A Calderon Multiplicative Preconditioner for the PMCHWT Equation for Scattering by Chiral Objects

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Abstract—Scattering of time-harmonic electromagnetic waves by chiral structures can be modeled via an extension of the PMCHWT boundary integral equation for analyzing scattering by dielectric objects. The classical PMCHWT equation however suffers from dense discretization breakdown: the matrices resulting from its discretization become increasingly ill-conditioned when the mesh density increases. This contribution revisits the PMCHWT equation for chiral media. It is demonstrated that it also suffers from dense discretization breakdown. This dense discretization breakdown is mitigated by the construction of a Calderon multiplicative preconditioner. A stable discretization scheme is introduced, and the resulting algorithm’s accuracy and efficiency are corroborated by numerical examples.

Index Terms—chiral media, boundary integral equations, boundary element method, PMCHWT equation, dense discretization breakdown, Calderon multiplicative preconditioner

I. INTRODUCTION

Scattering of time-harmonic electromagnetic fields by homogeneous objects often is modeled using boundary integral equations (BIEs). The best-known BIEs that apply to scattering by perfect electric conductors are the electric and magnetic field integral equations (EFIE and MFIE). Prototypical BIEs that apply to penetrable objects are the Poggio-Miller-Chan-Harrington-Wu-Tsai (PMCHWT) [1] and Müller equations [2]. These equations can be regarded as analogues of the EFIE and MFIE, in that they exhibit similar spectral properties. More precisely, the spectra of the EFIE’s and the PMCHWT equation’s operators comprise two branches, one accumulating at zero, and the other at infinity. The spectra of the MFIE’s and the Müller equation’s operators, on the other hand, accumulate at a finite non-zero value.

All of the above BIEs can be solved numerically using the boundary element method: the surface of the scatterer is approximated by a mesh, and the unknown field quantities are expanded in a finite number of basis functions defined on this mesh. This approach reduces the BIE to a finite set of linear equations in the field expansion coefficients, which often is solved using iterative methods. Because the EFIE’s and PMCHWT equation’s operators have unbounded spectra, the corresponding system matrices have very large condition numbers when the mesh parameter (i.e. the length of the shortest edge) decreases. This phenomenon is called dense discretization breakdown and can be resolved by applying Calderon multiplicative preconditioners (CMPs) [3]–[5].

In [6], the authors have presented the successful application of the CMP to the chiral extension of the PMCHWT equation. It is the aim of this paper to elaborate on the theoretical fundamentals of the chiral CMP, and to present further numerical experiments corroborating the accuracy and the efficiency of the technique.

Section II offers a quick overview of electromagnetic fields in chiral media. Following this, the PMCHWT equation for chiral media is presented in section III. While this is not new material, it is included for self-containedness and to introduce the notations used throughout the following sections.

In section IV, the self-regularizing property of the chiral PMCHWT operator is studied. While this is analogous to the nonchiral case, two difficulties arise: the spectral properties of a composite operator involving three different wavenumbers must be studied, and the chiral PMCHWT operator requires a diagonalization. Once it is established that the operator is indeed self-regularizing, the CMP is formed by applying a suitable discretization scheme.

In the last section, numerical experiments testify to the success of the CMP. The accuracy is tested by comparing the results to the Mie series and to ab initio simulations of chiral metamaterials. The efficiency is shown by comparing the condition number of the system matrix with and without CMP, and the required number of iterations.

II. ELECTROMAGNETIC FIELDS IN CHIRAL MEDIA

For time-harmonic electromagnetic fields, the electric and magnetic field (resp. \( e \) and \( h \)) are linked to the electric and magnetic displacement field (resp. \( d \) and \( j \)) by the Maxwell equations

\[
\begin{align*}
\nabla \times e &= -j\omega b - j_m, \\
\nabla \times h &= j\omega d + j,
\end{align*}
\]
The interaction of the electromagnetic fields with the medium in which they propagate is modeled by constitutive equations. The lack of reflection symmetry, which is the defining characteristic for chiral media, must therefore be incorporated into the constitutive equations. This can be done using the Drude-Born-Fedorov (DBF) model [7]. However, for notational simplicity, the following equivalent constitutive equations are assumed [8]:

\[
\begin{pmatrix}
  d \\
  b
\end{pmatrix} = \begin{pmatrix}
  \varepsilon \\
  j\kappa \sqrt{\varepsilon \mu}
\end{pmatrix} \begin{pmatrix}
  e \\
  h
\end{pmatrix},
\]

where \( \varepsilon \) is the permittivity, \( \mu \) is the permeability and \( \kappa \) is the dimensionless chirality parameter. The constitutive equations (3) introduce extra coupling between electric and magnetic field quantities. This coupling can be removed, however, by application of the so-called Bohren transform:

\[
\begin{pmatrix}
  \mathcal{E}_\pm \\
  \mathcal{H}_\pm
\end{pmatrix} = P^\pm \begin{pmatrix}
  e \\
  h
\end{pmatrix}, \quad P^\pm = \frac{1}{2} \begin{pmatrix}
  1 & \mp j\eta \\
  j\eta & 1
\end{pmatrix}.
\]

Here \( \eta = \sqrt{\mu/\varepsilon} \) is the characteristic impedance of the medium. The matrices \( P^\pm \) are projection matrices, satisfying \( P^+ + P^- = 1 \). The inverse Bohren transform is

\[
e = \mathcal{E}_+ + \mathcal{E}_-, \quad h = \mathcal{H}_+ + \mathcal{H}_-.
\]

A similar transformation applies to the electric and magnetic sources:

\[
\begin{pmatrix}
  \mathcal{J}_\pm \\
  \mathcal{M}_\pm
\end{pmatrix} = \frac{1}{2} \begin{pmatrix}
  1 & \mp j\eta \\
  j\eta & 1
\end{pmatrix} \begin{pmatrix}
  j \\
  j m
\end{pmatrix}.
\]

The fields resulting from the Bohren transforms (4) and (6) are governed by equations formally identical to Maxwell equations in the absence of chirality:

\[
\nabla \times \mathcal{E}_\pm = -j\omega\mu (1 \pm \kappa) \mathcal{H}_\pm - \mathcal{M}_\pm, \quad \nabla \times \mathcal{H}_\pm = j\omega\varepsilon (1 \pm \kappa) \mathcal{E}_\pm + \mathcal{J}_\pm.
\]

Equation (4) decomposes the electromagnetic fields \((e, h)\) into two contributions: \((\mathcal{E}_+, \mathcal{H}_+)\) and \((\mathcal{E}_-, \mathcal{H}_-). In the absence of external sources,

\[
\nabla \times \mathcal{E}_\pm = \pm \gamma_\pm \mathcal{E}_\pm, \quad \gamma_\pm = \omega \sqrt{\varepsilon \mu} (1 \pm \kappa).
\]

Therefore, \( \mathcal{E}_+ \) and \( \mathcal{E}_- \) are Beltrami fields. For \(-1 < \kappa < 1 \) (which is the case for realistic materials), the two “modes” \( \mathcal{E}_+ \) and \( \mathcal{E}_- \) have opposite helicity, and the operators \( P^+ \) and \( P^- \) project the electromagnetic fields upon their components with positive and negative helicity, respectively. When applied to plane wave solutions, the component with positive helicity \((\mathcal{E}_+, \mathcal{H}_+)\) is right-handed circularly polarized, while the component with negative helicity \((\mathcal{E}_-, \mathcal{H}_-)\) is left-handed circularly polarized. If the chirality parameter \( \kappa \) is nonzero, these components propagate with different wavenumbers \( \gamma_\pm \). This is the cause of the well-known phenomenon of optical activity.

### III. The Chiral PMCHWT Equation

The Bohren transform allows for the expansion of the electromagnetic field in a chiral medium into two components, each fulfilling the Maxwell equations in a nonchiral medium. These components thus obey all the usual equations and identities of electromagnetics. This property can be exploited to construct BIEs describing scattering by chiral objects. In this section, the extension of the PMCHWT equation for the modeling of scattering by nonchiral objects to the chiral PMCHWT equation for the modeling of scattering by chiral structures is revisited.

#### A. The Stratton-Chu Representation Theorem

Consider a homogeneous, isotropic, penetrable object \( \Omega \) characterized by permittivity \( \varepsilon \), permeability \( \mu \), impedance \( \eta = \sqrt{\mu/\varepsilon} \) and wavenumber \( k = \omega \sqrt{\mu/\varepsilon} \). It is embedded in a background medium with permittivity \( \varepsilon_0 \), permeability \( \mu_0 \), impedance \( \eta_0 = \sqrt{\mu_0/\varepsilon_0} \) and wavenumber \( k_0 = \omega \sqrt{\mu_0/\varepsilon_0} \). The boundary of \( \Omega \) is denoted \( \Gamma \), and its exterior normal vector is denoted \( \hat{n} \). An external electromagnetic field \((e^i, h^i)\) is applied. The tangential traces of the electromagnetic field just inside \( \Omega \), denoted \((e^-, h^-)\), satisfy the Stratton-Chu representation formula [9]:

\[
\begin{pmatrix}
  -\hat{n} \times e^- \\
  \hat{n} \times h^-
\end{pmatrix} = S^{\text{int}}(\eta, k) \begin{pmatrix}
  -\hat{n} \times e^- \\
  \hat{n} \times h^-
\end{pmatrix},
\]

where

\[
S^{\text{int}}(\eta, k) = \begin{pmatrix}
  \frac{1 - K_k}{1 - 2\kappa \eta T_k} & \frac{\eta T_k}{1 - 2\kappa \eta T_k} \\
  -\frac{T_k}{1 - 2\kappa \eta T_k} & \frac{1 - K_k}{1 - 2\kappa \eta T_k}
\end{pmatrix}.
\]

is the internal Stratton-Chu operator. A similar result holds for the traces of the electromagnetic field just outside \( \Omega \), denoted \((e^+, h^+)\):

\[
\begin{pmatrix}
  -\hat{n} \times e^+ \\
  \hat{n} \times h^+
\end{pmatrix} = S^{\text{ext}}(\eta_0, k_0) \begin{pmatrix}
  -\hat{n} \times e^+ \\
  \hat{n} \times h^+
\end{pmatrix} + \begin{pmatrix}
  -\hat{n} \times e^- \\
  \hat{n} \times h^-
\end{pmatrix},
\]

where

\[
S^{\text{ext}}(\eta_0, k_0) = \begin{pmatrix}
  \frac{1}{1 - 2\kappa \eta_0 T_{k_0}} + K_{k_0} & -\eta_0 T_{k_0} \\
  -\frac{T_{k_0}}{1 - 2\kappa \eta_0 T_{k_0}} & \frac{1}{1 - 2\kappa \eta_0 T_{k_0}} + K_{k_0}
\end{pmatrix}.
\]

is the external Stratton-Chu operator. The EFIE operator \( T_k \) (which is the sum of a weakly singular part \( T_s \) and a hypersingular part \( T_h \)) and the MIE operator \( K_k \) are

\[
T_k f(r) = T_{S,k} f(r) + T_{H,k} f(r),
\]

\[
T_{H,k} f(r) = -jk \hat{n} \times \int_G \frac{e^{-jkR}}{4\pi R} f(r') ds',
\]

where \( p.v. \) indicates that the integral should be interpreted as a Cauchy principal value, and \( R = |r - r'| \).

By imposing continuity of the tangential traces of \((e^-, h^-)\) and \((e^+, h^+)\), and subtracting (11) from (13), the PMCHWT equation [1] is obtained:

\[
Q(\eta_0, k_0; \eta, k) \begin{pmatrix}
  -\hat{n} \times e^- \\
  \hat{n} \times h^-
\end{pmatrix} = - \begin{pmatrix}
  -\hat{n} \times e^i \\
  \hat{n} \times h^i
\end{pmatrix}.
\]
where the PMCHWT operator is
\[ Q(\eta_0, k_0; \eta, k) = S^{\text{ext}}(\eta_0, k_0) - S^{\text{int}}(\eta, k) \]
\[ = \left( K_{k_0} + K_k - \eta_0 T_{k_0} - \eta T_k \right) \left( T_{k_0}/\eta_0 + T_k/\eta \right), \] (20)

\[ \left( \hat{n} \times \mathcal{E}_\pm \right) = S^{\text{int}}(\eta, \gamma_\pm) \left( \hat{n} \times \mathcal{H}_\pm \right), \] (21)

B. The PMCHWT Equation for Chiral Media

If the medium filling \( \Omega \) is chiral, equation (11) does not hold. However, the Bohren transform has shown that in chiral media, the field comprises two components \( (\mathcal{E}_\pm, \mathcal{H}_\pm) \) that do not couple (except at boundaries). They act as though they propagate through a nonchiral medium with characteristic impedance \( \eta \) and wavenumbers \( \gamma_\pm \). Therefore, they obey the Stratton-Chu representation formula (11):
\[ \left( \hat{n} \times \mathcal{E}_\pm \right) = S^{\text{int}}(\eta, \gamma_\pm) \left( \hat{n} \times \mathcal{H}_\pm \right), \]

Transforming this back to \( e \) and \( h \) using (4) and (5) results in
\[ \left( \hat{n} \times e^- \right) = S^c_{\text{int}}(\eta, \gamma_-, \gamma_+) \left( \hat{n} \times h^- \right), \]
\[ \left( \hat{n} \times h^- \right) = S^c_{\text{int}}(\eta, \gamma_-, \gamma_+) \left( \hat{n} \times e^- \right), \] (22)

\[ S^c_{\text{int}}(\eta, \gamma_-, \gamma_+) = S^{\text{int}}(\eta, \gamma_+) P^- + S^{\text{int}}(\eta, \gamma_-) P^+. \]

The pairing of \( \gamma_+ \) with \( P^- \) and \( \gamma_- \) with \( P^+ \) stems from
\[ \left( \mathcal{E}_\pm / \mathcal{H}_\pm \right) = P^\pm \left( e / h \right) \left( \hat{n} \times \mathcal{E}_\pm \right) = P^\pm \left( \hat{n} \times \mathcal{H}_\pm \right). \] (23)

The chiral PMCHWT equation is obtained by again imposing continuity of the tangential traces of \( (e^-, h^-) \) and \( (e^+, h^+), \) and subtracting (13) from (22):
\[ Q_c(\eta_0, k_0; \eta, \gamma_-, \gamma_+) \left( \hat{n} \times e^- \right) = \left( \hat{n} \times e^i \right) \left( \hat{n} \times h^i \right) \] (24)

where the chiral PMCHWT operator is
\[ Q_c(\eta_0, k_0; \eta, \gamma_-, \gamma_+) = \left( S^{\text{ext}}(\eta_0, k_0) - S^{\text{int}}(\eta, \gamma_-, \gamma_+) \right) \]
\[ = \left( \mathcal{K}_{k_0} + \mathcal{K}_k \right) - \left( \eta_0 T_{k_0} - \eta T_k \right) \]
\[ = \left( \mathcal{K}_{k_0} + \mathcal{K}_k \right) - \eta_0 T_{k_0} - \eta T_k. \] (25)

Expressions for the operators \( Q_{11}, Q_{12}, Q_{21} \) and \( Q_{22} \) are obtained by combining (4), (12) and (14):
\[ Q_{11} = Q_{22} = \mathcal{K}_{k_0} + \mathcal{K}_k - j T^-, \]
\[ Q_{12} = -\eta_0 T_{k_0} - \eta (T^+ + j K^-), \]
\[ Q_{21} = T_{k_0}/\eta_0 + (T^- + j K^+)/\eta. \] (26)

Here the notation
\[ K^\pm = \frac{1}{2} \left( K_{\gamma_-} \pm K_{\gamma_+} \right), \quad T^\pm = \frac{1}{2} \left( T_{\gamma_-} \pm T_{\gamma_+} \right) \]
was used.

The chiral PMCHWT equation is obtained by performing the following substitution in the nonchiral PMCHWT equation:
\[ K_k \rightarrow K^+ - j T^- \quad T_k \rightarrow T^+ + j K^- \]

Note that the compact contributions \( K_k \) from the nonchiral PMCHWT equation are perturbed by discontinuous contributions \( j T^- \). This implies that no matter how small the chirality parameter \( \kappa \), there always is a mesh parameter \( h_0 \) such that when the actual mesh parameter \( h \) is smaller than \( h_0 \), the spectra of the matrices resulting upon discretization of the nonchiral and chiral PMCHWT equation will differ qualitatively. This is symptomatic to the introduction of “new physics” in the system.

The chiral PMCHWT equation (24) is equivalent to that presented in [10], and is a special case of the integral equations constructed for inhomogeneous chiral structures in [11]. A similar boundary integral equation has been derived for scattering by chiral objects above a lossy half space [12], [13]. The chiral PMCHWT equation can also be applied to chiral scatterers in chiral background media [14].

C. Numerical Solution of the Chiral PMCHWT equation

To solve (24) via the boundary element method, the unknown quantities \( \hat{n} \times e \) and \( \hat{n} \times h \) are expanded in a set of basis functions \( f_i \):
\[ \hat{n} \times e = \sum_{i=1}^N c_i f_i, \quad \hat{n} \times h = \sum_{i=1}^N d_i f_i. \] (27)

These expansions are inserted into (24), and the resulting equations are tested with a set of testing functions \( \hat{f}_i \) (i.e. multiplied by \( \hat{f}_i \) and integrated over \( \Gamma \)). This results in the following set of linear equations (in matrix form):
\[ \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix} \begin{pmatrix} c \\ d \end{pmatrix} = \begin{pmatrix} e^i \\ -h^i \end{pmatrix} \] (28)

with
\[ (Q_{ij})_{mn} = \left( \hat{f}_m, Q_{ij} f_n \right), \]
\[ e^i_m = \left( \hat{f}_m, \hat{n} \times e^i \right), \]
\[ h^i_m = \left( \hat{f}_m, \hat{n} \times h^i \right), \]
\[ (x, y) = \int_\Gamma x(r) \cdot y(r) ds. \]

This set of \( 2N \) linear equations can be solved using a Krylov iterative solver.

The accuracy of the solution obtained by the boundary element method depends upon the spectral properties of the PMCHWT operator, as well as the choice of expansion and testing functions [15]. In our implementation, following standard practice [3], [4], the surface \( \Gamma \) is approximated by a triangle mesh. The expansion functions \( f_i \) are chosen to be div-conforming RWG functions [16], while the testing functions \( \hat{f}_i \) are chosen to be curl-conforming rotated RWG functions \( \hat{n} \times f_i \). The accuracy of the solution (27) then depends upon the density of the triangle mesh, which is measured by the mesh parameter (i.e. the minimum edge length).
IV. THE CALDERÓN MULTIPLICATIVE PRECONDITIONER

A. Dense Discretization Breakdown

The numerical solution of the EFIE suffers from dense discretization breakdown: when the mesh is made denser, the condition number of the system matrix in (28) grows quadratically as a function of the inverse of the mesh parameter. This renders the iterative solution of the discretized EFIE increasingly hard and time consuming.

The cause of this phenomenon is rooted in the mathematical properties of the EFIE operator. Its spectrum comprises two branches: one accumulating at zero, the other at infinity. As the discretization is made denser, eigenfunctions corresponding to eigenvalues accumulating at zero and infinity both can be resolved. This renders the system matrix ill-conditioned, and the iterative solution inefficient.

As the nonchiral PMCHWT operator (20) contains the EFIE operator as one of its constituents, it is not surprising that it too is susceptible to dense discretization breakdown [4].

Equation (25) indicates that the chiral PMCHWT operator is intimately connected with the nonchiral PMCHWT operator. Its spectrum can therefore also be expected to be unbounded, resulting in dense discretization breakdown.

To mitigate this problem, the EFIE and the PMCHWT equation have been regularized by Calderón multiplicative preconditioners (CMPs) [4], [5], [17]. In the next sections, this regularization procedure is elucidated and extended to the chiral PMCHWT equation.

B. Regularizing the EFIE

Dense discretization breakdown of the EFIE is caused by the unbounded spectrum of the EFIE operator $\mathcal{T}_k$. However, it is known that for smooth surfaces $\Gamma$, the eigenvalues of the MFIE operator $\mathcal{K}_k$ accumulate at zero (i.e. the operator is compact) [18]. The Calderón identities

\[
\mathcal{K}_k^2 - \mathcal{T}_k^2 = \frac{1}{4}, \quad (29)
\]

\[
\mathcal{T}_k\mathcal{K}_k + \mathcal{K}_k\mathcal{T}_k = 0, \quad (30)
\]

imply that the EFIE operator is self-regularizing: the eigenvalues of its square accumulate at $-\frac{1}{4}$, and its spectrum therefore is bounded. Moreover, if the scatterer does not support an internal resonance at the wave number $k$, the spectrum is bounded away from zero. Upon discretization, such an operator results in a well-conditioned set of equations, even when the discretization is made denser. This fact inspired the introduction of the CMP EFIE in [17]:

\[
\eta\mathcal{T}_k^2 (j) = -\mathcal{T}_k (\hat{n} \times e^i). \quad (31)
\]

In [3], it has been shown that this equation, which involves a product of two operators, can be discretized in a conforming and stable manner by leveraging both RWG and BC functions and the introduction of the corresponding inverse Gram matrix.

C. Regularizing the Nonchiral PMCHWT Equation

In [4], it has been shown that the PMCHWT equation’s operator too exhibits a self-regularizing property. In particular, it has been show that the CMP PMCHWT equation

\[
Q(\eta_0, k_0; \eta, k)^2 \left( -\hat{n} \times e^i \over \hat{n} \times \mathbf{h}^i \right) = -Q(\eta_0, k_0; \eta, k) \left( -\hat{n} \times e^i \over \hat{n} \times \mathbf{h}^i \right)
\]

involves an operator whose spectrum accumulates at finite non-zero values. In addition to the Calderón identities, the proof requires the determination of the accumulation points of the spectra of the following two-wavenumber operators:

\[
\mathcal{T}_{k_1}\mathcal{T}_{k_2} \rightarrow -k_1 \frac{k_2}{4k_2} \quad \text{and} \quad -k_2 \frac{k_1}{4k_1},
\]

For $k_1 = k_2$, this simply follows from the Calderón identities (29), (30). Ignoring all compact operators, it is then found that

\[
Q(\eta_0, k_0; \eta, k)^2 \left( \frac{1}{2} - \frac{\eta}{\eta_0} \mathcal{T}_{k_0}\mathcal{T}_{k} - \frac{\eta_0}{\eta} \mathcal{T}_{k_0}\mathcal{T}_{k} \right) \left( \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right)
\]

where the arrow “→” must be understood as an equality modulo compact contribution. This shows that the eigenvalues of the squared nonchiral PMCHWT operator will accumulate at finite nonzero values. Thus, upon discretization, the system matrix will be well-conditioned, uniformly with regard to the mesh parameter.

D. Regularizing the Chiral PMCHWT Equation

The results in [3], [4] suggest the introduction of the following CMP for the chiral PMCHWT equation (24):

\[
Q_c(\eta_0, k_0; \eta, \gamma, \gamma+, \gamma_+)^2 \left( -\hat{n} \times e^i \over \hat{n} \times \mathbf{h}^i \right) = -Q_c(\eta_0, k_0; \eta, \gamma, \gamma+, \gamma_+) \left( -\hat{n} \times e^i \over \hat{n} \times \mathbf{h}^i \right).
\]

(34)

The occurrence of a nonzero chirality parameter however complicates the spectral analysis. Two difficulties arise:

- Explicit computation of the operators in the operator block matrix $Q_c^2$ reveals the presence of a new type of operator: the three-wavenumber operator $\mathcal{T}_{k_0}\mathcal{K}^- - \mathcal{K}^- \mathcal{T}_{k_0}$. To characterize the spectrum of $Q_c^2$, the spectrum of this three-wavenumber operator needs to be understood. In section IV-D1, it will be shown that the three-wavenumber operator is compact. This operator therefore does not qualitatively affect the spectrum of $Q_c^2$.

- The explicit expression of $Q_c^2$ contains noncompact contributions in both the on- and off-diagonal blocks, complicating the study of the spectrum of the operator as a whole. To alleviate this difficulty, a suitable diagonalizing transformation (up to compact contributions) will be introduced in section IV-D2.

1) Spectrum of the three-wavenumber operator: Compactness of the three-wavenumber operator $\mathcal{T}_{k_0}\mathcal{K}^- - \mathcal{K}^- \mathcal{T}_{k_0}$ can be demonstrated for spherical scatterers of unit radius. It is known that the operators $\mathcal{T}_k$ and $\mathcal{K}_k$ are (skew-)diagonal in the basis of vector spherical harmonics $X_{lm} = \text{curl}_S Y_{lm}$ and $Y_{lm} = \text{grad}_S Y_{lm}$, with curl$S$ and grad$S$ the surface curl and...
Spectral accumulation points

\[ T_k X_{lm} = -jJ_l(k\eta)Y_{lm}, \quad (35a) \]
\[ T_k Y_{lm} = jJ_l(k\eta)X_{lm}, \quad (35b) \]
\[ K_k X_{lm} = \left( jJ_l(k\eta)H_l(k) - \frac{1}{2} \right) X_{lm}, \quad (35c) \]
\[ K_k Y_{lm} = -\left( jJ_l(k\eta)H_l(k) + \frac{1}{2} \right) Y_{lm} \quad (35d) \]

where \( J_l(k) \) and \( H_l(k) \) are the Riccati Bessel and Hankel functions, respectively. They are related to the spherical Bessel function \( j_l(k) \) and the spherical Hankel function of the first kind \( h_l^{(1)}(k) \) as
\[ J_l(k) = kj_l(k), \]
\[ H_l(k) = kh_l^{(1)}(k). \]

Using (35), it is found that
\[ (T_k K^c - K^c T_k) X_{lm} = \begin{pmatrix} 0 & a_{lm} \end{pmatrix} \begin{pmatrix} X_{lm} \\ Y_{lm} \end{pmatrix}, \quad (36) \]
with
\[ a_{lm} = -\frac{j}{2} (J_l(\gamma_1)H_l(\gamma_1) - J_l(\gamma_2)H_l(\gamma_2))' (J_l(k_0)H_l(k_0)''(k_0) - J_l(k_0)H_l(k_0)'(k_0)) \]

From (36), it follows that the eigenvalues of \( T_k K^c - K^c T_k \) are \( \pm \sqrt{a_{lm}b_{lm}} \) for large \( l \), these eigenvalues tend to [19]
\[ \pm \sqrt{a_{lm}b_{lm}} \rightarrow \pm \frac{k^2 k}{4 \ell^4} + \mathcal{O}(1^{-4}) \quad (37) \]
and hence accumulate at zero. The operator \( T_k K^c - K^c T_k \) is therefore compact. This conclusion is not limited to spherical objects: the numerical examples at the end of this paper will show that it also holds for non-spherical ones.

2) Diagonalization of the squared PMCHWT operator: Non-compact operators appear in the off-diagonal elements of \( Q_c \), which makes it difficult to make conclusive statements regarding the behavior of its spectrum. This complication can be resolved by expressing the chiral CMP PMCHWT equation (34) in terms of the circularly polarized components of the electromagnetic fields outside the scatterer, \( e_1 \) and \( e_2 \), as
\[ \begin{pmatrix} e \\ h \end{pmatrix} = \begin{pmatrix} \frac{1}{\eta_0} & 1 \\ -\frac{1}{\eta_0} & \frac{1}{\eta_0} \end{pmatrix} \begin{pmatrix} e_1 \\ e_2 \end{pmatrix}. \quad (38) \]
(Note the difference between (38) and the Bohren transform (4): in (38) the vacuum impedance \( \eta_0 \) is used instead of the impedance of the chiral medium \( \eta \).) Transformation (38) on the fields induces the following transformation on the traces:
\[ \begin{pmatrix} -\hat{n} \times e \\ \hat{n} \times h \end{pmatrix} = \begin{pmatrix} \frac{1}{\eta_0} & 1 \\ -\frac{1}{\eta_0} & \frac{1}{\eta_0} \end{pmatrix} \begin{pmatrix} \hat{n} \times e_1 \\ \hat{n} \times e_2 \end{pmatrix}. \]
The chiral CMP PMCHWT equation (34) can therefore be expressed as
\[ \begin{pmatrix} 1 & 1 \\ \frac{1}{\eta_0} & \frac{1}{\eta_0} \end{pmatrix}^{-1} Q_c^2 \begin{pmatrix} 1 & 1 \\ \frac{1}{\eta_0} & \frac{1}{\eta_0} \end{pmatrix} \begin{pmatrix} \hat{n} \times e_1 \\ \hat{n} \times e_2 \end{pmatrix} \]
\[ = -\begin{pmatrix} 1 & 1 \\ \frac{1}{\eta_0} & \frac{1}{\eta_0} \end{pmatrix}^{-1} Q_c \begin{pmatrix} 1 & 1 \\ \frac{1}{\eta_0} & \frac{1}{\eta_0} \end{pmatrix} \begin{pmatrix} \hat{n} \times e_1' \\ \hat{n} \times e_2' \end{pmatrix} \]

where the dependence of \( Q_c \) on material parameters has been left out to simplify the notation.

From a physical point of view, it is clear that this reformulation cannot change the essential properties of the PMCHWT operator. From an algebraic point of view, the matrix
\[ R = \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix} = \begin{pmatrix} 1 & \eta_0 \\ -\eta_0 & -\eta_0 \end{pmatrix}^{-1} Q_c^2 \begin{pmatrix} 1 & \eta_0 \\ -\eta_0 & -\eta_0 \end{pmatrix} \]
is connected to \( Q_c^2 \) by a similarity transformation, and therefore has an identical spectrum. Up to compact contributions (such as the three-wavenumber operator discussed in the previous subsection), it is found that
\[ R_{11} \rightarrow 1 - \frac{\eta_0}{\eta} T_k \hat{T}^+ \cdot \frac{\eta}{\eta_0} T_k^+ T_k \]
\[ + (\hat{T} T_k + T_k T'), \]
\[ R_{12} \rightarrow 0, \]
\[ R_{21} \rightarrow 0, \]
\[ R_{22} \rightarrow 1 - \frac{\eta_0}{\eta} T_k \hat{T}^+ \cdot \frac{\eta}{\eta_0} T_k^+ T_k \]
\[ - (\hat{T} T_k + T_k T'). \]

The eigenvalues of the diagonal elements accumulate at a finite number of finite nonzero values, while the off-diagonal elements are compact (for an overview of the accumulation points, see table 1). Therefore, it can be concluded that the spectrum of \( R \), and thus the spectrum of the squared chiral PMCHWT operator, is bounded from above and below and thus allows an unconditionally stable discretization, which will be discussed in the next subsection.

E. Stable Discretization

The chiral CMP PMCHWT equation is formed by action of the block operator \( Q_c \) on the left and right hand sides of the chiral PMCHWT equation (24):
\[ \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix} \left( -\hat{n} \times e \right) = -\begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix} \left( -\hat{n} \times e' \right). \quad (39) \]

The squared PMCHWT operator can be discretized elegantly by introducing a second set of expansion functions \( g_i \) and testing functions \( \tilde{g}_i \). The following system is obtained (in block matrix form):
\[ \begin{pmatrix} Q'_{11} & Q'_{12} \\ Q'_{21} & Q'_{22} \end{pmatrix} \left( \frac{1}{G} \right)^{-1} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix} \begin{pmatrix} c \\ d \end{pmatrix} \]
\[ = \begin{pmatrix} Q'_{11} & Q'_{12} \\ Q'_{21} & Q'_{22} \end{pmatrix} \left( \frac{1}{G} \right)^{-1} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} e' \\ -h' \end{pmatrix} \quad (40) \]

\[ \textbf{TABLE I OVERVIEW OF SPECTRAL ACCUMULATION POINTS} \]

<table>
<thead>
<tr>
<th>Operator</th>
<th>Spectral accumulation points</th>
</tr>
</thead>
<tbody>
<tr>
<td>( T_k^2 )</td>
<td>- \frac{k_1}{\eta_0^2} - \frac{k_2}{\eta_0^2}</td>
</tr>
<tr>
<td>( T_{k_1} T_{k_2} )</td>
<td>0</td>
</tr>
<tr>
<td>( K_{k_1} K_{k_2} )</td>
<td>0</td>
</tr>
<tr>
<td>( T_{k_1} K_{k_2} + K_{k_2} T_{k_1} )</td>
<td>0</td>
</tr>
<tr>
<td>( T_{k_0} K^c - K^c T_{k_0} )</td>
<td>0</td>
</tr>
</tbody>
</table>
with
\[
\begin{align*}
\mathbf{(Q_{ij})_{mn}} &= \left(f_m, Q_{ij} f_n \right), \\
\mathbf{(Q'_{ij})_{mn}} &= \left(g_m, Q_{ij} g_n \right), \\
\mathbf{G_{mn}} &= \left(f_m, g_n \right).
\end{align*}
\]

\(Q_{ij}\) results from discretizing the operator with the first set of basis and testing functions, and \(Q'_{ij}\) is obtained using the second set. The Gram matrix \(G\) relates the first set of testing functions to the second set of expansion functions. The matrix \(\mathbf{Q'G^{-1}}\) acts as a multiplicative preconditioner.

In order to obtain accurate results, both sets of expansion functions must be div-conforming, and both sets of testing functions must be curl-conforming. Secondly, the Gram matrix \(G\) must be well-conditioned. Finally, the operators \(Q_{ij}\) must be well-tested in \(Q_{ij}\) as well as \(Q'_{ij}\).

For a triangular mesh, a suitable choice was presented in [3] and [4]. There, \(Q\) is computed using divergence-conforming RWG functions \(f\) and curl-conforming rotated RWG functions \(g\) and [16]. \(\mathbf{Q'}\) is computed using div-conforming Buffa-Christiansen (BC) functions \(g\) and curl-conforming rotated BC functions \(\hat{n} \times g\) [20]. This discretization scheme will also be used in the numerical examples in the following section.

This discretization scheme can be extended to curvilinear [21] as well as higher-order triangular elements [22]. A general procedure not restricted to triangular meshes is described in [23].

In the next section, the beneficial properties of the CMP will be corroborated by numerical examples.

V. NUMERICAL EXAMPLES

A. Scattering by a Chiral Sphere

As presented in [6], the accuracy of the chiral CMP PMCHWT equation and the proposed discretization scheme can be tested by comparing numerical results to analytical solutions for scattering by a chiral sphere [24]. For example, consider a sphere with radius 1 meter and material parameters \(\epsilon = 2\epsilon_0, \mu = \mu_0\), and \(\kappa = 0.5\). It is embedded in vacuum, and illuminated by a circularly polarized plane wave propagating along the \(z\) axis with frequency 90 MHz:

\[
\begin{align*}
\mathbf{e^\pm(x, y, z)} &= p \exp(-jk_0z), \\
\mathbf{h^\pm(x, y, z)} &= \pm \frac{j}{k_0} e^\mp(x, y, z), \\
p &= \mathbf{1_x} + j\mathbf{1_y}.
\end{align*}
\]

\((e^+, h^+)\) corresponds to a right-hand circularly polarized wave, and \((e^-, h^-)\) corresponds to a left-hand circularly polarized wave. The radar cross section (RCS) of the chiral CMP PMCHWT method (with \(N = 1398\) RWG expansion functions) is compared to the results from the Mie series in Fig. 1, and seen to be in excellent agreement.

While the sphere is geometrically fully symmetrical, left-right symmetry in the scattered field is broken by the microscopic chiral structure of the material. This causes the sphere to react differently upon illumination by left- and right-handed circularly polarized waves. This asymmetry is only exhibited when \(\kappa \neq 0\).

When solving the chiral PMCHWT method without the CMP, dense discretization breakdown occurs. To illustrate this, the condition number of the system matrix in (28) is plotted in Fig. 2 for increasingly dense discretizations alongside the number of iterations needed to reach convergence (arbitrarily defined as a relative residual smaller than \(10^{-6}\) using the TFQMR method) when the sphere is illuminated by a linearly polarized plane wave.

However, when employing the CMP, the system matrix remains well-conditioned, no matter how small the mesh parameter. The condition number of the system matrix of (40) and the number of iterations needed to reach convergence for this scattering problem are shown in Fig. 3. It is clear that dense discretization breakdown is effectively cured by the CMP.

B. Compactness of the three-wavenumber operator

In section IV-D, we claimed that the three-wavenumber operator \(\mathbf{T_{k_0}\mathcal{K}^- - \mathcal{K}^- T_{k_0}}\) is compact, and proved this assertion for spherical scatterers. Now, the spectrum of this operator applied to a cube will be calculated by solving the eigenvalue equation

\[
\left(\mathbf{T_{k_0}\mathcal{K}^- - \mathcal{K}^- T_{k_0}}\right) \mathbf{f}(\lambda) = \lambda \mathbf{f}(\lambda).
\]

(41)
The eigenfunctions $f^{(\lambda)}$ are approximated using RWG expansion functions:

$$f^{(\lambda)} = \sum_{i=1}^{N} a_i^{(\lambda)} f_i,$$  (42)

By applying the discretization scheme used for the construction of the CMP, the eigenvalue equation (41) becomes

$$\left( T_{k_0} G^{-1} K^\ast - K^\ast G^{-1} T_{k_0} \right) a^{(\lambda)} = -\lambda G^{T} a^{(\lambda)}$$  (43)

with

\[
\begin{align*}
(T_{k_0})_{mn} &= (\hat{n} \times f_m, T_{k_0} f_n), \\
(K^-)_{mn} &= (\hat{n} \times f_m, K^- f_n), \\
(K^\ast)_{mn} &= (\hat{n} \times f_m, K^\ast f_n), \\
G_{mn} &= (\hat{n} \times f_m, g_n).
\end{align*}
\]

Thus, the spectrum of the operator $T_{k_0} K^\ast - K^\ast T_{k_0}$ is approximated by the spectrum of the matrix

$$-\left( G^{T} \right)^{-1} \left( T_{k_0} G^{-1} K^\ast - K^\ast G^{-1} T_{k_0} \right) ,$$  (44)

which can easily be calculated numerically.

For example, consider a cube with side 1 meter, $\epsilon = 2\epsilon_0$, $\mu = \mu_0$, and $\kappa = 0.5$. The surface of the cube is discretized using 1800 expansion functions. The matrix (44) and its eigenvalues are computed for a frequency of 150 MHz (Fig. 4). The eigenvalues accumulate at zero, thus supporting the assertion that $T_{k_0} K^\ast - K^\ast T_{k_0}$ is compact.

C. Application of the PMCHWT Equation to a Chiral Metamaterial

As a last example, the chiral CMP PMCHWT simulation technique is applied to the chiral metamaterial presented in [25]. Chiral particles (Fig. 5) with diameter 2.202 mm are mixed randomly to create an isotropic chiral metamaterial. The inclusion density is 34.5 cm$^{-3}$.

When the T-matrix of a spherical ensemble of chiral particles is known, it is possible to derive a closed form expression of the material parameters of an equivalent homogeneous sphere. Using this technique, the authors found that at a frequency of 5.98 GHz (corresponding to a wavelength $\lambda = 5$ cm), this metamaterial can be described by the following parameters: $\epsilon = 1.6347\epsilon_0$, $\mu = 1.1072\mu_0$, and $\kappa = 0.1511$.

The bistatic radar cross section of a cuboid of this material with dimensions 10 cm $\times$ 10 cm $\times$ 5 cm is computed in the xy-plane (Fig. 7). The incoming electric field is linearly polarized along the z axis and propagates along the directions $\phi^{inc} = 0$ and $\phi^{inc} = \pi/4$. The comparison of the condition number and the required number of iterations (averaged over the dipole and the plane wave excitations) with and without CMP again testifies to the success of the CMP (Fig. 8). Without CMP, dense discretization breakdown occurs for mesh parameters $h \leq \lambda/8$. With CMP, the condition number as well as the required number of iterations remain constant.

Next, the cuboid is excited by two different sources: a dipole located in the symmetry plane of the block, and one residing

![Fig. 3. The condition number of the system matrix and the number of iterations required to reach convergence with the CMP, as a function of the mesh parameter (in meters).](image)

![Fig. 4. Location of the eigenvalues of the three-wavenumber operator $T_{k_0} K^\ast - K^\ast T_{k_0}$ in the complex plane, applied to a cube. The left panel contains all eigenvalues. The middle and right panel are zoomed in around 0, where the eigenvalues are seen to accumulate.](image)

![Fig. 5. A chiral particle [25].](image)

![Fig. 6. Definition of the angle $\phi$.](image)
in its top plane (Fig. 9). In [25], the field scattered by this configuration was computed “ab initio”, that is by accounting for each and every spiral by using the NSPW-MLFMA T-matrix method. This approach required the solution of a set of linear equations with 347,400 unknowns.

The calculation is now repeated using both the classic chiral PMCHWT and the chiral CMP PMCHWT method by modeling the block as a homogeneous chiral medium, and covering its surface with 2048 expansion functions (the mesh parameter being $\lambda/8$). As is to be expected, the use of the CMP does not alter the results (up to numerical precision). The efficiency of the CMP is once again proven: for the symmetrical excitation, the required number of iterations to reach a relative residual of $10^{-6}$ is reduced from 247 to 16, and for the asymmetric one from 254 to 17.

In order to compare the results to the ab initio simulation data provided by the authors of [25], the electromagnetic fields are calculated at a distance of 40 cm from the center of the block (Fig. 6). The $h_x$-component is shown in the top and middle panels of Figs. 10 and 11 for the symmetric and the asymmetric excitations, respectively.

A remark concerning the approximate agreement between
the results of the ab initio simulation and the chiral PMCHWT method is in order. The constitutive equations (3) describe a homogeneous, continuous medium. However, in this particular example, the microscopic building blocks are relatively large (with dimensions of about $\lambda/20$). Therefore, constitutive equations can only provide an approximate model of the medium. When characterization of the chiral medium by a macroscopic parameter $\kappa$ is warranted, however, the modeling of scattering by such chiral objects obviously can be performed much more efficiently by the chiral CMP PMCHWT than by an ab initio simulation which takes into account the microscopic structure of the material.

The inclusion of a nonzero chirality parameter however does provide a good prediction of the order of magnitude of the different field components. The scattered field computed using the nonchiral PMCHWT method (with the same permittivity and permeability) is shown in the bottom panel of Figs. 10 and 11. For the symmetric excitation, the $h_z$-component vanishes (up to the iterative solver’s tolerance) for all $\phi$. For the asymmetric excitation, it vanishes at $\phi = 0$ and $\phi = \pi$. This is due to incorrect assumptions about the symmetry of the medium. This error is corrected by the inclusion of a nonzero chirality parameter.

VI. Conclusions

In this paper, numerical methods for analyzing scattering of electromagnetic fields by chiral media were studied. The main theoretical tool is the Bohren transform, which allows for a far-reaching analogy between chiral media and nonchiral dielectrics. By exploiting this analogy, boundary integral equations for dielectric structures can be extended to chiral objects. The extension of the PMCHWT equation was revisited in detail.

An accurate numerical solution of the chiral PMCHWT equation can be obtained with straightforward discretization schemes using RWG expansion functions. However, as is the case for the nonchiral PMCHWT equation and the EFIE, the condition number of the resulting set of equations quickly grows as the discretization becomes denser; that is, dense discretization breakdown occurs.

By studying two- and three-wavenumber extensions to the Calderón identities used in the Calderón preconditioning of the EFIE for analyzing PEC scattering, it is shown that the square of the chiral PMCHWT operator possesses a bounded spectrum and is therefore not susceptible to dense discretization breakdown. By applying a stable discretization scheme involving both RWG and BC functions to the squared chiral PMCHWT operator, a Calderón multiplicative preconditioner for the chiral PMCHWT equation, which effectively resolves the problem of dense discretization breakdown, was constructed.

Finally, three numerical experiments were performed. First, the accuracy of the chiral PMCHWT method and the efficacy of the CMP were corroborated by comparison of the result they yield, to the analytical solution for scattering by a spherical object. Second, the spectrum of the chiral PMCHWT operator was studied for nonsmooth surfaces. Third, the chiral CMP PMCHWT method was applied to the analysis of scattering by a metamaterial. These experiments show that the CMP PMCHWT method is able to efficiently and accurately solve scattering problems involving chiral media, provided that these media can be described using constitutive equations, i.e. if they can be considered as homogeneous and isotropic.

References

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