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Mathematical analysis of electromagnetic scattering by dielectric nanoparticles with high refractive indices

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Abstract

In this work, we are concerned with the mathematical modeling of the electromagnetic (EM) scattering by arbitrarily shaped non-magnetic nanoparticles with high refractive indices. When illuminated by visible light, these particles can exhibit a very strong isotropic magnetic response, in addition to the electric resonance, resulting from the coupling of the incident wave with the circular displacement currents of the EM fields. We shall first introduce the mathematical concept of dielectric (subwavelength) resonances, then perform the asymptotic analysis in terms of the small particle size and the high contrast parameter. This enables us to derive the a priori estimates for the leading-order terms of dielectric resonances and the associated resonant modes, by making use of a Helmholtz decomposition for divergence-free vector fields. It turns out that these dielectric resonant fields are almost transverse electric in the quasi-static and high contrast regime, and hence present the feature of the magnetostatic fields. To address the existence of resonances, we apply the Gohberg-Sigal theory under a physical condition for the contrast, and show that there exist finitely many physically meaningful resonances in the fourth quadrant. The second part of this work is for the quantitative investigation of the enhancement of the scattered field and the cross sections when the dielectric resonance occurs. In doing so, we develop a novel multipole radiation framework that directly separates the electric and magnetic multipole moments and allows us to clearly see their orders of magnitude and blow-up rates. We show that at the dielectric subwavelength resonant frequencies, the nanoparticles with high refractive indices behave like the coupling of an electric dipole with a resonant magnetic dipole. By using the spherical multipole expansion, we further show how to explicitly calculate the quasi-static dielectric resonance and the approximate scattered field which helps validate our general results and formulas.

Introduction

In the past decades, the plasmonic resonant nanostructures with localized surface plasmons have been extensively studied in nanophotonics and used as the building blocks to make novel optical devices and complex metamaterials [41]. The plasmonic materials that are usually made of metals may have the negative real permittivity in the visible spectral range and can be strongly coupled with the electric part of the incident field, inducing the light enhancement and confinement [33, 17]. It has been mathematically demonstrated that the quasi-static plasmonic resonance can be treated as an eigenvalue problem of the Neumann-Poincaré operator [2, 8, 7, 13, 14]. However, the metal structures suffer from a significant heat dissipation caused by the imaginary part of the electric permittivity and the anisotropic magnetic response. These physical properties severely limit the efficiency and functionality of the optical plasmonic nanodevice, which motivate the search for the alternatives to the metal subwavelength resonators [18, 27].

There is an immensely increasing interest in recent years on the study of the dielectric and semiconductor resonators with high refractive indices. These dielectric resonant structures have low absorbing properties and isotropic magnetic responses, making it possible to complement the plasmonic elements in many potential applications [36, 35]. In particular, the silicon nanoparticle has emerged as a popular choice of the subwavelength resonator for designing the dielectric metamaterials because of its high electric permittivity and very low dissipative loss [42]. It was observed experimentally [27, 36] that for an individual spherical silicon nanoparticle, when the wavelength inside the particle is comparable to its diameter, the electric and magnetic dipole radiations can have comparable strengths, and the magnetic dipole resonance can be excited in the visible region. Nevertheless, compared to considerable evidence from engineering and physics literature, the mathematical understanding of the origin of the dielectric resonance and the mechanism underlying the strong magnetic response is still limited, apart from the case of spherical nanoparticles which has been well-illustrated and studied by the Mie scattering theory [43]. In [1], the authors considered the Helmholtz equation and used asymptotic analysis to characterize the quasi-static dielectric resonant frequencies for

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the high contrast nanoparticles of arbitrary shape and obtained the corresponding first-order corrections. In [37], the case of the nonlinear scatterers of the Kerr type was investigated and the corresponding asymptotic formulas for the resonances were derived.

This work is devoted to modeling the EM scattering of strongly coupled nanoparticles with high refractive indices by using the full Maxwell system. We shall provide a solid mathematical framework generalizing the existing ones for the scalar case [37, 1, 20] to analyze the dielectric resonances and the scattered field enhancement. The new results may help confirm the aforementioned physical effects that are unique to the electromagnetic wave rigorously from the mathematical point of view.

For a general medium scattering problem, the dielectric resonance may appear under the name of scattering resonance. They are mathematically formulated as the poles of the meromorphic continuation of the scattering resolvent (Green's function) to the whole complex plane, which play crucial roles in many areas of mathematics and physics since their real parts can capture the rates of oscillation of waves while their imaginary parts capture the decay rates [45]. It is generally very hard to obtain the full knowledge of the distribution of all resonances for a system, but, as we shall demonstrate, it is possible in the quasi-static and high contrast regime.

If we represent the resolvent in terms of the Lippmann-Schwinger integral equation, the scattering resonance problem can be view as a nonlinear eigenvalue problem [31, 37]. For our problem, the nonlinear eigenproblem that is associated with the integral operator $\mathcal{T}_D^\omega$ is of central importance; see Definition 2.2. In [23, 24, 25], the authors gave a complete characterization of the essential spectrum of various integral operators arising from the EM scattering problems for both smooth and non-smooth (Lipschitz) domains. Along this direction, we showed in [5] that the spectrum of $\mathcal{T}_D^\omega$ is a disjoint union of the essential spectrum on the real axis and the eigenvalues of finite type in the upper-half plane with the essential spectrum being its possible accumulation points, and derived the pole-pencil decomposition of the resolvent $(\lambda - \mathcal{T}_D^\omega)^{-1}$ near its poles. We emphasize that all the aforementioned results concern the linear eigenproblem of the operator $\mathcal{T}_D^\omega$ and the corresponding research is far from being complete. Here we still consider the analytic family $(\lambda - \mathcal{T}_D^\omega)^{-1}$ but with ω being a complex variable, and hence we are facing a nonlinear eigenproblem. By the known spectral results of $\mathcal{T}_D^\omega$, we can readily conclude from the analytic Fredholm theory that there are at most finitely many possible dielectric resonances in the quasi-static regime for a given contrast parameter (cf. Theorem 3.8). Nevertheless, it is highly nontrivial to perform the asymptotic expansion for $\mathcal{T}_D^\omega$ with respect to small ω in an analogous manner to the scalar case [37, 1], in order to determine the limiting eigenvalue problem and further calculate the quasi-static resonances and their first-order corrections. The main difficulty comes from the fact that the leading-order part of $\mathcal{T}_D^\omega$ has an infinite-dimensional kernel consisting of magnetostatic fields (cf. Lemma 3.5). To cope with this technical issue, we shall utilize a Helmholtz decomposition for divergence-free functions to reformulate the considered operator-valued analytic function as a spectrally equivalent analytic family of operator matrices (cf. (3.15)). Then we perform standard asymptotic analysis to derive the a priori estimates for the subwavelength resonances and the corresponding resonant modes. We show that the first-order correction for a quasi-static resonance is zero and the quasi-static resonant mode is transverse electric; see Theorems 3.11 and 3.12. This is exactly the origin of the strong magnetic responses of the high contrast nanoparticles under visible light illumination [27]. The remaining question is whether the dielectric subwavelength resonances exist for a given small characteristic size δ and high contrast τ. The answer depends on the region we search for the resonances; see Remark 3.18. When the contrast τ is high in terms of a certain order of δ^{-1} (cf. (3.36)), which is a quantitative version of the experimentally observed resonance condition (cf. [36]) that the wavelength inside the particles is comparable to the size of particles, we are able to apply the Gohberg-Sigal theory (generalized argument principle and generalized Rouché's theorem) to ensure the existence of dielectric resonances; see Theorem 3.16.

To understand the structure of the scattering amplitude, we propose a new approach based on a Helmholtz decomposition for divergence-free functions to systematically investigate the multipolar response of nanoparticles of arbitrary shape. This is closely related to the classical Cartesian multipole moment expansion [32], but very different in spirit; see Remark 4.3. The main disadvantage of the classical approach is that one has to separate the electric and magnetic moments for each term in the Taylor expansion (cf. (4.2)) of the scattering amplitude by using different and complicated algebraic relations. Our new approach takes the advantage of the Helmholtz decomposition which helps us to disentangle the physically different moments with electric and magnetic nature from the beginning and can be applied to all the orders in the same manner. Compared with the known result in the classical electrodynamics that the subwavelength nanoparticles typically behave like an electric dipole that scatters light symmetrically [26], we can rigorously show (cf. Theorems 4.9 and 4.12) that in the high contrast regime, the magnetic multipole radiation provides a dominant contribution in the scattered amplitude and the scattering cross section when the incident frequency ω is near the resonance. This is realized by means of a new class of electric and magnetic multipole moments (cf. Definition 4.2) and the pole-pencil expansion of the leading-order operator of the Lippmann-Schwinger equation.

In particular, in the quasi-static limit, the nanoparticles with high refractive indices can be approximated by the coupling of an electric dipole with a magnetic dipole, but it is the magnetic dipole that is resonant at the resonant frequency and the blow-up of the electric dipole only becomes apparent at high orders; see Theorem 4.11. We shall also present an explicit calculation in the case of a single spherical nanoparticle, which serves to validate our general results for particles of arbitrary shape. It is interesting to note that for the case of a spherical domain, the quasi-static resonances can be characterized by the zeros of spherical Bessel functions.

The paper is organized as follows. In Section 2, we formally introduce the EM scattering problem by nanoparticles with high refractive indices and the dielectric subwavelength resonances. Sections 3 and 4 are devoted to the resonance analysis and far-field analysis respectively. The explicit calculations for the special spherical domain that complements our general framework are provided in Section 5. We end this paper with some concluding remarks and discussions.

In the remaining of this work, for a vector $x \in \mathbb{R}^3$, we denote its polar form by $(|x|, \hat{x})$ with $\hat{x} := x/|x| \in S$. S is the two dimensional unit sphere in $\mathbb{R}^3$, and S_r is the sphere with radius r centered at the origin. We also need the tensor product operation $\otimes$ of tensors. In particular, given two vectors $u \in \mathbb{R}^n$ and $v \in \mathbb{R}^m$, $u \otimes v$ is a $n \times m$ matrix given by $(u \otimes v)_{ij} = u_i v_j$. And we always let vector operators act on matrices column by column. For a Banach space X and its topological dual X', we introduce the dual pairing $\langle l, x \rangle_X := l(x)$. We reserve the notation $(\cdot,\cdot)_H$ and $\oplus$ for the inner product and the orthogonal direct sum for a Hilbert space H, respectively.

Problem setting and definition

In this section, we introduce the EM scattering problem by a system of strongly coupled nanoparticles with high refractive indices embedded in the free space, and mathematically define the dielectric subwavelength resonance.

Suppose D is a bounded smooth open set that is occupied by a set of dielectric nanoparticles with a characteristic size δ. By taking the center of the particle system as the origin of the coordinate system, we can choose a reference bounded open set B, containing the origin, with a smooth boundary ∂B and an the exterior unit normal vector ν such that $D = \delta B$. We assume that B has m connected components denoted by B_i, $1 \le i \le m$ $(m \ge 1)$, i.e., $B = \cup_{i=1}^m B_i$ to represent that the particle system has m nanoparticles. We like to point out that $B^c := \mathbb{R}^3 \backslash \bar{B}$ may also be a disconnected open set with connected components B_j^c, $0 \le j \le n$ $(n \ge 0)$, i.e., $B^c = \cup_{j=0}^n B_j^c$, where B_0^c is the unbounded one.

We denote by ε_0 the electric permittivity, by μ_0 the magnetic permeability, and by $c_0 = (\varepsilon_0\mu_0)^{-1/2}$ the speed of EM wave in the free space. Then the physical properties of the nanoparticles can be characterized by the relative electric permittivity ε_r and magnetic permeability μ_r. By choosing the appropriate physical units, we let ε_0 and μ_0 be the constant. We also let the nanoparticle be non-magnetic, i.e., $\mu_r = 1$, and ε_r is a constant. For our subsequent analysis, we introduce a dimensionless contrast parameter $\tau := \varepsilon_r - 1$ and assume

$$\mathfrak{Re}\tau \gg 1 \text{ and } \mathfrak{Im}\tau \ge 0\,, \tag{2.1}$$

throughout this work; see Figure A.1 for the possible values of τ (or ε_r) of silicon and the rationality of the above assumption. Then the refractive index $n(x)$ in $\mathbb{R}^3$ is given by

$$n(x) = \sqrt{\varepsilon_r \chi_D(x) + \chi_{\mathbb{R}^3\backslash D}(x)} = \sqrt{\tau\chi_D(x) + 1}\,, \quad x \in \mathbb{R}^3\backslash\partial D\,,$$

where χ_D and $\chi_{\mathbb{R}^3\backslash D}$ are the characteristic functions of the open sets D and $\mathbb{R}^3\backslash\bar{D}$ respectively. Here and throughout, we consider the principal branch of $\sqrt{\cdot}$ on the slit plane $\mathbb{C}\backslash(-\infty, 0]$.

Let (E^i, H^i) be the incident plane wave:

$$E^i = \mathbf{E}_0^i e^{i\omega\mathbf{d}\cdot x}, \quad H^i = \frac{1}{i\omega}\nabla \times E^i = \mathbf{d} \times \mathbf{E}_0^i e^{i\omega\mathbf{d}\cdot x}\,, \tag{2.2}$$

with the complex frequency ω, the unit incident direction $\mathbf{d} \in S$, and the unit polarization vector $\mathbf{E}_0^i \in S$ such that $\mathbf{E}_0^i \cdot \mathbf{d} = 0$. In this work, we focus on the quasi-static regime:

$$\left\{\omega \in \mathbb{C}\,;\ |\omega| \ll 2\pi\delta^{-1}\right\}\,, \tag{2.3}$$

namely, the wavelength in the free space is much lager than the characteristic size of the particle. With these notions, the EM scattering problem, by the subwavelength nanoparticles with high refractive indices, can be modelled by

$$\begin{cases} \nabla \times E = i\omega H & \text{in } \mathbb{R}^3\backslash\partial D\,, \\ \nabla \times H = -i\omega n^2 E & \text{in } \mathbb{R}^3\backslash\partial D\,, \\ [\nu \times E] = 0\,,\ [\nu \times H] = 0 & \text{on } \partial D\,, \end{cases} \tag{2.4}$$

where $[\cdot] = \cdot|_- - \cdot|_+$ is the jump across the boundary and the subscripts $\pm$ denote the limits from outside and inside D respectively. The system (2.4) is further complemented by the outgoing Silver-Müller radiation condition for the scattered wave $(E^s, H^s) := (E - E^i, H - H^i)$:

$$\lim_{|x|\to\infty} |x| \cdot (H^s \times \hat{x} - E^s) = 0\,,$$

for real frequency ω. When ω is complex, one may specify the outgoing condition by the analytic continuation of the scattering resolvent from the real axis [31] or, equivalently, let it be inherited from the Green's function [37]. Eliminating the magnetic field H from the system (2.4), we can reformulate problem (2.4) as a second-order equation:

$$\nabla \times \nabla \times E^s - \omega^2 E^s = \omega^2 \tau \chi_D E \,, \tag{2.5}$$

with the transmission boundary conditions: $[\nu \times E^s] = 0$ and $[\nu \times \nabla \times E^s] = 0$ on ∂D, and the outgoing radiation condition for E^s at infinity.

We next use the Lippmann-Schwinger representation formula to work out the relations between the various parameters in different regimes and the scattered field E^s. To do so, let us first introduce the fundamental solution:

$$g(x, \omega) = \frac{e^{i\omega|x|}}{4\pi|x|}, \quad \omega \in \mathbb{C} \,,$$

to the Helmholtz operator $-\Delta - \omega^2$ in the free space and the associated vector potential $\mathcal{K}_D^\omega : L^2(D, \mathbb{R}^3) \to H^2_{loc}(\mathbb{R}^3, \mathbb{R}^3)$:

$$\mathcal{K}_D^\omega[\varphi] = \int_D g(x - y, \omega)\varphi(y) dy \quad \text{for } x \in \mathbb{R}^3 \,. \tag{2.6}$$

Then we can introduce a key volume integral operator corresponding the EM scattering problem.

Definition 2.1. *The operator* $\mathcal{T}_D^\omega : L^2(D, \mathbb{R}^3) \longrightarrow H_{loc}(\mathrm{curl}, \mathbb{R}^3)$ *is given by*

$$\mathcal{T}_D^\omega[\varphi](x) = (\omega^2 + \nabla \mathrm{div})\mathcal{K}_D^\omega[\varphi](x) \quad \textit{for } x \in \mathbb{R}^3 \textit{ and } \varphi \in L^2(D, \mathbb{R}^3) \,. \tag{2.7}$$

When restricted to D*,* $\mathcal{T}_D^\omega$ *is viewed as an operator:*

$$\mathcal{T}_D^\omega : L^2(D, \mathbb{R}^3) \to L^2(D, \mathbb{R}^3) \,, \ \textit{or } \mathcal{T}_D^\omega : H(\mathrm{div}0, D) \to H(\mathrm{div}0, D) \,.$$

Using $\mathcal{T}_D^\omega$, we can readily write the Lippmann-Schwinger equation for the system (2.5) as

$$E^s(x) = E(x) - E^i(x) = \tau \mathcal{T}_D^\omega[E](x) \,, \quad x \in \mathbb{R}^3 \,, \tag{2.8}$$

which directly gives us the electric field inside D:

$$E(x) = (1 - \tau \mathcal{T}_D^\omega)^{-1}[E^i] \,, \quad x \in D \tag{2.9}$$

if $1 - \tau\mathcal{T}_D^\omega$ is invertible (cf. [5, Theorem 3.2]), and the scattered field outside D:

$$E^s(x) = \tau \mathcal{T}_D^\omega[E](x) \,, \quad x \in \mathbb{R}^3 \backslash \bar{D} \,. \tag{2.10}$$

As indicated in the introduction, the scattering resonance problem for the nanoparticles with high refractive indices can be mathematically treated as a nonlinear eigenvalue problem, that is, find the complex frequencies $\omega(\tau, D) \in \mathbb{C}$ such that there exists a nontrivial field $E \in L^2(D, \mathbb{R}^3)$ satisfying

$$(1 - \tau \mathcal{T}_D^\omega)E = 0 \,. \tag{2.11}$$

Note that we are only interested in those resonant frequencies that lie in the quasi-static regime (2.3). Via the density argument and the integration by parts, we have $\mathrm{div}\mathcal{T}_D^\omega[E] = -\mathrm{div}E$. This fact, together with the assumption (2.1) for τ, yields that the eigenfunction in (2.11) must be divergence-free, by taking the divergence on both sides of (2.11). Therefore, we are led to the following formal definition for the dielectric subwavelength resonance.

Definition 2.2. ω *is said to be a dielectric subwavelength resonance if it holds that* $|\omega| \ll 2\pi/\delta$ *and*

$$\tau^{-1} \in \sigma_p(\mathcal{T}_D^\omega) \,, \quad \textit{equivalently} \,, \ \tau^{-1} \in \sigma_p(\mathcal{T}_B^{\delta\omega}) \,, \tag{$\mathscr{P}$}$$

for $\mathcal{T}_D^\omega : H(\mathrm{div}0, B) \to H(\mathrm{div}0, B)$ *defined by* (2.7)*.*

In the above definition, we have used the scaling property that can be easily checked:

$$\mathcal{T}_D^\omega[E](x) = \mathcal{T}_D^\omega[E](\delta\widetilde{x}) = \mathcal{T}_B^{\delta\omega}[\widetilde{E}](\widetilde{x}) \,, \quad \text{with } x = \delta\widetilde{x} \,, \ \widetilde{E}(\widetilde{x}) := E(\delta\widetilde{x}) \,.$$

Remark 2.3. *The eigenvalue problem* ($\mathscr{P}$) *is equivalent to a transmission eigenvalue problem: find* ω *in the quasi-static regime* (2.3) *such that there exists a nontrivial* $E \in H_{loc}(\mathrm{curl}, \mathbb{R}^3)$ *solving the equation:*

$$\nabla \times \nabla \times E(x) - \delta^2\omega^2(\tau\chi_B + 1)E(x) = 0 \quad \textit{in } \mathbb{R}^3 \,,$$

with an appropriate boundary condition at infinity; see [5, Lemma 3.1]. Then the nontrivial solution E *automatically satisfies the following transmission boundary condition for its normal trace:*

$$(\tau + 1)E|_- \cdot \nu = E|_+ \cdot \nu \,.$$

This suggests that when the contrast parameter τ *is very high, the normal trace of the resonant field* E *inside the nanoparticles shall almost vanish, namely,* $E|_- \cdot \nu \approx 0$*. This simple but crucial observation will be rigorously verified in the next section and plays a key role therein.*

Dielectric subwavelength resonance

In this section, we first derive the a priori estimates for the dielectric subwavelength resonances and the associated eigenfunctions. We then address the existence of subwavelength resonances by using the Gohberg-Sigal theory when the contrast τ is high in terms of a certain order of δ^{-1}. As it will be revealed, there always exist finitely many dielectric resonant frequencies in the fourth quadrant near some characteristic points on a ray starting at the origin, when δ is small enough.

Let us prepare some analysis tools and recall some known related spectral results before proving the main results of this section. To start with, we give the asymptotics of the operators $\mathcal{K}_B^{\delta\omega}$ and $\mathcal{T}_B^{\delta\omega}$ in the following lemma by using the Taylor expansion of the Green's function $g(x, \delta\omega)$:

$$g(x,\delta\omega) = \sum_{n=0}^{\infty} (\delta\omega)^n g_n(x) \quad \text{with } g_n(x) = \frac{i^n |x|^{n-1}}{4\pi n!}\,. \tag{3.1}$$

Lemma 3.1. *It holds for the bounded linear operators $\mathcal{K}_B^{\delta\omega}$ and $\mathcal{T}_B^{\delta\omega}$ on $L^2(B, \mathbb{R}^3)$ that*

$$\mathcal{K}_B^{\delta\omega} = \sum_{n=0}^{\infty} (\delta\omega)^n \mathcal{K}_{B,n}\,, \quad \mathcal{T}_B^{\delta\omega} = \sum_{n=0}^{\infty} (\delta\omega)^n \mathcal{T}_{B,n}\,,$$

where the series converge in the operator norm and both $\mathcal{K}_B^{\delta\omega}$ and $\mathcal{T}_B^{\delta\omega}$ are analytic in $\delta\omega$. The operators $\mathcal{K}_{B,n}, n \geq 0$ are given by

$$\mathcal{K}_{B,n}[\varphi] = \int_B g_n(x-y)\varphi(y)dy\,,$$

where g_n are given in (3.1)*, while the operators $\mathcal{T}_{B,n}, n \geq 0$ are given by*

$$\begin{aligned} &\mathcal{T}_{B,0}[\varphi] = \nabla \mathrm{div} \int_B \frac{1}{4\pi|x-y|}\varphi(y)dy\,, \quad \mathcal{T}_{B,1}[\varphi] = i\nabla\mathrm{div}\frac{1}{4\pi}\int_B \varphi(y)dy = 0\,, \\ &\mathcal{T}_{B,n}[\varphi] = \mathcal{K}_{B,n-2}[\varphi] + \nabla\mathrm{div}\mathcal{K}_{B,n}[\varphi]\,, \quad n \geq 2\,. \end{aligned} \tag{3.2}$$

For the case $n = 0$, we shall denote $\mathcal{T}_{B,0}$ and $\mathcal{K}_{B,0}$ by $\mathcal{T}_B$ and $\mathcal{K}_B$ for simplicity of notation. We then have the asymptotic expansion of the operator $1 - \tau\mathcal{T}_B^{\delta\omega}$ from the above lemma:

$$1 - \tau\mathcal{T}_B^{\delta\omega} = 1 - \tau\mathcal{T}_B - \tau(\delta\omega)^2\mathcal{T}_{B,2} - \tau(\delta\omega)^3\mathcal{T}_{B,3} + O(\tau(\delta\omega)^4) \quad \text{as } \delta \to 0\,. \tag{3.3}$$

Here we deliberately express the high contrast parameter τ explicitly in the remainder term to indicate the possible implicit relation between τ and δ that should be met for the excitation of the dielectric subwavelength resonance, since the relative order of the rates of τ^{-1} and δ approaching zero can essentially change the asymptotic behavior of $1 - \tau\mathcal{T}_B^{\delta\omega}$ in (3.3).

As it was stated in the Introduction, there is a major technical difficulty that the leading-order part of $\mathcal{T}_B^{\delta\omega}$ has an infinite-dimensional kernel. Instead of performing the perturbation argument based on (3.3) to analyze the dielectric resonances directly, we shall first use the L^2-Helmholtz decomposition for divergence-free functions to transform the operator $\mathcal{T}_B^{\delta\omega}$ into an operator matrix and then conduct the asymptotic analysis. This allows us to see the clear asymptotic properties of $\mathcal{T}_B^{\delta\omega}$ on different components of an L^2-vector field and the impact of the parameters δ and τ. We adopted the same technique earlier in [5] for the spectral analysis of the integral operator $\mathcal{T}_D^{\omega}$ beyond the quasi-static regime.

We now briefly summarize the Helmholtz decomposition that we studied in [5, Appendix A] and review the definitions of various related operators for our later use.

Proposition 3.2. *All divergence-free vector fields from $H(\mathrm{div}0, B)$ have the L^2-orthogonal decomposition:*

$$H(\mathrm{div}0, B) = H_0(\mathrm{div}0, B) \oplus W = \mathrm{curl}X_N^0(B) \oplus K_T(B) \oplus W\,, \tag{3.4}$$

where W is the space consisting of the gradients of harmonic H^1-functions, the space $X_N^0(B)$ is given by

$$X_N^0(B) = H_0(\mathrm{curl}, B) \bigcap H(\mathrm{div}0, B)\,,$$

and $K_T(B)$ is the tangential cohomology space with a dimension being equal to the genus of B, defined by

$$K_T(B) = \{u \in H_0(\mathrm{div}, B)\,;\, \nabla \times u = 0,\ \mathrm{div}u = 0 \text{ in } B\}.$$

A field ϕ in $\mathrm{curl}X_N^0(B)$ can uniquely determine a potential A in the quotient space $\widetilde{X}_N^0(B) := X_N^0(B)/K_N(B)$ such that $\phi = \nabla \times A$, where $K_N(B) := \{u \in H_0(\mathrm{curl}, B)\,;\, \nabla \times u = 0,\ \mathrm{div}u = 0 \text{ in } B\}$ is the normal cohomology space.

We further introduce the Neumann Poincaré operator $\mathcal{K}^*_{\partial B}: H^{-1/2}(\partial B) \to H^{-1/2}(\partial B)$ and the single layer potential $\mathcal{S}_{\partial B}: H^{-1/2}(\partial B) \to H^{1/2}(\partial B)$ by

$$\mathcal{K}^*_{\partial B}[\varphi] = \int_{\partial B} \frac{\partial}{\partial \nu_x} \frac{1}{4\pi|x-y|}\varphi(y)d\sigma(y) \quad \text{and} \quad \mathcal{S}_{\partial B}[\varphi] = \int_{\partial B} \frac{1}{4\pi|x-y|}\varphi(y)d\sigma(y)\,, \tag{3.5}$$

respectively. Then the following normal trace formula for $\nabla \mathcal{S}_{\partial B}$ is well-known [3]:

$$\frac{\partial}{\partial \nu}\mathcal{S}_{\partial B}[\varphi]_{\pm} = (\mp\frac{1}{2} + \mathcal{K}^*_{\partial B})[\varphi]\,, \quad \varphi \in H^{-\frac{1}{2}}(\partial B)\,. \tag{3.6}$$

We shall often need the properties of the traces of functions in $H(\mathrm{div}, B)$. For this, we denote by $\gamma_n \varphi = \nu \cdot \varphi$ the normal trace mapping for all $\varphi \in H(\mathrm{div}, B)$, and by $H^{-1/2}_{00}(\partial B)$ the subspace of $H^{-1/2}(\partial B)$ consisting of the elements with the mean zero on the boundary of each of the connected components of B:

$$H^{-\frac{1}{2}}_{00}(\partial B) = \{u \in H^{-\frac{1}{2}}(\partial B)\,;\ \int_{\partial B_i} u d\sigma = 0\,,\ \text{for } 1 \le i \le m\}\,.$$

When γ_n is restricted on the space W (cf.(3.4)), denoted by $\widetilde{\gamma}_n$, we have the following results.

Lemma 3.3. *$\widetilde{\gamma}_n$ is an isomorphism from W to $H^{-1/2}_{00}(\partial B)$, and $\widetilde{\gamma}_n^{-1}[\phi]$ can be represented by the layer potential $\nabla \mathcal{S}_{\partial B}(\frac{1}{2} + \mathcal{K}^*_{\partial B})^{-1}[\phi]$, which is the gradient of a solution u to the interior Neumann problem:*

$$\Delta u = 0 \text{ in } B\,, \quad \frac{\partial u}{\partial \nu} = \phi \text{ on } \partial B\,. \tag{3.7}$$

The spectral properties of the leading-order operator $\mathcal{T}_B$ in the asymptotics of $\mathcal{T}^{\delta\omega}_B$ was clearly characterized in [24, Theorem 3.2]; see also the earlier work [29] where the variational framework was used. We shall give an improved variant of the existing results in [24], but with more desired properties for our purpose here, based on the following lemma about the Neumann Poincaré operator [3].

Lemma 3.4. *For the compact operator $\mathcal{K}^*_{\partial B}$ defined as above, we have $\sigma(\mathcal{K}^*_{\partial B}) \subset [-\frac{1}{2}, \frac{1}{2}]$ with*

$$\dim\ker\big(\frac{1}{2} + \mathcal{K}^*_{\partial B}\big) = m\,, \quad \dim\ker\big(-\frac{1}{2} + \mathcal{K}^*_{\partial B}\big) = n\,.$$

Moreover, $H^{-1/2}_{00}(\partial B)$ is an invariant subspace of $\mathcal{K}^*_{\partial B}$, and $\frac{1}{2} + \mathcal{K}^*_{\partial B}$ is invertible on $H^{-1/2}_{00}(\partial B)$.

Combining this lemma with Lemma 3.3 and [24, Theorem 3.2], we arrive at the following results.

Proposition 3.5. *$\mathcal{T}_B$ is self-adjoint with W and $H_0(\mathrm{div}0, B)$ being its invariant subspaces. $\mathcal{T}_B$ vanishes in $H_0(\mathrm{div}0, B)$, and has the representation that $\mathcal{T}_B[\cdot] = -\widetilde{\gamma}_n^{-1}(\frac{1}{2} + \mathcal{K}^*_{\partial B})\widetilde{\gamma}_n[\cdot]$ in W. The spectrum of $\mathcal{T}_B|_W$ is contained in the range $[-1, 0)$, i.e., $\sigma(\mathcal{T}_B|_W) \subset [-1, 0)$. Furthermore, we know that $-\frac{1}{2}$ is the only possible accumulation point of $\sigma(\mathcal{T}_B)$, and*

$$\dim\ker(\mathcal{T}_B|_W) = 0\,, \quad \dim\ker(1 + \mathcal{T}_B) = \dim\ker(1 + \mathcal{T}_B|_W) = n\,.$$

From the above proposition and Lemma 3.3, we see that $\mathcal{T}_B|_W$ is isomorphic with a shifted Neumann Poincaré operator, and invertible on W with the following layer potential representation for its inverse:

$$(\mathcal{T}_B|_W)^{-1}[\varphi] = -\nabla \mathcal{S}_{\partial B}(\frac{1}{2} + \mathcal{K}^*_{\partial B})^{-2}[\nu \cdot \varphi]\,, \quad \varphi \in W\,,$$

with the explicit expression of the operator norm that is of order one:

$$\big\|(\mathcal{T}_B|_W)^{-1}\big\| = \frac{1}{\min_{\lambda \in \sigma(\mathcal{T}_B|_W)} |\lambda|}\,. \tag{3.8}$$

The above connection between the integral operator $\mathcal{T}_B$ and the Neumann Poincaré operator $\mathcal{K}^*_{\partial B}$ was exploited in [6] to develop a new approach for analyzing the plasmonic resonances. From the physical perspective, W corresponds to the electric component of the EM fields (see the discussion below), and hence it is the strong coupling between the metallic nanoparticles and the electric component of the incident wave that induces plasmonic resonances [41, 27].

By contrast, for the dielectric nanoparticles with high refractive indices, we claim that the dielectric subwavelength resonance is excited by the magnetic component of the incident EM fields (cf. Theorems 3.10 and 3.16). To give a glimpse of this important difference between the plasmonic resonance and the dielectric resonance, we recall from the Helmholtz decomposition (3.4) that for an open set B with trivial topology, $K_T(B)$ is a null space and then a divergence-free vector field $\psi \in H(\mathrm{div}0, B)$ has the decomposition:

$$\psi = \nabla \times A + \nabla \phi , \quad A \in \widetilde{X}_N^0(B) , \quad \phi \in H^1(B) . \tag{3.9}$$

These two components match exactly the forms of the electrostatic and magnetostatic fields, with A being the so-called magnetic vector potential and ϕ being the electric scalar potential. Thus, the orthogonal projections associated with the decomposition (3.4):

$$\mathbb{P}_{\mathrm{d}} : H(\mathrm{div}0, B) \to H_0(\mathrm{div}0, B) , \quad \mathbb{P}_{\mathrm{w}} : H(\mathrm{div}0, B) \to W$$

may be regarded as the projections from a divergence-free vector field to its magnetic and electric component respectively. We shall see that it is the space $H_0(\mathrm{div}0, B)$ (the kernel of $\mathcal{T}_B$) that is responsible for the excitation of the dielectric resonance and support the resonant modes in the quasi-static limit.

For the sake of simplicity, we use the shorthand notations $\mathcal{T}^{\mathrm{s,t}}$ for $\mathbb{P}_{\mathrm{s}}\mathcal{T}\mathbb{P}_{\mathrm{t}}$ for a bounded linear operator $\mathcal{T}$ on $H(\mathrm{div}0, B)$ and $\mathrm{s}, \mathrm{t} = \mathrm{d}, \mathrm{w}$ in the remaining representation. For operators $\mathcal{T}_{B,n} (n \geq 2)$, although the space $H_0(\mathrm{div}0, B)$ (unlike the case $n = 0$) is not an invariant space anymore, we have the useful relation:

$$(\phi, \mathcal{T}_{B,n}[\varphi])_{L^2(B)}(B) = (\phi, (\mathcal{K}_{B,n-2} + \nabla \mathrm{div} \mathcal{K}_{B,n})[\varphi])_{L^2(B)} = (\phi, \mathcal{K}_{B,n-2}[\varphi])_{L^2(B)} \tag{3.10}$$

for $\phi \in L^2(B, \mathbb{R}^3)$, $\varphi \in H_0(\mathrm{div}0, B)$, or $\varphi \in L^2(B, \mathbb{R}^3)$, $\phi \in H_0(\mathrm{div}0, B)$, by using the definition of $\mathcal{T}_{B,n}$ in (3.2) and an integration by parts. The above relation enables us to write

$$\mathcal{K}_{B,n-2}^{\mathrm{s,t}} = \mathbb{P}_s \mathcal{T}_{B,n} \mathbb{P}_t \quad \text{for } \mathrm{s}, \mathrm{t} = \mathrm{d}, \mathrm{w} \text{ except } \mathrm{s}, \mathrm{t} = \mathrm{w} . \tag{3.11}$$

In particular, for the case $n = 2$, we have the following useful spectral result for the operator $\mathcal{K}_B^{\mathrm{d,d}} = \mathbb{P}_{\mathrm{d}} \mathcal{T}_{B,2} \mathbb{P}_{\mathrm{d}}$ by the standard spectral theory of compact self-adjoint operators.

Proposition 3.6. $\mathcal{K}_B^{\mathrm{d,d}}$ *is a compact self-adjoint operator from* $H_0(\mathrm{div}0, B)$ *to* $H_0(\mathrm{div}0, B)$ *with the following spectral resolution:*

$$\mathcal{K}_B^{\mathrm{d,d}}[E] = \sum_{n=0}^{\infty} \lambda_n (E, E_n)_{L^2(B)} E_n , \quad E \in H_0(\mathrm{div}0, B) ,$$

where $\lambda_0 \geq \lambda_1 \geq ... \geq \lambda_n \cdots > 0$ *are the eigenvalues of* $\mathcal{K}_B^{\mathrm{d,d}}$*, counted with their multiplicities, with* 0 *as the only possible accumulation point, and* $\{E_n\}_{n \geq 0}$ *consists of a complete orthogonal normalized system in* $H_0(\mathrm{div}0, B)$*.*

It is worth mentioning that in the above proposition, we conclude that $0 \notin \sigma_p(\mathcal{K}_B^{\mathrm{d,d}})$ and $\mathcal{K}_B^{\mathrm{d,d}}$ is positive semidefinite, which does not directly follow from the standard spectral theory. The first point will be observed later in the proof of Proposition 5.1, while the second point follows from the following fact that

$$(u, \mathcal{K}_B[u])_{L^2(B)} = \lim_{\eta \to 0^+} (u, \mathcal{K}_B^{i\eta}[u])_{L^2(B)} = \lim_{\eta \to 0^+} (\mathcal{F}[u\chi_B], \frac{1}{4\pi^2 |\xi|^2 + \eta^2} \mathcal{F}[u\chi_B])_{L^2(\mathbb{R}^3)} \geq 0 , \quad u \in L^2(B) ,$$

where η is a small real parameter and $\mathcal{F}$ denotes the L^2-Fourier transform [28].

For the case $n = 3$, we have the following useful result from (3.10) and (3.11):

$$\mathcal{K}_{B,1}^{\mathrm{s,t}} = \mathbb{P}_s \mathcal{T}_{B,3} \mathbb{P}_t = 0 \quad \text{for } \mathrm{s}, \mathrm{t} = \mathrm{d}, \mathrm{w} \text{ except } \mathrm{s}, \mathrm{t} = \mathrm{w} , \tag{3.12}$$

by noting

$$\mathcal{K}_{B,1}[\varphi](x) = \frac{i}{4\pi} \int_B \varphi(y) dy ,$$

and making use of the Green's formula:

$$\int_B \varphi(y) dy = - \int_B y \mathrm{div} \varphi(y) dy + \int_{\partial B} \varphi(y) \cdot \nu y d\sigma(y) , \quad \varphi \in H(\mathrm{div}, B) . \tag{3.13}$$

A priori estimate

This subsection aims for the priori information on the location of the dielectric resonance. For ease of exposition, we view $\delta\omega$ in $(\mathscr{P})$ as a whole and define an operator-valued analytic function $\mathcal{A}(\tau, \omega) = \frac{1}{\tau} - \mathcal{T}_B^{\omega}$ on the space $H(\mathrm{div}0, B)$ with the complex variable ω. Then the dielectric subwavelength resonance defined in $(\mathscr{P})$ can be reformulated.

Definition 3.7. ω *is said to be a dielectric subwavelength resonance if* $\omega \in B(0, \delta_0) \subset \mathbb{C}$ *for a given small enough* δ_0*, and is a characteristic value of the analytic function* $\mathcal{A}(\tau, \omega) = \tau^{-1} - \mathcal{T}_B^{\omega}$*, that is, there exists a eigenfunction* $E \in H(\mathrm{div}0, B)$ *such that* $\mathcal{A}(\tau, \omega)E = 0$*.*

We shall analyze the dielectric subwavelength resonances ω according to the above definition. It has been shown in [24, 5] that the essential spectrum of $\mathcal{T}_B^\omega$ for any $\omega \in \mathbb{C}$ is given by

$$\sigma_{ess}(\mathcal{T}_B^\omega) = \{-1, -\frac{1}{2}, 0\}\,.$$

Hence, for a given high contrast τ with (2.1), τ^{-1} will never touch the essential spectrum of $\mathcal{T}_B^\omega$, and we can conclude that $\mathcal{A}(\tau,\omega)$ is an analytic family of Fredholm operators on $H(\mathrm{div}0, B)$. We also observe from Lemma 3.5 that $\mathcal{A}(\tau, 0) = \tau^{-1} - \mathcal{T}_B$ is invertible if the contrast τ has a positive real part. A direct application of the analytic Fredholm theorem [30] gives us the following result.

Theorem 3.8. *For a given contrast τ with* (2.1)*, there exists a discrete set Ω (countable and with no accumulation point in $\mathbb{C}$) consisting of the characteristic values of $\mathcal{A}(\tau,\omega)$ such that $\mathcal{A}(\tau,\omega)$ is invertible for $\omega \in \mathbb{C}\backslash\Omega$. Moreover, $\mathcal{A}(\tau,\omega)^{-1}$ can be extended to a meromorphic function on $\mathbb{C}$ with Ω being the set of poles. For each $\omega \in \Omega$, the Fredholm index* $\mathrm{ind}\mathcal{A}(\tau,\omega)$ *vanishes and the associated eigenspace* $\ker \mathcal{A}(\tau,\omega)$ *is finite-dimensional.*

As a corollary, the analytic function $\mathcal{A}(\tau,\omega)$, when restricted to $B(0,\delta_0) \subset \mathbb{C}$, has at most finitely many characteristic values, i.e., we can only have finitely many possible dielectric resonances for a given δ_0, by Definition 3.7. To further analyze the dielectric resonant frequencies ω, we now write the operator function $\mathcal{A}(\tau,\omega)$ as an analytic family of operator matrices by the Helmholtz decomposition. In contrast to the statement in [5], we provide a more general perspective for this procedure here, by using the concept of global equivalence from [30] . It generalizes the concept of similarity for the linear operator and is applied to a nonlinear eigenproblem.

Definition 3.9. *Suppose U is an open set in $\mathbb{C}$, and $T(\lambda) : X_1 \to Y_1$ and $S(\lambda) : X_2 \to Y_2$ are bounded linear operators acting on Banach spaces for each $\lambda \in U$. The operator-valued functions $T(\cdot)$ and $S(\cdot)$ are called globally equivalent on U if there exist operator-valued analytic functions $P : U \to \mathcal{L}(X_1, X_2)$ and $Q : U \to \mathcal{L}(Y_2, Y_1)$, which are invertible for each $\lambda \in U$, such that*

$$T(\lambda) = P(\lambda)S(\lambda)Q(\lambda), \quad \lambda \in U\,.$$

We readily see from the above definition that if two analytic operator functions are globally equivalent on some open set U, then these two analytic functions must have same characteristic values on U. For our purpose, we introduce the product space corresponding to the orthogonal direct sum (3.4):

$$\mathbb{X} := H_0(\mathrm{div}0, B) \times W\,,$$

with the induced inner product $(\cdot,\cdot)_{\mathbb{X}}$, which is isomorphic with $H(\mathrm{div}0, B)$ via the mapping $\varphi \to [\mathbb{P}_{\mathrm{d}}\varphi, \mathbb{P}_{\mathrm{w}}\varphi]$. We immediately see that $\mathcal{A}(\tau,\omega)$ is globally equivalent to

$$\begin{bmatrix} \mathbb{P}_{\mathrm{d}}\mathcal{A}(\tau,\omega)\mathbb{P}_{\mathrm{d}} & \mathbb{P}_{\mathrm{d}}\mathcal{A}(\tau,\omega)\mathbb{P}_{\mathrm{w}} \\ \mathbb{P}_{\mathrm{w}}\mathcal{A}(\tau,\omega)\mathbb{P}_{\mathrm{d}} & \mathbb{P}_{\mathrm{w}}\mathcal{A}(\tau,\omega)\mathbb{P}_{\mathrm{w}} \end{bmatrix}\,. \tag{3.14}$$

We further transform the system (3.14) to the following one that is also globally equivalent to $\mathcal{A}(\tau,\omega)$:

$$\mathbb{A}(\tau,\omega) := \begin{bmatrix} 1 - \tau\mathbb{P}_{\mathrm{d}}\mathcal{T}_B^\omega\mathbb{P}_{\mathrm{d}} & -\tau\mathbb{P}_{\mathrm{d}}\mathcal{T}_B^\omega\mathbb{P}_{\mathrm{w}} \\ -\mathbb{P}_{\mathrm{w}}\mathcal{T}_B^\omega\mathbb{P}_{\mathrm{d}} & \frac{1}{\tau} - \mathbb{P}_{\mathrm{w}}\mathcal{T}_B^\omega\mathbb{P}_{\mathrm{w}} \end{bmatrix}\,, \tag{3.15}$$

by multiplying the first row of (3.14) by the factor τ.

We remark that the choice of the form of $\mathbb{A}(\tau,\omega)$ is not crucial for the analysis in this section, but as we can see in Section 3.2, the form of $\mathbb{A}(\tau,\omega)$ in (3.15) is the most appropriate one for the argument therein, compared to the form in (3.14) and the other possible choices. We specify it here mainly for the consistency of our presentation.

At first glance, it still seems very difficult to find the characteristic values of the system (3.15) due to its dense structure. However, in the quasi-static and high contrast limit, this system actually has a hidden upper triangular structure; see (3.38). More precisely, $H_0(\mathrm{div}0, B)$ is nearly an invariant subspace of $1 - \tau\mathcal{T}_B^\omega$ for $\delta \ll 1$ and $|\tau| \gg 1$, and the upper left block in (3.14), i.e., $1 - \tau\mathbb{P}_{\mathrm{d}}\mathcal{T}_B^\omega\mathbb{P}_{\mathrm{d}}$ can essentially determine the resonant behavior of the whole system. These observations provide us some intuition for the following arguments, and will become clearer and more rigorous in Section 3.2.

We now state and prove the main results of this section.

Theorem 3.10. *Given a small enough constant δ_0 and a contrast $\tau \in \mathbb{C}$ with* (2.1)*, for any complex characteristic value $\omega(\tau, B)$ of the analytic function $\mathcal{A}(\tau,\omega)$ in $B(0,\delta_0) \subset \mathbb{C}$, there exists an eigenvalue λ_i of $\mathcal{K}_B^{\mathrm{d,d}}$, depending on $\omega(\tau, B)$, such that the following a priori estimate holds,*

$$|\frac{1}{\tau\omega^2} - \lambda_i| \lesssim |\omega| + |\tau|^{-1}\,. \tag{3.16}$$

The dominant part of the associated eigenfunction E^ω is given by $\mathbb{P}_{\mathrm{d}}E^\omega$ in the sense that

$$\mathbb{P}_{\mathrm{w}}E^\omega = E^\omega - \mathbb{P}_{\mathrm{d}}E^\omega = O(\tau^{-1}) + O(\omega^2)\,.$$

Proof. Consider an eigenpair $(\omega, E^\omega) \in \mathbb{C} \times H(\mathrm{div}0, B)$ associated with $\omega(\tau, B)$ that satisfies the equation:

$$\mathbb{A}(\tau,\omega)\begin{bmatrix}\mathbb{P}_{\mathrm{d}}E^\omega \\ \mathbb{P}_{\mathrm{w}}E^\omega\end{bmatrix} = 0 \quad \text{with} \ \|E^\omega\|_{L^2(B)} = 1\,, \tag{3.17}$$

where $\mathbb{A}(\tau,\omega)$ is given in (3.15). We first show that $\mathbb{P}_{\mathrm{w}}E^\omega$ is a higher-order term in terms of the small parameters τ^{-1} and δ. To do so, we apply the asymptotics of $\mathcal{T}_B^\omega$ in Lemma 3.1 to the second equation in (3.17) and see the following estimate:

$$\frac{1}{\tau}\mathbb{P}_{\mathrm{w}}E^\omega - \mathcal{T}_B[\mathbb{P}_{\mathrm{w}}E^\omega] - \omega^2\mathbb{P}_{\mathrm{w}}\mathcal{T}_{B,2}[E^\omega] = O(\omega^3)\,, \tag{3.18}$$

where we have used $\mathcal{T}_B|_{H_0(\mathrm{div}0,B)} = 0$. Since $\mathcal{T}_B$ is invertible on W with (3.8), we obtain by applying $(\mathcal{T}_B|_W)^{-1}$ on both sides of (3.18) that

$$\mathbb{P}_{\mathrm{w}}E^\omega = O(\tau^{-1}) + O(\omega^2)\,, \tag{3.19}$$

which directly indicates that the projection of E^ω on $H_0(\mathrm{div}0, B)$ is of order one, that is, we can find a positive constant $r(\omega,\tau)$ less than one such that

$$r(\omega,\tau) \le \|\mathbb{P}_{\mathrm{d}}E^\omega\|^2_{L^2(B)} \le 1\,, \ \text{and}\ |1 - r(\omega,\tau)| \lesssim |\omega|^4 + |\tau|^{-2}\,. \tag{3.20}$$

We next derive the a priori estimate (3.16) for the resonant frequency ω with the above observations. By the first equation in (3.17) and the fact $\mathcal{T}_B|_{H_0(\mathrm{div}0,B)} = 0$, as well as the asymptotics of $\mathcal{T}_B^\omega$, we can derive

$$\mathbb{P}_{\mathrm{d}}E^\omega - \tau\omega^2\mathcal{K}_B^{\mathrm{d,d}}[E^\omega] - \tau\omega^2\mathcal{K}_B^{\mathrm{d,w}}[E^\omega] = O(\tau\omega^3)\,. \tag{3.21}$$

Moreover, by the estimate (3.19) for $\mathbb{P}_{\mathrm{w}}E^\omega$, we readily see

$$\tau\omega^2\mathcal{K}_B^{\mathrm{d,w}}[E^\omega] = O(\tau\omega^4) + O(\omega^2)\,,$$

which, along with (3.21), further implies

$$\mathbb{P}_{\mathrm{d}}E^\omega - \tau\omega^2\mathcal{K}_B^{\mathrm{d,d}}[E^\omega] = O(\omega^2) + O(\tau\omega^3)\,. \tag{3.22}$$

Then, by using the spectral resolution of $\mathcal{K}_B^{\mathrm{d,d}}$ in Proposition 3.6 and dividing two sides of (3.22) by $\tau\omega^2$, we obtain

$$\sum_{j=0}^{\infty}\Big(\frac{1}{\tau\omega^2} - \lambda_j\Big)(E^\omega, E_j)_{L^2(B)}E_j = O(\tau^{-1}) + O(\omega)\,.$$

Further, an application of the Parseval's identity allows the following estimate:

$$\sum_{j=0}^{\infty}\Big|\Big(\frac{1}{\tau\omega^2} - \lambda_j\Big)(E^\omega, E_j)_{L^2(B)}\Big|^2 = O(\omega^2) + O(\tau^{-2})\,. \tag{3.23}$$

Similarly, by the Parseval's identity, the estimate (3.20) gives us

$$r(\omega,\tau) \le \sum_{j=0}^{\infty}\big|(E^\omega, E_j)_{L^2(B)}\big|^2 \le 1\,.$$

By the above estimate together with (3.20), it readily follows from (3.23) that

$$\inf_j\Big|\frac{1}{\tau\omega^2} - \lambda_j\Big|^2 = O(\omega^2) + O(\tau^{-2})\,. \tag{3.24}$$

Since the sequence $\{\lambda_j\}$ has only 0 as its possible accumulation point, the infimum is actually attainable and then we can conclude that there exists a finite index $i \in \mathbb{N}$ such that

$$\Big|\frac{1}{\tau\omega^2} - \lambda_i\Big| = \inf_j\Big|\frac{1}{\tau\omega^2} - \lambda_j\Big| \lesssim |\omega| + |\tau|^{-1}\,. \tag{3.25}$$

□

By the above Theorem 3.10, we have rigorously confirmed the observation: $E \cdot \nu \approx 0$ in Remark 2.3 in the sense that

$$\|\mathbb{P}_{\mathrm{w}} E^\omega\|_{L^2(B)} \lesssim |\tau|^{-1} + |\omega|^2 \to 0 \quad \text{as } |\omega| \to 0\,,\ |\tau| \to \infty\,.$$

In general, it is unclear that the eigenvalues λ_j of $\mathcal{K}_B^{\mathrm{d,d}}$ satisfying the estimate (3.16) are unique, that is, there may exist many eigenvalues λ_j of $\mathcal{K}_B^{\mathrm{d,d}}$ in a given small neighborhood of $(\tau\omega^2)^{-1}$ with a diameter of order $|\omega| + |\tau|^{-1}$. In this case, the dominant part $\mathbb{P}_{\mathrm{d}} E^\omega$ of the eigenfunction E^ω will be approximated by a mixture of multiple excited resonant modes. To be more specific, let ω be a complex dielectric resonance and r_0 be a constant of order one. We define

$$\Sigma := \big\{\lambda_j \in \sigma(\mathcal{K}_B^{\mathrm{d,d}})\,;\ \big|\frac{1}{\tau\omega^2} - \lambda_j\big| \ge r_0\big\}\,, \tag{3.26}$$

and the corresponding L^2-projection on $H_0(\mathrm{div}0, B)$:

$$\mathbb{P}_\Sigma[\cdot] = \sum_{\lambda_j \in \Sigma} (\cdot, E_j)_{L^2(B)} E_j\,.$$

Then, acting with $\mathbb{P}_\Sigma$ on both sides of (3.22) and using the definition of Σ, a very similar argument to the one for (3.23) gives us

$$\|\mathbb{P}_\Sigma E^\omega\|_{L^2(B)} \lesssim |\omega| + |\tau|^{-1}\,. \tag{3.27}$$

If r_0 can be suitably chosen such that the region $\{\lambda \in \mathbb{C}\,;\ |\lambda - \tau^{-1}\omega^{-2}| < r_0\}$ does not include the origin, there would be only finitely many possible eigenvalues λ_j inside and E^ω can be approximated by a finite sum of the associated resonant modes with an error of order $|\omega| + |\tau|^{-1}$.

The above observations hint that some additional condition should be included, in order to obtain a sharper a priori information for ω and make a clearer and simpler structure of the eigenfunction E^ω. We actually have the following theorems (Theorems 3.11 and 3.12) which tell us that the subwavelength resonance ω and the eigenfunction E^ω can be approximated by $(\lambda_i\tau)^{-1/2}$ and $\mathbb{P}_{\lambda_i} E^\omega$ for some index i with the errors of orders $O(\omega^3)$ and $O(\omega)$ respectively.

For the sake of clarity, we introduce the eigen-projection $\mathbb{P}_\lambda$ for the eigenvalue λ of $\mathcal{K}_B^{\mathrm{d,d}}$:

$$\mathbb{P}_\lambda[\cdot] = \sum_{\lambda_j = \lambda} (\cdot, E_j)_{L^2(B)} E_j\,.$$

Theorem 3.11. *Under the same conditions as in Theorem 3.10, if we further assume*

$$\inf_j \big|\frac{1}{\tau\omega^2} - \lambda_j\big|^2 = \min_{j=0,1,\cdots,N} \big|\frac{1}{\tau\omega^2} - \lambda_j\big|^2\,, \tag{3.28}$$

with a preset positive integer N independent of τ and ω, then the following a priori estimate holds,

$$|\omega - \frac{1}{\sqrt{\lambda_i\tau}}| \lesssim \omega^2\,, \tag{3.29}$$

and we have

$$E^\omega = \mathbb{P}_{\lambda_i}[E^\omega] + O(\omega)\,. \tag{3.30}$$

Proof. By the a priori estimate (3.16), we readily have that if the condition (3.28) holds, then there exist constants C_1 and C_2 of order one, depending on N, such that

$$C_1|\omega|^{-2} \le |\tau| \le C_2|\omega|^{-2}\,. \tag{3.31}$$

Moreover, when ω is small enough, we can find constants C_3 and C_4 of order one such that the following estimates hold for $i \in \{0, 1, \cdots, N\}$:

$$C_3 \le \big|\frac{1}{\tau\omega^2} - \lambda_j\big| \le C_4 \quad \text{for } \lambda_j \ne \lambda_i\,. \tag{3.32}$$

To obtain the estimate (3.29), we let ω_i be $(\lambda_i\tau)^{-1/2}$ and define a complex-valued function $f(s)$ on $[0,1]$ by

$$f(s) = \frac{1}{\tau(\omega_i + s(\omega - \omega_i))^2}\,,$$

with its derivative given by

$$f'(s) = \frac{-2}{\tau(\omega_i + s(\omega - \omega_i))^3}(\omega - \omega_i)\,.$$

With these auxiliary functions, we readily see from (3.16), by using the mean-value theorem and the estimate for τ in (3.31), that

$$|f(1) - f(0)| = |f'(\xi)| \lesssim |\omega|\,,$$

which yields

$$|\omega - \omega_i| \lesssim |\omega| \cdot |\tau| \cdot (|\omega_i| + |\xi| \cdot |\omega - \omega_i|)^3 \lesssim |\omega|^2\,,$$

where $\xi \in (0,1)$ is a real constant and we have also used an easy observation from (3.31) that

$$|\tau| \cdot (|\omega_i| + |\xi| \cdot |\omega - \omega_i|)^2 = O(1)\,.$$

Finally, the estimate (3.30) is a direct consequence of (3.27) and (3.32), by noting that

$$\mathbb{P}_{\mathrm{d}}[\cdot] = \mathbb{P}_{\lambda_i}[\cdot] + \mathbb{P}_{\Sigma}[\cdot]\,,$$

where $\mathbb{P}_{\Sigma}$ is as defined in (3.26) with r_0 chosen as

$$r_0 = \min_{\lambda_j \neq \lambda_i} |\frac{1}{\tau\omega^2} - \lambda_j|\,.$$

The proof is now completed. ☐

We observe from the estimate (3.29) that the quasi-static approximation for the dielectric subwavelength resonance ω is given by $(\lambda_i\tau)^{-1/2}$ for some i. The above approach can be easily generalized to derive the higher-order estimate for ω as well as the eigenfunction E^ω. We consider the first-order correction of the quasi-static approximation for the dielectric resonance ω below, which shows a remarkable result that $(\lambda_i\tau)^{-1/2}$ is actually an $O(\omega^3)$ approximation for the subwavelength resonance.

Theorem 3.12. *Under the same conditions as in Theorem 3.11, the following sharper a priori estimate holds for the resonance ω:*

$$|\omega - \frac{1}{\sqrt{\lambda_i\tau}}| \lesssim |\omega|^3\,. \tag{3.33}$$

Proof. By the assumptions of the theorem, we have $\tau \sim \omega^{-2}$. We then have from (3.3) that

$$(1 - \tau\mathcal{T}_B - \tau\omega^2\mathcal{T}_{B,2} - \tau\omega^3\mathcal{T}_{B,3})[E^\omega] = O(\omega^2)\,.$$

To get an equation for the resonant frequency ω, we take the inner product of the above equation with $\mathbb{P}_{\lambda_i}E^\omega$, and then obtain

$$(1 - \tau\omega^2\lambda_i)(\mathbb{P}_{\lambda_i}E^\omega, E^\omega)_{L^2(B)} - \tau\omega^3(\mathbb{P}_{\lambda_i}E^\omega, \mathcal{T}_{B,3}[E^\omega])_{L^2(B)} = O(\omega^2)\,, \tag{3.34}$$

which implies, by the formula (3.12),

$$(1 - \tau\omega^2\lambda_i)(\mathbb{P}_{\lambda_i}E^\omega, E^\omega)_{L^2(B)} = O(\omega^2)\,. \tag{3.35}$$

It further follows from the estimates $1 - \tau\omega^2\lambda_i = O(\omega)$ and (3.30) that $1 - \tau\omega^2\lambda_i = O(\omega^2)$. Similarly, the desired result follows from the mean-value theorem. ☐

Existence and asymptotics of dielectric resonances

In the previous section, we provide an a priori estimates for the dielectric resonance and the associated eigenfunctions in the quasi-static regime when the contrast τ is very high. Nevertheless, it is still unknown whether there exist subwavelength resonant frequencies ω for the eigenvalue problem $(\mathscr{P})$ for a given size parameter δ and contrast τ. We note that the analytic function $\mathcal{A}(+\infty,\omega) = -\mathcal{T}_B^\omega$ has a unique characteristic value 0 with an infinite-dimensional eigenspace. The Gohberg-Sigal theory can not be applied to $\mathcal{A}(\tau,\omega)$ (a small perturbation of the analytic function $\mathcal{A}(+\infty,\omega)$) to guarantee the existence of resonances near the origin.

To get some motivation for this section, we see from Theorem 3.12 that for $\tau \sim \delta^{-2}$ (a condition equivalent to (3.28)), there exists $\lambda_i \in \sigma(\mathcal{K}_B^{\mathrm{d};\mathrm{d}})$ for a dielectric subwavelength resonance ω such that

$$|\omega - \frac{1}{\delta\sqrt{\lambda_i\tau}}| \lesssim \delta^2\omega^3\,,$$

if we separate the size parameter δ and the frequency ω. The (resonance) condition $\tau \sim \delta^{-2}$ means that the wavelength inside the nanoparticle is comparable with its characteristic size, in which case the dielectric resonances have actually been experimentally observed [36].

This section is devoted to rigorously showing the existence of the dielectric subwavelength resonances under such circumstances. For this, we consider the eigenvalue problem ($\mathscr{P}$) and make the assumption $\tau \sim \delta^{-2}$ more precise. We assume $\tau(\delta)$ is a meromorphic function of δ with the following Laurent expansion:

$$\tau(\delta) = c_\tau \delta^{-2} + \sum_{i=-1}^{\infty} c_i \delta^i \quad \text{with } c_\tau \in \mathbb{C}\,, c_i \in \mathbb{R} \text{ and } \mathfrak{Re} c_\tau > 0\,, \mathfrak{Im} c_\tau \geq 0\,. \tag{3.36}$$

By abuse of notation and Lemma 3.1, we write $\mathbb{A}(\delta,\omega)$ as

$$\mathbb{A}(\delta,\omega) := \mathbb{A}(\tau(\delta),\delta\omega) = \begin{bmatrix} 1-\tau(\delta)\mathbb{P}_{\mathrm{d}}\mathcal{T}_B^{\delta\omega}\mathbb{P}_{\mathrm{d}} & -\tau(\delta)\mathbb{P}_{\mathrm{d}}\mathcal{T}_B^{\delta\omega}\mathbb{P}_{\mathrm{w}} \\ -\mathbb{P}_{\mathrm{w}}\mathcal{T}_B^{\delta\omega}\mathbb{P}_{\mathrm{d}} & \frac{1}{\tau(\delta)} - \mathbb{P}_{\mathrm{w}}\mathcal{T}_B^{\delta\omega}\mathbb{P}_{\mathrm{w}} \end{bmatrix}, \tag{3.37}$$

with the asymptotic expansion: $\mathbb{A}(\delta,\omega) = \mathbb{A}_0(\omega) + \delta\mathbb{A}_1(\omega) + O(\delta^2)$, where the operators $\mathbb{A}_0(\omega)$ and $\mathbb{A}_1(\omega)$ can be computed, by using the relation (3.12), as follows:

$$\mathbb{A}_0(\omega) = \begin{bmatrix} 1 - c_\tau\omega^2\mathcal{K}_B^{\mathrm{d,d}} & -c_\tau\omega^2\mathcal{K}_B^{\mathrm{d,w}} \\ 0 & -\mathcal{T}_B \end{bmatrix}, \quad \mathbb{A}_1(\omega) = -\begin{bmatrix} c_{-1}\omega^2\mathcal{K}_B^{\mathrm{d,d}} & c_{-1}\omega^2\mathcal{K}_B^{\mathrm{d,w}} \\ 0 & 0 \end{bmatrix}. \tag{3.38}$$

For the sake of simplicity, from now on, we identify the space $H_0(\mathrm{div}0,B)\times\{0\}$ (resp., $\{0\}\times W$) with $H_0(\mathrm{div}0,B)$ (resp., W), and do not distinguish between the projection from $\mathbb{X}$ to $H_0(\mathrm{div}0,B)\times\{0\}$ (resp., $\{0\}\times W$) and the projection from $H(\mathrm{div}0,B)$ to $H_0(\mathrm{div}0,B)$ (resp., W). Both of them are denoted by $\mathbb{P}_{\mathrm{d}}$ (resp., $\mathbb{P}_{\mathrm{w}}$).

Then, for the leading-order operator $\mathbb{A}_0(\omega)$, we immediately see from the invertibility of $\mathcal{T}_B|_W$ and Proposition 3.6 that $H_0(\mathrm{div}0,B)$ is an invariant subspace of $\mathbb{A}_0(\omega)$, and $\mathbb{A}_0(\omega)^{-1}$ is a meromorphic function well-defined on $\mathbb{C}$ with all the poles given by $\pm\omega_i := \pm(c_\tau\lambda_i)^{-1/2}$ $(i=0,1,2,\cdots)$, counted with their multiplicities. To proceed, without loss of generality, we consider the local behavior of $\mathbb{A}_0(\omega)^{-1}$ near the pole ω_0. By a simple matrix computation, we can derive

$$\mathbb{A}_0(\omega)^{-1}\begin{bmatrix} f \\ g \end{bmatrix} = \begin{bmatrix} (1-c_\tau\omega^2\mathcal{K}_B^{\mathrm{d,d}})^{-1}[f - c_\tau\omega^2\mathcal{K}_B^{\mathrm{d,w}}\mathcal{T}_B^{-1}g] \\ -\mathcal{T}_B^{-1}g \end{bmatrix}$$

for $(f,g)\in\mathbb{X}$ and ω in a small punctured neighborhood of ω_0, which can be further factorized as

$$\begin{aligned}\mathbb{A}_0(\omega)^{-1}\begin{bmatrix} f \\ g \end{bmatrix} &= \begin{bmatrix} (1-c_\tau\omega^2\mathcal{K}_B^{\mathrm{d,d}})^{-1} & 0 \\ 0 & I \end{bmatrix}\begin{bmatrix} I & -c_\tau\omega^2\mathcal{K}_B^{\mathrm{d,w}}\mathcal{T}_B^{-1} \\ 0 & -\mathcal{T}_B^{-1} \end{bmatrix}\begin{bmatrix} f \\ g \end{bmatrix} \\ &= \begin{bmatrix} \frac{-\omega_0}{2(\omega-\omega_0)}\mathbb{P}_{\lambda_0} + \mathcal{R}_{\mathrm{w}}^{\lambda_0}(\omega) & 0 \\ 0 & I \end{bmatrix}\begin{bmatrix} I & -c_\tau\omega^2\mathcal{K}_B^{\mathrm{d,w}}\mathcal{T}_B^{-1} \\ 0 & -\mathcal{T}_B^{-1} \end{bmatrix}\begin{bmatrix} f \\ g \end{bmatrix},\end{aligned} \tag{3.39}$$

where we have used the spectral resolution of $\mathcal{K}_B^{\mathrm{d,d}}$ in Proposition 3.6 and the identity:

$$\frac{1}{1-c_\tau\omega^2\lambda_0} = \frac{\omega_0^2}{\omega_0^2-\omega^2} = \frac{-\omega_0}{2(\omega-\omega_0)} + \mathcal{R}(\omega)\,.$$

Here and throughout this work, $\mathcal{R}(\omega)$ is a general (operator-valued) analytic function on a suitable domain that may have a different meaning in different contexts.. In particular, $\mathcal{R}_{\mathrm{w}}^{\lambda_i}(\omega)$ (resp., $\mathcal{R}^{\lambda_i}(\omega)$) denotes a class of operator-valued analytic functions that satisfy the property that for each ω, the range of $\mathcal{R}_{\mathrm{w}}^{\lambda_i}(\omega)$ (resp., $\mathcal{R}^{\lambda_i}(\omega)$) is orthogonal to $\ker(\lambda_i - \mathcal{K}_B^{\mathrm{d,d}})\oplus W$ (resp., $\ker(\lambda_i - \mathcal{K}_B^{\mathrm{d,d}})$).

We summarize the above facts about $\mathbb{A}_0(\omega)$ in the following proposition.

Proposition 3.13. *The leading-order operator $\mathbb{A}_0(\omega):\mathbb{X}\to\mathbb{X}$ of $\mathbb{A}(\delta,\omega)$ has the following inverse:*

$$\mathbb{A}_0(\omega)^{-1} = \begin{bmatrix} (1-c_\tau\omega^2\mathcal{K}_B^{\mathrm{d,d}})^{-1} & 0 \\ 0 & I \end{bmatrix}\begin{bmatrix} I & -c_\tau\omega^2\mathcal{K}_B^{\mathrm{d,w}}\mathcal{T}_B^{-1} \\ 0 & -\mathcal{T}_B^{-1} \end{bmatrix}, \tag{3.40}$$

which is a meromorphic function on $\mathbb{C}$ with the simple poles $\pm\omega_i = \pm\sqrt{\lambda_i c_\tau}^{-1}$, $i=0,1,2,\cdots$. Moreover, the pole-pencil expansion of the inverse associated with the pole ω_0 is given by

$$\mathbb{A}_0(\omega)^{-1} = \frac{1}{\omega-\omega_0}\mathcal{L}_0 + \mathcal{R}^{\lambda_0}(\omega)\,, \tag{3.41}$$

for ω in a small punctured neighborhood of ω_0, where the residue $\mathcal{L}_0$ of $\mathbb{A}_0^{-1}$ at the isolated singularity ω_0 is given by

$$\mathcal{L}_0 = -\frac{\omega_0}{2}\begin{bmatrix} \mathbb{P}_{\lambda_0} & -c_\tau\mathbb{P}_{\lambda_0}\omega_0^2\mathcal{K}_B^{\mathrm{d,w}}\mathcal{T}_B^{-1} \\ 0 & 0 \end{bmatrix}. \tag{3.42}$$

Suppose that the eigenspace of $\mathcal{K}_B^{\mathrm{d},\mathrm{d}}$ associated with λ_0 has dimension m and is spanned by $E_{0,j} \in H_0(\mathrm{div}0, B)$ with $\|E_{0,j}\|_{L^2(B)} = 1$, $1 \le j \le m$. Thus, we have

$$\ker\left(\mathbb{A}_0(\omega_0)\right) = \mathrm{span}\left\{E_{0,1}, \cdots, E_{0,m}\right\}, \tag{3.43}$$

and the geometric multiplicity of $\mathbb{A}_0(\omega)$ at ω_0 is m. Since ω_0 is a simple pole of $\mathbb{A}_0(\omega)$, the geometric multiplicity of ω_0 is equal to the algebraic multiplicity $M(\mathbb{A}_0(\omega), \Gamma_0)$ [3, 30], which can be computed, by the generalized argument principle [3, Theorem 1.12]:

$$M(\mathbb{A}_0(\omega), \Gamma_0) = \frac{1}{2\pi i}\,\mathrm{tr}\int_{\Gamma_0} \mathbb{A}_0(\omega)^{-1}\mathbb{A}_0'(\omega)dw\,, \tag{3.44}$$

where Γ_0 is a Cauchy contour enclosing only the singularity ω_0 among all the poles of $\mathbb{A}_0(\omega)^{-1}$. In fact, in our case, the fact that $m = M(\mathbb{A}_0(\omega), \Gamma_0)$ can be verified by a direct calculation following the framework in Appendix B for computing the trace of a finite rank operator. By (3.44) and the pole-pencil decomposition (3.41), as well as the analyticity of $\mathcal{R}^{\lambda_0}(\omega)\mathbb{A}_0'(\omega)$, we obtain

$$\begin{aligned}
M(\mathbb{A}_0(\omega), \Gamma_0) &= \frac{1}{2\pi i}\,\mathrm{tr}\int_{\Gamma_0} \mathbb{A}_0(\omega)^{-1}\mathbb{A}_0'(\omega)d\omega \\
&= \frac{1}{2\pi i}\,\mathrm{tr}\int_{\Gamma_0} \frac{1}{\omega-\omega_0}\mathcal{L}_0\mathbb{A}_0'(\omega)d\omega \\
&= \frac{1}{2\pi i}\sum_{j=1}^{m}\int_{\Gamma_0} \frac{1}{\omega-\omega_0}\left(\begin{bmatrix}E_{0,j}\\0\end{bmatrix}, \mathcal{L}_0\mathbb{A}_0'(\omega)\begin{bmatrix}E_{0,j}\\0\end{bmatrix}\right)_{\mathbb{X}} d\omega\,.
\end{aligned} \tag{3.45}$$

From the above formula, we readily observe that only the $(1,1)$-block of $\mathcal{L}_0\mathbb{A}_0'(\omega)$:

$$(\mathcal{L}_0\mathbb{A}_0'(\omega))_{1,1} = (-\frac{\omega_0}{2})\cdot(-2c_\tau\omega)\mathbb{P}_{\lambda_0}\mathcal{K}_B^{\mathrm{d},\mathrm{d}} = c_\tau\omega_0\omega\lambda_0\mathbb{P}_{\lambda_0}\,, \tag{3.46}$$

is needed for computing $M(\mathbb{A}_0(\omega), \Gamma_0)$. Substituting (3.46) back into (3.45), we have

$$M(\mathbb{A}_0(\omega), \Gamma_0) = \frac{1}{2\pi i}\sum_{j=1}^{m}\int_{\Gamma_0} \frac{c_\tau\omega_0\omega\lambda_0}{\omega-\omega_0}(E_{0,j}, \mathbb{P}_{\lambda_0}E_{0,j})_{L^2(B)}d\omega = m\,. \tag{3.47}$$

We are now well prepared to use the Gohberg-Sigal theory to find the subwavelength resonances near the simple poles of $\mathbb{A}_0(\omega)^{-1}$. By Proposition 3.13 and the relation (3.47), the following result follows readily from the generalized Rouché's theorem [3, Theorem 1.15].

Theorem 3.14. *Let C_r be a constant of order one and let n_0 be a finite index (if exists) such that*

$$\Omega_0 := \{\pm\omega_i\,;\ i = 0,1,\cdots,n_0\} = \{\pm\omega_i\,;\ i = 0,1,\cdots\}\bigcap B(0, C_r)\,.$$

Since Ω_0 is a finite set, we can choose a small constant ε_0 such that $B(\pm\omega_i, \varepsilon_0) \subset B(0, C_r)$ for each $i \in \{0,1,\cdots,n_0\}$, and $\pm\omega_i$ is the only singularity of $\mathbb{A}_0(\omega)^{-1}$ inside $B(\pm\omega_i, \varepsilon_0)$. Then there exists a small constant $\delta(\varepsilon_0)$ such that $|\delta(\varepsilon_0)C_r| \ll 2\pi$, and for any $\delta \in (-\delta(\varepsilon_0), \delta(\varepsilon_0))$, it holds that

$$\left\|\left(\mathbb{A}(\delta,\omega) - \mathbb{A}_0(\omega)\right)\mathbb{A}_0(\omega)^{-1}\right\| < 1\,, \quad \forall\, \omega \in \partial B(\pm\omega_i, \varepsilon_0)\,,\ i = 0,1,\cdots,n_0\,,$$

and

$$M(\mathbb{A}(\delta,\omega), \partial B(\pm\omega_i, \varepsilon_0)) = M(\mathbb{A}_0(\omega), \partial B(\pm\omega_i, \varepsilon_0)) = \dim\ker(\lambda_i - \mathcal{K}_B^{\mathrm{d},\mathrm{d}}) \quad \text{for } i = 0,1,\cdots,n_0\,.$$

Here, $M(\mathbb{A}(\delta,\omega), \partial B(\pm\omega_i, \varepsilon_0))$ is given by

$$M(\mathbb{A}(\delta,\omega), \partial B(\pm\omega_i, \varepsilon_0)) = \frac{1}{2\pi i}\,\mathrm{tr}\int_{\partial B(\pm\omega_i,\varepsilon_0)} \mathbb{A}(\delta,\omega)^{-1}\frac{\partial}{\partial\omega}\mathbb{A}(\delta,\omega)d\omega\,.$$

From the above theorem, we can conclude that for any $\delta \in (-\delta(\varepsilon_0), \delta(\varepsilon_0))$, there are $m_i := \dim\ker(\lambda_i - \mathcal{K}_B^{\mathrm{d},\mathrm{d}})$ isolated singularities of $\mathbb{A}(\delta,\omega)^{-1}$ in each $B(\pm\omega_i, \varepsilon_0)$, counted with algebraic multiplicity, which are "splitted" from $\pm\omega_i$. These singular points of $\mathbb{A}(\delta,\omega)^{-1}$ (characteristic values of $\mathbb{A}(\delta,\omega)$) are exactly the dielectric subwavelength resonances according to Definition 2.2.

However, we emphasize that Definition 2.2 (or Definition 3.7) makes sense only mathematically, since for a practical incident wave with $\mathfrak{Re}\omega > 0\,,\ \mathfrak{Im}\omega \ge 0$, the resonant frequencies in the left-half plane has no possibility of being approached by the incident frequency ω. To select those physically meaningful dielectric subwavelength resonances, we need to make use of the knowledge of the distribution of the characteristic values of $\mathbb{A}(\delta,\omega)$ in $B(0,C_r)$. If the contrast τ satisfying (3.36) has a positive imaginary part, then the simple poles $\pm\omega_i$ are distributed on the line like $\{\alpha\exp\{-i\frac{\arg c_\tau}{2}\};\ \alpha\in\mathbb{R}\}$. Therefore, when δ is small enough, we know by Theorem 3.14 that the characteristic values of $\mathbb{A}(\delta,\omega)$ perturbed from ω_i will be completely in the fourth quadrant while those from $-\omega_i$ will be in the second quadrant. If τ is real, we obtain the following precise characterization about the distribution of the characteristic values of $\mathcal{A}(\tau,\omega)$, from which we can still guarantee that the singularities of $\mathbb{A}(\delta,\omega)^{-1}$ perturbed from ω_i are in the fourth quadrant.

Proposition 3.15. *For the case where τ is real and large enough, all the characteristic values of the analytic function $\mathcal{A}(\tau,\omega)=\tau^{-1}-\mathcal{T}_B^\omega$ on $\mathbb{C}$ are located in the lower half-plane $\{\omega\in\mathbb{C};\ \mathfrak{Im}\omega<0\}$, and symmetric with respect to the imaginary axis.*

Proof. The symmetry of the characteristic values is a direct consequence of the following relation:

$$\overline{\mathcal{A}(\tau,\omega)[E]}=\left(\tau^{-1}-\mathcal{T}_B^{-\bar\omega}\right)\left[\bar E\right]=\mathcal{A}(\tau,-\bar\omega)\left[\bar E\right]\,,$$

from which we have that if ω is a characteristic value, then so is $-\bar\omega$. And we have proved in [5, Theorem 3.2] that there is no characteristic values of $\mathcal{A}(\tau,\omega)$ on the real axis for a real high contrast τ. To finish the proof of the proposition, we show that if $(\omega,E^\omega)\in\mathbb{C}\times H(\mathrm{div}0,B)$ satisfies $\mathcal{A}(\tau,\omega)[E^\omega]=0$ with $\mathfrak{Im}\omega>0$, then the associated eigenfunction E^ω must be zero. We let $u(x)=\mathcal{T}_B^\omega[E](x)$ for $x\in\mathbb{R}^3$, which exponentially decays when $|x|\to\infty$, due to the positive imaginary part of ω. Then, an integration by parts inside and outside the domain helps us to write

$$\int_{\mathbb{R}^3\backslash\bar B}|\nabla\times u|-\omega^2|u|^2dx=\int_{\partial B}\nu\times\nabla\times u\cdot\bar u d\sigma(x)\,, \tag{3.48}$$

and

$$\int_B|\nabla\times u|^2-\omega^2(1+\tau)|u|^2dx=-\int_{\partial B}\nu\times\nabla\times u\cdot\bar u d\sigma(x)\,, \tag{3.49}$$

respectively. We hence have, by taking the imaginary parts of both sides of (3.48) and (3.49),

$$\mathfrak{Im}\int_{\partial B}\nu\times\nabla\times u\cdot\bar u d\sigma(x)=-\mathfrak{Im}\omega^2\int_{\mathbb{R}^3\backslash\bar B}|u|^2dx=\mathfrak{Im}\omega^2(1+\tau)\int_B|u|^2dx=0\,.$$

If $\omega\neq i$ ($\mathfrak{Im}\omega^2\neq0$), the above formula directly yields $u=0$. If $\omega=i$, then we observe from (3.48) and (3.49) that

$$\int_{\mathbb{R}^3\backslash\bar B}|\nabla\times u|+|u|^2dx=\int_B|\nabla\times u|^2+(1+\tau)|u|^2dx=0\,,$$

which implies that $u=0$. The proof is complete. □

The second issue we would like to emphasize is that it is nontrivial to show if the characteristic values $\omega_{i,j}(\delta)(1\le j\le m_i)$ of $\mathbb{A}(\delta,\omega)$ in $B(\omega_i,\varepsilon_0)$ is analytic with respect to δ. In general, $\{\omega_{i,j}\}_{j=1}^{m_i}$ consist of branches of one or several analytic functions that may have algebraic singularities at $\delta=0$ [9, 34]. However, in the case $m_i=1$, the analyticity of $\omega_i(\delta)(=\omega_{i,1}(\delta))$ easily follows from the formula:

$$\omega_i(\delta)-\omega_i=\frac{1}{2\pi i}\operatorname{tr}\int_{\partial B(\omega_i,\varepsilon_0)}(\omega-\omega_i)\mathbb{A}(\delta,\omega)^{-1}\frac{d}{d\omega}\mathbb{A}(\delta,\omega)d\omega\,, \tag{3.50}$$

which is derived from generalized argument principle. Furthermore, it is easy to observe that we can set the index N in Theorem 3.12 to n_0, and then the scaled resonances $\delta\omega_{i,j}(\delta)$ satisfy the conditions in Theorem 3.12 for small enough δ, which directly yields the following estimates:

$$|\omega_{i,j}(\delta)-\frac{1}{\delta\sqrt{\lambda_i\tau}}|\lesssim\delta^2\quad\text{for } 0\le i\le n_0\,, 1\le j\le m_i \text{ and } \delta\ll1\,.$$

If we substitute the expansion (3.36) into the above estimates, we shall have the following asymptotics for $\omega_{i,j}(\delta)$, by a simple Taylor expansion:

$$|\omega_{i,j}(\delta)-\omega_i+\delta\frac{\omega_i c_{-1}}{2c_\tau}|\lesssim\delta^2\quad\text{for } 0\le i\le n_0\,, 1\le j\le m_i \text{ and } \delta\ll1\,. \tag{3.51}$$

It follows that $\omega_{i,j}(\delta)$ is differentiable at $\delta=0$, although may not be analytic. We summarize the above discussions in the following theorem.

Theorem 3.16. *Let C_r and n_0 be the same as in Theorem 3.14. For small enough δ, we have exactly $\sum_{i=0}^{n_0} m_i$ physically meaningful dielectric subwavelength resonances $\omega_{i,j}(\delta) \subset B(0, C_r)$, $0 \le i \le n_0$, $1 \le j \le m_i$ in the fourth quadrant $\{\omega \in \mathbb{C}\,;\ \mathfrak{Re}\omega > 0\,,\ \mathfrak{Im}\omega < 0\}$, counted with algebraic multiplicity, where $m_i = \dim\ker(\lambda_i - \mathcal{K}_B^{\mathrm{d,d}})$ and $\omega_{i,j}(\delta)$ are characteristic values of $\mathbb{A}(\delta,\omega)$ near ω_i. For each i, j, the perturbed resonance $\omega_{i,j}(\delta)$ is differentiable at $\delta = 0$ with the asymptotic estimate* (3.51).

We end this section with several remarks. In particular, Remarks 3.19 and 3.20 have some physical significance.

Remark 3.17. *By the asymptotic formulas* (3.51) *for the resonances $\omega_{i,j}(\delta)$, we see that the splitting of ω_i only becomes apparent at high orders (≥ 2) in the expansion of $\omega_{i,j}(\delta)$. The same asymptotic formula for the average of $\omega_{i,j}(\delta)$ can also be obtained by the formula* (3.50) *for $m_i \ge 1$ [3, 9] (by a similar argument to the one for the formula* (3.47)*):*

$$\sum_{j=1}^{m_i}(\omega_{i,j}(\delta) - \omega_i) = \frac{1}{2\pi i}\operatorname{tr}\int_{\partial B(\omega_i,\varepsilon_0)}(\omega - \omega_0)\mathbb{A}(\delta,\omega)^{-1}\frac{d}{d\omega}\mathbb{A}(\delta,\omega)d\omega$$
$$= -\delta\frac{1}{2\pi i}\operatorname{tr}\int_{\partial B(\omega_i,\varepsilon_0)}\mathbb{A}_0(\omega)^{-1}\mathbb{A}_1(\omega)d\omega + O(\delta^2) = -\delta\frac{m_i c_{-1}\omega_i}{2c_\tau} + O(\delta^2)\,.$$

Remark 3.18. *By Theorem 3.14, the existence of resonances depends on the choice of C_r. If C_r is not large enough, the set Ω_0 would be empty and then there is no resonances in the admissible domain $B(0, C_r)$ for the frequency. On the other hand, C_r can also not be too large, since we need to satisfy the quasi-static regime* (2.3)*. The above discussion theoretically predicts that only lowest few characteristic values of $1 - \tau\mathcal{T}_B^{\delta\omega}$ can be excited, and in the physics experiments [36], it is indeed the case.*

Remark 3.19. *If we fix the size parameter δ and the admissible domain $B(0, C_r)$ such that $|\delta C_r| \ll 2\pi$, we see that when the refractive index n increases ($|c_\tau|$ increases), the index n_0 in Theorem 3.14 will also increases. Hence, we may expect that the ability of the nanoparticle to concentrate EM energy is enhanced in this case [27], since more resonant modes can be excited.*

Remark 3.20. *We can clearly observe from the a priori estimate* (3.33) *that with increasing the particle size, the resonant frequencies are expected to have the red-shift phenomenon, as reported in [27].*

Multipole radiation and scattering enhancement

In this section, we shall carry out some quantitative analysis of the enhancement of the scattered field and the cross sections when the dielectric resonance occurs. To do so, we develop a new and systematic approach to derive the full Cartesian multipole expansion and apply it to analyze the scattering amplitude of the fields to the problem (2.4). We will also compute the corresponding extinction and scattering cross sections and analyze their blow-up rates.

It is known [22] that for any EM radiating field E, we can define its scattering amplitude E_∞, which is an analytic tangential vector field on the unit sphere S, by the asymptotic behavior:

$$E = \frac{e^{i\omega|x|}}{|x|}E_\infty(\hat{x}) + O\left(\frac{1}{|x|^2}\right) \quad \text{as } |x| \to \infty\,.$$

We follow the framework established in Section 3.2 and work under the condition (3.36) for the contrast τ. Without loss of generality, we suppose that the incident frequency ω is real and near ω_0 (so that the operator $\mathbb{A}(\delta,\omega)$ is invertible since ω will not hit its singularities by Theorem 3.16). We also assume, for simplicity, that the particles B have genus zero and ω_0 has multiplicity one, with the corresponding normalized eigenfunction being denoted by E_0.

Multipole expansion for the scattering amplitude

For our purpose, we first observe, from the Lippmann-Schwinger representation (2.10) for the scattered wave E^s, the following integral representation for the scattering amplitude E^s_∞:

$$E^s_\infty(\hat{x}) = \frac{\tau\omega^2}{4\pi}(\mathbb{I} - \hat{x}\otimes\hat{x})\int_D e^{-i\omega\hat{x}\cdot y}E(y)dy\,, \tag{4.1}$$

with the matrix $\mathbb{I} - \hat{x}\otimes\hat{x}$ being the projection on the tangent space of the unit sphere S at $\hat{x}$. Here we have exploited the far-field expansion of the EM Green's tensor [22]:

$$(\mathbb{I} + \frac{1}{\omega^2}\nabla_x\mathrm{div}_x)g(x-y,\omega) = \frac{e^{i\omega|x|}}{4\pi|x|}e^{-i\omega\hat{x}\cdot y}(\mathbb{I} - \hat{x}\otimes\hat{x}) + O\left(\frac{1}{|x|^2}\right) \quad \text{as } |x| \to \infty\,.$$

It then follows from the Taylor series expansion for $e^{-i\omega\hat{x}\cdot y}$ and the change of variables $y=\delta\widetilde{y}$ that

$$E^s_\infty(\hat{x}) = \frac{\tau\omega^2}{4\pi}(\mathbb{I}-\hat{x}\otimes\hat{x})\int_B\sum_{n=0}^\infty \delta^{n+3}\frac{(-i\omega\hat{x}\cdot\widetilde{y})^n}{n!}\widetilde{E}(\widetilde{y})d\widetilde{y} \quad \text{with } \widetilde{E}(\widetilde{y}) := E(\delta\widetilde{y})\,, \tag{4.2}$$

which is used in physics [32, 26] as a starting point for deriving the classical multipole moment expansion; see (4.11) below. Nevertheless, as pointed out in [32], to arrive at (4.11), one needs different calculation techniques to disentangle the electric and magnetic multipole fields from each term in the expansion (4.2), and the details and technicalities involved become increasingly prohibitive when the order n increases. Instead, we take a different approach for the multipole moment expansion, motivated by the Helmholtz decomposition (3.4), and along with the help of the following formulae. The big advantage of this approach is that it can handle all the orders in a unified manner.

Lemma 4.1. *For $\varphi\in H_0(\mathrm{curl},B)$, we have*

$$\int_B(\hat{x}\cdot y)^l\nabla\times\varphi(y)dy = \int_B l(\hat{x}\cdot y)^{l-1}\varphi(y)dy\times\hat{x}\,,\quad l\geq 1\,. \tag{4.3}$$

For the case where the open set B has genus zero, we have written the following decomposition for $\psi\in H(\mathrm{div}0,B)$ in (3.9):

$$\psi = \mathbb{P}_{\mathrm{d}}\psi+\mathbb{P}_{\mathrm{w}}\psi\,,\quad \text{with } \mathbb{P}_{\mathrm{d}}\psi = \nabla\times\varphi \text{ and } \mathbb{P}_{\mathrm{w}}\psi = \nabla p\,, \tag{4.4}$$

where φ is uniquely determined in $\widetilde{X}^0_N(B)$ and $p\in H^1(B)$ is unique up to some constants [5, Appendix A]. Since the right side of (4.3) is independent of the representative of the equivalent class φ, the left side of (4.3) is well-defined for the elements in the quotient space $\widetilde{X}^0_N(B)$.

In view of the decomposition (4.4) and the physical explanations provided after (3.9), it is natural for us to separate the physically different electric and magnetic radiations by writing

$$\int_B(\hat{x}\cdot\widetilde{y})^l\widetilde{E}(\widetilde{y})d\widetilde{y} = \int_B(\hat{x}\cdot\widetilde{y})^l\left(\mathbb{P}_{\mathrm{d}}\widetilde{E}(\widetilde{y})+\mathbb{P}_{\mathrm{d}}\widetilde{E}(\widetilde{y})\right)d\widetilde{y}\,, \tag{4.5}$$

and introduce the following new class of electric and magnetic multipole moments, based on Lemma 4.1.

Definition 4.2. *For a divergence-free vector field $\psi\in H(\mathrm{div}0,B)$ with the Helmholtz decomposition (4.4), the associated magnetic $l-$moment is $l-$tensor on the $l-$ary Cartesian power of $\mathbb{R}^3$: $\Pi^l\mathbb{R}^3$, defined by*

$$\mathbf{M}^\psi_l := \int_B l\varphi(y)\otimes\left(\otimes^{l-1}y\right)dy\,,\qquad l=1,2,\cdots\,,$$

and $\mathbf{M}^\psi_l=0$ for $l=0$. The associated electric $l-$moment is $(l+1)-$tensor on $\Pi^{l+1}\mathbb{R}^3$ define by

$$\mathbf{Q}^\psi_l := \int_B\nabla p(y)\otimes\left(\otimes^l y\right)d\sigma(y)\,,\quad l=0,1,\cdots\,.$$

Remark 4.3. *Our definition provides a new interpretation, as well as a new derivation, for those EM moments occurring in the physics literature. For instance, in classical electrodynamics, given a current distribution* J*, the corresponding electric dipole moment* $\mathbf{p}$ *and magnetic dipole moment* $\mathbf{m}$ *are typically given by*

$$\mathbf{p} = \frac{1}{i\omega}\int x\mathrm{div}\mathrm{J}(x)dx\,,\ \textit{and}\ \mathbf{m} = \frac{1}{2}\int x\times\mathrm{J}(x)dx\,,$$

respectively; see [32, Chapter 9]. If we ignore the boundary condition on J *and write it as $J=\nabla\times A+\nabla p$, a formal integration by parts allows us to see*

$$\mathbf{p} = -\frac{1}{i\omega}\int\mathrm{J} = -\frac{1}{i\omega}\int\nabla p\,,\quad \mathbf{m} = \frac{1}{2}\int x\times(\nabla\times A) = \int A\,,$$

due to $\int\nabla\times A=0$ and $\int x\times\nabla p=0$. Thus these physically defined dipole moments are indeed equal to our newly introduced EM moments $\mathbf{Q}^\psi_0$ and $\mathbf{M}^\psi_1$, up to a constant factor. A similar formal verification can be conducted for the higher-order moments.

We remark that an $l-$tensor is a multilinear function on the product vector space and we identify the dual space of $\mathbb{R}^3$ with itself. Thus, we do not distinguish between the linear mapping $\mathbf{M}^\psi_l(\cdot,\Pi^{l-1}\hat{x})$ on $\mathbb{R}^3$ and the vector:

$$\sum_{i=1}^3\mathbf{M}^\psi_l(\mathbf{e}_i,\underbrace{\hat{x},\cdots,\hat{x}}_{l-1})\mathbf{e}_i\,,$$

and similarly between the linear function $\mathbf{Q}_l^{\psi}(\cdot, \Pi^l \hat{x})$ and

$$\sum_{i=1}^{3} \mathbf{Q}_l^{\psi}(\mathbf{e}_i, \underbrace{\hat{x}, \cdots, \hat{x}}_{l})\mathbf{e}_i \,.$$

With the help of these notions, we immediately have

$$\int_B (\hat{x}\cdot\widetilde{y})^l \widetilde{E}(\widetilde{y})d\widetilde{y} = \mathbf{M}_l^{\widetilde{E}}(\cdot, \Pi^{l-1}\hat{x}) \times \hat{x} + \mathbf{Q}_l^{\widetilde{E}}(\cdot, \Pi^l \hat{x})\,, \tag{4.6}$$

from the formula (4.5), and obtain the following proposition by the expansion (4.2).

Proposition 4.4. *The scattering amplitude $E^s_\infty(\hat{x})$ corresponding to the problem* (2.5) *has the following multipole moment expansion:*

$$E^s_\infty(\hat{x}) = \frac{\tau\omega^2\delta^3}{4\pi}(\mathbb{I} - \hat{x}\otimes\hat{x}) \sum_{l=0}^{\infty} \frac{(-i\delta\omega)^l}{l!} \Big(\mathbf{M}_l^{\widetilde{E}}(\cdot, \Pi^{l-1}\hat{x}) \times \hat{x} + \mathbf{Q}_l^{\widetilde{E}}(\cdot, \Pi^l \hat{x}) \Big)\,, \tag{4.7}$$

where the field $\widetilde{E}$ on B is the solution to the equation:

$$(1 - \tau T_B^{\delta\omega})[\widetilde{E}] = \widetilde{E}^i \quad \textit{with } \widetilde{E}^i(\widetilde{x}) = E^i(\delta\widetilde{x})\,. \tag{4.8}$$

Generally, it appears necessary to consider all the terms in the expansion (4.2) in order to fully understand the properties of the scattered wave. However, since we are working in the quasi-static regime, the first several terms are sufficient to essentially determine the behavior of E^s in the far field. To approximate E^s_∞ with a certain order, we note from the Parseval's identity and the Green's formula (3.13) that

$$\left\| \mathbb{P}_{\mathrm{d}} \widetilde{E}^i \right\|^2_{L^2(B)} = \sum_{n=0}^{\infty} \left| \Big(\widetilde{E}^i - \widetilde{E}^i(0), E_n \Big)_{L^2(B)} \right|^2 ,$$

which implies $\mathbb{P}_{\mathrm{d}}\widetilde{E}^i = O(\delta)$. Combining this with the following system that is equivalent to (4.8):

$$\mathbb{A}(\delta,\omega) \begin{bmatrix} \mathbb{P}_{\mathrm{d}}\widetilde{E} \\ \mathbb{P}_{\mathrm{w}}\widetilde{E} \end{bmatrix} = \begin{bmatrix} \mathbb{P}_{\mathrm{d}}\widetilde{E}^i \\ \tau^{-1}\mathbb{P}_{\mathrm{w}}\widetilde{E}^i \end{bmatrix}, \tag{4.9}$$

we readily obtain $\widetilde{E} = O(\delta)$ by the condition (3.36), i.e., $\tau \sim \delta^{-2}$. Then the following result follows from the expansion (4.2).

Lemma 4.5. *In the high contrast regime, $\tau \sim \delta^{-2}$, the scattering amplitude E^s_∞ can be approximated by*

$$E^{s,app}_\infty := \frac{\tau\omega^2\delta^3}{4\pi}(\mathbb{I} - \hat{x}\otimes\hat{x}) \left\{ \int_B \widetilde{E}(\widetilde{y})d\widetilde{y} - i\delta\omega \int_B \hat{x}\cdot\widetilde{y}\widetilde{E}(\widetilde{y})d\widetilde{y} - \frac{\delta^2\omega^2}{2} \int_B (\hat{x}\cdot\widetilde{y})^2 \widetilde{E}(\widetilde{y})d\widetilde{y} \right\}, \tag{4.10}$$

with an error of order δ^5.

Remark 4.6. *If τ is only a constant of order one, we will have $\widetilde{E} = O(1)$ and the error in the approximation* (4.10) *would be of order δ^6. By using* (4.6) *to separate the electric and magnetic multipoles, we can derive the following formula usually used in the physics community [32, 26]:*

$$E^s_\infty(\hat{x}) \approx \frac{\omega^2}{4\pi} \{ \underbrace{\hat{x}\times(\mathbf{p}\times\hat{x})}_{O(\delta^3)} + \underbrace{\mathbf{m}\times\hat{x} + \hat{x}\times(\hat{x}\times\mathbf{Q}\hat{x})}_{O(\delta^4)} + \underbrace{\hat{x}\times\mathbf{M}\hat{x} + \hat{x}\times(\hat{x}\times\mathbf{O}(\cdot,\hat{x},\hat{x}))}_{O(\delta^5)} \}\,, \tag{4.11}$$

where the electric dipole (ED) $\mathbf{p}$, magnetic dipole (MD) $\mathbf{m}$, electric quadrupole (EQ) $\mathbf{Q}$, magnetic quadrupole (MQ) $\mathbf{M}$ and electric octupole (EO) $\mathbf{O}$ are given by $\mathbf{Q}_0^{\widetilde{E}}$, $\mathbf{M}_1^{\widetilde{E}}$, $\mathbf{Q}_1^{\widetilde{E}}$, $\mathbf{M}_2^{\widetilde{E}}$ and $\mathbf{Q}_2^{\widetilde{E}}$, up to some constant factors.

The approximation (4.11) *permits us to conclude that in the quasi-static regime, any dielectric nanoparticle behaves like a electric dipole in the far field, and the corresponding magnetic dipole radiation is a higher-order term. However, we shall see soon (cf. Theorem 4.8) that the high contrast τ can essentially change the orders of these lower-order moments, and this kind of changes does not rely on the excitation of dielectric resonances.*

We proceed to approximate the scattering amplitude E^s_∞ with an error term of order $O(\delta^5)$ by using Lemma 4.5. For this, we need to compute the second-order approximation of the solution $\widetilde{E}$ to the system (4.9), and, in particular, the third-order approximation of $\mathbb{P}_{\rm w}\widetilde{E}$, since it holds that

$$\int_B \mathbb{P}_{\rm d}\widetilde{E}d\widetilde{y} = 0\,. \tag{4.12}$$

It requires us to expand $\mathbb{A}(\delta,\omega)^{-1}$ by the Neumann series to the second order:

$$\begin{aligned}\mathbb{A}(\delta,\omega)^{-1} =&(I+\delta\mathbb{A}_0^{-1}\mathbb{A}_1+\delta^2\mathbb{A}_0^{-1}\mathbb{A}_2+O(\delta^3))^{-1}\mathbb{A}_0^{-1}\\ =&(I-\delta\mathbb{A}_0^{-1}\mathbb{A}_1-\delta^2\mathbb{A}_0^{-1}\mathbb{A}_2+\delta^2(\mathbb{A}_0^{-1}\mathbb{A}_1)^2)\mathbb{A}_0^{-1}+O(\delta^3)\\ =&\mathbb{A}_0^{-1}-\delta\mathbb{A}_0^{-1}\mathbb{A}_1\mathbb{A}_0^{-1}-\delta^2\left(\mathbb{A}_0^{-1}\mathbb{A}_2\mathbb{A}_0^{-1}-(\mathbb{A}_0^{-1}\mathbb{A}_1)^2\mathbb{A}_0^{-1}\right)+O(\delta^3)\,.\end{aligned} \tag{4.13}$$

We actually have the following result by acting each term in the expansion (4.13) on $(\mathbb{P}_{\rm d}\widetilde{E}^i,\tau^{-1}\mathbb{P}_{\rm w}\widetilde{E}^i)$.

Proposition 4.7. *In the high contrast regime, $\tau\sim\delta^{-2}$, for real ω in a small neighborhood of ω_0, the solution to the equation* (4.9) *has the following representation:*

$$\begin{cases}\mathbb{P}_{\rm d}\widetilde{E} = C_{\rm m}\mathbb{P}_{\lambda_0}\widetilde{E}^i + \dfrac{\omega_0 c_\tau\tau^{-1}}{2(\omega-\omega_0)}\omega^2\mathbb{P}_{\lambda_0}\mathcal{K}_B^{\rm d,w}(\mathcal{T}_B|_W)^{-1}\mathbb{P}_{\rm w}\left[\widetilde{E}^i\right] + \mathcal{R}_{\rm w}^{\lambda_0}\mathbb{P}_{\rm d}\widetilde{E}^i + \mathbb{P}_{\rm d}O\left(\dfrac{\delta^3}{(\omega-\omega_0)^3}\right),\\ \mathbb{P}_{\rm w}\widetilde{E} = -\tau^{-1}(\mathcal{T}_B|_W)^{-1}\mathbb{P}_{\rm w}\left[\widetilde{E}^i\right] + \dfrac{\delta^2\omega^2\omega_0}{2(\omega-\omega_0)}(\mathcal{T}_B|_W)^{-1}\mathcal{K}_B^{\rm w,d}\mathbb{P}_{\lambda_0}\left[\widetilde{E}^i\right] + O(\delta^2)\mathbb{P}_{\rm w}\mathcal{R}(\omega)\mathbb{P}_{\rm d}\left[\widetilde{E}^i\right] + \mathbb{P}_{\rm w}O\left(\dfrac{\delta^4}{(\omega-\omega_0)^2}\right),\end{cases} \tag{4.14}$$

where $C_{\rm m}$ is a blow-up coefficient defined as

$$C_{\rm m} = \frac{-\omega_0}{2(\omega-\omega_0)} + \delta\frac{\omega_0^2 c_{-1}\omega^2\lambda_0}{4(\omega-\omega_0)^2}\,. \tag{4.15}$$

The detailed proof of the above proposition is given in Appendix E. From the representation formula (4.14), we clearly see the structures of the $H_0(\mathrm{div}0,B)$ and W components of $\widetilde{E}$, and the blow-up rate and the order of the amplitude of each term involved in it. After we remove the higher-order remainder terms and ignore the regular part (analytic part) in the low-order terms, we come to the dominant part of $\widetilde{E}$:

$$\begin{cases}\mathbb{P}_{\rm d}\widetilde{E} \sim C_{\rm m}\mathbb{P}_{\lambda_0}\widetilde{E}^i + \dfrac{\omega_0 c_\tau\tau^{-1}}{2(\omega-\omega_0)}\omega^2\mathbb{P}_{\lambda_0}\mathcal{K}_B^{\rm d,w}(\mathcal{T}_B|_W)^{-1}\mathbb{P}_{\rm w}\left[\widetilde{E}^i\right],\\ \mathbb{P}_{\rm w}\widetilde{E} \sim -\tau^{-1}(\mathcal{T}_B|_W)^{-1}\mathbb{P}_{\rm w}\left[\widetilde{E}^i\right] + \dfrac{\delta^2\omega^2\omega_0}{2(\omega-\omega_0)}(\mathcal{T}_B|_W)^{-1}\mathcal{K}_B^{\rm w,d}\mathbb{P}_{\lambda_0}\left[\widetilde{E}^i\right].\end{cases} \tag{4.16}$$

It is worth emphasizing that the dominant part of $\mathbb{P}_{\rm w}\widetilde{E}$ involves two terms, one is of order δ^2 while the other is of order δ^3 but with a blow-up rate $(\omega-\omega_0)^{-1}$.

We are now in a position to give the main results of this section based on the above results and discussions. We first observe from Proposition 4.7 that

$$\mathbb{P}_{\rm d}\widetilde{E} = O(\delta)\,,\quad \mathbb{P}_{\rm w}\widetilde{E} = O(\delta^2)\,,$$

which are nontrivial, essentially resulting from the upper triangular structure of $\mathbb{A}_0^{-1}$. Then it follows from Definition 4.2 that

$$\mathbf{M}_l^{\widetilde{E}} = O(\delta) \text{ for } l=1,2,\cdots\,,\quad \mathbf{Q}_l^{\widetilde{E}} = O(\delta^2) \text{ for } l=0,1,2,\cdots\,.$$

Thus, by Proposition 4.4 and Lemma 4.5, there are four moments involved, i.e., $\mathbf{Q}_l^{\widetilde{E}}$, $l=0,1$ and $\mathbf{M}_l^{\widetilde{E}}$, $l=1,2$, in order to achieve a fourth-order approximation of E^s_∞. This is summarized below.

Theorem 4.8. *In the high contrast regime, $\tau\sim\delta^{-2}$, the scattering amplitude E^s_∞ has the asymptotics:*

$$E^s_\infty(\hat{x}) = \frac{\tau\omega^2\delta^3}{4\pi}(\mathbb{I}-\hat{x}\otimes\hat{x})\Big\{\underbrace{\left(\mathbf{Q}_0^{\widetilde{E}} - i\delta\omega\mathbf{M}_1^{\widetilde{E}}\times\hat{x}\right)}_{O(\delta^2)} - \underbrace{\left(i\delta\omega\mathbf{Q}_1^{\widetilde{E}}\hat{x} + \frac{\delta^2\omega^2}{2}\mathbf{M}_2^{\widetilde{E}}(\cdot,\hat{x})\times\hat{x}\right)}_{O(\delta^3)}\Big\} + O(\delta^5)\,. \tag{4.17}$$

Theorem 4.8 helps us to clearly see the change of the orders of the multipole moments compared to those in the asymptotics (4.11), and theoretically justify the experimentally observed phenomenon [36]: when the wavelength inside the particle has the same order as its size (equivalently, $\tau\sim\delta^{-2}$), the electric and magnetic dipole radiations have the comparable strengths; see the first term in (4.17).

To consider the scattered wave from resonant nanoparticles with high refractive indices, we first observe from (4.16) that when the incident frequency ω approaches the resonance ω_0, compared to the strong singularity of $\mathbb{P}_{\rm d}\widetilde{E}$, the blow-up only occurs in the higher-order terms in the asymptotic expansion of $\mathbb{P}_{\rm w}\widetilde{E}$. In view of this fact, the high contrast nanoparticles are expected to exhibit a strong magnetic response at the dielectric resonant frequencies. This is in sharp contrast with the approximation derived in [10] in the non-resonant case.

By substituting (4.16) into the representation (4.17) and using Definition 4.2, we can conclude the following results.

Theorem 4.9. *Under the high contrast condition* (3.36), *for real incident frequency ω near the resonance ω_0, the principal part of E^s_∞ is given by*

$$E^s_\infty(\hat{x}) \sim \frac{\tau\omega^2\delta^3}{4\pi}(\mathbb{I}-\hat{x}\otimes\hat{x})\Big\{\underbrace{-i\delta\omega\widehat{\mathbf{M}}_1^{\widetilde{E}}\times\hat{x}}_{O(\delta^2)}+\underbrace{\widehat{\mathbf{Q}}_0^{\widetilde{E}}-\frac{\delta^2\omega^2}{2}\widehat{\mathbf{M}}_2^{\widetilde{E}}(\cdot,\hat{x})\times\hat{x}}_{O(\delta^3)}\Big\},$$

where the approximate moments $\widehat{\mathbf{Q}}_0^{\widetilde{E}}$, $\widehat{\mathbf{M}}_1^{\widetilde{E}}$ and $\widehat{\mathbf{M}}_2^{\widetilde{E}}$ are defined as

$$\begin{aligned}
\widehat{\mathbf{Q}}_0^{\widetilde{E}} &:= -\int_{\partial B} y(\frac{1}{2}+\mathcal{K}^*_{\partial B})^{-1}\big[\nu\cdot\hat{\phi}\big]d\sigma(y)\,, \quad \textit{with } \hat{\phi} = \frac{\delta^2\omega^2\omega_0}{2(\omega-\omega_0)}\mathcal{K}_B^{\rm w,d}\mathbb{P}_{\lambda_0}\big[\widetilde{E}^i\big]\,,\\
\widehat{\mathbf{M}}_1^{\widetilde{E}} &:= \widehat{C}_{\rm m}\int_B \varphi_0(y)dy\,, \quad \textit{with } \widehat{C}_{\rm m} = C_{\rm m}(\widetilde{E}^i,E_0)_{L^2(B)} + \frac{\omega^2\omega_0 c_\tau\tau^{-1}}{2(\omega-\omega_0)}(\mathcal{K}_B E_0, (\mathcal{T}_B|_W)^{-1}\mathbb{P}_{\rm w}\big[\widetilde{E}^i\big])\,,\\
\widehat{\mathbf{M}}_2^{\widetilde{E}} &:= \frac{-\omega_0}{(\omega-\omega_0)}(\widetilde{E}^i,E_0)_{L^2(B)}\int_B \varphi_0(y)\otimes y dy\,,
\end{aligned} \tag{4.18}$$

and the blow-up coefficient $C_{\rm m}$ is given in (4.15).

To find the principal part (4.18) of multipole moments, again we have omitted the terms of order larger than four and regular terms of lower order in (4.17). We have also utilized the following formula derived from the Green's formula (3.13),

$$\int_B (\mathcal{T}_B|_W)^{-1}[\varphi]dy = -\int_{\partial B} y(\frac{1}{2}+\mathcal{K}^*_{\partial B})^{-1}[\varphi\cdot\nu]d\sigma(y)\,, \quad \varphi\in W\,,$$

and the representations for $\mathbb{P}_{\lambda_0}$ and $\mathbb{P}_{\rm d}\widetilde{E}$:

$$\mathbb{P}_{\lambda_0}[\cdot] = (\cdot,E_0)_{L^2(B)}E_0\,, \quad \mathbb{P}_{\rm d}\widetilde{E} = \nabla\times\varphi_0\,, \text{ with } \varphi_0\in X_N^0(B)\,. \tag{4.19}$$

Remark 4.10. *We have assumed that the open set B has a trivial topology at the beginning of this section. To generalize the above analysis and results to the case where B has genus L greater than zero, it is sufficient to note from [38, Theorem 3.44] that any element ϕ from the orthogonal complement $K_T(B)$ of* $\mathrm{curl}X_N^0(B)$ *in* $H_0(\mathrm{div}0,B)$ *can be represented as*

$$\phi = \nabla p \quad \textit{for some } p\in H^1(B^0)\,.$$

Here B^0 is constructed by removing some interior cuts from B such that B^0 is a union of simply-connected domains; see [38, 12] for more details. Thus, $K_T(B)$ plays a very similar role to W in the scattering amplitude but generates a radiating field of order $O(\delta)$, and we can define the associated electric multipole moments like the ones in Definition 4.2. Then, with minor modifications, our main results and conclusions in this section still hold for the nanoparticles with a nontrivial topology.

On account of the formula (4.19) and the plane wave form of E^i, it follows that

$$(\widetilde{E}^i,E_0)_{L^2(B)} = i\delta\omega(\mathbf{d}\times\mathbf{E}_0^i e^{i\delta\omega\mathbf{d}\cdot x},\varphi_0)_{L^2(B)} = i\delta\omega(\mathbf{d}\times\mathbf{E}_0^i,\varphi_0)_{L^2(B)} + O(\delta^2)\,.$$

Then, as a direct corollary of Proposition 4.7, Theorem 4.8, we have the following quasi-static limit (leading-order approximation) of the scattering amplitude near the dielectric resonance ω_0, which will be used in the next section, and whose proof is omitted as it is similar to the one for Theorem 4.9.

Theorem 4.11. *Under the same assumptions as in Theorem 4.9, the scattering amplitude has the form:*

$$E^s_\infty = \frac{\omega^2}{4\pi}\{\hat{x}\times(\mathbf{p}\times\hat{x})+\mathbf{m}\times\hat{x}\}+O(\delta^4)\,, \tag{4.20}$$

where the approximate electric dipole $\mathbf{p}$ is given by

$$\mathbf{p} = \delta^3\int_{\partial B} y\otimes(\frac{1}{2}+\mathcal{K}^*_{\partial B})^{-1}[\nu]d\sigma(y)\mathbf{E}_0^i\,,$$

and the approximate magnetic dipole $\mathbf{m}$ *has the following pole-pencil expansion,*

$$\mathbf{m} = c_\tau \omega^2 \delta^3 \left\{ \frac{-\omega_0}{2(\omega-\omega_0)} \Big(\int_B \varphi_0 \otimes \int_B \overline{\varphi_0} \Big) \mathbf{d} \times \mathbf{E}_0^i + \mathcal{R}(\omega)\mathbf{E}_0^i \right\},$$

for ω *near the resonant frequency* ω_0*. Here* $\mathcal{R}(\omega)$ *is analytic matrix in a small neighborhood of* ω_0*.*

Scattering and absorption cross sections

This section is devoted to the estimates of the scattering and extinction rate, as well as the blow-up in the case where the particle is at a resonant state.

For this purpose, let us first briefly review some basic physical concepts from [19] for the description of the energy flow. We define the time-averaged Poynting vector $\langle \mathbf{S} \rangle$ for the electromagnetic field E and the associated averaged outward energy flow $\mathcal{W}$ through the large sphere S_R by

$$\langle \mathbf{S} \rangle := \mathfrak{Re}\left\{ E \times \overline{H} \right\}, \quad \mathcal{W} := \int_{S_R} \langle \mathbf{S} \rangle \cdot \nu d\sigma \,,$$

respectively. By the decomposition: $E = E^i + E^s$, we can write $\mathcal{W}$ as $\mathcal{W} = \mathcal{W}^i + \mathcal{W}^s + \mathcal{W}'$, where

$$\begin{aligned} \mathcal{W}^i &:= \int_{S_R} \mathfrak{Re}\left\{ E^i \times \overline{H^i} \right\} \cdot \nu d\sigma \,, \qquad \mathcal{W}^s := \int_{S_R} \mathfrak{Re}\left\{ E^s \times \overline{H^s} \right\} \cdot \nu d\sigma \,, \\ \mathcal{W}' &:= \int_{S_R} \mathfrak{Re}\left\{ E^i \times \overline{H^s} + E^s \times \overline{H^i} \right\} \cdot \nu d\sigma \,. \end{aligned}$$

It follows from a simple calculation that the energy flow $\mathcal{W}^i$ for the incident plane wave is zero. Then the conservation of energy gives us the rate of absorption $\mathcal{W}^a = -\mathcal{W} = -\mathcal{W}^s - \mathcal{W}'$. Therefore, $\mathcal{W}'$ is nothing but the rate at which the energy is dissipated by heat and scattering, referred to as the extinction rate. By the normalization to the incident energy flux, we define the scattering cross section Q^s, the absorption cross section Q^a and the extinction cross section Q', respectively, by

$$Q^s := \frac{\mathcal{W}^s}{|\langle \mathbf{S}^i \rangle|}, \quad Q^a := \frac{\mathcal{W}^a}{|\langle \mathbf{S}^i \rangle|}, \quad Q' := \frac{\mathcal{W}'}{|\langle \mathbf{S}^i \rangle|}\,,$$

where $|\langle \mathbf{S}^i \rangle| = \mathfrak{Re}\{E^i \times \bar{H}^i\}$. For the incident plane wave, we have $|\langle \mathbf{S}^i \rangle| = |\mathbf{E}_0^i|^2 = 1$, due to our assumption that $\mathbf{E}_0^i \in S$.

Note that in the far field, the scattered magnetic wave H^s has the form:

$$H^s(x) = \frac{e^{i\omega|x|}}{|x|} H^s_\infty(\hat{x}) + O\left(\frac{1}{|x|^2}\right), \text{ with } H^s_\infty(\hat{x}) = \hat{x} \times E^s_\infty(\hat{x}) \quad \text{as } |x| \to \infty \,.$$

Then we can compute and estimate Q^s directly as follows,

$$\begin{aligned} Q^s &= \int_{S_R} \mathfrak{Re}\left\{ E^s_\infty(\hat{x}) \times \overline{H}^s_\infty(\hat{x}) \right\} \cdot \nu(x) \frac{1}{R^2} d\sigma(x) + O\left(\frac{1}{R}\right) \\ &= \int_S |E^s_\infty(\hat{x})|^2 d\sigma(\hat{x}) + O\left(\frac{1}{R}\right) \quad \text{as } R \to \infty \,. \end{aligned} \tag{4.21}$$

The well-known optical cross section theorem [19] shows the following representation of the extinction rate:

$$Q' = \frac{4\pi}{\omega} \mathfrak{Im}\left\{ \mathbf{E}_0^i \cdot E^s_\infty(\mathbf{d}) \right\}. \tag{4.22}$$

With these preparations, we can now give the upper bounds of the cross sections.

Theorem 4.12. *Suppose that* τ *satisfies the condition* (3.36)*. When the incident frequency* ω *is near the resonance* ω_0*, the principal parts of the leading-order terms of the averages over the orientations of the scattering and extinction cross sections of a randomly oriented nanoparticle are given by*

$$Q^s_m \sim |c_\tau|^2 \delta^6 \frac{|\omega_0|^2 |\omega|^8}{|\omega-\omega_0|^2} \frac{4\pi}{27} \left| \int_B \varphi_0(y) dy \right|^4, \quad Q'_m \sim c_\tau \delta^3 \frac{-\omega_0 \omega^3}{\omega - \omega_0} \frac{16\pi^2}{9} \left| \int_B \varphi_0 dy \right|^2 .$$

Proof. By Theorem 4.11, when it is near the resonance ω_0, the scattering amplitude E^s_∞ is dominated by the resonant magnetic dipole moment, i.e.,

$$E^s_\infty(\hat{x}) \sim \frac{\omega^2}{4\pi}\hat{\mathbf{m}} \times \hat{x}\,, \tag{4.23}$$

where $\hat{\mathbf{m}}$ is the principal part of the magnetic dipole defined by

$$\hat{\mathbf{m}} = c_\tau \omega^2 \delta^3 \frac{-\omega_0}{2(\omega-\omega_0)}\Big(\int_B \varphi_0 \otimes \int_B \varphi_0\Big)\mathbf{d} \times \mathbf{E}^i_0\,. \tag{4.24}$$

We start with the computation of the scattering cross section Q^s. Noting from (4.21) and (4.23) that

$$Q^s = \int_S |E^s_\infty(\hat{x})|^2 d\sigma(\hat{x}) \sim \frac{|\omega|^4}{16\pi^2}\int_S |\hat{\mathbf{m}} \times \hat{x}|^2 d\sigma(\hat{x}) = \frac{|\omega|^4}{16\pi^2}\int_S |\hat{x} \times (\hat{\mathbf{m}} \times \hat{x})|^2 d\sigma(\hat{x})\,,$$

and $\hat{x} \times (\hat{\mathbf{m}} \times \hat{x}) = \hat{\mathbf{m}} - (\hat{x}\cdot\hat{\mathbf{m}})\hat{x}$, we derive

$$Q^s \sim \frac{|\omega|^4}{16\pi^2}\int_S |\hat{\mathbf{m}}|^2 - |(\hat{x}\cdot\hat{\mathbf{m}})|^2 d\sigma(\hat{x}) = \frac{|\omega|^4}{16\pi^2}\int_S |\hat{\mathbf{m}}|^2 - \hat{x}_j\hat{\mathbf{m}}^j\hat{x}^i\hat{\mathbf{m}}_i d\sigma(\hat{x}) = \frac{|\omega|^4}{6\pi}|\hat{\mathbf{m}}|^2\,,$$

where we have used the Einstein summation convention and the formula:

$$\int_S \hat{x}_i\hat{x}_j d\sigma(\hat{x}) = \frac{4\pi}{3}\delta_{ij}. \tag{4.25}$$

Then, it follows from the formula (4.24) that the average of the scattering cross section Q^s over all the directions of $\mathbf{E}^i_0$ and $\mathbf{d}$ can be estimated by

$$\begin{aligned} Q^s_m &\sim \frac{|\omega|^4}{6\pi}\int_S\int_S \left|\hat{\mathbf{m}}\left(\mathbf{d},\mathbf{E}^i_0\right)\right|^2 d\sigma(\mathbf{d})d\sigma(\mathbf{E}^i_0) \\ &= |c_\tau|^2|\omega|^4\delta^6\frac{|\omega_0|^2}{4|\omega-\omega_0|^2}\frac{|\omega|^4}{6\pi}\int_S\int_S |\mathbf{A}(\varphi)\mathbf{d}\times\mathbf{e}|^2 d\sigma(\mathbf{d})d\sigma(\mathbf{e})\,, \end{aligned} \tag{4.26}$$

where $\mathbf{A}(\varphi) := \int_B \varphi_0 \otimes \int_B \varphi_0$. To calculate this integral, we introduce the Levi-Civita symbol ε_{kij} to avoid the complicated vector and matrix calculations. First, we have the important property for the symbol ε_{kij}:

$$\varepsilon_{kij}\varepsilon^{kpq} = \delta^p_i\delta^q_j - \delta^p_j\delta^q_i\,. \tag{4.27}$$

Using this, we can derive for a general matrix $\mathbf{A} := (a_{ij})$:

$$\begin{aligned} &\frac{1}{(4\pi)^2}\int_S\int_S |\mathbf{A}\mathbf{d}\times\mathbf{e}|^2 d\sigma(\mathbf{d})d\sigma(\mathbf{e}) = \frac{1}{(4\pi)^2}\int_S\int_S a^{sk}\varepsilon_{kij}d^ie^ja_{sr}\varepsilon^{rpq}d_pe_q \\ =&\frac{1}{9}a^{sk}\varepsilon_{kij}\delta^i_p\delta^j_q a_{sr}\varepsilon^{rpq} = \frac{1}{9}a^{sk}a_{sr}\varepsilon_{kpq}\varepsilon^{rpq} = \frac{2}{9}a^{sk}a_{sr}\delta^r_k = \frac{2}{9}\operatorname{tr}\left(\mathbf{A}\mathbf{A}^T\right)\,, \end{aligned}$$

where we have used (4.27). For our special rank-one matrix $\mathbf{A}(\varphi)$, we have

$$\operatorname{tr}(\mathbf{A}(\varphi)\mathbf{A}(\varphi)^T) = \left|\int_B \varphi_0(y)dy\right|^4\,.$$

Combining the above formulas with (4.26), we immediately derive the desired estimate:

$$Q^s_m \sim |c_\tau|^2\delta^6\frac{|\omega_0|^2|\omega|^8}{|\omega-\omega_0|^2}\frac{4\pi}{27}\left|\int_B \varphi_0(y)dy\right|^4\,.$$

To consider the extinction cross section, we first observe from (4.22) and (4.23) that

$$Q' \sim \omega\,\mathfrak{Im}\left\{\mathbf{E}^i_0\cdot(\hat{\mathbf{m}}\times\mathbf{d})\right\}. \tag{4.28}$$

With the help of (4.24), we are led to the following approximation by taking the average of the scattering cross section Q^s over all the directions for $\mathbf{E}^i_0$ and $\mathbf{d}$:

$$Q'_m \sim c_\tau\omega^3\delta^3\frac{-\omega_0}{2(\omega-\omega_0)}\mathfrak{Im}\int_S\int_S \mathbf{E}^i_0\cdot\left(\left(\mathbf{A}(\varphi)\mathbf{d}\times\mathbf{E}^i_0\right)\times\mathbf{d}\right)d\sigma(\mathbf{d})d\sigma(\mathbf{E}^i_0)\,.$$

Similarly, by using Levi-Civita symbol, (4.27) and a direct calculation, we derive

$$\begin{aligned}
&\frac{1}{(4\pi)^2}\int_S\int_S \mathbf{e}\cdot((\mathbf{A}\mathbf{d}\times\mathbf{e})\times\mathbf{d})d\sigma(\mathbf{d})d\sigma(\mathbf{e}) = \frac{1}{(4\pi)^2}\int_S\int_S e_r\varepsilon^{rst}a_{sk}\varepsilon^{kij}d_ie_jd_t \\
=&\frac{1}{9}\varepsilon^{rst}a_{sk}\varepsilon^{kij}\delta_{it}\delta_{rj} = \frac{1}{9}\varepsilon^{rst}a_{sk}\varepsilon^{ktr} = \frac{2}{9}\operatorname{tr}(\mathbf{A})\,,
\end{aligned}$$

for a general matrix $\mathbf{A}$, which, along with (4.28), completes the estimate for Q'_m. □

Remark 4.13. *The above theorem considers only the contribution of the resonant magnetic dipole to the cross sections. A similar but much more involved calculation allows us to take into account of more multipole moments and derive sharper estimates for the cross sections.*

Explicit formulas for a spherical nanoparticle

In this section, we provide some explicit calculations for the special case of a single spherical nanoparticle to validate the general quasi-static approximation results for the dielectric subwavelength resonances and the scattering amplitude we established in the previous two sections (cf. Theorems 3.11 and 4.9) for nanoparticles of arbitrary shape.

Quasi-static dielectric resonance

This section is devoted to finding the explicit formulas for the dielectric resonances and the associated resonant modes for a spherical nanoparticle in the quasi-static limit, equivalently, solving the eigenvalue problem associated with the operator $\mathcal{K}_B^{\mathrm{d,d}}$. The calculations are carried out by using the spherical multipole expansion and the following proposition.

Proposition 5.1. *Suppose that B is a bounded smooth open set. $\lambda > 0$ is an eigenvalue of $\mathcal{K}_B^{\mathrm{d,d}}$ if and only if the following system has a nontrivial solution in $H^2_{loc}(\mathbb{R}^3,\mathbb{R}^3)$ with $k^2 = \lambda^{-1}$,*

$$\begin{cases}
\nabla\times\nabla\times u = 0\,,\ \operatorname{div} u = 0 & \text{in } \mathbb{R}^3\backslash\bar{B}\,,\\
\nabla\times\nabla\times(u - \widetilde{\gamma}_n^{-1}\gamma_n u) = k^2(u - \widetilde{\gamma}_n^{-1}\gamma_n u) & \text{in } B\,,\\
[\nu\times u] = 0\,,\ [\nu\cdot u] = 0\,,\ [\nu\times\nabla\times u] = 0 & \text{on } \partial B\,,\\
u = O(|x|^{-2}) & \text{as } |x|\to\infty\,.
\end{cases} \tag{5.1}$$

Moreover, for a solution u to the above system, $u - \widetilde{\gamma}_n^{-1}\gamma_n u$ is an eigenfunction of $\mathcal{K}_B^{\mathrm{d,d}}$ associated with the eigenvalue $\lambda = k^{-2}$.

Proof. Suppose that $(\lambda, E) \in \mathbb{C}\times H_0(\operatorname{div}0, B)$ is an eigenpair for the operator $\mathcal{K}_B^{\mathrm{d,d}}$ and define $u = \mathcal{K}_B[E] \in H^2_{loc}(\mathbb{R}^3,\mathbb{R}^3)$. By the density argument and an integration by parts, we readily have $\operatorname{div} u = 0$ on the whole space $\mathbb{R}^3$ and

$$\mathcal{K}_B[E](x) = \int_B\left(\frac{1}{4\pi|x-y|} - \frac{1}{4\pi|x|}\right)E(y)dy = O\left(\frac{1}{|x|^2}\right) \quad \text{as } |x|\to\infty\,,$$

due to (4.12) and the mean-value theorem. We can then verify that u satisfies

$$\begin{cases}
-\Delta u = E\chi_B,\ \operatorname{div} u = 0 & \text{in } \mathbb{R}^3\,,\\
\quad u = O(|x|^{-2}) & \text{as } |x|\to\infty\,.
\end{cases} \tag{5.2}$$

By means of the vector identity curlcurl $= \nabla\mathrm{div} - \Delta$, we can reformulate the equation (5.2) as

$$\begin{cases}
\nabla\times\nabla\times u = E\chi_B,\ \operatorname{div} u = 0 & \text{in } \mathbb{R}^3\,,\\
u = O(|x|^{-2}) & \text{as } |x|\to\infty\,.
\end{cases} \tag{5.3}$$

To proceed, we note from the above system that

$$\nabla\times\nabla\times\mathcal{K}_B[E] = \nabla\times\nabla\times\lambda E = E\chi_B \quad \text{in } B\,,$$

since $\nabla\times\mathcal{K}_B[E] = \nabla\times\mathcal{K}_B^{\mathrm{d,d}}[E]$ and $\mathcal{K}_B^{\mathrm{d,d}}[E] = \lambda E$ hold on B, which further implies that 0 is not an eigenvalue of $\mathcal{K}_B^{\mathrm{d,d}}$. Then, by using the formula $\mathcal{K}_B^{\mathrm{d,d}}[E] = \mathcal{K}_B[E] - \widetilde{\gamma}_n^{-1}\gamma_n\mathcal{K}_B[E]$ in B for $E\in H_0(\operatorname{div}0, B)$, it follows from the system (5.3) that u solves the following equation in the variational sense:

$$\begin{cases} \nabla\times\nabla\times u = 0\,,\ \operatorname{div} u = 0 & \text{in } \mathbb{R}^3\backslash\bar{B}\,, \\ \nabla\times\nabla\times(u-\widetilde{\gamma}_n^{-1}\gamma_n u) = \dfrac{1}{\lambda}(u-\widetilde{\gamma}_n^{-1}\gamma_n u) & \text{in } B\,, \\ [\nu\times u]=0\,,\ [\nu\cdot u]=0\,,\ [\nu\times\nabla\times u]=0 & \text{on } \partial B\,, \\ u = O(|x|^{-2}) & \text{as } |x|\to\infty\,. \end{cases} \tag{5.4}$$

Letting λ in the above system be k^{-2} for some non-zero real k due to the positive-definiteness of $\mathcal{K}_B^{\mathrm{d,d}}$, we obtain the desired equivalent system (5.1). Conversely, if u satisfies (5.4) in the variational sense with $\lambda > 0$, then curl$u$, curlcurl$u$ and div$u$ are globally well-defined on $\mathbb{R}^3$ with locally L^2-regularities. Thus, we have $u \in H^2_{loc}(\mathbb{R}^3,\mathbb{R}^3)$ solves

$$\begin{cases} -\Delta u = \dfrac{1}{\lambda}(u-\widetilde{\gamma}_n^{-1}\gamma_n u)\chi_B,\ \operatorname{div} u = 0 & \text{in } \mathbb{R}^3\,, \\ \quad u = O(|x|^{-2}) & \text{as } |x|\to\infty\,, \end{cases} \tag{5.5}$$

where we have used the fact [12] that the space $H_{loc}(\mathrm{curl},\mathbb{R}^3)\bigcap H_{loc}(\mathrm{div},\mathbb{R}^3)$ is contained in $H^1_{loc}(\mathbb{R}^3,\mathbb{R}^3)$. The proof is completed by the uniqueness of the solution to the system (5.2) for a given $E \in H_0(\mathrm{div}0, B)$. □

We emphasize that the above proposition can be applied to nanoparticles with arbitrary shape and the form of equation (5.1) is chosen mainly for the purpose of explicit calculation. By Proposition 5.1, once we obtain the nontrivial solutions to the system (5.1) and the associated k^2, we can determine the eigenstructure of $\mathcal{K}_B^{\mathrm{d,d}}$.

For this, we shall use the series expansions of the solution. By the entire electric multipole fields (cf. (C.6)-(C.7)), we assume that for a nontrivial solution $u \in H^2_{loc}(\mathbb{R}^3,\mathbb{R}^3)$ to (5.1), $u-\widetilde{\gamma}_n^{-1}\gamma_n u$ has the following form inside B:

$$u(x)-\widetilde{\gamma}_n^{-1}\gamma_n u(x) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n}\alpha_{n,m}\widetilde{E}^{TE}_{n,m}(k,x)+\beta_{n,m}\widetilde{E}^{TM}_{n,m}(k,x)\,,\quad x\in B\,. \tag{5.6}$$

Moreover, by Lemma 3.3, $\widetilde{\gamma}_n^{-1}\gamma_n u$ is the gradient of a solution v to the interior Neumann problem (3.7) with boundary condition $\frac{\partial}{\partial\nu}v = \nu\cdot u$. We hence have the following series representation for $\widetilde{\gamma}_n^{-1}\gamma_n u$:

$$\begin{aligned} \widetilde{\gamma}_n^{-1}\gamma_n u(x) &= \sum_{n=1}^{\infty}\sum_{m=-n}^{n}\frac{c_{n,m}}{n}\nabla\left(|x|^n Y_n^m(\hat{x})\right) \\ &= \sum_{n=1}^{\infty}\sum_{m=-n}^{n}\frac{c_{n,m}}{n}\left(|x|^{n-1}\nabla_S Y_n^m(\hat{x})+n|x|^{n-1}Y_n^m(\hat{x})\hat{x}\right)\,,\quad x\in B\,. \end{aligned} \tag{5.7}$$

For the field u outside the domain B, by making use of some multipole fields $\{E^h_{n,m}\}$ (see the construction in Appendix D and Proposition D.1), we can assume that it has the following ansatz:

$$u = \sum_{n=1}^{\infty}\sum_{m=-n}^{n}\gamma_{n,m}E^h_{n,m}+\eta_{n,m}\nabla\times E^h_{n,m}\,,\quad x\in\mathbb{R}^3\backslash\bar{B}\,, \tag{5.8}$$

due to $\int_S \nu\cdot u d\sigma$ following from div$u = 0$ on $\mathbb{R}^3$. Here, $\alpha_{n,m},\beta_{n,m},\gamma_{n,m},\eta_{n,m},c_{n,m}$ in (5.6), (5.7) and (5.8) are complex coefficients to be further determined by matching the traces of the field u inside and outside B.

Then we have the main result of this section, whose proof is given in Appendix F.

Theorem 5.2. *Suppose that $\{k_{n,s}\}_{s=0}^{\infty}$ are the positive zeros of $j_n(z)$, $n \geq 0$, such that $k_{n,1}\leq k_{n,2}\leq\cdots$. For the spherical nanoparticle $B(0,1)$, the eigenvalues of $\mathcal{K}_B^{\mathrm{d,d}}$ is given by $1/k^2_{n,s}$, $n = 0,1,2,3,\cdots$ and $s = 1,2,\cdots$. The associated eigenspace is spanned by $\{\widetilde{E}^{TE}_{n+1,m}(k_{n,s},x)\}_{m=-(n+1)}^{n+1}$ and $\{\widetilde{E}^{TM}_{n,m}(k_{n,s},x)\}_{m=-n}^{n}$ for $n\geq 1$. For the case $n = 0$, the associated eigenspace is spanned by $\{\widetilde{E}^{TE}_{1,m}(k_{0,s},x)\}_{m=-1}^{1}$.*

Remark 5.3. *By the interlacing of zeros of Bessel functions J_ν [44], we have that $1/k^2_{0,1} = 1/\pi^2$ and $1/k^2_{1,1}$ are the first and second largest eigenvalues of $\mathcal{K}_B^{\mathrm{d,d}}$, i.e., λ_0 and λ_1 in Proposition 3.6, corresponding to the magnetic and electric dipole resonances by the Mie theory.*

Remark 5.4. *The approach developed in [15] can be generalized to compute the first Hadamard variation of the dielectric resonances.*

Validation of the quasi-static approximation

We revisit the scattering problem (2.4), with $D = B(0,\delta)$ with a high contrast τ satisfying (3.36). We first recall the Jacobi-Anger expansion for the plane wave (2.2):

$$E^i(x) = e^{i\omega \mathbf{d}\cdot x}\mathbf{E}_0^i = -\sum_{n=1}^{\infty}\frac{4\pi i^n}{\sqrt{n(n+1)}}\sum_{m=-n}^{n}\widetilde{E}_{n,m}^{TE}(\omega,x)\overline{V_n^m}(\mathbf{d})\cdot\mathbf{E}_0^i + \widetilde{E}_{n,m}^{TM}(\omega,x)\overline{U_n^m}(\mathbf{d})\cdot\mathbf{E}_0^i\,,\quad x\in\mathbb{R}^3\,.$$

Denoting by ω_τ the wave number $\omega\sqrt{1+\tau}$ inside the particle, we have the following result by Mie scattering theory, which was proved in [8, Lemma A.2].

Lemma 5.5. *The scattered wave $E^s = E - E^i$ has the following representation: for $|x| > \delta$,*

$$E^s(x) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n}\gamma_{n,m}E_{n,m}^{TE}(\omega,x) + \eta_{n,m}E_{n,m}^{TM}(\omega,x)\,,$$

where the coefficients $\gamma_{n,m}$ and $\eta_{n,m}$ are given by

$$\begin{aligned}\gamma_{n,m} &= \frac{4\pi i^n\overline{V_n^m}(\mathbf{d})\cdot\mathbf{E}_0^i}{\sqrt{n(n+1)}}\cdot\frac{-j_n(\delta\omega_\tau)\mathcal{J}_n(\delta\omega)+\mathcal{J}_n(\delta\omega_\tau)j_n(\delta\omega)}{h_n^{(1)}(\delta\omega)\mathcal{J}_n(\delta\omega_\tau)-j_n(\delta\omega_\tau)\mathcal{H}_n(\delta\omega)}\,,\\ \eta_{n,m} &= \frac{4\pi i^n\overline{U_n^m}(\mathbf{d})\cdot\mathbf{E}_0^i}{\sqrt{n(n+1)}}\,\frac{\frac{1}{1+\tau}\mathcal{J}_n(\delta\omega_\tau)j_n(\delta\omega)-j_n(\delta\omega_\tau)\mathcal{J}_n(\delta\omega)}{\frac{1}{1+\tau}h_n^{(1)}(\delta\omega)\mathcal{J}_n(\delta\omega_\tau)-j_n(\delta\omega_\tau)\mathcal{H}_n(\delta\omega)}\,.\end{aligned}\tag{5.9}$$

Remark 5.6. *The multipole fields $\widetilde{E}_{n,m}^{TE}$ and $\widetilde{E}_{n,m}^{TM}$ are usually referred to as the magnetic (transverse electric) multipole modes and electric (transverse magnetic) multipole modes, specifying the EM radiations from the electric-charge density and the magnetic-moment density of order (n,m), respectively [32, Section 9.7]. For this reason, the coefficients $\gamma_{n,m}$ and $\eta_{n,m}$ may be called the magnetic and electric coefficients respectively [43].*

From Lemma 5.5, we clearly see that the dielectric resonances are characterized by the complex zeros of denominators of $\gamma_{n,m}$ and $\eta_{n,m}$, that is,

$$\begin{aligned}&h_n^{(1)}(\delta\omega)/\mathcal{H}_n(\delta\omega)\mathcal{J}_n(\delta\omega_\tau)-j_n(\delta\omega_\tau)=0\,,\\ &(1+\tau)^{-1}h_n^{(1)}(\delta\omega)/\mathcal{H}_n(\delta\omega)\mathcal{J}_n(\delta\omega_\tau)-j_n(\delta\omega_\tau)=0\,.\end{aligned}$$

If the condition (3.36) holds, letting δ in the above formulas tend to zero permits us to see

$$-n^{-1}\mathcal{J}_n(\widetilde{\omega}c_\tau^{-1/2})-j_n(\widetilde{\omega}c_\tau^{-1/2})=0\,,\ \text{and}\ j_n(\widetilde{\omega}c_\tau^{-1/2})=0\,,\tag{5.10}$$

respectively, since $h_n^{(1)}(\delta\omega)/\mathcal{H}_n(\delta\omega)\to -n^{-1}$ as $\delta\to 0$. Here $\widetilde{\omega}$ is the quasi-static limit of ω, i,e, $\widetilde{\omega}=\lim_{\delta\to 0}\omega(\delta)$. As we shall see from the proof of Theorem 5.2 in Appendix F, the formula (5.10) has actually validated our quasi-static approximation for the dielectric resonances. To numerically verify the order of the approximation, we consider the lowest dielectric resonance, which is perturbed from π; see Remark 5.3. We plot the zeros of $f(\omega) := h_n^{(1)}(\delta\omega)\mathcal{J}_n(\delta\omega_\tau)-j_n(\delta\omega_\tau)\mathcal{H}_n(\delta\omega)$, using the Muller's method [3] with the initial value π, for $\tau=\delta^{-2}$ and $\delta\in(0,0.22)$ in Figure 1.

We then immediately observe from Figure 1 the red-shift phenomenon for the resonance $\omega(\delta)$ with increasing δ (see Remark 3.20), and that the error between the quasi-static resonance ω and the dielectric resonant frequency $\omega(\delta)$ is bounded by a term of order $O(\delta^2)$ as $\delta\to 0$.

To proceed our validation of the quasi-static approximate formula (4.20) for the scattering amplitude near the lowest dielectric resonance, we have the following asymptotic estimates for the coefficients $\gamma_{n,m}$ and $\eta_{n,m}$ in the regime $\tau\sim\delta^{-2}$ (cf. (C.14)-(C.16)):

$$\gamma_{n,m}=\frac{4\pi i^n\overline{V_n^m}(\mathbf{d})\cdot\mathbf{E}_0^i}{\sqrt{n(n+1)}}\cdot\begin{cases}\dfrac{i}{3}(\delta\omega)^3\dfrac{-2j_1(\delta\omega_\tau)+\mathcal{J}_1(\delta\omega_\tau)}{\mathcal{J}_1(\delta\omega_\tau)+j_1(\delta\omega_\tau)}+O\left(\dfrac{\delta^5}{\mathcal{J}_1(\delta\omega_\tau)+j_1(\delta\omega_\tau)}\right) & n=1\,,\\ O\left(\dfrac{\delta^{2n+1}}{\frac{1}{n}\mathcal{J}_n(\delta\omega_\tau)+j_n(\delta\omega_\tau)}\right) & n\geq 2\,,\end{cases}\tag{5.11}$$

and

$$\eta_{n,m}=\frac{4\pi i^n\overline{U_n^m}(\mathbf{d})\cdot\mathbf{E}_0^i}{\sqrt{n(n+1)}}\cdot\left\{\frac{\mathcal{J}_n(\delta\omega)}{\mathcal{H}_n(\delta\omega)}+O\left(\frac{\delta^{2n+3}}{j_n(\delta\omega_\tau)}\right)\right\}\,,\quad n\geq 1\,.\tag{5.12}$$

We remark that the above estimates do not depend on whether the dielectric subwavelength resonances are excited. It is evident from the estimates (5.11) and (5.12) that when $\delta\omega_\tau$ approaches the positive zeros of $j_0(z)$, $\gamma_{1,m}$ will blow up

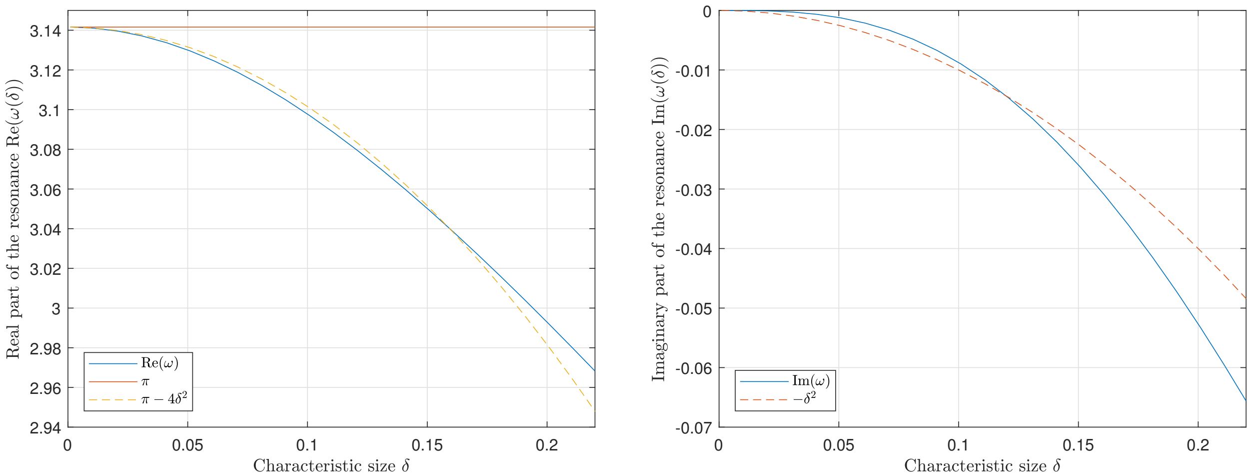


Figure 1: Dielectric subwavelength resonances ω for a spherical nanoparticle with radius $\delta \in (0, 0.22)$ and the contrast $\tau = \delta^{-2}$.

with an order of $\delta^3 / j_0(\delta\omega_\tau)$ while other coefficients remain regular; when $\delta\omega_\tau$ approaches the positive zeros of $j_n(z)$, $n \geq 1$, both coefficients $\gamma_{n,m}$ and $\eta_{n,m}$ blow up but the blow-up of $\eta_{n,m}$ occurs only at a higher order. It is analogous to the finding in the previous section that the blow-up of $\mathbb{P}_{\mathrm{w}}\widetilde{E}$ is from the higher-order terms in its asymptotic form; see the discussion before Theorem 4.9.

By estimates (5.11) and (5.12), Lemma 5.5 gives us the following quasi-static approximation for E^s and its principle part when $\delta\omega_\tau$ is near $k_{0,1} = \pi$:

$$E^s = \sum_{m=-1}^{1} \gamma_{1,m} E^{TE}_{1,m} + \eta_{1,m} E^{TM}_{1,m} + O(\delta^5) \sim \sum_{m=-1}^{1} \hat{\gamma}_m E^{TE}_{1,m} \,,$$

where $\hat{\gamma}_m$ is defined by ignoring the higher-order remainder term of $\gamma_{1,m}$:

$$\hat{\gamma}_m = -(\delta\omega)^3 \frac{2\sqrt{2}\pi}{3} \cdot \frac{-2j_1(\delta\omega_\tau) + \mathcal{J}_1(\delta\omega_\tau)}{\mathcal{J}_1(\delta\omega_\tau) + j_1(\delta\omega_\tau)} \overline{V_1^m}(\mathbf{d}) \cdot \mathbf{E}_0^i \,. \tag{5.13}$$

Then the scattering amplitude can be approximated by (cf. (C.12))

$$\hat{E}^s_\infty(\hat{x}) = \sum_{m=-1}^{1} \frac{\sqrt{2}}{\omega} \hat{\gamma}_m V_1^m(\hat{x}) \,.$$

Recalling the definition of the vector spherical harmonics (C.1) and denoting by $\mathbf{Y}_j$ the vector $\nabla(|x| Y_1^j(\hat{x}))$ (cf. (C.5)), then we have

$$\hat{E}^s_\infty(\hat{x}) = \sum_{m=-1}^{1} \frac{1}{\omega} \hat{\gamma}_m \hat{x} \times \mathbf{Y}_m \,.$$

Comparing with the form (4.20), we obtain the approximate magnetic dipole for a spherical nanoparticle:

$$\widetilde{\mathbf{m}} = -\sum_{j=-1}^{1} \frac{4\pi}{\omega^3} \hat{\gamma}_j \mathbf{Y}_j \,,$$

which, along with (5.13), gives us

$$\widetilde{\mathbf{m}} = \delta^3 \frac{8\pi^2}{3} \cdot \frac{2j_1(\delta\omega_\tau) - \mathcal{J}_1(\delta\omega_\tau)}{\mathcal{J}_1(\delta\omega_\tau) + j_1(\delta\omega_\tau)} \sum_{j=-1}^{1} \mathbf{Y}_j \otimes \overline{\mathbf{Y}}_j (\mathbf{d} \times \mathbf{E}_0^i) \,, \tag{5.14}$$

where we have used

$$\overline{V_1^m}(\mathbf{d}) \cdot \mathbf{E}_0^i = -\frac{1}{\sqrt{2}} \overline{\mathbf{Y}}_m \cdot (\mathbf{d} \times \cdot \mathbf{E}_0^i) \,.$$

The explicit representation for the magnetic dipole (5.14) motives us to define a scattering function:

$$\widetilde{s}_m(\omega) = \frac{8\pi^2}{3} \cdot \frac{2j_1(\delta\omega_\tau) - \mathcal{J}_1(\delta\omega_\tau)}{\mathcal{J}_1(\delta\omega_\tau) + j_1(\delta\omega_\tau)} \,. \tag{5.15}$$

We shall numerically compare it with the one derived from the general formula in Theorem 4.11. By generalizing Theorem 4.11 to the case of multidimensional eigenspace, we obtain the following representation for the approximate magnetic dipole:

$$\hat{\mathbf{m}} = c_\tau \omega^2 \delta^3 \frac{-\omega_0}{2(\omega-\omega_0)} \sum_{j=-1}^{1} \Big(\int_{B(0,1)} \varphi_j \otimes \int_{B(0,1)} \overline{\varphi_j} \Big) \mathbf{d} \times \mathbf{E}_0^i \,, \tag{5.16}$$

where φ_j are the potentials chosen from X_N^0 such that $\nabla \times \varphi_j = \widetilde{E}_{1,j}^{TE} / \left\| \widetilde{E}_{1,j}^{TE} \right\|_{L^2(B)}$. Here, ω_0 is the quasi-static resonance, i.e., $\omega_0 = (c_\tau)^{-1/2} k_{0,1} = (c_\tau)^{-1/2}\pi$. Recalling the definition of $\widetilde{E}_{1,j}^{TE}$ (C.6)), we know

$$\int_{B(0,1)} |\widetilde{E}_{1,j}^{TE}(\pi, x)|^2 dx = \int_0^1 2 j_1(\pi r) j_1(\pi r) r^2 dr = \frac{1}{\pi^2} \,,$$

by the Lommel's integral [44]: $\int_0^1 j_n(ar) j_n(ar) r^2 dr = \frac{1}{2}\big(j_n^2(a) - j_{n+1}(a) j_{n-1}(a)\big)$, and then introduce $\varphi_j \in X_N^0$ as follows:

$$\varphi_j(x) = \pi x j_1(\pi |x|) Y_1^j(\hat{x}) + \nabla p_j \,.$$

Here, $p_j \in H_0^1(B(0,1))$ is constructed such that $\mathrm{div}\varphi_j = 0$, by solving a Laplacian Dirichlet problem (cf. [5, Appendix A]). It further follows that, by (C.2)-(C.4) and (4.25),

$$\int_{B(0,1)} \varphi_j dx = \pi \int_0^1 r^3 j_1(\pi r) dr \int_S \hat{x} Y_1^j(\hat{x}) d\sigma(\hat{x}) = \frac{4}{\pi} \mathbf{Y}_j \,,$$

due to $\int_{B(0,1)} \nabla p_j dx = 0$. By substituting the above formula into (5.16), we obtain

$$\hat{\mathbf{m}} = c_\tau \omega^2 \delta^3 \frac{-\omega_0}{2(\omega-\omega_0)} \frac{16}{\pi^2} \sum_{j=-1}^{1} \mathbf{Y}_j \otimes \overline{\mathbf{Y}}_j \mathbf{d} \times \mathbf{E}_0^i \,, \tag{5.17}$$

which gives us another scattering function:

$$\hat{s}_m(\omega) = -\frac{8}{\pi^2} \frac{\omega^2 \omega_0 c_\tau}{\omega - \omega_0} \,. \tag{5.18}$$

We plot the scattering functions $\widetilde{s}_m$ and $\hat{s}_m$ in Figure 2 with $c_\tau = 1$, $c_i = 0$ in (3.36) and $\delta = 0.15$, from which we see that the explicit scattering function $\widetilde{s}_m$ agrees very well with $\hat{s}_m$ derived from our general results (cf. Theorem 4.11).

Concluding remarks and discussions

In this work, we have provided a comprehensive investigation of the EM scattering by a strongly-coupled non-magnetic nanoparticles system with high refractive indices. The geometry of the particles can be of very general shape, e.g., a torus with a hole. We have observed that both the surface plasmon resonance and the dielectric subwavelength resonance are closely related to the integral operator $\mathcal{T}_D^\omega$, but with very different underlying mechanism. For the dielectric resonances, we have showed, under the condition $\tau \sim \delta^{-2}$ (see [36] for the experimental evidence), that a dielectric resonance $\omega(\delta,\tau)$ can be approximated by $(\lambda_i \delta^2 \tau)^{-1/2}$ with a second-order accuracy and the corresponding resonant mode behaves like a magnetostatic field. The existence of the dielectric resonance has also been guaranteed by using the Gohberg-Sigal theory under the essentially same but more precise condition. Because of the low losses of dielectric nanostructures ($\mathfrak{Im}\tau \ll 1$; see Figure A.1), the dielectric resonance $\omega(\delta,\tau) \approx (\lambda_i \delta^2 \tau)^{-1/2}$ can have a very high quality factor $Q = |\mathfrak{Re}\omega / \mathfrak{Im}\omega|$, which is a desirable property in many potential applications and gives rise to the superior performance of the all-dielectric metamaterials over the lossy plasmonic devices.

To explore the behavior of the scattering amplitude, we have proposed a new approach to derive the electromagnetic multipole moment expansion based on the Helmholtz decomposition, which is reported in the literature for the first time, to the best of our knowledge. We have theoretically found that the high contrast can weaken the electric responses of the nanoparticles and correspondingly the magnetic responses are enhanced. These points have been illustrated by Theorems 4.8 and 4.9. In particular, at the resonant frequency, the scattered field by nanoparticles with high refractive indices is dominated by the resonant magnetic dipole radiation (cf. Theorem 4.11), which is different

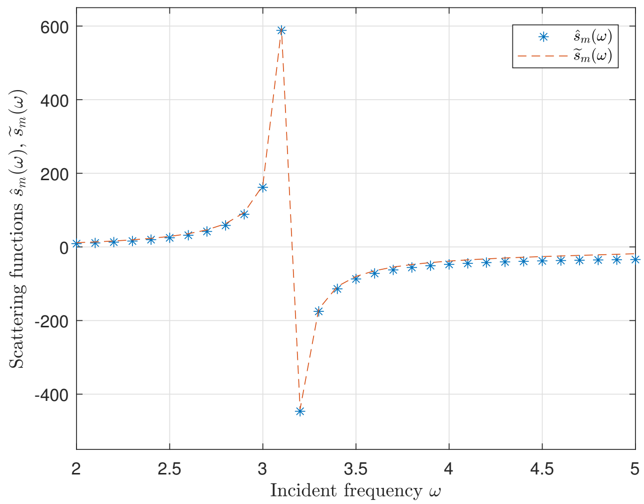


Figure 2: Scattering functions $\widetilde{s}_m(\omega)$ and $\hat{s}_m(\omega)$ for incident frequencies near the quasi-static resonance $\omega_0 = \pi$ with $\delta = 0.15$ and $\tau = 0.15^{-2}$.

from the plasmonic case where the non-magnetic particles are approximated by a resonant electric dipole [8]. We have also expressed the scattering and absorption cross sections in terms of quasi-static resonant potentials and considered their enhancement.

In a forthcoming paper, we plan to combine the results obtained in this paper on the subwavelength resonances in dielectric nanoparticles with high refractive index together with the effective medium approaches in [11, 4, 21] for the design of all-dielectric, electromagnetic metamaterials.

Justification of the asymptotic regime

To verify the quasi-static regime where we do the asymptotic analysis and the high contrast relation $\tau = O(\delta^{-2})$ we obtain theoretically, we give the values of the physical parameters used in the practical experiment [36, 27], where the dielectric resonance and the strong magnetic response are observed. For the scattering by a silicon nanoparticle in the free space, we have

$$\mu_{\mathrm{m}} \sim 12 \times 10^{-7}\mathrm{H} \cdot \mathrm{m}^{-1}\,,\ \varepsilon_{\mathrm{m}} \sim 9 \times 10^{-12}\mathrm{F} \cdot \mathrm{m}^{-1}\,,\ c \sim 3 \times 10^{8}\mathrm{m} \cdot \mathrm{s}^{-1}$$

for the background medium;

$$\mu_r \sim 1\,,\ \varepsilon_r \sim [10, 50]\,;\ \delta \sim [50, 200] \times 10^{-9}\mathrm{m}$$

for the silicon nanoparticle;

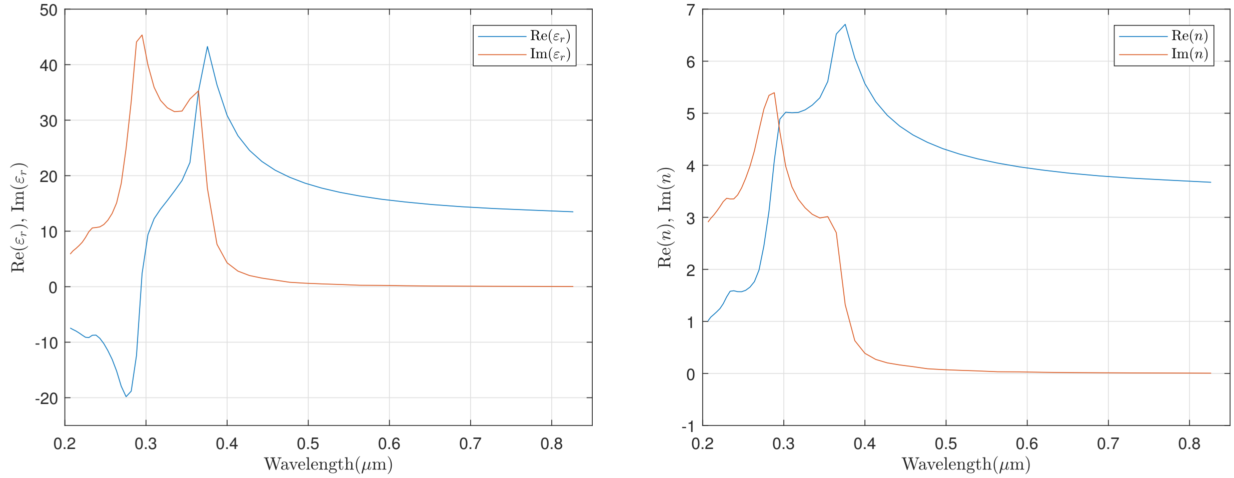
$$\omega \sim 2\pi \times [350, 650] \times 10^{12}\mathrm{Hz}\,,\ \lambda = \frac{2\pi c}{\omega} \sim [461, 850] \times 10^{-9}\mathrm{m}$$

for in the incident wave. Then, we see that when the resonance happens, the wavelength inside the particle is comparable with the particle size, equivalently, $\delta/\lambda \sim \varepsilon_r^{-1/2}$. We also plot in Figure A.1 the experimentally measured values of the relative electric permittivity, as well as the refractive index, of silicon as a function of the incident wavelength [16]. We see that in the visible region, the refractive index n has a very small imaginary part and is nearly the real constant 4.

Trace of the finite rank operator

We provide a framework to calculate the trace of a finite rank operator T on a Banach space X. Suppose that the range of $T : X \to X$ is spanned by the basis $\{v_k\}_{k=1}^n \subset X$, with its dual set in X^* given by $\{v_k^*\}_{k=1}^n$, i.e., $\langle v_i^*, v_j\rangle_X = \delta_i^j$. Then, the following representation of T readily follows,

$$Tx = \sum_{k=1}^{n} \langle v_k^*, Tx\rangle_X v_k\,.$$



(a) Relative electric permittivity

(b) Refractive index

Figure A.1: Relative electric permittivity and refractive index for silicon.

With the help of the above representation, the trace of T is given by

$$\mathrm{tr}(T) = \sum_{k=1}^{n} \langle v_k^*, T v_k \rangle_X . \tag{B.1}$$

By some fundamental algebraic calculations, we can check that the definition in (B.1) is independent of the choice of the basis $\{v_k\}$. If X is a Hilbert space, we may replace the dual pairing $\langle \cdot, \cdot \rangle_X$ in the above formulas with the inner product $(\cdot, \cdot)_X$. In this case, v_i^* is given by v_i if v_i is normalized, i.e., $\|v_i\|_X = 1$.

Some definitions, asymptotics and estimates

- Let $Y_n^m(\hat{x})$, $n = 0, 1, 2, \cdots$, $m = -n, \cdots, n$, be the spherical harmonics on the unit sphere S, which are the eigenfunctions of the Laplace-Beltrami operator: $\Delta_S Y_n^m(\hat{x}) + n(n+1) Y_n^m(\hat{x}) = 0$. Define the vector spherical harmonics as follows:

$$U_n^m = \frac{1}{\sqrt{n(n+1)}} \nabla_S Y_n^m , \quad V_n^m = \hat{x} \times U_n^m , \; n = 1, 2, \cdots , \; m = -n, \cdots, n . \tag{C.1}$$

For $n = 1$, $m = -1, 0, 1$, the spherical harmonics $Y_n^m(\hat{x})$ can be explicitly represented as:

$$Y_1^{-1}(\hat{x}) = \frac{1}{2}\sqrt{\frac{3}{2\pi}} \sin\theta e^{-i\varphi} = \frac{1}{2}\sqrt{\frac{3}{2\pi}} (\hat{x}_1 - i\hat{x}_2) , \tag{C.2}$$

$$Y_1^{1}(\hat{x}) = -\frac{1}{2}\sqrt{\frac{3}{2\pi}} \sin\theta e^{i\varphi} = -\frac{1}{2}\sqrt{\frac{3}{2\pi}} (\hat{x}_1 + i\hat{x}_2) , \tag{C.3}$$

$$Y_1^{0}(\hat{x}) = \frac{1}{2}\sqrt{\frac{3}{\pi}} \cos\theta = \frac{1}{2}\sqrt{\frac{3}{\pi}} \hat{x}_3 , \tag{C.4}$$

with azimuthal angle $0 \le \varphi \le 2\pi$ and polar angle: $0 \le \theta \le \pi$. By above formulas, we further have the explicit formulas for the gradients of the homogeneous harmonic polynomials of degree one:

$$\nabla\left(|x| Y_1^{-1}(\hat{x})\right) = \frac{1}{2}\sqrt{\frac{3}{2\pi}} \begin{bmatrix} 1 \\ -i \\ 0 \end{bmatrix} , \quad \nabla\left(|x| Y_1^{1}(\hat{x})\right) = -\frac{1}{2}\sqrt{\frac{3}{2\pi}} \begin{bmatrix} 1 \\ i \\ 0 \end{bmatrix} , \quad \nabla\left(|x| Y_1^{0}(\hat{x})\right) = \frac{1}{2}\sqrt{\frac{3}{2\pi}} \begin{bmatrix} 0 \\ 0 \\ \sqrt{2} \end{bmatrix} . \tag{C.5}$$

- Define the entire electric multipole fields $\widetilde{E}_{n,m}^{TE}(k, x)$ and $\widetilde{E}_{n,m}^{TM}(k, x)$ on $\mathbb{R}^3$ with wave number k for $n = 1, 2, \cdots$

and $m=-n,\cdots,n$:

$$\widetilde{E}_{n,m}^{TE}(k,x)=\nabla\times\{xj_n(k|x|)Y_n^m(\hat{x})\}=-\sqrt{n(n+1)}j_n(k|x|)V_n^m(\hat{x}), \tag{C.6}$$

$$\begin{aligned}\widetilde{E}_{n,m}^{TM}(k,x)&=-\frac{1}{ik}\nabla\times\widetilde{E}_{n,m}^{TE}(k,x)\\&=-\frac{\sqrt{n(n+1)}}{ik|x|}\mathcal{J}_n(k|x|)U_n^m(\hat{x})-\frac{n(n+1)}{ik|x|}j_n(k|x|)Y_n^m(\hat{x})\hat{x}\,,\end{aligned} \tag{C.7}$$

where $j_n(t)$ is the spherical Bessel function of the first kind and of order n, and $\mathcal{J}_n(t)$ is given by $\mathcal{J}_n(t):=j_n(t)+tj_n'(t)$. The radiating electric multipole fields $E_{n,m}^{TE}(k,x)$ and $E_{n,m}^{TM}(k,x)$ on $\mathbb{R}^3\backslash\{0\}$ can be introduced similarly with $j_n(t)$ and $\mathcal{J}_n(t)$ in (C.6) and (C.7) replaced by the spherical Hankel function of the first kind $h_n^{(1)}(t)$ and $\mathcal{H}_n(t):=h_n^{(1)}(t)+t(h_n^{(1)})'(t)$.

- When $t\to0$, the following asymptotics for spherical Bessel functions and Hankel functions hold [32, 8]:

$$j_n(t)=\frac{t^n}{(2n+1)!!}\big(1-\frac{1}{2(2n+3)}t^2+O(t^4)\big)\,, \tag{C.8}$$

$$h_n^{(1)}(t)=-i\frac{(2n-1)!!}{t^{n+1}}\big(1+\frac{1}{2(2n-1)}t^2+O(t^4)\big)\,, \tag{C.9}$$

$$\mathcal{J}_n(t)=\frac{t^n}{(2n+1)!!}\big(n+1-\frac{n+3}{2(2n+3)}t^2+O(t^4)\big)\,, \tag{C.10}$$

$$\mathcal{H}_n(t)=-i\frac{(2n-1)!!}{t^{n+1}}\big(-n-\frac{n-2}{2(2n-1)}t^2+O(t^4)\big)\,. \tag{C.11}$$

- Wave functions $E_{n,m}^{TE}$ and $E_{n,m}^{TM}$ have the following far-field behaviors: when $|x|\to\infty$,

$$E_{n,m}^{TE}(\omega,x)=-\sqrt{n(n+1)}\frac{e^{i\omega|x|}}{\omega|x|}e^{-i\frac{n+1}{2}\pi}V_n^m(\hat{x})+O\left(\frac{1}{|x|^2}\right)\,, \tag{C.12}$$

$$E_{n,m}^{TM}(\omega,x)=-\sqrt{n(n+1)}\frac{e^{i\omega|x|}}{\omega|x|}e^{-i\frac{n+1}{2}\pi}U_n^m(\hat{x})+O\left(\frac{1}{|x|^2}\right)\,. \tag{C.13}$$

- By using the asymptotic forms in (C.8)-(C.11), in the regimes, $\tau=O(\delta^{-2})$, $\omega=O(1)$ and $\delta\ll1$, we have the following estimates used in (5.11) and (5.12): as $\delta\to0$,

$$\begin{aligned}&\frac{-j_n(\delta\omega_\tau)\mathcal{J}_n(\delta\omega)+\mathcal{J}_n(\delta\omega_\tau)j_n(\delta\omega)}{h_n^{(1)}(\delta\omega)\mathcal{J}_n(\delta\omega_\tau)-j_n(\delta\omega_\tau)\mathcal{H}_n(\delta\omega)}\\=&\frac{-j_n(\delta\omega_\tau)\mathcal{J}_n(\delta\omega)/\mathcal{H}_n(\delta\omega)+\mathcal{J}_n(\delta\omega_\tau)j_n(\delta\omega)/\mathcal{H}_n(\delta\omega)}{h_n^{(1)}(\delta\omega)/\mathcal{H}_n(\delta\omega)\mathcal{J}_n(\delta\omega_\tau)-j_n(\delta\omega_\tau)}\\=&\frac{-j_n(\delta\omega_\tau)O(\delta^{2n+1})+\mathcal{J}_n(\delta\omega_\tau)O(\delta^{2n+1})}{-\frac{1}{n}\mathcal{J}_n(\delta\omega_\tau)-j_n(\delta\omega_\tau)+O(\delta^2)}=O\left(\frac{\delta^{2n+1}}{-\frac{1}{n}\mathcal{J}_n(\delta\omega_\tau)-j_n(\delta\omega_\tau)}\right)\,,\end{aligned} \tag{C.14}$$

and

$$\begin{aligned}&\frac{\frac{1}{1+\tau}\mathcal{J}_n(\delta\omega_\tau)j_n(\delta\omega)-j_n(\delta\omega_\tau)\mathcal{J}_n(\delta\omega)}{\frac{1}{1+\tau}h_n^{(1)}(\delta\omega)\mathcal{J}_n(\delta\omega_\tau)-j_n(\delta\omega_\tau)\mathcal{H}_n(\delta\omega)}\\=&\frac{\frac{1}{1+\tau}\mathcal{J}_n(\delta\omega_\tau)j_n(\delta\omega)/\mathcal{H}_n(\delta\omega)-j_n(\delta\omega_\tau)\mathcal{J}_n(\delta\omega)/\mathcal{H}_n(\delta\omega)}{\frac{1}{1+\tau}h_n^{(1)}(\delta\omega)/\mathcal{H}_n(\delta\omega)\mathcal{J}_n(\delta\omega_\tau)-j_n(\delta\omega_\tau)}\\=&\frac{\mathcal{J}_n(\delta\omega_\tau)O(\delta^{2n+3})-j_n(\delta\omega_\tau)\mathcal{J}_n(\delta\omega)/\mathcal{H}_n(\delta\omega)}{O(\delta^2)-j_n(\delta\omega_\tau)}=\frac{\mathcal{J}_n(\delta\omega)}{\mathcal{H}_n(\delta\omega)}+O\left(\frac{\delta^{2n+3}}{j_n(\delta\omega_\tau)}\right)\,.\end{aligned} \tag{C.15}$$

In particular, for $n=1$, we have the following explicit estimate for the first one by using (C.8)-(C.11):

$$\frac{-j_1(\delta\omega_\tau)\mathcal{J}_1(\delta\omega)+\mathcal{J}_1(\delta\omega_\tau)j_1(\delta\omega)}{h_1^{(1)}(\delta\omega)\mathcal{J}_1(\delta\omega_\tau)-j_1(\delta\omega_\tau)\mathcal{H}_1(\delta\omega)}=\frac{i}{3}(\delta\omega)^3\frac{\mathcal{J}_1(\delta\omega_\tau)-2j_1(\delta\omega_\tau)}{\mathcal{J}_1(\delta\omega_\tau)+j_1(\delta\omega_\tau)}+O\left(\frac{\delta^5}{\mathcal{J}_1(\delta\omega_\tau)+j_1(\delta\omega_\tau)}\right)\,. \tag{C.16}$$

Multipole expansion for the Laplacian vector field

We consider a three-dimensional vector field E satisfying

$$\begin{cases} \Delta E = 0\,,\ \operatorname{div} E = 0\,, & |x| > 1\,, \\ E = O(|x|^{-2})\,, & |x| \to \infty\,. \end{cases} \tag{D.1}$$

By the elliptic regularity, we have that E is analytic on $|x| > 1$. We shall find the multipole expansion for E via the Debye potential. Since many calculations involved are similar to the case of Maxwell's equations and can be found in [38, pp.235-236], we will not repeat all the details and only give a sketch of these steps.

Given a smooth scalar function u, the associated Debye potential is given by $E_u = \nabla \times (ux)$. It is easy to check, by a direct calculation, that if u is harmonic, i.e., $\Delta u = 0$, then the Debye potential E_u satisfies

$$\nabla \times \nabla \times E_u = 0\,.$$

This, along with $\operatorname{div} E_u = 0$, indicates that E_u is harmonic, i.e., $\Delta E_u = 0$.

Moreover, for any scalar harmonic function u in a neighborhood of infinity, we can expand it by

$$r^{-(n+1)} Y_n^m(\hat{x})\,, \quad n = 0, 1, 2, \cdots\,,\ m = -n, \cdots, n\,,$$

with $r = |x|$. The corresponding Debye potentials and their curl's are given by

$$E_{n,m}^h(x) = \nabla \times \left(\frac{1}{r^{n+1}} Y_n^m(\hat{x}) x \right)\,, \quad \nabla \times E_{n,m}^h(x) = \nabla \times \nabla \times \left(\frac{1}{r^{n+1}} Y_n^m(\hat{x}) x \right)\,,$$

for $n = 1, 2, \cdots\,,\ m = -n, \cdots, n$, which can be calculated explicitly:

$$E_{n,m}^h(x) = -\sqrt{n(n+1)} \frac{1}{r^{n+1}} V_n^m(\hat{x})\,, \tag{D.2}$$

$$\nabla \times E_{n,m}^h(x) = \frac{n(n+1)}{r^{n+2}} Y_n^m(\hat{x})\hat{x} - \sqrt{n(n+1)} \frac{n}{r^{n+2}} U_n^m(\hat{x})\,, \tag{D.3}$$

see the end of this section for the detailed calculations. To summarize, for any harmonic function u, the Debye potential E_u and its curl solve the equation (D.1), and can be spanned by $E_{n,m}^h$ and $\nabla \times E_{n,m}^h$ defined in (D.2) and (D.3). We remark that $\nabla \times E_{n,m}^h$ is nothing but, up to a factor $-n$, the electrostatic multipole fields $\nabla \left(r^{-(n+1)} Y_n^m(\hat{x}) \right)$.

Proposition D.1. *Any solution to the equation* (D.1) *has the following series expansion:*

$$E(x) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \gamma_{n,m} E_{n,m}^h(x) + \eta_{n,m} \nabla \times E_{n,m}^h(x) + d_0 \frac{\hat{x}}{r^2}\,,$$

where $\gamma_{n,m}$, $\eta_{n,m}$ *and* d_0 *are complex constants.*

Proof. Since $\{V_n^m\}$ and $\{U_n^m\}$ form an orthogonal basis for $L_T^2(S)$, we can assume that the solution E has the following expansion for its tangential trace on S,

$$\hat{x} \times E(x)|_S = \sum_{n=1}^{\infty} \sqrt{n(n+1)} \sum_{m=-n}^{n} \gamma_{n,m} U_n^m(\hat{x}) - n\eta_{n,m} V_n^m(\hat{x})\,. \tag{D.4}$$

We define the constant d_0 as

$$d_0 = \frac{1}{4\pi} \int_S \hat{x} \cdot E(x) d\sigma(\hat{x})\,.$$

Then we can conclude the desired result by showing that E has the following expression:

$$\widetilde{E} := \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \gamma_{n,m} E_{n,m}^h(x) + \eta_{n,m} \nabla \times E_{n,m}^h(x) + d_0 \frac{\hat{x}}{r^2}\,.$$

For this, by the first vector Green's formula: for any fields E, F,

$$\int_D \overline{E} \cdot \Delta F + \overline{\nabla \times E} \cdot \nabla \times F + \overline{\operatorname{div} E} \operatorname{div} F dx = \int_{\partial D} (\nu \times \overline{E}) \cdot \nabla \times F + \nu \cdot \overline{E} \operatorname{div} F d\sigma\,,$$

we have

$$\int_{1\le|x|\le R} |\nabla\times(E-\widetilde{E})|^2 dx = \int_{S_R} \nu\times\overline{E}\cdot\nabla\times E d\sigma \tag{D.5}$$

for the field $E-\widetilde{E}$, since $\hat{x}\times(E-\widetilde{E})|_S = 0$. To proceed, since each Cartesian component of E is harmonic at infinity, we know from [28, Proposition 2.75] that $\partial_j E_i = O(|x|^{-2})$. It then follows from (D.5) that

$$\int_{1\le|x|\le R} |\nabla\times(E-\widetilde{E})|^2 dx = O\left(\frac{1}{R^2}\right) \quad \text{as } R\to\infty\,, \tag{D.6}$$

which, along with [38, Theorem 3.37] and $\nu\times\nabla\phi|_S = 0$, yields

$$E-\widetilde{E} = \nabla\phi \quad \text{for some } \phi\in H^1_{loc}(\mathbb{R}^3\backslash\bar{B}(0,1)) \text{ with } \phi|_S = \text{constant}\,.$$

We now prove that ϕ must be zero. Note that ϕ solves the exterior Dirichlet problem for the Laplacian. The harmonic function ϕ has the form:

$$\phi = c_0\frac{1}{r}Y_0^0(\hat{x})\,,\quad c_0\in\mathbb{C}\,.$$

By the above formula, we derive

$$0 = \int_S \hat{x}\cdot(E-\widetilde{E})d\sigma(\hat{x}) = -c_0\int_S \frac{1}{r^2}Y_0^0(\hat{x})d\sigma(\hat{x})\,,$$

which implies that $c_0 = 0$, hence complete the proof. □

We end this section with the detailed calculations for formulas (D.2) and (D.3), which mainly rely on the following fundamental formula for the curl operator [39, p.187]:

$$\nabla\times E = \nabla_{S_r}\cdot(E\times\hat{x})\hat{x} + \vec{\text{curl}}_{S_r}(E\cdot\hat{x}) - \frac{\partial}{\partial r}(E\times\hat{x}) - \frac{1}{r}(E\times\hat{x})\,.$$

For $E^h_{n,m}$, we have

$$\begin{aligned} E^h_{n,m}(x) =& \nabla\times\left(\frac{1}{r^{n+1}}Y_n^m(\hat{x})x\right) = \vec{\text{curl}}_{S_r}\left(\frac{1}{r^{n+1}}Y_n^m(\hat{x})r\right) \\ =& \frac{1}{r^n}\vec{\text{curl}}_{S_r}Y_n^m(\hat{x}) = \frac{1}{r^{n+1}}\nabla_S Y_n^m(\hat{x})\times\hat{x} = -\sqrt{n(n+1)}\frac{1}{r^{n+1}}V_n^m(\hat{x})\,. \end{aligned}$$

Similarly, it holds for $\nabla\times E^h_{n,m}$ that

$$\begin{aligned} -\frac{1}{\sqrt{n(n+1)}}\nabla\times E^h_{n,m}(x) =& \nabla\times(\frac{1}{r^{n+1}}V_n^m(\hat{x})) \\ =& \frac{1}{r^{n+2}}\nabla_S\cdot U_n^m(\hat{x})\hat{x} - \frac{\partial}{\partial r}\left(\frac{1}{r^{n+1}}U_n^m(\hat{x})\right) - \frac{1}{r}\frac{1}{r^{n+1}}U_n^m(\hat{x}) \\ =& -\sqrt{n(n+1)}\frac{1}{r^{n+2}}Y_n^m(\hat{x})\hat{x} + \frac{n}{r^{n+2}}U_n^m(\hat{x})\,. \end{aligned}$$

Proof of Proposition 4.7

We first prepare for the determination of $\mathbb{P}_{\mathrm{d}}\widetilde{E}$ to the second order. By the formula (3.39) with (f,g) given by $(\mathbb{P}_{\mathrm{d}}\widetilde{E}^i, \tau^{-1}\mathbb{P}_{\mathrm{w}}\widetilde{E}^i)$, we can derive

$$\begin{aligned} \mathbb{A}_0(\omega)^{-1}\begin{bmatrix}\mathbb{P}_{\mathrm{d}}\widetilde{E}^i \\ \tau^{-1}\mathbb{P}_{\mathrm{w}}\widetilde{E}^i\end{bmatrix} =& \begin{bmatrix}\frac{-\omega_0}{2(\omega-\omega_0)}\mathbb{P}_{\lambda_0} + \mathcal{R}_{\mathrm{w}}^{\lambda_0}(\omega) & 0 \\ 0 & I\end{bmatrix}\begin{bmatrix} I & -c_\tau\omega^2\mathcal{K}_B^{\mathrm{d,w}}\mathcal{T}_B^{-1} \\ 0 & -\mathcal{T}_B^{-1}\end{bmatrix}\begin{bmatrix}\mathbb{P}_{\mathrm{d}}\widetilde{E}^i \\ \tau^{-1}\mathbb{P}_{\mathrm{w}}\widetilde{E}^i\end{bmatrix} \\ =& \begin{bmatrix}\frac{-\omega_0}{2(\omega-\omega_0)}\mathbb{P}_{\lambda_0} + \mathcal{R}_{\mathrm{w}}^{\lambda_0}(\omega) & 0 \\ 0 & I\end{bmatrix}\begin{bmatrix}\mathbb{P}_{\mathrm{d}}\widetilde{E}^i - c_\tau\tau^{-1}\omega^2\mathcal{K}_B^{\mathrm{d,w}}\mathcal{T}_B^{-1}\mathbb{P}_{\mathrm{w}}\widetilde{E}^i \\ -\tau^{-1}\mathcal{T}_B^{-1}\mathbb{P}_{\mathrm{w}}\widetilde{E}^i\end{bmatrix} \\ =& \begin{bmatrix}\frac{-\omega_0}{2(\omega-\omega_0)}\mathbb{P}_{\lambda_0}\widetilde{E}^i + \frac{\omega_0 c_\tau\tau^{-1}}{2(\omega-\omega_0)}\omega^2\mathbb{P}_{\lambda_0}\mathcal{K}_B^{\mathrm{d,w}}\mathcal{T}_B^{-1}\mathbb{P}_{\mathrm{w}}\widetilde{E}^i + \mathcal{R}_{\mathrm{w}}^{\lambda_0}\mathbb{P}_{\mathrm{d}}\widetilde{E}^i + O(\delta^2) \\ -\tau^{-1}\mathcal{T}_B^{-1}\mathbb{P}_{\mathrm{w}}\widetilde{E}^i\end{bmatrix}\,. \end{aligned} \tag{E.1}$$

Due to $\tau = O(\delta^2)$, the above formula further yields

$$\mathbb{A}_0(\omega)^{-1}\begin{bmatrix}\mathbb{P}_{\rm d}\widetilde{E}^i\\ \tau^{-1}\mathbb{P}_{\rm w}\widetilde{E}^i\end{bmatrix} = \frac{-\omega_0}{2(\omega-\omega_0)}\mathbb{P}_{\lambda_0}\widetilde{E}^i + \mathcal{R}_{\rm w}^{\lambda_0}\mathbb{P}_{\rm d}\widetilde{E}^i + O\left(\frac{\delta^2}{\omega-\omega_0}\right). \tag{E.2}$$

To proceed, by (E.2) and (3.38), a direct calculation implies

$$\begin{aligned}\mathbb{A}_0^{-1}\mathbb{A}_1\mathbb{A}_0^{-1}\begin{bmatrix}\mathbb{P}_{\rm d}\widetilde{E}^i\\ \tau^{-1}\mathbb{P}_{\rm w}\widetilde{E}^i\end{bmatrix} =&\mathbb{A}_0^{-1}\mathbb{A}_1\left(\frac{-\omega_0}{2(\omega-\omega_0)}\mathbb{P}_{\lambda_0}\widetilde{E}^i + \mathcal{R}_{\rm w}^{\lambda_0}\mathbb{P}_{\rm d}\widetilde{E}^i + O\left(\frac{\delta^2}{\omega-\omega_0}\right)\right)\\
=&c_{-1}\omega^2\mathbb{A}_0^{-1}\mathcal{K}_B^{\rm d,d}\left(\frac{\omega_0}{2(\omega-\omega_0)}\mathbb{P}_{\lambda_0}\widetilde{E}^i + \mathcal{R}_{\rm w}^{\lambda_0}\mathbb{P}_{\rm d}\widetilde{E}^i\right) + \mathbb{A}_0^{-1}\mathbb{P}_{\rm d}O\left(\frac{\delta^2}{\omega-\omega_0}\right)\\
=&-c_{-1}\omega^2\lambda_0\frac{\omega_0^2}{4(\omega-\omega_0)^2}\mathbb{P}_{\lambda_0}\widetilde{E}^i + \mathcal{R}_{\rm w}^{\lambda_0}\mathbb{P}_{\rm d}\widetilde{E}^i + \mathbb{P}_{\rm d}O\left(\frac{\delta^2}{(\omega-\omega_0)^2}\right),\end{aligned} \tag{E.3}$$

where we have used the fact that $\ker(\lambda_0 - \mathcal{K}_B^{\rm d,d}) \oplus W$ is an invariant space of $\mathbb{A}_0^{-1}\mathcal{K}_B^{\rm d,d}$ to help us write

$$\mathcal{R}_{\rm w}^{\lambda_0} = \mathbb{A}_0^{-1}\mathcal{K}_B^{\rm d,d}\mathcal{R}_{\rm w}^{\lambda_0}.$$

For the approximation of $\mathbb{P}_{\rm w}\widetilde{E}$, by the upper triangular form of $\mathbb{A}_0^{-1}$ and the fact $(\mathbb{A}_1(\omega)[\cdot])_2 = 0$, it is easy to see that the second components of the values of the second operator and the fourth operator in (4.13) always vanish, namely,

$$\left(\mathbb{A}_0^{-1}\mathbb{A}_1\mathbb{A}_0^{-1}[\cdot]\right)_2 = 0 \quad \left((\mathbb{A}_0^{-1}\mathbb{A}_1)^2\mathbb{A}_0^{-1}[\cdot]\right)_2 = 0. \tag{E.4}$$

Hence, it suffices to consider $\mathbb{A}_0^{-1}\mathbb{A}_2\mathbb{A}_0^{-1}$ to find the third-order approximation for $\mathbb{P}_{\rm w}\widetilde{E}$. In fact, we have

$$\begin{aligned}\left(\mathbb{A}_0^{-1}\mathbb{A}_2\mathbb{A}_0^{-1}\begin{bmatrix}\mathbb{P}_{\rm d}\widetilde{E}^i\\ \tau^{-1}\mathbb{P}_{\rm w}\widetilde{E}^i\end{bmatrix}\right)_2 =& -(\mathcal{T}_B|_W)^{-1}\left(\mathbb{A}_2\mathbb{A}_0^{-1}\begin{bmatrix}\mathbb{P}_{\rm d}\widetilde{E}^i\\ \tau^{-1}\mathbb{P}_{\rm w}\widetilde{E}^i\end{bmatrix}\right)_2\\
=& -(\mathcal{T}_B|_W)^{-1}\left\{(\mathbb{A}_2)_{2,1}\left(\mathbb{A}_0^{-1}\begin{bmatrix}\mathbb{P}_{\rm d}\widetilde{E}^i\\ \tau^{-1}\mathbb{P}_{\rm w}\widetilde{E}^i\end{bmatrix}\right)_1 + (\mathbb{A}_2)_{2,2}\left(\mathbb{A}_0^{-1}\begin{bmatrix}\mathbb{P}_{\rm d}\widetilde{E}^i\\ \tau^{-1}\mathbb{P}_{\rm w}\widetilde{E}^i\end{bmatrix}\right)_2\right\}\\
=& -(\mathcal{T}_B|_W)^{-1}\left\{(\mathbb{A}_2)_{2,1}\left(\frac{-\omega_0}{2(\omega-\omega_0)}\mathbb{P}_{\lambda_0}\widetilde{E}^i + \mathcal{R}_{\rm w}^{\lambda_0}\mathbb{P}_{\rm d}\widetilde{E}^i\right) + O\left(\frac{\delta^2}{\omega-\omega_0}\right)\right\},\end{aligned} \tag{E.5}$$

where we have used (E.1). We note from (3.37) that $(\mathbb{A}_2(\omega))_{2,1} = -\omega^2\mathcal{K}_B^{\rm w,d}$. Then it follows readily from (E.5) that

$$\left(\mathbb{A}_0^{-1}\mathbb{A}_2\mathbb{A}_0^{-1}\begin{bmatrix}\mathbb{P}_{\rm d}\widetilde{E}^i\\ \tau^{-1}\mathbb{P}_{\rm w}\widetilde{E}^i\end{bmatrix}\right)_2 = -\frac{\omega^2\omega_0}{2(\omega-\omega_0)}(\mathcal{T}_B|_W)^{-1}\mathcal{K}_B^{\rm w,d}\mathbb{P}_{\lambda_0}\widetilde{E}^i + \mathbb{P}_{\rm w}\mathcal{R}(\omega)\mathbb{P}_{\rm d}\widetilde{E}^i + \mathbb{P}_{\rm w}O\left(\frac{\delta^2}{\omega-\omega_0}\right). \tag{E.6}$$

Collecting the formulas (E.1), (E.3), (E.4) and (E.6), we obtain the desired formula for the solution $\widetilde{E}$ from the expansion (4.13) and the estimate $(\mathbb{P}_{\rm d}\widetilde{E}^i, \tau^{-1}\mathbb{P}_{\rm w}\widetilde{E}^i) = O(\delta)$.

Proof of Theorem 5.2

By the series representations (5.6), (5.7) and (5.8), we first calculate the tangential traces of u inside and outside $B(0,1)$ as

$$\hat{x}\times u(x)|_- = \sum_{n=1}^{\infty}\sqrt{n(n+1)}\sum_{m=-n}^{n}\left(\frac{c_{n,m}}{n} - \frac{\beta_{n,m}}{ik}\mathcal{J}_n(k)\right)V_n^m(\hat{x}) + \alpha_{n,m}j_n(k)U_n^m(\hat{x}),$$

and

$$\hat{x}\times u(x)|_+ = \sum_{n=1}^{\infty}\sqrt{n(n+1)}\sum_{m=-n}^{n}\gamma_{n,m}U_n^m(\hat{x}) - n\eta_{n,m}V_n^m(\hat{x}),$$

respectively. Similarly, we have the following tangential traces for $\nabla\times u$ on S:

$$\hat{x}\times\nabla\times u(x)|_- = \sum_{n=1}^{\infty}\sqrt{n(n+1)}\sum_{m=-n}^{n}\mathcal{J}_n(k)\alpha_{n,m}V_n^m(\hat{x}) + ikj_n(k)\beta_{n,m}U_n^m(\hat{x}),$$

and

$$\hat{x} \times \nabla \times E(x)|_{+} = -\sum_{n=1}^{\infty} \sqrt{n(n+1)} \sum_{m=-n}^{n} n\gamma_{n,m} V_n^m(\hat{x}) \,.$$

Matching the tangential traces of u and $\nabla \times u$ allows us to write

$$\begin{bmatrix} j_n(k) & -1 \\ \mathcal{J}_n(k) & n \end{bmatrix} \begin{bmatrix} \alpha_{n,m} \\ \gamma_{n,m} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} , \tag{F.1}$$

and

$$\begin{bmatrix} j_n(k) & 0 \\ (ik)^{-1}\mathcal{J}_n(k) & -n \end{bmatrix} \begin{bmatrix} \beta_{n,m} \\ \eta_{n,m} \end{bmatrix} = \begin{bmatrix} 0 \\ n^{-1}c_{n,m} \end{bmatrix} . \tag{F.2}$$

To complement the second linear system, we match the normal traces of u inside and outside the domain, which gives us $c_{n,m} = \eta_{n,m} n(n+1)$. Then, by substituting it into (F.2), we obtain

$$\begin{bmatrix} j_n(k) & 0 \\ (ik)^{-1}\mathcal{J}_n(k) & -2n-1 \end{bmatrix} \begin{bmatrix} \beta_{n,m} \\ \eta_{n,m} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} . \tag{F.3}$$

It is easy to observe that the equation (5.1) has nontrivial solutions if and only if one of the linear systems (F.1) and (F.3) is singular for some n, m. More precisely, if

$$n j_n(k) + \mathcal{J}_n(k) = 0 \,, \tag{F.4}$$

holds for some n, then the systems (F.1) and (5.1) shall have nontrivial solutions and hence the eigenspace of $\mathcal{K}_B^{\mathrm{d,d}}$ associated with the eigenvalue $\lambda = k^{-2}$ contains a linear space spanned by $\{\widetilde{E}_{n,m}^{TE}\}_{m=-n}^{n}$. Similarly, in the case when $j_n(k) = 0$, we can conclude that the system (F.3) is singular and $\widetilde{E}_{n,m}^{TM}, m = -n, \cdots, n$ are the linearly independent eigenfunctions of $\mathcal{K}_B^{\mathrm{d,d}}$ for the eigenvalue k^{-2}.

To proceed, by the following recurrence relation of the Bessel function:

$$j_n'(k) = j_{n-1}(k) - \frac{n+1}{k} j_n(k) \,, \tag{F.5}$$

we can write (F.4) as

$$0 = (n+1) j_n(k) + k j_{n-1}(k) - (n+1) j_n(k) \,,$$

which is equivalent to $j_{n-1}(k) = 0$.

To conclude, we have shown that if $k \neq 0$ is a zero of a Bessel function j_n for some nonnegative integer n which must be real and simple, then $k^{-2} > 0$ is an eigenvalue of $\mathcal{K}_B^{\mathrm{d,d}}$ with the eigenspace containing linearly independent eigenfunctions:

$$\left(\bigcup_{m=-n-1}^{n+1} \widetilde{E}_{n+1,m}^{TE} \right) \bigcup \left(\bigcup_{m=-n}^{n} \widetilde{E}_{n,m}^{TM} \right) , \quad \text{for } n \geq 1 \,,$$

and

$$\bigcup_{m=-1}^{1} \widetilde{E}_{1,m}^{TE} \,, \quad \text{for } n = 0 \,.$$

To prove that the above eigenfunctions exactly span the corresponding eigenspace, we need to investigate the common zeros of Bessel functions, which is a quite important and classical problem [40]. One existing answer is the Bourgets hypothesis [44], which states that the Bessel function of the first kind $J_\mu(z)$ and $J_{\mu+m}(z)$, where μ is rational and m is a positive integer, can not have common zeros except at $z = 0$. It immediately implies that $j_n(z), n \geq 0$ have no common zeros that are nonzero, hence completes the proof.

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