

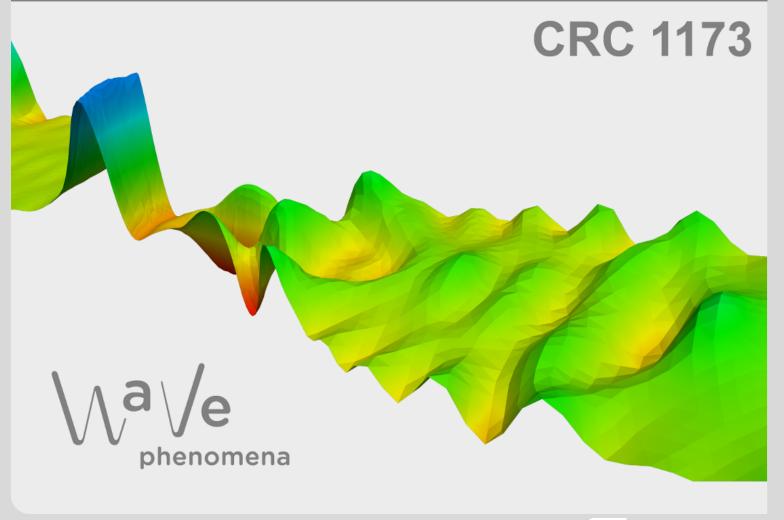


The definition and measurement of electromagnetic chirality

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The Definition and Measurement of Electromagnetic Chirality

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Abstract

The notion of Electromagnetic Chirality, recently introduced in the Physics literature, is investigated in the framework of scattering of time-harmonic electromagnetic waves by bounded scatterers. This type of chirality is defined as a property of the far field operator. The relation of this novel notion of chirality to that of geometric chirality of the scatterer is explored. It is shown for several examples of scattering problems that electromagnetic achirality is a more general property than geometric chirality. On the other hand, a chiral material law, as for example given by the Drude-Born-Fedorov model, yields an electromagnetically chiral scatterer. Electromagnetic chirality also allows the definition of a measure. Scatteres invisible to fields of one helicity turn out to be maximally chiral with respect to this measure. For a certain class of electromagnetically chiral scatters, we provide numerical calculations of the measure of chirality through solutions of scattering problems computed by a boundary element method.

1 Introduction

The fundamental laws governing the propagation of electromagnetic waves are Maxwell's equations. To obtain a full modell, these equations have to be complemented by a set of constitutive relations describing the interplay of the electromagnetic fields with the medium they propagate through. Although most materials can be described by simple linear laws involving scalar coefficients – the electric permittivity and the magnetic permeability – more complicated laws may lead to a much more interesting interaction of fields and material. One particularly interesting example is optical activity which includes effects due to anisotropy and chirality.

One possibility to obtain such material laws may be from a homogenization process with the material being made up of a large number of tightly packed individual scatterer. The present paper is concerned with the description of the chiral properties of one such individual object. In the accepted definition, a scatterer is called *achiral* if its response to fields of purely one helicity may be obtained by fields of the opposite helicity incident upon an appropriately rotated and translated mirror image of this object. Any scatterer without this property will be called *chiral*. As this definition is a purely binary criterium, it offers no possibility of establishing an ordering of chiral scatterers: Is there a way to consistently decide whether one object is more or less chiral than another object.

In the past, a number of attempts have been made to establish such an ordering based on a purely geometric definition of chiral objects [4, 10, 20]. However, these attempts have led to inconsistencies or undesired properties of the proposed measures of chirality. Recently, for scattering of electromagnetic waves, in [9] a measure of chirality was proposed that is based on the impact of the scatterer on the fields rather than on geometric properties. To distinguish this measure and the corresponding notion of chirality from the established definition the term *electromagnetically chiral (em-chiral)* was coined.

In this paper, we investigate this notion of em-chirality and its corresponding measure in a specific mathematical setting describing the scattering of a time-harmonic electromagnetic field by a bounded obstacle. The obstacle may be either penetrable or inpenetrable. The incident field is assumed to be a Herglotz wave pair. Then, the mathematical object completely describing the scattering response of the obstacle is the *far field operator* which has been well studied in the theory of qualitative methods in inverse scattering theory (see the monographs [6, 13] and the extensive literature cited therein). We prove that in this setting, the concept of em-chirality extends that of geometric chirality in that geometrically achiral scatterers are also em-achiral. In the measure of em-chirality introduced in [9], scatterers invisible to fields of one helicity turn out to be exactly those that are maximally chiral provided reciprocity holds. Given this measure, we are also able to give examples of em-chiral scatterers both by an analytic and a numerical calculation.

Ultimately the results established in the present work are meant to serve as a basis of a future study on constructing scatterers which are (close to) invisible to fields of one helicity by shape optimization. As such scatterers are the maximizers of the appropriately normalized measure of chirality, it is natural to use this measure as the basis of a corresponding objective functional. As can be seen from our analytical construction, we have to expect this measure to be non-smooth, in particular in the extremal points, and to have many local extrema.

We will start in Section 2 with a rewiev of the concept of helicity of electromagnetic waves and give a precise definition of electromagnetic chirality. In Section 3, we will investigate the relation of this definition to the one purely relying on geometry. We give some examples indicating that em-chirality is the more general concept in the sense that geometrically achiral scatterers are also em-achiral. The notion of electromagnetic chirality gives rise to a measure of chirality as first introduced in [9]. This measure will be defined in our context in Section 4 and the relation of maximizing it in a certain sense to the invisibility of the corresponding scatterer to fields of one helicity will be explored. In Section 5, we present a first concrete example of an em-chiral scatterer by analytically solving the problem of scattering by a penetrable sphere made of a material obeying a chiral material law. Finally, in Section 6, we will present an example of an em-chiral perfectly conducting scatterer. The results presented were obtained by numerically solving scattering problems using boundary element methods.

2 Helicity and Electro-Magnetic Chirality

An optically active material will produce a response to an electromagnetic wave propagating through it that depends on the circular polarization state of the wave, i.e. on its *helicity*. In macroscopic models, such materials require *bianisotropic* or, in a more restrictive model, *chiral* material laws [16]. On the other hand, chirality may be caused by the geometry of an individual scatterer. We will discuss a recently proposed definition of chirality [9] for scattering of electromagnetic waves that includes both aspects and moreover allows to measure *how chiral* a given scatterer is.

Let us consider a relatively simple situation for the background medium surrounding the scatterer. Under appropriate normalizations, the spatial part of a time-harmonic electromagnetic wave of circular frequency ω propagating in a homogeneous, isotropic material characterized by the electric permittivity ε and the magnetic permeability μ is a solution to the Maxwell system

$$\operatorname{curl} E - \mathrm{i} \, k \, H = 0 \,, \qquad \operatorname{curl} H + \mathrm{i} \, k \, E = 0 \,. \tag{1}$$

Here, the wave number is given by $k = \sqrt{\varepsilon \mu} \omega$. A Herglotz wave pair is a solution to this system given by

$$V[A](x) = \begin{pmatrix} E^0[A] \\ H^0[A] \end{pmatrix}(x) = \int_{\mathbb{S}^2} \begin{pmatrix} A(d) \\ d \times A(d) \end{pmatrix} e^{i k \, d \cdot x} \, ds(d) \,, \tag{2}$$

where $A \in L^2_t(\mathbb{S}^2)$, the space of square-integrable tangential fields on the unit sphere. In [8] it is proved that in any compact set $B \subset \mathbb{R}^3$, the Herglotz wave pairs form a dense sub-space of the space of solutions to the Maxwell system (1) with respect to the H(curl)-norm. Hence, any possible weak solution to (1) in B can be approximated arbitrarily well by Herglotz wave pairs.

A plane wave

$$E(x) = A e^{ikd \cdot x}, \qquad H(x) = (d \times A) e^{ikd \cdot x}, \qquad x \in \mathbb{R}^3,$$

with amplitude vector $A \in \mathbb{C}^3$, $A \cdot d = 0$, is said to be left or right circularly polarized if along a line in the direction of propagation the amplitude performs an anti-clockwise or clockwise circular motion, respectively. This corresponds to the relations $id \times A = \pm A$. Generalizing this notion to Herglotz wave pairs we arive at the following definition.

Definition 2.1 A Herglotz wave pair V[A], $A \in L^2_t(\mathbb{S}^2)$, is called **left (or right) circularly** polarized if A is an eigenfunction for the eigenvalue +1 (or -1, respectively) of the operator $C: L^2_t(\mathbb{S}^2) \to L^2_t(\mathbb{S}^2)$ where $CA(d) = i d \times A(d), d \in \mathbb{S}^2$.

Remark 2.2 The eigenspaces of C for the eigenvalues ± 1 are given exactly by

$$V^{\pm} = \left\{ A \pm \mathcal{C}A : A \in L^2_t(\mathbb{S}^2) \right\}.$$

This follows easily from $C^2A(d) = -d \times (d \times A(d)) = A(d)$. Additionally, from

$$\int_{\mathbb{S}^2} \mathcal{C}A \cdot \overline{B} \, \mathrm{d}s = \int_{\mathbb{S}^2} \mathrm{i} \left(d \times A(d) \right) \cdot \overline{B(d)} \, \mathrm{d}s(d) = \int_{\mathbb{S}^2} -\mathrm{i} \left(d \times \overline{B(d)} \right) \cdot A(d) \, \mathrm{d}s(d) = \int_{\mathbb{S}^2} A \cdot \mathcal{C}\overline{B} \, \mathrm{d}s(d) = \int_{\mathbb{S}^2} A \cdot$$

we see that C is self adjoint. As

$$A = \frac{1}{2} \left(A + \mathcal{C}A \right) + \frac{1}{2} \left(A - \mathcal{C}A \right)$$

we have that $L_t^2(\mathbb{S}^2) = V^+ \oplus V^-$ where these two subspaces are orthogonal and the orthogonal projections $\mathcal{P}^{\pm} : L_t^2(\mathbb{S}^2) \to V^{\pm}$ are given by $\mathcal{P}^{\pm} = (\mathcal{I} \pm \mathcal{C})/2$, respectively.

A straightforward calculation shows that if $A \in V^{\pm}$, then $A(-\cdot)$, $\overline{A} \in V^{\mp}$, where the overline signifies complex conjugation.

Adapting a notion from physics, we say that the Herglotz wave pair V[A] has **helicity** ± 1 if $A \in V^{\pm}$.

Remark 2.3 The decomposition of Herglotz wave pairs by helicity corresponds to the well known Riemann-Silberstein linear combinations. Let $B \subseteq \mathbb{R}^3$ denote a bounded open set and consider the two subspaces of Beltrami fields

$$W^{\pm}(B) = \{ U \in H(\operatorname{curl}, B) : \operatorname{curl} U = \pm k U \}$$

With the Riemann-Silberstein linear combinations $E^+ = E + iH \in U^+$ and $E^- = E - iH \in U^$ of solutions of (1), we obtain the decomposition

$$E = \frac{1}{2} \left(E^+ + E^- \right),$$

which is orthogonal with respect to the inner product

$$\langle u, v \rangle = \int_B \left(\operatorname{curl} u \cdot \operatorname{curl} \overline{v} + k^2 \, u \cdot \overline{v} \right) \mathrm{d}x \qquad on \ H(\operatorname{curl}, B)$$

With $A \in V^{\pm}$ we observe that $V[A] \in W^{\pm}(B) \times W^{\pm}(B)$ for the corresponding Herglotz wave pairs.

Let us consider the fairly general problem that an incident Herglotz wave pair V[A] is scattered by some bounded scatterer $D \subseteq \mathbb{R}^3$. Thus, scattering by an inpenetrable scatterer where the total field satisfies some boundary condition as well as scattering by a pentrable medium can be considered. We only assume that the presence of D gives rise to some scattererd field (E^s, H^s) which is a solution to (1) in $\mathbb{R}^3 \setminus \overline{D}$ and that it satisfies the Silver-Müller radiation condition at infinity, i.e.

$$E^{s}(x) - H^{s}(x) \times \frac{x}{|x|}$$

$$H^{s}(x) + E^{s}(x) \times \frac{x}{|x|}$$

$$= O\left(\frac{1}{|x|^{2}}\right), \qquad |x| \to \infty,$$

$$(3)$$

uniformly with respect to $x/|x| \in \mathbb{S}^2$. As consequence of (3), the scattered field has the asymptotic representation

$$\begin{pmatrix} E^s \\ H^s \end{pmatrix}(x) = \frac{\mathrm{e}^{\mathrm{i}k\,|x|}}{4\pi\,|x|} \left[\begin{pmatrix} E^\infty \\ H^\infty \end{pmatrix}(\hat{x}) + \mathrm{O}\left(\frac{1}{|x|}\right) \right], \qquad |x| \to \infty$$

Here $\hat{x} = x/|x| \in \mathbb{S}^2$. The functions E^{∞} and H^{∞} are called the *electric and magnetic far* field pattern, respectively. They are analytic tangential fields on \mathbb{S}^2 and also satisfy $H^{\infty}(\hat{x}) = \hat{x} \times E^{\infty}(\hat{x})$. The far field patterns also uniquely define (E^s, H^s) in $\mathbb{R}^3 \setminus \overline{D}$ (see e.g. [7, Theorem 6.9]).

In inverse scattering problems, it is a common technique to characterize the scattering behaviour of D by its scattering response to plane waves. Denote by $(E^{\infty}, H^{\infty})(\hat{x}, d, A)$, the far field pattern of the scattered field observed in direction \hat{x} for an incident plane wave with direction $d \in \mathbb{S}^2$ and amplitude $A \in \mathbb{C}^3$ where $A \cdot d = 0$. Note that $A \mapsto (E^{\infty}, H^{\infty})(\cdot, d, A)$ is linear. Then, the electric far field pattern of the scattered field due to an incident Herglotz wave pair V[A] is $\mathcal{F}A$ where we have used the *far field operator* $\mathcal{F} : L^2_t(\mathbb{S}^2) \to L^2_t(\mathbb{S}^2)$ given by

$$\mathcal{F}A(\hat{x}) = \int_{\mathbb{S}^2} E^{\infty}(\hat{x}, d, A(d)) \,\mathrm{d}s(d) \,, \qquad \hat{x} \in \mathbb{S}^2 \,, A \in L^2_t(\mathbb{S}^2) \,. \tag{4}$$

As the far field patterns are analytic, \mathcal{F} is a compact linear operator in $L^2_t(\mathbb{S}^2)$. As below, we will formulate a number of specific problems for the magnetic field, we also note

$$\mathcal{F}A(\hat{x}) = -\hat{x} \times \int_{\mathbb{S}^2} H^{\infty}(\hat{x}, d, A(d)) \,\mathrm{d}s(d) \,, \qquad \hat{x} \in \mathbb{S}^2 \,, A \in L^2_t(\mathbb{S}^2) \,. \tag{5}$$

In the same way that we characterize the helicity of a Herglotz wave pair V[A] by $A \in V^{\pm}$, we can characterize the helicity of the scattered fields through the fact that their far fields are in V^{\pm} :

Theorem 2.4 The far field patterns E^{∞} , H^{∞} are elements of V^{\pm} if and only if for any bounded open set B such that $\overline{B} \subseteq \mathbb{R}^3 \setminus \overline{D}$ we have E^s , $H^s \in W^{\pm}(B)$.

Proof: Let $E^{\infty} \in V^+$. Then $E^{\infty}(\hat{x}) = i\hat{x} \times E^{\infty}(\hat{x}) = iH^{\infty}(\hat{x})$. As the map $E^s \mapsto E^{\infty}$ is linear and injective [7, Theorem 6.9], we conclude

$$E^s = iH^s = i\frac{1}{ik}\operatorname{curl} E^s = \frac{1}{k}\operatorname{curl} E^s.$$

Thus $E^s \in W^+(B)$ for any bounded open set B with $\overline{B} \subseteq \mathbb{R}^3 \setminus \overline{D}$. The argument is analogous for $H^s \in V^+$ and for $E^s, H^s \in V^-$.

Suppose now E^s , $H^s \in W^+(B)$ for any bounded open set B with $\overline{B} \subseteq \mathbb{R}^3 \setminus \overline{D}$. In particular, consider an open ball $B_R(0)$ of radius R such that $\overline{D} \subset B_R(0)$ and let B denote an open neighborhood of $\partial B_R(0)$. Then by a boundary integral representation of the far field (see [7, Theorem 6.8]),

$$\begin{split} \mathbf{i}\hat{x} \times E^{\infty}(\hat{x}) &= \mathbf{i}H^{\infty}(\hat{x}) = -k\,\hat{x} \times \int_{|y|=R} \left(\hat{y} \times H^{s}(y) - \left[\hat{y} \times E^{s}(y)\right] \times \hat{x}\right) \mathrm{e}^{-\mathbf{i}k\hat{x} \cdot y} \,\mathrm{d}s(y) \\ &= -\hat{x} \times \int_{|y|=R} \left(\hat{y} \times \mathrm{curl}\, H^{s}(y) - \left[\hat{y} \times \mathrm{curl}\, E^{s}(y)\right] \times \hat{x}\right) \mathrm{e}^{-\mathbf{i}k\hat{x} \cdot y} \,\mathrm{d}s(y) \\ &= \mathbf{i}k\,\hat{x} \times \int_{|y|=R} \left(\hat{y} \times E^{s}(y) + \left[\hat{y} \times H^{s}(y)\right] \times \hat{x}\right) \mathrm{e}^{-\mathbf{i}k\hat{x} \cdot y} \,\mathrm{d}s(y) = E^{\infty}(\hat{x})\,. \end{split}$$

Thus $E^{\infty} \in V^+$. Again, the proof is analogous for H^{∞} and also for the case E^s , $H^s \in W^-(B)$.

In order to identify corresponding contributions of different helicities in the far field operator, using the orthogonal projections defined in Remark 2.2, we can decompose \mathcal{F} into four operators,

$$\mathcal{F}^{++} = P^+ \mathcal{F} P^+, \quad \mathcal{F}^{+-} = P^+ \mathcal{F} P^-, \quad \mathcal{F}^{-+} = P^- \mathcal{F} P^+, \quad \mathcal{F}^{--} = P^- \mathcal{F} P^-,$$
(6)

so that

$$\mathcal{F} = \mathcal{F}^{++} + \mathcal{F}^{+-} + \mathcal{F}^{-+} + \mathcal{F}^{--}$$

In [9] it was proposed to define achirality of a scatterer by the fact that certain relations exist between these four components of \mathcal{F} .

Definition 2.5 The scatterer D is called **electromagnetically achiral (em-achiral)** if there exist unitary operators $\mathcal{U}^{(j)}$ in $L^2_t(\mathbb{S}^2)$ with $\mathcal{U}^{(j)}\mathcal{C} = -\mathcal{C}\mathcal{U}^{(j)}$, $j = 1, \ldots, 4$, such that

$$\mathcal{F}^{++} = \mathcal{U}^{(1)} \mathcal{F}^{--} \mathcal{U}^{(2)}, \qquad \mathcal{F}^{-+} = \mathcal{U}^{(3)} \mathcal{F}^{+-} \mathcal{U}^{(4)}.$$

If this is not the case, we call the scatterer D em-chiral.

3 Examples of EM-Achiral Scatterers

It is not a priori clear how Definition 2.5 of chirality relates to previous notions based on handedness. Thus, in the following paragraphs we want to discuss some of these relations. We will start by considering scattering problems for intuitively achiral objects and show that such scatterers are also em-achiral. The arguments for different types of scatterers are essentially similar and rely on the following lemma.

Lemma 3.1 Suppose that for a scattering problem with far field operator \mathcal{F} there exists a unitary operator \mathcal{D} in $L^2_t(\mathbb{S}^2)$ such that

$$\mathcal{CD} = -\mathcal{DC}$$
 and $\mathcal{FD} = \mathcal{DF}$

Then the scatterer is em-achiral.

Proof: The conditions of the lemma imply

$$\mathcal{F}^{++} = \frac{1}{4} \left(I + \mathcal{C} \right) \mathcal{F} \left(I + \mathcal{C} \right) = \frac{1}{4} \left(I + \mathcal{C} \right) \mathcal{D} \mathcal{F} \mathcal{D}^{-1} \left(I + \mathcal{C} \right)$$
$$= \frac{1}{4} \mathcal{D} \left(I - \mathcal{C} \right) \mathcal{F} \left(I - \mathcal{C} \right) \mathcal{D}^{-1} = \mathcal{D} \mathcal{F}^{--} \mathcal{D}^{-1},$$

and likewise for $\mathcal{F}^{+-} = \mathcal{D} \mathcal{F}^{-+} \mathcal{D}^{-1}$. Thus the scatterer is em-achiral.

Consider first the scattering of a Herglotz wave pair V[A] by a perfect conducting scatterer D, where D is assumed to be a bounded Lipschitz domain in \mathbb{R}^3 with simply connected exterior. In this case, the scattering problem can be written as an exterior boundary value problem for the magnetic field,

$$\operatorname{curl}\operatorname{curl} H - k^2 H = 0 \qquad \text{in } \mathbb{R}^3 \setminus \overline{D},$$
$$(\operatorname{curl} H) \times \nu = 0 \qquad \text{on } \partial D,$$

 $H^s = H - H^0[A]$ satisfies the Silver-Müller radiation condition (with $E^s = -1/(ik) \operatorname{curl} H^s$).

Here ν denotes the outward drawn unit normal vector to ∂D .

Unique solvablity of this scattering problem can be shown in various function space settings (see e.g. [14]). By the Stratton-Chu formulas, the solution has the representation

$$H(x) = H^{0}[A](x) + \operatorname{curl} \int_{\partial D} \nu(y) \times H(y) \Phi(x, y) \, \mathrm{d}s(y) \,, \qquad x \in \mathbb{R}^{3} \setminus \partial D \,,$$

where by Φ we denote the Green's function for the Helmholtz equation with wave number k in free field conditions,

$$\Phi(x,y) = \frac{\mathrm{e}^{\mathrm{i}k|x-y|}}{4\pi |x-y|}, \qquad x,y \in \mathbb{R}^3, \quad x \neq y.$$

Consequently, the far field pattern of the scattered field is given by

$$H^{\infty}(\hat{x}) = \mathrm{i}k\,\hat{x} \times \int_{\partial D} \nu(y) \times H(y) \,\mathrm{e}^{-\mathrm{i}k\,\hat{x}\cdot y} \,\mathrm{d}s(y)\,, \qquad \hat{x} \in \mathbb{S}^2\,.$$
(7)

We will call a scatterer D geometrically achiral, if there exists $x_0 \in \mathbb{R}^3$ and an orthogonal matrix $J \in \mathbb{R}^{3\times 3}$ with det J = -1 such that $D = x_0 + JD$. This means that D is invariant under some reflection by a plane combined with translations and rotations. In the arguments to follow, it is essential to know how the field changes under such a transformation. In order to make implicit the dependence of the fields on the density of the Herglotz wave pair by writing H[A] for the total field and $H^{\infty}[A]$ for the far field pattern. Using the identity

$$Bx \times By = \det(B) B(x \times y)$$

for any orthogonal matrix B, an elementary calculation shows that under the transformation $x = x_0 + J\tilde{x}$, the Herglotz wave pair transforms by

$$H^{0}[A](x) = H^{0}[A](x_{0} + J\tilde{x}) = -J H^{0}[\mathcal{D}A](\tilde{x}),$$

with $\mathcal{D}: L^2_t(\mathbb{S}^2) \to L^2_t(\mathbb{S}^2)$ defined by

$$\mathcal{D}A(d) = e^{ik x_0 \cdot Jd} J^{\top} A(Jd), \qquad d \in \mathbb{S}^2, \quad A \in L^2_t(\mathbb{S}^2).$$

Likewise, the total field transforms by

$$H[A](x) = -J H[\mathcal{D}A](\tilde{x}).$$
(8)

It is easy to see, that \mathcal{D} is unitary in $L^2_t(\mathbb{S}^2)$. Moreover, \mathcal{D} anticommutes with \mathcal{C} as can be seen from

$$\mathcal{CD}A(d) = i e^{ik x_0 \cdot Jd} d \times J^{\top} A(Jd) = \det(J) e^{ik x_0 \cdot Jd} J^{\top} (i Jd \times A(Jd)) = \det(J) \mathcal{DC}A(d),$$

Thus we have

$$\mathcal{FD}A(\hat{x}) = -\hat{x} \times H^{\infty}[\mathcal{D}A](\hat{x}), \quad \text{while} \quad \mathcal{D}\mathcal{F}A(\hat{x}) = -e^{ikx_0 \cdot J\hat{x}} J^{\top} \left(J\hat{x} \times H^{\infty}[A](J\hat{x})\right).$$
(9)

Theorem 3.2 If the perfect conductor D is geometrically achiral then it is also em-achiral.

Proof: Let D be geomtrically achiral. From (7) and substituting $y = x_0 + J\tilde{y}$ in the integral, we see

$$e^{ikx_0 \cdot J\hat{x}} H^{\infty}[A](J\hat{x}) = ik e^{ikx_0 \cdot J\hat{x}} J\hat{x} \times \int_{\partial D} \nu(y) \times H[A](y) e^{-ikJ\hat{x} \cdot y} ds(y)$$
$$= ik J\hat{x} \times \int_{\partial D} \nu(x_0 + J\tilde{y}) \times H[A](x_0 + J\tilde{y}) e^{-ikJ\hat{x} \cdot J\tilde{y}} ds(\tilde{y}).$$

An elementary calculation shows $\nu(x_0 + J\tilde{y}) = J\nu(\tilde{y})$ and together with (8) we conclude

$$\begin{split} \mathrm{e}^{\mathrm{i}kx_{0}\cdot J\hat{x}} H^{\infty}[A](J\hat{x}) &= \mathrm{i}k \, J\hat{x} \times \int_{\partial D} J\nu(\tilde{y}) \times JH[\mathcal{D}A](\tilde{y}) \, \mathrm{e}^{-\mathrm{i}k\hat{x}\cdot\tilde{y}} \, \mathrm{d}s(\tilde{y}) \\ &= \frac{-\mathrm{i}k}{\det(J)^{2}} \, J\left[\hat{x} \times \int_{\partial D} \nu(\tilde{y}) \times H[\mathcal{D}A](\tilde{y}) \, \mathrm{e}^{-\mathrm{i}k\hat{x}\cdot\tilde{y}} \, \mathrm{d}s(\tilde{y})\right] \\ &= -JH^{\infty}[\mathcal{D}A](\hat{x}) \, . \end{split}$$

Hence from (9),

$$\mathcal{DF}A(\hat{x}) = J^{\top} \left[J\hat{x} \times JH^{\infty}[\mathcal{D}A](\hat{x}) \right] = \det(J)\,\hat{x} \times H^{\infty}[\mathcal{D}A](\hat{x}) = \mathcal{FD}A(\hat{x})\,.$$

Thus \mathcal{D} commutes with \mathcal{F} and the assertion follows from Lemma 3.1.

Next consider the scattering of a Herglotz wave pair V[A] by a penetrable scatterer D with a non-magnetic and non-conductive isotropic linear material. In this case, the total magnetic field H is seen to satisfy the equation

$$\operatorname{curl}\left(\frac{1}{\varepsilon_r}\operatorname{curl} H\right) - k^2 H = 0 \quad \text{in } D,$$

with some positive function ε_r with $\operatorname{supp}(1 - \varepsilon_r) = D$. We will assume that $\varepsilon_r \in C^{1,\alpha}(\mathbb{R}^3)$ such that the problem is uniquely solvable [7, Chapter 9]. The scattering problem can be equivalently formulated as a Lippmann-Schwinger type integro-differential equation

$$H(x) = H^{0}[A](x) + \operatorname{curl} \int_{D} [q(y) \operatorname{curl} H(y)] \Phi(x, y) \,\mathrm{d}y \,, \qquad x \in D \,. \tag{10}$$

Here $q = 1 - 1/\varepsilon_r$. For the derivation of (10) as well as the solvability theory in $H(\operatorname{curl}, D)$ as well as in $L^2(D, \mathbb{C}^3)$ under suitable assumptions on ε_r see [7, 12, 15]. The magnetic far field pattern can be seen to be

$$H^{\infty}(\hat{x}) = \mathrm{i}k\hat{x} \times \int_{D} q(y) \operatorname{curl} H(y) \operatorname{e}^{-\mathrm{i}k\hat{x}\cdot y} \mathrm{d}y.$$
(11)

In this case, we call the scatterer $D = \operatorname{supp} q$ geometrically achiral if there exists $x_0 \in \mathbb{R}^3$ and an orthogonal matrix $J \in \mathbb{R}^{3 \times 3}$ with det J = -1 such that $q(x) = q(x_0 + Jx)$. In particular, this implies $D = x_0 + JD$, as for the perfect conductor case.

Theorem 3.3 If the penetrable scatterer D is geometrically achiral then it is also em-achiral.

Proof: Let $x_0 \in \mathbb{R}^3$ and $J \in \mathbb{R}^{3\times 3}$ denote the point and orthogonal matrix, respectively, such that $q(x) = q(x_0 + Jx)$. For $x \in \mathbb{R}^3$, let $\tilde{x} \in \mathbb{R}^3$ be defined by $x = x_0 + J\tilde{x}$. As an additional argument, we here require a formula for the curl operator under this transformation. From (8) using Corollary 3.58 from [19], we obtain

$$\operatorname{curl}_{x} H[A](x) = -\frac{1}{\det(J)} J \operatorname{curl}_{\tilde{x}} H[\mathcal{D}A](\tilde{x})$$

Hence, from (8), (11) and the transform of the curl operation we observe using the substitution $y = x_0 + J\tilde{y}$,

$$\begin{aligned} \mathrm{e}^{\mathrm{i}kx_0 \cdot J\hat{x}} \, H^{\infty}[A](J\hat{x}) &= \mathrm{i}k \, \mathrm{e}^{\mathrm{i}kx_0 \cdot J\hat{x}} \, J\hat{x} \times \int_D q(y) \, \mathrm{curl}_y \, H[A](y) \, \mathrm{e}^{-\mathrm{i}kJ\hat{x} \cdot y} \, \mathrm{d}y \\ &= \mathrm{i}k \, J\hat{x} \times \int_D q(\tilde{y}) \, \mathrm{curl}_y \, H[A](x_0 + J\tilde{y}) \, \mathrm{e}^{-\mathrm{i}kJ\hat{x} \cdot J\tilde{y}} \, \mathrm{d}\tilde{y} \\ &= \frac{-\mathrm{i}k}{\det(J)} \, J\hat{x} \times \int_D q(\tilde{y}) \, J \, \mathrm{curl}_{\tilde{y}} \, H[\mathcal{D}A](\tilde{y}) \, \mathrm{e}^{-\mathrm{i}kJ\hat{x} \cdot J\tilde{y}} \, \mathrm{d}\tilde{y} \\ &= \mathrm{i}k \, J \left[\hat{x} \times \int_D q(\tilde{y}) \, \mathrm{curl}_{\tilde{y}} \, H[\mathcal{D}A](\tilde{y}) \, \mathrm{e}^{-\mathrm{i}k\hat{x} \cdot \tilde{y}} \, \mathrm{d}\tilde{y} \right] \\ &= -JH^{\infty}[\mathcal{D}A](\hat{x}) \,, \end{aligned}$$

As in the proof of Theorem 3.2 we see that \mathcal{D} and \mathcal{F} commute, and the assertion again follows from Lemma 3.1.

4 Measuring of EM-Chirality

The central tool in this section are singular systems for the operator \mathcal{F} and its four helicity components. We denote by (σ_j, G_j, H_j) a singular system for \mathcal{F} , with the convention that the singular values form a decreasing sequence. Likewise, we denote by $(\sigma_j^{pq}, G_j^{pq}, H_j^{pq})$ a singular system for \mathcal{F}^{pq} , $p, q \in \{+, -\}$. In the case where any of these operators are finite dimensional, to simplify arguments below, we extend the corresponding finite sequence of positive singular values by a sequence of zeros.

As pointed out in [9], for an em-achiral scatterer, Definition 2.5 has important consequences for the singular systems of the helicity components of \mathcal{F} . Indeed,

$$\mathcal{F}^{++}G = \mathcal{U}^{(1)}\mathcal{F}^{--}\mathcal{U}^{(2)}G = \sum_{j} \sigma_{j}^{--} \langle \mathcal{U}^{(2)}G, G_{j}^{--} \rangle \mathcal{U}^{(1)}H_{j}^{--} = \sum_{j} \sigma_{j}^{--} \langle G, \mathcal{U}^{(2)*}G_{j}^{--} \rangle \mathcal{U}^{(1)}H_{j}^{--}$$

for all $G \in L^2_t(\mathbb{S}^2)$. As $\mathcal{U}^{(k)}$, k = 1, 2, are unitary, we conclude that $(\sigma_j^{--}, \mathcal{U}^{(2)*}G_j^{--}, \mathcal{U}^{(1)}H_j^{--})$ is a singular system for \mathcal{F}^{++} . Thus $\sigma_j^{++} = \sigma_j^{--}$, $j \in \mathbb{N}$, and the analogous result $\sigma_j^{+-} = \sigma_j^{-+}$ is obtained in the same way.

For a chiral scatterer it is hence plausible to characterize the deviation from achirality by a measure of the difference of these sequences of singular value. The far field operator is an integral operator with an analytic kernel, hence its singular values are known to decay rapidly [18]. They in particular form sequences in the space ℓ^2 so that the following definition is well posed. **Definition 4.1** For a scatterer characterized by a far field operator \mathcal{F} , the **measure of chi**rality $\chi(\mathcal{F})$ is defined as

$$\chi(\mathcal{F}) = \left(\| (\sigma_j^{++}) - (\sigma_j^{--}) \|_{\ell^2}^2 + \| (\sigma_j^{+-}) - (\sigma_j^{-+}) \|_{\ell^2}^2 \right)^{1/2}$$

As a measure of the responsiveness of the scatterer to any type of incident field, the authors of [9] also introduce the **total interaction cross section** of the scatterer by

$$C_{\text{int}}(\mathcal{F}) = \sum_{j} \sigma_j^2 = \sum_{j} \|\mathcal{F}G_j\|^2 = \sum_{j,k} |\langle \mathcal{F}G_j, H_k \rangle|^2.$$

In the following two lemmas, we rigorously prove two results from [9] in our specific setting.

Lemma 4.2 For any scatterer there holds $\chi(\mathcal{F})^2 \leq C_{int}(\mathcal{F})$. If the scatterer does not scatter fields of one helicity, then $\chi(\mathcal{F})^2 = C_{int}(\mathcal{F})$, i.e. then the scatterer has maximal measure of chirality among all scatterers with the same total interaction cross section.

Proof: We begin by showing

$$C_{\rm int}(\mathcal{F}) = \sum_{p,q \in \{+,-\}} \sum_{j} [\sigma_j^{pq}]^2 \,.$$
(12)

Consider first the case p = q = +. Denote by L the closed subspace of V^+ such that

 $V^{+} = \overline{\operatorname{span}\{G_{j}^{++}\}} + \left(\ker \mathcal{F} \cap V^{+}\right) + L$

and L is orthogonal to the other two spaces. Note that $L \subseteq \ker \mathcal{F}^{++}$. Choose a complete orthonormal system $\{\tilde{G}_m\}$ in L. Then

$$\mathcal{P}^+ G_k = \sum_j \langle G_k, G_j^{++} \rangle G_j^{++} + \sum_m \langle G_k, \tilde{G}_m \rangle \tilde{G}_m ,$$

and

$$\langle \mathcal{P}^+G_k, \mathcal{P}^+G_l \rangle = \sum_j \langle G_k, G_j^{++} \rangle \,\overline{\langle G_l, G_j^{++} \rangle} + \sum_m \langle G_k, \tilde{G}_m \rangle \,\overline{\langle G_l, \tilde{G}_m \rangle} \,.$$

We write

$$\sum_{j} [\sigma_{j}^{++}]^{2} = \sum_{j} \|\mathcal{F}^{++}G_{j}^{++}\|^{2} + \sum_{m} \|\mathcal{F}^{++}\tilde{G}_{m}\|^{2} = \sum_{j} \|\mathcal{P}^{+}\mathcal{F}G_{j}^{++}\|^{2} + \sum_{m} \|\mathcal{P}^{+}\mathcal{F}\tilde{G}_{m}\|^{2}$$

and apply the singular value decomposition of \mathcal{F} to obtain

$$\sum_{j} [\sigma_{j}^{++}]^{2} = \sum_{k,l} \sigma_{k} \sigma_{l} \left(\sum_{j} \langle G_{k}, G_{j}^{++} \rangle \overline{\langle G_{l}, G_{j}^{++} \rangle} + \sum_{m} \langle G_{k}, \tilde{G}_{m} \rangle \overline{\langle G_{l}, \tilde{G}_{m} \rangle} \right) \langle \mathcal{P}^{+} H_{k}, \mathcal{P}^{+} H_{l} \rangle$$
$$= \sum_{k,l} \sigma_{k} \sigma_{l} \langle \mathcal{P}^{+} G_{k}, \mathcal{P}^{+} G_{l} \rangle \langle \mathcal{P}^{+} H_{k}, \mathcal{P}^{+} H_{l} \rangle = \sum_{k,l} \sigma_{k} \sigma_{l} \langle \mathcal{P}^{+} G_{k}, \mathcal{P}^{+} G_{l} \rangle \langle \mathcal{P}^{+} H_{k}, H_{l} \rangle,$$

where the last identity is just the characterization of an orthogonal projection. The same calculation for \mathcal{F}^{-+} gives

$$\sum_{j} [\sigma_{j}^{-+}]^{2} = \sum_{k,l} \sigma_{k} \sigma_{l} \left\langle \mathcal{P}^{+} G_{k}, \mathcal{P}^{+} G_{l} \right\rangle \left\langle \mathcal{P}^{-} H_{k}, H_{l} \right\rangle$$

Adding both equations and using orthonormality of the functions H_k yields

$$\sum_{j} \left([\sigma_{j}^{++}]^{2} + [\sigma_{j}^{-+}]^{2} \right) = \sum_{k} \sigma_{k}^{2} \|\mathcal{P}^{+}G_{k}\|^{2}.$$

Repeating this argument for \mathcal{F}^{+-} and \mathcal{F}^{--} , we arrive at (12).

From the definition of the measure of chirality, we now conclude

$$\chi(\mathcal{F})^2 = C_{\rm int}(\mathcal{F}) - 2\sum_j \left(\sigma_j^{++}\sigma_j^{--} + \sigma_j^{+-}\sigma_j^{-+}\right) \,. \tag{13}$$

Hence $\chi(\mathcal{F})^2 \leq C_{\text{int}}$ follows, with equality when the sum vanishes.

Suppose now without loss of generality that the scatterer does not scatter fields of helicity +. This implies that $\mathcal{F}^{++} = 0$ and $\mathcal{F}^{-+} = 0$ and the corresponding singular values σ_j^{++} and σ_j^{-+} , respectively, are also zero. Hence the sum vanishes in this case.

In general, the reverse conclusion is only true if the scatterer is *reciprocal*. Recall the notation $E^{\infty}(\hat{x}, d, A)$ from the definition of the far field operator (4). A scatterer is said to satisfy the **reciprocity relation** if the equation

$$A \cdot E^{\infty}(\hat{x}, \hat{y}, B) = B \cdot E^{\infty}(-\hat{y}, -\hat{x}, A)$$
(14)

holds for all $\hat{x}, \hat{y} \in \mathbb{S}^2$, $A, B \in \mathbb{C}^3 \setminus \{0\}, A \cdot \hat{x} = 0, B \cdot \hat{y} = 0$. For the far field operator and any $A, B \in L^2_t(\mathbb{S}^2)$, this implies

$$(\mathcal{F}A, B)_{L^2_t(\mathbb{S}^2)} = \int_{\mathbb{S}^2} \int_{\mathbb{S}^2} E^{\infty}(\hat{x}, \hat{y}, A(\hat{y})) \cdot \overline{B(\hat{x})} \, \mathrm{d}s(\hat{y}) \, \mathrm{d}s(\hat{x})$$

$$= \int_{\mathbb{S}^2} \int_{\mathbb{S}^2} A(\hat{y}) \cdot E^{\infty}(-\hat{y}, -\hat{x}, \overline{B(\hat{x})}) \, \mathrm{d}s(\hat{y}) \, \mathrm{d}s(\hat{x})$$

$$= \int_{\mathbb{S}^2} \int_{\mathbb{S}^2} A(-\hat{y}) \cdot E^{\infty}(\hat{y}, \hat{x}, \overline{B(-\hat{x})}) \, \mathrm{d}s(\hat{x}) \, \mathrm{d}s(\hat{y}) = \left(\mathcal{F}\overline{B(-\cdot)}, \overline{A(-\cdot)}\right)_{L^2_t(\mathbb{S}^2)}$$
(15)

Lemma 4.3 If a scatterer satisfies the reciprocity relation and $\chi(\mathcal{F})^2 = C_{int}(\mathcal{F})$ holds, then the scatterer is invisible to incident fields of one helicity.

Proof: From (13), we see that $\sum_{j} \left(\sigma_{j}^{++} \sigma_{j}^{--} + \sigma_{j}^{+-} \sigma_{j}^{-+} \right) = 0$. Recall that the sequences (σ_{j}^{pq}) are non-negative and monotonically decreasing. Consider just the first term in the sum: Either $\sigma_{1}^{++} = 0$ or $\sigma_{1}^{--} = 0$ and either $\sigma_{1}^{+-} = 0$ or $\sigma_{1}^{-+} = 0$. Then also the entire corresponding sequences (σ_{j}^{pq}) vanish.

Let $A \in V^+$, $B \in V^-$. From Remark 2.2, we then see $\overline{A(-\cdot)} \in V^+$, $\overline{B(-\cdot)} \in V^-$. Assume $\mathcal{F}^{+-} = 0$. Then

$$\left(\mathcal{F}^{-+}A,B\right)_{L^2_t(\mathbb{S}^2)} = \left(\mathcal{F}A,B\right)_{L^2_t(\mathbb{S}^2)} = \left(\mathcal{F}\overline{B(-\cdot)},\overline{A(-\cdot)}\right)_{L^2_t(\mathbb{S}^2)} = \left(\mathcal{F}^{+-}\overline{B(-\cdot)},\overline{A(-\cdot)}\right)_{L^2_t(\mathbb{S}^2)} = 0.$$

As A, B where chosen arbitrarily, we conclude $\mathcal{F}^{-+} = 0$. The argument works exactly the same for the other direction, thus $\mathcal{F}^{+-} = 0 = \mathcal{F}^{-+}$. As either $\mathcal{F}^{++} = 0$ or $\mathcal{F}^{--} = 0$, we conclude that the scatterer is invisible to fields of one helicity.

5 EM-Chirality via Material Laws

Examples for em-chiral scatterers with maximal measure of em-chirality can be constructed using media with chiral material laws. Such laws are given by the Drude-Born-Fedorov model [17, 21]. This model has also been used in [2, 3] when studying the formal mathematical solution of a scattering problem for a homogeneous chiral medium by boundary integral equations and in [11] in an analysis of the application of the factorization method to a chiral scattering problem. The material inside a bounded open domain $\Omega \subseteq \mathbb{R}^3$ is characterized by an electric permittivity $\varepsilon_D > 0$, a magnetic permeability $\mu_D > 0$ and a chirality $\beta \in \left(-1/(\sqrt{\varepsilon_r \mu_r k}), 1/(\sqrt{\varepsilon_r \mu_r k})\right)$. Keeping in mind our normalization of the electromagnetic field, the Drude-Born-Fedorov constitutive relations are of the form

$$\frac{1}{\sqrt{\varepsilon_0}} D = \varepsilon_r \left(E + \beta \operatorname{curl} E \right) , \qquad \frac{1}{\sqrt{\mu_0}} B = \mu_r \left(H + \beta \operatorname{curl} H \right) .$$

where we have set $\varepsilon_r = \varepsilon_D/\varepsilon_0$, $\mu_r = \mu_D/\mu_0$. In Ω , the electromagnetic field satisfies the equations

$$\operatorname{curl} E - \operatorname{i} k \,\mu_r \left(H + \beta \,\operatorname{curl} H \right) = 0 \,, \qquad \operatorname{curl} H + \operatorname{i} k \,\varepsilon_r (E + \beta \,\operatorname{curl} E) = 0 \,. \tag{16}$$

At the interface $\partial \Omega$ the tangential components of the electric and the magnetic field are continuous,

$$[\nu \times E] = 0, \qquad [\nu \times H] = 0 \qquad \text{on } \partial\Omega, \qquad (17)$$

where ν denotes the outward directed unit normal vector to $\partial\Omega$ and by [.] we denote the jump across $\partial\Omega$.

Recalling Remark 2.3, we consider the Riemann-Silberstein linear combinations

$$E^{\pm} = E \pm \mathrm{i} H$$

instead of the fields E, H. One then finds [2] that these fields both satisfy equations

$$\operatorname{curl}\operatorname{curl} E^{\pm} - k_{\pm}^2 E^{\pm} = 0 \qquad \text{in } \mathbb{R}^3 \,,$$

with

$$k_{\pm} = \begin{cases} k & \text{in } \mathbb{R}^3 \setminus \overline{\Omega} \\ \frac{\sqrt{\varepsilon_r \, \mu_r} \, k}{1 \mp \sqrt{\varepsilon_r \, \mu_r} \, k \, \beta} & \text{in } \Omega \, . \end{cases}$$

Note that when $k = k_+$ or $k = k_-$, i.e. when

$$\beta = \beta_{\rm crit}^+ = -\frac{\sqrt{\varepsilon_r \,\mu_r} - 1}{\sqrt{\varepsilon_r \,\mu_r} \,k} \qquad \text{or} \qquad \beta = \beta_{\rm crit}^- = +\frac{\sqrt{\varepsilon_r \,\mu_r} - 1}{\sqrt{\varepsilon_r \,\mu_r} \,k} \,, \tag{18}$$

the equation for the corresponding Beltrami field is the same inside and outside of Ω , so that Ω is invisible to fields of this helicity. We expect a maximal measure of em-chirality relative to the total interaction cross section in this case.

For the case where Ω is a ball, the fields E^{\pm} and consequently the far field operator can be computed analytically using expansions in vector spherical harmonics. Such calculations have been carried out by S. HEUMANN [11, Chapter IV]. Given the vector spherical harmonics

$$U_n^m(\hat{x}) = \frac{1}{\sqrt{n(n+1)}} \operatorname{Grad}_{\mathbb{S}^2} Y_n^m(\hat{x}), \qquad V_n^m(\hat{x}) = \hat{x} \times U_n^m(\hat{x}), \qquad \hat{x} \in \mathbb{S}^2,$$
(19)

for $n = 1, 2, 3, \ldots, m = -n, \ldots n$, one defines the linear combinations

$$A_n^m = U_n^m + i V_n^m, \qquad B_n^m = U_n^m - i V_n^m.$$
 (20)

The sets $\{A_n^m\}$ and $\{B_n^m\}$ then form complete orthogonal systems in V^+ and V^- , respectively. Expanding a tangential field $A \in L_t^2(\mathbb{S}^2)$ as

$$A = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left(a_n^m A_n^m + b_n^m B_n^m \right),$$

For the unit ball $\Omega = \{|x| = 1\}$, Heumann finds the expression

$$\mathcal{F}A(\hat{x}) = \frac{(4\pi)^2 \,\mathrm{i}}{k} \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left(\gamma_n(\kappa^+) \, a_n^m A_n^m + \gamma_n(\kappa^-) \, b_n^m \, B_n^m \right)$$

for the far field operator, with

$$\gamma_n(\kappa) = \frac{\operatorname{Re} d_n(\kappa)}{d_n(\kappa)}, \quad d_n(\kappa) = \left(\frac{1}{\kappa} - \frac{1}{k}\right) j_n(\kappa) h_n^{(1)}(k) + h_n^{(1)}(k) j_n'(\kappa) - j_n(\kappa) h_n^{(1)'}(k).$$

Here j_n denotes the spherical Bessel functions of order n and $h_n^{(1)}$ the spherical Hankel functions of order n and of the first kind. Thus the chiral ball as a scatterer preserves helicity and the eigenvalues of its far field operator are $(16\pi^2 i/k) \gamma_n(\kappa^+)$ with eigenfunctions A_n^m and $(16\pi^2 i/k) \gamma_n(\kappa^-)$ with eigenfunctions B_n^m , respectively. Its measure of em-chirality is

$$\chi(\Omega) = \frac{16\pi^2}{k} \left(\sum_{n=1}^{\infty} (2n+1) \left[|\gamma_n(\kappa^+)| - |\gamma_n(\kappa^-)| \right]^2 \right)^{1/2}$$

We plot $\chi(\Omega)^2/C_{\text{int}}$ as a function of β in Figure 1. As expected, this quantity attains a maximum value of 1 exactly at $\beta = \beta_{\text{crit}}^+$. It appears that in a number of points, but particularly in the maximal point β_{crit}^+ , the function $\chi(\Omega)^2/C_{\text{int}}$ is not differentiable. Indeed, in the present example $\gamma_n(\kappa^{\pm})$ is a smooth function of β , but $\chi(\Omega)$ depends on $|\gamma_n(\kappa^{\pm})|$. Whenever $\gamma_n(\kappa^{\pm})$ has a zero, which is true in particular in β_{crit}^+ , we cannot in general expect differentiability. Even though the singular values of a chirality component of the far field operator may be smooth functions of some parameter, the singular values will then not be differentiable in the parameter value where they become zero. This has to be taken into account in algorithms where $\chi(\Omega)^2/C_{\text{int}}$ is used as the basis of the objective functional in a shape optimization procedure to develop maximally em-chiral scatterers.

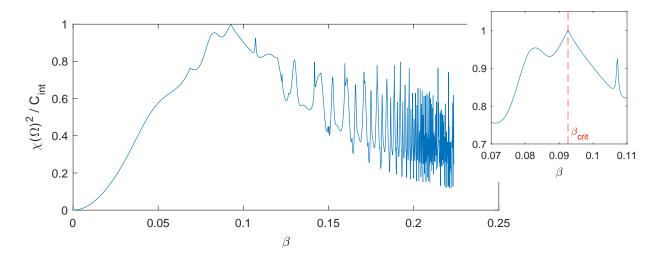


Figure 1: Plot of $\chi(\Omega)^2/C_{\text{int}}$ against β for $k = \sqrt{10}$, $\varepsilon_r = 2$ and $\mu_r = 1$. The inset is an enlarged view of the plot around $\beta_{\text{crit}}^+ \approx 0.0926$.

6 EM-Chirality for a Perfect Conducting Geometrically Chiral Scatterer

Analytic calculations of $\chi(D)$ as presented in the previous section are only possible in the case of simple geometries where exact solutions to Maxwell's equations are available. For more complex geometries, appropriate numerical methods have to be employed for the calculation of a discretization of \mathcal{F} and its singular values are approximated by the singular values of this discretization.

In this section, we will consider a perfectly conducting scatterer and present calculations carried out with the boundary element package BEM++ (http://www.bempp.org, [22,23]). For a bounded scatterer $D \subseteq \mathbb{R}^3$ and after normalization, the boundary value problem reads as

$$\operatorname{curl} E - \mathrm{i}kH = 0 \quad \text{in } \mathbb{R}^3 \setminus \overline{D},$$
$$\operatorname{curl} H + \mathrm{i}kE = 0 \quad \text{in } \mathbb{R}^3 \setminus \overline{D},$$
$$\nu \times E = 0 \quad \text{on } \partial D.$$

The fields (E, H) decompose into $(E, H) = (E^i + E^s, H^i + H^s)$, where (E^i, H^i) are incoming waves, i.e. solutions of the first two equations and (E^s, H^s) the scattered fields which satisfy the Silver-Müller radiation condition. Following the notation of BUFFA/HIPTMAIR [5], we have $E^s = -\Psi_{SL}\lambda$ with the Neumann or magnetic trace $\lambda = \gamma_N E^s$ and the electric single layer potential

$$\Psi_{SL}\mu(x) = k \int_{\partial D} \Phi(x, y) \,\mu(y) \,\mathrm{d}s(y) + \frac{1}{k} \,\mathrm{grad}_x \int_{\partial D} \Phi(x, y) \,\mathrm{Div} \,\mu(y) \,\mathrm{d}s(y)$$

for $\mu \in H^{-\frac{1}{2}}(\text{Div}, \partial D)$. This leads to the electric field integral equation (EFIE)

4

$$S\lambda = -\gamma_t E^i = -\nu \times E^i$$

where S is the associated boundary operator.

We will briefly outline, how we represent the far field operator in these numerical calculations. Define

$$M_n^m(x) = -j_n(k|x|) V_n^m(\hat{x}), \qquad x \in \mathbb{R}^3, \quad n = 1, 2, 3, \dots, \quad m = -n, \dots n.$$

where $\hat{x} = x/|x|$, j_n denotes the spherical Bessel function of order n and V_n^m was introduced in (19). Expanding a plane wave with polarization vector $p \in \mathbb{C}^3$ in terms of these functions and their curls,

$$p e^{ikd \cdot x} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left[\alpha_n^m M_n^m(x) + \beta_n^m \frac{1}{ik} \operatorname{curl} M_n^m(x) \right] \,,$$

orthogonality of the vector spherical harmonics gives

$$\alpha_n^m = -\frac{(p e^{ikr d \cdot \hat{x}}, V_n^m)_{L^2(\mathbb{S}^2)}}{j_n(kr)}, \qquad \beta_n^m = -\frac{i kr (p e^{ikr d \cdot \hat{x}}, U_n^m)_{L^2(\mathbb{S}^2)}}{(r j_n(kr))'}$$

The scalar products in the enumerators are Herglotz wave functions. Thus, letting $r \to \infty$, from the asymptotic behaviour of these functions (see e.g. [1]), we obtain

$$p e^{ikd \cdot x} = -4\pi \sum_{n=1}^{\infty} i^n \sum_{m=-n}^n \left[\left(p \cdot V_n^{-m}(d) \right) M_n^m(x) - \left(p \cdot U_n^{-m}(d) \right) \frac{1}{ik} \operatorname{curl} M_n^m(x) \right].$$

Inserting this representation in (2), one derives a corresponding expansion for the Herglotz wave pairs. Expanding a tangential field on the unit sphere in vector spherical harmonics

$$A = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left(u_n^m \, U_n^m + v_n^m \, V_n^m \right),$$

we obtain

$$E^{i}(x) = E^{0}[A](x) = -4\pi \sum_{n=1}^{\infty} i^{n} \sum_{m=-n}^{n} \left[v_{n}^{m} M_{n}^{m}(x) - u_{n}^{m} \frac{1}{ik} \operatorname{curl} M_{n}^{m}(x) \right].$$

We use this representation to evaluate the incident field on the boundary of the obstacle. Likewise expanding the far field pattern E^{∞} with respect to U_n^m , V_n^m leads to a representation of the far field operator with respect to this basis. Recalling the definition of A_n^m , B_n^m in (20), we easily obtain corresponding representations of the four component operators \mathcal{F}^{pq} , p, $q \in \{+, -\}$. For the numerical approximation, in all these representations, the series over nare cut off at $N \in \mathbb{N}$.

As the scatterer, we consider 4 perfectly conducting spheres with different diameters located on the corner points of a tetrahedron. With this type of object, it is possible to obtain a good approximation to the exact solution by a sum of expansions around the center of each sphere. It is thus well suited as a benchmark problem for the boundary element code. We fix three of the radii at $r_1 = 1/2$, $r_2 = 1/\sqrt{2}$ and $r_3 = 2$ while varying r_4 in the interval $[r_1, r_2]$. A typical geometric configuration is shown in Figure 2 (a). All calculations where carried out

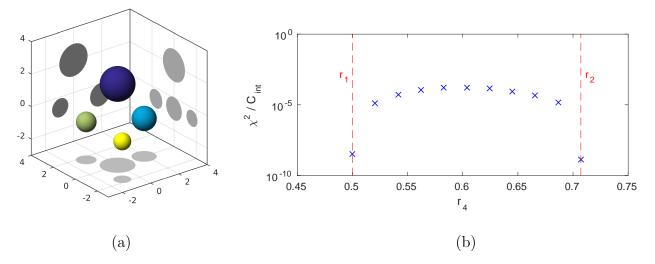


Figure 2: Scattering by four perfectly conducting spheres. (a) Typical geometric configuration. (b) Plot of $\chi(\Omega)^2/C_{int}$ against the radius r_4 of the third largest (green) ball.

at $k = \sqrt{10}$. When r_4 coincides with r_1 or r_2 , the scatterer is geometrically achiral and thus em-achiral by Theorem 3.2, so we expect the measure of em-chirality to be zero in these cases.

Calculations were carried out for N = 5, i.e. the far field operator was approximated by a matrix in $\mathbb{C}^{70\times70}$. The boundary element meshes were generated with a maximum mesh size of h = 0.1. The exact number of unknowns for each boundary integral equation varies between 10 080 for $r_4 = r_1$ and 11 517 for $r_4 = r_2$.

Indeed, our numerical computations meet the expectation that the measure of em-chirality is much smaller when the scatterer is geometrically achiral as in the cases when is is geometrically chiral, as shown in Figure 2 (b). Overall, the measure of em-chirality is relative small, as each combination of three spheres forms an achiral scatterer with a stronger scattering response than the entire ensemble of four spheres.

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References

 T. ARENS AND J. SYLVESTER, Born non-scattering electromagnetic media, Journal of Inverse and Ill-posed Problems, published online (https://doi.org/10.1515/jiip-2016-0054) (2016).

- [2] C. ATHANASIADIS, P.A. MARTIN AND I.G. STRATIS, Electromagnetic scattering by a homogeneous chiral obstacle: Boundary integral equations an low-chirality approximations, SIAM J. Appl. Math., 59, 1745–1762 (1999).
- [3] C. ATHANASIADIS, P.A. MARTIN AND I.G. STRATIS, Electromagnetic scattering by a homogeneous chiral obstacle: Scattering relations and the far-field operator, *Math. Meth. Appl. Sci.*, 22, 1175–1188 (1999).
- [4] ANDRZEJ B. BUDA, THOMAS AUF DER HEYDE AND KURT MISLOW, On quantifying chirality, Angewandte Chemie International Edition in English, **31**, 989–1007 (1992).
- [5] ANNALISA BUFFA AND RALF HIPTMAIR, Galerkin boundary element methods for electromagnetic scattering, in *Topics in Computational Wave Propagation, Direct and Inverse Problems* (M. AINSWORTH, P. DAVIES, D. DUNCAN, P. MARTIN AND B. RYNNE, eds.), volume 31 of *Lecture Notes in Computational Science and Engineering*, 83–124, Springer, Berlin, 2003.
- [6] F. CAKONI AND D. COLTON, A Qualitative Approach to Inverse Scattering Theory, Springer, Berlin, 2006.
- [7] D. COLTON AND R. KRESS, *Inverse Acoustic and Electromagnetic Scattering Theory*, Springer, 1998, 2nd edition.
- [8] DAVID COLTON AND RAINER KRESS, On the denseness of Herglotz wave functions and electromagnetic Herglotz pairs in Sobolev spaces, *Math. Meth. Appl. Sci.*, 24, 1289–1303 (2001).
- [9] IVAN FERNANDEZ-CORBATON, MARTIN FRUHNERT AND CARSTEN ROCKSTUHL, Objects of maximum electromagnetic chirality, *Phys. Rev. X*, **6**, 031013 (2016).
- [10] P.W. FOWLER, Quantification of chirality: Attempting the impossible, Symmetry: Culture and Science, 16, 321–334 (2005).
- [11] SVEN HEUMANN, The Factorization Method for Inverse Scattering from Chiral Media, Ph.D. thesis, Karlsruhe Institute of Technology (2012).
- [12] A. KIRSCH, An integral equation for Maxwell's equations in a layered medium with an application to the Factorization Method, J. Integral Equations Appl., 19, 333–358 (2007).
- [13] A. KIRSCH AND N. GRINBERG, *The Factorization Method for Inverse Problems*, Oxford Lecture Series in Mathematics and its Applications 36, Oxford University Press, 2008.
- [14] A. KIRSCH AND F. HETTLICH, The Mathematical Theory of Time-Harmonic Maxwell's Equations, Springer, 2015.
- [15] A. KIRSCH AND A. LECHLEITER, The operator equations of Lippmann-Schwinger type for acoustic and electromagnetic scattering problems in L²., *Applicable Analysis*, 4, 749– 769 (2009).
- [16] JIN AU KONG, *Electromagnetic Wave Theory*, Wiley-Interscience, New York, 1990, second edition edition.

- [17] A. LAKHTAKIA, V.K. VARADAN AND V.V. VARADAN, Time Harmonic Electromagnetic Fields in Chiral Media, number 335 in Lecture Notes in Physics, Springer, Berlin, Heidelberg, New York, 1989.
- [18] S. LITTLE AND J.B. READE, Eigenvalues and analytic kernels, SIAM J. Math. Anal., 15, 133–136 (1984).
- [19] P. MONK, Finite Element Methods for Maxwell's Equations, Oxford Science Publications, Oxford, 2003.
- [20] ANDRÉ RASSAT AND PATRICK W. FOWLER, Is there a 'most chiral tetrahedron'?, Chemistry – A European Journal, 10, 6575–6580 (2004).
- [21] G.F. ROACH, I.G. STRATIS AND A.N. YANNACOPOULOS, Mathematical Analysis of Deterministic and Stochastic Problems in Complex Media Electromagnetics, Princeton Series in Applied Mathematics, Princeton University Press, 2012.
- [22] MATTHEW SCROGGS, TIMO BETCKE, ERIK BURMAN, ŚMIGAJ WOJCIECH AND ELWIN VAN'T WOUT, Software frameworks for integral equations in electromagnetic scattering based on Calderón identities, submitted for publication.
- [23] W. ŚMIGAJ, S. ARRIDGE, T. BETCKE, J. PHILLIPS AND M. SCHWEIGER, Solving boundary integral problems with BEM++, ACM Trans. Math. Software, 41, 6:1–6:40 (2015).