mathbf{E}^{(\gamma)}(\mathbf{r}, t) = i \left[ \omega A_x + \gamma \frac{c^2}{\omega} \partial_x (\nabla_\perp \cdot \mathbf{A}_\perp) \right] \hat{x} + i \left[ \omega A_y + \gamma \frac{c^2}{\omega} \partial_y (\nabla_\perp \cdot \mathbf{A}_\perp) \right] \hat{y} - \left[ \frac{\omega}{q_z} + \gamma \frac{c^2 q_z}{\omega} \right] (\nabla_\perp \cdot \mathbf{A}_\perp) \hat{z}
\]

where \(\mathbf{A}_i = \mathbf{A}_i(\mathbf{r}, t)\) and \(A_\perp\) is the transverse part of the vector potential (either LG or BB) and \(\gamma = 1 - \gamma\).

In order to model head-on ion-OV interaction experiments –such as that from Ref.\(^{27}\) we approximate the field Eq. \(^2\) up to first order in the paraxial ratio \(q_r/q_z\), and look for its values in the neighborhood of \(r = 0\) (where the atom is placed), keeping up to first order in \(q_r/r\). A lengthy but straightforward calculation reveals
that all LG and Bessel beams of the type described by Eq. 2 with $|\ell| = 1$ are of the same form

\[ \sigma = +1 : \tilde{E}^{(r)}(r) = E_0 \left( r e^{i\delta} e_+ + i \frac{\sqrt{2}}{q_z} e_z \delta_{\ell, -1} \right) \]  
\[ \sigma = -1 : \tilde{E}^{(\gamma)}(r) = E_0 \left( r e^{i\delta} e_- + i \frac{\sqrt{2}}{q_z} e_z \delta_{\ell, +1} \right) \]

irrespective of the value of $\gamma$. In Eq. (1) $E = E \exp [i (q_z z - \omega t)]$, with $\{r, \varphi, z\}$ cylindrical coordinates. To this level of approximation, one clearly sees that parallel OV (first equation) are transverse.

We have reached the main point of this report: Equations 3-4 has the same structure as Eqs. 1a-1b; that is, the electric field of all general OV here considered are indistinguishable when $q_z/q_\perp$ is small and one looks close to the phase singularity. Therefore, any antiparallel OV under the same conditions stated above will yield the same results as presented in Table 1. We conclude that the PA fails in general to describe the interaction of antiparallel $|\ell| = 1$ OV with atoms.

**CONCLUSIONS**

We have demonstrated that the PA fails not only for LG beams but also for a large family of OV -including LG and Bessel- that have antiparallel spin and orbital angular momenta. All these beams share the same mathematical structure close to the phase singularity and, based on a conclusive experiment plus theory, the full vector character of the light field has to be taken into account, such that the longitudinal component of the electrical field is correctly included and the OV-atom interaction is properly described. Our findings have practical consequences in new applications that make use of light-matter interaction. Examples from AMO physics include the excitation of single trapped ions, e.g. for quantum optical experiments of for accurate frequency standards or of single trapped atoms. In the field of solid state application we see the excitions of magnetic transitions in impurities such as Eu$^{3+}$ or quantum dots as highly relevant cases.

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