Maximizing the electromagnetic chirality for metallic nanowires in the visible spectrum

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Abstract

Electromagnetic chirality describes differences in the interaction of scattering objects with electromagnetic fields of different helicity. If the scattering behavior of an object with respect to incident waves of one helicity cannot be reproduced with incident fields of the opposite helicity, then the object is said to be electromagnetically chiral (em-chiral), otherwise it is called em-achiral. Em-chirality can be quantified by chirality measures that attain the value 0 for an em-achiral object and the value 1 for a maximally em-chiral object. We investigate a shape optimization problem, where the goal is to construct thin metallic nanowires that exhibit large measures of em-chirality at a given frequency. We present a gradient based optimization method, based on an asymptotic representation formula for approximating scattered fields due to thin metallic scattering objects.

Keywords: Electromagnetic chirality, shape optimization, asymptotic representation formula

1 Scattering from metallic wires

Let $\omega > 0$ denote the angular frequency and let $\varepsilon_0, \mu_0 > 0$ denote the electric permittivity and magnetic permeability in free space. We define the wave number $k > 0$ in free space to be $k = \omega\sqrt{\varepsilon_0\mu_0} > 0$. Let the pair of incident fields $(\boldsymbol{E}^i, \boldsymbol{H}^i)$ be entire solutions of time harmonic Maxwell's equation in homogeneous space, i.e.

$$\begin{aligned} \mathbf{curl}\, \boldsymbol{E}^i - \mathrm{i}\,\omega\mu_0 \boldsymbol{H}^i = 0 \quad &\text{in } \mathbb{R}^3, \\ \mathbf{curl}\, \boldsymbol{H}^i + \mathrm{i}\,\omega\varepsilon_0 \boldsymbol{E}^i = 0 \quad &\text{in } \mathbb{R}^3\,. \end{aligned}$$

We assume that the incident field is scattered by a non-magnetic scattering object D, for which we assume a constant electric permittivity $\varepsilon_1 \in \mathbb{C}$ with $\mathrm{Re}(\varepsilon_1) < 0$ and $\mathrm{Im}(\varepsilon_1) > 0$. These electric permittivites are observed in the study of metallic scattering objects like silver and gold, especially for wavelengths in the visible electromagnetic spectrum. We define the permittivity distribution $\varepsilon = \varepsilon_1\chi_D + \varepsilon_0\chi_{\mathbb{R}^3\setminus\overline{D}}$ and consider the scattering problem in full space, which is to find the total fields $(\boldsymbol{E}, \boldsymbol{H}) = (\boldsymbol{E}^i + \boldsymbol{E}^s, \boldsymbol{H}^i + \boldsymbol{H}^s)$ satisfying

$$\begin{aligned} \mathbf{curl}\, \boldsymbol{E} - \mathrm{i}\,\omega\mu_0 \boldsymbol{H} = 0 \qquad &\text{in } \mathbb{R}^3, \\ \mathbf{curl}\, \boldsymbol{H} + \mathrm{i}\,\omega\varepsilon \boldsymbol{E} = 0 \qquad &\text{in } \mathbb{R}^3\,, \end{aligned}$$

together with the Silver-Müller radiation condition (SMR). The scattered field $\boldsymbol{E}^s$ satisfies a far field expansion, which reads

$$\boldsymbol{E}^s(\boldsymbol{x}) = \frac{e^{\mathrm{i}\,k|\boldsymbol{x}|}}{4\pi|\boldsymbol{x}|}\left(\boldsymbol{E}^\infty(\widehat{\boldsymbol{x}}) + \mathcal{O}(|\boldsymbol{x}|^{-1})\right)$$

as $|\boldsymbol{x}| \to \infty$ uniformly with respect to all directions $\widehat{\boldsymbol{x}} = \boldsymbol{x}/|\boldsymbol{x}| \in S^2$.

In this talk we focus on thin tubular scattering objects D_ρ having an elliptical cross section that possibly rotates around the center curve Γ. Here, the parameter $\rho > 0$ represents the radius of the elliptical cross section. The space of admissible parametrizations is denoted by $\mathcal{U}_{\mathrm{ad}}$. The rotation function is further denoted by θ. In our work (see [3]) we establish an asymptotic representation formula for electric fields scattered by D_ρ.

Theorem 1 *For a thin tubular scatterer with elliptical cross section with semiaxes lengths $a = \rho\tilde{a}$ and $b = \rho\tilde{b}$, the far field of $\boldsymbol{E}^s_\rho$ satisfies*

$$\begin{aligned} \boldsymbol{E}^\infty_\rho(\widehat{\boldsymbol{x}}) \;=\; & abk^2\pi \int_\Gamma (\varepsilon_r - 1)e^{-\mathrm{i}k\widehat{\boldsymbol{x}}\cdot\boldsymbol{y}} \\ & \big((\widehat{\boldsymbol{x}} \times \mathbb{I}_3) \times \widehat{\boldsymbol{x}}\big)\mathbb{M}^\varepsilon_\theta(\boldsymbol{y})\boldsymbol{E}^i(\boldsymbol{y})\;\mathrm{d}s(\boldsymbol{y}) + o(|D_\rho|) \end{aligned}$$

as $\rho \to 0$. The matrix valued function $\mathbb{M}^\varepsilon_\theta \in L^2(\Gamma, \mathbb{C}^{3\times 3})$ is the so-called electric polarization tensor.

2 Maximizing electromagnetic chirality

We define the far field operator

$$(\mathcal{F}_D\boldsymbol{A})(\widehat{\boldsymbol{x}}) = \int_{S^2} \boldsymbol{E}^\infty(\widehat{\boldsymbol{x}}, \boldsymbol{d}, \boldsymbol{A}(\boldsymbol{d}))\;\mathrm{d}s(\boldsymbol{d}).$$

Electromagnetic chirality describes the interaction of a scattering object D with fields of different helicities. As shown in [2], helicity of either an incident Herglotz field $\boldsymbol{E}^i[\boldsymbol{A}]$ or the corresponding scattered field $\boldsymbol{E}^s[\boldsymbol{A}]$ can be characterized by the assignment of the representative field $\boldsymbol{A} \in L^2_t(S^2, \mathbb{C}^3)$ to spaces V^+ or V^- with $V^+ \oplus V^- = L^2_t(S^2, \mathbb{C}^3)$ where

$$V^\pm = \{\boldsymbol{A} \pm \mathcal{C}\boldsymbol{A} \;:\; \boldsymbol{A} \in L^2_t(S^2, \mathbb{C}^3)\}$$

and $(\mathcal{C}\boldsymbol{A})(\boldsymbol{\theta}) = \mathrm{i}\,\boldsymbol{\theta} \times \boldsymbol{A}(\boldsymbol{\theta})$ for $\boldsymbol{\theta} \in S^2$. Using orthogonal projections, it is possible to derive a decomposition of the far field operator

$$\mathcal{F}_D = \mathcal{F}^{++} + \mathcal{F}^{+-} + \mathcal{F}^{-+} + \mathcal{F}^{--}, \qquad (1)$$

where $\mathcal{F}^{pq}$ characterizes the helicity contribution of the p incident field to the q scattered field for $p, q \in \{+, -\}$. For a thin scatterer D_ρ we employ theorem 1 to approximate the far field operator. Introducing the operator

$$(\mathcal{T}_{D_\rho}\boldsymbol{A})(\widehat{\boldsymbol{x}}) := abk^2\pi \int_\Gamma (\varepsilon_r - 1)e^{-\mathrm{i}k\widehat{\boldsymbol{x}}\cdot\boldsymbol{y}} \big((\widehat{\boldsymbol{x}} \times \mathbb{I}_3) \times \widehat{\boldsymbol{x}}\big)\mathbb{M}^\varepsilon_\theta(\boldsymbol{y})\boldsymbol{E}^i[\boldsymbol{A}](\boldsymbol{y}) \,\mathrm{d}s(\boldsymbol{y})$$

consequently gives that $\mathcal{F}_D = \mathcal{T}_{D_\rho} + o((k\rho)^2)$ as $\rho \to 0$ and the term $o((k\rho)^2)$ is such that $\|o((k\rho)^2)\|_{\mathrm{HS}}/(k\rho)^2$ converges to zero. Here, $\|\cdot\|_{\mathrm{HS}}$ denotes the Hilbert-Schmidt norm. We define the nonlinear operator $T_\rho : \mathcal{U}_{\mathrm{ad}} \times [0,1] \to \mathrm{HS}(L^2_t(S^2, \mathbb{C}^3))$ by

$$T_\rho(\Gamma, \theta) = \mathcal{T}_{D_\rho}, \qquad (2)$$

where D_ρ is the thin tubular scatterer characterized by the center curve Γ and the rotation function θ. The operators $T_\rho(\Gamma, \theta)^{pq}$ for $p, q \in \{+, -\}$ are defined analogously to $\mathcal{F}^{pq}$ and consitute a decomposition of T_ρ, equally to (1). These operators are now used to approximate the relative chirality measure introduced in [4]. In our setting, this approximation is denoted by $J_2 : \mathcal{U}_{\mathrm{ad}} \times [0,1] \to [0,1]$, with

$$J_2 = \frac{\sqrt{\|(\sigma_j^{++}) - (\sigma_j^{--})\|^2_{\ell^2} + \|(\sigma_j^{+-}) - (\sigma_j^{-+})\|^2_{\ell^2}}}{\|T_\rho\|_{\mathrm{HS}}},$$

where (σ_j^{pq}) denote the singular values of $\mathcal{F}^{pq}$. The functional J_2 takes the value 1 for a maximally em-chiral object and the value 0 for an em-achiral object. Since the function J_2 is not smooth, we consider a smooth relaxation of J_2, denoted by J_{HS}. Moreover, we introduce penalty terms and regularization parameters, denoted by Λ and α, respectively, in order to stabilize the optimization functional. Thus, we define the regularized functional $F(\Gamma, \theta) = J_{\mathrm{HS}}(\Gamma, \theta) - \alpha\Lambda(\Gamma, \theta)$, that we aim to maximize with respect to the center curve Γ and the rotation θ of the elliptical cross section around Γ. For this purpose, we apply the BFGS method to F. The far field operator approximation in (2) allows an explicit computation of the Fréchet derivative of F with respect to Γ and θ, resulting in an efficient optimization scheme. An example of such an optimization can be found in Figure 1. The initial guess on the left, a 4 turn helix with an elliptical cross section, is iteratively deformed by the optimization scheme. The algorithm stops after 26 steps, returning the nano-structure in the right plot of figure 1. This object has a comparatively large measure of em-chirality. This talk is based on joint work with T. Arens, I. Fernandez-Corbaton, R. Griesmaier and C. Rockstuhl.

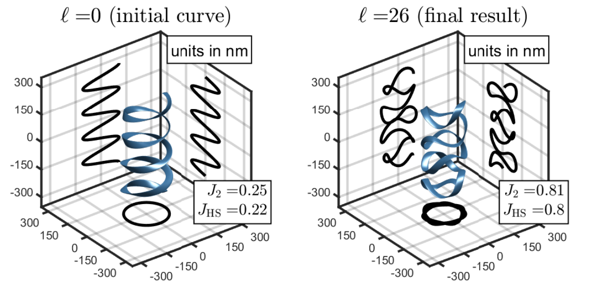

Figure 1: Maximizing electromagnetic chirality for a silver scatterer at 555THz.

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