Implementation of Various Bessel Beams in the Framework of the Discrete Dipole Approximation

Stefania A. Glukhova^{1, 2, a)} and Maxim A. Yurkin^{1, 2}

¹Voevodsky Institute of Chemical Kinetics and Combustion, SB RAS, Institutskaya 3, 630090 Novosibirsk, Russia ²Novosibirsk State University, Pirogova 2, 630090 Novosibirsk, Russia

^{a)}Corresponding author: : <u>stefgluhova@gmail.com</u>

Abstract. In this work we generalize the classical framework of Mueller (or amplitude) scattering matrices for the Bessel beams (BBs). For that we extend the rotation relations of BBs (considering 'vortex' additional phase factor) for an arbitrary angle, which are useful for solving the scattering problem in a rotated coordinate system. Thus, we rework the existing classification of the BBs and their polarizations with the focus on rotation relations between them. We have already implemented all BB types with arbitrary polarizations/rotations in a separate branch of ADDA, and are working on testing the code. As a result, it should be trivial for anyone to simulate the scattering of Bessel beams by arbitrary inhomogeneous particles, including randomly orientated ones.

INTRODUCTION

In recent years the Bessel beams (BBs) are gaining popularity [1]. The area of Bessel beam applications contains optical levitation and manipulation, laser materials processing, non-linear optics, optical acceleration, optical guiding and alignment, microscopic imaging, and so on [2–8]. They belong to the class of non-diffraction beams, which do not spread out during propagation (like an unbounded plane wave). While the scattering of these beams by particles of simple shapes, such as spheres, has been considered in the literature [9], it is rarely done for complex particles.

The discrete dipole approximation (DDA) is a popular method to simulate scattering and absorption of electromagnetic waves by particles of arbitrary shape and internal structure [10]. In principle, the DDA and the corresponding computer codes are applicable to arbitrary incident fields. However, the practical simulations for any beam types are much more accessible to the practitioners if these beams are built into the code. Thus, the final goal of this work is the implementation of BBs in the open-source ADDA code [11].

KNOWN BESSEL-BEAM TYPES

It is convenient to use Hertz vector potentials Π_e and Π_m to describe BB types [12]. The electric and magnetic fields are then expressed as:

$$\mathbf{E} = \nabla \times \nabla \times \mathbf{\Pi}_{\mathrm{e}} - \nabla \times \partial \mathbf{\Pi}_{\mathrm{m}} / \partial t, \tag{1}$$

$$\mathbf{H} = \nabla \times \nabla \times \mathbf{\Pi}_{\mathrm{m}} - \nabla \times \partial \mathbf{\Pi}_{\mathrm{e}} / \partial t.$$
⁽²⁾

Note that these vector potentials are not unique for given fields. For BBs the amplitudes of both Π_e and Π_m take the following form in the cylindrical coordinate system

$$\Pi \stackrel{\text{\tiny def}}{=} J_n(k_t \rho) e^{in\varphi} e^{-ik_z z},\tag{3}$$

where J_n is the Bessel function of the first kind (*n* is the order of BB), $k_t \stackrel{\text{def}}{=} k \sin \alpha_0$ and $k_z \stackrel{\text{def}}{=} k \cos \alpha_0$ are the transverse and longitudinal components of the wave vector *k*, respectively, and α_0 is the half cone angle (Fig. 1). Varying the direction of the Hertz vector potentials, we obtain different types of BBs.

5th International Conference on Metamaterials and Nanophotonics METANANO 2020 AIP Conf. Proc. 2300, 020037-1–020037-5; https://doi.org/10.1063/5.0032030 Published by AIP Publishing. 978-0-7354-4034-0/\$30.00



FIGURE 1 Geometry of BB generation using an axicon (conical lens) [12].

TE and TM (transverse electric and magnetic) BBs are obtained from $\Pi_{\rm m} = \Pi \mathbf{e}_z$, $\Pi_{\rm e} = 0$ and $\Pi_{\rm e} = \Pi \mathbf{e}_z$, $\Pi_{\rm m} = 0$, respectively. where \mathbf{e}_z is the unit vector along the propagation direction. We denote the corresponding fields $\mathbf{E}_{\rm TE}$ and $\mathbf{H}_{\rm TM}$, respectively; they have zero z-components. The accompanying fields $\mathbf{H}_{\rm TE}$ and $\mathbf{E}_{\rm TM}$ have no zero components. These BB types are very convenient in reflection and transmission problems [13]. Also, TE and TM BBs of zero order are connected to the azimuthal and radial BB polarizations [14].

BB with linearly polarized electric and magnetic fields (LE and LM, respectively) are obtained from $\Pi_m = \Pi \mathbf{e}_t$, $\Pi_e = 0$ and $\Pi_e = \Pi \mathbf{e}_t$, $\Pi_m = 0$, respectively. Here \mathbf{e}_t is a polarization vector perpendicular to \mathbf{e}_z ; \mathbf{e}_t directed along y or x axes leads to so-called x- or y-linear polarizations of the corresponding fields: $\mathbf{E}_m^{(x)}$, $\mathbf{E}_m^{(y)}$ and $\mathbf{H}_e^{(x)}$, $\mathbf{H}_e^{(y)}$ for LE and LM fields, respectively (here subscripts m and e correspond to beam type) [14]. More specifically, these fields still have longitudinal components, i.e. the electric (for LE type) or magnetic (for LM type) field has zero components only along \mathbf{e}_t . The accompanying magnetic $\mathbf{H}_m^{(x)}$, $\mathbf{H}_m^{(y)}$ and electric fields $\mathbf{E}_c^{(x)}$, $\mathbf{E}_c^{(y)}$, have no zero components at all.

only along \mathbf{e}_t . The accompanying magnetic $\mathbf{H}_m^{(x)}$, $\mathbf{H}_m^{(y)}$ and electric fields $\mathbf{E}_e^{(x)}$, $\mathbf{E}_e^{(y)}$, have no zero components at all. Circularly symmetric (CS) BB types are defined by $\mathbf{\Pi}_m = \Pi \mathbf{e}_y/2$, $\mathbf{\Pi}_e = -\Pi \mathbf{e}_x/2$ and $\mathbf{\Pi}_m = -\Pi \mathbf{e}_x/2$, $\mathbf{\Pi}_e = -\Pi \mathbf{e}_y/2$ leading to two BB polarizations $\mathbf{E}_{cs}^{(1,0)}$ and $\mathbf{E}_{cs}^{(0,1)}$ (subscript CS is usually omitted in the literature) with circularly symmetric time-averaged Pointing vector. This BB type can also be produced using angular spectrum representation (ASR) [12]. One can also generalize these definitions to

$$\mathbf{E}_{\mathrm{CS}}^{(\alpha,\beta)} \stackrel{\text{def}}{=} \alpha \, \mathbf{E}_{\mathrm{CS}}^{(1,0)} + \beta \, \mathbf{E}_{\mathrm{CS}}^{(0,1)},\tag{4}$$

$$\mathbf{E}_{m,e}^{(\alpha,\beta)} \stackrel{\text{def}}{=} \alpha \, \mathbf{E}_{m,e}^{(x)} + \beta \, \mathbf{E}_{m,e}^{(y)},\tag{5}$$

$$|\alpha|^2 + |\beta|^2 = 1. \tag{6}$$

In particular, $\mathbf{E}_{m,e}^{(1,\pm i)}$ can be considered as generalizations of circularly-polarized plane waves, while both real α and β are similarly correspond rotated linear polarizations of a plane wave.

BESSEL BEAMS IN SCATTERING PROBLEMS

Additional complication arises from the fact that most light-scattering codes (including ADDA) are tailored for the calculation of the Mueller (or amplitude) scattering matrices, which requires simulations for two polarizations (commonly linear) of the incident field. Thus, we extended this approach to BBs, defining two basis polarizations for each BB type. It is natural to require these polarizations to be connected by $\pi/2$ rotation

$$\mathbf{E}^{\parallel} \propto \mathcal{R}_{\pi/2} \mathbf{E}^{\perp}(\mathbf{r}) = \mathbf{R}_{\pi/2} \mathbf{E}^{\perp}(\mathbf{R}_{-\pi/2} \mathbf{r}), \tag{7}$$

where \mathcal{R}_{χ} is the rotation operator (acting on a field) and \mathbf{R}_{χ} is a 3×3 rotation matrix (acting on a vector), both over angle χ around the beam propagation axis (positive value – in counterclockwise direction). Parallel and perpendicular polarizations are considered with respect to the scattering plane, as typically used for scattering matrices [15]. For a plane wave the rotation transformation of \mathbf{r} in Eq. (7) is redundant, and the proportionality can be replaced by equality. By contrast, BB is generally a vortex beam (i.e. its phase depends on azimuthal angle φ) leading to the additional phase factor discussed below.

Redefined Bessel-beam polarizations

We already have two polarizations for each of LE, LM, and CS BBs: $\mathbf{E}_{m}^{(x)}$, $\mathbf{E}_{m}^{(y)}$; $\mathbf{E}_{e}^{(x)}$, $\mathbf{E}_{e}^{(y)}$; and $\mathbf{E}_{cs}^{(1,0)}$, $\mathbf{E}_{cs}^{(0,1)}$, respectively. Here and further we discuss only the electric fields, since they are sufficient for light-scattering simulations of non-magnetic materials. The relations for magnetic fields can be obtained analogously, if needed. The only missing component is the polarizations for TE and TM types, since these types are almost axisymmetric, leading to trivial transformations under rotations:

$$\mathcal{R}_{\chi} \mathbf{E}_{\mathrm{TE,TM},n} = e^{-in\chi} \mathbf{E}_{\mathrm{TE,TM},n},\tag{8}$$

where we explicitly specify the order of BB as a subscript to avoid confusion.

Therefore, we introduce $\mathbf{E}_{\text{TE},n-1}^{(x)}$, $\mathbf{E}_{\text{TE},n-1}^{(y)}$, $\mathbf{E}_{\text{TM},n-1}^{(x)}$, $\mathbf{E}_{\text{TM},n-1}^{(y)}$ determined by the following equations:

$$\mathbf{E}_{\text{TE,TM},n} = \mathbf{E}_{\text{TE,TM},n-1}^{(x)} + i \, \mathbf{E}_{\text{TE,TM},n-1}^{(y)},\tag{9}$$

$$\mathcal{R}_{\pi/2} \mathbf{E}_{\text{TE,TM},n}^{(x)} = e^{-in\pi/2} \mathbf{E}_{\text{TE,TM},n}^{(y)}, \tag{10}$$

and have the following explicit expressions:

$$\mathbf{E}_{\mathrm{TE},n}^{(x,y)} = -\csc\alpha_0 \left(\mathbf{E}_{\mathrm{e},n}^{(x,y)} - \mathrm{i}\cos\alpha_0 \ \mathbf{E}_{\mathrm{m},n}^{(x,y)} \right),\tag{11}$$

$$\mathbf{E}_{\mathrm{TM},n}^{(x,y)} = -\csc\alpha_0 \left(\mathbf{E}_{\mathrm{m},n}^{(x,y)} + i\cos\alpha_0 \mathbf{E}_{\mathrm{e},n}^{(x,y)} \right). \tag{12}$$

Thus, similarly to Eqs. (4)–(6) we can determine general polarizations (α , β) for TE and TM BB types.

Rotation relations

Many light-scattering codes (including ADDA) allow one to rotate the particle and/or the incident beam by arbitrary angles. The corresponding rotation relations are well-known for plane waves [16], but need to be re-derived for the BBs. The ingenuity of the above definition of BB polarizations implies universal rotation transformation over the beam axis

$$\mathcal{R}_{\chi} \mathbf{E}_{n}^{(\alpha,\beta)} = e^{-\mathrm{i}n\chi} \Big(\cos\chi \, \mathbf{E}_{n}^{(\alpha,\beta)} + \sin\chi \, \mathbf{E}_{n}^{(-\beta,\alpha)} \Big), \tag{13}$$

for arbitrary (α, β) and each BB type (subscripts m, e, CS, TE, TM). Note that by definition $\mathbf{E}_n^{(-1,0)} = -\mathbf{E}_n^{(1,0)}$. Moreover, Eq. (13) implies Eq. (10) and trivial relations

$$\mathcal{R}_{\pi} \mathbf{E}_{n}^{(\alpha,\beta)} = (-1)^{n+1} \mathbf{E}_{n}^{(\alpha,\beta)},$$

$$\mathcal{R}_{2\pi} \mathbf{E}_{n}^{(\alpha,\beta)} = \mathbf{E}_{n}^{(\alpha,\beta)},$$

(14)

which are also satisfied by $\mathbf{E}_{\text{TE},n}$ and $\mathbf{E}_{\text{TM},n}$ (without superscripts), as follows from Eq. (8).

Scattering matrices

Overall, Eq. (13) is the most straightforward generalization of rotation relations for plane waves (corresponding to n = 0), since the dependence on n is localized into a common phase factor. For any scattering plane there exist real α and β such that for a plane wave $\mathbf{E}^{\perp} = \mathbf{E}^{(\alpha,\beta)}$, $\mathbf{E}^{\parallel} = \mathbf{E}^{(-\beta,\alpha)}$ (e.g., $\alpha = 1$, $\beta = 0$ for yz scattering plane and default propagation direction along the z-axis). And we postulate the same definitions for each of the five BB types, i.e. α and β are determined by the scattering plane the same way as for plane waves. This leads to the definition of the amplitude scattering matrix for BBs, i.e. it is a matrix with columns, describing the scattered field due to incident $\mathbf{E}^{\parallel}(\mathbf{r})$ and $\mathbf{E}^{\perp}(\mathbf{r})$, respectively (Eq. (3.12) of [15]). Two values in each column correspond to the projections of the scattered field parallel and perpendicular to the scattering plane, respectively, but for this part the specifics of the incident wave are completely irrelevant.

Next, we define the Mueller matrix for BBs using the standard transformation from the amplitude one (Eq. (3.16) of [15]). As usually, it relates the Stokes vectors of the incident and scattered fields, but the Stokes vector of the incident BBs does not have a clear physical meaning. Still we postulate this vector by standard expressions (Eq. (2.84) of [15]), using the expansion coefficient of the incident field into $\mathbf{E}^{||}(\mathbf{r})$ and $\mathbf{E}^{\perp}(\mathbf{r})$. Importantly, any linear combination of the above components, e.g., $\mathbf{E}^{(\alpha,\beta)}$, can be represented through this Stokes vector.

Therefore, once the light-scattering problem is solved for two polarizations of the specific BB, the solution for any their combination, i.e. $\mathbf{E}^{(\alpha,\beta)}$ of the same BB type, can be obtained for free. The corresponding scattered fields and Stokes vectors can be, most directly, obtained through the generalized amplitude and Mueller matrices, respectively.

The immediate benefit of this linearity is related to the simulation of scattering for randomly oriented particles. Generally, in the DDA (or similar methods) the particle orientation need to be sampled over three Euler angles [17], and the scattering problem need to be solved for each orientation independently. For plane waves (that are naturally axisymmetric) – the well-known trick is to replace the rotation over the first Euler angle by the rotation of the scattering plane (i.e. varying azimuthal scattering angle) [11]. The corresponding values are each obtained from a simulation for single particle orientation.

The above analysis shows that the same optimization remains valid for BBs, since the scattered field in a rotated scattering plane can be obtained from Eq. (13) (assuming that the rotation center lies on the beam axis). Moreover, the resulting expressions for scattered Stokes vector (to be averaged over particle orientations) are exactly the same as that for the plane wave, since the factor $e^{-in\chi}$ cancels out.

NUMERICAL SIMULATIONS

We have already implemented all BBs with arbitrary polarizations/rotations in a separate branch of ADDA – https://github.com/stefanyagl/adda, and are working on testing the code. First simulation results are shown in Fig. 2. The scattering intensity in H-plane (yz-plane) expressed through Mueller matrix elements

$$I_{\perp} = S_{11} - S_{12},\tag{15}$$

is plotted in comparison with the results of [18]. Further numerical results and comparison with reference methods will be presented at the conference.



FIGURE 2 The comparison of the scattering intensities I_{\perp} in *yz*-plane obtained with the DDA (our results) and SIEM [18] for scattering of zero-order CS BB with $\alpha_0 = 15^\circ$ and $\lambda = 0.6328 \,\mu\text{m}$ by a coated sphere (inner core with m = 1.55 and radius 0.5λ , outer shell with m = 1.33 and radius λ), centered on a beam axis. In the DDA we used 64 dipoles per λ .

CONCLUSION

We have extended the definitions of polarizations of various BB types to be consistent with the classical framework of amplitude and Mueller scattering matrices, commonly employed for plane waves. Apart from conceptual simplicity, this allows one to keep optimizations of orientation averaging, developed for plane waves. The implementation of BBs in the open-source code ADDA allows anyone to easily simulate the scattering of BBs by arbitrary inhomogeneous particles.

ACKNOWLEDGMENTS

We thank Gérard Gouesbet and James A. Lock for insightful discussions. This work is supported by the Russian Science Foundation (Grant No. 18-12-00052).

REFERENCES

- 1. J.J. Wang, T. Wriedt, J.A. Lock, and Y.C. Jiao, J. Quant. Spectrosc. Radiat. Transfer 195, 8–17 (2017).
- 2. D. McGloin and K. Dholakia, Contemp. Phys. 46, 15–28 (2005).
- 3. V. Garcés-Chávez, D. McGloin, H. Melville, W. Sibbett, and K. Dholakia, Nature 419, 145–147 (2002).
- 4. R. Stoian, M.K. Bhuyan, G. Zhang, G. Cheng, R. Meyer, and F. Courvoisier, Advanced Optical Technologies 7, 165–174 (2018).
- 5. F. He, J. Yu, Y. Tan, W. Chu, C. Zhou, Y. Cheng, and K. Sugioka, Sci Rep 7, 40785 (2017).
- 6. M. Duocastella and C.B. Arnold, Laser & Photonics Reviews 6, 607–621 (2012).
- 7. G. Antonacci, D. Caprini, and G. Ruocco, Applied Physics Letters 114, 013502 (2019).
- T.A. Planchon, L. Gao, D.E. Milkie, M.W. Davidson, J.A. Galbraith, C.G. Galbraith, and E. Betzig, Nat Methods 8, 417–423 (2011).
- 9. F.G. Mitri, R.X. Li, L.X. Guo, and C.Y. Ding, Annals of Physics 361, 120–147 (2015).
- 10. M.A. Yurkin and A.G. Hoekstra, J. Quant. Spectrosc. Radiat. Transfer 106, 558–589 (2007).
- 11. M.A. Yurkin and A.G. Hoekstra, J. Quant. Spectrosc. Radiat. Transfer 112, 2234–2247 (2011).
- 12. J.J. Wang, T. Wriedt, J.A. Lock, and L. Mädler, J. Quant. Spectrosc. Radiat. Transfer 184, 218-232 (2016).
- 13. M.A. Salem and H. Bağcı, J. Opt. Soc. Am. A 29, 139 (2012).
- 14. Y. Wang, W. Dou, and H. Meng, Optics Express 22, 7821 (2014).
- 15. C.F. Bohren and D.R. Huffman, Absorption and Scattering of Light by Small Particles (Wiley, New York, 1983).
- 16. M.I. Mishchenko, L.D. Travis, and A.A. Lacis, *Scattering, Absorption, and Emission of Light by Small Particles* (Cambridge University Press, Cambridge, 2002).
- 17. M.I. Mishchenko and M.A. Yurkin, Opt. Lett. 42, 494–497 (2017).
- 18. Z. Chen, Y. Han, Z. Cui, and X. Shi, J. Opt. 16, 055701 (2014).