Hybridisation in coupled-dipole chiral meta-atoms

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Abstract

We analyse the optical activity in twisted dimers, the meta-atoms of a chiral metamaterial, by introducing a simple yet accurate model for the coupling between them. The near-field interaction coefficients are derived from a Lagrangian model and include the effects of retardation, whereas the far-field radiation is based on a multipole expansion. Our approach is accurate over a wide frequency range, including the resonant regions with the highest optical activity. In contrast to other models of near-field interaction, it requires no fitted parameters or homogenization procedure and is directly applicable to a wide variety of resonant particles.

1. Introduction

We study optical activity in a twisted wire dimer, showing that the resonant lineshapes can be easily predicted. This enables accurate modelling of the far-field scattering, clearly showing the polarisation rotation in all regimes, including at resonance where the effect is strongest. This is performed with a semi-analytical hybridisation model [1] of the coupled resonators, using coefficients derived from the numerically obtained charge and current distributions [2], and a multi-pole expansion of far-field radiation. In contrast to point-dipole based models [3], our approach is applicable to the close spacing typically used in twisted dimers.

2. Coupling of twisted dipoles

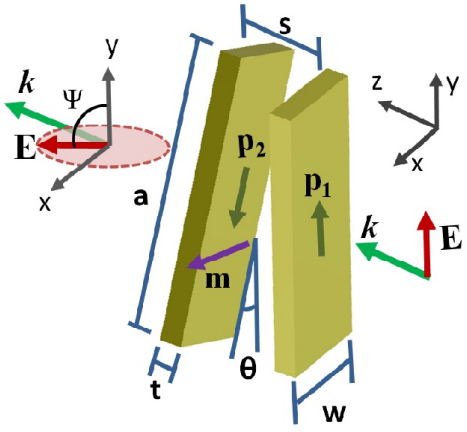

Fig. 1: Schematic layout of the twisted cut-wire pair. The two cut-wires locate on the plane $z = -s/2$ and $z = s/2$, respectively, with a twist angle θ between them. We set their central points lying on the z axis. The impinging wave propagates in the z direction.

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The twisted cut-wire pair is illustrated in Fig. 1. The first cut-wire is located on the plane $z = -s/2$, oriented along the y direction, and the second cut-wire is on the plane $z = s/2$, rotated about the z axis by angle θ. Our model starts from the Lagrangian description [1] of the metallic structures, which provides an intuitive picture of the coupling and can predict the resonant frequencies as well as the polarization change in twisted SRRs [4]. We utilise physically-meaningful coupling parameters based on the calculated charge and current distribution [2]. Including retardation effects in the calculation of the interaction constants allows the phase shift between coupled elements to be correctly predicted [5,6].

As described in Ref. [2], we numerically find the charge $\rho(t, \mathbf{r})$ and current distribution $\mathbf{J}(t, \mathbf{r})$ for a single wire, and separate them into a time-dependent mode amplitude $Q(t)$ and spatially dependent charge density $q(\mathbf{r})$ and current density $\mathbf{j}(\mathbf{r})$. Following Ref. [4], the Lagrangian of the twisted cut-wire pair excited by a plane-wave is written as

$$\mathcal{L} = \frac{L}{2}(\dot{Q}_1^2 + \dot{Q}_1^2 + 2\kappa_M \dot{Q}_1 \dot{Q}_2) - \frac{1}{2C}(Q_1^2 + Q_2^2 + 2\kappa_E Q_1 Q_2) - \mathbf{p}_1 \cdot \mathbf{E}_i - \mathbf{p}_2 \cdot \mathbf{E}_i \exp(i\varphi). \quad (1)$$

where Q_m, $\dot{Q}_m$ describe the time-dependent amplitudes of the charge and current on wire m ($m = 1, 2$). L and C are the self-inductance and self-capacitance of a single cut-wire; κ_M and κ_E are magnetic and electric interaction coefficients, which are functions of s and θ. The last two terms of Eq. (1) describe the interaction energy between the cut-wire pair and the external field. $\mathbf{E}_i$ is the electric field of the incident wave, and $\varphi = \omega s/c$ is the phase difference in excitation of the wires due to retardation. $\mathbf{p}_m = Q_m \mathbf{l}_{\mathit{eff}}$ is the electric dipole moment of cut-wire m, where $l_{\mathit{eff}} = |\mathbf{l}_{\mathit{eff}}| = |\int_{V_m} q(\mathbf{r})\mathbf{r}\mathrm{d}^3\mathbf{r}|$ is the effective dipole length, which can be calculated by making a volume integral over cut-wire m once $q(\mathbf{r})$ is known. According to the symmetry of the charge distribution, we can easily get $\mathbf{p}_1 = Q_1 l_{\mathit{eff}} \cdot \hat{\mathbf{y}}$ and $\mathbf{p}_2 = Q_2 l_{\mathit{eff}}(-\sin\theta \cdot \hat{\mathbf{x}} + \cos\theta \cdot \hat{\mathbf{y}})$. To obtain the solution for Q_m, we substitute Eq. (1) into the Euler-Lagrange equations. Taking $\exp(-i\omega t)$ time dependence, the solution is

$$\begin{aligned}
Q_1 &= (F_{mut}F_2 - F_{self}F_1)/(F_{self}^2 - F_{mut}^2) && (2)\\
Q_2 &= (F_{mut}F_1 - F_{self}F_2)/(F_{self}^2 - F_{mut}^2) && (3)\\
F_{self} &= (\omega_0^2 - \omega^2) \qquad F_{mut} = (\omega_0^2\kappa_E - \omega^2\kappa_M) &&\\
F_1 &= \tfrac{l_{\mathit{eff}}}{L} E_{i,y} \qquad F_2 = \tfrac{l_{\mathit{eff}}}{L} e^{i\varphi}(E_{i,x}\sin\theta + E_{i,y}\cos\theta) &&
\end{aligned}$$

$\omega_0 = 1/\sqrt{LC}$, and $E_{i,x}$ and $E_{i,y}$ denote the x and y components of the incident electric field. The coupling constants κ_E and κ_M can be determined by calculating the mutual electric and magnetic interaction energies including the retardation terms [5].

3. Far-field scattering

We use the modal amplitudes Q_1 and Q_2 to investigate the scattering properties, taking into account the three dominant multipole terms: electric dipole $\mathbf{p}$, electric quadrupole $\overline{\overline{\mathbf{q}}}$ and magnetic dipole $\mathbf{m}$. The radiated electric field at the far-field point $\mathbf{R}$ can be written explicitly as

$$\mathbf{E}(\mathbf{R}) = \frac{\exp(ik_0R)}{4\pi\epsilon_0 c^2 R}\left\{\frac{-\omega^2\mathbf{R}\times(\mathbf{R}\times\mathbf{p})}{R^2} + \frac{i\omega^3\mathbf{R}\times[\mathbf{R}\times(\mathbf{R}\cdot\overline{\overline{\mathbf{q}}})]}{2cR^3} - \frac{\omega^2\mathbf{R}\times\mathbf{m}}{cR}\right\}. \quad (4)$$

From the symmetry of the charge and the current distribution, we can express the electric dipole, quadrupole and magnetic dipole in terms of Q_m, θ and l_{eff}:

$$\begin{aligned}
\mathbf{p} &= l_{\mathit{eff}}\left[-Q_2\sin\theta\cdot\hat{\mathbf{x}} + (Q_1 + Q_2\cos\theta)\cdot\hat{\mathbf{y}}\right],\\
\overline{\overline{\mathbf{q}}} &= \frac{s\, l_{\mathit{eff}}}{2}\left[(Q_2\cos\theta - Q_1)(\hat{\mathbf{y}}\hat{\mathbf{z}} + \hat{\mathbf{z}}\hat{\mathbf{y}}) - Q_2\sin\theta(\hat{\mathbf{x}}\hat{\mathbf{z}} + \hat{\mathbf{z}}\hat{\mathbf{x}})\right]\\
\mathbf{m} &= \frac{i\omega s}{4}\, l_{\mathit{eff}}\left[(Q_2\cos\theta - Q_1)\cdot\hat{\mathbf{x}} + Q_2\sin\theta\cdot\hat{\mathbf{y}}\right] \quad (5)
\end{aligned}$$

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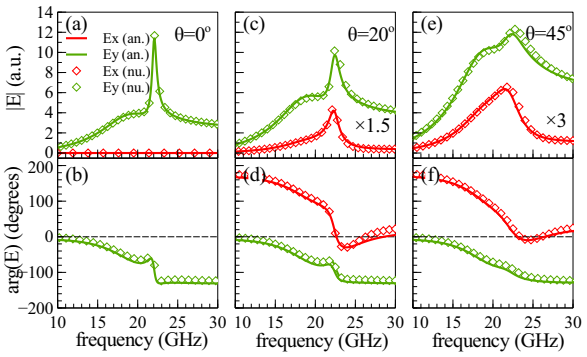

Fig. 2: Amplitudes and phases of the electric field of forward radiated wave at (0,0,z), under different twist angle. (a,b) $\theta = 0°$, (c,d) $\theta = 20°$, (e,f) $\theta = 45°$. The results from analytical model (an.) and numerical simulation (nu.) are plotted in (—) and (⋄), respectively.

To test our model, we compare the results of full wave simulation from CST Microwave Studio. We compared the forward far-field radiation spectra, as shown in Fig. 2. When cut-wire 2 is twisted by an angle θ, a cross component E_x is observed in the radiated wave. For clarity, the electric field amplitudes of radiation are multiplied by 1.5 and 3 in Fig. 2(c) and (e), respectively. The excellent agreement between our method and numerical simulation is evident. Under a certain twist angle, the strongest cross polarization conversion occurs near the antisymmetric resonance, when Q_2 becomes maximum. This is consistent with Eq. (4): when $\mathbf{R} = (0, 0, z)$, $E_x(\omega, R) = -\omega^2 Q_2 l_{eff} \sin\theta \left[1 - i\omega s/(2c)\right] \exp\left(ik_0 z\right) / \left(4\pi\epsilon_0 c^2 z\right)$.

4. Conclusion

To conclude, we propose a semi-analytical method to study the resonant and scattering properties of chiral metallic structures based on Lagrange model and multipole approximation. In this method, all the parameters can be obtained deterministically by considering the near-field interaction and the retardation effect. A twisted cut-wire pair is studied to test the model; both the resonant lineshapes and far-field results show a good agreement with full-wave simulation. This method can be further extended as an efficient tool for the future exploring on other chiral and hybrid structures. The approach can also be extended to include the coupling between neighbouring elements in an array.

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