A framework for the finite series method of the generalized Lorenz-Mie theory and its application to freely-propagating Laguerre-Gaussian beams

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Abstract

In face of a revival of interest in the finite series (FS) method due to recent developments upon generalized Lorenz-Mie theories (GLMTs), a more general, understandable, and systematic formulation is proposed. Possibly due to an apparent lack of flexibility in the FS method's earlier statements, there has been a void in its use since the 1990s. Particularly, the method demands some degree of mathematical labor each time it is applied to a different kind of field profile. Furthermore, the algebraic complexity of its earlier occurrences might also have weighted upon the method's historical shunning. Dissecting the later works reclaiming the FS, several possibilities for generalization, simplification, and organization were found. Accordingly, with the intent to render the method more approachable and to encourage its use, this work derives an alternative path suitable for both understanding and implementation. Applying the procedure, expressions for the beam shape coefficients of freely propagating Laguerre-Gaussian beams are obtained in closed form in a more straightforward manner when compared to previous formulations – this time not relying on recursions.

Keywords: Finite series, Generalized Lorenz-Mie theory, Laguerre-Gaussian beams

1. Introduction

An effective class of approaches for solving problems in electromagnetic scattering is commonly known as T-matrix methods [1–3]. These generically consist of formulations equivalent to expressing fields in a basis of vector spherical wave functions (VSWFs) to model scattering phenomena through transformations described by matrix operators in the function space [4]. Within this category lie the generalized Lorenz-Mie theories (GLMTs) [4–6]. Still, there is a variety of GLMTs to choose, and, among them, the GLMT *stricto sensu*, which refers to the scattering by a single homogeneous sphere of arbitrary refractive index. In broad strokes, the GLMT *stricto sensu* – which shall be addressed as "*the* GLMT" throughout this work – mainly consists of modeling scattering phenomena in terms of beam-shape coefficients (BSCs) which factor in the multipole expansion of the incident field from Bromwich scalar potentials [5] or in terms of VSWFs [4]. Therefore, once the BSCs are known, scattering events can be studied in depth through the GLMT.

Since finding BSCs for a specific kind of wave arrangement is usually not a trivial task, the subject has been studied in depth throughout the years. Thus several different methods may be found in the literature. Usual examples include: quadrature methods [5, 7, 8]; the (integral) localized approximation (LA) [9–13]; the finite series (FS) method [7, 14]; or the angular spectrum decomposition (ASD), e.g. Sections 3 and 4 in [15]. Each procedure features its own set of advantages and disadvantages. As one might expect, localized approximations generally do not deliver the exact coefficients of Maxwellian beams, even though they are often more time-efficient than, say, numerical quadrature methods [16, 17]. On the other hand, quadrature methods do entail integral expressions that indeed represent the exact BSCs, which may even be faster than the LA when such quadratures are given by explicit solutions. The FS method for finding BSCs, which, like quadratures, is mathematically rigorous in the sense that it delivers the exact BSCs, plays a central role in this article. Nevertheless, FS have historically been put aside due to their intricate mathematical formulation which might seem rather baffling to the untrained eye. This resulted in a hiatus of decades in its use since its inception in the 1980s by Gouesbet, Gréhan & Maheu [7, 14]. Furthermore, unlike numerical quadrature methods, the FS tends to lack flexibility, potentially demanding an undesirable load of algebraic effort each time it is applied to a new sort of wave.

More recently, the FS method has been brought back to model relevant classes of waves other than regular Gaussian beams in the GLMT, such as: Bessel beams [18], freely propagating Laguerre-Gaussian (LG) beams [17, 19], lens-focused LG beams [20, 21], and Bessel-Gaussian beams [22], Hermite-Gaussian beams [23], Ince-Gaussian beams [24], etc. Such families of "Gaussian-like" beams have been shown to benefit quite considerably from the FS, delivering exact BSCs while outperforming numerical quadratures in computational efficiency [17, 21]. Closely watching each of these later FS formulations, improving upon a generalization by Ambrosio [18], we have been able to hone the FS method's mathematical formalism in a cleaner, yet no less systematic, layout, better suited to aid its following computational implementation. Moreover, the FS framework here presented should serve as a more understandable guideline to anybody interested in applying it in real problems.

To illustrate the value in this new procedure, we refer to a recent FS formulation, in retrospect, of freely propagating LG beams by Gouesbet, Votto & Ambrosio [19] which relied on recursions, demanding some degree of care in its implementation [17]. This time, however, we arrive at closed form expressions for these LG BSCs eliminating recursions and mitigating eventual issues with respect to the numerical error propagation which tends to occur for Gaussian-like beams under the FS. Such closed-form expressions were already obtained in Ref. [17], but this time they are deduced in a significantly more straightforward manner illustrating the importance of such a framework for the method. Given the relevance of such beams due to their ability to transfer angular momentum to illuminated objects, such improvements are in order [25–35].

In short, this article is organized in the following set of sections. Section 2 derives the main expressions, stating the general FS method. In Section 3, the LG BSCs are found in closed form through the FS procedure. In most numerical experiences with the FS method, some peculiarities have been found; Section 4 then shows some results for LG BSCs paying attention to any issues involving error propagation. Finally, we give our closing remarks in Section 5.

2. Finite series method

2.1. The Neumann expansion theorem in context

In works regarding the finite series method, the **Neumann Expansion Theorem (NET)** is usually presented as a special case of Gegenbauer's generalization of Neumann's expansion [36, Section 16.13]. Its statement is often presented as follows.

Theorem (NET)**.** *Let $g : (0, \infty) \to \mathbb{C}$ be a map that satisfies the Bessel function Neumann expansion*

$$x^{\frac{1}{2}} g(x) = \sum_{n=0}^{\infty} c_n J_{n+1/2}(x), \tag{2.1}$$

and the Maclaurin series

$$g(x) = \sum_{n=0}^{\infty} b_n x^n, \tag{2.2}$$

both convergent. One then may write the Neumann coefficients c_n in (2.1) *in terms of the Maclaurin coefficients b_n in* (2.2) *– through a* "finite series"*:*

$$c_n = \left(n + \frac{1}{2}\right) \sum_{p=0}^{\leq n/2} 2^{\frac{1}{2}+n-2p} \frac{\Gamma\left(\frac{1}{2} + n - p\right)}{p!} b_{n-2p}. \tag{2.3}$$

Even though this statement of the NET could be used to derive the FS method as it is, it might be preferable to equivalently adapt it to the subsequent GLMT steps before. Matching usual GLMT field expressions [5], we do so in terms of spherical Bessel functions of the first kind j_n instead of the half-integer order Bessel functions $J_{n+\frac{1}{2}}$ in (2.1). From the definition of spherical Bessel functions,

$$J_{n+1/2}(x) = \sqrt{\frac{2x}{\pi}} j_n(x), \tag{2.4}$$

the Bessel function Neumann expansion in (2.1) may be written as a **spherical Bessel function Neumann series**:

$$x^{\frac{1}{2}} g(x) = \sum_{n=0}^{\infty} c_n x^{\frac{1}{2}} \sqrt{\frac{2}{\pi}} j_n(x), \tag{2.5}$$

$$g(x) = \sum_{n=0}^{\infty} \alpha_n j_n(x), \tag{2.6}$$

where $\alpha_n = c_n \sqrt{2/\pi}$. Therefore, in order to pave the way for a more understandable definition of the FS method, the NET may be alternately stated as below.

Theorem (Adapted NET)**.** *Let $f : (0, \infty) \to \mathbb{C}$ admitting convergent spherical Bessel function Neumann series and Maclaurin series such that*

$$f(x) = \sum_{n=0}^{\infty} \alpha_n j_n(x) = \sum_{n=0}^{\infty} b_n x^n, \tag{2.7}$$

then its Neumann coefficients α_n may be written in terms of the Maclaurin coefficients b_n as

$$\alpha_n = \frac{2n+1}{\sqrt{\pi}} \sum_{p=0}^{\leq n/2} 2^{n-2p} \frac{\Gamma\left(\frac{1}{2} + n - p\right)}{p!} b_{n-2p}. \tag{2.8}$$

As a side note, see that we maintain the notation for the the Maclaurin coefficients b_n found in other works employing the FS method, even though their expressions may not be identical due to the fact that the adapted NET now concerns the coefficients α_n instead of c_n [18–20, 22]. Since these b_n do play the same role in both versions of the method, producing the same BSCs overall, their notation is kept the same.

2.2. Finite series: throwing the NET into the GLMT

Here, we assemble the FS from the adapted NET. Throughout the literature, it is usual to address the following set of steps as "the NET procedure" [5, 19]. In brief, the FS method allows writing BSCs through weighted sums of Maclaurin coefficients of a function that depends on the field profile in a subset of $\mathbb{R}^3$. Throughout this paper, we denote the spherical coordinates by (r, θ, ϕ), where θ gives polar angles, and ϕ azimuth angles.

Consider a monochromatic beam of wave number k, whose BSCs are $g_{n,\mathrm{TM}}^m$ and $g_{n,\mathrm{TE}}^m$, to compose an electric field $\mathbf{E}$ and a magnetic field $\mathbf{H}$. We wish to determine any such beam's BSC $g_{n,\mathrm{TX}}^m$, where TX is either the transverse magnetic TM or the transverse electric TE mode, given that the radial components of the electromagnetic fields are known. In order to find each $g_{n,\mathrm{TX}}^m$, define X_r to be such that the pair (X_r, TX) is either (E_r, TM) or (H_r, TE), and fix $\theta = \theta_0$. For each m, let the function $f_m : (0, \infty) \to \mathbb{C}$, defined as

$$f_m(kr) = \frac{kr}{X_0} \int_0^{2\pi} X_r\left(r, \theta_0, \phi\right) e^{-\mathrm{i}m\phi}\, \mathrm{d}\phi, \tag{2.9}$$

assume convergent Maclaurin series as in (2.7) from the adapted NET. This definition of f_m in (2.9) shall be justified further ahead. We claim that, applying the NET to the GLMT incident field expressions, the TX BSCs $g_{n,\mathrm{TX}}^m$ may be given in terms of these Maclaurin coefficients b_j through the finite sum

$$g_{n,\mathrm{TX}}^m = \sum_{q=0}^{\leq n/2} F_{n,q}^m b_{n-2q}. \tag{2.10}$$

This is a generic way to state the FS method, with the $F_{n,q}^m$ coefficients as determined further ahead.

More simply, to compute a BSC $g_{n,\mathrm{TX}}^m$ through the FS method is to:

(i) express the incident field's radial component X_r at $\theta = \theta_0$,

(ii) find the function $f_m(x = kr)$ as in (2.9),

(iii) calculate the Maclaurin coefficients b_n of f_m,

(iv) apply the NET to find the TX BSC $g_{n,\mathrm{TX}}^m$ through (2.10).

The brief description above is more valuable than it may seem at first glance. Essentially, it shows that writing the Maclaurin expansion for a chosen θ_0 allows finding any BSC through the coefficients $F_{n,q}^m$ once they are determined. Moreover, it is a manageable frame for further implementing the FS method in a programming language. With respect to code, this formulation serves as a basis for an abstract class that implements the FS in Votto's open-source Python package for the GLMT, *glmtech* [37]. With the $F_{n,q}^m$ as deduced below, the Python class solely requires a method for evaluating the Maclaurin coefficients b_j, as in step (iii) above, to then return any desired BSC. Generic expressions for FS BSCs as in (2.10), in terms of the Maclaurin coefficients of their specific f_m functions, are given below.

Again, as we shall soon see, whereas the TM and TE BSC equations derived below may not seem identical to other FS formulations, they do represent the same exact BSCs. That is, even though our adaptation preserves the notation for the coefficients b_j, their definition does slightly differ for the sake of algebraic simplification as explained above.

2.2.1. TM mode

According to the GLMT (see [5, Eq. (3.10)] or [20, Eq. (47)]), the electric field's radial component may be laid in the form

$$\begin{aligned} E_r = &\sum_{n=1}^{\infty} \sum_{m=-n}^{n} E_0 (-\mathrm{i})^{n+1} \frac{2n+1}{kr} g_{n,\mathrm{TM}}^m \\ &\times j_n(kr) P_n^{|m|}(\cos\theta) \exp(\mathrm{i}m\phi), \end{aligned} \tag{2.11}$$

where j_n denotes the spherical Bessel functions of the first kind, and $P_n^{|m|}$ denotes the associated Legendre functions using Hobson's notation. Similar to the quadrature method [5], we integrate from 0 to 2π with respect to ϕ in order to eliminate the inner m-sum with the following orthogonality relation in mind:

$$\int_0^{2\pi} e^{\mathrm{i}m\phi} e^{-\mathrm{i}p\phi} \mathrm{d}\phi = 2\pi \delta_m^p, \tag{2.12}$$

where δ is the Kronecker delta – $\delta_a^b = 1$ if $a = b$ and $\delta_a^b = 0$ otherwise. Fixing m, multiplying by $\exp(-\mathrm{i}m\phi)$, and integrating both sides of (2.11), we obtain

$$\begin{aligned} &\int_0^{2\pi} E_r \exp(-\mathrm{i}m\phi) \mathrm{d}\phi \\ &\quad = \sum_{n=1}^{\infty} 2\pi E_0 (-\mathrm{i})^{n+1} \frac{2n+1}{kr} g_{n,\mathrm{TM}}^m \\ &\quad \times P_n^{|m|}(\cos\theta) j_n(kr). \end{aligned} \tag{2.13}$$

Note it suffices to fix a value for θ to obtain a Neumann series as in Section 2.1. Then, let $\theta = \theta_0$,

$$\begin{aligned} f_m(kr) &= \frac{kr}{E_0} \int_0^{2\pi} E_r|_{\theta=\theta_0} \exp(-\mathrm{i}m\phi) \mathrm{d}\phi \\ &= \sum_{n=1}^{\infty} \underbrace{\left[2\pi(-\mathrm{i})^{n+1}(2n+1) P_n^{|m|}(\cos\theta_0) g_{n,\mathrm{TM}}^m\right]}_{\alpha_n} j_n(kr) \\ &= \sum_{n=1}^{\infty} \alpha_n j_n(kr) = \sum_{n=0}^{\infty} b_n (kr)^n. \end{aligned} \tag{2.14}$$

Now, if $x = kr$, we have a Neumann series in the same form of (2.7), where

$$f_m(x) = \frac{x}{E_0} \int_0^{2\pi} E_r\left(\frac{x}{k}, \theta_0, \phi\right) e^{-\mathrm{i}m\phi} \mathrm{d}\phi, \tag{2.15a}$$

$$\alpha_n = 2\pi(-\mathrm{i})^{n+1}(2n+1) P_n^{|m|}(\cos\theta_0) g_{n,\mathrm{TM}}^m, \tag{2.15b}$$

for $n \geq 1$, in which we note $\alpha_0 = 0$.

Should we know the Maclaurin coefficients b_n for $f_m(x)$ beforehand, we may use the FS expression in (2.8) for the Neumann coefficients α_n to then obtain from (2.15b) that, if $P_n^{|m|}(\cos\theta_0) \neq 0$,

$$g_{n,\mathrm{TM}}^m = \frac{\mathrm{i}^{n+1}}{2\pi^{\frac{3}{2}} P_n^{|m|}(\cos\theta_0)} \times \sum_{p=0}^{\leq n/2} 2^{n-2p} \frac{\Gamma\left(\frac{1}{2}+n-p\right)}{p!} b_{n-2p}. \tag{2.16}$$

2.2.2. TE mode

The starting point is very similar to the TM mode's (2.11) [5, 20]

$$H_r = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} H_0 (-\mathrm{i})^{n+1} \frac{2n+1}{kr} g_{n,\mathrm{TE}}^m \times j_n(kr) P_n^{|m|}(\cos\theta) \exp(\mathrm{i}m\phi). \tag{2.17}$$

Consequently, fixing $\theta = \theta_0$ gives

$$f_m(x) = \frac{x}{H_0} \int_0^{2\pi} H_r\left(\frac{x}{k}, \theta_0, \phi\right) e^{-\mathrm{i}m\phi} \mathrm{d}\phi, \tag{2.18a}$$

$$\alpha_n = 2\pi(-\mathrm{i})^{n+1}(2n+1) P_n^{|m|}(\cos\theta_0) g_{n,\mathrm{TE}}^m, \tag{2.18b}$$

for $n \geq 1$, and $\alpha_0 = 0$.

As in the TM mode, if f_m's Maclaurin coefficients b_n are known, from (2.8) and (2.18b):

$$g_{n,\mathrm{TE}}^m = \frac{\mathrm{i}^{n+1}}{2\pi^{\frac{3}{2}} P_n^{|m|}(\cos\theta_0)} \times \sum_{p=0}^{\leq n/2} 2^{n-2p} \frac{\Gamma\left(\frac{1}{2}+n-p\right)}{p!} b_{n-2p}, \tag{2.19}$$

but only if $P_n^{|m|}(\cos\theta_0) \neq 0$.

From the deductions above, one may notice that both TM and TE modes only differ on how the f_m function is evaluated. That is, their $F_{n,q}^m$ coefficients from (2.10) are the same:

$$F_{n,q}^m = \frac{\mathrm{i}^{n+1} 2^{n-2q-1}}{\pi^{3/2} P_n^{|m|}(\cos\theta_0) q!} \Gamma\left(\frac{1}{2}+n-q\right), \tag{2.20}$$

for $P_n^{|m|}(\cos\theta_0) \neq 0$.

2.3. The choice of θ_0

So long as the singularity conditions are satisfied, the FS method leaves the choice of θ_0 open. That is, Eqs. (2.16) and (2.19) only hold strictly under the condition that $P_n^{|m|}(\cos\theta_0) \neq 0$. Historically, it has been usual to adopt $\cos\theta_0 = 0$, with the caveat that singularity conditions cannot be satisfied for odd $(n-m)$ where $P_n^m(0) = 0$. In such cases, nevertheless, it is possible to evaluate closed-form expressions for Maclaurin coefficients by adopting a complementary procedure. We therefore now deal with the deviant case when $\cos\theta_0 = 0$, i.e. $\theta_0 = \pi/2$. For this, we split the BSC expressions into two different cases depending on what $g_{n,\mathrm{TX}}^m$ is evaluated: when $(n-m)$ is (i) even, and (ii) odd. Suitably, with reference to equations below, (2.16) for TM BSCs becomes (2.24) for even $(n-m)$ and (2.29) whenever it is odd. Likewise, (2.19) for TE BSCs splits into (2.30) and (2.32).

For this specific case where $\theta_0 = \pi/2$ the associated Legendre special values at the origin are, for $(n-m)$ even [38],

$$P_n^m(0) = (-1)^{\frac{n+m}{2}} \frac{(n+m-1)!!}{2^{\frac{n-m}{2}} \left(\frac{n-m}{2}\right)!}, \tag{2.21}$$

and $P_n^m(0) = 0$ otherwise. Note that for odd natural numbers n [39, Eq. 6.1.12]

$$n!! = \prod_{p=1}^{\frac{n+1}{2}} (2p-1) = \frac{2^{\frac{n+1}{2}}}{\sqrt{\pi}} \Gamma\left(\frac{n}{2}+1\right) \tag{2.22}$$

is the semi-factorial of n; then for even $(n-m)$,

$$P_n^m(0) = (-1)^{\frac{n+m}{2}} \frac{2^m}{\sqrt{\pi}} \frac{\Gamma\left(\frac{n+m+1}{2}\right)}{\left(\frac{n-m}{2}\right)!}. \tag{2.23}$$

It then becomes possible to rewrite (2.16) for even $(n-m)$ as

$$g_{n,\mathrm{TM}}^m = \frac{(-\mathrm{i})^{|m|-1}}{2^{|m|+1}\pi} \frac{\left(\frac{n-|m|}{2}\right)!}{\Gamma\left(\frac{n+|m|+1}{2}\right)} \times \sum_{p=0}^{\leq n/2} 2^{n-2p} \frac{\Gamma\left(\frac{1}{2}+n-p\right)}{p!} b_{n-2p}. \tag{2.24}$$

For odd $(n-m)$ when $\theta_0 = \pi/2$, the function $f_m(x)$ should be defined differently, meaning that the expressions for Maclaurin coefficients are not identical to (2.24). The first derivative of associated Legendre functions also holds the following special values at $\cos\theta = 0$ [38]:

$$\frac{\mathrm{d}P_n^m(0)}{\mathrm{d}\cos\theta} = (-1)^{\frac{n+m-1}{2}} \frac{(n+m)!!}{2^{\frac{n-m-1}{2}} \left(\frac{n-m-1}{2}\right)!}, \tag{2.25}$$

for odd $(n-m)$, while it equals zero otherwise. Substituting the semi-factorial, we obtain

$$\frac{\mathrm{d}P_n^m(0)}{\mathrm{d}\cos\theta} = \frac{(-1)^{\frac{n+m-1}{2}} 2^{m+1}}{\sqrt{\pi}} \frac{\Gamma\left(\frac{n+m}{2}+1\right)}{\left(\frac{n-m-1}{2}\right)!} \tag{2.26}$$

for odd $(n-m)$.

In this case, the FS expressions should be:

$$f_m(x) = \frac{x}{E_0} \int_0^{2\pi} \frac{\partial E_r\left(\theta = \frac{\pi}{2}\right)}{\partial\cos\theta} \exp(-\mathrm{i}m\phi) \mathrm{d}\phi = \sum_{n=0}^{\infty} b_n x^n, \tag{2.27}$$

$$\alpha_n = 2\pi(-\mathrm{i})^{n+1}(2n+1) \frac{\mathrm{d}P_n^{|m|}(0)}{\mathrm{d}\cos\theta} g_{n,\mathrm{TM}}^m, \tag{2.28}$$

with $\alpha_0 = 0$. Then, from Eqs. (2.8) and (2.28):

$$\begin{aligned} g_{n,\mathrm{TM}}^m &= \frac{(-\mathrm{i})^{|m|-2}}{2^{|m|+2}\pi} \frac{\left(\frac{n-|m|-1}{2}\right)!}{\Gamma\left(\frac{n+|m|}{2}+1\right)} \\ &\times \sum_{p=0}^{\leq n/2} 2^{n-2p} \frac{\Gamma\left(\frac{1}{2}+n-p\right)}{p!} b_{n-2p} \end{aligned} \tag{2.29}$$

for odd $(n-m)$.

Expressions for the TE mode are analogous and are given below. For $(n-m)$ even:

$$\begin{aligned} f_m(x) &= \frac{x}{H_0} \int_0^{2\pi} H_r\left(\theta = \frac{\pi}{2}\right) e^{-\mathrm{i}m\phi} \mathrm{d}\phi \\ &= \sum_{n=0}^{\infty} b_n x^n, \\ g_{n,\mathrm{TE}}^m &= \frac{(-\mathrm{i})^{|m|-1}}{2^{|m|+1}\pi} \frac{\left(\frac{n-|m|}{2}\right)!}{\Gamma\left(\frac{n+|m|+1}{2}\right)} \\ &\times \sum_{p=0}^{\leq n/2} 2^{n-2p} \frac{\Gamma\left(\frac{1}{2}+n-p\right)}{p!} b_{n-2p}. \end{aligned} \tag{2.30}$$

and, for $(n-m)$ odd,

$$\begin{aligned} f_m(x) &= \frac{x}{H_0} \int_0^{2\pi} \frac{\partial H_r\left(\theta = \frac{\pi}{2}\right)}{\partial \cos\theta} \exp(-\mathrm{i}m\phi) \mathrm{d}\phi \\ &= \sum_{n=0}^{\infty} b_n x^n, \end{aligned} \tag{2.31}$$

$$\begin{aligned} g_{n,\mathrm{TE}}^m &= \frac{(-\mathrm{i})^{|m|-2}}{2^{|m|+2}\pi} \frac{\left(\frac{n-|m|-1}{2}\right)!}{\Gamma\left(\frac{n+|m|}{2}+1\right)} \\ &\times \sum_{p=0}^{\leq n/2} 2^{n-2p} \frac{\Gamma\left(\frac{1}{2}+n-p\right)}{p!} b_{n-2p}. \end{aligned} \tag{2.32}$$

3. Laguerre-Gaussian beams

The freely propagating LG beams here studied are composed of LG modes, solutions to the scalar paraxial wave equation in cylindrical coordinates. Assuming propagation in the z-direction, their linearly polarized electric field phasors are then given by

$$\mathbf{E}(\mathbf{r}) = \hat{\mathbf{x}} \mathrm{LG}(\mathbf{r}) \exp(-\mathrm{i}kz), \tag{3.1}$$

with its corresponding instantaneous field given by $\mathbf{E}(\mathbf{r}, t) = \mathrm{Re}\{\mathbf{E}(\mathbf{r})\exp(+\mathrm{i}\omega t)\}$, where ω is the angular frequency and k is the wave number. Since the scalar approximation is employed, the field $\mathbf{E}$ does not satisfy Maxwell's equations; see that $\boldsymbol{\nabla} \cdot \mathbf{E} \neq 0$ in general for non-trivial solutions. This is what we mean by saying that such LG beam formulation is non-Maxwellian, which carries some implications when applying the GLMT that shall be explained in the next section. For now, we focus on obtaining LG BSCs through the FS steps deduced in Section 2.

First of all, since the BSCs of a (p, l) order LG beam satisfy the properties [19]

$$g_{n,\mathrm{TE}}^{l\pm 1} = \mp \mathrm{i} g_{n,\mathrm{TM}}^{l\pm 1}, \tag{3.2}$$

$$g_{n,\mathrm{TE}}^m = g_{n,\mathrm{TM}}^m = 0, \text{ for all } m \neq l \pm 1, \tag{3.3}$$

it suffices to find only TM BSCs. LG beams, in the formulation presented below, are an example where it is preferable to adopt $\theta_0 = \pi/2$, even though it implies finding two sets of Maclaurin coefficients.

As emphasized, in order to evaluate TM BSCs $g_{n,\mathrm{TM}}^m$, it suffices to find Maclaurin coefficients b_j for the two cases where $(n-m)$ is even or odd. Orderly, to find closed-form BSCs, for even $(n-m)$:

(1.i) express E_r at $\theta = \pi/2$,

(1.ii) find the respective f_m function,

(1.iii) calculate the Maclaurin coefficients b_j of f_m,

(1.iv) substitute the b_j coefficients in Eq. (2.24);

and for odd $(n-m)$:

(2.i) express $\partial E_r / \partial \cos\theta$ at $\theta = \pi/2$,

(2.ii) find the respective f_m function,

(2.iii) calculate the Maclaurin coefficients b_j of f_m,

(2.iv) substitute the b_j coefficients in Eq. (2.29).

3.1. Formulation

A z-propagating (p, l) LG mode, solution to the scalar paraxial wave equation in cylindrical coordinates (ρ, ϕ, z), may be defined by its wave number k, beam waist radius w_0, degree p and topological charge l. Let the Rayleigh length be $z_\mathrm{R} = kw_0^2/2$. In an on-axis configuration, the mode can be expressed as [40]

$$\begin{aligned} \mathrm{LG}_{p,l} &= \frac{C_{p,l}}{w} \left(\frac{\rho}{w}\sqrt{2}\right)^l L_p^l \left(2\frac{\rho^2}{w^2}\right) \exp(\mathrm{i}l\phi) \exp\left(-\frac{\rho^2}{w^2}\right) \\ &\times \exp\left[-\mathrm{i}k\frac{\rho^2}{2R} + \mathrm{i}(2p+l+1)\psi\right], \end{aligned} \tag{3.4}$$

where L_p^l are associated Laguerre polynomials, the beam radius w is

$$w = w(z) = w_0\sqrt{1 + \frac{z^2}{z_\mathrm{R}^2}}, \tag{3.5}$$

radius of curvature

$$R = R(z) = \frac{z^2 + z_\mathrm{R}^2}{z}, \tag{3.6}$$

fundamental Gouy phase

$$\psi = \psi(z) = \arctan\left(\frac{z}{z_{\mathrm{R}}}\right), \tag{3.7}$$

and normalization factor $C_{p,l}$ specific to the mode being

$$C_{p,l} = \sqrt{\frac{2p!}{\pi(1+\delta_l^0)(p+l)!}}, \tag{3.8}$$

so that $\langle \mathrm{LG}_{p,l}, \mathrm{LG}_{p',l'}\rangle = \iint_{-\infty}^{\infty} \mathrm{LG}_{p,l}\mathrm{LG}^*_{p',l'}\,\mathrm{d}x\mathrm{d}y = \delta_p^{p'}\delta_l^{l'}$ fixing $z = 0$. The associated Laguerre polynomials are given in closed form by [39, Section 22.3]

$$L_p^l(x) = \sum_{u=0}^{p} \frac{(-1)^u}{u!}\binom{p+l}{p-u}x^u \tag{3.9}$$

for $l > -1$.

Assume that the corresponding non-Maxwellian electric field is

$$\mathbf{E} = \hat{\mathbf{x}}\mathrm{LG}_{p,l}\exp(-\mathrm{i}kz), \tag{3.10}$$

then its radial component is

$$E_r = \mathrm{LG}_{p,l}\exp(-\mathrm{i}kz)\sin\theta\cos\phi. \tag{3.11}$$

The electric field's radial component is, therefore, given in spherical coordinates by:

$$\begin{aligned} E_r(r,\theta,\phi) = E_0\frac{C_{p,l}}{w}&\left(\sqrt{2}\frac{r}{w}\sin\theta\right)^l L_p^l\left(2\frac{r^2}{w^2}\sin^2\theta\right) \\ &\times \exp\left[-\mathrm{i}k\frac{r^2}{2R}\sin^2\theta + \mathrm{i}(2p+l+1)\psi + \mathrm{i}l\phi\right] \\ &\times \exp\left(-\frac{r^2}{w^2}\sin^2\theta\right) \\ &\times \exp\left(-\mathrm{i}kr\cos\theta\right)\sin\theta\cos\phi. \end{aligned} \tag{3.12}$$

Note that (3.12) may be shown to be equivalent, up to re-normalization, to Eq. (22) in [41] and Eq. (17) in [19].

Since each mode shall be reproduced separately, it is unnecessary to our purposes to carry the normalization factor $C_{p,l}$ through the calculations here forth. Therefore, we incorporate $C_{p,l}$ into the amplitudes E_0 or H_0 from now on.

3.2. Applying the finite series method

As stated before, since we shall choose $\theta_0 = \pi/2$, the FS procedure is split into two different cases: case 1, where $(n-m)$ is even, and case 2, otherwise. The BSCs themselves are finally determined by plugging the Maclaurin coefficients b_j: (i) from (3.23) into (2.24) in case 1, and (ii) from (3.38) into (2.29) in case 2.

3.2.1. Case 1

For $x = kr$ and $s = 1/kw_0$, and noting that $w = w_0$ for $\theta = \pi/2$, the radial electric field of the LG beam at $\theta = \pi/2$ is given, according to (3.12), as

$$\begin{aligned} E_r\left(\frac{x}{k},\frac{\pi}{2},\phi\right) = E_0ks\left(\sqrt{2}sx\right)^l L_p^l\left(2s^2x^2\right) \\ \times \exp\left(-s^2x^2\right)e^{\mathrm{i}l\phi}\cos\phi \end{aligned} \tag{3.13}$$

so that, for $m \in \mathbb{Z}$

$$\begin{aligned} f_m(x) &= \frac{x}{E_0}\int_0^{2\pi} E_r\left(\theta = \frac{\pi}{2}\right)e^{-\mathrm{i}m\phi}\,\mathrm{d}\phi \\ &= \pi ksx\left(\sqrt{2}sx\right)^l L_p^l\left(2s^2x^2\right) \\ &\quad\times \exp\left(-s^2x^2\right)\left(\delta_m^{l+1} + \delta_m^{l-1}\right), \end{aligned} \tag{3.14}$$

so that $g_{n,\mathrm{TM}}^m = 0$ for all $m \neq l\pm1$. Therefore, for $m = l\pm1$ and omitting the sub-index,

$$f(x) = \pi k2^{l/2}L_p^l\left(2s^2x^2\right)s^{l+1}x^{l+1}\exp(-s^2x^2), \tag{3.15}$$

which we want to Maclaurin-expand.

Now, to write the associated Laguerre polynomials in closed-form, define (see, e.g. Eq. (18.59) of Ref. [42]):

$$\begin{aligned} \alpha_{p,u}^l &= \frac{(-1)^u}{u!}\binom{p+l}{p-u}2^us^{2u} \\ &= \frac{(-1)^u}{u!}\frac{(p+l)!}{(p-u)!(l+u)!}2^us^{2u} \end{aligned} \tag{3.16}$$

so that, from (3.9),

$$L_p^l(2s^2x^2) = \sum_{u=0}^{p}\alpha_{p,u}^l x^{2u}. \tag{3.17}$$

Substituting (3.17) into (3.15),

$$f(x) = \pi k2^{l/2}s^{l+1}\sum_{u=0}^{p}\alpha_{p,u}^l\left[x^{2u+l+1}\exp\left(-s^2x^2\right)\right]. \tag{3.18}$$

Consider the following Maclaurin expansion:

$$x^\mu\exp\left(-s^2x^2\right) = \sum_{j=0}^{\infty}\frac{(-1)^j}{j!}s^{2j}x^{2j+\mu}, \tag{3.19}$$

and change the index in the sum in (3.19) so that we have a proper x^j term, i.e.

$$\begin{aligned} x^\mu\exp\left(-s^2x^2\right) &= \sum_{\substack{j=\mu \\ (j-\mu)\text{ even}}}^{\infty}\frac{(is)^{j-\mu}}{\left(\frac{j-\mu}{2}\right)!}x^j \\ &= \sum_{j=0}^{\infty}\beta(j,\mu)x^j \end{aligned} \tag{3.20}$$

by defining

$$\beta(j,\mu) = \begin{cases} \frac{(\mathrm{i}s)^{j-\mu}}{\left(\frac{j-\mu}{2}\right)!}, & j \geq \mu,\ (j-\mu) \text{ even}, \\ 0, & \text{otherwise.} \end{cases} \tag{3.21}$$

Substituting (3.20) into (3.18),

$$\begin{aligned} f(x) &= \sum_{j=0}^{\infty} \left[\pi k 2^{l/2} s^{l+1} \sum_{u=0}^{p} \alpha_{p,u}^{l} \beta(j, 2u+l+1) \right] x^j \\ &= \sum_{j=0}^{\infty} b_j x^j, \end{aligned} \tag{3.22}$$

the Maclaurin coefficients b_j become evident:

$$b_j = \pi k 2^{l/2} s^{l+1} \sum_{u=0}^{p} \alpha_{p,u}^{l} \beta(j, 2u+l+1), \tag{3.23}$$

for even $(n-m)$, so that the corresponding TM BSCs $g_{n,\mathrm{TM}}^{m}$ are readily obtained from Eq. (2.24).

3.2.2. Case 2

From (3.12),

$$\begin{aligned} \frac{\partial E_r \left(\theta = \frac{\pi}{2}\right)}{\partial \cos\theta} &= E_0 \mathrm{i} k 2^{\frac{l}{2}} L_p^l \left(2s^2 x^2\right) \\ &\times \left[2s^2 \left(2p+l+1-s^2x^2\right) - 1\right] \\ &\times (sx)^{l+1} \exp\left(-s^2x^2\right) e^{\mathrm{i}l\phi} \cos\phi. \end{aligned} \tag{3.24}$$

For $(n-m)$ odd, define f_m as

$$f_m(x) = \frac{x}{E_0} \int_0^{2\pi} \frac{\partial E_r \left(\theta = \frac{\pi}{2}\right)}{\partial \cos\theta} e^{-\mathrm{i}m\phi} \mathrm{d}\phi, \tag{3.25}$$

then

$$\begin{aligned} f_m(x) &= \mathrm{i}kx 2^{l/2} L_p^l \left(2s^2x^2\right) \left[2s^2 \left(2p+l+1-s^2x^2\right) - 1\right] \\ &\times s^{l+1} x^{l+1} \exp\left(-s^2x^2\right) \pi \left(\delta_m^{l+1} + \delta_m^{l-1}\right). \end{aligned} \tag{3.26}$$

So, we should only consider the two cases where $m = l \pm 1$, for which $f_m(x)$ is the same. Let

$$A = \mathrm{i}\pi k 2^{l/2} \left[2s^2(2p+l+1) - 1\right] s^{l+1}, \tag{3.27}$$

$$B = -2\mathrm{i}\pi k 2^{l/2} s^{l+5}, \tag{3.28}$$

then, omitting the sub-index,

$$f(x) = \left(A + Bx^2\right) L_p^l \left(2s^2x^2\right) x^{l+2} \exp\left(-s^2x^2\right). \tag{3.29}$$

Making use of the notation established in Eqs. (3.16), (3.21) we shall expand f. Rewriting Laguerre polynomials as in (3.17),

$$f(x) = \sum_{u=0}^{p} \left(A + Bx^2\right) \alpha_{p,u}^{l} \left[x^{2u+l+2} \exp\left(-s^2x^2\right)\right]. \tag{3.30}$$

Also consider $f(x) = f^A(x) + f^B(x)$ with

$$f^A(x) = A \sum_{u=0}^{p} \alpha_{p,u}^{l} \left[x^{2u+l+2} \exp\left(-s^2x^2\right)\right] = \sum_{j=0}^{\infty} b_j^A x^j, \tag{3.31}$$

$$f^B(x) = B \sum_{u=0}^{p} \alpha_{p,u}^{l} \left[x^{2u+l+4} \exp\left(-s^2x^2\right)\right] = \sum_{j=0}^{\infty} b_j^B x^j, \tag{3.32}$$

then

$$f(x) = \sum_{j=0}^{\infty} b_j x^j = \sum_{j=0}^{\infty} \left(b_j^A + b_j^B\right) x^j. \tag{3.33}$$

Through (3.20),

$$f^A(x) = \sum_{j=0}^{\infty} \left[A \sum_{u=0}^{p} \alpha_{p,u}^{l} \beta(j, 2u+l+2) \right] x^j, \tag{3.34}$$

$$f^B(x) = \sum_{j=0}^{\infty} \left[B \sum_{u=0}^{p} \alpha_{p,u}^{l} \beta(j, 2u+l+4) \right] x^j. \tag{3.35}$$

It then becomes evident that

$$b_j^A = A \sum_{u=0}^{p} \alpha_{p,u}^{l} \beta(j, 2u+l+2), \tag{3.36}$$

$$b_j^B = B \sum_{u=0}^{p} \alpha_{p,u}^{l} \beta(j, 2u+l+4), \tag{3.37}$$

such that finally

$$\begin{aligned} b_j &= b_j^A + b_j^B \\ &= \sum_{u=0}^{p} \alpha_{p,u}^{l} \left[A\beta\left(j, 2u+l+2\right) + B\beta\left(j, 2u+l+4\right)\right] \end{aligned} \tag{3.38}$$

for odd $(n-m)$, so that the corresponding TM BSCs $g_{n,\mathrm{TM}}^{m}$ are readily obtained from Eq. (2.29).

4. Results

Before anything else, it should be noticed that the FS method is prone to severe numerical error propagation when depicting BSCs $g_{n,\mathrm{TX}}^{m}$ for high n values so that the numerical precision must be managed accordingly [21]. For better illustration this section is divided into two parts. Subsection 4.1 shows results with parameters with higher degree of paraxiality, avoiding numerical abnormalities, making it possible to study the features that arise in the remodelling of non-Maxwellian beams. It might be pertinent to address that the BSCs in Subsection 4.1 should still blow up for some n, but that value is much higher than the values computed there. Subsection 4.2 depicts the FS blowups that arise for Gaussian-like beams which come into being in two kinds: one due to numerical precision, another due to deeper mathematical implications of the method, the latter is yet to be better understood in works solely dedicated to them.

4.1. Remodelling aspects

Results here shown assume monochromatic LG beams with wavelength $\lambda = 632.8\,\text{nm}$, and waist parameter $s = 1/kw_0 = 0.01$. All BSCs featured in this subsection have been evaluated with 15 decimal places (dps) of precision without showing any numerical abnormalities such as values blowing up or behaving chaotically.

Fig. 1 depicts TM BSCs of three different orders of LG beam. Computationally, the runtimes of closed-form coefficients deduced above do not significantly differ from those of the recursive FS BSCs shown by Gouesbet, Votto & Ambrosio [17, 19]. Assuming that factorials and Γ functions are evaluated at linear time complexity in the worst case, it is clear, from expressions (3.23) and (3.38), that Maclaurin coefficients b_n corresponding to a $\text{LG}_{p,l}$ beam are evaluated at a time complexity of $\mathcal{O}(np)$. Therefore, from (2.10), the respective BSC $g^m_{n,\text{TX}}$ should have time complexity of $\mathcal{O}(n^2p)$, or simply $\mathcal{O}(n^2)$ since p should not scale significantly when compared to n. This is the same implied by the previous FS recursive method [17, 19]. Even though both time complexities are asymptotically equivalent, eliminating recursion evidently reduces memory complexity since there is no recursion call stack to store.

Now, due to the field decomposition into Maxwellian spherical wave functions, the GLMT must necessarily reproduce fields that are solutions to Maxwell's equations. However, as emphasized in Section 3, the LG BSC expressions were obtained through an electric vector field which ultimately is non-Maxwellian. Therefore, one cannot expect the GLMT-reconstructed fields to exactly match the paraxial formulation everywhere in space. This, nevertheless, indicates no contradiction in the FS method. That is, the method itself only "sees" radial components at a specific region in the space **regardless of the vector field** they pertain to. Fundamentally, the FS method shows that, once E_r (resp. H_r) is known at a locus $\theta = \theta_0$ for some fixed $\theta_0 \in (0, \pi)$, the set of all TM BSCs $g^m_{n,\text{TM}}$ (resp. TE BSCs $g^m_{n,\text{TE}}$) becomes uniquely determined, thus representing a unique TM (resp. TE) solution to Maxwell's equations.

In the case of the LG BSCs deduced above, whilst the radial components of the electromagnetic field must exactly match the paraxial approximation fed to the FS algorithm, it should not be the case for the other field components, since the original paraxial field does not satisfy Maxwell's equations. In Fig. 2, the x, y, and z electric field components are reconstructed with the computed BSCs. Whereas the x-polarized paraxial approximation, given by $\mathbf{E} = \hat{\mathbf{x}}\text{LG}_{p,l}\exp(-ikz)$ from (3.4), should only have a non-zero electric field x-component, we may see from Fig. 2 that the GLMT-reconstructed fields at least bear an additional non-zero z-component so that $\nabla \cdot \mathbf{E} = 0$ is satisfied along with a non-zero y-component due to Ampère's law: note that $\partial H_z/\partial x$ is not guaranteed to be equal to zero when taking the y-component of $\nabla \times \mathbf{H}$ into account for determining E_y.

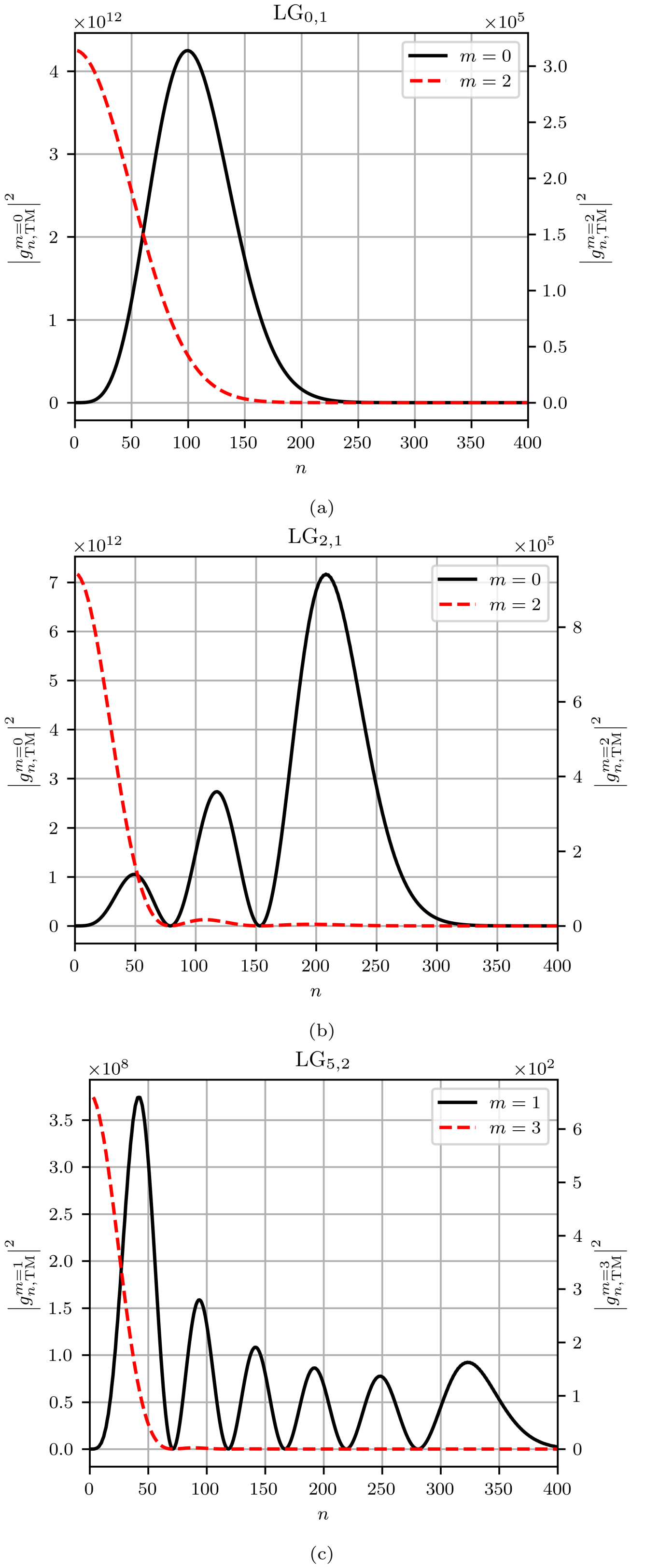
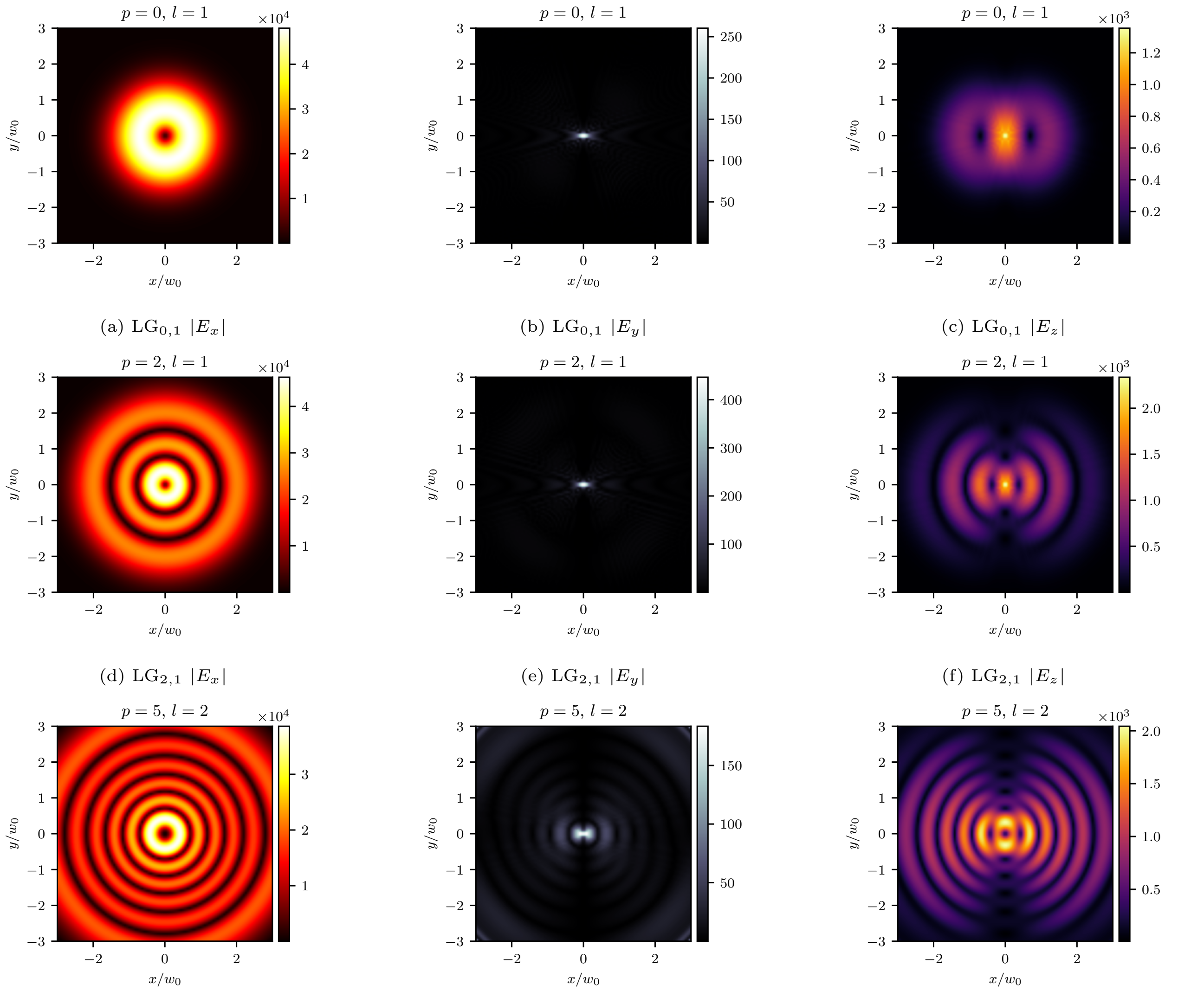


Figure 1: TM BSC square magnitude for several orders of LG modes $\text{LG}_{p,l}$ of wavelength $\lambda = 632.8\,\text{nm}$ and waist parameter $s = (kw_0)^{-1} = 0.01$. All plots feature values for both $m = l - 1$ in the black continuous curves whose values may be seen in the axes at the left-hand side, and $m = l + 1$ in the red dashed lines, the values of which are in the right-hand side.



(a) $\mathrm{LG}_{0,1}$ $|E_x|$ (b) $\mathrm{LG}_{0,1}$ $|E_y|$ (c) $\mathrm{LG}_{0,1}$ $|E_z|$

(d) $\mathrm{LG}_{2,1}$ $|E_x|$ (e) $\mathrm{LG}_{2,1}$ $|E_y|$ (f) $\mathrm{LG}_{2,1}$ $|E_z|$

(g) $\mathrm{LG}_{5,2}$ $|E_x|$ (h) $\mathrm{LG}_{5,2}$ $|E_y|$ (i) $\mathrm{LG}_{5,2}$ $|E_z|$

Figure 2: GLMT-reconstructed electric field rectangular components magnitudes $|E_x|$, $|E_y|$, $|E_z|$ for LG beams of several orders.

4.2. Numerical aspects

The FS method may exhibit a peculiar behaviour when applied to Gaussian-like beams. It is also relevant to mention that the remodelling of paraxial Gaussian-like beams into Maxwellian solutions may also cause diverging behaviours [43], which is the case for the FS for higher n values, depending on the beam waist w_0. Wherever the paraxial approximation starts to lose its validity, this is more prone to take place. Nevertheless, this is a complex subject of our study deserving its own place in other works to be published analysing both the numerical and mathematical aspects of the issue meticulously.

Results shown in this subsection assume wavelength of $\lambda = 1064\,\mathrm{nm}$ and beam-waist parameter $s = 0.05$. Fig. 3 depicts the TM BSCs of the $\mathrm{LG}_{0,1}$ mode evaluated with several degrees of numerical precision. We may see that the BSCs behave differently depending on the number of decimal places used: if precision is too low, the BSCs blow up earlier. The BSCs seem to behave the same, nonetheless, for high enough precision, but they still blow up at the same place, which is still observed for precisions higher than 2000 dps. Therefore, we see that, indeed, the blowups that come from a mathematical failure of convergence due to the remodelling have been depicted in Fig. 3.

5. Conclusion

In sum, in face of the FS method's capability of acquiring BSCs that are both exact and, for several classes of fields, time-efficient, such procedure would not deserve to be put aside as has been the case since the late 1980's. Addressing such issues, this work presents the FS method in a more approachable, algorithmic, manner, while illustrating its usefulness by deducing new closed-form expressions of freely-propagating LG BSCs. Consequently, such reformulation has allowed a more general implementation of the

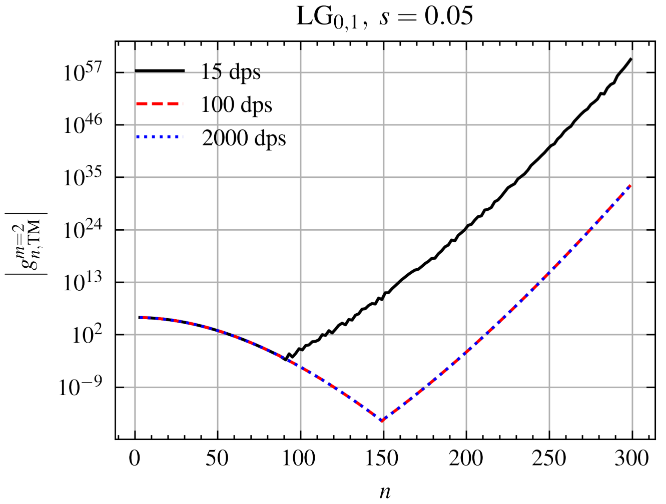


Figure 3: Absolute value of the $LG_{0,1}$ mode TM BSCs with $m = 2$ evaluated with 15, 100, and 2000 decimal places of precision. Values in logarithmic scale.

method, as it may be seen in the `glmtech` Python package by Votto [37].

In contrast with previous descriptions of LG VSWF expansion coefficients [17, 19, 44], which heavily relied on recursions, here BSCs are presented in closed form obtained with significantly more straightforward steps. That is, if the reader were to compare the deduction of such expressions in this work with the ones in Ref. [17], they would see that the same results are here obtained in half the number of pages. This illustrates the need for a more systematic and more approachable framework of the FS method. Given the importance of LG beams for electromagnetic scattering applications, it is relevant to seek accurate and efficient methods for their decomposition into VSWFs. Moreover, a straightforward description of FS LG BSCs should seem even more important when considering that they allow the inclusion of other high-order Gaussian beams, such as Hermite-Gaussian beams [23] and Ince-Gaussian beams [24], into the GLMT, since they form a complete orthogonal basis of solutions to the paraxial wave equation [40, 44].

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