Domain Derivatives in Electromagnetism and Optimal Design of Chiral Objects

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Abstract

The concept of electromagnetic chirality allows the quantification of the difference in interaction of objects with electromagnetic fields of the two handednesses. Objects of high em-chirality are desirable in many technical applications. Domain derivatives are required to analyse the effect of variations of the shape of an obstacle on the scattered fields. They have been used both for inverse shape reconstruction problems as well as for optimal design. In the talk, their use in designing scatteres of (close to) maximal em-chirality is discussed.

Keywords: Electromagnetic scattering, chirality, inverse scattering, shape design.

1 Introduction

In nature, chirality is a phenomenon with important implications in physics, chemistry or biology. One field of interest is the interaction of chiral matter with electromagnetic fields. In applications, one is naturally interested in materials that interact very differently with fields of opposite helicity (e.g. circular polarization).

The traditional geometric definition of chirality does not allow for quantification. In Physics, this has lead to the concept of *electromagnetic chirality (em-chirality)* [3] and a corresponding scalar measure of this quantity. From a mathematical perspective, this was first discussed in [2]. Scatterers that have maximal measure of em-chirality, relative to all others with the same norm of the farfield operator, have special and desirable properties: at least in the case that reciprocity holds, they are invisible to incident fields of one helicity.

2 EM-Chirality

We consider a scattering problem for a penetrable object illuminated by a time-harmonic electromagnetic wave. The electromagnetic field (E, H) is a solution to the Maxwell system

$$\begin{aligned} \operatorname{curl} E - \mathrm{i}\omega\mu H = 0 \\ \operatorname{curl} H + \mathrm{i}\omega\varepsilon E = 0 \end{aligned} \qquad \text{in } \mathbb{R}^3 . \tag{1}$$

We assume that the material parameters ε, μ are equal to constant background parameters ε_0, $\mu_0 > 0$ outside of some bounded (Lipschitz) domain D. Inside of D they are also assumed constant with $\mu > 0$ and $\arg(\varepsilon) \in [0, \pi)$. The incident field (E^i, H^i) is assumed to be a solution of (1) for ε_0, μ_0 in $\mathbb{R}^3$. The scattered field $(E^s, H^s) = (E, H) - (E^i, H^i)$ satisfies the Silver-Müller radiation condition at infinity. The standard asymptotics for scattered fields give rise to the far field operator $\mathbf{F} : L^2_t(\mathbb{S}^2) \to L^2_t(\mathbb{S}^2)$, given by

$$\mathbf{F}g(\hat{x}) = \int_{\mathbb{S}^2} E^\infty(\hat{x}, \hat{y}, g(\hat{y}))\, \mathrm{d}s(\hat{y}), \quad g \in L^2_t(\mathbb{S}^2) .$$

Here, $E^\infty(\hat{x}, \hat{y}, g(\hat{y}))$ is the farfield of E^s for an incident plane wave propagating in direction $\hat{y}$ with amplitude $g(\hat{y})$, observed in direction $\hat{x}$. $L^2_t(\mathbb{S}^{2^2})$ denotes the space of square integrable tangential vector fields on the unit sphere.

A field is said to have *helicity* λ, if it is an eigenfunction with eigenvalue λ of the operator $\frac{1}{\omega\sqrt{\varepsilon\mu}}$ curl. For constant ε, μ, a solution (E, H) to the Maxwell system can always be represented as a linear combination of two such eigenfunctions for the eigenvalues ± 1, the *Beltrami fields* $E \pm \mathrm{i}\sqrt{\mu/\varepsilon}\, H$. For a plane wave, this is just the well known decomposition into left and right circularly polarized components. By approximation with Herglotz wave pairs in the case of an entire field, or through the far field in case of a radiating field, this decomposition extends to $L^2_t(\mathbb{S}^2)$ and hence to $\mathbf{F}$: the far field operator is split into

$$\mathbf{F} = \mathbf{F}^+_+ + \mathbf{F}^+_- + \mathbf{F}^-_+ + \mathbf{F}^-_- ,$$

with $\mathbf{F}^p_q$, p, $q \in \{+, -\}$ describing the scattering of fields of helicity q onto fields of helicity p. Denote by (σ^p_q) the sequences of singular values of $\mathbf{F}^p_q$. The scatterer is called *em-achiral* if $(\sigma^+_+) = (\sigma^-_-)$ and $(\sigma^+_-) = (\sigma^-_+)$. Otherwise it is called *em-chiral*, and the relative measure of chirality

$$\chi = \frac{\|(\sigma^+_+) - (\sigma^-_-)\|^2_{\ell^2} + \|(\sigma^+_-) - (\sigma^-_+)\|^2_{\ell^2}}{\|\mathbf{F}\|^2_*}$$

was proposed in [3]. Here, $\|\cdot\|_*$ denotes the Hilbert-Schmidt norm.

3 Domain Derivatives

Consider the map $\mathcal{F}: \partial D \to E^\infty$ for a fixed incident field (E^i, H^i). The Fréchet derivative of $\mathcal{F}$ with respect to variations of ∂D is called the *domain derivative* and may be computed by solving a transmission problem of the same type as the original scattering problem [6]. This derivative can be used in regularized Gauss-Newton schemes for solving the inverse scattering problem of reconstructing the shape of ∂D from measurements of E^∞ for one incident wave. The method was implemented for star-shaped obstacles and electromagnetic transmission problems in [5].

When only star-shaped scatterers are considered, the set of admissable parametrizations for ∂D is a subset of a linear space. Obstacles for which high em-chirality can be expected are typically described by more complicated parameterizations with a non-linear dependence on the optimization variables. When discretizing the domain derivative in this case, a detailed derivation of corresponding expressions subject to the chosen class of parameterizations is required. A particular application, helicical scatterers, and corresponding inverse problems, will be presented in the talk. Such scatterers are constructed as C^1-smooth surfaces from a center curve given as a B-spline and function specifying the diameter along the curve. Smooth caps close the surface at the two ends.

4 Optimal Design of EM-Chiral Objects

For problem of optimally designing a scatterer with respect to its em-chirality, one requires the Frécht differentiability of an appropriately chosen measure of chirality with respect to variations of ∂D. It has been shown that χ as defined above does not have the required smoothness [4]. Hence the related measure

$$\hat{\chi} = \frac{(\|\mathbf{F}_+^+\|_* - \|\mathbf{F}_-^-\|_*)^2 + (\|\mathbf{F}_-^+\|_* - \|\mathbf{F}_+^-\|_*)^2}{\|\mathbf{F}\|_*^2}$$

has been proposed [4] and used in a related optimal design scheme based on an asymptotic representation formula of the scattered field [1]. Note that $\hat{\chi} \le \chi$ for all scatterers and that, in particular, $\hat{\chi}$ attains the maximal value 1 if and only if χ does.

An expressions for the Fréchet derivative of $\|\mathbf{F}\|_*^2$ and corresponding terms for the other operators are readily obtained from the definition of $\mathbf{F}$ as a linear integral operator. One only requires variants of the estimates in [6] that make explicit the uniform bound on the $H(\text{curl})$-norm of the incident field. The implementation of the algorithm for the class of helicical scatterers discussed in the previous section is subject to ongoing research.

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