Scattering of generalized Bessel beams simulated with the discrete dipole approximation

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Abstract. We consider the simulation of scattering of the high-order vector Bessel beams in the discrete dipole approximation framework (DDA). For this purpose, a new general classification of all existing Bessel beam types was developed based on the superposition of transverse Hertz vector potentials. Next, we implemented these beams in ADDA code – an open-source parallel implementation of the DDA. The code enables easy and efficient simulation of Bessel beams scattering by arbitrary-shaped particles. Moreover, these results pave the way for the following research related to the Bessel beam scattering near a substrate and optical forces.

1. Introduction
Today Bessel beams are at the frontier of structured light with orbital angular momentum. One of the most prominent advantages of Bessel beams is its diffractionless, i.e., the ability to propagate while maintaining the profile near the beam axis. These beams are actively used in such areas as optical manipulation (tweezing), material proceeding, imaging, etc. In many physical problems, it is crucial to consider the scattering of Bessel beams, which is predominantly studied for spherical particles with the use of the generalized Lorenz-Mie theory (GLMT) [1] than for arbitrary particles. Moreover, various types of Bessel beams exist that only have been named [2], lacking a complete picture of how they relate to one another. In this regard, this work has two goals: the classification of various types of high-order vector Bessel beams and the development of the capability to simulate the scattering of such beams by arbitrary particle using the discrete dipole approximation.

2. Bessel beam generalization
The scalar Bessel beam was obtained by J. Durnin [3] as a solution of the scalar Helmholtz equation in a cylindrical coordinate system. Meanwhile, vector Bessel beams are vectorial solutions of the Helmholtz equation and they can be presented in several different forms or types. These types differ by their polarizations, field, and energy configurations. Among them are beams with circularly symmetric energy density (CS type), with transverse electric and magnetic fields – TE and TM types, respectively, and LE and LM – beams with linear polarizations of electric and magnetic fields, respectively.

To derive the expressions of various types, it is convenient to use Hertz vector potentials (so-called Davis approach). This approach has been applied to the Bessel beams [4], but we have extended it further, making it possible to obtain all relationships between different beam types and their polarizations. Also, we managed to relate beams of other orders using the rotation and duality operators.
2.1. Matrix representation of Hertz vector potentials
This section outlines the derivation of generalized Bessel beams in a homogeneous isotropic medium (with absolute permittivity \(\varepsilon\), permeability \(\mu\), and wave impedance \(\eta \equiv \sqrt{\mu/\varepsilon}\)) in SI units. The symmetry of Maxwell equations allows one to consider only the electric field, but it is more convenient to consider a pair \(\{\mathbf{E}, \mathbf{H}\}\) taking into account a duality transformation \(\mathbf{P}_{\chi}(\mathbf{E}, \mathbf{H})\) of duality rotation by the angle \(\chi\), similar to the standard rotation matrix \(\mathbf{R}_{\chi}\) given by

\[
P_{\chi} \equiv \begin{pmatrix} \cos \chi & -\eta \sin \chi \\ \eta^{-1} \sin \chi & \cos \chi \end{pmatrix}, \quad \mathbf{R}_{\chi} \equiv \begin{pmatrix} \cos \chi & -\sin \chi \\ \sin \chi & \cos \chi \end{pmatrix}.
\]  

Electric and magnetic fields of any beam can be obtained starting from the Hertz vector potentials of electric and magnetic types [5]. We relate the pairs \(\{\mathbf{E}, \mathbf{H}\}\) and \(\{\mathbf{\Pi}_e, \mathbf{\Pi}_m\}\) in matrix form using an operator \(\mathcal{L}\) given by

\[
\begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix} = \mathcal{L} \begin{pmatrix} \mathbf{\Pi}_e \\ \mathbf{\Pi}_m \end{pmatrix}, \quad \mathcal{L} \equiv \nabla \times \left( \nabla \times \frac{i k \eta}{\nabla} \right) = \nabla \times \left( -i k \mathbf{P}_{\pi/2} + \nabla \times \right).
\]  

Note that both pairs satisfy Maxwell equations. For Bessel beams propagating along the \(z\)-axis the expressions for \(\mathbf{\Pi}_e\) and \(\mathbf{\Pi}_m\) are significantly simpler than that for the fields. The potentials have, up to the constant vector, the following concise functional form in the cylindrical coordinate system [4]

\[
f_n(\mathbf{r}) = f_n(k_t \rho) e^{i n \varphi} e^{i k z},
\]  

where \(f_n\) is the Bessel function of the first kind (\(n\) is the order of BB), \(k_t \equiv k \sin \alpha_0\) and \(k_z \equiv k \cos \alpha_0\) are the transverse and longitudinal components of the wave vector \(k\), and \(\alpha_0\) is the half cone angle.

The direction of Hertz vector potentials determines Bessel beam type and polarization. More specifically, a matrix \(\mathbf{M}\) represents any superposition of the transverse potentials

\[
\begin{pmatrix} \mathbf{\Pi}_e \\ \mathbf{\Pi}_m \end{pmatrix} = \begin{pmatrix} \Pi_{e,x} \\ \Pi_{m,x} \\ \Pi_{e,y} \\ \Pi_{m,y} \end{pmatrix} \begin{pmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{pmatrix} = \Pi_0 \begin{pmatrix} 1 & 0 \\ 0 & \eta^{-1} \end{pmatrix} \mathbf{M} \begin{pmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{pmatrix} f_n.
\]  

We have shown that all known Bessel beam types: LE, LM, CS, TE, and TM are presented this way. Moreover, the corresponding matrix \(\mathbf{M}\) has a simple form for most of these Bessel beams. This description clarifies relationships between various types and polarizations. It does not explicitly include longitudinal potentials, since any potential of the form \(f_n \mathbf{e}_z\) is equivalent to the superposition of transverse potentials of orders \(n \pm 1\).

2.2. Relations between beam types and polarizations
The ingenuity of the above matrix representation allows one to easily relate polarizations of one beam type and different types of Bessel beams. The expressions in Table 1 demonstrate some examples of these relationships based on polarization and duality transformations. Naturally, the polarization rotation transforms matrix \(\mathbf{M}\) into the matrix of the same beam matrix but with different polarization. By contrast, duality rotation relates different beam types. For example, LE and LM Bessel beams are coupled since the electric field of one type equal to a magnetic field of the other (up to a constant).
The discrete dipole approximation, including

\[ k = M \cdot f_k + i - \frac{1}{\varepsilon} - \frac{1}{\varepsilon} \left( \frac{1}{2} - k_x ( \mathbf{M}_{x} + i \mathbf{M}_{y} ) \right) f_{n+1} + \left[ -i k ( \mathbf{M}_{x} + i \mathbf{M}_{y} ) \right] f_{n-1} \].

### Table 1. Relations between LE, LM, and CS beam types and their polarizations expressed in terms of matrix \( \mathbf{M} \).

| Type | Field | \( \mathbf{M} \) | Polarization rotation | Duality rotation |
|------|-------|----------------|----------------------|-----------------|
| LE   | \( \mathbf{E}_{(x)}^{(x)} \) | \( \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \) | \( \mathbf{M}_{LE}^{(y)} R_\pi/2 = \mathbf{M}_{LE}^{(x)} \) |                    |
|      | \( \mathbf{E}_{(x)}^{(y)} \) | \( \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix} \) | \( \mathbf{R}_\pi/2 \mathbf{M}_{LM}^{(xy)} = \mathbf{M}_{LE}^{(xy)} \) |                    |
| LM   | \( \mathbf{E}_{(x)}^{(x)} \) | \( \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \) | \( \mathbf{M}_{LM}^{(y)} R_\pi/2 = \mathbf{M}_{LM}^{(x)} \) |                    |
|      | \( \mathbf{E}_{(x)}^{(y)} \) | \( \begin{pmatrix} 1 & 0 \\ -1 & 0 \end{pmatrix} \) | |                    |
| CS   | \( \mathbf{E}_{CS}^{(0,1)} \) | \( \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \) | \( \mathbf{M}_{CS}^{(0,1)} R_\pi/2 = \mathbf{M}_{CS}^{(1,0)} \) | \( \mathbf{R}_\pi/2 \mathbf{M}_{CS}^{(0,1)} = \mathbf{M}_{CS}^{(1,0)} \) |

The electric field \( \mathbf{E} \) of a generalized Bessel beam with matrix \( \mathbf{M} \) is the following:

\[
E_x = \frac{E_0}{k^2} \left( \frac{k^2 + k_x^2}{2} \mathbf{M}_{e,x} + k_x \mathbf{M}_{m,y} \right) f_n - \frac{k_x^2}{4} \left( \mathbf{M}_{e,x} + i \mathbf{M}_{e,y} \right) f_{n-2} + \left( \mathbf{M}_{e,x} - i \mathbf{M}_{e,y} \right) f_{n+2} \right) \),
\[
E_y = \frac{E_0}{k^2} \left( \frac{k^2 + k_y^2}{2} \mathbf{M}_{e,y} - k_x \mathbf{M}_{m,x} \right) f_n - \frac{k_y^2}{4} \left( \mathbf{M}_{e,x} + i \mathbf{M}_{e,y} \right) f_{n-2} - \left( \mathbf{M}_{e,x} - i \mathbf{M}_{e,y} \right) f_{n+2} \right) \),
\[
E_z = -\frac{E_0 k_t}{2k^2} \left[ k_x \left( \mathbf{M}_{e,x} - i \mathbf{M}_{e,y} \right) + i k \left( \mathbf{M}_{m,x} - i \mathbf{M}_{m,y} \right) \right] f_{n+1} + \left[ k_x \left( \mathbf{M}_{e,x} + i \mathbf{M}_{e,y} \right) \right] f_{n-1} \right) \).

Corresponding expressions for the magnetic field were obtained using duality transformation.

### 3. Numerical simulations

The above theoretical results were applied to generalize the Mueller calculus (involving Muller and amplitude scattering matrices) to vortex beams, i.e. beams with non-zero orbital angular momentum. The Mueller calculus is used in many implementations of the discrete dipole approximation, including a popular open-source ADDA package [6]. Besides the standard Bessel beam types (LE, LM, CS, TEC, and TMC – they are used to generate TE and TM modes [7] effectively), we have implemented a generalized Bessel beam specified by a matrix \( \mathbf{M} \) (4 complex values) in ADDA. The latter correspond to a linear combination of 4 basis beams (x- and y-polarizations of LE and LM types). We successfully validated this implementation against the reference results of GLMT for spheres [8]. Currently, the code is available at a separate fork of ADDA: https://github.com/stefaniagl/adda.

![Figure 1](image-url) Geometry of scattering of high-order Bessel beam by the Chebyshev particle with \( n = 8, \varepsilon = 0.1 \).
The scattering intensity in H-plane (yz-plane) and E-plane (xz-plane) are expressed with the Mueller matrix elements as

\[ I_\perp = S_{11} - S_{12}, \quad I_\parallel = S_{11} + S_{12}. \]  

(9)

The results in (Figure 2) show the scattering intensities of various high-order Bessel beam types by the Chebyshev particle (expressed in spherical coordinates as \( r = [1 + \epsilon \cos(n\theta)] \) with \( \epsilon = 0.1 \) and \( n = 8 \)). The scheme in (Figure 1) depicts particle geometry and position.

4. Conclusion

The theoretical results clarify the general idea and relationships between various types of Bessel beams. Similar derivations can potentially be applied to other complex light beams. The implementation of these beams in the open-source ADDA code enables one to simulate the scattering of various Bessel beams by particles with arbitrary shape and internal structure. Future research directions include scattering Bessel beams by particles near a substrate and calculating optical forces.

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