Modal approximation for plasmonic resonators in the time domain

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Abstract

We study the electromagnetic field scattered by a metallic nanoparticle with dispersive material parameters in a resonant regime. We consider the particle placed in a homogeneous medium in a low-frequency regime. We define modes for the non-Hermitian problem as perturbations of electro-static modes, and obtain a modal approximation of the scattered field in the frequency domain. The poles of the expansion correspond to the eigenvalues of a singular boundary integral operator and are shown to lie in a bounded region near the origin of the lower-half complex plane. Finally, we show that this modal representation gives a very good approximation of the field in the time domain. We present numerical simulations in two dimensions to corroborate our results.

Keywords: Plasmonic resonance · Time-domain modal expansion · Subwavelength resonators · Quasi-normal modes

Main results

The starting point is the *Electric Field Integral Equation* (or Lippman-Schwinger equation) in the scatterer D:

$$\left(I - \gamma^{-1}(\omega)\mathcal{T}^{\omega}\right)\mathbf{E} = \mathbf{E}^{\mathrm{in}} \qquad \text{in } D, \tag{1}$$

where $\mathcal{T}^{\omega}$ is a singular integral operator and γ is a non-linear function of ω that depends on the permittivity model for the scatterer D. We assume D has characteric size δ with $\frac{\delta\omega}{c} \ll 1$ where c is the speed of light in the background. Building on the previous spectral analysis of $\mathcal{T}$ [3] and classic results on the compact symmetrisable *Neumann-Poincaré operator*, we exhibit a complete modal basis for the static transmission problem:

Theorem 1 *When $\omega\delta c^{-1} \to 0$, the electric field inside the particle converges to:*

$$\mathbf{E}^0 = \sum_{n=0}^{\infty} \frac{\gamma(\omega)}{\gamma(\omega) - \gamma_n} \left\langle \mathbf{E}^{\mathrm{in}}, \mathbf{e}_n \right\rangle_{L^2(D,\mathbb{R}^3)} \mathbf{e}_n \qquad \textit{in } D, \tag{2}$$

where $(\mathbf{e}_n)_{n\in\mathbb{N}}$ is an orthonormal basis of $\mathbf{W}(D)$ for the usual $L^2(D,\mathbb{R}^3)$ scalar product, eigenvectors of $\mathcal{T}^0$ associated with the eigenvalue γ_n. The space $\mathbf{W}(D)$ is the space of gradients of harmonic H^1 fields on D.

We show that, under the assumption that the particle is strictly convex, the excitation coefficients of the eigenfunctions exhibit superpolynomial decay with the order of the mode, and therefore the field can be well approximated by a finite number of modes. Using elementary perturbative analysis, we then show in Proposition 2 that the resolvent for the dynamic problem ($\omega \neq 0$) can be approximated by a perturbed resolvent of a finite-dimensional operator (the truncated static operator):

Proposition 2 *There exists a sequence with superpolynomial decay $\left(\epsilon_N(\mathbf{E}^{\mathrm{in}})\right)_{N\in\mathbb{N}}$ depending only on $\mathbf{E}^{\mathrm{in}}$ and B, and a sequence of open complex neighbourhood of the origin $\mathcal{V}(N) \ni 0$ such that for $\omega\delta c^{-1} \in \mathcal{V}(N) \cap \mathbb{R}$ the electric field solution of (1) satisfies:*

$$\mathbf{E} = \sum_{n=0}^{N} \frac{\gamma(\omega)\left\langle \mathbf{E}^{\mathrm{in}}, \mathbf{e}_n \right\rangle_{L^2(D,\mathbb{R}^3)}}{\gamma(\omega) - \gamma_n(\frac{\omega\delta}{c})} \mathbf{e}_n + \mathcal{O}\left(\frac{\epsilon_N(\mathbf{E}^{\mathrm{in}})}{f\left(\left| \Im\gamma(\omega) - \widetilde{C}_D\left(\omega\delta c^{-1}\right)^3 \right| \right)} \right),$$

in D and $f(x) := xe^{x^{-2}}$ and $\gamma_n(\frac{\omega\delta}{c})$ are eigenvalues of $\mathcal{T}_D^{\omega}$ obtained via classic perturbative spectral theory applied to $\mathcal{T}_D^0$.

Next, using Rouché's theorem, we prove the existence of poles for this approximated resolvent and give a *resonance-like* expansion for the electric field inside the particle:

Theorem 3 *For a given $\mathbf{E}^{\mathrm{in}}$ there exists N (depending on $\mathbf{E}^{\mathrm{in}}$), $\delta_{max}(N)$ such that for all $\delta < \delta_{max}(N)$, there exists $\omega_{max} = \mathcal{O}\left(c\delta^{-1}\right)$ such that for all $\omega \in \mathbb{R}$ satisfying $|\omega| < \omega_{max}$ the* *following holds:*

$$\mathbf{E} = \sum_{n=0}^{N} \frac{\gamma(\omega)}{\gamma(\omega) - \gamma_n\left(\Omega_n(\delta)\right)} \left\langle \mathbf{E}^{\text{in}}, \mathbf{e}_n \right\rangle_{L^2(D,\mathbb{R}^3)} \mathbf{e}_n + \epsilon_{int} \text{ in } D,$$

and

$$\mathbf{E}(x) - \mathbf{E}^{\text{in}}(x) = \sum_{n=0}^{N} \frac{\left\langle \mathbf{E}^{\text{in}}, \mathbf{e}_n \right\rangle_{L^2(D,\mathbb{R}^3)}}{\gamma(\omega) - \gamma_n\left(\Omega_n(\delta)\right)} \left(\frac{\omega}{c}\right)^2 \int_D \mathbf{\Gamma}^{\frac{\omega}{c}}(x,y)\mathbf{e}_n(y)\mathrm{d}y + \epsilon_{ext}(x) \text{ in } \mathbb{R}^3 \backslash \overline{D},$$

and $\gamma_n(\Omega_n(\delta))$ *are the eigenvalues of* $\mathcal{T}_D^{\frac{\omega}{c}}$ *at the dynamic plasmonic resonant frequency* $\omega = \Omega_n(\delta)$ *on* $\mathbf{W}(D)$ *associated with the eigenvectors* $\mathbf{e}_n$*, and* $\mathbf{\Gamma}^{\frac{\omega}{c}}(x,y)$ *the outgoing Green function associated with Maxwell's equation in* $\mathbb{R}^3$*. The error terms* ϵ_{int} *and* ϵ_{ext} *depend mainly onthe incident wave and the number of modes considered.*

From this expansion we construct the so-called *quasi-normal modes* found in the physics literature. Finally, using elementary complex analysis tools, we give an expansion for the *low-frequency part* of the electromagnetic field in the time domain and we show that the the truncated inverse Fourier transform (low frequency only, $\omega < \rho$) has the form:

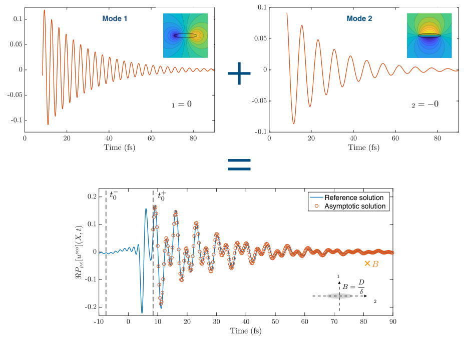
$$P_\rho\left[\mathbf{E}^{sca}\right](x,t) = \sum_{1}^{N} C_n \mathbf{E}_n(x) e^{-i\Omega_n(\delta)t} + \epsilon(x,t)$$

for $t \geq t_0^+$ where

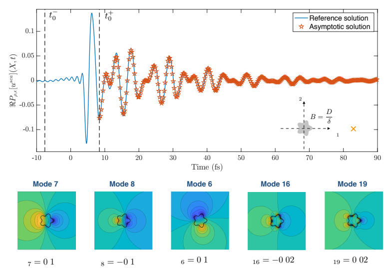
$$t_0^{\pm}(s,x) := \frac{1}{c}\left(|s-z| + |x-z| \pm 2\delta\right),$$

is the time it takes to the signal to reach first the scatterer from source point s and then observation point x, and $\mathbf{E}_n$ the generalised (exponentially diverging) eigenvectors, the so-called *quasi normal modes*. The error term $\epsilon(x,t)$ can be analyzed precisely. By doing so, we show that in the time domain causality ensures that the electromagnetic field does not diverge exponentially in space. Similar results were obtained in [4] for a non-dispersive dielectric spherical scatterer in any frequency range.

In the scalar case, we numerically study the quality of the approximation in a two dimensional setting for different shapes of scatterers. The real part of the field scattered by the ellipse and observed at some fixed observation point is the superposition of two dipoles modes :



We also show that the approximation is valid well outside of the restrictive theoretical hypotheses from the paper, for example the approximation seems to be valid for non convex scatterers.



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