Blowing-ups of beam shape coefficients of Gaussian beams using finite series in generalized Lorenz-Mie theory

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Abstract

Compact closed-form expressions of the beam shape coefficients (BSCs) of Gaussian beams are obtained in the generalized Lorenz-Mie theory through the finite series (FS) method. As a result, such expressions have made it possible to more deeply understand the behaviour of the BSCs and, therefore, the scattering of Gaussian beams beyond the paraxial approximation. The blowing up, in particular, of FS BSCs which has been observed for several paraxial beams is now mathematically justified as a phenomenon that is independent of numerical precision. Furthermore, numerical results demonstrate how such blow ups are related to the ratio between the beam waist radius and its wavelength.

Keywords: light scattering, lasers, Mie theory

1. Introduction

Multipole decomposition is a valuable procedure in the study of light scattering, for instance making it possible to develop T-matrix techniques [1], among which are the generalized Lorenz-Mie theories (GLMTs) [2, 3]. In this paper, we shall refer to the study of electromagnetic scattering by a single homogeneous spherical obstacle centred at the origin of a coordinate system as *the* GLMT. The factors of the multipole decomposition coefficients which depend of the incident field profile are called beam shape coefficients (BSCs). Briefly, the GLMT gives detailed information on the field scattering having only the BSCs as input along with the scatterer parameters encoded in Mie coefficients. Therefore, obtaining such BSCs for a given incident field is a crucial process which may be done through several methods such as quadratures, the integral localized approximation, angular spectrum decomposition or the finite series (FS) method.

Regarding accuracy, computation time, or even mathematical complexity, each method for obtaining BSCs features its own advantages and disadvantages depending on the incident field profile. Thus, the method must be chosen accordingly. In particular, the FS method has shown remarkable performance when applied to solutions to the paraxial wave equation: compositions of Gaussian, Laguerre-Gaussian [4, 5, 6], Hermite-Gaussian beams [7], and so on [8, 9, 10]. Examining the works on these families of beams, a few unexpected behaviours were observed in the numerical evaluations of the FS expressions, which did not arise for other kinds of electromagnetic fields. Despite being a time-efficient exact method, the FS for such paraxial beams had its BSCs blowing up in magnitude when numerically evaluated at higher orders with no immediate explanation to be found within the sometimes convoluted mathematical expressions. It was unclear whether it was a strictly numerical phenomenon or if there was a deeper mathematical explanation behind it.

What made it difficult to assess the actual source of the FS paraxial blow ups was that the BSC expressions were not always given in closed form – they were often obtained by recursive relations or non-trivial iterative algorithms. In this work, we deduce compact closed-form expressions for the FS BSCs of a zeroth-order Gaussian beam which are put in terms of special functions known as the generalized Bessel polynomials. Subsequently, the mathematical analysis of the BSCs may be done with much more rigorous support given the thorough knowledge available on such polynomials [11, 12]. In fact, we use known asymptotic relations of these special functions in order to prove that the absolute value of Gaussian BSCs $g_{n,\mathrm{TM}}^{\pm 1}$ are bound to indefinitely increase for high enough n. We note that this is compatible with the observations of the non-paraxial corrections given in the series originally found by Lax, Louisell & McKnight [13]. Furthermore, such behaviour is related to the divergence of the Davis scheme of approximations which is in turn based on such series of corrections [14, 15].

In the study of beam propagation beyond the paraxial approximation, Wünsche found transition operators, through functional analysis, between the space of solutions to the paraxial wave equation and the space of solutions of the Helmholtz equation [16]. Therein, the author explains that the series that define the transition operators have issues with convergence for more tightly focused beams, where the paraxial approximation starts to lose its validity. Partial sums of the divergent Lax series up to more terms have been evaluated without loss of physical meaning [17, 18]. Therefore, the blowing up of the FS BSCs is indeed to be expected, but it was not yet proven up to now.

In Section 2 we briefly deduce the FS method expressions for general beam shapes. In Section 3, we employ the FS to the boundary conditions of fundamental Gaussian beams and retrieve closed-form expressions for their BSCs. Section 4 introduces the generalized Bessel polynomials and puts the closed-form BSC expressions in terms of them, then we use known asymptotic relations to prove the blow ups. Numerical results are shown in Section 5, revealing the relation of the blow ups with the beam-waist factor. Section 6 is the conclusion.

2. Finite series method

There is a range of methods one may employ in order to obtain the BSCs of a given electromagnetic field, each one presenting advantages and disadvantages depending on the shape of the field. Among such techniques is the FS method, which retrieves the exact BSCs of the field given its radial component at a given region in space. That is, given such boundary conditions, the FS method gives the multipole decomposition of an exact solution to Maxwell's equations: a Maxwellian field. Consequently, the method is a valid approach to survey the mathematical properties of non-trivial Maxwellian fields. In this section, we briefly derive the FS method in the GLMT for its application further ahead when we examine Maxwellian counterparts of paraxial Gaussian beams.

2.1. Neumann expansion theorem

The Neumann expansion theorem (NET) is an elegant result whose demonstration may be found in Watson's work [19, Section 16.13].

Theorem 1 (Neumann Expansion Theorem)**.** *If a map $f : (0, \infty) \to \mathbb{C}$ admits, at the same time, a half-integer-order Bessel function Neumann ex-*

pansion

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

and Maclaurin series

$$f(x) = \sum_{n=0}^{\infty} b_n x^n \tag{2}$$

that are both convergent, then

$$c_n = \left(n + \frac{1}{2}\right) \sum_{q=0}^{\leq n/2} \frac{2^{n-2q+1/2}}{q!} \Gamma\left(n - q + \frac{1}{2}\right) b_{n-2q}. \tag{3}$$

In short, one may write the Neumann coefficients c_n of f from (1) in terms of a *finite series* of its Maclaurin coefficients b_n in (2) through (3).

2.2. Applying the theorem in the generalized Lorenz-Mie theory

According to the GLMT [3], an electromagnetic field may be decomposed into partial spherical wave functions (multipoles) in spherical coordinates (r, θ, ϕ). Consider a monochromatic electric field of wavenumber k and angular frequency ω so that it may admit a phasor $\mathbf{E}$ adopting the time-harmonic convention $\exp(+i\omega t)$. The phasor radial component E_r may be expanded as (see [3, Eq. (3.10)] or [8, Eq. (47)]):

$$E_r = E_0 \sum_{n=1}^{\infty} \sum_{m=-n}^{n} (-i)^{n+1} \frac{2n+1}{kr} g_{n,\mathrm{TM}}^m j_n(kr) P_n^{|m|}(\cos\theta) e^{im\phi} \tag{4}$$

where E_0 is a (complex) amplitude constant, the $g_{n,\mathrm{TM}}^m$ are the transverse magnetic (TM) beam shape coefficients (BSCs), j_n are spherical Bessel functions of first kind, and $P_n^{|m|}$ are associated Legendre functions following Hobson's notation [20].

First, since the exponential function satisfies the orthogonality relation

$$\int_0^{2\pi} e^{im\phi} e^{-ip\phi} \mathrm{d}\phi = 2\pi \delta_{mp}, \tag{5}$$

where δ is the Kronecker delta, we may fix m, multiply both sides of (4) by $\exp(-im\phi)$, and integrate with respect to ϕ so that the summation over m is eliminated:

$$\int_0^{2\pi} E_r e^{-im\phi} \mathrm{d}\phi = 2\pi E_0 \sum_{n=1}^{\infty} (-i)^{n+1} \frac{2n+1}{kr} g_{n,\mathrm{TM}}^m j_n(kr) P_n^{|m|}(\cos\theta). \tag{6}$$

Now, see that

$$j_n(x) = \sqrt{\frac{\pi}{2x}} J_{n+1/2}(x). \tag{7}$$

Thus, letting $x = kr$ and fixing $\theta = \theta_0$, we obtain

$$\begin{aligned} x^{1/2} \frac{x}{E_0} \int_0^{2\pi} E_r\left(\frac{x}{k}, \theta_0, \phi\right) e^{-im\phi} \mathrm{d}\phi = \sum_{n=1}^{\infty} &\pi\sqrt{2\pi}(-i)^{n+1}(2n+1) \\ &\times P_n^{|m|}(\cos\theta_0) g_{n,\mathrm{TM}}^m J_{n+1/2}(x). \end{aligned} \tag{8}$$

It is then evident that (8) features a Neumann expansion similar to (1). That is, for the fixed m and θ_0, define a function $f_m : (0,\infty) \to \mathbb{C}$ such that

$$f_m(x) = \frac{x}{E_0} \int_0^{2\pi} E_r\left(\frac{x}{k}, \theta_0, \phi\right) e^{-im\phi} \mathrm{d}\phi, \tag{9}$$

then f_m admits a Neumann expansion just like f in (1):

$$\begin{aligned} x^{1/2} f_m(x) &= \sum_{n=1}^{\infty} \pi\sqrt{2\pi}(-i)^{n+1}(2n+1) P_n^{|m|}(\cos\theta_0) g_{n,\mathrm{TM}}^m J_{n+1/2}(x) \\ &= \sum_{n=0}^{\infty} c_n J_{n+1/2}(x). \end{aligned} \tag{10}$$

Finally, if f_m has a Maclaurin expansion

$$f_m(x) = \sum_{n=0}^{\infty} b_n^{(m)} x^n, \tag{11}$$

we may apply the NET and find the TM BSC $g_{n,\mathrm{TM}}^m$. In some more detail, since, from (10), the Neumann coefficients of $x^{1/2} f_m(x)$ are given by

$$c_n = \pi\sqrt{2\pi}(-i)^{n+1}(2n+1) P_n^{|m|}(\cos\theta_0) g_{n,\mathrm{TM}}^m \tag{12}$$

for $n \geq 1$ and $c_0 = 0$, we apply the NET relating the such coefficients with the Maclaurin coefficients $b_n^{(m)}$ through (3) so that

$$g_{n,\mathrm{TM}}^{m} = \frac{i^{n+1}}{2\pi^{3/2} P_n^{|m|}(\cos\theta_0)} \sum_{q=0}^{\leq n/2} \frac{2^{n-2q}}{q!} \Gamma\left(n - q + \frac{1}{2}\right) b_{n-2q}^{(m)}, \tag{13}$$

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

2.3. The choice of θ_0

See that (13) imposes a restriction over the choice of θ_0 such that $P_n^{|m|}(\cos\theta_0)$ cannot be equal to zero. That is, the choice of θ_0 matters not only for defining the function f_m to be Maclaurin-expanded, but may also make it so that (13) would not be valid anymore for finding the BSCs $g_{n,\mathrm{TM}}^{m}$. [6, 21]

The value $\theta_0 = \pi/2$ is an usual choice for making it possible to find, for more complicated electromagnetic fields, functions f_m with Maclaurin coefficients $b_n^{(m)}$ that are actually possible to compute. However, since $P_n^{|m|}(0) = 0$ for odd $(n - m)$, (13) would only hold for even $(n - m)$, in which case [22]

$$P_n^m(0) = (-1)^{(n+m)/2} \frac{2^m}{\sqrt{\pi}} \frac{\Gamma\left(\frac{n+m+1}{2}\right)}{\left(\frac{n-m}{2}\right)!}. \tag{14}$$

Therefore, we may rewrite (13) for $\theta_0 = \pi/2$ so that

$$g_{n,\mathrm{TM}}^{m} = \frac{(-i)^{|m|-1}}{2^{|m|+1}\pi} \frac{\left(\frac{n-|m|}{2}\right)!}{\Gamma\left(\frac{n+|m|+1}{2}\right)} \sum_{q=0}^{\leq n/2} \frac{2^{n-2q}}{q!} \Gamma\left(n - q + \frac{1}{2}\right) b_{n-2q}^{(m)} \tag{15}$$

for even $(n - m)$.

For the odd $(n - m)$ case, see Appendix A.

3. Modelling Gaussian beams through the finite series method

Following the rationale behind the model by Agrawal and Pattanayak [23], we assume the electromagnetic field in the xy-plane to be given by

$$\mathbf{E}(x, y, 0) = \hat{\mathbf{x}} E_0 \exp\left(-\frac{x^2 + y^2}{w_0^2}\right), \tag{16}$$

$$\mathbf{H}(x, y, 0) = \hat{\mathbf{y}} H_0 \exp\left(-\frac{x^2 + y^2}{w_0^2}\right), \tag{17}$$

with $H_0 = (\varepsilon/\mu)^{1/2} E_0$ where μ and ε are respectively the permeability and the permittivity of the medium so that $k = \omega(\mu\varepsilon)^{1/2}$. Thus, the electric field radial component at $\theta = \pi/2$ is

$$E_r\left(r, \frac{\pi}{2}, \phi\right) = E_0 \exp\left(\frac{-r^2}{w_0^2}\right) \cos\phi \tag{18}$$

so that, for $x = kr$ and beam waist parameter $s = (kw_0)^{-1}$,

$$E_r\left(\frac{x}{k}, \frac{\pi}{2}, \phi\right) = E_0 \exp\left(-s^2 x^2\right) \cos\phi. \tag{19}$$

Now we may find a function f_m to Maclaurin-expand as in (9), that is

$$\begin{aligned} f_m(x) &= x \int_0^{2\pi} \exp(-s^2 x^2) \cos\phi e^{-im\phi} \mathrm{d}\phi \\ &= \pi x \exp(-s^2 x^2) \left(\delta_{m,1} + \delta_{m,-1}\right), \end{aligned} \tag{20}$$

so that $f_m = 0$ for any $m \neq \pm 1$, and $f_{\pm 1}(x) = \pi x \exp(-s^2 x^2)$. Hence, expanding the exponential function in (20), we have

$$f_{\pm 1}(x) = \pi \sum_{n=0}^{\infty} \frac{(-s^2)^n}{n!} x^{2n+1} = \pi \sum_{n \text{ odd}} \frac{(-s^2)^{(n-1)/2}}{\left(\frac{n-1}{2}\right)!} x^n, \tag{21}$$

so that we may determine the Maclaurin coefficients $b_n^{(\pm 1)}$. Indeed, let

$$f_{\pm 1}(x) = \sum_{n=0}^{\infty} b_n^{(\pm 1)} x^n, \tag{22}$$

then, $b_{2n+1}^{(\pm 1)} = \pi(-s^2)^n/n!$, or

$$b_n^{(\pm 1)} = \begin{cases} \pi \dfrac{(-s^2)^{(n-1)/2}}{\left(\frac{n-1}{2}\right)!}, & n \text{ odd}, \\ 0, & \text{otherwise}. \end{cases} \tag{23}$$

For $m = \pm 1$, forcing $(n-m)$ to be even implies that n is odd, so let $n = 2p+1$ for non-negative integers p. This way, the Maclaurin coefficients as shown inside the summation in (15) would be

$$b_{n-2q} = b_{2p+1-2q} = b_{2(p-q)+1} = \pi \frac{(-s^2)^{p-q}}{(p-q)!}. \tag{24}$$

Therefore, the TM BSCs $g_{2p+1,\mathrm{TM}}^{\pm 1}$ of an EM field with radial electric field component $E_r(\theta = \pi/2)$ at the xy-plane as in (19) may be given, from (15), by

$$g_{2p+1,\mathrm{TM}}^{\pm 1} = \frac{1}{2} \sum_{q=0}^{p} \frac{p!}{q!(p-q)!} \frac{\Gamma(2p-q+3/2)}{\Gamma(p+3/2)} (-4s^2)^{p-q}. \tag{25}$$

Since reversing the terms of a summation does not change it, i.e. $\sum_{q=0}^{p} a_q = \sum_{q=0}^{p} a_{p-q}$, we have

$$g_{2p+1,\mathrm{TM}}^{\pm 1} = \frac{1}{2} \sum_{q=0}^{p} \frac{p!}{(p-q)!q!} \frac{\Gamma(p+3/2+q)}{\Gamma(p+3/2)} (-4s^2)^{q}. \tag{26}$$

Let $\binom{p}{q} = p!/q!(p-q)!$ be the binomial coefficient and $(a)_q = \Gamma(a+q)/\Gamma(a)$ be the Pochhammer symbol, then the TM BSCs for odd $n = 2p+1$ are

$$g_{2p+1,\mathrm{TM}}^{\pm 1} = \frac{1}{2} \sum_{q=0}^{p} \binom{p}{q} \left(p + \frac{3}{2}\right)_q \left(-4s^2\right)^q. \tag{27}$$

It should be noted that Eq. (26) for $g_{n,\mathrm{TM}}^{m}$ for $n = 2p+1$, and $m = \pm 1$ corresponds to Eq. (6.151) for g_{2p+1} in [3] with a difference by a factor of 1 / 2 due to the relationship between uni-index BSC g_n and the bi-index BSC g_n^m, see Eq. (6.2) in [3]. Similarly, Eq. (A.18) corresponds to Eq. (6.152) in [3].

4. Analysis of the beam shape coefficients

Here, we introduce a class of polynomials that shall be important for analysing the fundamental Gaussian BSCs found in the previous section: the generalized Bessel polynomials. For deeper insight on such functions, we refer to the works of Krall & Frink [11], and Grosswald [12].

A generalized Bessel polynomial $y_p(x; a, b)$ is defined to be the polynomial of degree p with constant term equal to unity that satisfies the differential equation

$$x^2 \frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + (ax + b) \frac{\mathrm{d}y}{\mathrm{d}x} = p(p + a - 1)y, \tag{28}$$

where a is not a negative integer nor zero, and b is not zero. In fact, we shall denote such polynomials as $y_p(x; a) = y_p(x; a, 2)$ taking $b = 2$ as is usual in the literature. This implies that the generalized Bessel polynomials may be expressed by the explicit formula

$$y_p(x; a) = \sum_{q=0}^{p} \binom{p}{q} (p + a - 1)_q \left(\frac{x}{2}\right)^q . \tag{29}$$

At this stage, the reader might already have recognized that the TM BSCs $g_{2p+1,\mathrm{TM}}^{\pm 1}$ in (27) may be readily written in terms of a generalized Bessel polynomial:

$$g_{2p+1,\mathrm{TM}}^{\pm 1} = \frac{1}{2} y_p \left(-8s^2; \frac{5}{2} \right) . \tag{30}$$

Such representation shall be useful as it immediately identifies the odd BSCs with a generalized Bessel polynomial so that its mathematical properties – such as recurrence relations and asymptotic behaviour – are properly recognizable. **In fact, (30) reveals that, for large enough p, the BSCs $g_{2p+1,\mathrm{TM}}^{\pm 1}$ must indefinitely increase in magnitude.** This is a consequence of the result that, for a fixed $z \neq 0$, a neither a negative integer nor zero, and large p [12, Chapter 13, Theorem 3],

$$y_p(z; a) = \left(\frac{2z}{e} p \right)^p 2^{a-3/2} e^{1/z} \left[1 + \mathcal{O}\left(\frac{1}{p} \right) \right] . \tag{31}$$

5. Results

In Section 4 it has been shown that, from some n onward, the BSCs $g_{n,\mathrm{TX}}^m$, TX being TM or TE, start to blow up, which has been numerically verified throughout many works which remodel paraxial beams with the FS method, see in particular [3], pp. 164-171. The usual behaviour that has been observed in these studies is that an increase to numerical precision would make the threshold where the BSCs blow up be higher, up to an extent in which arbitrary precision does not seem to make a difference anymore. In this manner, it was unclear until now whether the BSC expressions – many times given by recursive relations – were mathematically bound to blow up, or if there was still major numerical error propagation taking place. In particular, blowing-ups due to a loss of significant digits have been indeed observed in

[9] and [24] (the attribution of such blowing-ups to numerical inaccuracies has been confirmed by complementary calculations using an infinite precision mode, private communication from Jianqi Shen). Here, the analysis of the closed-form expressions finally shows that it is indeed a mathematical property of the Gaussian FS BSCs to blow up for high enough n. However, we are still left with the question of exactly up to what n one may safely compute BSCs before values grow out of control, or even if this depends on beam parameters.

Numerical results shown in this paper assume beams with wavelength of $\lambda = 1064\,\text{nm}$. Then, to better understand if the blowing up behaviour depends on the beam waist w_0, or the beam-waist parameter $s = 1/kw_0$ more specifically, define $N(s)$ to be the smallest $n > 1$ such that the FS BSC $g_{n,\text{TM}}^1$ has absolute value greater than $g_{1,\text{TM}}^1 = 1/2$. For instance, Fig. 1 shows the magnitude of FS BSCs of a lowest-order Gaussian beam calculated assuming $s = 0.01$ showing the corresponding $N(0.01)$th BSC with a red dot. In this case, we calculated $N(0.01) = 5584$ with numerical precision of 2000 decimal places (dps). Notice that employing low numerical precision causes the BSCs to blow up earlier, before $N(s)$, due to catastrophic cancellation. For example, with only 15 dps, we would have found that the first BSC greater than 1/2 was with $n = 629$ for $s = 0.01$, whereas, with 1500 dps, 2000 dps, or higher, the value of $n = N(0.01) = 5584$ is always obtained.

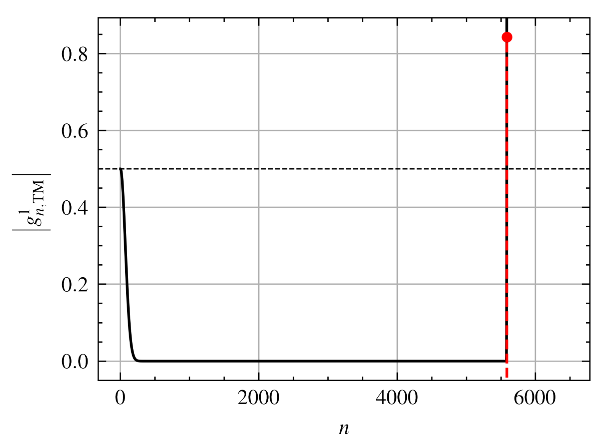

Figure 1: Absolute value of the FS BSCs for $s = 0.01$. The red dot represents $N(0.01)$ whose corresponding BSC is greater than $g_{1,\text{TM}}^1 = 1/2$ in magnitude. The wavelength is $\lambda = 1064\,\text{nm}$.

In Fig. 2 we show the BSCs as in Fig. 1 but for a range of beam waist radii w_0 between 5 µm and 20 µm while maintaining a fixed wavelength of $\lambda = 1064\,\text{nm}$. The red dashed line depicts the values of $N(1/kw_0)$ for each w_0 as defined above. For visualization purposes, values that rose higher than a given threshold were masked out of the plot. Fig. 3, similar to Fig. 2, shows such magnitudes in logarithmic scale within the shorter range of 1 µm up to 10 µm with the same red dashed line of Fig. 2. s

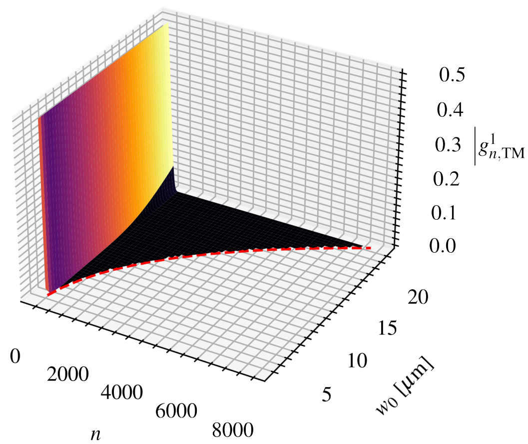

Figure 2: Absolute value of the FS BSCs for several values of w_0 computed at 2000 dps between 5 µm and 10 µm and fixed wavelength $\lambda = 1064\,\text{nm}$. The red dashed line represents $N(1/kw_0)$ whose corresponding BSC is greater than 1/2 in magnitude.

The red dashed lines in Figs. 2 and 3 appear to form a parabola – i.e. $N(1/k/w_0)$ seems to directly depend of w_0^2 – corroborating the results of Gouesbet, Shen and Ambrosio [15] that the non-paraxial correction series in the Davis scheme is always invalid beyond a certain $n \sim 1/s^2$.

6. Conclusion

In face of the results presented above, expressing the BSCs of fundamental Gaussian beams explicitly in terms of generalized Bessel polynomials has made it possible to better understand the behaviour of the remodelling of scalar paraxial beams to a vector Maxwellian framework. To begin with, such FS BSCs, before, were generally obtained through recursive methods which were difficult to translate to iterative counterparts, so not much insight could be obtained merely through the method's expressions.

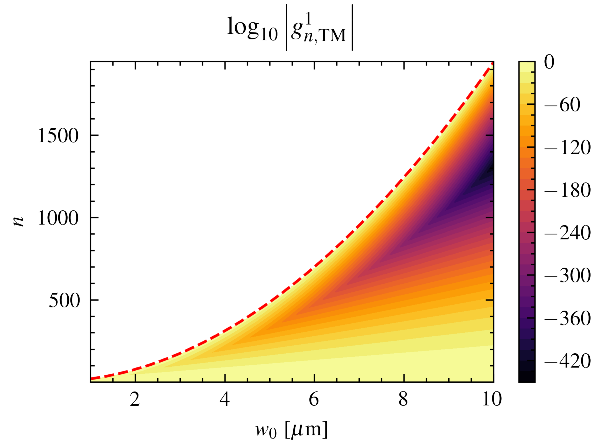

Figure 3: Detail of Fig. 2 in logarithmic scale ranging from 1 μm to 10 μm.

Favorably, the closed-form expressions do more rigorously elucidate some outstanding patterns with no clear mathematical explanation at the time – and so could have been thought to be strictly numerical phenomena. For instance, we have shown that, even though catastrophic cancellation may occur if lower numerical precision is employed, the non-zero FS BSCs $g^{\pm 1}_{n,\mathrm{TX}}$ of Gaussian beams are mathematically bound to indefinitely increase in magnitude from some n onward. This was unproven until now, even though it was suspected to be the case on the basis of empirical evidence, e.g. page 169 of [3].

The FS method once again was a valuable asset to better understand physical and mathematical properties of electromagnetic waves subject to multipole decomposition. The diverging character of representations of electromagnetic beams beyond the paraxial approximation has been observed ever since the Lax series [13] was numerically evaluated for higher terms [17]. Complementary to this, the evaluation of exact multipole decomposition coefficients through the FS method in the GLMT has mathematically shown that such divergence is bound to occur when remodelling the propagation of Gaussian beams using non-Maxwellian descriptions. Whether this should occur as well when using Maxwellian descriptions may be an open subject of research.

Appendix A. The finite series odd case

Appendix A.1. TM BSC expression

When finding the TM BSC FS expression (13) we saw that the only restriction for the choice of θ_0 was that $P_n^{|m|}(\cos\theta_0) \neq 0$ for the concerning n and m. Then, in Section (2.3), we have derived closed form expressions for these BSCs $g_{n,\mathrm{TM}}^m$ when $\theta_0 = \pi/2$ with the caveat that such expressions must only hold when $(n-m)$ is even. We now show that it is still possible to find BSCs for $\theta_0 = \pi/2$ and odd $(n-m)$ by making a minor change to the FS setup. For this, we note that [22]

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

for odd $(n-m)$ and $(P_n^m)'(0) = 0$ otherwise.

Hence, in order to obtain valid FS expressions, we may work with the derivative of the radial electric field component with respect to $\cos\theta$ at $\theta = \pi/2$ when deducing the FS expressions. In short, one may see that we now work with a function

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

to be Maclaurin-expanded with coefficients $b_n^{(m)}$, and where the Neumann coefficients of $x^{1/2}f_m(x)$ are given by

$$c_n = \pi\sqrt{2\pi}(-i)^{n+1}(2n+1)(P_n^{|m|})'(0)g_{n,\mathrm{TM}}^m \tag{A.3}$$

for $n \geq 1$ and $c_0 = 0$. Next, applying the NET to relate c_n and $b_n^{(m)}$ as in (3) and substituting $(P_n^m)'(0)$ with (A.1), we have that

$$g_{n,\mathrm{TM}}^m = \frac{(-i)^{|m|-2}}{2^{|m|+2}\pi}\frac{\left(\frac{n-|m|-1}{2}\right)!}{\Gamma\left(\frac{n+|m|}{2}+1\right)}\sum_{q=0}^{\leq n/2}\frac{2^{n-2q}}{q!}\Gamma\left(n-q+\frac{1}{2}\right)b_{n-2q} \tag{A.4}$$

for odd $(n-m)$.

Appendix A.2. Gaussian beam odd BSC expression

In Section 3, we have deduced the fundamental Gaussian BSCs $g_{n,\mathrm{TM}}^{m}$ for even $(n-m)$. We shall see how to proceed for the remaining odd $(n-m)$ case. We remind that it is assumed that, in the xy-plane, $\theta=\pi/2$, the EM fields are

$$\mathbf{E}(x,y,0)=\hat{\mathbf{x}}E_0\exp\left(-\frac{x^2+y^2}{w_0^2}\right), \tag{A.5}$$

$$\mathbf{H}(x,y,0)=\hat{\mathbf{y}}H_0\exp\left(-\frac{x^2+y^2}{w_0^2}\right), \tag{A.6}$$

where $H_0=(\varepsilon/\mu)^{1/2}E_0$. Moreover, such fields are bound to Maxwell's equations; more specifically Faraday's law

$$\boldsymbol{\nabla}\times\mathbf{E}=-i\omega\mu\mathbf{H}. \tag{A.7}$$

To obtain the function f_m in (A.2) concerning such field, we must find the derivative of the radial electric field component with respect to $\cos\theta$ when $\theta=\pi/2$. Seeing that $E_r=E_r(\rho,z)$ for $\rho=(x^2+y^2)^{1/2}$ due to symmetry, we may verify that, if $\gamma=\cos\theta$ so that $z=r\gamma$ and $\rho=r(1-\gamma^2)^{1/2}$, then

$$\frac{\partial E_r}{\partial\cos\theta}=\frac{\partial E_r}{\partial\gamma}=\frac{\partial\rho}{\partial\gamma}\frac{\partial E_r}{\partial\rho}+\frac{\partial z}{\partial\gamma}\frac{\partial E_r}{\partial z}. \tag{A.8}$$

At $\theta=\pi/2$, $\partial z/\partial\gamma=\rho=r$ and $\partial\rho/\partial\gamma=0$, meaning

$$\frac{\partial E_r}{\partial\cos\theta}\left(\theta=\frac{\pi}{2}\right)=r\frac{\partial E_r}{\partial z}\left(\theta=\frac{\pi}{2}\right). \tag{A.9}$$

Consequently, it suffices to find the z-derivative to obtain the $\cos\theta$-derivative at the xy-plane.

From Faraday's law expressed in cylindrical coordinates, we have that

$$-i\omega\mu H_\phi=\frac{\partial E_\rho}{\partial z}-\frac{\partial E_z}{\partial\rho}, \tag{A.10}$$

so that, at $\theta=\pi/2$, where $E_\rho=E_r$,

$$-i\omega\mu H_\phi\left(\theta=\frac{\pi}{2}\right)=\frac{\partial E_r}{\partial z}\left(\theta=\frac{\pi}{2}\right). \tag{A.11}$$

From (A.6), $H_\phi = H_0 \exp\left(-r^2/w_0^2\right)\cos\phi$ in the waist plane, so, since $k = \omega(\mu\varepsilon)^{1/2}$, and let $x = kr$, $s = (kw_0)^{-1}$,

$$\frac{\partial E_r}{\partial \cos\theta}\left(\theta = \frac{\pi}{2}\right) = -ixE_0 \exp\left(-s^2x^2\right)\cos\phi. \tag{A.12}$$

Now the odd case f_m may be found from (A.2):

$$f_m(x) = -i\pi x^2 \exp(-s^2x^2)\left(\delta_{m,1} + \delta_{m,-1}\right), \tag{A.13}$$

such that $f_m = 0$ if $m \neq \pm 1$. Thus, we may expand $f_{\pm 1}$ in power series as

$$f_m(x) = \sum_{n=0}^{\infty} -i\pi \frac{(-s^2)^n}{n!} x^{2n+2} = \sum_{n=0}^{\infty} b_n x^n, \tag{A.14}$$

with $b_{2n+2} = -i\pi(-s^2)^n/n!$, or

$$b_n = \begin{cases} -i\pi \dfrac{(-s^2)^{-1+n/2}}{\left(\frac{n}{2}-1\right)!}, & \text{for even } n > 0, \\ 0, & \text{otherwise.} \end{cases} \tag{A.15}$$

The FS expression (A.4) requires having the Maclaurin coefficients as b_{n-2q}, which, taking $n = 2p + 2$ for non-negative integers p, are

$$b_{n-2q} = b_{2(p-q)+2} = -i\pi \frac{(-s^2)^{p-q}}{(p-q)!}, \tag{A.16}$$

so substituting in (A.4) gives

$$g_{2p+2,\mathrm{TM}}^{\pm 1} = \frac{1}{2}\frac{p!}{\Gamma\left(p+\frac{5}{2}\right)} \sum_{q=0}^{p+1} \frac{2^{2(p-q)}}{q!} \Gamma\left(2p - q + \frac{5}{2}\right) \frac{(-s^2)^{p-q}}{(p-q)!}, \tag{A.17}$$

or

$$g_{2p+2,\mathrm{TM}}^{\pm 1} = \frac{1}{2}\sum_{q=0}^{p+1} \binom{p}{q} \frac{\Gamma\left(2p - q + \frac{5}{2}\right)}{\Gamma\left(p + \frac{5}{2}\right)} \left(-4s^2\right)^{p-q}. \tag{A.18}$$

Now, since $\binom{p}{p+1} = 0$, we may eliminate the $q = p + 1$ summation term. Furthermore, if we reverse the summation – $\sum_{q=0}^{p} a_q = \sum_{q=0}^{p} a_{p-q}$ –, we arrive at

$$g_{2p+2,\mathrm{TM}}^{\pm 1} = \frac{1}{2}\sum_{q=0}^{p} \binom{p}{q} \left(p + \frac{5}{2}\right)_q \left(-4s^2\right)^q. \tag{A.19}$$

In terms of a generalized Bessel polynomial, we have

$$g_{2p+2,\mathrm{TM}}^{\pm 1} = \frac{1}{2} y_p \left(-8s^2; \frac{7}{2} \right). \tag{A.20}$$

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