Accurate Computation and Tabulation of the Scalar Green Function for Bi-anisotropic Media and its Derivatives

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Abstract: A novel numerical scheme is presented for the computation and tabulation of the scalar Green function in bi-anisotropic media and its derivatives. The main idea in the proposed scheme is to expand the scalar Green function into Gegenbauer polynomials. Besides quite naturally yielding a storage scheme for the scalar Green function, this approach allows a unique trick for computing its derivatives. The trick is based on the fact that the polynomial expansion coefficients for plane waves are analytically known in terms of Bessel functions. This allows the numerical computation of polynomial expansion coefficients that are much smaller than the machine precision. This in turn allows the derivatives of the scalar Green function to be accurately and robustly computed as the derivatives of polynomials.

Keywords: Bi-anisotropic Media, Scalar Green Function, Derivatives, Accurate Computation, Tabulation

1. Introduction

Bi-anisotropic media are the most general media that can be described using linear constitutive equations. These media have received much attention in the past, because of the plethora of applications in various microwave components such as depolarizers, polarimeters and directional couplers [1]. In addition, the bi-anisotropy of materials is of importance in the study of metamaterials.

From a computational point of view, however, bi-anisotropic media present many difficulties. The sheer number of parameters in the constitutive equations allows for many potentially troublesome cases, and no numerical technique can be expected to work for all possible materials. Nevertheless, it is rather straightforward to formally extend the Finite Element Method (FEM) to bi-anisotropic media [1]. For Boundary Integral Equation (BIE) techniques, such an extension is much more difficult because of two major problems. The first problem is that the Green dyadics of the used medium need to be computed one way or another. There are four Green dyadics: one for each possible combination of current type (electric or magnetic) and field type (also electric or magnetic). The need for the Green dyadics has resulted in much research into the construction of explicit formulas for these Green dyadics [2,3]. Despite dramatic progress, however, the class of media for which explicit formulas are available is still a small subset of the full parameter space. The second problem is the computation of the impedance integrals required in the discretization of the integral equation. Since there are no analytical expressions for the Green dyadics in the general case, mainstream techniques such as singularity extraction cannot be used. Arguably, these two problems are the prime reasons why BIEs have only scarcely been applied to bi-anisotropic media.

In this contribution, the first problem will be tackled. As has been shown in the literature [4], the computation of the Green dyadics can be reduced to the computation of one scalar Green function that

satisfies a fourth-order partial differential equation. The Green dyadics can then be obtained from this scalar Green function by means of at most fourth-order derivatives. Here, a novel numerical scheme for the evaluation and tabulation of the scalar Green function in bi-anisotropic media is presented. It relies on the expansion of the scalar Green function into Gegenbauer polynomials. This approach leads to an exponentially converging representation of the scalar Green function, which means that only a moderate number of polynomial coefficients need to be stored to get a highly accurate result. In addition, the properties of the Gegenbauer polynomials can be leveraged to allow the numerically stable computation of the expansion coefficients, even if they are much smaller than the machine precision (relative to the leading expansion coefficient). In the following, the established theory behind the scalar Green function will be summarized, followed by the derivation of the Gegenbauer polynomial coefficients and some numerical results.

2. The Scalar Green Function

Maxwell's curl equations in the frequency domain are given by

$$\boldsymbol{\nabla} \times \boldsymbol{e}(\boldsymbol{r}) = -j\omega \boldsymbol{b}(\boldsymbol{r}) - \boldsymbol{m}(\boldsymbol{r}), \tag{1}$$

$$\boldsymbol{\nabla} \times \boldsymbol{h}(\boldsymbol{r}) = j\omega \boldsymbol{d}(\boldsymbol{r}) + \boldsymbol{j}(\boldsymbol{r}), \tag{2}$$

with constitutive equations

$$\boldsymbol{d}(\boldsymbol{r}) = \bar{\bar{\varepsilon}} \cdot \boldsymbol{e}(\boldsymbol{r}) + \bar{\bar{\xi}} \cdot \boldsymbol{h}(\boldsymbol{r}), \tag{3}$$

$$\boldsymbol{b}(\boldsymbol{r}) = \bar{\bar{\zeta}} \cdot \boldsymbol{e}(\boldsymbol{r}) + \bar{\bar{\mu}} \cdot \boldsymbol{h}(\boldsymbol{r}). \tag{4}$$

A medium is called anisotropic when the magneto-electric coupling tensors, i.e. $\bar{\bar{\xi}}$ and $\bar{\bar{\zeta}}$, are zero. In the isotropic case, all parameter tensors are scalars. For the computation of the fields generated by the currents, the bi-anisotropic medium is assumed to be homogeneous and to extend to infinity in all directions. A spatial Fourier transform of these equations then replaces $\boldsymbol{\nabla}$ with $j\boldsymbol{k}$. This allows Maxwell's equations to be written in a concise matrix form

$$-j\omega \mathsf{P} \cdot \begin{bmatrix} \boldsymbol{e}(\boldsymbol{r}) \\ \boldsymbol{h}(\boldsymbol{r}) \end{bmatrix} = \begin{bmatrix} \boldsymbol{j}(\boldsymbol{r}) \\ \boldsymbol{m}(\boldsymbol{r}) \end{bmatrix}, \tag{5}$$

with

$$\mathsf{P} = \begin{bmatrix} \bar{\bar{\varepsilon}} & \bar{\bar{\xi}} - \boldsymbol{s} \times \mathbb{1} \\ \bar{\bar{\zeta}} + \boldsymbol{s} \times \mathbb{1} & \bar{\bar{\mu}} \end{bmatrix}. \tag{6}$$

Here, $\boldsymbol{s}$ denotes the slowness, defined by $\boldsymbol{k} = \omega \boldsymbol{s}$. Solving the system of linear equations (5) can be done by means of the adjugate matrix of P:

$$\mathsf{P}^{-1} = \frac{\mathrm{Adj}(\mathsf{P})}{\mathrm{Det}(\mathsf{P})}. \tag{7}$$

The denominator is usually called the Helmholtz determinant $D(\boldsymbol{s})$ and defines the scalar Green function by means of the inverse Fourier transform

$$G_\omega(\boldsymbol{r}) = \frac{1}{8\pi^3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{e^{j\boldsymbol{k}\cdot\boldsymbol{r}}}{D(\frac{\boldsymbol{k}}{\omega})} \mathrm{d}\boldsymbol{k} = \omega^3 G(\omega \boldsymbol{r}). \tag{8}$$

A convenient frequency-independent Green function was introduced here, which is given by

$$G(\boldsymbol{r}) = \frac{1}{8\pi^3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{e^{j\boldsymbol{s}\cdot\boldsymbol{r}}}{D(\boldsymbol{s})} \mathrm{d}\boldsymbol{s}. \tag{9}$$

Taking the inverse Fourier transform of equation (5) shows that the fields are basically the convolution of the inverse Fourier transform of P^{-1} with the currents. Therefore, the inverse Fourier transform of P^{-1} can be interpreted as a concatenation of the four Green dyadics. When studying formula (7), it can be seen that the elements of P's adjugate are polynomials of degree four in the components of $\boldsymbol{k}$. The inverse Fourier transform maps this adjugate matrix to an operator containing only spatial derivatives. Therefore it can be concluded that the inverse Fourier transform of P^{-1}, i.e. the four Green dyadics, can be numerically computed if the scalar Green function and its derivatives (up to fourth order) can be computed. This shows why it is important to be able to accurately compute derivatives of the scalar Green function.

3. Computing the Gegenbauer Polynomial Coefficients

The Gegenbauer polynomials $C_k^{\nu}(t)$ (sometimes also called the ultraspherical polynomials) are the family of orthogonal polynomials associated with the weighting function $(1-t^2)^{\nu-\frac{1}{2}}$ on the interval [-1,1]. These polynomials satisfy the following addition theorem [5]

$$e^{ivt} = \frac{2^{\nu}\Gamma(\nu)}{v^{\nu}} \sum_{k=0}^{\infty} (\nu+k) i^k J_{\nu+k}(v)\, C_k^{\nu}(t), \forall \nu \neq \{0,-1,-2,...\}, \tag{10}$$

which is valid on the interval [-1,1]. However, using elementary manipulations, it can be modified to

$$e^{ivt} = e^{ivc} \frac{2^{\nu}\Gamma(\nu)}{(va)^{\nu}} \sum_{k=0}^{\infty} (\nu+k) i^k J_{\nu+k}(va)\, C_k^{\nu}\left(\frac{t-c}{a}\right). \tag{11}$$

This expression is valid on the interval [c-a,c+a]. The parameter ν can be freely chosen within the limitations given in equation (10).

Now, the exponential in the integral representation of the frequency-independent Green function (9) can be split into three factors, one for each Cartesian coordinate. When each of these factors is expanded into Gegenbauer polynomials using equation (11), the following is obtained

$$G(\boldsymbol{r}) = \left(\frac{2^{\nu}\Gamma(\nu)}{2\pi}\right)^3 \sum_{k_x=0}^{\infty} B_{k_x,k_y,k_z} C_{k_x}^{\nu}\left(\frac{x-c_x}{a_x}\right) C_{k_y}^{\nu}\left(\frac{y-c_y}{a_y}\right) C_{k_z}^{\nu}\left(\frac{z-c_z}{a_z}\right), \tag{12}$$

with the coefficients

$$B_{k_x,k_y,k_z} = (\nu+k_x)(\nu+k_y)(\nu+k_z) i^{k_x+k_y+k_z} \int\int\int \frac{e^{j\boldsymbol{s}\cdot\boldsymbol{c}}}{D(\boldsymbol{s})} \left[\frac{J_{\nu+k_x}(s_x a_x)}{(s_x a_x)^{\nu}} \frac{J_{\nu+k_y}(s_y a_y)}{(s_y a_y)^{\nu}} \frac{J_{\nu+k_z}(s_z a_z)}{(s_z a_z)^{\nu}}\right] \mathrm{d}\boldsymbol{s}. \tag{13}$$

Expansion (12) is valid in a rectangular region with center $\boldsymbol{c}$ and sides $[a_x, a_y, a_z]$ in the three Cartesian coordinate directions.

It is worthwhile to point out that the normal procedure for expanding a function into orthogonal polynomials is the computation of inner products between the function and the polynomials (with the correct weighting function). In the case of the scalar Green function, this would mean that a six-fold integral would have to be computed for each coefficient. Thanks to addition theorem (10), however, this prohibitively expensive operation is avoided.

In addition, if the inner products would be computed numerically, their absolute error would be inherently limited to around the machine precision. Because the Bessel functions in equation (13) converge to zero very quickly once their order exceeds their argument, this would result in large relative errors, which would show up in the computation of the derivatives. This problem is solved by using equation (13), because there exist efficient and accurate computation routines for the Bessel functions that fully capture this convergence to zero (up till the point where underflow occurs). For example, the Matlab routines for computing Bessel functions have no problems producing values that are much smaller than the machine precision. The fact that this is possible is crucial for the accurate computation of the

polynomial coefficients that have a small magnitude.

Finally, the triple integral in equation (9) has to be evaluated. Since it is easy to show that the factor between square brackets in equation (13) is actually an entire function, it is possible to do one integration analytically by means of complex contour integration. The remaining two integrations can then be done using adaptive quadrature.

3. Numerical Results

For the numerical tests, $\nu = 0.5$ was chosen. In this case, the Gegenbauer polynomials reduce to the Legendre polynomials. In [6], closed form expressions are given for various Green functions. From these results, the frequency-independent scalar Green function for a uniaxially anisotropic medium can be found. For this example, the medium dyadics where chosen as

$$\bar{\bar{\varepsilon}} = \begin{bmatrix} \varepsilon_t & 0 & 0 \\ 0 & \varepsilon_t & 0 \\ 0 & 0 & \varepsilon_z \end{bmatrix}, \; \bar{\bar{\mu}} = \begin{bmatrix} \mu_t & 0 & 0 \\ 0 & \mu_t & 0 \\ 0 & 0 & \mu_z \end{bmatrix}, \; \bar{\bar{\xi}} = \bar{\bar{\zeta}} = 0. \tag{14}$$

with the parameters having numerical values $\varepsilon_t = 2.0 - 0.01i$, $\varepsilon_z = 1.0 - 0.01i$, $\mu_t = 1.5 - 0.01i$, $\mu_z = 2.5 - 0.01i$.

Figure 1 shows a comparison between the numerically computed scalar Green function and the analytical expression for points on a line between [1,1,1] and [1,1,3]. The tolerance for the adaptive integration was set to 1.0e-12, and the highest degree of the Legendre polynomials that were used was 36. Excellent agreement between the curves for the numerically and analytically computed Green function can be observed. Indeed, the relative error between the two is less than 1.0e-13 for this example. It should be pointed out that, even though the magnitude of the Green function does not change much in the plot, the phase does change. The relative error on all derivatives up to fourth order is also shown, again confirming the accuracy of the approach.

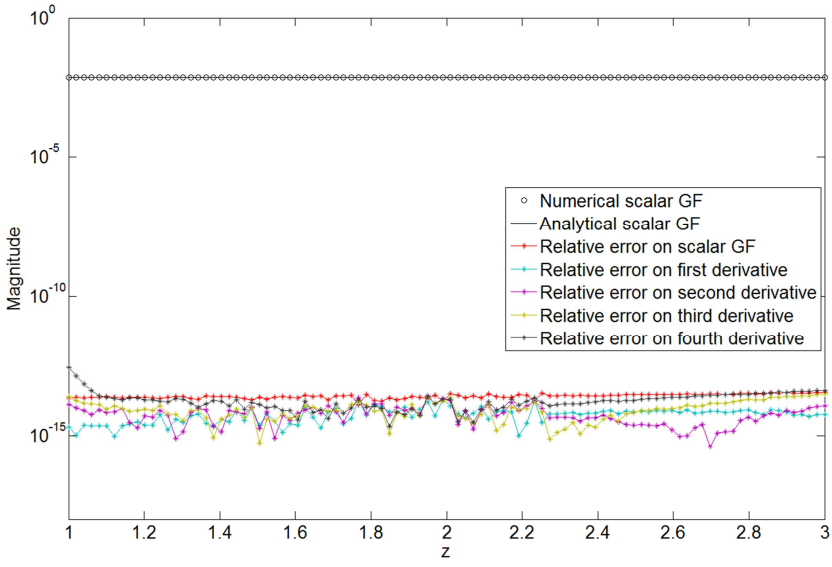

Figure 1: Comparison of the numerically computed scalar Green function (GF) with the analytical result. Excellent accuracy is obtained for the scalar Green function and its derivatives.

7. Conclusions

A novel scheme for the computation and tabulation of the scalar Green function for bi-anisotropic media has been developed. Leveraging the unique properties of the Gegenbauer polynomials allows the accurate computation and tabulation of both the scalar Green function and its derivatives, thereby opening the door to the investigation of boundary integral methods in bi-anisotropic media.

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