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On an infinite number of quadratures to evaluate beam shape coefficients in generalized Lorenz-Mie theory and the Extended Boundary Condition Method for structured EM beams.

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Abstract

When dealing with light scattering theories such as the T-matrix methods for structured laser beams, e.g. Generalized Lorenz-Mie Theory (GLMT) or the Extended Boundary Condition Method (EBCM), EM fields are expanded over a set of Vector Spherical Wave Functions (VSWFs) involving spherical Bessel functions, with expansion coefficients expressed in terms of Beam Shape Coefficients (BSCs). Although spherical Bessel functions are orthogonal over the range $(-\infty, +\infty)$, the GLMT may be expressed using a non-orthogonal set of spherical Bessel functions defined over $(0, +\infty)$, allowing one to generate an infinite number of quadratures for evaluating the BSCs. This paper points out the difference between orthogonal and non-orthogonal spherical Bessel functions, establishes the infinite number of quadratures and discusses its properties.

Keywords : Generalized Lorenz-Mie Theory; Extended Boundary Condition Method; T-matrix; Beam Shape Coefficients; Vector Spherical Wave Functions.

1 Introduction.

The description of electromagnetic structured beams may be carried out in terms of expansions over Vector Spherical Wave Functions (VSWFs), e.g. in the framework of light scattering theories such as Generalized Lorenz-Mie Theory (GLMT) [1], [2], [3] or the Extended Boundary Condition Method (EBCM) [4], [5] for structured beams [6]. In these frameworks, expansion coefficients over the VSWFs can be expressed in terms of sub-coefficients known as Beam Shape Coefficients (BSCs) usually denoted as $g_{n, TM}^m$ and $g_{n, TE}^m$ (TM: Transverse Magnetic; TE: Transverse Electric) although, originally, BSCs were introduced in the framework of the Bromwich formalism [7]. VSWFs involve spherical Bessel functions which are orthogonal over $(-\infty, +\infty)$. However, the GLMT may be expressed in terms of a non-orthogonal set of spherical Bessel functions defined over the range $(0, \infty)$ instead of being defined over the range $(-\infty, +\infty)$. We examine the implications of the use of a non-orthogonal set of spherical Bessel functions, in particular the fact that BSCs may be evaluated in an infinite number of ways under the form of an infinite number of quadratures, and discuss whether these different ways are equivalent or not. We shall restrict our discussion to the TM-BSCs $g_{n, TM}^m$ insofar as the case of TE-BSCs would be treated similarly.

2 Non-orthogonality of spherical Bessel functions over $(0, +\infty)$ and their consequences.

In the Bromwich formulation, the TM-BSCs $g_{n, TM}^m$ allow one to express the radial component E_r of the electric field according to, e.g. Eq.(3.10) in [3]:

$$E_r = E_0 \sum_{n=1}^{\infty} \sum_{m=-n}^{+n} c_n^{pw} g_{n, TM}^m \frac{n(n+1)}{r} \Psi_n^{(1)}(kr) P_n^{|m|}(\cos \theta) \exp(im\varphi) \quad (1)$$

in which $P_n^{|m|}$ are associated Legendre functions defined according to Hobson's notation, which is also used by Arfken and Weber [8] with an extra-prefactor $(-1)^m$ introduced, $\Psi_n^{(1)}(kr)$ are spherical Bessel functions of the first kind also denoted as $j_n(kr)$, and c_n^{pw} , with pw standing for "plane wave" are plane wave coefficients which occur in the Bromwich formulation of the usual Lorenz-Mie theory [9] and which do not need to be specified in the present paper.

The usual way to isolate the BSCs is as follows. First, use the orthogonality relation for exponentials to get rid of the azimuthal angle φ :

$$\int_0^{2\pi} \exp[i(m - m')\varphi] d\varphi = 2\pi \delta_{mm'} \quad (2)$$

Afterward, use the orthogonality relation for the associated Legendre functions $P_n^m(\cos \theta)$ to get rid of the polar angle θ :

$$\int_0^\pi P_n^m(\cos \theta) P_l^m(\cos \theta) \sin \theta d\theta = \frac{2}{2n+1} \frac{(n+m)!}{(n-m)!} \delta_{nl} \quad (3)$$

To take advantage of Eqs.2 and 3, Eq.1 is successively multiplied by integral operators $\int_0^{2\pi} (\cdot) \exp(-im'\varphi) d\varphi$ and $\int_0^\pi (\cdot) P_{n'}^{|m|} \sin \theta d\theta$ to obtain:

$$g_{n, TM}^m = \frac{1}{E_0 c_n^{pw}} \frac{2n+1}{4\pi n(n+1)} \frac{(n-|m|)!}{(n+|m|)!} \frac{r}{\Psi_n^{(1)}(kr)} \quad (4)$$

$$\int_0^\pi \int_0^{2\pi} E_r P_n^{|m|}(\cos \theta) \exp(-im\varphi) \sin \theta d\theta d\varphi$$

It is to be noted that Eq.4 contains an r -dependent term $r/\Psi_n^{(1)}(kr)$. This does not prevent the BSCs from being complex numbers, as they should, because the integrals in Eq.4 are proportional to an inverse factor $\Psi_n^{(1)}(kr)/r$, e.g. [10] for the case of a plane wave propagating along the z -axis, [11], [12] for oblique propagation and [13] for any beam perfectly satisfying Maxwell's equations. Furthermore, the double quadrature expression of Eq.4 pertains to what has been called the F1-formulation in [14]. It must also be noted that this F1-formulation does not need any orthogonality property of spherical Bessel functions, and works independently of whether the spherical Bessel functions are orthogonal or not. This is because the only integrals which have to be used in the F1-formulation are the ones over θ and φ .

Another way to obtain expressions of BSCs, known as the F2-formulation [14] is by using triple quadratures instead of using double quadratures. For this, we shall use [15], p. 412:

$$\int_0^\infty \Psi_n^{(1)}(kr) \Psi_{n'}^{(1)}(kr) d(kr) = \frac{\pi}{2(2n+1)} \text{ for } n = n' \quad (5)$$

in which the integration interval is from 0 to ∞ , which is natural since this is the range of the radial variable r . Then, rearranging Eq.4 in an obvious way and applying the operator $\int_0^\infty (\cdot) \Psi_n^{(1)}(kr) d(kr)$, we obtain:

$$g_{n, TM}^m = \frac{(2n+1)^2}{2\pi^2 n(n+1) c_n^{pw}} \frac{(n-|m|)!}{(n+|m|)!} \quad (6)$$

$$\int_0^\pi \int_0^{2\pi} \int_0^\infty \frac{Er}{E_0} r \Psi_n^{(1)}(kr) P_n^{|m|}(\cos\theta) \exp(-im\varphi) \sin\theta d\theta d\varphi d(kr)$$

Eqs.4 and 6 are strictly equivalent when the field descriptions exactly satisfy Maxwell's equations, and provide two different ways to evaluate the BSCs. The first way (double quadratures) does not explicitly eliminate the spherical Bessel functions and therefore does not need to specify whether they constitute a set of orthogonal functions or not. Conversely, the second set explicitly eliminates the spherical Bessel functions. These functions are orthogonal over the range $(-\infty, +\infty)$, according to [8], p. 732:

$$\int_{-\infty}^{\infty} \Psi_n^{(1)}(kr) \Psi_{n'}^{(1)}(kr) d(kr) = \frac{\pi}{2n+1} \delta_{nn'} \quad (7)$$

However, Eq.5 is defined over $(0, +\infty)$ instead of over $(-\infty, +\infty)$ and is therefore restricted to a non-orthogonal set of spherical Bessel functions. Eq.5 is then to be completed by [15], p. 412:

$$\int_0^\infty \Psi_n^{(1)}(kr) \Psi_{n'}^{(1)}(kr) d(kr) = \frac{\sin[(n-n')\pi/2]}{n(n+1) - n'(n'+1)} \text{ for } n \neq n' \quad (8)$$

The fact that the spherical Bessel functions $\Psi_n^{(1)}(x)$ are not orthogonal over the interval $(0, +\infty)$ is reminiscent of contravariant and covariant components in tensor calculus. For instance, let us consider a point P in an Euclidean plane spanned by two linear non-orthogonal axes \mathbf{x} and \mathbf{y} crossing with an angle $\gamma \neq 0$ at point O. We may then introduce a vector $\mathbf{V} = \overrightarrow{OP}$ using an intrinsic notation. The vector \mathbf{V} may then receive two different index representations, named the contravariant and the covariant representations. In the contravariant representation, \mathbf{V} is projected onto the axes parallel to them, then defining a contravariant vector $V^i = (x_\parallel, y_\parallel)^+$ in which x_\parallel and y_\parallel are the contravariant components of the contravariant vector V^i , and the cross (+) denotes a

transpose. Conversely, in the covariant representation, \mathbf{V} is projected onto the axes perpendicularly to them, then defining a covariant vector $V_i = (x_\perp, y_\perp)$ in which x_\perp and y_\perp are the covariant components of the covariant vector V_i . But, because the axes \mathbf{x} and \mathbf{y} are not orthogonal, we have $(x_\parallel, y_\parallel) \neq (x_\perp, y_\perp)$.

Similarly, in the F2-formulation, the BSCs may be viewed as components over a set of basis functions involving non-orthogonal spherical Bessel functions. The analogy with contravariant and covariant vectors, although very loose, was a motivation that led us to a careful examination of uniqueness properties of the BSCs in the framework of the F2-formulation.

Then, let us multiply both sides of Eq.1 by r and apply:

$$\int_0^\infty r \Psi_{n'}^{(1)}(kr) dk r \quad (9)$$

to obtain, after using Eq.8, for $n \neq n'$:

$$\int_0^\infty r E_r \Psi_{n'}^{(1)}(kr) dk r = E_0 \sum_{n=1}^\infty \sum_{m=-n}^{+n} c_n^{pw} g_{n, TM}^m \frac{n(n+1) \sin[(n-n')\pi/2]}{n(n+1) - n'(n'+1)} P_n^{|m|}(\cos \theta) e^{im\varphi} \quad (10)$$

Next, we use Eq.2, to obtain, after a change of m' to m :

$$\frac{1}{2\pi} \int_0^\infty \int_0^{2\pi} r E_r \Psi_{n'}^{(1)}(kr) e^{-im\varphi} dk r d\varphi = E_0 \sum_{n=1}^\infty c_n^{pw} g_{n, TM}^m \frac{n(n+1) \sin[(n-n')\pi/2]}{n(n+1) - n'(n'+1)} P_n^{|m|}(\cos \theta) \quad (11)$$

Next, we use Eq.3 and, after a change $l \mapsto n$, and rearranging, we obtain for $n \neq n'$:

$$g_{n, TM}^m \sin[(n-n')\pi/2] = \frac{1}{4\pi E_0 c_n^{pw}} \frac{n(n+1) - n'(n'+1)}{n(n+1)} (2n+1) \frac{(n-|m|)!}{(n+|m|)!} \quad (12)$$

$$\int_0^\infty \int_0^\pi \int_0^{2\pi} r E_r \Psi_{n'}^{(1)}(kr) P_n^{|m|}(\cos \theta) \sin \theta e^{-im\varphi} dk r d\theta d\varphi$$

If $(n-n')$ is even, i.e. $(n-n') = 2k$, then $\sin[(n-n')\pi/2] = 0$, and Eq.12 implies:

$$\int_0^\infty \int_0^\pi \int_0^{2\pi} r E_r \Psi_{n'}^{(1)}(kr) P_n^{|m|}(\cos \theta) \sin \theta e^{-im\varphi} dk r d\theta d\varphi = 0 \text{ for } (n-n') \text{ even, } n \neq n' \quad (13)$$

Inserting the expression of Eq.1 into the l.h.s. of Eq.13, and using Eq.8 for $(n - n')$ even, $n \neq n'$, allows one to check the validity of Eq.13 whenever the function $E_r(r, \theta, \varphi)$ represents the radial component of an EM field. But, if $(n - n')$ is odd, i.e. $(n - n') = 2k + 1$, then $\sin[(n - n')\pi/2] = \pm 1$, and Eq.12 leads to:

$$[g_{n, TM}^m]_{n \neq n'} = \frac{1}{4\pi E_0 c_n^{pw}} \frac{n(n+1) - n'(n'+1)}{n(n+1) \sin[(n-n')\pi/2]} (2n+1) \frac{(n-|m|)!}{(n+|m|)!} \quad (14)$$

$$\int_0^\infty \int_0^\pi \int_0^{2\pi} r E_r \Psi_{n'}^{(1)}(kr) P_n^{|m|}(\cos \theta) \sin \theta e^{-im\varphi} dk r d\theta d\varphi \text{ for } (n - n') \text{ odd}$$

for a given value of n and with $n' \neq n$ being arbitrary, for $(n - n')$ odd. Thus we appear to have an infinite number of ways to compute BSCs, depending on the value chosen for n' , as expected from the above-mentioned analogy. With the idea that the F1- and F2-formulations are actually equivalent, and that the set of BSCs is unique, we now have to compare the different sets of BSCs that we obtain, either from Eq.4 or from Eq.14, $(n - n')$ odd. To do this, we rewrite Eq.14 as:

$$[g_{n, TM}^m]_{n \neq n'} = \frac{1}{4\pi E_0 c_n^{pw}} \frac{n(n+1) - n'(n'+1)}{n(n+1) \sin[(n-n')\pi/2]} (2n+1) \frac{(n-|m|)!}{(n+|m|)!} \quad (15)$$

$$\int_0^\infty r \Psi_{n'}^{(1)}(kr) d(kr) \left\{ \int_0^\pi \int_0^{2\pi} E_r P_n^{|m|}(\cos \theta) \sin \theta e^{-im\varphi} d\theta d\varphi \right\} \text{ for } (n - n') \text{ odd}$$

The $\{.\}$ -term may however be taken from Eq.4 to obtain:

$$[g_{n, TM}^m]_{n \neq n'} = \frac{n(n+1) - n'(n'+1)}{\sin[(n-n')\pi/2]} g_{n, TM}^m \int_0^\infty \Psi_{n'}^{(1)}(kr) \Psi_n^{(1)}(kr) d(kr) \quad (16)$$

which by virtue of Eq.8 implies:

$$[g_{n, TM}^m]_{n \neq n'} = g_{n, TM}^m \quad (17)$$

independently of the value of n' ($n - n'$ odd).

TE-BSCs would be treated similarly allowing one to similarly obtain:

$$[g_{n,TE}^m]_{n \neq n'} = g_{n,TE}^m \quad (18)$$

therefore assuring the uniqueness of BSCs.

Strictly speaking, the uniqueness of BSCs has here been demonstrated in the framework of quadrature formulations. The result obtained could have been however expected insofar as the uniqueness of BSCs may be shown to be valid whatever the method used. The demonstration goes on as follows. Let us assume that Eq.1 is valid as well for an alternative set of BSCs $\overline{g_{n,TM}^m}$ according to:

$$E_r = E_0 \sum_{n=1}^{\infty} \sum_{m=-n}^{+n} c_n^{pw} \overline{g_{n,TM}^m} \frac{n(n+1)}{r} \Psi_n^{(1)}(kr) P_n^{|m|}(\cos \theta) \exp(im\varphi) \quad (19)$$

Hence, by subtraction:

$$0 = E_0 \sum_{n=1}^{\infty} \sum_{m=-n}^{+n} c_n^{pw} [g_{n,TM}^m - \overline{g_{n,TM}^m}] \frac{n(n+1)}{r} \Psi_n^{(1)}(kr) P_n^{|m|}(\cos \theta) \exp(im\varphi) \quad (20)$$

Next, applying Eqs.2 and 3 to Eq.20 to successively get rid of the exponentials and of the associated Legendre functions, we obtain:

$$0 = [g_{n,TM}^m - \overline{g_{n,TM}^m}] \Psi_n^{(1)}(kr) \quad (21)$$

which exhibits the particular role played by the spherical Bessel functions and implies:

$$g_{n,TM}^m = \overline{g_{n,TM}^m} \quad (22)$$

with a similar demonstration for the TE-coefficients.

As a final remark, let us note that the present work complements our understanding of the description of structured beams in terms of BSCs, but have no implication concerning the numerical efficiency of the theory. Indeed, in any

case, triple quadratures of the form of Eq.14 will be more time-consuming than the double quadratures of the form of Eq.4. Let us also take the opportunity of this remark to recall that even the double quadratures of Eq.4 are numerically too time-consuming to constitute an efficient way of evaluating the BSCs, except when they can be analytically solved to obtain closed-form solutions, e.g. for zeroth-order Bessel beams [16], higher-order Bessel beams [17], and superpositions of Bessel beams, either for "frozen waves" [18], [19], [20], [21], or for Mathieu beams which are expressed as well as superpositions of Bessel beams [22].

Otherwise, the arsenal of methods usable to evaluate BSCs also contains localized approximations (with several variants) which may speed up the computations by several orders of magnitude, e.g. [23] to be complemented by [24], [25], [26], and finite series which, after having been forgotten for several decades, has been recently used again due to the limitations encountered when dealing with localized approximations in the case of beams exhibiting axicon angles and/or topological charges, e.g. [27], [28], [29], and references therein. It is also possible to use an angular spectrum decomposition into elementary plane waves either (i) by computing the scattering response of each plane wave and summing up all the responses over the plane waves present in the decomposition, a process which requires the use of GLMT for each tilted plane wave, e.g. [30] or (ii) evaluating the BSCs of each plane wave and summing up to obtain the BSCs of the whole beam, before entering GLMT computations, e.g. without pretending to exhaustiveness [31], [32], [33], [34], [35], [36], [37], [38], [39] and [40] for a variant relying on the use of a Whittaker integral formalism. See also [41] for the relationship between BSCs and plane wave spectra.

3 Conclusion.

BSCs in GLMT may be derived by using a non-orthogonal subset of spherical Bessel functions. Motivated by an analogy concerning the difference between contravariant and covariant vectors, we noted that there appears to exist an infinite number of different quadratures to evaluate the BSCs. We have demonstrated that the BSCs obtained by the different ways of evaluating them are identical, so that the decomposition of E_r over VSWFs is indeed unique, as expected, and demonstrated in a general framework. As a by-product, we have established a new equation, namely Eq.13.

More generally, the present paper complements our understanding of the structure of the GLMT in the sense that the fact that we may use a non-orthogonal version of spherical Bessel functions by restricting the range of definition of the spherical Bessel functions to $(0, +\infty)$ has not been explicitly noted previously, nor has it been perceived that it implies the existence of an infinite number of quadratures to evaluate the BSCs.

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