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MATHEMATICAL ANALYSIS OF ELECTROMAGNETIC PLASMONIC METASURFACES*

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Abstract. We study the anomalous electromagnetic scattering in the homogenization regime, by a subwavelength thin layer consisting of periodically distributed plasmonic nanoparticles on a perfectly conducting plane. By using quasi-periodic layer potential techniques, we derive the asymptotic expansion of the electromagnetic field away from the thin layer and quantitatively analyze the field enhancement induced by the excitation of the mixed collective plasmonic resonances, which can be characterized by the spectra of two types of periodic Neumann–Poincaré operators. Based on the asymptotic behavior of the scattered field in the macroscopic scale, characterize the reflection scattering matrix for the thin layer and demonstrate that the optical effect of this metasurface can be effectively approximated by a Leontovich impedance boundary condition, which is uniformly valid no matter whether the incident frequency is near the resonant range. The quantitative approximation clearly shows the blow-up of the field energy and the conversion of the field polarization when the resonance occurs, resulting in a significant change of the reflection property of the conducting plane. These results confirm essential physical changes of electromagnetic metasurface at resonances mathematically, whose occurrence was verified earlier for the acoustic case and the transverse magnetic case.

Key words. plasmonic resonance, array of nanoparticles, biperiodic Green's tensor, metasurfaces, Neumann–Poincaré operator

AMS subject classifications. 35R30, 35C20

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1. Introduction.

The study of the electromagnetic scattering by a thin layer composed of periodic subwavelength resonators that can strongly interact with the incident wave has received considerable attention recently for the possibilities of realizing the full control of the reflected and transmitted waves [20, 49, 50, 30]. Such thin layers of composite material, usually referred to as the ultrathin metasurfaces in the physical and engineering literature, have a macroscopic effect on the scattered wave although the layer thickness, or the size of cell structure, is negligible with respect to the operating wavelength [26, 27, 35, 34, 16, 39, 40]. We refer the readers to [48] for a systematic review of the electromagnetic metasurfaces and their potential applications. Great effort has also been made recently by the mathematical community to develop a universal theory for a better understanding of the mechanism underlying the metasurfaces. It turns out that these anomalous scattering phenomena typically have a close relation with the multiscale nature of the subwavelength cell structures and the excitation of various resonances. A systematic study was carried out in [38, 39, 40, 41, 37] to understand the electromagnetic scattering by the perfectly conducting slab patterned with the subwavelength narrow slits under varying

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regimes and periodic patterns. It was shown in [43] that the scattering effect of a novel metasurface made of periodically corrugated cylindrical waveguides can be approximated by smooth cylindrical waveguides with an effective metamaterial surface impedance.

In this work, we consider the full set of Maxwell's equations and investigate the electromagnetic scattering from an array of periodically distributed subwavelength plasmonic nanoparticles mounted on a perfectly conducting plane in the homogenization regime where the period of the microstructure is of the same order as the characteristic size of the nanoparticles but is much smaller than the incident wavelength. Plasmonic nanoparticles such as gold and silver have unique optical capabilities of confining charge density oscillations (localized surface plasmons) and hence are popular and ideal choices for the subwavelength resonators in the electromagnetic setting [44]. We shall see that even a thin layer of the plasmonic nanoparticles can significantly influence the wave propagation pattern and our mathematical findings may theoretically verify the possibility of the ultrathin electromagnetic plasmonic metasurface.

It has been shown in [5] that at the quasi-static limit, a single nanoparticle can exhibit the plasmonic resonances at some specific frequencies that are essentially related to the spectra of the Neumann–Poincaré operators. We refer to [5, 12, 10] for a complete mathematical analysis of the plasmonic nanoparticles. In our case where the nanoparticles are periodically distributed in the homogenization regime, we shall prove that the anomalous electromagnetic scattering can result from the occurrence of the mixed and collective plasmonic resonances, which are very different from the case of a single plasmonic nanoparticle in free space. It is worth mentioning that if the thin layer is made of normal dielectric materials with biperiodic conducting inclusions covering a cylindrical body, a Leontovich boundary condition was derived in [1] to approximate the effect of the layer. Such grating problems and boundary layer effects have been extensively studied by matched asymptotic expansion techniques; see, e.g., [15, 3, 2, 4, 24, 25]. Nevertheless, as we shall characterize, the cell problem here is nearly singular at some frequencies if the nanoparticles are plasmonic. In this case, the standard homogenization is not applicable and the effective reflection coefficient (matrix) for the thin layer may blow up. Therefore, we must seek new analytical tools for deriving the exact blow-up order and mathematically justifying the validity of the approximation of the Leontovich-type boundary conditions at the resonance frequencies. In the present work, we use the layer potential techniques to study the reflection properties of electromagnetic plasmonic metasurfaces and to provide a rigorous homogenization theory for our singular subwavelength diffraction grating, which is more general than the framework recently proposed in [11] for the Helmholtz equation. A similar technique was used in [6] to illustrate the superabsorption of acoustic waves with bubble metascreens experimentally observed in [36].

For our purpose, we shall introduce two quasi-periodic Green's tensors for Maxwell's equations with the vanishing tangential components and the vanishing normal components on the planar interface, respectively, which further allow us to define the corresponding quasi-periodic layer potentials. It turns out that both types of operators with different boundary conditions are necessary for our new representation formula of the scattered electric field (cf. (4.1)). We then perform the asymptotic analysis and analyze the spectral properties of the leading-order potentials that can be written as the sum of the periodic layer potentials and remainder terms depending on the incident angle (incident direction). We shall prove that these incident angle-

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dependent remainder terms actually have no essential effect on the spectral structures of the involved operators and the associated resolvents, compared to the unperturbed periodic ones. This fact is crucial for the subsequent analysis for the blow-up of the field and the technical calculations for approximating the scattered wave. The main idea behind the calculations is that we first separate the propagative part and the evanescent part of the scattered wave and then use the asymptotic analysis and the various algebraic relations to compute the approximation of the propagative scattered wave. All these facts make our arguments and calculations significantly different from the scalar case [11, 6] and the single-particle case [5, 12].

We would like to stress that the assumption of the perfectly conducting half-space is not physical in the range of visible and near-infrared frequencies. In practice, a plasmonic metasurface typically consists of a thin subwavelength metallic grating mounted on a dielectric substrate [33]. We will elaborate in section 5 on how to apply our newly developed mathematical framework to generalize the main results obtained to the more realistic case of the penetrable half-space. Moreover, our results and analysis in this work also apply to other important physical settings where the involved physical scales, namely, the distances between multiple thin layers of plasmonic nanoparticles, the incident wavelength, sizes of nanoparticles, and the period of the lattice, are of very different orders of magnitude, such as

$$\text{size of particle} \ll \text{period} \ll \text{distance} \sim \text{wavelength or}$$
$$\text{size of particle} \ll \text{period} \sim \text{distance} \ll \text{wavelength}.$$

Another important assumption that needs to be pointed out is that in our following analysis, we consider the possibility of plasmonic nanoparticles possessing negative permeability and showing a magnetic response. But in fact the natural metallic (plasmonic) nanoparticle is generally nonmagnetic at optical frequencies. The recent developments of the material science and the mathematical homogenization have made it possible to design and manufacture the double negative composite medium and produce artificial magnetism from dielectric structures [47, 31, 21, 17], although there is still a distance to reach the nanoscale. For the sake of mathematical generality and completeness, instead of only considering the negative electric permittivity, we allow both permittivity and permeability to take the negative values.

The paper is organized as follows. In the next section, we describe our model mathematically and introduce some notation and definitions. In section 3, we introduce the quasi-periodic layer potentials and derive the corresponding asymptotic expansions, and then recall some basic results concerning the Neumann–Poincaré operators and establish the resolvent estimates for the leading-order potentials. Section 4 is the main contribution of this work, devoted to the calculation of the far-field asymptotic expansion of the scattered wave and a boundary condition approximation under the excitation of plasmons. We shall end this work with some concluding and extension remarks.

2. Problem descriptions and preliminaries. This section is devoted to the basic setup and the mathematical formulation of the electromagnetic scattering problem. We shall write (x', x_3) for $\mathbf{x} = (x_1, x_2, x_3) \in \mathbb{R}^3$ with $x' = (x_1, x_2) \in \mathbb{R}^2$ and $x_3 \in \mathbb{R}$, and $\Gamma := \{x \in \mathbb{R}^3 | x_3 = 0\}$ for the reflective plane, and $\mathbb{R}^3_\pm := \{\mathbf{x} \in \mathbb{R}^3 | \pm x_3 > 0\}$ for the upper and lower half-spaces. We denote by $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ the usual Cartesian basis of $\mathbb{R}^3$. For a multi-index $\alpha \in \mathbb{N}^3$, we write $\mathbf{x}^\alpha = x_1^{\alpha_1} x_2^{\alpha_2} x_3^{\alpha_3}$ and $\partial^\alpha = \partial_1^{\alpha_1} \partial_2^{\alpha_2} \partial_3^{\alpha_3}$ with $\partial_j = \partial/\partial x_j$. We shall always use $B \in \mathbb{R}^3_+$ to denote a C^2-smooth bounded domain with a connected boundary and a characteristic size of

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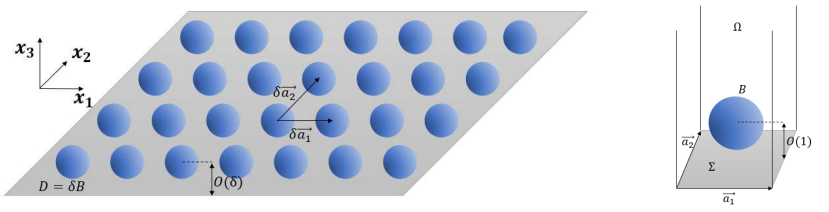

(a) Array of nanoparticles (b) Cell structure

FIG. 1. *Periodically distributed plasmonic nanoparticles $\mathcal{D}$ and the associated cell structure.*

order one and use $D := \delta B$ to describe a single nanoparticle. We denote by $\mathcal{D}$ the collection of plasmonic nanoparticles periodically distributed along the lattice Λ^δ,

$$\Lambda^\delta = \left\{ \mathrm{R}^\delta \in \Gamma;\, \mathrm{R}^\delta = n_1 \delta \mathbf{a}_1 + n_2 \delta \mathbf{a}_2 \,,\ n_i \in \mathbb{Z} \right\} ,$$

in which $\mathbf{a}_1, \mathbf{a}_2$ are linearly independent vectors lying on Γ with $|\mathbf{a}_1| \sim |\mathbf{a}_2| \sim 1$. Then we can write $\mathcal{D} = \bigcup_{\mathrm{R}^\delta \in \Lambda^\delta} (D + \mathrm{R}^\delta)$; see Figure 1(a). For convenience, we shall simply denote Λ^1 by Λ, and then we can see $\mathcal{D} = \bigcup_{\mathrm{R} \in \Lambda} \delta(B + \mathrm{R})$. We now define the cells Σ, Ω in Γ and in $\mathbb{R}^3_+$ by

$$\Sigma = \left\{ \mathbf{a} \in \Gamma;\, \mathbf{a} = c_1 \mathbf{a}_1 + c_2 \mathbf{a}_2 \,,\ c_i \in \left(-\frac{1}{2}, \frac{1}{2} \right) \right\} , \quad \Omega = \Sigma \times (0, \infty) ,$$

respectively. We further assume that B is contained in Ω with a distance of order one from the reflective plane Γ (see Figure 1(b)), and the dimensionless quantity δ is much less than one, since we are interested in the homogenization regime. For any $\widetilde{\mathbf{x}} \in \partial B$, we have $\mathbf{x} = \delta \widetilde{\mathbf{x}} \in \partial D$. Then for a function $\varphi(\mathbf{x})$ defined on ∂D, its pull back $\widetilde{\varphi}(\widetilde{\mathbf{x}}) := \varphi(\delta \widetilde{\mathbf{x}}) = \varphi(\mathbf{x})$ is defined on ∂B. This convention is adopted throughout this work. In particular, if we denote by $\nu(\mathbf{x})$ the exterior normal vector of ∂D, then its pull back $\widetilde{\nu}(\widetilde{\mathbf{x}})$ is the normal vector of ∂B. But we may also simply write ν for a normal vector without specifying its definition domain when no confusion is caused. For the sake of exposition, we often refer to $\widetilde{\mathbf{x}}$, B, and Ω as the reference variable, reference domain, and reference cell, respectively.

The explicit formulas for the electric permittivity $\varepsilon_c(\omega)$ and the magnetic permeability $\mu_c(\omega)$ of the nanoparticle may be available in terms of the Drude model and the Kramers–Kronig relations [5, 10, 44]. However, in this work, we generally assume that both μ_c and ε_c are complex numbers with $\mathfrak{Im}\mu_c, \mathfrak{Im}\varepsilon_c \geq 0$ and may depend on the frequency ω of the incident wave. We denote the permittivity and permeability of the background medium by ε and μ and further assume them to be the constant one after an appropriate scaling. Then the wave numbers $k_c(\omega)$ for the nanoparticle and k for the background are given by

$$k_c(\omega) = \omega \sqrt{\varepsilon_c(\omega) \mu_c(\omega)} \text{ and } k = \omega \sqrt{\varepsilon \mu} = \omega \,.$$

We are now ready to formulate the scattering problem of our interest as follows:

$$\begin{cases} \nabla \times E = ik \mu_{\mathcal{D}} H & \text{in } \mathbb{R}^3_+ \backslash \partial \mathcal{D} \,, \\ \nabla \times H = -ik \varepsilon_{\mathcal{D}} E & \text{in } \mathbb{R}^3_+ \backslash \partial \mathcal{D} \,, \\ [\nu \times E] = [\nu \times H] = 0 & \text{on } \partial \mathcal{D} \,, \\ \mathbf{e}_3 \times E = 0 & \text{on } \Gamma \,, \end{cases} \tag{2.1}$$

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where $E-E^i$ and $H-H^i$ satisfy certain outgoing radiation conditions, $\varepsilon_{\mathcal{D}} := \chi_{\mathbb{R}^3_+\setminus\mathcal{D}} + \varepsilon_c\chi_{\mathcal{D}}$ and $\mu_{\mathcal{D}} := \chi_{\mathbb{R}^3_+\setminus\mathcal{D}} + \mu_c\chi_{\mathcal{D}}$ with $\chi_{\mathbb{R}^3_+\setminus\mathcal{D}}$ and $\chi_{\mathcal{D}}$ being the standard characteristic functions. Throughout the work, we use $[\cdot] := \cdot|_- - \cdot|_+$ to denote the jump across the interface $\partial\mathcal{D}$ and the subscripts $\pm$ to denote the limits taken from outside and inside $\mathcal{D}$, respectively. The incident plane wave (E^i, H^i) is given by

$$E^i = \mathbf{p}e^{ik\mathbf{d}\cdot\mathbf{x}} - \mathbf{p}^* e^{ik\mathbf{d}^*\cdot\mathbf{x}}\,, \quad H^i = \mathbf{d}\times\mathbf{p}e^{ik\mathbf{d}\cdot\mathbf{x}} - \mathbf{d}^*\times\mathbf{p}^* e^{ik\mathbf{d}^*\cdot\mathbf{x}}\,,$$

where $\mathbf{d}$ is the unit incident direction with $d_3 < 0$ and $\mathbf{p}$ is the polarization vector. Here and in what follows we often use the superscript $*$ to denote the reflection of a vector with respect to Γ, e.g., $\mathbf{d}^* = (d', -d_3)$ is the reflection of $\mathbf{d}$. But the notation $*$ may have other meanings on different occasions, so we will illustrate the actual meaning of $*$ whenever it may cause confusion. Denote by $\mathbf{k} = k\mathbf{d}$ and $\mathbf{k}^* = k\mathbf{d}^*$ the wave vector and its reflection, respectively. We are interested in finding a quasi-periodic solution (E, H) to the system (2.1), that is,

$$E(\mathbf{x}+\mathrm{R}^\delta) = e^{i\mathbf{k}\cdot\mathrm{R}^\delta}E(\mathbf{x})\,, \quad H(\mathbf{x}+\mathrm{R}^\delta) = e^{i\mathbf{k}\cdot\mathrm{R}^\delta}H(\mathbf{x})\,.$$

Hence we have the usual Rayleigh–Bloch expansion for the scattered field in the domain above the layer of nanoparticles. As in [6], we impose the outgoing radiation condition on the solutions to the system (2.1) by assuming that all the modes in the Rayleigh–Bloch expansion are either decaying exponentially or propagating along the x_3-direction. Under the subwavelength assumption, the period of the lattice is of order δ and the scattered wave consists of only a single propagative mode in the far field:

$$E^r := E - E^i \sim \mathbf{p}^r e^{ik'\cdot x'} e^{-ik_3 x_3} \quad \text{as } x_3 \to \infty \quad (\text{for some polarization vector } \mathbf{p}^r)\,.$$

One of the main tasks of this work is to determine the structure of $\mathbf{p}^r$ (cf. (4.59)).

The remaining part of this section is devoted to introducing more notation and definitions and recalling some basic results concerning the surface differential operators and function spaces that are frequently used in the paper. For $s \in \mathbb{R}$, we denote by $H^s(\partial B)$ and $H^s_T(\partial B)$ the usual Sobolev space of order s of scalar functions and tangential vector fields on ∂B, respectively, and denote by $H^s_0(\partial B)$ the zero mean subspace of $H^s(\partial B)$. Also, the Sobolev spaces $H^s(B)$ and $H^s_{loc}(\Omega\backslash B)$ are needed, as well as the trace operator $\gamma_0 : H^s(B) \to H^{s-1/2}(\partial B)$ for $s > 1/2$. We introduce the surface gradient $\nabla_{\partial B}$ and the surface vector curl (written as $\vec{\mathrm{curl}}_{\partial B}$) in the standard way [46], which map $H^{1/2}(\partial B)$ to $H_T^{-1/2}(\partial B)$. Their corresponding adjoint operators are the surface divergence $\nabla_{\partial B}\cdot$ and the surface scalar curl, i.e., $\mathrm{curl}_{\partial B}$: $H_T^{1/2}(\partial B) \to H^{-1/2}(\partial B)$. And it holds in $H^{-1/2}(\partial B)$ that

$$\ker(\nabla_{\partial B}) = \ker(\vec{\mathrm{curl}}_{\partial B}) = \mathbb{R}\,. \tag{2.2}$$

The Laplace–Beltrami operator $\Delta_{\partial B} := \nabla_{\partial B}\cdot\nabla_{\partial B} = -\mathrm{curl}_{\partial B}\vec{\mathrm{curl}}_{\partial B}$ shall also be used. For a vector field $u \in H_T^{-1/2}(\partial B)$, we will often need its tangential component $r(u) := \nu\times u$. It is easy to check by using the definition and duality relations that each of the following identities holds for a suitable function φ:

$$\vec{\mathrm{curl}}_{\partial B}\varphi = -r(\nabla_{\partial B}\varphi)\,, \quad \mathrm{curl}_{\partial B}\varphi = -\nabla_{\partial B}\cdot(r\varphi)\,, \tag{2.3}$$

$$\nabla_{\partial B}\cdot\vec{\mathrm{curl}}_{\partial B}\varphi = 0\,, \quad \mathrm{curl}_{\partial B}\nabla_{\partial B}\varphi = 0\,. \tag{2.4}$$

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Moreover, we introduce the spaces $H(\mathrm{curl}, B)$, $H_{loc}(\mathrm{curl}, \Omega\backslash\bar{B})$, $H(\mathrm{div}, B)$, and $H_{loc}(\mathrm{div}, \Omega\backslash\bar{B})$ of (locally) square integrable vector fields with (locally) square integrable curl and divergence, respectively. We will frequently use the normal trace $\gamma_n(u) := u\cdot\nu|_{\partial B}$, the tangential trace $\gamma_t(u) := \nu\times u|_{\partial B}$, and the tangential component trace $\pi_t(u) := (\nu\times u)\times\nu|_{\partial B}$ for appropriately smooth vector fields u. Indeed, γ_n, γ_t, and π_t can be extended to linear continuous mappings from $H(\mathrm{div}, B)$ to $H^{-1/2}(\partial B)$, $H(\mathrm{curl}, B)$ to $H_T^{-1/2}(\mathrm{div}, \partial B)$, and $H(\mathrm{curl}, B)$ to $H_T^{-1/2}(\mathrm{curl}, \partial B)$, respectively, where

$$H_T^{-\frac{1}{2}}(\mathrm{div}, \partial B) = \left\{\varphi \in H_T^{-\frac{1}{2}}(\partial B);\ \nabla_{\partial B}\cdot\varphi \in H^{-\frac{1}{2}}(\partial B)\right\},$$
$$H_T^{-\frac{1}{2}}(\mathrm{curl}, \partial B) = \left\{\varphi \in H_T^{-\frac{1}{2}}(\partial B);\ \mathrm{curl}_{\partial B}\varphi \in H^{-\frac{1}{2}}(\partial B)\right\}.$$

It is known that $H_T^{-1/2}(\mathrm{curl}, \partial B)$ can be identified with the dual space of $H_T^{-1/2}(\mathrm{div}, \partial B)$ with the duality pairing $\langle\psi, \varphi\rangle := \int_{\partial B}\psi\cdot\varphi d\sigma$ for smooth vector fields ψ, φ (cf. [45, 18]). For $f \in H^1(B)$, we have

$$\nabla_{\partial B}\gamma_0(f) = \pi_t(\nabla f). \tag{2.5}$$

Similarly, it holds for $u \in H(\mathrm{curl}, B)$ that

$$\mathrm{curl}_{\partial B}\pi_t(u) = \gamma_n(\nabla\times u). \tag{2.6}$$

For our subsequent analysis, the Helmholtz decomposition of $H_T^{-1/2}(\mathrm{div}, \partial B)$ is useful (cf. [18]):

$$H_T^{-\frac{1}{2}}(\mathrm{div}, \partial B) = \nabla_{\partial B}H_0^{\frac{3}{2}}(\partial B) \oplus \vec{\mathrm{curl}}_{\partial B}H_0^{\frac{1}{2}}(\partial B). \tag{2.7}$$

In this work, we denote by $\otimes$ the tensor product operation of two vectors, i.e., given two vectors $\mathbf{a} \in \mathbb{R}^n$ and $\mathbf{b} \in \mathbb{R}^m$, $\mathbf{a}\otimes\mathbf{b}$ is an $n\times m$ matrix given by $(\mathbf{a}\otimes\mathbf{b})_{ij} = a_ib_j$, and let vector operators act on matrices column by column. For any two Banach spaces X and Y, we write by $\mathcal{L}(X, Y)$ the set of all linear continuous mappings from X to Y, or simply by $\mathcal{L}(X)$ if $Y = X$. We write $\|\cdot\|_X$ for the norm defined on the space X and ${}_{X^*}\langle\cdot,\cdot\rangle_X$ for the natural duality pairing between X and its dual space X^*. However, we may simply write $\|\cdot\|$ and $\langle\cdot,\cdot\rangle$ without specifying the subscripts when no confusion is caused. We will not identify the dual spaces of Hilbert spaces with themselves, instead we always regard them as the subspaces of distributions. Hence all the adjoint operators in this work are introduced by their natural duality pairings. We end this section by introducing the expression $x \lesssim y$, which means $x \le Cy$ for some generic constant C. If $x \gtrsim y$ and $x \lesssim y$ holds simultaneously, then we write $x \approx y$.

3. Layer potential techniques. Before considering the scattering problem, we introduce in this section the quasi-periodic layer potentials and present some analysis tools. We shall first define the quasi-periodic Green's tensors satisfying certain boundary conditions and derive their asymptotic expansions with respect to δ. Then we study the associated layer potentials, as well as their asymptotics. After that, we turn our attention to the spectral properties of the leading-order potentials and the resolvent estimates of the Neumann–Poincaré-type operators. These results will be fundamental for the far-field asymptotics and approximation error estimate conducted in section 4.

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3.1. Quasi-periodic Green's tensors and basic properties. Following the notation in [6], we start with the scalar quasi-periodic Green's function $G^{\mathbf{k}}_{\#}$ with respect to the lattice Λ, which is the solution to

$$(\Delta + k^2)G^{\mathbf{k}}_{\#}(\mathbf{x}) = \sum_{\mathrm{R}\in\Lambda} e^{ik'\cdot x'}\delta_{\mathrm{R}}(\mathbf{x}) = \sum_{\mathrm{R}\in\Lambda} e^{ik'\cdot \mathrm{R}}\delta_{\mathrm{R}}(\mathbf{x})\,, \quad k\in\mathbb{C} \text{ with } \mathfrak{Im}k \geq 0\,, \tag{3.1}$$

and satisfies a certain outgoing condition. In the distribution sense, $G^{\mathbf{k}}_{\#}$ is well-defined and given by

$$G^{\mathbf{k}}_{\#}(\mathbf{x}) = \sum_{\mathrm{R}\in\Lambda} e^{ik'\cdot \mathrm{R}} G^k(\mathbf{x},\mathrm{R})\,, \tag{3.2}$$

where $G^k(\mathbf{x},\mathbf{y}) := -\frac{e^{ik|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|}$ is the fundamental solution to the Helmholtz operator $\Delta + k^2$ in the free space. We further define $G^{\mathbf{k}}_{\#}(\mathbf{x},\mathbf{y}) := G^{\mathbf{k}}_{\#}(\mathbf{x}-\mathbf{y})$. For our interested subwavelength diffraction grating problem, we consider the quasi-periodic Green's function $G^{\mathbf{k}}_{\#^\delta}(\mathbf{x})$ with respect to the lattice Λ^δ. With the help of the reference variable $\widetilde{\mathbf{x}}$, we easily observe the following useful scaling property:

$$G^{\mathbf{k}}_{\#^\delta}(\mathbf{x}) = \sum_{\mathrm{R}^\delta\in\Lambda^\delta} e^{ik'\cdot \mathrm{R}^\delta} G^k(\mathbf{x},\mathrm{R}^\delta) = \frac{1}{\delta}\sum_{\mathrm{R}\in\Lambda} e^{i\delta k'\cdot \mathrm{R}} G^{\delta k}(\widetilde{\mathbf{x}},\mathrm{R})\,, \tag{3.3}$$

that is,

$$G^{\mathbf{k}}_{\#^\delta}(\mathbf{x}) = \frac{1}{\delta} G^{\delta\mathbf{k}}_{\#}(\widetilde{\mathbf{x}})\,. \tag{3.4}$$

Let Λ^* be the reciprocal lattice of Λ (cf. [42]) and τ be the volume of the unit cell Σ of Λ. Then the explicit formula of $G^{\mathbf{k}}_{\#}$ in the homogenization regime, i.e., $|k| \ll \tau \sim 1$, is available in [6, Lemma 3.2].

THEOREM 3.1. *Let $k\in\mathbb{C}$ be the complex wave number with $\mathfrak{Im}k \geq 0$. Suppose that $|k|$ is small enough; then the quasi-periodic Green's function $G^{\mathbf{k}}_{\#}$ has the following representation:*

$$G^{\mathbf{k}}_{\#}(\mathbf{x}) = \frac{i}{2\tau k_3} e^{ik'\cdot x' - ik_3|x_3|} - \frac{1}{2\tau}\sum_{\xi\in\Lambda^*\setminus\{0\}} \frac{1}{\sqrt{|\xi+k'|^2-k^2}} e^{i(\xi+k')\cdot x'} e^{-\sqrt{|\xi+k'|^2-k^2}|x_3|}\,, \tag{3.5}$$

where $\sqrt{z}$ is viewed as an analytic function defined by $\sqrt{z} = |z|^{1/2}e^{i\arg z/2}$ for $z\in\mathbb{C}\setminus\{-it, t\geq 0\}$. In particular, when $k=0$, it holds that

$$G^0_{\#}(\mathbf{x}) = \frac{|x_3|}{2\tau} - \frac{1}{2\tau}\sum_{\xi\in\Lambda^*\setminus\{0\}} \frac{1}{|\xi|} e^{i\xi\cdot x'} e^{-|\xi|\cdot|x_3|}\,. \tag{3.6}$$

We readily observe from the representation formula (3.6) the symmetry property of $G^0_{\#}$:

$$G^0_{\#}(\pm x', \pm x_3) = G^0_{\#}(x', x_3)\,. \tag{3.7}$$

A direct application of Taylor's expansion gives us the asymptotics of $G^{\delta\mathbf{k}}_{\#}$ in terms of δ:

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$$G_{\#}^{\delta\mathbf{k}}(\mathbf{x}) = \frac{i}{2\delta k_3 \tau} + G_{0,\#}(\mathbf{x}) + \sum_{n=1}^{\infty} (\delta k)^n G_{n,\#}(\mathbf{x})\,. \tag{3.8}$$

We remark that each term $G_{n,\#}$ in the expansion (3.8) can be computed explicitly (cf. [6] for more details). In particular, for the leading-order term, we have

$$G_{0,\#}(\mathbf{x}) = \frac{k_3|x_3| - k'\cdot x'}{2k_3\tau} - \frac{1}{2\tau}\sum_{\xi\in\Lambda^*\setminus\{0\}} \frac{1}{|\xi|} e^{i\xi\cdot x'} e^{-|\xi|\cdot|x_3|} = G_{\#}^{0}(\mathbf{x}) - \frac{k'\cdot x'}{2k_3\tau}\,. \tag{3.9}$$

Recalling from the definition of $G_{\#}^{\delta\mathbf{k}}$ that

$$(\Delta + \delta^2 k^2) G_{\#}^{\delta\mathbf{k}}(\mathbf{x}) = \sum_{\mathrm{R}\in\Lambda} e^{i\delta k'\cdot x'}\delta_{\mathrm{R}}(\mathbf{x})\,,$$

we obtain, by substituting the expansion (3.8) into the above formula,

$$\begin{aligned}&\Delta G_{0,\#}(\mathbf{x}) + \delta k\left(\Delta G_{1,\#}(\mathbf{x}) + \frac{i}{2d_3\tau}\right) + \sum_{n=2}^{\infty}\delta^n k^n(\Delta G_{n,\#}(\mathbf{x}) + G_{n-2,\#}(\mathbf{x}))\\ &\quad = \sum_{n=0}^{\infty}\delta^n k^n \sum_{\mathrm{R}\in\Lambda}\frac{(id'\cdot x')^n}{n!}\delta_{\mathrm{R}}(\mathbf{x})\,,\end{aligned}$$

which implies (with notation $G_{-1,\#} = \frac{i}{2d_3\tau}$)

$$\Delta G_{0,\#}(\mathbf{x}) = \sum_{\mathrm{R}\in\Lambda}\delta_{\mathrm{R}}(\mathbf{x})\,,\ \text{and}\ \Delta G_{n,\#}(\mathbf{x}) + G_{n-2,\#}(\mathbf{x}) = \sum_{\mathrm{R}\in\Lambda}\frac{(id'\cdot \mathrm{R})^n}{n!}\delta_{\mathrm{R}}(\mathbf{x})\quad \text{for } n\geq 1\,. \tag{3.10}$$

The quasi-periodic Green's functions with Dirichlet and Neumann boundary conditions are defined by

$$G_{\mathrm{e}}^{\mathbf{k}}(\mathbf{x},\mathbf{y}) := G_{\#}^{\mathbf{k}}(\mathbf{x}-\mathbf{y}) - G_{\#}^{\mathbf{k}}(\mathbf{x}-\mathbf{y}^*)\,,\quad G_{\mathrm{m}}^{\mathbf{k}}(\mathbf{x},\mathbf{y}) := G_{\#}^{\mathbf{k}}(\mathbf{x}-\mathbf{y}) + G_{\#}^{\mathbf{k}}(\mathbf{x}-\mathbf{y}^*)\,, \tag{3.11}$$

respectively. Then it directly follows from (3.8) that

$$G_{\mathrm{e/m}}^{\delta\mathbf{k}}(\mathbf{x},\mathbf{y}) = \sum_{n=-1}^{\infty}(\delta k)^n G_{n,\mathrm{e/m}}(\mathbf{x},\mathbf{y})\,, \tag{3.12}$$

where $G_{n,\mathrm{e/m}}(\mathbf{x},\mathbf{y})$ are given by

$$G_{n,\mathrm{e/m}}(\mathbf{x},\mathbf{y}) := G_{n,\#}(\mathbf{x}-\mathbf{y}) \mp G_{n,\#}(\mathbf{x}-\mathbf{y}^*)\quad \text{for } n\geq -1\,. \tag{3.13}$$

In particular, $G_{-1,\mathrm{e}} = 0$ and $G_{-1,\mathrm{m}} = i/(d_3\tau)$. For ease of exposition, here and in what follows, we use the subscript e/m to include two cases, e.g., (3.12) actually represents two equations, obtained by replacing e/m by e and m, respectively, in (3.12). Similarly, we shall also use m/e frequently. We note that $\delta_{\mathrm{R}}(x'-y') = 0$ holds for all $\mathrm{R}\neq 0$ and $\mathbf{x},\mathbf{y}\in\bar{B}$, and then obtain from (3.10) and the definition of $G_{n,\mathrm{e/m}}$ (3.13) that

$$\Delta G_{0,\mathrm{e/m}}(\mathbf{x},\mathbf{y}) = \delta_0(\mathbf{x}-\mathbf{y})\ \text{and}\ \Delta G_{n,\mathrm{e/m}}(\mathbf{x},\mathbf{y}) + G_{n-2,\mathrm{e/m}}(\mathbf{x},\mathbf{y}) = 0\quad \text{for } n\geq 1\,. \tag{3.14}$$

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The above recurrence relations shall be used in the calculations for the asymptotic expansions of layer potential operators. According to the reciprocity (3.7) of the periodic Green's function, we have

$$G^0_{\mathrm{e/m}}(\mathbf{x},\mathbf{y}) = G^0_{\mathrm{e/m}}(\mathbf{y},\mathbf{x}).$$

Combining the above observation with (3.9) and (3.13), we readily see the reciprocity does not hold for $G_{0,\mathrm{m}}(\mathbf{x},\mathbf{y})$ anymore since

$$G_{0,\mathrm{m}}(\mathbf{x},\mathbf{y}) = G^0_{\mathrm{m}}(\mathbf{x},\mathbf{y}) - \frac{k'\cdot(x'-y')}{k_3\tau}\,, \tag{3.15}$$

while $G_{0,\mathrm{e}}(\mathbf{x},\mathbf{y})$ still satisfies the reciprocity due to

$$G_{0,\mathrm{e}}(\mathbf{x},\mathbf{y}) = G^0_{\mathrm{e}}(\mathbf{x},\mathbf{y})\,. \tag{3.16}$$

Another important difference between $G^{\delta\mathbf{k}}_{\mathrm{m}}$ and $G^{\delta\mathbf{k}}_{\mathrm{e}}$ worth mentioning is that there is a singularity $O(\delta^{-1})$ for $G^{\delta\mathbf{k}}_{\mathrm{m}}$ as δ goes to 0 (cf. (3.8) and (3.11)). This fact, together with the nonsymmetry of $G_{0,\mathrm{m}}(\mathbf{x},\mathbf{y})$, makes some of our subsequent analysis technical and difficult. We finally introduce the conjugate kernels $\hat{G}_{0,\mathrm{e/m}}$ of $G_{0,\mathrm{e/m}}$,

$$\hat{G}_{0,\mathrm{e}}(\mathbf{x},\mathbf{y}) = G_{0,\mathrm{e}}(\mathbf{y},\mathbf{x}) = G^0_{\mathrm{e}}(\mathbf{x},\mathbf{y})\,, \tag{3.17}$$

$$\hat{G}_{0,\mathrm{m}}(\mathbf{x},\mathbf{y}) = G_{0,\mathrm{m}}(\mathbf{y},\mathbf{x}) = G^0_{\mathrm{m}}(\mathbf{x},\mathbf{y}) + \frac{k'\cdot(x'-y')}{k_3\tau}\,, \tag{3.18}$$

for our later use, by setting $\hat{G}_{0,\mathrm{e/m}}(\mathbf{x},\mathbf{y}) := G_{0,\mathrm{e/m}}(\mathbf{y},\mathbf{x})$.

We are now ready to introduce the electromagnetic Green's tensors:

$$\mathbb{G}^{\mathbf{k}}_{\mathrm{e/m}}(\mathbf{x},\mathbf{y}) = \left(1 + \frac{1}{k^2}\nabla_{\mathbf{x}}\nabla_{\mathbf{x}}\cdot\right)\Pi^{\mathbf{k}}_{\mathrm{e/m}}(\mathbf{x},\mathbf{y})\,, \tag{3.19}$$

where the matrix-valued functions $\Pi^{\mathbf{k}}_{\mathrm{e/m}}$ are given by

$$\Pi^{\mathbf{k}}_{\mathrm{e/m}}(\mathbf{x},\mathbf{y}) = \left[G^{\mathbf{k}}_{\mathrm{e/m}}\mathbf{e}_1,\quad G^{\mathbf{k}}_{\mathrm{e/m}}\mathbf{e}_2,\quad G^{\mathbf{k}}_{\mathrm{m/e}}\mathbf{e}_3\right](\mathbf{x},\mathbf{y})\,. \tag{3.20}$$

It is easy to check that $\mathbb{G}^{\mathbf{k}}_{\mathrm{e/m}}$ solve Maxwell's equations,

$$\nabla_{\mathbf{x}}\times\nabla_{\mathbf{x}}\times\mathbb{G}^{\mathbf{k}}_{\mathrm{e/m}}(\mathbf{x},\mathbf{y}) - k^2\mathbb{G}^{\mathbf{k}}_{\mathrm{e/m}}(\mathbf{x},\mathbf{y}) = -\sum_{\mathrm{R}\in\Lambda} e^{ik'\cdot\mathrm{R}}\delta_{\mathrm{R}}(\mathbf{x}-\mathbf{y})\mathbb{I}_3\,,$$

and satisfy the boundary conditions,

$$\mathbf{e}_3\times\mathbb{G}^{\mathbf{k}}_{\mathrm{e}}(\mathbf{x},\mathbf{y}) = 0 \text{ and } \mathbf{e}_3\cdot\mathbb{G}^{\mathbf{k}}_{\mathrm{m}}(\mathbf{x},\mathbf{y}) = 0 \quad \text{for } \mathbf{x}\in\Gamma\,,\ \mathbf{y}\in\mathbb{R}^3_+\,,$$

respectively. As a direct consequence of (3.12), we have the asymptotic expansions of $\Pi^{\delta\mathbf{k}}_{\mathrm{e/m}}$:

$$\Pi^{\delta\mathbf{k}}_{\mathrm{e/m}}(\mathbf{x},\mathbf{y}) = \sum_{n=-1}^{\infty}(\delta k)^n\Pi_{n,\mathrm{e/m}}(\mathbf{x},\mathbf{y})\,. \tag{3.21}$$

Then we readily see, from the above formula and the definition of $\mathbb{G}^{\mathbf{k}}_{\mathrm{e/m}}$ in (3.19), the following expansion:

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$$\mathbb{G}^{\delta\mathbf{k}}_{\mathrm{e/m}}(\mathbf{x},\mathbf{y}) = \frac{1}{\delta k}\mathbb{G}_{-1,\mathrm{e/m}}(\mathbf{x},\mathbf{y}) + \sum_{n=0}^{\infty}(\delta k)^n \mathbb{G}_{n,\mathrm{e/m}}(\mathbf{x},\mathbf{y})\,, \tag{3.22}$$

where $\mathbb{G}_{n,\mathrm{e/m}}(\mathbf{x},\mathbf{y})$ are given by

$$\mathbb{G}_{n,\mathrm{e/m}}(\mathbf{x},\mathbf{y}) = \Pi_{n,\mathrm{e/m}}(\mathbf{x},\mathbf{y}) + \nabla_{\mathbf{x}}\nabla_{\mathbf{x}}\cdot\Pi_{n+2,\mathrm{e/m}}(\mathbf{x},\mathbf{y})\,.$$

We end this subsection with some basic but very useful observations:

$$\frac{\partial}{\partial x_i}G^{\mathbf{k}}_{\mathrm{e}} = -\frac{\partial}{\partial y_i}G^{\mathbf{k}}_{\mathrm{e}}(i=1,2)\,,\quad \frac{\partial}{\partial x_3}G^{\mathbf{k}}_{\mathrm{e}} = -\frac{\partial}{\partial y_3}G^{\mathbf{k}}_{\mathrm{m}}\,,$$
$$\frac{\partial}{\partial x_i}G^{\mathbf{k}}_{\mathrm{m}} = -\frac{\partial}{\partial y_i}G^{\mathbf{k}}_{\mathrm{m}}(i=1,2)\,,\quad \frac{\partial}{\partial x_3}G^{\mathbf{k}}_{\mathrm{m}} = -\frac{\partial}{\partial y_3}G^{\mathbf{k}}_{\mathrm{e}}\,,$$

which lead to the following reciprocity:

$$(\nabla_{\mathbf{x}}\times\Pi^{\mathbf{k}}_{\mathrm{e/m}}(\mathbf{x},\mathbf{y}))^T = \nabla_{\mathbf{y}}\times\Pi^{\mathbf{k}}_{\mathrm{m/e}}(\mathbf{x},\mathbf{y})\,. \tag{3.23}$$

Here the superscript T denotes the transport of a matrix.

3.2. Integral operators and their asymptotics. With the help of the Green's tensors introduced in the last subsection, we define the following vector layer potentials with the density φ on ∂B [29, 22]:

$$\mathcal{A}^{\mathbf{k}}_{B,\mathrm{e/m}} : H_T^{-\frac{1}{2}}(\mathrm{div},\partial B) \longrightarrow H(\mathrm{curl},B) \text{ or } H_{loc}(\mathrm{curl},\Omega\backslash\bar{B}),$$
$$\varphi \longmapsto \mathcal{A}^{\mathbf{k}}_{B,\mathrm{e/m}}[\varphi](\mathbf{x}) = \int_{\partial B}\Pi^{\mathbf{k}}_{\mathrm{e/m}}(\mathbf{x},\mathbf{y})\varphi(\mathbf{y})d\sigma\,;$$
$$\mathcal{M}^{\mathbf{k}}_{B,\mathrm{e/m}} : H_T^{-\frac{1}{2}}(\mathrm{div},\partial B) \longrightarrow H_T^{-\frac{1}{2}}(\mathrm{div},\partial B),$$
$$\varphi \longmapsto \mathcal{M}^{\mathbf{k}}_{B,\mathrm{e/m}}[\varphi](\mathbf{x}) = \int_{\partial B}\nu(\mathbf{x})\times\nabla_{\mathbf{x}}\times\Pi^{\mathbf{k}}_{\mathrm{e/m}}(\mathbf{x},\mathbf{y})\varphi(\mathbf{y})d\sigma\,;$$
$$\mathcal{L}^{\mathbf{k}}_{B,\mathrm{e/m}} : H_T^{-\frac{1}{2}}(\mathrm{div},\partial B) \longrightarrow H_T^{-\frac{1}{2}}(\mathrm{div},\partial B),$$
$$\varphi \longmapsto \mathcal{L}^{\mathbf{k}}_{B,\mathrm{e/m}}[\varphi](\mathbf{x}) = \nu(\mathbf{x}) \times\left(k^2\mathcal{A}^{\mathbf{k}}_{B,\mathrm{e/m}}[\varphi](\mathbf{x}) + \nabla\mathcal{S}^{\mathbf{k}}_{B,\mathrm{e/m}}[\nabla_{\partial B}\cdot\varphi](\mathbf{x})\right).$$

Further, we define the single layer potential,

$$\mathcal{S}^{\mathbf{k}}_{B,\mathrm{e/m}} : H^{-\frac{1}{2}}(\partial B) \longrightarrow H^{\frac{1}{2}}(\partial B),$$
$$\varphi \longmapsto \mathcal{S}^{\mathbf{k}}_{B,\mathrm{e/m}}[\varphi](\mathbf{x}) = \int_{\partial B}G^{\mathbf{k}}_{\mathrm{e/m}}(\mathbf{x},\mathbf{y})\varphi(\mathbf{y})d\sigma\,,$$

the double layer potential,

$$\mathcal{K}^{\mathbf{k}}_{B,\mathrm{e/m}} : H^{\frac{1}{2}}(\partial B) \longrightarrow H^{\frac{1}{2}}(\partial B),$$
$$\varphi \longmapsto \mathcal{K}^{\mathbf{k}}_{B,\mathrm{e/m}}[\varphi](\mathbf{x}) = \int_{\partial B}\frac{\partial}{\partial\nu_{\mathbf{y}}}G^{\mathbf{k}}_{\mathrm{e/m}}(\mathbf{x},\mathbf{y})\varphi(\mathbf{y})d\sigma\,,$$

and the Neumann–Poincaré operator,

$$\mathcal{K}^{\mathbf{k},*}_{B,\mathrm{e/m}} : H^{-\frac{1}{2}}(\partial B) \longrightarrow H^{-\frac{1}{2}}(\partial B),$$
$$\varphi \longmapsto \mathcal{K}^{\mathbf{k},*}_{B,\mathrm{e/m}}[\varphi](\mathbf{x}) = \int_{\partial B}\frac{\partial}{\partial\nu_{\mathbf{x}}}G^{\mathbf{k}}_{\mathrm{e/m}}(\mathbf{x},\mathbf{y})\varphi(\mathbf{y})d\sigma\,.$$

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These integral operators will be used for the integral formulation of the scattering problem (2.1) and the further mathematical analysis of the integral formulation in section 4. It follows from the definitions that $\mathcal{S}^{\mathbf{k}}_{B,\mathrm{e}}$ and $\mathcal{S}^{\mathbf{k}}_{B,\mathrm{m}}$ satisfy the Dirichlet and Neumann boundary conditions on the reflective plane Γ, respectively, while $\mathcal{A}^{\mathbf{k}}_{B,\mathrm{e}}$ and $\mathcal{A}^{\mathbf{k}}_{B,\mathrm{m}}$ satisfy the boundary conditions:

$$\mathbf{e}_3 \times \mathcal{A}^{\mathbf{k}}_{B,\mathrm{e}}[\varphi](\mathbf{x}) = 0\,,\ \mathbf{e}_3 \cdot \mathcal{A}^{\mathbf{k}}_{B,\mathrm{m}}[\varphi](\mathbf{x}) = 0 \quad \text{on } \Gamma\,.$$

When $k = 0$, we omit the subscript B in all the potentials defined above for simplicity, e.g., we write $\mathcal{S}^0_{\mathrm{e/m}}$ for $\mathcal{S}^0_{B,\mathrm{e/m}}$. We emphasize that all of the above definitions depend on the lattice Λ and the domain B in the unit cell Ω. For the scaled lattice Λ^δ and the domain D, the associated operators can be defined similarly.

It can be shown that $\nabla \times \mathcal{A}^k_{B,\mathrm{e/m}}$ defines a bounded linear operator from $H_T^{-1/2}(\mathrm{div}, \partial B)$ into $H(\mathrm{curl}, B)$ or $H(\mathrm{curl}, \Omega\backslash\bar{B})$ (cf. [22]). Since $G^{\mathbf{k}}_{\mathrm{e/m}}(\mathbf{x}) - G^k(\mathbf{x})$ is a smooth function defined in Ω, the trace formulas related to $\mathcal{A}^{\mathbf{k}}_{B,\mathrm{e/m}}$ follow directly from the standard results [7, Lemma 2.96],

$$(\nu \times \nabla \times \mathcal{A}^{\mathbf{k}}_{B,\mathrm{e/m}})|_\pm = \mp\frac{1}{2} + \mathcal{M}^{\mathbf{k}}_{B,\mathrm{e/m}}\,, \tag{3.24}$$

$$(\nu \times \nabla \times \nabla \times \mathcal{A}^{\mathbf{k}}_{B,\mathrm{e/m}})|_\pm = \mathcal{L}^{\mathbf{k}}_{B,\mathrm{e/m}}\,. \tag{3.25}$$

Moreover, it holds for $\mathcal{S}^{\mathbf{k}}_{B,\mathrm{e/m}}$ that

$$\left(\frac{\partial}{\partial \nu_{\mathbf{x}}} \mathcal{S}^{\mathbf{k}}_{B,\mathrm{e/m}}\right)|_\pm = \pm\frac{1}{2} + \mathcal{K}^{\mathbf{k},*}_{B,\mathrm{e/m}}\,. \tag{3.26}$$

Recalling the asymptotic expansions (3.12) and (3.21), we may define the potentials $\mathcal{A}_{n,\mathrm{e/m}}$ and $\mathcal{S}_{n,\mathrm{e/m}}$ associated with $\Pi_{n,\mathrm{e/m}}$ and $G_{n,\mathrm{e/m}}$, respectively, and $\mathcal{K}_{n,\mathrm{e/m}}$ and $\mathcal{K}^*_{n,\mathrm{e/m}}$ as well. Then we can directly see that the following expansions hold for any density φ on ∂D:

$$\mathcal{A}^{\mathbf{k}}_{D,\mathrm{e/m}}[\varphi](\mathbf{x}) = \delta \mathcal{A}^{\delta\mathbf{k}}_{B,\mathrm{e/m}}[\widetilde{\varphi}](\widetilde{\mathbf{x}}) = \sum_{n=-1}^{\infty} \delta^{n+1} k^n \mathcal{A}_{n,\mathrm{e/m}}[\widetilde{\varphi}](\widetilde{\mathbf{x}})\,, \tag{3.27}$$

$$\mathcal{S}^{\mathbf{k}}_{D,\mathrm{e/m}}[\varphi](\mathbf{x}) = \delta \mathcal{S}^{\delta\mathbf{k}}_{B,\mathrm{e/m}}[\widetilde{\varphi}](\widetilde{\mathbf{x}}) = \sum_{n=-1}^{\infty} \delta^{n+1} k^n \mathcal{S}_{n,\mathrm{e/m}}[\widetilde{\varphi}](\widetilde{\mathbf{x}})\,, \tag{3.28}$$

and

$$\mathcal{K}^{\mathbf{k}}_{D,\mathrm{e/m}}[\varphi](\mathbf{x}) = \sum_{n=0}^{\infty} \delta^n k^n \mathcal{K}_{n,\mathrm{e/m}}[\widetilde{\varphi}](\widetilde{\mathbf{x}}), \quad \mathcal{K}^{\mathbf{k},*}_{D,\mathrm{e/m}}[\varphi](\mathbf{x}) = \sum_{n=0}^{\infty} \delta^n k^n \mathcal{K}^*_{n,\mathrm{e/m}}[\widetilde{\varphi}](\widetilde{\mathbf{x}}).$$

Furthermore, by the above asymptotic expansions, arguments similar to the ones for [12, Lemmas 3.1–3.2] yield the following two lemmas.

LEMMA 3.2. *For $\phi \in H_T^{-1/2}(\mathrm{div}, \partial D)$, $\mathcal{M}^{\mathbf{k}}_{D,\mathrm{e/m}}[\phi]$ has the following asymptotic expansion:*

$$\mathcal{M}^{\mathbf{k}}_{D,\mathrm{e/m}}[\phi](\delta\widetilde{\mathbf{x}}) = \mathcal{M}^{\delta\mathbf{k}}_{B,\mathrm{e/m}}[\widetilde{\phi}](\widetilde{\mathbf{x}}) = \sum_{n=0}^{\infty} (\delta k)^n \mathcal{M}_{n,\mathrm{e/m}}[\widetilde{\phi}](\widetilde{\mathbf{x}})\,, \tag{3.29}$$

where

$$\mathcal{M}_{n,\mathrm{e/m}}[\widetilde{\phi}](\widetilde{\mathbf{x}}) = \int_{\partial B} \nu(\widetilde{\mathbf{x}}) \times \nabla_{\widetilde{\mathbf{x}}} \times \Pi_{n,\mathrm{e/m}}(\widetilde{\mathbf{x}}, \widetilde{\mathbf{y}}) \phi(\widetilde{\mathbf{y}}) d\sigma\,, \quad n \geq 0\,,$$

has an uniform bound in $\mathcal{L}(H_T^{-1/2}(\mathrm{div}, \partial B))$. Moreover, $\mathcal{M}^{\mathbf{k}}_{D,\mathrm{e/m}}$ is analytic in δ.

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LEMMA 3.3. *For $\phi \in H_T^{-1/2}(\mathrm{div}, \partial D)$, $\mathcal{L}^{\mathbf{k}}_{D,\mathrm{e/m}}[\phi]$ has the asymptotic expansion:*

$$\mathcal{L}^{\mathbf{k}}_{D,\mathrm{e/m}}[\phi](\delta\widetilde{\mathbf{x}}) - \mathcal{L}^{\mathbf{k}_c}_{D,\mathrm{e/m}}[\phi](\delta\widetilde{\mathbf{x}}) = \sum_{n=1}^{\infty} \delta^{n-1}(k^n - k_c^n)\mathcal{L}_{n,\mathrm{e/m}}[\widetilde{\phi}](\widetilde{\mathbf{x}})\,,$$

where

$$\mathcal{L}_{n,\mathrm{e/m}}[\widetilde{\phi}](\widetilde{\mathbf{x}}) = \nu \times \mathcal{A}_{n-2,\mathrm{e/m}}[\widetilde{\phi}](\widetilde{\mathbf{x}}) + \nu \times \nabla \mathcal{S}_{n,\mathrm{e/m}}[\nabla_{\partial B} \cdot \widetilde{\phi}](\widetilde{\mathbf{x}})\,.$$

In particular, it holds that

$$\begin{aligned}
\mathcal{L}_{1,\mathrm{e}}[\widetilde{\phi}](\widetilde{\mathbf{x}}) &= -\frac{i}{\tau d_3}\nu(\widetilde{\mathbf{x}}) \times \int_{\partial B} \widetilde{y}_3 \mathbf{e}_3 \nabla_{\partial B} \cdot \widetilde{\phi}(\widetilde{\mathbf{y}}) d\sigma \\
&\quad + \nu(\widetilde{\mathbf{x}}) \times \nabla \int_{\partial B} G_{1,\mathrm{e}}(\widetilde{\mathbf{x}}, \widetilde{\mathbf{y}}) \nabla_{\partial B} \cdot \widetilde{\phi}(\widetilde{\mathbf{y}}) d\sigma\,, \\
\mathcal{L}_{1,\mathrm{m}}[\widetilde{\phi}](\widetilde{\mathbf{x}}) &= -\frac{i}{\tau d_3}\nu(\widetilde{\mathbf{x}}) \times \int_{\partial B} (\widetilde{y}', 0)^t \nabla_{\partial B} \cdot \widetilde{\phi}(\widetilde{\mathbf{y}}) d\sigma \\
&\quad + \nu(\widetilde{\mathbf{x}}) \times \nabla \int_{\partial B} G_{1,\mathrm{m}}(\widetilde{\mathbf{x}}, \widetilde{\mathbf{y}}) \nabla_{\partial B} \cdot \widetilde{\phi}(\widetilde{\mathbf{y}}) d\sigma\,.
\end{aligned}$$

Moreover, $\mathcal{L}_{n,\mathrm{e/m}}$ has an uniform bound in $\mathcal{L}(H_T^{-1/2}(\mathrm{div}, \partial B))$, and $\mathcal{L}^{\mathbf{k}}_{D,\mathrm{e/m}}$ is analytic in δ.

For the sake of simplicity, we write $\mathcal{M}_{\mathrm{e/m}}$, $\mathcal{K}_{\mathrm{e/m}}$, and $\mathcal{K}^*_{\mathrm{e/m}}$ for the leading-order terms in the asymptotic expansions of $\mathcal{M}^{\delta\mathbf{k}}_{B,\mathrm{e/m}}$, $\mathcal{K}^{\delta\mathbf{k}}_{B,\mathrm{e/m}}$, and $\mathcal{K}^{\delta\mathbf{k},*}_{B,\mathrm{e/m}}$, respectively. We emphasize that we only need the surface divergence of density $\widetilde{\phi}$ to evaluate $\mathcal{L}_{1,\mathrm{e/m}}[\widetilde{\phi}]$, which immediately implies

$$\vec{\mathrm{curl}}_{\partial B} H_0^{\frac{1}{2}}(\partial B) \subset \mathbb{H} \subset \ker(\mathcal{L}_{1,\mathrm{e/m}})\,,$$

where $\mathbb{H}$ denotes the divergence-free space:

$$\mathbb{H} := \left\{ \varphi \in H_T^{-\frac{1}{2}}(\mathrm{div}, \partial B)\,;\ \nabla_{\partial B} \cdot \varphi = 0 \right\}. \tag{3.30}$$

This observation shall be used repeatedly in section 4 to simplify our calculation. For a better understanding of the terms involved in the expansions, we present the following lemma.

LEMMA 3.4. *For any $\widetilde{\phi} \in H_T^{-1/2}(\mathrm{div}, \partial B)$, it holds that*

(i) $\nabla_{\partial B} \cdot \mathcal{L}_{n,\mathrm{e/m}}[\widetilde{\phi}] = \nabla_{\partial B} \cdot (\nu \times \mathcal{A}_{n-2,\mathrm{e/m}})[\widetilde{\phi}]$ *for $n \geq 1$, in particular, $\nabla_{\partial B} \cdot \mathcal{L}_{1,\mathrm{e/m}}[\widetilde{\phi}] = 0$;*

(ii) $\nabla_{\partial B} \cdot \mathcal{M}_{n,\mathrm{e/m}}[\widetilde{\phi}] = -\mathcal{K}^*_{n,\mathrm{e/m}}[\nabla_{\partial B} \cdot \widetilde{\phi}] - \nu \cdot \mathcal{A}_{n-2,\mathrm{e/m}}[\widetilde{\phi}]$ *for $n \geq 1$, while for $n = 0$,*

$$\nabla_{\partial B} \cdot \mathcal{M}_{\mathrm{e/m}}[\widetilde{\phi}] = -\mathcal{K}^*_{\mathrm{e/m}}[\nabla_{\partial B} \cdot \widetilde{\phi}].$$

Proof. We first note that $\nabla \mathcal{S}_{n,\mathrm{e/m}}[\nabla_{\partial B} \cdot \widetilde{\phi}] \in H(\mathrm{curl}, B)$. Then by the formulas (2.3) and (2.6), we see that $\nabla_{\partial B} \cdot (\nu \times \nabla \mathcal{S}_{n,\mathrm{e/m}}[\nabla_{\partial B} \cdot \widetilde{\phi}]) = 0$, which, along with Lemma 3.3, yields the property (i). To show the second property, again by (2.3) and (2.6), we obtain

$$\begin{aligned}
\nabla_{\partial B} \cdot \mathcal{M}_{n,\mathrm{e/m}}[\widetilde{\phi}] &= \nabla_{\partial B} \cdot (\nu \times \pi_t(\nabla \times \mathcal{A}_{n,\mathrm{e/m}}))[\widetilde{\phi}] \\
&= \mathrm{curl}_{\partial B} \pi_t(\nabla \times \mathcal{A}_{n,\mathrm{e/m}})[\widetilde{\phi}] = -\gamma_n(\nabla \times \nabla \times \mathcal{A}_{n,\mathrm{e/m}})[\widetilde{\phi}] \\
&= -\mathcal{K}^*_{n,\mathrm{e/m}}[\nabla_{\partial B} \cdot \widetilde{\phi}] - \nu(\widetilde{x}) \cdot \mathcal{A}_{n-2,\mathrm{e/m}}[\widetilde{\phi}]\,, \quad n \geq 1\,.
\end{aligned}$$

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We should be more careful to deal with the case $n = 0$ due to the jump formulas (3.24) and (3.26). A calculation similar to the one presented above gives us $\nabla_{\partial B} \cdot \mathcal{M}_{\mathrm{e/m}}[\widetilde{\phi}] = -\mathcal{K}^*_{\mathrm{e/m}}[\nabla_{\partial B} \cdot \widetilde{\phi}]$. ∎

Before we move on to the next subsection on the spectral analysis, we further investgate the leading-order terms and prepare some tools for later use. By the formulas (3.15) and (3.16), we find that $\mathcal{K}^*_{\mathrm{e}}$ is identical to $\mathcal{K}^{0,*}_{\mathrm{e}}$ with the adjoint operator given by $\mathcal{K}_{\mathrm{e}} = \mathcal{K}^0_{\mathrm{e}}$. Nevertheless, $\mathcal{K}^*_{\mathrm{m}}$ can only be identified with $\mathcal{K}^{0,*}_{\mathrm{m}}$ on $H_0^{-1/2}(\partial B)$. We remark that $\mathcal{K}_{\mathrm{m}}$ here is not the adjoint operator of $\mathcal{K}^*_{\mathrm{m}}$. Indeed, the adjoint operators of $\mathcal{K}^*_{\mathrm{m}}$ and $\mathcal{K}_{\mathrm{m}}$ are defined by

(3.31)
$$\hat{\mathcal{K}}_{\mathrm{m}}[\varphi](\mathbf{x}) = \int_{\partial B} \frac{\partial}{\partial \nu_{\mathbf{y}}} \hat{G}_{0,\mathrm{m}}(\mathbf{x},\mathbf{y})\varphi(\mathbf{y}) d\sigma \quad \text{and} \quad \hat{\mathcal{K}}^*_{\mathrm{m}}[\varphi](\mathbf{x}) = \int_{\partial B} \frac{\partial}{\partial \nu_{\mathbf{x}}} \hat{G}_{0,\mathrm{m}}(\mathbf{x},\mathbf{y})\varphi(\mathbf{y}) d\sigma$$

for smooth functions φ, respectively; see formulas (3.17) and (3.18) for the definition of $\hat{G}_{0,\mathrm{e/m}}$. To find the adjoint operator of $\mathcal{M}_{\mathrm{e/m}}$, we introduce the conjugate matrix-valued function $\hat{\Pi}_{\mathrm{e/m}}$ of $\Pi_{\mathrm{e/m}}$,

$$\hat{\Pi}_{\mathrm{e/m}}(\mathbf{x},\mathbf{y}) = \left[\hat{G}_{0,\mathrm{e/m}}\mathbf{e}_1, \quad \hat{G}_{0,\mathrm{e/m}}\mathbf{e}_2, \quad \hat{G}_{0,\mathrm{m/e}}\mathbf{e}_3\right](\mathbf{x},\mathbf{y}),$$

and the associated layer potential $\hat{\mathcal{M}}_{\mathrm{e/m}}$,

$$\hat{\mathcal{M}}_{\mathrm{e/m}}[\varphi](\mathbf{x}) = \int_{\partial B} \nu(\mathbf{x}) \times \nabla_{\mathbf{x}} \times \hat{\Pi}_{\mathrm{e/m}}(\mathbf{x},\mathbf{y})\varphi(\mathbf{y}) d\sigma,$$

which is a bounded linear operator from $H_T^{-1/2}(\mathrm{div}, \partial B)$ to $H_T^{-1/2}(\mathrm{div}, \partial B)$. Then, the adjoint operator of $\mathcal{M}_{\mathrm{e/m}}$, denoted by $\mathcal{M}^*_{\mathrm{e/m}}$, is given by

$$\mathcal{M}^*_{\mathrm{e/m}} = r\hat{\mathcal{M}}_{\mathrm{m/e}} r : H_T^{-\frac{1}{2}}(\mathrm{curl}, \partial B) \to H_T^{-\frac{1}{2}}(\mathrm{curl}, \partial B). \tag{3.32}$$

To see this fact, by a standard density argument, it suffices to verify it on the smooth function space. Indeed, using (3.23) and Fubini's theorem, we have

$$\begin{aligned}
\langle \psi, \mathcal{M}_{\mathrm{e/m}}[\phi] \rangle &= \int_{\partial B} \int_{\partial B} \psi(\mathbf{x}) \cdot \nu(\mathbf{x}) \times \nabla_{\mathbf{x}} \times (\Pi_{\mathrm{e/m}}(\mathbf{x},\mathbf{y})\phi(\mathbf{y})) d\sigma(\mathbf{y}) d\sigma(\mathbf{x}) \\
&= \int_{\partial B} \int_{\partial B} (\nabla_{\mathbf{x}} \times \Pi_{\mathrm{e/m}}(\mathbf{x},\mathbf{y}))^T (\psi(\mathbf{x}) \times \nu(\mathbf{x})) \cdot \phi(\mathbf{y}) d\sigma(\mathbf{y}) d\sigma(\mathbf{x}) \\
&= \int_{\partial B} \int_{\partial B} (\nabla_{\mathbf{y}} \times \hat{\Pi}_{\mathrm{m/e}}(\mathbf{y},\mathbf{x}))(\psi(\mathbf{x}) \times \nu(\mathbf{x})) \cdot \phi(\mathbf{y}) d\sigma(\mathbf{x}) d\sigma(\mathbf{y}) \\
&= \langle r\hat{\mathcal{M}}_{\mathrm{m/e}} r[\psi], \phi \rangle
\end{aligned}$$

for smooth functions ψ and ϕ. Similarly, we can get the adjoint operator $\hat{\mathcal{M}}^*_{\mathrm{e/m}} : H_T^{-1/2}(\mathrm{curl}, \partial B) \to H_T^{-1/2}(\mathrm{curl}, \partial B)$ of $\hat{\mathcal{M}}_{\mathrm{e/m}}$:

$$\hat{\mathcal{M}}^*_{\mathrm{e/m}} = r\mathcal{M}_{\mathrm{m/e}} r. \tag{3.33}$$

Recall that we have proven in Lemma 3.4 that it holds that

$$\nabla_{\partial B} \cdot \mathcal{M}_{\mathrm{e/m}}[\varphi] = -\mathcal{K}^*_{\mathrm{e/m}}[\nabla_{\partial B} \cdot \varphi] = -\mathcal{K}^{0,*}_{\mathrm{e/m}}[\nabla_{\partial B} \cdot \varphi], \tag{3.34}$$

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where we have utilized the fact that $\nabla_{\partial B}\cdot\varphi$ is from the space $H_0^{-\frac{1}{2}}(\partial B)$ on which $\mathcal{K}_{\mathrm{e/m}}$ and $\mathcal{K}_{\mathrm{e/m}}^{0,*}$ are identical to each other. By exactly the same arguments, we obtain

$$\nabla_{\partial B}\cdot\hat{\mathcal{M}}_{\mathrm{e/m}}[\varphi]=-\hat{\mathcal{K}}_{\mathrm{e/m}}^{*}[\nabla_{\partial B}\cdot\varphi]=-\mathcal{K}_{\mathrm{e/m}}^{0,*}[\nabla_{\partial B}\cdot\varphi]\,. \tag{3.35}$$

Furthermore, taking the adjoint on the both sides of (3.35) and using (3.33) allow us to see

$$\mathcal{M}_{\mathrm{m/e}}\vec{\mathrm{curl}}_{\partial B}=\vec{\mathrm{curl}}_{\partial B}\mathcal{K}_{\mathrm{e/m}}^{0}\,. \tag{3.36}$$

3.3. Spectral analysis of integral operators. In this subsection, we are going to consider the spectral properties of Neumann–Poincaré-type operators, which is essential for the subsequent analysis for the singular behavior of the scattered field.

Let us start with the analysis for the periodic Neumann–Poincaré operators. Considering the single layer potential $\mathcal{S}_{\mathrm{e/m}}^{0}$, it is easy to observe that $\mathcal{S}_{\mathrm{e/m}}^{0}: H^{-1/2}(\partial B)\to H^{1/2}(\partial B)$ is self-adjoint, i.e., $\langle\psi,\mathcal{S}_{\mathrm{e/m}}^{0}[\phi]\rangle=\langle\mathcal{S}_{\mathrm{e/m}}^{0}[\psi],\phi\rangle$, and the Calderón identity

$$\mathcal{S}_{\mathrm{e/m}}^{0}\mathcal{K}_{\mathrm{e/m}}^{0,*}=\mathcal{K}_{\mathrm{e/m}}^{0}\mathcal{S}_{\mathrm{e/m}}^{0} \tag{3.37}$$

holds in $H^{-1/2}(\partial B)$. Nevertheless, since $\mathcal{S}_{\mathrm{m}}^{0}$ is generally neither injective nor invertible on $H^{-1/2}(\partial B)$, the standard symmetrization technique (cf. [7, 9, 11]) via Calderón identity (3.37) cannot be applied directly to symmetrize the operator $\mathcal{K}_{\mathrm{m}}^{0}$.

Before proceeding to remedy the aforementioned difficulty, we sketch the proof of the claim that $\mathcal{S}_{\mathrm{e}}^{0}$ is injective on $H^{-1/2}(\partial B)$, while $\mathcal{S}_{\mathrm{m}}^{0}$ is injective only on $H_0^{-1/2}(\partial B)$ and the dimension of the kernel of $\mathcal{S}_{\mathrm{m}}^{0}$ in $H^{-1/2}(\partial B)$ is at most one (under the assumption that ∂B is connected), for the sake of completeness. Some technical estimates shall also be useful in section 4. For this, we first observe the far-field behavior of $\mathcal{S}_{\mathrm{e/m}}^{0}[\phi]$ from (3.6), i.e., it holds for $\phi\in H^{-1/2}(\partial B)$ and large enough x_3 that

$$\mathcal{S}_{\mathrm{e/m}}^{0}[\phi](\mathbf{x})=c_{0,\mathrm{e/m}}(\phi)+\sum_{\xi\in\Lambda^*\backslash\{0\}}\frac{1}{|\xi|}c_{\xi,\mathrm{e/m}}(\phi)e^{i\xi\cdot x'}e^{-|\xi|x_3}\,, \tag{3.38}$$

where $c_{\xi,\mathrm{e/m}}$ for $\xi\in\Lambda^*\backslash\{0\}$ are linear functionals on $H^{-1/2}(\partial B)$, and in particular the coefficients $c_{0,\mathrm{e}}(\phi)$ and $c_{0,\mathrm{m}}(\phi)$ are given by

$$c_{0,\mathrm{e}}(\phi)=-\frac{1}{\tau}\int_{\partial B}y_3\phi(\mathbf{y})d\sigma(\mathbf{y})\,,\quad c_{0,\mathrm{m}}(\phi)=\frac{x_3}{\tau}\langle\phi,1\rangle\,. \tag{3.39}$$

Then, by using integration by parts, we have

$$\int_{\Sigma\times(0,L)}\left|\nabla\mathcal{S}_{\mathrm{e/m}}^{0}[\phi]\right|^2d\mathbf{x}=-\int_{\partial B}\phi\cdot\overline{\mathcal{S}_{\mathrm{e/m}}^{0}}[\phi]d\sigma+\int_{\Sigma\times\{L\}}\frac{\partial\mathcal{S}_{\mathrm{e/m}}^{0}[\phi]}{\partial\nu}\cdot\overline{\mathcal{S}_{\mathrm{e/m}}^{0}}[\phi]d\sigma\,,$$

which, combined with (3.38) and (3.39), implies that, by letting L tend to infinity,

$$\int_{\Omega}\left|\nabla\mathcal{S}_{\mathrm{e}}^{0}[\phi]\right|^2d\mathbf{x}=-\int_{\partial B}\phi\cdot\overline{\mathcal{S}_{\mathrm{e}}^{0}}[\phi]d\sigma\geq 0 \tag{3.40}$$

holds for all $\phi\in H^{-1/2}(\partial B)$. If $\mathcal{S}_{\mathrm{e}}^{0}$ is replaced by $\mathcal{S}_{\mathrm{m}}^{0}$ in the above formula, then (3.40) holds only for $\phi\in H_0^{-1/2}(\partial B)$. We further see from (3.40) that if $\mathcal{S}_{\mathrm{e/m}}^{0}[\phi]$ vanishes, then $\nabla\mathcal{S}_{\mathrm{e/m}}^{0}[\phi]$ must be zero, which yields that ϕ is also zero by the jump formula

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(3.26). Hence we can conclude that $\mathcal{S}_{\rm e}^0$ is injective on $H^{-1/2}(\partial B)$ and $\mathcal{S}_{\rm m}^0$ is injective only on $H_0^{-1/2}(\partial B)$. As a consequence of the fact that the orthogonal complement of $H_0^{-1/2}(\partial B)$ in $H^{-1/2}(\partial B)$ is a one-dimensional space, we know that the dimension of the kernel of $\mathcal{S}_{\rm m}^0$ in $H^{-1/2}(\partial B)$ is at most one.

A standard approach [7] to overcome the difficulty that $\mathcal{S}_{\rm m}^0$ may not be invertible on $H^{-1/2}(\partial B)$ is to consider the bounded operator $A_{\rm e/m} : H^{-\frac{1}{2}}(\partial B)\times\mathbb{C} \to H^{\frac{1}{2}}(\partial B)\times\mathbb{C}$ defined by

$$A_{\rm e/m}(\phi, a) := (\mathcal{S}_{\rm e/m}^0[\phi] + a, \langle\phi, 1\rangle)\,,$$

which can be shown to have a bounded inverse. In fact, since the Fredholm index is stable under the compact perturbation and $\mathcal{S}_{\rm e/m}^0$ is a Fredholm operator with index zero, we can conclude that the operator $A_{\rm e/m}$ is also Fredholm with index zero. Hence it suffices to prove the injectivity of $A_{\rm e/m}$ to establish its invertibility, which follows from exactly the same proof as the one for [8, Theorem 2.26]; see also [32, 13]. Then we can prove that $\mathcal{S}_{\rm e/m}^0$ is invertible if and only if $\mathcal{S}_{\rm e/m}^0[\varphi_0^{\rm e/m}] \neq 0$ (cf. [13]), where $\varphi_0^{\rm e/m}$ is the eigenfunction of $\mathcal{K}_{\rm e/m}^{0,*}$ associated with the eigenvalue $\frac{1}{2}$, satisfying $\langle\varphi_0^{\rm e/m}, 1\rangle = -1$. We define

$$\widetilde{\mathcal{S}}_{\rm e/m}^0[\psi] = \begin{cases} \mathcal{S}_{\rm e/m}^0[\psi] & \text{if } \ \langle\psi, 1\rangle = 0\,, \\ 1 & \text{if } \ \psi = \varphi_0^{\rm e/m}\,. \end{cases}$$

Then $\widetilde{\mathcal{S}}_{\rm e/m}^0$ is a bijection from $H^{-1/2}(\partial B)$ to $H^{1/2}(\partial B)$, and the generalized Calderón identity

$$\widetilde{\mathcal{S}}_{\rm e/m}^0\mathcal{K}_{\rm e/m}^{0,*} = \mathcal{K}_{\rm e/m}^0\widetilde{\mathcal{S}}_{\rm e/m}^0$$

holds. This allows us to define two new inner products (equivalent to the original one) on $H^{-1/2}(\partial B)$:

$$(\phi, \psi)_{\mathcal{H}_{\rm e/m}^*} = -\langle\phi, \widetilde{\mathcal{S}}_{\rm e/m}^0[\psi]\rangle\,.$$

We denote by $\mathcal{H}_{\rm e/m}^*$ the space $H^{-1/2}(\partial B)$ equipped with these two new inner products, respectively. Then we can symmetrize $\mathcal{K}_{\rm e/m}^{0,*}$ as follows.

LEMMA 3.5. *For a C^2-smooth bounded domain B with a connected boundary, we have as follows:*

(i) *$\mathcal{K}_{\rm e/m}^{0,*}$ is compact and self-adjoint on the Hilbert space $\mathcal{H}_{\rm e/m}^*$.*

(ii) *Suppose that $\{(\lambda_j^{\rm e/m}, \varphi_j^{\rm e/m})\}_{j\geq 0}$ are the eigenpairs of $\mathcal{K}_{\rm e/m}^{0,*}$ with $\lambda_0^{\rm e/m} = \frac{1}{2}$ and normalized eigenfunctions: $\|\varphi_j^{\rm e/m}\|_{\mathcal{H}_{\rm e/m}^*} = 1$; then $\lambda_j^{\rm e/m} \in (-\frac{1}{2}, \frac{1}{2}]$ for $j \geq 0$ with $\lambda_j^{\rm e/m} \to 0$ as $j \to \infty$.*

(iii) *$\{\varphi_j^{\rm e/m}\}_{j\geq 0}$ forms a complete orthogonal basis on $\mathcal{H}_{\rm e/m}^*$ with $\mathcal{H}_{\rm e/m}^* = \mathcal{H}_{0,\rm e/m}^* \oplus \{\mu\varphi_0^{\rm e/m},\, \mu \in \mathbb{C}\}$, where $\mathcal{H}_{0,\rm e/m}^*$ is the zero mean subspace of $\mathcal{H}_{\rm e/m}^*$ spanned by $\{\varphi_j^{\rm e/m}\}_{j\neq 0}$.*

(iv) *The following spectral decomposition holds:*

$$\mathcal{K}_{\rm e/m}^{0,*}[\phi] = \sum_{j=0}^{\infty} \lambda_j^{\rm e/m} \left(\phi,\, \varphi_j^{\rm e/m}\right)_{\mathcal{H}_{\rm e/m}^*} \varphi_j^{\rm e/m} \quad \text{for } \phi \in \mathcal{H}_{\rm e/m}^*\,. \tag{3.41}$$

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Similarly, we can define the inner products on $H^{1/2}(\partial B)$ by

$$-\left\langle \left(\widetilde{\mathcal{S}}^0_{\mathrm{e/m}}\right)^{-1}[\psi],\, \phi \right\rangle$$

and denote by $\mathcal{H}_{\mathrm{e/m}}$ the Hilbert space $H^{1/2}(\partial B)$ equipped with these two inner products, respectively, both of which are equivalent to the original space. Note that $\widetilde{\mathcal{S}}^0_{\mathrm{e/m}}$ is a unitary operator from $\mathcal{H}^*_{\mathrm{e/m}}$ to $\mathcal{H}_{\mathrm{e/m}}$, hence $\{\widetilde{\mathcal{S}}^0_{\mathrm{e/m}}[\varphi_j]\}_{j\geq 0}$ forms an orthonormal basis on $\mathcal{H}_{\mathrm{e/m}}$. We remark that $\widetilde{\mathcal{S}}^0_{\mathrm{e/m}}[\varphi_j]$, $j \geq 0$, are also the eigenfunctions of $\mathcal{K}^0_{\mathrm{e/m}}$.

We are now ready to consider the leading-order terms $\mathcal{K}^*_{\mathrm{e/m}}$ and $\mathcal{K}_{\mathrm{e/m}}$ in the expansions of $\mathcal{K}^{\delta\mathbf{k},*}_{B,\mathrm{e/m}}$ and $\mathcal{K}^{\delta\mathbf{k}}_{B,\mathrm{e/m}}$, which can be regarded as the corrections of $\mathcal{K}^{0,*}_{\mathrm{e/m}}$ and $\mathcal{K}^0_{\mathrm{e/m}}$ due to the incident direction $\mathbf{d}$. In fact, recalling the definitions of $\mathcal{K}_{\mathrm{e/m}}$ and $\mathcal{K}^*_{\mathrm{e/m}}$ and using formulas (3.15) and (3.16), we obtain

$$\mathcal{K}_{\mathrm{e}} = \mathcal{K}^0_{\mathrm{e}}\,, \quad \mathcal{K}_{\mathrm{m}}[\phi] = \mathcal{K}^0_{\mathrm{m}} + \frac{1}{d_3\tau}\langle d'\cdot\nu'\phi, 1\rangle\,, \tag{3.42}$$

$$\mathcal{K}^*_{\mathrm{e}} = \mathcal{K}^{0,*}_{\mathrm{e}}\,, \quad \mathcal{K}^*_{\mathrm{m}}[\phi] = \mathcal{K}^{0,*}_{\mathrm{m}} - \frac{d'\cdot\nu'}{d_3\tau}\langle \phi, 1\rangle\,. \tag{3.43}$$

Hence the spectral structure of $\mathcal{K}^*_{\mathrm{e}}$ can be completely characterized by Lemma 3.5. In the following, we shall only pay attention to the operator $\mathcal{K}^*_{\mathrm{m}}$. It turns out that the spectra of $\mathcal{K}^*_{\mathrm{m}}$ has nothing to do with the incident angle (or $\mathbf{d}$) although there are remaining items in (3.42) and (3.43) involving $\mathbf{d}$.

We next introduce some standard notation and present several spectral results. For a compact operator K, we denote by $\sigma(K)$ its spectrum set and by $(\lambda I - K)^{-1}$ its resolvent operator with $\lambda \in \mathbb{C}\backslash\sigma(K)$ being the regular values. For a point p and a set F in the complex plane $\mathbb{C}$, we define their distance by $d(p, F) := \inf_{q\in F}|p - q|$.

THEOREM 3.6. *The operators $\mathcal{K}^*_{\mathrm{m}}$ and $\mathcal{K}^{0,*}_{\mathrm{m}}$ have the same spectra. For $\lambda_j \in \sigma(\mathcal{K}^*_{\mathrm{m}})\backslash\{0\}$, we further have* $\dim\ker(\lambda_j - \mathcal{K}^*_{\mathrm{m}}) = \dim\ker(\lambda_j - \mathcal{K}^{0,*}_{\mathrm{m}})$.

Proof. It is known that $\mathcal{K}^*_{\mathrm{m}}$ is a compact operator with the adjoint operator $\hat{\mathcal{K}}_{\mathrm{m}}$; see (3.31). It then follows from Gauss's lemma (cf. [28, Proposition 3.19]) that $\hat{\mathcal{K}}_{\mathrm{m}}[1] = 1/2$ holds, which implies that $1/2$ is also an eigenvalue of $\mathcal{K}^*_{\mathrm{m}}$. Combining this with the fact that $\mathcal{K}^*_{\mathrm{m}} = \mathcal{K}^{0,*}_{\mathrm{m}}$ on $H_0^{-1/2}(\partial B)$, we have $\sigma(\mathcal{K}^{0,*}_{\mathrm{m}}) \subset \sigma(\mathcal{K}^*_{\mathrm{m}})$. Suppose $\lambda \in \sigma(\mathcal{K}^*_{\mathrm{m}})\backslash\{0, 1/2\}$ and that ϕ is the associated eigenfunction; then we obtain, by using $\hat{\mathcal{K}}_{\mathrm{m}}[1] = 1/2$, that

$$0 = \int_{\partial B}(\lambda I - \mathcal{K}^*_{\mathrm{m}})[\phi]d\sigma = \left(\lambda - \frac{1}{2}\right)\int_{\partial B}\phi d\sigma\,,$$

which further yields $\phi \in H_0^{-1/2}(\partial B)$. We thus have $\sigma(\mathcal{K}^{0,*}_{\mathrm{m}}) = \sigma(\mathcal{K}^*_{\mathrm{m}})$ and the desired result follows. ∎

We next consider the spectral decomposition of $\mathcal{K}^*_{\mathrm{m}}$ and $\mathcal{K}_{\mathrm{m}}$ and the corresponding resolvent estimates. Suppose that $\phi \in \mathcal{H}^*_{\mathrm{m}}$ has the following decomposition with respect to the orthonormal basis $\{\varphi_j\}_{j\geq 0}$ given by the eigensystem $\{(\lambda_j, \varphi_j)\}_{j\geq 0}$ of $\mathcal{K}^{0,*}_{\mathrm{m}}$:

$$\phi = \sum_{j=0}^{\infty}(\phi, \varphi_j)_{\mathcal{H}^*_{\mathrm{m}}}\varphi_j\,. \tag{3.44}$$

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Here we have omitted the superscript m of $\left(\lambda_j^{\mathrm{m}}, \varphi_j^{\mathrm{m}}\right)$ for simplicity. By writing the Fourier coefficients $(\phi, \varphi_j)_{\mathcal{H}_{\mathrm{m}}^*}$ as $\hat{\phi}(j)$ and using Lemma 3.5, Theorem 3.6, and the formula (3.43), we can derive

$$\mathcal{K}_{\mathrm{m}}^*[\phi] = \hat{\phi}(0)\mathcal{K}_{\mathrm{m}}^*[\varphi_0] + \sum_{n=1}^{\infty} \hat{\phi}(j)\lambda_j\varphi_j = \hat{\phi}(0)\left(\frac{1}{2}\varphi_0 + \sum_{j=1}^{\infty}\iota_j\varphi_j\right) + \sum_{j=1}^{\infty}\hat{\phi}(j)\lambda_j\varphi_j$$

$$= \sum_{j=0}^{\infty}\lambda_j\hat{\phi}(j)\varphi_j + \hat{\phi}(0)\sum_{j=1}^{\infty}\iota_j\varphi_j\,, \tag{3.45}$$

where the constants $\{\iota_j\}_{j=1}^{\infty}$ are obtained by applying the decomposition (3.44) to $-\frac{d'\cdot\nu'}{d_3\tau}\langle\varphi_0, 1\rangle$, i.e.,

$$-\frac{d'\cdot\nu'}{d_3\tau}\langle\varphi_0, 1\rangle = \frac{d'\cdot\nu'}{d_3\tau} = \sum_{j=1}^{\infty}\iota_j\varphi_j\,.$$

PROPOSITION 3.7. *For the operators $\mathcal{K}_{\mathrm{e/m}}^*$, the following resolvent estimates hold:*

$$\left\|\left(\lambda I - \mathcal{K}_{\mathrm{e/m}}^*\right)^{-1}[f]\right\|_{\mathcal{H}_{\mathrm{e/m}}^*} \lesssim \frac{\|f\|_{\mathcal{H}_{\mathrm{e/m}}^*}}{d\left(\lambda, \sigma\left(\mathcal{K}_{\mathrm{e/m}}^{0,*}\right)\right)}\,, \quad \lambda \in \mathbb{C}\backslash\sigma\left(\mathcal{K}_{\mathrm{e/m}}^*\right),\ f \in H^{-\frac{1}{2}}(\partial B)\,.$$

Proof. The resolvent estimate for $\mathcal{K}_{\mathrm{e}}^*$ follows directly from the fact that $\mathcal{K}_{\mathrm{e}}^*$ is a compact self-adjoint operator on $\mathcal{H}_{\mathrm{e}}^*$. For $\mathcal{K}_{\mathrm{m}}^*$, considering the equation $(\lambda I - \mathcal{K}_{\mathrm{m}}^*)[\phi] = f$, we obtain from (3.45) that

$$\sum_{j=0}^{\infty}(\lambda - \lambda_j)\hat{\phi}(j)\varphi_j - \hat{\phi}(0)\sum_{j=1}^{\infty}\iota_j\varphi_j = \sum_{j=0}^{\infty}\hat{f}(j)\varphi_j\,.$$

For $\lambda \notin \sigma(\mathcal{K}_{\mathrm{m}}^{0,*})$, $\hat{\phi}(j)$ can be uniquely determined by

$$\hat{\phi}(0) = \frac{1}{\lambda - \frac{1}{2}}\hat{f}(0)\,; \quad \hat{\phi}(j) = \frac{\hat{f}(j) + \hat{\phi}(0)\iota_j}{\lambda - \lambda_j} = \frac{\hat{f}(j)}{\lambda - \lambda_j} + \frac{\hat{f}(0)\iota_j}{(\lambda - \lambda_j)(\lambda - \frac{1}{2})} \quad \text{for} \ \ j \geq 1\,.$$

Using the above formulas, we then derive

$$\|\phi\|_{\mathcal{H}_{\mathrm{m}}^*} \lesssim \frac{\|f\|_{\mathcal{H}_{\mathrm{m}}^*}}{d\left(\lambda, \sigma\left(\mathcal{K}_{\mathrm{m}}^{0,*}\right)\right)} + \frac{|\langle f, 1\rangle|}{d\left(\lambda, \sigma\left(\mathcal{K}_{\mathrm{m}}^{0,*}\right)\backslash\{\frac{1}{2}\}\right)\cdot|\lambda - \frac{1}{2}|} \lesssim \frac{\|f\|_{\mathcal{H}_{\mathrm{m}}^*}}{d\left(\lambda, \sigma\left(\mathcal{K}_{\mathrm{m}}^{0,*}\right)\right)}\,. \qquad \square$$

For convenience, we shall define $\check{\psi}(j) := (\psi, \widetilde{\mathcal{S}}_{\mathrm{m}}^0[\varphi_j])_{\mathcal{H}_{\mathrm{m}}}$ for $\psi \in \mathcal{H}_{\mathrm{m}}$. Then we can write the following decomposition:

$$\psi = \sum_{j=0}^{\infty}\check{\psi}(j)\widetilde{\mathcal{S}}_{\mathrm{m}}^0[\varphi_j]\,. \tag{3.46}$$

Again we have omitted the superscript m of $\left(\lambda_j^{\mathrm{m}}, \varphi_j^{\mathrm{m}}\right)$ for simplicity. Using the above decomposition and arguments similar to the ones for the above proposition, we can obtain the resolvent estimate of $\mathcal{K}_{\mathrm{e/m}}$.

PROPOSITION 3.8. *For the operators $\mathcal{K}_{\mathrm{e/m}}$, the following resolvent estimates hold:*

$$\left\|\left(\lambda I - \mathcal{K}_{\mathrm{e/m}}\right)^{-1}[g]\right\|_{\mathcal{H}_{\mathrm{e/m}}} \lesssim \frac{\|g\|_{\mathcal{H}_{\mathrm{e/m}}}}{d\left(\lambda, \sigma\left(\mathcal{K}_{\mathrm{e/m}}^{0}\right)\right)}\,, \quad \lambda \in \mathbb{C}\backslash\sigma\left(\mathcal{K}_{\mathrm{e/m}}\right),\ g \in H^{\frac{1}{2}}(\partial B)\,.$$

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Proof. We only prove the estimate for $\mathcal{K}_{\rm m}$. It follows from the formulas (3.42) and (3.46) that

$$\begin{aligned}\mathcal{K}_{\rm m}[\psi] &= \sum_{j=0}^{\infty} \check{\psi}(j)\lambda_j \widetilde{\mathcal{S}}^0_{\rm m}[\varphi_j] + \frac{1}{d_3\tau}\sum_{j=0}^{\infty}(-d'\cdot\nu', \varphi_j)_{\mathcal{H}^*_{\rm m}}\check{\psi}(j)\\ &= \sum_{j=0}^{\infty} \check{\psi}(j)\lambda_j \widetilde{\mathcal{S}}^0_{\rm m}[\varphi_j] - \sum_{j=1}^{\infty}\iota_j\check{\psi}(j)\,.\end{aligned}$$

Considering the equation $(\lambda I - \mathcal{K}_{\rm m})[\psi] = g$ and using (3.46), we have

$$\sum_{j=1}^{\infty}(\lambda-\lambda_j)\check{\psi}(j)\widetilde{\mathcal{S}}^0_{\rm m}[\varphi_j] + \sum_{n=1}^{\infty}\iota_n\check{\psi}(n) = \check{g}(0) + \sum_{n=1}^{\infty}\check{g}(n)\widetilde{\mathcal{S}}^0_{\rm m}[\varphi_n]\,.$$

For $\lambda \notin \sigma(\mathcal{K}^0_{\rm m})$, $\check{\psi}(n)$ can be uniquely determined by

$$\begin{aligned}\check{\psi}(n) = \frac{\check{g}(n)}{\lambda-\lambda_n}, \quad n\geq 1\,; \quad \check{\psi}(0) &= \frac{1}{\lambda-\frac{1}{2}}\left(\check{g}(0) - \sum_{n=1}^{\infty}\iota_n\check{\psi}(n)\right)\\ &= \frac{1}{\lambda-\frac{1}{2}}\left(\check{g}(0) - \sum_{n=1}^{\infty}\iota_n\frac{\check{g}(n)}{\lambda-\lambda_n}\right).\end{aligned}$$

Then we can obtain the desired estimate:

$$\|\psi\|_{\mathcal{H}_{\rm m}} \lesssim \frac{\|g\|_{\mathcal{H}_{\rm m}}}{d\left(\lambda, \sigma\left(\mathcal{K}^0_{\rm m}\right)\right)} + \frac{\|g\|_{\mathcal{H}_{\rm m}}}{d\left(\lambda, \sigma\left(\mathcal{K}^0_{\rm m}\right)\backslash\{\frac{1}{2}\}\right)\cdot|\lambda-\frac{1}{2}|} \lesssim \frac{\|g\|_{\mathcal{H}_{\rm m}}}{d\left(\lambda, \sigma\left(\mathcal{K}^0_{\rm m}\right)\right)}\,. \qquad \square$$

The above spectral results suggest to us that in most cases, there is no need to distinguish between $\mathcal{K}_{\rm e/m}$ and $\mathcal{K}^0_{\rm e/m}$, as well as between $\mathcal{K}^*_{\rm e/m}$ and $\mathcal{K}^{0,*}_{\rm e/m}$, since they have the same spectrum and have the same resolvent estimates. We are now in a position to study the spectral structure of the compact operator $\mathcal{M}_{\rm e/m}$ (see [22, p. 208], and also [12, Lemma 2.3], for the compactness). For each $u \in H_T^{-1/2}(\mathrm{div}, \partial B)$, we recall the Helmholtz decomposition (2.7) to write it as

$$u = \nabla_{\partial B} u^{(1)} + \vec{\mathrm{curl}}_{\partial B} u^{(2)} \tag{3.47}$$

with two functions $u^{(1)} \in H_0^{3/2}(\partial B)$ and $u^{(2)} \in H_0^{1/2}(\partial B)$. We shall adopt this notation throughout this work and may not always specify the subspaces $H_0^{3/2}(\partial B)$ and $H_0^{1/2}(\partial B)$ when we use $u^{(1)}$ and $u^{(2)}$. By utilizing the invertibility of the Laplace–Beltrami operator $\Delta_{\partial B} : H_0^{3/2}(\partial B) \to H_0^{-1/2}(\partial B)$ and the inverse mapping theorem, we obtain an isomorphism between $H_T^{-1/2}(\mathrm{div}, \partial B)$ and $H_0^{3/2} \times H_0^{1/2}$ via the decomposition (3.47), which further induces an equivalent norm on $H_T^{-1/2}(\mathrm{div}, \partial B)$:

$$\|\phi\|_{H_T^{-\frac{1}{2}}(\mathrm{div}, \partial B)} \approx \|\Delta_{\partial B}\phi^{(1)}\|_{H^{-\frac{1}{2}}(\partial B)} + \|\phi^{(2)}\|_{H^{\frac{1}{2}}(\partial B)}\,.$$

THEOREM 3.9. *The spectra $\sigma\left(\mathcal{M}_{\rm e/m}\right)$ and $\sigma\left(\mathcal{M}^0_{\rm e/m}\right)$ of the operators $\mathcal{M}^0_{\rm e/m}$ and $\mathcal{M}_{\rm e/m}$ are given by*

$$\sigma\left(\mathcal{M}_{\rm e/m}\right) = \sigma\left(\mathcal{M}^0_{\rm e/m}\right) = \left(-\sigma\left(\mathcal{K}^{0,*}_{\rm e/m}\right)\bigcup\sigma\left(\mathcal{K}^{0,*}_{\rm m/e}\right)\right)\setminus\left\{-\frac{1}{2}, \frac{1}{2}\right\}. \tag{3.48}$$

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Proof. We shall only consider the spectrum of $\mathcal{M}_{\mathrm{e/m}}$, as the analysis for $\mathcal{M}^0_{\mathrm{e/m}}$ is similar and even simpler. Denote by $F_{\mathrm{e/m}}$ the set in the right-hand side of (3.48). Define

$$\sigma^1_{\mathrm{e/m}} := F_{\mathrm{e/m}} \bigcap \sigma\big(\mathcal{K}^{0,*}_{\mathrm{m/e}}\big), \quad \sigma^2_{\mathrm{e/m}} := F_{\mathrm{e/m}} \backslash \sigma\big(\mathcal{K}^{0,*}_{\mathrm{m/e}}\big)\,.$$

Since $\mathcal{M}_{\mathrm{e/m}}$ is a compact operator, it suffices to consider the equation, for a given $\lambda \in \mathbb{C}\backslash\{0\}$,

$$(\lambda I - \mathcal{M}_{\mathrm{e/m}})[\phi] = 0\,, \tag{3.49}$$

and prove that the above equation has nontrivial solutions if and only if $\lambda \in \sigma^1_{\mathrm{e/m}} \bigcup \sigma^2_{\mathrm{e/m}}$. By the decomposition (3.47), we can write

$$\phi = \nabla_{\partial B}\phi^{(1)} + \vec{\mathrm{curl}}_{\partial B}\phi^{(2)}\,.$$

For nonzero $\lambda \in \sigma^1_{\mathrm{e/m}}$, we first note from (3.36) that

$$(\lambda I - \mathcal{M}_{\mathrm{e/m}})[\vec{\mathrm{curl}}_{\partial B}\phi^{(2)}] = \lambda \vec{\mathrm{curl}}_{\partial B}\phi^{(2)} - \vec{\mathrm{curl}}_{\partial B}\mathcal{K}^0_{\mathrm{m/e}}[\phi^{(2)}]\,, \tag{3.50}$$

which directly implies that $(\lambda, \vec{\mathrm{curl}}_{\partial B}\phi^{(2)})$ is an eigenpair of $\mathcal{M}_{\mathrm{e/m}}$ if $\phi^{(2)}$ is an eigenfunction of $\mathcal{K}^0_{\mathrm{m/e}}$ associated with λ. If $\lambda \in \sigma^2_{\mathrm{e/m}}$, we readily obtain, by using the surface divergence for (3.49), that

$$\nabla_{\partial B} \cdot \left(\lambda I - \mathcal{M}_{\mathrm{e/m}}\right)[\phi] = \left(\lambda I + \mathcal{K}^{0,*}_{\mathrm{e/m}}\right)[\nabla_{\partial B} \cdot \phi] = \left(\lambda I + \mathcal{K}^{0,*}_{\mathrm{e/m}}\right)[\Delta_{\partial B}\phi^{(1)}] = 0\,. \tag{3.51}$$

Since the eigenfunction of $-\mathcal{K}^{0,*}_{\mathrm{e/m}}$ associated with $\lambda \in \sigma^2_{\mathrm{e/m}}$ has mean value zero and $\Delta_{\partial B}$ is an isomorphism from $H_0^{3/2}(\partial B)$ to $H_0^{-1/2}(\partial B)$, we have that there exists a nonconstant function $\phi^{(1)}$ satisfying (3.51). We then reduce (3.49) via (3.50) to

$$\lambda \vec{\mathrm{curl}}_{\partial B}\phi^{(2)} - \vec{\mathrm{curl}}_{\partial B}\mathcal{K}^0_{\mathrm{m/e}}[\phi^{(2)}] = -(\lambda I - \mathcal{M}_{\mathrm{e/m}})[\nabla_{\partial B}\phi^{(1)}]\,.$$

Taking the surface curl on both sides of the above equation, we then find that it is solvable, by the invertibility of $\Delta_{\partial B}$ and $\lambda I - \mathcal{K}^0_{\mathrm{m/e}}$. Hence, there exists a nontrivial ϕ satisfying (3.49) for $\lambda \in \sigma^2_{\mathrm{e/m}}$. We next consider the last case: $\lambda \in \mathbb{C}\backslash\big(\sigma^1_{\mathrm{e/m}} \bigcup \sigma^2_{\mathrm{e/m}}\big)$. By the invertibility of $\lambda I + \mathcal{K}^{0,*}_{\mathrm{e/m}}$ on $H_0^{-1/2}(\partial B)$, it is easy to derive that ϕ must be $\vec{\mathrm{curl}}_{\partial B}\phi^{(2)}$ for some $\phi^{(2)}$. Then the reduced equation from (3.50) reads

$$(\lambda I - \mathcal{K}^0_{\mathrm{m/e}})[\phi^{(2)}] = C$$

by the fact that $\Delta_{\partial B}$ is invertible, where C is some constant. Without loss of generality, we consider two cases: $C = 1$ or 0. If $\lambda = 1/2$, we must have $C = 0$ in order to guarantee the existence of $\phi^{(2)}$ due to the Fredholm alternative. In this case, we have $\phi = \vec{\mathrm{curl}}_{\partial B}\phi^{(2)} = 0$. If $\lambda \neq 1/2$, we can find a constant C' such that

$$(\lambda I - \mathcal{K}^0_{\mathrm{m/e}})[\phi^{(2)} + C'] = 0\,,$$

which yields $\phi^{(2)}$ is a constant. Hence, if $\lambda \in \mathbb{C}\backslash(\sigma^1_{\mathrm{e/m}} \bigcup \sigma^2_{\mathrm{e/m}})$, we can conclude $\phi = 0$. The proof is complete. ∎

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4. Approximation of the scattered wave.

4.1. Integral formulation and asymptotic analysis. With the help of the analytical tools and results established in the previous section, in this subsection, we shall first reformulate the system (2.1) as a boundary integral equation and then build up a norm estimate of the associated solution operator, from which we can predict the occurrence of the resonance phenomenon. To do so, we take advantage of the vector potential $\mathcal{A}^{\mathbf{k}}_{D,\mathrm{e/m}}$ given in section 3.2 and assume that the electric field solution to (2.1) has the following ansatz:

$$E = \begin{cases} E^i + \nabla \times \mathcal{A}^{\mathbf{k}}_{D,\mathrm{m}}[\phi] + \nabla \times \nabla \times \mathcal{A}^{\mathbf{k}}_{D,\mathrm{e}}[\psi]\,, & \mathbf{x} \in \mathbb{R}^3 \backslash \mathcal{D}\,, \\ \mu_c \nabla \times \mathcal{A}^{\mathbf{k}_c}_{D,\mathrm{m}}[\phi] + \nabla \times \nabla \times \mathcal{A}^{\mathbf{k}_c}_{D,\mathrm{e}}[\psi]\,, & \mathbf{x} \in \mathcal{D}\,. \end{cases} \tag{4.1}$$

It can be directly checked that the field E given above solves Maxwell's equations in both $\mathcal{D}$ and $\mathbb{R}^3_+ \backslash \mathcal{D}$ and satisfies the perfectly conducting boundary condition on Γ. Then by the jump formula (3.24), the original scattering problem can be equivalently written as a boundary integral equation on ∂D:

$$\begin{bmatrix} \frac{\mu_c+1}{2} + \mu_c \mathcal{M}^{\mathbf{k}_c}_{D,\mathrm{m}} - \mathcal{M}^{\mathbf{k}}_{D,\mathrm{m}} & \mathcal{L}^{\mathbf{k}_c}_{D,\mathrm{e}} - \mathcal{L}^{\mathbf{k}}_{D,\mathrm{e}} \\ \mathcal{L}^{\mathbf{k}_c}_{D,\mathrm{m}} - \mathcal{L}^{\mathbf{k}}_{D,\mathrm{m}} & \frac{k^2}{2}(\varepsilon_c+1)I + k^2(\varepsilon_c \mathcal{M}^{\mathbf{k}_c}_{D,\mathrm{e}} - \mathcal{M}^{\mathbf{k}}_{D,\mathrm{e}}) \end{bmatrix} \begin{bmatrix} \phi \\ \psi \end{bmatrix} = \begin{bmatrix} \nu \times E^i \\ ik\nu \times H^i \end{bmatrix}.$$

By setting $\mathbf{x} = \delta \widetilde{\mathbf{x}}$, we obtain the integral equation defined on ∂B

$$\mathcal{W}_{\delta,B} \begin{bmatrix} \widetilde{\phi} \\ \widetilde{\psi} \end{bmatrix} = \begin{bmatrix} \nu(\widetilde{\mathbf{x}}) \times \widetilde{E}^i \\ ik\nu(\widetilde{\mathbf{x}}) \times \widetilde{H}^i \end{bmatrix}, \tag{4.2}$$

where the block coefficient matrix is given by

$$\mathcal{W}_{\delta,B} = \begin{bmatrix} \frac{\mu_c+1}{2} + \mu_c \mathcal{M}^{\delta\mathbf{k}_c}_{B,\mathrm{m}} - \mathcal{M}^{\delta\mathbf{k}}_{B,\mathrm{m}} & \mathcal{L}^{\mathbf{k}_c}_{\mathrm{e},\delta} - \mathcal{L}^{\mathbf{k}}_{\mathrm{e},\delta} \\ \mathcal{L}^{\mathbf{k}_c}_{\mathrm{m},\delta} - \mathcal{L}^{\mathbf{k}}_{\mathrm{m},\delta} & k^2(\frac{\varepsilon_c+1}{2} I + \varepsilon_c \mathcal{M}^{\delta\mathbf{k}_c}_{B,\mathrm{e}} - \mathcal{M}^{\delta\mathbf{k}}_{B,\mathrm{e}}) \end{bmatrix}.$$

By Lemmas 3.2 and 3.3, we have the asymptotic expansion of $\mathcal{W}_{\delta,B}$:

$$\mathcal{W}_{\delta,B} = \sum_{n=0}^{\infty} \delta^n \mathcal{W}_{n,B},$$

where

$$\mathcal{W}_{0,B} = \begin{bmatrix} \frac{\mu_c+1}{2} + (\mu_c - 1)\mathcal{M}_{\mathrm{m}} & (k_c - k)\mathcal{L}_{1,\mathrm{e}} \\ (k_c - k)\mathcal{L}_{1,\mathrm{m}} & k^2 \frac{\varepsilon_c+1}{2} I + k^2(\varepsilon_c - 1)\mathcal{M}_{\mathrm{e}} \end{bmatrix},$$

and

$$\mathcal{W}_{n,B} = \begin{bmatrix} (k_c^n - k^n)\mathcal{M}_{n,\mathrm{m}} & (k_c^{n+1} - k^{n+1})\mathcal{L}_{n+1,\mathrm{e}} \\ (k_c^{n+1} - k^{n+1})\mathcal{L}_{n+1,\mathrm{m}} & k^2(\varepsilon_c k_c^n - k^n)\mathcal{M}_{n,\mathrm{e}} \end{bmatrix} \quad \text{for } n \geq 1\,.$$

We now investigate the invertibility of the leading-order operator $\mathcal{W}_{0,B}$. We introduce two contrast parameters $\lambda_\mu(\omega)$ and $\lambda_\varepsilon(\omega)$:

$$\lambda_\mu(\omega) = \frac{1 + \mu_c(\omega)}{2(1 - \mu_c(\omega))}, \quad \lambda_\varepsilon(\omega) = \frac{1 + \varepsilon_c(\omega)}{2(1 - \varepsilon_c(\omega))}\,.$$

The main result of this subsection is given as follows.

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THEOREM 4.1. *Suppose $\lambda_\mu(\omega)$, $\lambda_\varepsilon(\omega) \notin \sigma(\mathcal{M}_{\mathrm{e/m}})$; then $\mathcal{W}_{0,B}$ is invertible with the estimate:*

$$\left\|\mathcal{W}_{0,B}^{-1}\right\| \lesssim \frac{1}{d_\sigma d_\sigma^*}\,, \tag{4.3}$$

where the two constants d_σ and d_σ^* are defined by

$$d_\sigma = \min\left\{d\left(\lambda_\mu, \sigma\big(\mathcal{K}_{\mathrm{e}}^0\big)\right), d\left(\lambda_\varepsilon, \sigma\big(\mathcal{K}_{\mathrm{m}}^0\big)\right)\right\},$$

$$d_\sigma^* = \min\left\{d\left(\lambda_\mu, -\sigma\big(\mathcal{K}_{\mathrm{m}}^{0,*}\big)\right), d\left(\lambda_\varepsilon, -\sigma\big(\mathcal{K}_{\mathrm{e}}^{0,*}\big)\right)\right\}.$$

Proof. Without loss of generality, we assume $\mu_c \neq 1$, $\varepsilon_c \neq 1$ (the analysis for these two cases would be direct and simple) and consider the system

$$\mathcal{W}_{0,B}\begin{bmatrix}\phi\\ \psi\end{bmatrix} = \begin{bmatrix}(1-\mu_c)f\\ (1-\varepsilon_c)g\end{bmatrix}$$

for given $f, g \in H_T^{-1/2}(\mathrm{div}, \partial B)$, which is equivalent to the following two equations:

$$(\lambda_\mu I - \mathcal{M}_{\mathrm{m}})[\phi] + \frac{k_c - k}{1-\mu_c}\mathcal{L}_{1,\mathrm{e}}[\psi] = f\,, \quad \frac{k_c - k}{k^2(1-\varepsilon_c)}\mathcal{L}_{1,\mathrm{m}}[\phi] + (\lambda_\varepsilon I - \mathcal{M}_{\mathrm{e}})[\psi] = g\,. \tag{4.4}$$

Similarly to the proof of Theorem 4.1, we shall reduce (4.4) to some easily solvable subproblems by using the Helmholtz decomposition. To do so, we take the surface divergence on both sides of two equations in (4.4) and then use the formula (3.34) to obtain

$$\left(\lambda_\mu + \mathcal{K}_{\mathrm{m}}^{0,*}\right)[\nabla_{\partial B}\cdot\phi] = \nabla_{\partial B}\cdot f\,, \quad \left(\lambda_\varepsilon + \mathcal{K}_{\mathrm{e}}^{0,*}\right)[\nabla_{\partial B}\cdot\psi] = \nabla_{\partial B}\cdot g\,, \tag{4.5}$$

which, along with the fact that $\nabla_{\partial B}\cdot u = \Delta_{\partial B}u^{(1)}$ for any $u \in H_T^{-1/2}(\mathrm{div}, \partial B)$, yields

$$\phi^{(1)} = \Delta_{\partial B}^{-1}\left(\lambda_\mu + \mathcal{K}_{\mathrm{m}}^{0,*}\right)^{-1}\left(\Delta_{\partial B} f^{(1)}\right), \quad \psi^{(1)} = \Delta_{\partial B}^{-1}\left(\lambda_\varepsilon + \mathcal{K}_{\mathrm{e}}^{0,*}\right)^{-1}\left(\Delta_{\partial B} g^{(1)}\right).$$

Then it directly follows from Proposition 3.7 that

$$\|\Delta_{\partial B}\phi^{(1)}\|_{\mathcal{H}_{\mathrm{m}}^*} \lesssim \frac{\|\Delta_{\partial B} f^{(1)}\|_{\mathcal{H}_{\mathrm{m}}^*}}{d\big(\lambda_\mu, -\sigma\big(\mathcal{K}_{\mathrm{m}}^{0,*}\big)\big)}\,, \quad \|\Delta_{\partial B}\psi^{(1)}\|_{\mathcal{H}_{\mathrm{e}}^*} \lesssim \frac{\|\Delta_{\partial B} g^{(1)}\|_{\mathcal{H}_{\mathrm{e}}^*}}{d\big(\lambda_\varepsilon, -\sigma\big(\mathcal{K}_{\mathrm{e}}^{0,*}\big)\big)}\,.$$

We next solve the second component $\phi^{(2)}$. For this purpose, we use the formula (3.36) and write the first equation in (4.4) as

$$\begin{aligned}(\lambda_\mu I - \mathcal{M}_{\mathrm{m}})[\vec{\mathrm{curl}}_{\partial B}\phi^{(2)}] &= \vec{\mathrm{curl}}_{\partial B}\left(\lambda_\mu I - \mathcal{K}_e^0\right)[\phi^{(2)}]\\ &= f - \frac{k_c - k}{1-\mu_c}\mathcal{L}_{1,\mathrm{e}}[\psi] - (\lambda_\mu I - \mathcal{M}_{\mathrm{m}})[\nabla_{\partial B}\phi^{(1)}]\,.\end{aligned}$$

Then taking the surface scalar curl on both sides of the equation and using Proposition 3.8 give us

$$\begin{aligned}\|\phi^{(2)}\|_{\mathcal{H}_{\mathrm{e}}} \lesssim\ & \frac{\|f^{(2)}\|_{\mathcal{H}_{\mathrm{e}}}}{d\Big(\lambda_\mu, \sigma\big(\mathcal{K}_{\mathrm{e}}^0\big)\Big)} + \frac{\|\Delta_{\partial B} g^{(1)}\|_{\mathcal{H}_{\mathrm{e}}^*}}{d\Big(\lambda_\mu, \sigma\big(\mathcal{K}_{\mathrm{e}}^0\big)\Big)\cdot d\left(\lambda_\varepsilon, -\sigma\big(\mathcal{K}_{\mathrm{e}}^{0,*}\big)\right)}\\ &+ \frac{\|\Delta_{\partial B} f^{(1)}\|_{\mathcal{H}_{\mathrm{m}}^*}}{d\Big(\lambda_\mu, \sigma\big(\mathcal{K}_{\mathrm{e}}^0\big)\Big)\cdot d\left(\lambda_\mu, -\sigma\big(\mathcal{K}_{\mathrm{m}}^{0,*}\big)\right)}\,.\end{aligned}$$

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Similarly, we can compute $\psi^{(2)}$ and derive the estimate

$$\|\psi^{(2)}\|_{\mathcal{H}_{\mathrm{m}}} \lesssim \frac{\|g^{(2)}\|_{\mathcal{H}_{\mathrm{m}}}}{d\Big(\lambda_\varepsilon, \sigma\big(\mathcal{K}_{\mathrm{m}}^0\big)\Big)} + \frac{\|\Delta_{\partial B} f^{(1)}\|_{\mathcal{H}_{\mathrm{m}}^*}}{d\Big(\lambda_\mu, -\sigma\big(\mathcal{K}_{\mathrm{m}}^{0,*}\big)\Big) \cdot d\Big(\lambda_\varepsilon, \sigma\big(\mathcal{K}_{\mathrm{m}}^0\big)\Big)} + \frac{\|\Delta_{\partial B} g^{(1)}\|_{\mathcal{H}_{\mathrm{e}}^*}}{d\left(\lambda_\varepsilon, -\sigma\big(\mathcal{K}_{\mathrm{e}}^{0,*}\big)\right) \cdot d\Big(\lambda_\varepsilon, \sigma\big(\mathcal{K}_{\mathrm{m}}^0\big)\Big)}.$$

In view of all the above arguments, we actually have obtained the unique solvability of the system (4.4) and the desired estimate (4.3). ∎

Remark 4.2. If we restrict the operator $\mathcal{W}_{0,B}$ on the space $\mathbb{H} \times \mathbb{H}$ (see (3.30) for the definition of $\mathbb{H}$), then $\mathcal{W}_{0,B}$ shall have a diagonal form:

$$\mathcal{W}_{0,B} = \begin{bmatrix} \frac{\mu_c+1}{2} I + (\mu_c - 1)\mathcal{M}_{\mathrm{m}}^0 & 0 \\ 0 & k^2 \frac{\varepsilon_c+1}{2} I + k^2(\varepsilon_c - 1)\mathcal{M}_{\mathrm{e}}^0 \end{bmatrix}.$$

Furthermore, $\mathcal{W}_{0,B}$ is an isomorphism on $\mathbb{H} \times \mathbb{H}$ with the estimate $\|\mathcal{W}_{0,B}^{-1}\| \lesssim 1/d_\sigma$ if $\lambda_\mu,\, \lambda_\varepsilon \notin \sigma\big(\mathcal{M}_{\mathrm{e/m}}\big)$.

By the recurrence relation (3.14) and the elliptic regularity, we conclude that $\mathcal{W}_{n,B}$ are uniformly bounded with respect to n. Then the uniform operator convergence follows:

$$\lim_{\delta \to 0} \mathcal{W}_{\delta,B}^{-1} = \mathcal{W}_{0,B}^{-1}.$$

Therefore, there exists a $\delta_0 > 0$ such that the following equivalence holds for $\delta \le \delta_0$:

$$\left\|\mathcal{W}_{\delta,B}^{-1}\right\| \approx \left\|\mathcal{W}_{0,B}^{-1}\right\|.$$

Combining the above estimate with Theorem 4.1, we directly observe that at some specified frequencies (characterized by the spectra of $\mathcal{M}_{\mathrm{e/m}}$), the solution operator $\mathcal{W}_{\delta,B}^{-1}$ can blow up with the order $(d_\sigma d_\sigma^*)^{-1}$, which indicates the existence of resonances.

4.2. Approximate scattered field. We are now in a position to approximate the scattered field with a certain order. In view of the complexities and technicalities of the detailed computations and relevant estimates, we split this section into three parts to make it more readable. The main result of this section is given in Theorem 4.7.

4.2.1. Approximate kernels and densities. Motivated by the well-known two-scale asymptotic expansion method in the standard homogenization theory [4], we shall first separate the propagative component from the scattered wave in the macroscopic scale. For this purpose, we observe from (3.5) that the quasi-periodic Green's function $G_{\mathrm{e/m}}^{\mathbf{k}}$ consists of a propagating mode,

$$G_{p,\mathrm{e/m}}^{\mathbf{k}}(\mathbf{x}, \mathbf{y}) = \frac{i}{2\tau k_3} e^{ik' \cdot (x' - y') - ik_3 |x_3 - y_3|} \pm \frac{i}{2\tau k_3} e^{ik' \cdot (x' - y') - ik_3 |x_3 + y_3|}, \tag{4.6}$$

and an exponentially decaying mode, $G_{e,\mathrm{e/m}}^{\mathbf{k}} := G_{\mathrm{e/m}}^{\mathbf{k}} - G_{p,\mathrm{e/m}}^{\mathbf{k}}$. Then the matrices $\Pi_{p,\mathrm{e/m}}^{\mathbf{k}}$ and $\Pi_{e,\mathrm{e/m}}^{\mathbf{k}}$ can be defined in the same way as $\Pi_{\mathrm{e/m}}^{\mathbf{k}}$ in (3.20), by replacing $G_{\mathrm{e/m}}^{\mathbf{k}}$ with $G_{p,\mathrm{e/m}}^{\mathbf{k}}$ and $G_{e,\mathrm{e/m}}^{\mathbf{k}}$. We can further decompose the operator $\mathcal{A}_{B,\mathrm{e/m}}^{\mathbf{k}}[\phi]$ as $\mathcal{A}_{B,\mathrm{e/m}}^{\mathbf{k}}[\phi] = \mathcal{A}_{p,\mathrm{e/m}}^{\mathbf{k}}[\phi] + \mathcal{A}_{e,\mathrm{e/m}}^{\mathbf{k}}[\phi]$, where

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$$\mathcal{A}^{\mathbf{k}}_{p,\mathrm{e/m}}[\phi] = \int_{\partial B} \Pi^{\mathbf{k}}_{p,\mathrm{e/m}}(\mathbf{x},\mathbf{y})\phi(\mathbf{y})d\sigma\,, \quad \mathcal{A}^{\mathbf{k}}_{e,\mathrm{e/m}}[\phi] = \int_{\partial B} \Pi^{\mathbf{k}}_{e,\mathrm{e/m}}(\mathbf{x},\mathbf{y})\phi(\mathbf{y})d\sigma\,.$$

We now define the propagative part and the evanescent part of the scattered wave in the reference space by

$$\widetilde{E}^r_p(\widetilde{\mathbf{x}}) = \nabla\times\mathcal{A}^{\delta\mathbf{k}}_{p,\mathrm{m}}[\widetilde{\phi}](\widetilde{\mathbf{x}}) + \frac{1}{\delta}\nabla\times\nabla\times\mathcal{A}^{\delta\mathbf{k}}_{p,\mathrm{e}}[\widetilde{\psi}](\widetilde{\mathbf{x}})\,, \tag{4.7}$$

$$\widetilde{E}^r_e(\widetilde{\mathbf{x}}) = \nabla\times\mathcal{A}^{\delta\mathbf{k}}_{e,\mathrm{m}}[\widetilde{\phi}](\widetilde{\mathbf{x}}) + \frac{1}{\delta}\nabla\times\nabla\times\mathcal{A}^{\delta\mathbf{k}}_{e,\mathrm{e}}[\widetilde{\psi}](\widetilde{\mathbf{x}})\,, \tag{4.8}$$

for densities $\widetilde{\phi}$ and $\widetilde{\psi}$ satisfying the system (4.2), respectively. We may see from the definition of $G^{\mathbf{k}}_{e,\mathrm{e/m}}$ that the structure of the evanescent wave is much more complicated than the one of the propagative part. Fortunately, we only care about the far-field behavior of the scattered wave, where the effect of the evanescent part can be ignored. Indeed, we have the following approximation estimate, whose proof is given in Appendix A.

LEMMA 4.3. *Let $L \in \mathbb{R}^+$ be a constant such that $|x_3| < L$ for all $\mathbf{x} \in D$. Then for small enough δ, there exists some positive constant c independent of δ such that*

$$\sup_{\mathbf{x}\in\mathbb{R}^2\times(L,+\infty)} \left|E^r(\mathbf{x}) - \widetilde{E}^r_p\left(\frac{\mathbf{x}}{\delta}\right)\right| = O\left(\delta^{-1}e^{-\frac{cL}{\delta}}\right)\,.$$

To further derive an approximation of the propagative scattered wave $\widetilde{E}^r_p$, we need to approximate the propagative kernel $\Pi^{\delta\mathbf{k}}_{p,\mathrm{e/m}}$ and the two densities $\widetilde{\psi},\widetilde{\phi}$. We consider the approximation of the integral kernel first, for which we define two linear operators $\hat{\mathcal{A}}^{\delta\mathbf{k}}_{p,\mathrm{e/m}}[\widetilde{\phi}]$ and $\mathcal{A}^{\delta\mathbf{k}}_{p,\mathrm{e/m},0}[\widetilde{\phi}]$ for $\widetilde{\phi} \in H_T^{-1/2}(\mathrm{div},\partial B)$:

$$\hat{\mathcal{A}}^{\delta\mathbf{k}}_{p,\mathrm{e/m}}[\widetilde{\phi}](\widetilde{\mathbf{x}}) := \int_{\partial B}[g_{\mathrm{e/m}}\mathbf{e}_1, g_{\mathrm{e/m}}\mathbf{e}_2, g_{\mathrm{m/e}}\mathbf{e}_3](\widetilde{\mathbf{y}})\widetilde{\phi}(\widetilde{\mathbf{y}})d\sigma\,,$$

$$\mathcal{A}^{\delta\mathbf{k}}_{p,\mathrm{e/m},0}[\widetilde{\phi}](\widetilde{\mathbf{x}}) := e^{i\delta\mathbf{k}^*\cdot\widetilde{\mathbf{x}}}\hat{\mathcal{A}}^{\delta\mathbf{k}}_{p,\mathrm{e/m}}[\widetilde{\phi}](\widetilde{\mathbf{x}})\,,$$

where $g_{\mathrm{e/m}}(\widetilde{\mathbf{y}})$ is given by

$$g_{\mathrm{e}}(\widetilde{\mathbf{y}}) = -\frac{\widetilde{y}_3}{\tau}\,, \quad g_{\mathrm{m}}(\widetilde{\mathbf{y}}) = \frac{i}{\tau\delta k_3} + \frac{d'\cdot\widetilde{y}'}{d_3\tau}\,.$$

We can see that $e^{i\delta\mathbf{k}^*\cdot\widetilde{\mathbf{x}}}g_{\mathrm{e/m}}(\widetilde{\mathbf{y}})$ are good approximations of $G^{\delta\mathbf{k}}_{p,\mathrm{e/m}}$ (cf. (4.6)), by noting the fact that

$$\frac{ie^{-i\delta\mathbf{k}^*\cdot\widetilde{\mathbf{y}}}}{2\tau\delta k_3} = \frac{i}{2\tau\delta k_3} + \frac{\mathbf{d}^*\cdot\widetilde{\mathbf{y}}}{2d_3\tau} + O(\delta).$$

Then by a direct estimate, we arrive at the following result.

LEMMA 4.4. *Let L be the same constant as in Lemma 4.3. Then for small enough δ, $x_3 \geq L$, and $\widetilde{\phi},\widetilde{\psi} \in H_T^{-1/2}(\mathrm{div},\partial B)$, it holds that*

$$\begin{aligned}&\left|\nabla\times\left(\mathcal{A}^{\delta\mathbf{k}}_{p,\mathrm{m}} - \mathcal{A}^{\delta\mathbf{k}}_{p,\mathrm{m},0}\right)[\widetilde{\phi}]\right|(\widetilde{\mathbf{x}}) + \frac{1}{\delta}\left|\nabla\times\nabla\times\left(\mathcal{A}^{\delta\mathbf{k}}_{p,\mathrm{e}} - \mathcal{A}^{\delta\mathbf{k}}_{p,\mathrm{e},0}\right)[\widetilde{\psi}]\right|(\widetilde{\mathbf{x}})\\ &\quad\lesssim \delta^2\left\{\left\|\widetilde{\phi}\right\|_{H_T^{-\frac{1}{2}}(\mathrm{div},\partial B)} + \left\|\widetilde{\psi}\right\|_{H_T^{-\frac{1}{2}}(\mathrm{div},\partial B)}\right\}.\end{aligned}$$

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To proceed with our approximation, we define the Green's tensor $\mathbb{G}_r^{\delta\mathbf{k}}(\widetilde{\mathbf{x}})$ associated with the propagative mode $g_r^{\delta\mathbf{k}}(\widetilde{\mathbf{x}}) = e^{i\delta\mathbf{k}^*\cdot\widetilde{\mathbf{x}}}$:

$$\mathbb{G}_r^{\delta\mathbf{k}}(\widetilde{\mathbf{x}}) = g_r^{\delta\mathbf{k}}(\widetilde{\mathbf{x}})\mathbb{I} + \frac{1}{\delta^2 k^2}\nabla^2 g_r^{\delta\mathbf{k}}(\widetilde{\mathbf{x}}) = (\mathbb{I} - \mathbf{d}^*\otimes\mathbf{d}^*)g_r^{\delta\mathbf{k}}(\widetilde{\mathbf{x}})\,. \tag{4.9}$$

We remark that the matrix $\mathbb{I}-\mathbf{d}^*\otimes\mathbf{d}^*$ is the projection on the orthogonal complement of the linear space spanned by $\mathbf{d}^*$. With the help of (4.9), we readily have that

$$\nabla\times\mathcal{A}_{p,\mathrm{m},0}^{\delta\mathbf{k}}[\widetilde{\phi}] = \nabla\times\mathbb{G}_r^{\delta\mathbf{k}}\hat{\mathcal{A}}_{p,\mathrm{m}}^{\delta\mathbf{k}}[\widetilde{\phi}]\,,\quad \nabla\times\nabla\times\mathcal{A}_{p,\mathrm{e},0}^{\delta\mathbf{k}}[\widetilde{\psi}] = (\delta k)^2\mathbb{G}_r^{\delta\mathbf{k}}\hat{\mathcal{A}}_{p,\mathrm{e}}^{\delta\mathbf{k}}[\widetilde{\phi}]\,,$$

which, together with (4.7) and Lemma 4.4, results in the asymptotic estimate:

$$\widetilde{E}_p^r = \nabla\times\mathbb{G}_r^{\delta\mathbf{k}}\hat{\mathcal{A}}_{p,\mathrm{m}}^{\delta\mathbf{k}}[\widetilde{\phi}] + \delta k^2\mathbb{G}_r^{\delta\mathbf{k}}\hat{\mathcal{A}}_{p,\mathrm{e}}^{\delta\mathbf{k}}[\widetilde{\phi}] + O(\delta^2)\,. \tag{4.10}$$

We next work out the leading-order terms of the densities $\widetilde{\phi}$ and $\widetilde{\psi}$. For this, using the Taylor expansion of the incident wave,

$$\begin{bmatrix}\nu(\widetilde{\mathbf{x}})\times\widetilde{E}^i(\widetilde{\mathbf{x}})\\ ik\nu(\widetilde{\mathbf{x}})\times\widetilde{H}^i(\widetilde{\mathbf{x}})\end{bmatrix} = \sum_\beta \frac{\delta^{|\beta|}}{\beta!}\begin{bmatrix}\nu(\widetilde{\mathbf{x}})\times\widetilde{\mathbf{x}}^\beta\partial^\beta E^i(0)\\ ik\nu(\widetilde{\mathbf{x}})\times\widetilde{\mathbf{x}}^\beta\partial^\beta H^i(0)\end{bmatrix},$$

we can have

$$\widetilde{\phi} = \sum_\beta \frac{\delta^{|\beta|}}{\beta!}\widetilde{\phi}_\beta\,,\quad \widetilde{\psi} = \sum_\beta \frac{\delta^{|\beta|}}{\beta!}\widetilde{\phi}_\beta\,, \tag{4.11}$$

by setting

$$\mathcal{W}_{\delta,B}\begin{bmatrix}\widetilde{\phi}_\beta\\ \widetilde{\psi}_\beta\end{bmatrix}(\widetilde{\mathbf{x}}) = \begin{bmatrix}\nu(\widetilde{\mathbf{x}})\times\widetilde{\mathbf{x}}^\beta\partial^\beta E^i(0)\\ ik\nu(\widetilde{\mathbf{x}})\times\widetilde{\mathbf{x}}^\beta\partial^\beta H^i(0)\end{bmatrix}. \tag{4.12}$$

We should note from (4.12) that ϕ_β and ψ_β still depend on δ. Indeed, recalling the expansion

$$\mathcal{W}_{\delta,B} = \sum_{n=0}^\infty \delta^n\mathcal{W}_{n,B} =: \mathcal{W}_{0,B} - \delta\mathcal{W}_{r,B}\,,$$

we can expand $\mathcal{W}_{\delta,B}^{-1}$ by the Neumann series in terms of δ,

$$\mathcal{W}_{\delta,B}^{-1} = (I - \delta\mathcal{W}_{0,B}^{-1}\mathcal{W}_{r,B})^{-1}\mathcal{W}_{0,B}^{-1} = \sum_{n=0}^\infty \delta^n(\mathcal{W}_{0,B}^{-1}\mathcal{W}_{r,B})^n\mathcal{W}_{0,B}^{-1}\,. \tag{4.13}$$

when $\delta/(d_\sigma d_\sigma^*)$ is small enough. It then follows that

$$\widetilde{\phi}_\beta = \sum_{j=0}^\infty \delta^j\widetilde{\phi}_{\beta,j}\,,\quad \widetilde{\psi}_\beta = \sum_{j=0}^\infty \delta^j\widetilde{\psi}_{\beta,j}\,. \tag{4.14}$$

We would like to emphasize that $\widetilde{\phi}_{\beta,j}$ and $\widetilde{\psi}_{\beta,j}$ are not simply determined by

$$(\mathcal{W}_{0,B}^{-1}\mathcal{W}_{r,B})^j\mathcal{W}_{0,B}^{-1}\begin{bmatrix}\nu(\widetilde{\mathbf{x}})\times\widetilde{\mathbf{x}}^\beta\partial^\beta E^i(0)\\ ik\nu(\widetilde{\mathbf{x}})\times\widetilde{\mathbf{x}}^\beta\partial^\beta H^i(0)\end{bmatrix},$$

since $\mathcal{W}_{r,B}$ still depends on δ. A more careful but direct calculation (expanding $\mathcal{W}_{r,B}$ in (4.13) and combining the terms of order $O(\delta^n)$) is needed to determine

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the coefficients of the terms of order $O(\delta^n)$ in the Neumann expansion (4.13). We shall write $\widetilde{\phi}_{\beta,0}$ with $|\beta| = 1$ below as $\widetilde{\phi}_{j,0}$ with $j = 1, 2, 3$ for simplicity. Then the expansions (4.11) and (4.14) give us

(4.15)
$$\widetilde{\phi} = \widetilde{\phi}_{0,0} + \delta\widetilde{\phi}_{0,1} + \delta\sum_{j=1}^{3}\widetilde{\phi}_{j,0} + O(\delta^2)\,, \quad \widetilde{\psi} = \widetilde{\psi}_{0,0} + \delta\widetilde{\psi}_{0,1} + \delta\sum_{j=1}^{3}\widetilde{\psi}_{j,0} + O(\delta^2)\,.$$

We remark that the error terms are measured in the space $H_T^{-1/2}(\mathrm{div}, \partial B)$.

Substituting the expansion (4.15) into the approximate scattered field (4.10), we readily obtain

$$\begin{aligned}
\widetilde{E}_p^r(\widetilde{\mathbf{x}}) &= \nabla\times\mathbb{G}_r^{\delta\mathbf{k}}\left(\int_{\partial B}\frac{i+\delta kd'\cdot\widetilde{y}'}{\tau\delta k_3}\left(\widetilde{\phi}',\,0\right)^t d\sigma - \int_{\partial B}\frac{\widetilde{y}_3}{\tau}\widetilde{\phi}_3\mathbf{e}_3 d\sigma\right)\\
&\quad + \delta k^2\mathbb{G}_r^{\delta\mathbf{k}}\left(\int_{\partial B} -\frac{\widetilde{y}_3}{\tau}\left(\widetilde{\psi}',\,0\right)^t d\sigma + \int_{\partial B}\frac{i+\delta kd'\cdot\widetilde{y}'}{\tau\delta k_3}\widetilde{\psi}_3\mathbf{e}_3 d\sigma\right) + O(\delta^2)\\
&= \nabla\times\mathbb{G}_r^{\delta\mathbf{k}}\Bigg(\frac{i}{\tau k_3}\int_{\partial B}\left(\widetilde{\phi}'_{0,1} + \sum_{j=1}^{3}\widetilde{\phi}'_{j,0},\,0\right)^t d\sigma + \int_{\partial B}\frac{d'\cdot\widetilde{y}'}{\tau d_3}\left(\widetilde{\phi}'_{0,0},\,0\right)^t d\sigma\\
&\qquad - \int_{\partial B}\frac{\widetilde{y}_3}{\tau}\left(\widetilde{\phi}_{0,0}\right)_3\mathbf{e}_3 d\sigma\Bigg)\\
&\quad + \delta k^2\mathbb{G}_r^{\delta\mathbf{k}}\Bigg(\int_{\partial B} -\frac{\widetilde{y}_3}{\tau}\left(\widetilde{\psi}'_{0,0},\,0\right)^t d\sigma + \int_{\partial B}\frac{d'\cdot\widetilde{y}'}{\tau d_3}\left(\widetilde{\psi}_{0,0}\right)_3\mathbf{e}_3 d\sigma\\
&\qquad + \frac{i}{\tau k_3}\int_{\partial B}\left(\widetilde{\psi}_{0,1}\right)_3\mathbf{e}_3 + \sum_{j=1}^{3}\left(\widetilde{\psi}_{j,0}\right)_3\mathbf{e}_3 d\sigma\Bigg) + O(\delta^2)\,,
\end{aligned} \tag{4.16}$$

where the superscript t denotes the transport of a vector.

4.2.2. Computing the leading-order densities. This subsection is devoted to finding the explicit formulas for the leading-order densities in (4.15), which is necessary in order to further compute each term in (4.16). For this purpose, we first see from (4.12) that the zero-order terms $\widetilde{\phi}_{\beta,0}$ and $\widetilde{\psi}_{\beta,0}$ in (4.14) satisfy the equation

$$\mathcal{W}_{0,B}\begin{bmatrix}\widetilde{\phi}_{\beta,0}\\ \widetilde{\psi}_{\beta,0}\end{bmatrix}(\widetilde{\mathbf{x}}) = \begin{bmatrix}\nu(\widetilde{\mathbf{x}})\times\widetilde{\mathbf{x}}^\beta\partial^\beta E^i(0)\\ ik\nu(\widetilde{\mathbf{x}})\times\widetilde{\mathbf{x}}^\beta\partial^\beta H^i(0)\end{bmatrix}, \tag{4.17}$$

which has been well studied in the proof of Theorem 4.1, where we can directly observe the solution:

$$\widetilde{\phi}_{\beta,0} = (\lambda_\mu - \mathcal{M}_{\mathrm{m}})^{-1}\left(\frac{\nu(\widetilde{\mathbf{x}})\times\widetilde{\mathbf{x}}^\beta\partial^\beta E^i(0)}{1-\mu_c} + f_\beta\right), \tag{4.18}$$

$$\widetilde{\psi}_{\beta,0} = (\lambda_\varepsilon - \mathcal{M}_{\mathrm{e}})^{-1}\left(\frac{i\nu(\widetilde{\mathbf{x}})\times\widetilde{\mathbf{x}}^\beta\partial^\beta H^i(0)}{k(1-\varepsilon_c)} + g_\beta\right). \tag{4.19}$$

Here f_β and g_β are defined by

$$f_\beta := \frac{k-k_c}{1-\mu_c}\mathcal{L}_{1,\mathrm{e}}[\widetilde{\psi}_{\beta,0}]\,, \quad g_\beta := \frac{k-k_c}{k^2(1-\varepsilon_c)}\mathcal{L}_{1,\mathrm{m}}[\widetilde{\phi}_{\beta,0}]\,.$$

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In particular, by the representation formulas (4.18) and (4.19), for $\beta = 0$, we know, from the facts that $\nabla_{\partial B} \cdot (\nu \times E^i(0)) = 0$ and $\nabla_{\partial B} \cdot (\nu \times H^i(0)) = 0$, that $\widetilde{\phi}_{0,0}$ and $\widetilde{\psi}_{0,0}$ are divergence-free. Further, by matching the terms of order $O(\delta)$ in both sides of (4.12), we have that the first-order terms $\widetilde{\phi}_{0,1}$ and $\widetilde{\psi}_{0,1}$ can be completely determined by the equation (once $\widetilde{\phi}_{0,0}$ and $\widetilde{\psi}_{0,0}$ are solved)

$$\mathcal{W}_{0,B} \begin{bmatrix} \widetilde{\phi}_{0,1} \\ \widetilde{\psi}_{0,1} \end{bmatrix} + \mathcal{W}_{1,B} \begin{bmatrix} \widetilde{\phi}_{0,0} \\ \widetilde{\psi}_{0,0} \end{bmatrix} = 0 \,,$$

which can also be written componentwise as

(4.20)
$$(\lambda_\mu - \mathcal{M}_{\rm m})[\widetilde{\phi}_{0,1}] + \frac{k_c - k}{1 - \mu_c} \mathcal{L}_{1,{\rm e}}[\widetilde{\psi}_{0,1}] + \frac{k_c - k}{1 - \mu_c} \mathcal{M}_{1,{\rm m}}[\widetilde{\phi}_{0,0}] + \frac{k_c^2 - k^2}{1 - \mu_c} \mathcal{L}_{2,{\rm e}}[\widetilde{\psi}_{0,0}] = 0 \,,$$

(4.21)
$$\frac{k_c - k}{k^2(1 - \varepsilon_c)} \mathcal{L}_{1,{\rm m}}[\widetilde{\phi}_{0,1}] + (\lambda_\varepsilon - \mathcal{M}_{\rm e})[\widetilde{\psi}_{0,1}] + \frac{k_c^2 - k^2}{k^2(1 - \varepsilon_c)} \mathcal{L}_{2,{\rm m}}[\widetilde{\phi}_{0,0}] + \frac{\varepsilon_c k_c - k}{1 - \varepsilon_c} \mathcal{M}_{1,{\rm e}}[\widetilde{\psi}_{0,0}] = 0 \,.$$

Nevertheless, it is not an easy task to fully solve the above equations. Fortunately, by the Green's formula

$$\int_{\partial B} \widetilde{\phi}(\widetilde{\mathbf{y}}) d\sigma = - \int_{\partial B} \widetilde{\mathbf{y}} \nabla_{\partial B} \cdot \phi(\widetilde{\mathbf{y}}) d\sigma \,, \tag{4.22}$$

it suffices to find the surface divergence of $\widetilde{\phi}_{0,1}$ and $\widetilde{\psi}_{0,1}$ to compute (4.16). For this, we take the surface divergence on both sides of (4.20) and (4.21) to deduce that

$$(\lambda_\mu + \mathcal{K}_{\rm m}^{0,*})[\nabla_{\partial B} \cdot \widetilde{\phi}_{0,1}] = \frac{k_c^2 - k^2}{1 - \mu_c} \gamma_n (\nabla \times \mathcal{A}_{\rm e}[\widetilde{\psi}_{0,0}]) \,, \tag{4.23}$$

$$(\lambda_\varepsilon + \mathcal{K}_{\rm e}^{0,*})[\nabla_{\partial B} \cdot \widetilde{\psi}_{0,1}] = \frac{k_c^2 - k^2}{k^2(1 - \varepsilon_c)} \gamma_n (\nabla \times \mathcal{A}_{\rm m}[\phi_{0,0}]) \tag{4.24}$$

by using Lemma 3.4. To facilitate our further computations, we follow the ideas of [5, Lemma 5.5] and introduce the following two harmonic systems with appropriate interface conditions:

$$\begin{cases} \Delta u = 0 & \text{in } \Omega \,, \\ (\nu \cdot \nabla u)|_- = (\nu \cdot \nabla u)|_+ & \text{on } \partial B \,, \\ \mu_c (\nu \times \nabla u)|_- - (\nu \times \nabla u)|_+ = \nu \times E^i(0) & \text{on } \partial B \,, \\ u - u_\infty \text{ is exponentially decaying} & \text{as } x_3 \to \infty \,, \\ u = 0 & \text{on } \Sigma \,, \\ u \text{ satisfies the periodic boundary condition} & \text{on } \partial\Omega \backslash \Sigma \,, \end{cases} \tag{4.25}$$

and

$$\begin{cases} \Delta v = 0 & \text{in } \Omega \,, \\ (\nu \cdot \nabla v)|_- = (\nu \cdot \nabla v)|_+ & \text{on } \partial B \,, \\ \varepsilon_c (\nu \times \nabla v)|_- - (\nu \times \nabla v)|_+ = \frac{i}{k} \nu \times H^i(0) & \text{on } \partial B \,, \\ v \text{ is exponentially decaying} & \text{as } x_3 \to \infty \,, \\ \frac{\partial v}{\partial x_3} = 0 & \text{on } \Sigma \,, \\ v \text{ satisfies the periodic boundary condition} & \text{on } \partial\Omega \backslash \Sigma \,, \end{cases} \tag{4.26}$$

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where u_∞ is a complex constant. The solutions to the above two systems shall be denoted by u^e and u^h, respectively, which may not necessarily be unique but have uniquely determined gradients. With these auxiliary systems, we can prove the following results.

LEMMA 4.5. *For $\nabla \times \mathcal{A}_{\rm m}[\widetilde{\phi}_{0,0}]$ and $\nabla \times \mathcal{A}_{\rm e}[\widetilde{\psi}_{0,0}]$, it holds that*

(4.27)
$$\nabla u^e = \nabla \times \mathcal{A}^0_{\rm m}[\widetilde{\phi}_{0,0}] = \begin{cases} \frac{1}{1-\mu_c}\nabla \mathcal{S}^0_{\rm e}\left(\lambda_\mu - \mathcal{K}^{0,*}_{\rm e}\right)^{-1}\left[\nu \cdot E^i(0)\right] & \text{in } \Omega\backslash B\,, \\ \frac{1}{\mu_c}E^i(0) + \frac{1}{\mu_c(1-\mu_c)}\nabla \mathcal{S}^0_e\left(\lambda_\mu - \mathcal{K}^{0,*}_{\rm e}\right)^{-1}\left[\nu \cdot E^i(0)\right] & \text{in } B, \end{cases}$$

and

(4.28)
$$\nabla u^h = \nabla \times \mathcal{A}^0_{\rm e}[\widetilde{\psi}_{0,0}] = \begin{cases} \frac{i}{k(1-\varepsilon_c)}\nabla \mathcal{S}^0_{\rm m}\left(\lambda_\varepsilon - \mathcal{K}^{0,*}_{\rm m}\right)^{-1}\left[\nu \cdot H^i(0)\right] & \text{in } \Omega\backslash B, \\ \frac{i}{k\varepsilon_c}H^i(0) + \frac{i}{k\varepsilon_c(1-\varepsilon_c)}\nabla \mathcal{S}^0_{\rm m}\left(\lambda_\varepsilon - \mathcal{K}^{0,*}_{\rm m}\right)^{-1}\left[\nu \cdot H^i(0)\right] & \text{in } B. \end{cases}$$

The above lemma enables us to represent the quantities $\nabla \times \mathcal{A}_{\rm e}[\widetilde{\psi}_{0,0}]$ and $\nabla \times \mathcal{A}_{\rm m}[\widetilde{\phi}_{0,0}]$ involved in (4.23) and (4.24) in terms of the gradients of scalar potentials. Its proof is rather technical and included in Appendix B. Combining Lemma 4.5 with the formulas (4.23) and (4.24), we see

(4.29)
$$\nabla_{\partial B}\cdot\widetilde{\phi}_{0,1} = \left(\lambda_\mu + \mathcal{K}^{0,*}_{\rm m}\right)^{-1}\left(\frac{k_c^2-k^2}{1-\mu_c}\frac{\partial u^h}{\partial \nu}\right), \quad \nabla_{\partial B}\cdot\widetilde{\psi}_{0,1} = \left(\lambda_\varepsilon + \mathcal{K}^{0,*}_{\rm e}\right)^{-1}\left(\frac{k_c^2-k^2}{k^2(1-\varepsilon_c)}\frac{\partial u^e}{\partial \nu}\right).$$

To calculate the approximate field $\widetilde{E}^r_p$ in (4.16), we still need to find the quantities $\int_{\partial B}\widetilde{\phi}_{j,0}d\sigma$ and $\int_{\partial B}\widetilde{y}_j\widetilde{\phi}_{0,0}d\sigma$ and the similar quantities associated with $\widetilde{\psi}$. The corresponding result is summarized in the following lemma, whose proof is given in Appendix C.

LEMMA 4.6. *The following identities hold:*

$$\int_{\partial B}\widetilde{y}_j\widetilde{\phi}_{0,0}(\widetilde{\mathbf{y}})d\sigma = |B|\mathbf{e}_j \times E^i(0) + (1-\mu_c)\mathbf{e}_j \times \int_{\partial B}\widetilde{\mathbf{y}}\frac{\partial u^e}{\partial \nu}(\widetilde{\mathbf{y}})d\sigma\,, \tag{4.30}$$

$$\int_{\partial B}\widetilde{y}_j\widetilde{\psi}_{0,0}(\widetilde{\mathbf{y}})d\sigma = \frac{i}{k}|B|\mathbf{e}_j \times H^i(0) + (1-\varepsilon_c)\mathbf{e}_j \times \int_{\partial B}\widetilde{\mathbf{y}}\frac{\partial u^h}{\partial \nu}(\widetilde{\mathbf{y}})d\sigma\,, \tag{4.31}$$

$$\int_{\partial B}\widetilde{\phi}_{j,0}(\widetilde{\mathbf{y}})d\sigma = \mathbf{e}_j \times \partial^j E^i(0)|B| + (1-\mu_c)\int_B \nabla \mathcal{S}^0_{\rm m}\left[\nabla_{\partial B}\cdot\widetilde{\phi}_{j,0}\right](\widetilde{\mathbf{y}})d\widetilde{\mathbf{y}}\,, \tag{4.32}$$

$$\int_{\partial B}\widetilde{\psi}_{j,0}(\widetilde{\mathbf{y}})d\sigma = \frac{i}{k}\mathbf{e}_j \times \partial^j H^i(0)|B| + (1-\varepsilon_c)\int_B \nabla \mathcal{S}^0_{\rm e}\left[\nabla_{\partial B}\cdot\widetilde{\psi}_{j,0}\right](\widetilde{\mathbf{y}})d\widetilde{\mathbf{y}}\,. \tag{4.33}$$

4.2.3. Computation of the approximate scattered wave. We are now well prepared to compute each term in (4.16) and prove our main result: Theorem 4.7. Recalling our conventional notation $\mathbf{d} = (d', d_3)$ for a vector $\mathbf{d} \in \mathbb{R}^3$, we shall identify the two-dimensional vector d' with $(d', 0) \in \mathbb{R}^3$ below for ease of exposition. We start with a direct consequence of Lemma 4.6:

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$$-\frac{1}{\tau}\int_{\partial B}\widetilde{y_3}\widetilde{\psi}_{0,0}(\widetilde{\mathbf{y}})d\sigma=-\frac{i}{k\tau}|B|\mathbf{e}_3\times H^i(0)+\frac{\varepsilon_c-1}{\tau}\mathbf{e}_3\times\int_{\partial B}\widetilde{\mathbf{y}}\frac{\partial u^h}{\partial\nu}(\widetilde{\mathbf{y}})d\sigma\,, \tag{4.34}$$

$$\int_{\partial B}\frac{d'\cdot\widetilde{y}'}{\tau d_3}\widetilde{\psi}_{0,0}(\widetilde{\mathbf{y}})d\sigma=\frac{i}{\tau k_3}|B|d'\times H^i(0)+\frac{1-\varepsilon_c}{\tau d_3}d'\times\int_{\partial B}\widetilde{\mathbf{y}}\frac{\partial u^h}{\partial\nu}(\widetilde{\mathbf{y}})d\sigma\,, \tag{4.35}$$

and

$$\int_{\partial B}\frac{d'\cdot\widetilde{y}'}{\tau d_3}\widetilde{\phi}_{0,0}(\widetilde{\mathbf{y}})d\sigma=\frac{d'\times E^i(0)|B|}{\tau d_3}+\frac{d'}{\tau d_3}\times\int_{\partial B}(1-\mu_c)\widetilde{\mathbf{y}}\frac{\partial u^e}{\partial\nu}(\widetilde{\mathbf{y}})d\sigma\,. \tag{4.36}$$

We remark that it is unnecessary for us to consider $\int_{\partial B}\frac{\widetilde{y_3}}{\tau}\widetilde{\phi}_{0,0}(\widetilde{\mathbf{y}})d\sigma$ since only its third component is needed in (4.16), which is known to be zero by the formula (4.30). It is easy to check that

$$\sum_{j=1}^{3}\mathbf{e}_j\times\partial^j E^i(0)=ikH^i(0)\text{ and }\sum_{j=1}^{3}\mathbf{e}_j\times\partial^j H^i(0)=-ikE^i(0) \tag{4.37}$$

hold. It then follows from the formulas (4.5) and (4.17) that

$$\begin{aligned}\sum_{j=1}^{3}\nabla_{\partial B}\cdot\widetilde{\phi}_{j,0}&=\sum_{j=1}^{3}\left(\lambda_\mu+\mathcal{K}_{\mathrm{m}}^{0,*}\right)^{-1}\left(\frac{\nabla_{\partial B}\cdot\nu(\widetilde{\mathbf{x}})\times\widetilde{x}_j\partial^j E^i(0)}{1-\mu_c}\right)\\&=\sum_{j=1}^{3}\left(\lambda_\mu+\mathcal{K}_{\mathrm{m}}^{0,*}\right)^{-1}\left(\frac{\nu(\widetilde{\mathbf{x}})\cdot\left(\mathbf{e}_j\times\partial^j E^i(0)\right)}{\mu_c-1}\right)\\&=\frac{ik}{\mu_c-1}\left(\lambda_\mu+\mathcal{K}_{\mathrm{m}}^{0,*}\right)^{-1}\left[\nu\cdot H^i(0)\right].\end{aligned} \tag{4.38}$$

Using (4.37) and (4.38), we can obtain the summation of (4.32) over j:

$$\begin{aligned}\frac{i}{\tau k_3}\int_{\partial B}\sum_{j=1}^{3}\widetilde{\phi}_{j,0}d\sigma&=-\frac{H^i(0)|B|}{\tau d_3}+\frac{1}{\tau d_3}\int_B\nabla\mathcal{S}_{\mathrm{m}}^{0,*}\left(\lambda_\mu+\mathcal{K}_{\mathrm{m}}^{0,*}\right)^{-1}\left[\nu\cdot H^i(0)\right]d\sigma\\&=-\frac{H^i(0)|B|}{\tau d_3}+\frac{1}{\tau d_3}\int_{\partial B}\widetilde{\mathbf{y}}\left(-\frac{1}{2}+\mathcal{K}_{\mathrm{m}}^{0,*}\right)\left(\lambda_\mu+\mathcal{K}_{\mathrm{m}}^{0,*}\right)^{-1}\left[\nu\cdot H^i(0)\right]d\sigma\\&=-\frac{H^i(0)|B|}{\tau d_3}+\frac{1}{\tau d_3(\mu_c-1)}\int_{\partial B}\widetilde{\mathbf{y}}\left(\lambda_\mu+\mathcal{K}_{\mathrm{m}}^{0,*}\right)^{-1}\left[\nu\cdot H^i(0)\right]d\sigma\,.\end{aligned} \tag{4.39}$$

A similar calculation gives us the summation of (4.33) over j:

$$\begin{aligned}\frac{i}{\tau k_3}\int_{\partial B}\sum_{j=1}^{3}\widetilde{\psi}_{j,0}d\sigma&=\frac{i}{\tau k_3}E^i(0)|B|-\frac{i}{\tau k_3}\int_B\nabla\mathcal{S}_{\mathrm{e}}^{0}\left(\lambda_\varepsilon+\mathcal{K}_{\mathrm{e}}^{0,*}\right)^{-1}\left[\nu\cdot E^i(0)\right]d\sigma\\&=\frac{i}{\tau k_3}E^i(0)|B|+\frac{i}{\tau k_3(1-\varepsilon_c)}\int_B\widetilde{\mathbf{y}}\left(\lambda_\varepsilon+\mathcal{K}_{\mathrm{e}}^{0,*}\right)^{-1}\left[\nu\cdot E^i(0)\right]d\sigma\,,\end{aligned} \tag{4.40}$$

by using (4.37) and the fact that

$$\sum_{j=1}^{3}\nabla_{\partial B}\cdot\widetilde{\psi}_{j,0}=\frac{1}{\varepsilon_c-1}\left(\lambda_\varepsilon+\mathcal{K}_{\mathrm{e}}^{0,*}\right)^{-1}\left[\nu\cdot E^i(0)\right]. \tag{4.41}$$

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Moreover, recalling (4.29) and the Green's formula (4.22), we have

$$\frac{i}{\tau k_3}\int_{\partial B}\widetilde{\phi}_{0,1}d\sigma = \frac{i}{\tau k_3}\int_{\partial B}\widetilde{\mathbf{y}}\frac{k^2-k_c^2}{1-\mu_c}\left(\lambda_\mu+\mathcal{K}_{\mathrm{m}}^{0,*}\right)^{-1}\frac{\partial u^h}{\partial\nu}(\widetilde{\mathbf{y}})d\sigma\,, \tag{4.42}$$

$$\frac{i}{\tau k_3}\int_{\partial B}\widetilde{\psi}_{0,1}d\sigma = -\frac{i}{\tau k_3}\int_{\partial B}\widetilde{\mathbf{y}}\frac{k_c^2-k^2}{k^2(1-\varepsilon_c)}\left(\lambda_\varepsilon+\mathcal{K}_{\mathrm{e}}^{0,*}\right)^{-1}\frac{\partial u^e}{\partial\nu}(\widetilde{\mathbf{y}})d\sigma\,. \tag{4.43}$$

We have now computed all the terms involved in (4.16). It is worth mentioning that we shall only need the first two components of the vector identities (4.34), (4.36), (4.39), and (4.42), as well as the third component of the identities (4.35), (4.40), and (4.43), to compute the approximate scattered wave. Before we apply all the expressions to (4.16), we make some further observations to simplify our subsequent calculations. We first consider the nonintegral terms in (4.34), (4.36), and (4.39) and find

$$\begin{aligned}
&\nabla\times\mathbb{G}_r^{\delta\mathbf{k}}\left(\frac{-H^i(0)|B|}{\tau d_3}+\frac{|B|d'\times E^i(0)}{\tau d_3}\right)+\delta k^2\mathbb{G}_r^{\delta\mathbf{k}}\left(-\frac{i}{k\tau}|B|\mathbf{e}_3\times H^i(0)\right)\\
&=\nabla\times\mathbb{G}_r^{\delta\mathbf{k}}\left(-\frac{2|B|}{\tau}\mathbf{e}_3\times\mathbf{p}\right)+\delta k^2\mathbb{G}_r^{\delta\mathbf{k}}\left(-\frac{i}{k\tau}|B|\mathbf{e}_3\times H^i(0)\right)\\
&=-i\delta k\frac{2|B|}{\tau}\mathbb{G}_r^{\delta\mathbf{k}}(-d_3\mathbf{p}^*)+\delta k^2\mathbb{G}_r^{\delta\mathbf{k}}\left(-\frac{i}{k\tau}|B|\mathbf{e}_3\times H^i(0)\right)\\
&=-i\delta k\frac{2|B|}{\tau}\mathbb{G}_r^{\delta\mathbf{k}}(-p_3\mathbf{d}^*)=0\,,
\end{aligned}$$

where we have used the definition of $\mathbb{G}_r^{\delta\mathbf{k}}$ (4.9) and a simple identity: $-H^i(0)+d'\times E^i(0)=2d_3(p_2,-p_1,0)$. In addition, we note that $d'\times H^i(0)+E^i(0)=0$. Therefore, the nonintegral terms in (4.35) and (4.40) can also be cancelled. Moreover, for any vector $\mathbf{a}\in\mathbb{R}^3$, we can check from (4.9) that

$$\nabla\times\mathbb{G}_r^{\delta\mathbf{k}}\mathbf{a}=i\delta k\mathbb{G}_r^{\delta\mathbf{k}}\mathbf{d}^*\times\mathbf{a}\,,\quad \nabla\times\mathbb{G}_r^{\delta\mathbf{k}}\mathbf{d}^*\times\mathbf{a}=-i\delta k\mathbb{G}_r^{\delta\mathbf{k}}\mathbf{a}\,, \tag{4.44}$$

and the vector identities:

$$\mathbf{d}^*\times a'=-d_3\mathbf{e}_3\times\mathbf{a}+(d'\times\mathbf{a})_3\mathbf{e}_3\,,\quad (d'\times\mathbf{a})'=\mathbf{d}^*\times(a_3\mathbf{e}_3)\,. \tag{4.45}$$

Now, recalling (4.34) and (4.35) and using (4.44) and (4.45), we can deduce

$$\begin{aligned}
&\delta k^2\mathbb{G}_r^{\delta\mathbf{k}}\frac{1-\varepsilon_c}{\tau d_3}\left(\left(d'\times\int_{\partial B}\widetilde{\mathbf{y}}\frac{\partial u^h}{\partial\nu}d\sigma\right)_3\mathbf{e}_3-d_3\mathbf{e}_3\times\int_{\partial B}\widetilde{\mathbf{y}}\frac{\partial u^h}{\partial\nu}d\sigma\right)\\
&=\delta k^2\mathbb{G}_r^{\delta\mathbf{k}}\frac{1-\varepsilon_c}{\tau d_3}\mathbf{d}^*\times\left(\int_{\partial B}\widetilde{\mathbf{y}}\frac{\partial u^h}{\partial\nu}d\sigma\right)'\\
&=\frac{ik(\varepsilon_c-1)}{\tau d_3}\nabla\times\mathbb{G}_r^{\delta\mathbf{k}}\left(\int_{\partial B}\widetilde{\mathbf{y}}\frac{\partial u^h}{\partial\nu}d\sigma\right)'.
\end{aligned}$$

Similarly, we can derive, by means of (4.44) and (4.45), that

$$\nabla\times\mathbb{G}_r^{\delta\mathbf{k}}\frac{1-\mu_c}{\tau d_3}\mathbf{d}^*\times\left(\int_{\partial B}\widetilde{\mathbf{y}}\frac{\partial u^e}{\partial\nu}d\sigma\right)_3\mathbf{e}_3=\delta k^2\mathbb{G}_r^{\delta\mathbf{k}}\frac{i}{\tau k_3}\left(\int_{\partial B}\widetilde{\mathbf{y}}(\mu_c-1)\frac{\partial u^e}{\partial\nu}d\sigma\right)_3\mathbf{e}_3\,.$$

Combining these observations above and substituting the expressions into (4.16), we can write the approximate scattered wave $\widetilde{E}_p^r$ as a sum of the electric dipole and the magnetic dipole:

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$$\widetilde{E}_p^r(\widetilde{\mathbf{x}}) = \nabla \times \mathbb{G}_r^{\delta\mathbf{k}}(\widetilde{\mathbf{x}})\mathbf{J}'_{\rm m} + \delta k^2 \mathbb{G}_r^{\delta\mathbf{k}}(\widetilde{\mathbf{x}})(\mathbf{J}_{\rm e})_3\mathbf{e}_3 + O(\delta^2)\,, \tag{4.46}$$

where $\mathbf{J}_{\rm m}$ and $\mathbf{J}_{\rm e}$ are defined by

$$\begin{aligned}\mathbf{J}_{\rm m} :=\ & \frac{i}{\tau k_3}\int_{\partial B}\widetilde{\mathbf{y}}k^2(\varepsilon_c-1)\frac{\partial u^h}{\partial\nu}d\sigma - \frac{i}{\tau k_3}\int_{\partial B}\widetilde{\mathbf{y}}\left(\lambda_\mu+\mathcal{K}_{\rm m}^{0,*}\right)^{-1}\frac{k_c^2-k^2}{1-\mu_c}\frac{\partial u^h}{\partial\nu}d\sigma \\ & + \frac{1}{\tau d_3(\mu_c-1)}\int_{\partial B}\widetilde{\mathbf{y}}\left(\lambda_\mu+\mathcal{K}_{\rm m}^{0,*}\right)^{-1}\left[\nu\cdot H^i(0)\right]d\sigma\,, \end{aligned}\tag{4.47}$$

$$\begin{aligned}\mathbf{J}_{\rm e} :=\ & \frac{i}{\tau k_3}\int_{\partial B}(\mu_c-1)\widetilde{\mathbf{y}}\frac{\partial u^e}{\partial\nu}d\sigma - \frac{i}{\tau k_3}\int_{\partial B}\frac{k_c^2-k^2}{k^2(1-\varepsilon_c)}\widetilde{\mathbf{y}}\left(\lambda_\varepsilon+\mathcal{K}_{\rm e}^{0,*}\right)^{-1}\frac{\partial u^e}{\partial\nu}d\sigma \\ & + \frac{i}{\tau k_3(1-\varepsilon_c)}\int_{\partial B}\widetilde{\mathbf{y}}\left(\lambda_\varepsilon+\mathcal{K}_{\rm e}^{0,*}\right)^{-1}\left[\nu\cdot E^i(0)\right]d\sigma\,. \end{aligned}\tag{4.48}$$

Next, we compute the above two dipoles, $\mathbf{J}_{\rm m}$ and $\mathbf{J}_{\rm e}$, respectively. For $\mathbf{J}_{\rm m}$, noting the relation

$$\begin{aligned} k^2(\varepsilon_c-1)(\lambda_\mu+\mathcal{K}_{\rm m}^{0,*}) + \frac{k^2-k_c^2}{1-\mu_c} &= k^2(\varepsilon_c-1)\left(\lambda_\mu+\mathcal{K}_{\rm m}^{0,*}+\frac{1-\varepsilon_c\mu_c}{(\varepsilon_c-1)(1-\mu_c)}\right) \\ &= k^2(\varepsilon_c-1)(-\lambda_\varepsilon+\mathcal{K}_{\rm m}^{0,*})\,, \end{aligned}\tag{4.49}$$

we add the first two terms in (4.47) to obtain

$$\frac{ik^2}{\tau k_3}\int_{\partial B}(\varepsilon_c-1)\widetilde{\mathbf{y}}(-\lambda_\varepsilon+\mathcal{K}_{\rm m}^{0,*})(\lambda_\mu+\mathcal{K}_{\rm m}^{0,*})^{-1}\frac{\partial u^h}{\partial\nu}d\sigma\,. \tag{4.50}$$

To proceed, by applying Lemma 4.5 and the jump formula (3.26) for $\mathbf{k}=0$, we have

$$\begin{aligned}\frac{\partial u^h}{\partial\nu} &= \frac{i}{k\varepsilon_c}\nu\cdot H^i(0) + \frac{i}{k\varepsilon_c(1-\varepsilon_c)}\left(-\frac{1}{2}+\lambda_\varepsilon-\lambda_\varepsilon+\mathcal{K}_{\rm m}^{0,*}\right)\left(\lambda_\varepsilon-\mathcal{K}_{\rm m}^{0,*}\right)^{-1}\left[\nu\cdot H^i(0)\right] \\ &= \frac{i}{k(\varepsilon_c-1)}\nu\cdot H^i(0) + \frac{i}{k(1-\varepsilon_c)^2}\left(\lambda_\varepsilon-\mathcal{K}_{\rm m}^{0,*}\right)^{-1}\left[\nu\cdot H^i(0)\right]. \end{aligned}\tag{4.51}$$

Then it follows from (4.50) that

$$\begin{aligned}&\frac{ik^2}{\tau k_3}\int_{\partial B}(\varepsilon_c-1)\widetilde{\mathbf{y}}(-\lambda_\varepsilon+\mathcal{K}_{\rm m}^{0,*})(\lambda_\mu+\mathcal{K}_{\rm m}^{0,*})^{-1}\frac{\partial u^h}{\partial\nu}d\sigma \\ &\quad= \frac{ik(\varepsilon_c-1)}{\tau d_3}\int_{\partial B}\widetilde{\mathbf{y}}(-\lambda_\varepsilon+\mathcal{K}_{\rm m}^{0,*})(\lambda_\mu+\mathcal{K}_{\rm m}^{0,*})^{-1}\frac{i}{k(\varepsilon_c-1)}\nu\cdot H^i(0)d\sigma \\ &\qquad+\frac{ik(\varepsilon_c-1)}{\tau d_3}\int_{\partial B}\widetilde{\mathbf{y}}(-\lambda_\varepsilon+\mathcal{K}_{m}^{0,*})(\lambda_\mu+\mathcal{K}_{\rm m}^{0,*})^{-1}\frac{i}{k(1-\varepsilon_c)^2}(\lambda_\varepsilon-\mathcal{K}_{\rm m}^{0,*})^{-1}\left[\nu\cdot H^i(0)\right]d\sigma \\ &\quad= \frac{1}{\tau d_3}\int_{\partial B}\widetilde{\mathbf{y}}(\lambda_\varepsilon+\lambda_\mu)(\lambda_\mu+\mathcal{K}_{\rm m}^{0,*})^{-1}\left[\nu\cdot H^i(0)\right] \\ &\qquad+\frac{1}{\tau d_3(\varepsilon_c-1)}\int_{\partial B}\widetilde{\mathbf{y}}(\lambda_\mu+\mathcal{K}_{\rm m}^{0,*})^{-1}\left[\nu\cdot H^i(0)\right]d\sigma\,. \end{aligned}\tag{4.52}$$

Combining the above results with the relation

$$-\lambda_\mu-\lambda_\varepsilon+\frac{1}{1-\varepsilon_c}+\frac{1}{1-\mu_c}=1\,, \tag{4.53}$$

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we arrive at the desired expression:

$$\mathbf{J}_{\mathrm{m}} = -\frac{1}{\tau d_3}\int_{\partial B}\widetilde{\mathbf{y}}(\lambda_\mu + \mathcal{K}_{\mathrm{m}}^{0,*})^{-1}\left[\nu\cdot H^i(0)\right]d\sigma\,. \tag{4.54}$$

We now compute $\mathbf{J}_{\mathrm{e}}$. Similarly to the results (4.49) and (4.51), we have

$$(\mu_c-1)(\lambda_\varepsilon+\mathcal{K}_{\mathrm{e}}^{0,*}) + \frac{k_c^2-k^2}{k^2(\varepsilon_c-1)} = (-\lambda_\mu+\mathcal{K}_{\mathrm{e}}^{0,*})(\mu_c-1) \tag{4.55}$$

and

$$\begin{aligned}\frac{\partial u^e}{\partial\nu} &= \frac{1}{\mu_c}\nu\cdot E^i((0) + \frac{1}{\mu_c(1-\mu_c)}(-\frac{1}{2}+\mathcal{K}_{\mathrm{e}}^{0,*})(\lambda_\mu-\mathcal{K}_{\mathrm{e}}^{0,*})^{-1}[\nu\cdot E^i(0)]\\ &= \frac{1}{\mu_c-1}\nu\cdot E^i(0) + \frac{1}{(1-\mu_c)^2}(\lambda_\mu-\mathcal{K}_{\mathrm{e}}^{0,*})^{-1}\left[\nu\cdot E^i(0)\right].\end{aligned} \tag{4.56}$$

Applying these two expressions and (4.53) yields

$$\mathbf{J}_{\mathrm{e}} = \frac{i}{\tau k_3}\int_{\partial B}\widetilde{\mathbf{y}}(\lambda_\varepsilon + \mathcal{K}_{\mathrm{e}}^{0,*})^{-1}\left[\nu\cdot E^i(0)\right]d\sigma\,. \tag{4.57}$$

Finally, by substituting (4.57) and (4.54) into (4.46) and using the relation (4.44), we come to the main result of this section, where the estimate of the remainder term (cf. (4.58)) follows from the Neumann expansion (4.13) and the expression (4.15), as well as Theorem 4.1, Remark 4.2, and the fact that $\widetilde{\phi}_{0,0}, \widetilde{\psi}_{0,0} \in \mathbb{H}$.

THEOREM 4.7. *Let L be the same constant as in Lemma 4.3 and let $\mathbb{G}_r^{\mathbf{k}}(\mathbf{x})$ be the propagative kernel defined by $(\mathbb{I}-\mathbf{d}^*\otimes\mathbf{d}^*)e^{i\mathbf{k}^*\cdot\mathbf{x}}$. When $\widetilde{\delta} := \delta/(d_\sigma d_\sigma^*)$ is sufficiently small, for $\mathbf{x}$ with $x_3 \geq L$, the scattered electric field $E^r = E - E^i$ has the following pointwise asymptotic expression as $\delta\to 0$:*

$$E^r(\mathbf{x}) = \delta k\mathbb{G}_r^{\mathbf{k}}(\mathbf{x})\,(i\mathbf{d}^*\times\mathbf{J}'_{\mathrm{m}} + k(\mathbf{J}_{\mathrm{e}})_3\mathbf{e}_3) + O\left(\frac{\widetilde{\delta}^2}{d_\sigma}\right), \tag{4.58}$$

which is uniformly valid with respect to the incident frequency. Here $\mathbf{J}_{\mathrm{e}}$ and $\mathbf{J}_{\mathrm{m}}$ are given by (4.57) and (4.54), respectively, and the parameters d_σ and d_σ^* are given in Theorem 4.1.

Remark 4.8. In our analysis, we assume that D is simply connected with a connected boundary for simplicity. Nevertheless, our arguments and results are actually very general and apply to the quite complicated geometry of the microstructure D of the thin layer, e.g., a domain with a hole or an open set with multiple connected components. In particular, Theorem 4.7 holds for the strongly coupled multilayer case, i.e., there are multiple layers of close-to-touching nanoparticles; see Figure 2.

We clearly see from the above theorem that the anomalous electromagnetic scattering results from the occurrence of the mixed collective plasmonic resonances. To make the statement more precise, let us define the electric and magnetic polarization tensors:

$$M_{\mathrm{e}}(\lambda_\varepsilon, B) = \int_{\partial B}\widetilde{\mathbf{y}}(\lambda_\varepsilon+\mathcal{K}_{\mathrm{e}}^{0,*})^{-1}[\nu]d\sigma\,,\quad M_{\mathrm{m}}(\lambda_\mu,B) = \int_{\partial B}\widetilde{\mathbf{y}}(\lambda_\mu+\mathcal{K}_{\mathrm{m}}^{0,*})^{-1}[\nu]d\sigma\,.$$

By the definition of $\mathbb{G}_r^{\mathbf{k}}(\mathbf{x})$ in Theorem 4.7, and with the help of projections $\mathbf{e}_3\otimes\mathbf{e}_3$ and $\mathbb{I}-\mathbf{e}_3\otimes\mathbf{e}_3$ and the relations

$$E^i(0) = -2\mathbf{e}_3\otimes\mathbf{e}_3\mathbf{p}^*\,,\quad H^i(0) = -2(\mathbb{I}-\mathbf{e}_3\otimes\mathbf{e}_3)\mathbf{d}^*\times\mathbf{p}^*\,,$$

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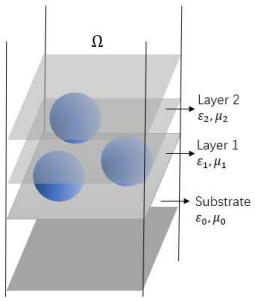

FIG. 2. *A generalized and physical configuration (cell structure Ω)* [33].

we can reformulate (4.58) in a concise form,

$$\begin{aligned} E^r(\mathbf{x}) &= \delta k(\mathbb{I} - \mathbf{d}^* \otimes \mathbf{d}^*) e^{i\mathbf{k}^*\cdot\mathbf{x}} (i\mathbf{d}^* \times \mathbf{J}'_{\mathrm{m}} + k(\mathbf{J}_{\mathrm{e}})_3 \mathbf{e}_3) + O(\delta^2) \\ &= \frac{2i\delta k}{\tau d_3} e^{i\mathbf{k}^*\cdot\mathbf{x}} \mathscr{R}\mathbf{p}^* + O(\delta^2)\,, \end{aligned} \tag{4.59}$$

where the reflection scattering matrix $\mathscr{R}$ is given by

$$\begin{aligned} \mathscr{R} = \big(\mathbb{I} - \mathbf{d}^* \otimes \mathbf{d}^*\big)\big(\mathbf{d}^* \times (\mathbb{I} - \mathbf{e}_3 \otimes \mathbf{e}_3) M_{\mathrm{m}}(\lambda_\mu, B)(\mathbb{I} - \mathbf{e}_3 \otimes \mathbf{e}_3)\mathbf{d}^* \\ \times \mathbb{I} - \mathbf{e}_3 \otimes \mathbf{e}_3 M_{\mathrm{e}}(\lambda_\varepsilon, B)\mathbf{e}_3 \otimes \mathbf{e}_3\big)\,. \end{aligned}$$

We remark that $\mathscr{R}$ should be regarded as a linear mapping defined on the two-dimensional subspace of $\mathbb{R}^3$ orthogonal to the vector $\mathbf{d}^*$, although it is a three by three matrix. Moreover, the matrix $\mathscr{R}$ essentially chacterizes the polarization conversion of the metasurface.

In the traditional optical systems, the scattering effect of such a subwavelength rough surface is almost negligible so that $\mathscr{R}$ plays a limited role in the far-field behavior of the reflected wave. However, due to the possible large negative permittivity and permeability of the plasmonic nanoparticles (as we have explained in the introduction, it is only an ideal assumption since the metallic nanoparticles typically do not possess the negative permeability at optical frequencies), λ_μ and λ_ε can approach the spectrum of $-\mathcal{K}_{\mathrm{m}}^{0,*}$ and $-\mathcal{K}_{\mathrm{e}}^{0,*}$ such that the elements in the tensors $M_{\mathrm{e}}(\lambda_\varepsilon, B)$ and $M_{\mathrm{m}}(\lambda_\mu, B)$ may blow up with an enhancement order $1/d_\sigma^*$. Therefore, following [5, 12, 10], we may define the collective plasmonic resonances by the frequencies ω satisfying

$$d(\lambda_\varepsilon(\omega), -\mathcal{K}_{\mathrm{e}}^{0,*}) \ll 1 \text{ or } d(\lambda_\mu(\omega), -\mathcal{K}_{\mathrm{m}}^{0,*}) \ll 1\,.$$

It is worth emphasizing that these frequencies generally are very different from the single-particle case. Physically, these periodically distributed plasmonic nanoparticles can resonate as a whole so that a nanoscale thin layer can significantly affect the wave propagation at the macroscale. We refer readers to [11] for some numerical evidence on collective plasmonic resonances. If the collective plasmonic resonances are excited, the effect of the reflection scattering matrix $\mathscr{R}$ can overcome the small size parameter δ and become visible, giving the possibility of achieving a desired far-field pattern. Nevertheless, our electromagnetic plasmonic metasurface, as all the nano-optic devices, still faces many fundamental limits. Actually, following [14],

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we may decompose $E^r(\mathbf{x})$ into two plane waves with orthogonal polarizations: one with the polarization vector $\mathbf{p}^*$ and the other with the polarization vector orthogonal to $\mathbf{p}^*$. We may further introduce the reflection coefficients and polarization conversion coefficients to measure the functionalities of the metasurface as in [14], and then analyze their bounds and fundamental relations via the holomorphic functional calculus [10].

4.3. Equivalent impedance boundary condition. The final goal of this work is to present an impedance boundary condition approximation for the plasmonic metasurface. For this, we first recall the surface scalar curl and the surface vector curl on the plane surface $\Gamma = \partial\mathbb{R}^3_+$, which have the explicit forms $\mathrm{curl}_\Gamma u = \frac{\partial u_2}{\partial x_1} - \frac{\partial u_1}{\partial x_2}$ for a vector function $\mathbf{u} = (u_1, u_2, 0)$ and $\vec{\mathrm{curl}}_\Gamma v = (\frac{\partial v}{\partial x_2}, -\frac{\partial v}{\partial x_1}, 0)$ for a scalar function v. We start with the simple but more realistic case: the plasmonic nanoparticles are nonmagnetic, i.e., $\mu_c = 1$. In this case, Theorem 4.7 indicates that in the far field, the total electric field can be approximated by

$$E^\delta := E^i + \delta k^2 \mathbb{G}^{\mathbf{k}}_r(\mathbf{J}_e)_3 \mathbf{e}_3 \,.$$

Introduce

$$\beta_{\mathrm{e}} := -\frac{1}{\tau}\int_{\partial B} y_3(\lambda_\varepsilon + \mathcal{K}^{0,*}_{\mathrm{e}})^{-1}[v_3]d\sigma \,.$$

Then, by applying the formula (4.9) and the fact $\mathbf{e}_3 \times E^i|_\Gamma = 0$, a simple calculation gives us

$$\begin{aligned}\mathbf{e}_3 \times E^\delta|_\Gamma &= -\delta k^2 \mathbf{e}_3 \times \mathbf{d}^* d_3 (\mathbf{J}_{\mathrm{e}})_3 e^{ikd'\cdot x'} \\ &= i\delta k 2p_3 \mathbf{e}_3 \times \mathbf{d}^* \beta_{\mathrm{e}} e^{ikd'\cdot x'} \\ &= \delta e^{ikd'\cdot x'}\,(ikd_2, -ikd_1, 0)\,\beta_{\mathrm{e}} 2p_3 \,.\end{aligned}$$

Hence we can derive that when $\delta/(d_\sigma d^*_\sigma) \to 0$, it holds that

$$\mathbf{e}_3 \times E^\delta|_\Gamma = \delta\beta_{\mathrm{e}} \vec{\mathrm{curl}}_\Gamma \mathbf{e}_3 \cdot E^i|_\Gamma = \delta\beta_{\mathrm{e}} \vec{\mathrm{curl}}_\Gamma \frac{i}{k}\mathrm{curl}_\Gamma (H^i)'|_\Gamma = \delta \frac{i\beta_{\mathrm{e}}}{k} \vec{\mathrm{curl}}_\Gamma \mathrm{curl}_\Gamma (H^\delta)'|_\Gamma + O(\delta^2)$$

by noting that $\mathrm{curl}_\Gamma (H^i)'|_\Gamma = -ik\mathbf{e}_3 \cdot E^i|_\Gamma$. The above formula further yields the equivalent (Leontovich) impedance boundary condition,

$$\mathbf{e}_3 \times E^\delta|_\Gamma = \delta \frac{i\beta_{\mathrm{e}}}{k} \vec{\mathrm{curl}}_\Gamma \mathrm{curl}_\Gamma (H^\delta)'|_\Gamma \,, \tag{4.60}$$

which can help us to approximate the far-field effect of the thin layer of the plasmonic nanoparticles, up to a second-order term. Moreover, we emphasize that the approximation is uniformly valid with respect to the incident frequency.

We now consider the magnetic plasmonic nanoparticles, i.e., μ_c has the possibility of taking negative values, and introduce a two by two matrix:

$$D_{\mathrm{m}} = \frac{1}{\tau}\int_{\partial B} y'(\lambda_\mu + \mathcal{K}^{0,*}_{\mathrm{m}})^{-1}[\nu']d\sigma \,.$$

According to Theorem 4.7, the total electric field can be approximated by

$$E^\delta = E^i + \delta k \mathbb{G}^{\mathbf{k}}_r(\mathbf{x})(i\mathbf{d}^* \times \mathbf{J}'_{\mathrm{m}} + k(\mathbf{J}_{\mathrm{e}})_3 \mathbf{e}_3) \,.$$

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In a manner similar to the nonmagnetic case, we can find that

$$\mathbf{e}_3 \times E^\delta|_\Gamma = \delta \frac{i\beta_{\rm e}}{k} \vec{\rm curl}_\Gamma {\rm curl}_\Gamma (H^\delta)'|_\Gamma - ik\delta D_{\rm m}(H^\delta)'|_\Gamma + O(\delta^2)$$

with the help of the following observation:

$$i\delta k \mathbf{e}_3 \times \left(\mathbb{G}_r^{\mathbf{k}} \mathbf{d}^* \times \mathbf{J}'_{\rm m}\right)|_\Gamma = i\delta k \mathbf{e}_3 \times \left(\mathbf{d}^* \times \mathbf{J}'_{\rm m}\right) e^{ikd'\cdot x'}|_\Gamma = -ik\delta D_{\rm m}(H^i)'|_\Gamma \,.$$

It then follows that we can use the effective (Leontovich) impedance boundary condition

$$\mathbf{e}_3 \times E^\delta|_\Gamma = \delta \frac{i\beta_{\rm e}}{k} \vec{\rm curl}_\Gamma {\rm curl}_\Gamma (H^\delta)'|_\Gamma - ik\delta D_{\rm m}(H^\delta)'|_\Gamma \tag{4.61}$$

to approximate the effect of the thin layer in the macroscopic scale, up to the second order term. Again, this approximation is uniformly valid with respect to the incident frequency and no matter whether the resonance is excited or not.

5. Concluding remarks and extensions. In this work, we have studied the scattering effect of the periodically distributed plasmonic nanoparticles in the homogenization regime. For the subwavelength structures of such patterns, the reflection scattering matrix (cf. (4.59)) and the Leontovich impedance boundary condition (cf. (4.61)) have been derived for the approximation of the scattered field in both magnetic and nonmagnetic cases. A similar problem setting was considered in [25, 24, 23], where the thin layer was made of dielectric particles and the standard variational approach applies. However, the variational framework breaks down in the resonant case, hence we have adopted the layer potential theories instead in this work to analyze the singularity and prove the uniform validation of the boundary condition approximations. Our results provide a relatively complete picture of the mechanism of the electromagnetic plasmonic metasurfaces and can be easily modified to cope with other regimes and boundary conditions. Therefore, this work may be viewed as a generalization of the standard homogenization theory to the resonant periodic microstructures. And our theoretical analysis and findings may help design a metasurface that can resonate at some specific dense set of frequencies to further realize the broadband wave modulation. In addition, it is also a very interesting and challenging topic to understand how to reconstruct the fine structures of thin layers in terms of the scattered field under the resonance.

Our analysis and results can also be easily extended to several physical and realistic regimes and applications, although we only consider the homogenization regime in this work since it is the most interesting and important case where the collective resonance can happen. First, our approach can be directly applied to other important regimes:

$$\text{size of particle} \ll \text{period} \sim \text{wavelength}, \quad \text{or} \quad \text{size of particle} \ll \text{period} \ll \text{wavelength}.$$

However, we may not expect the collective plasmonic resonances in the above two configurations, since the particles are essentially well separated though they are distributed in a certain pattern. In these two cases, the scattering field will be locally dominated by the resonance modes excited by the nearest single nanoparticle. In view of this fact, the thin layers under these regimes may not have the capability to realize the control of the electromagnetic wave in the macroscopic scale. Second,

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in this work, we have only considered the unrealistic perfectly conducting boundary conditions on the bottom surface Γ. Nevertheless, by replacing the Green's tensors defined in section 3 by the ones satisfying other appropriate boundary conditions, we can naturally modify the corresponding analysis and deal with the more physical case where the particles are periodically distributed on a supporting substrate; see Figure 2. Third, as we have pointed out in Remark 4.8, our results remain the same for the multiple close-to-touching thin layers. The generalization to the well-separated multilayer case

$$\text{size of particle} \sim \text{period} \ll \text{distance between two layers} \sim \text{wavelength} \sim 1$$

is also direct since the scattering effect of each layer can be considered independently due to the weak interactions between the arrays. More precisely, suppose that we have the approximate scattered waves $E_1^r, \ldots, E_n^r$ associated with n thin layers; then each approximate wave can be determined by Theorem 4.7. The total approximate scattered wave E_{app}^r for such a multilayer structure could be written as $E_{app}^r = E_1^r + \cdots + E_n^r$.

With these design flexibilities and extension remarks, our theoretical findings may shed light on the mathematical understanding of electromagnetic plasmonic metasurfaces and their related optimal design problems.

Appendix A. Proof of Lemma 4.3. By the scaling property (3.27) of $\mathcal{A}^{\mathbf{k}}_{D,\mathrm{e/m}}$, we have

$$\widetilde{E}^r(\widetilde{\mathbf{x}}) - \widetilde{E}^r_p(\widetilde{\mathbf{x}}) = \widetilde{E}^r_e(\widetilde{\mathbf{x}}) = \nabla \times \mathcal{A}^{\delta\mathbf{k}}_{e,\mathrm{m}}[\widetilde{\phi}](\widetilde{\mathbf{x}}) + \frac{1}{\delta}\nabla \times \nabla \times \mathcal{A}^{\delta\mathbf{k}}_{e,\mathrm{e}}[\widetilde{\psi}](\widetilde{\mathbf{x}})\,. \tag{A.1}$$

We next estimate the two terms in (A.1). To do so, for large enough $\widetilde{x}_3$, we separate the variables of the kernel $\Pi^{\delta\mathbf{k}}_{e,\mathrm{e/m}}$ involved in the definition of $\mathcal{A}^{\delta\mathbf{k}}_{e,\mathrm{e/m}}$:

$$\Pi^{\delta\mathbf{k}}_{e,\mathrm{e/m}}(\widetilde{\mathbf{x}},\widetilde{\mathbf{y}}) = -\frac{1}{2\tau}\sum_{\xi\in\Lambda^*\setminus\{0\}} \rho^{\delta\mathbf{k}}_{\xi}(\widetilde{\mathbf{x}})\pi^{\delta\mathbf{k}}_{\xi,\mathrm{e/m}}(\widetilde{\mathbf{y}})\,, \tag{A.2}$$

where $\rho^{\delta\mathbf{k}}_{\xi}(\widetilde{\mathbf{x}})$ is given by

$$\rho^{\delta\mathbf{k}}_{\xi}(\widetilde{\mathbf{x}}) := \frac{1}{\sqrt{|\xi+\delta k'|^2-(\delta k)^2}} e^{i(\xi+\delta k')\cdot\widetilde{x}'} e^{-\sqrt{|\xi+\delta k'|^2-(\delta k)^2}(\widetilde{x}_3-h)}\,. \tag{A.3}$$

Here, h is a constant satisfying $|\widetilde{x}_3| < h < \delta^{-1}L$ with $\widetilde{\mathbf{x}} \in B$ and $\pi^{\delta\mathbf{k}}_{\xi,\mathrm{e/m}}(\widetilde{\mathbf{y}})$ is naturally introduced by the formulas (A.2) and (A.3). We also note that $\Pi^{\delta\mathbf{k}}_{e,\mathrm{e/m}}$ is a diagonal matrix and all of its diagonal entries are smooth functions.

Then, for the first term in (A.1), we can write

$$\nabla \times \mathcal{A}^{\delta\mathbf{k}}_{e,\mathrm{m}}[\widetilde{\phi}](\widetilde{\mathbf{x}}) = \int_{\partial B} \nabla \times \Pi^{\delta\mathbf{k}}_{e,\mathrm{m}}(\widetilde{\mathbf{x}},\widetilde{\mathbf{y}})\widetilde{\phi}(\widetilde{\mathbf{y}})d\widetilde{\mathbf{y}}\,, \tag{A.4}$$

where

$$\nabla \times \Pi^{\delta\mathbf{k}}_{e,\mathrm{m}}(\widetilde{\mathbf{x}},\widetilde{\mathbf{y}}) = -\frac{1}{2\tau}\sum_{\xi\in\Lambda^*\setminus\{0\}} \nabla\rho^{\delta\mathbf{k}}_{\xi}(\widetilde{\mathbf{x}}) \times \pi^{\delta\mathbf{k}}_{\xi,\mathrm{m}}(\widetilde{\mathbf{y}})\,. \tag{A.5}$$

For $\rho^{\delta\mathbf{k}}_{\xi}(\widetilde{\mathbf{x}})$, we can see the existence of a positive constant c such that the following estimate holds for all $\xi \in \Lambda^*\setminus\{0\}$ and uniformly with respect to all small enough δ:

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$$\left|\partial_j \rho_\xi^{\delta\mathbf{k}}(\widetilde{\mathbf{x}})\right| \lesssim e^{-c|\xi|(\widetilde{x}_3-h)}\,.$$

Applying the above estimate and the trace inequality, we derive

$$\Big|\int_{\partial B} \nabla\rho_\xi^{\delta\mathbf{k}}(\widetilde{\mathbf{x}}) \times \pi_{\xi,\mathrm{m}}^{\delta\mathbf{k}}(\widetilde{\mathbf{y}})\phi(\widetilde{\mathbf{y}})d\sigma(\widetilde{\mathbf{y}})\Big| \lesssim e^{-c|\xi|(\widetilde{x}_3-h)} \|\phi\|_{H^{-\frac{1}{2}}(\partial B)} \sum_{j=1}^{3} \big\|(\pi_{\xi,\mathrm{m}}^{\delta\mathbf{k}})_j\big\|_{H^{\frac{1}{2}}(\partial B)}$$

$$\lesssim e^{-c|\xi|(\widetilde{x}_3-h)} \|\phi\|_{H^{-\frac{1}{2}}(\partial B)} \sum_{j=1}^{3} \big\|(\pi_{\xi,\mathrm{m}}^{\delta\mathbf{k}})_j\big\|_{H^1(B)} \lesssim e^{-c|\xi|(\widetilde{x}_3-h)} \|\phi\|_{H^{-\frac{1}{2}}(\partial B)}\,,$$

where we have used the uniform boundedness of $\|(\pi_{\xi,\mathrm{m}}^{\delta k})_j\|_{H^1(B)}$ with respect to $\xi \in \Lambda^*\backslash\{0\}$. Now it follows easily from the above estimate and the formulas (A.4) and (A.5) that

$$\left|\nabla \times \mathcal{A}_{e,\mathrm{m}}^{\delta k}[\widetilde{\phi}](\widetilde{\mathbf{x}})\right| \lesssim e^{-c(\widetilde{x}_3-h)} \|\phi\|_{H^{-\frac{1}{2}}(\partial B)}\,.$$

Similarly, we can establish the desired pointwise estimate of the second term in (A.1), and then the error estimate in Lemma 4.3 follows.

Appendix B. Proof of Lemma 4.5. We consider only the system (4.25) and show the formula (4.27). The proof of (4.28) is similar. We shall first prove that the right-hand side of (4.27) and $\nabla \times \mathcal{A}_{\mathrm{m}}^0[\widetilde{\phi}_{0,0}]$ are both the gradients of some solutions to (4.25) and then demonstrate that the gradients of the solutions to (4.25) are unique. For this purpose, recalling the far-field behavior of $\mathcal{S}_{\mathrm{e}}^0[\phi]$ (cf. (3.38) and (3.39)), we can verify that the function

$$u(\widetilde{\mathbf{x}}) := \begin{cases} \frac{1}{1-\mu_c}\mathcal{S}_{\mathrm{e}}^0\left(\lambda_\mu - \mathcal{K}_{\mathrm{e}}^{0,*}\right)^{-1}\left[\nu \cdot E^i(0)\right](\widetilde{\mathbf{x}}) & \text{in } \Omega\backslash B, \\ \frac{1}{\mu_c}E^i(0)\widetilde{\mathbf{x}} + \frac{1}{\mu_c(1-\mu_c)}\mathcal{S}_{\mathrm{e}}^0\left(\lambda_\mu - \mathcal{K}_{\mathrm{e}}^{0,*}\right)^{-1}\left[\nu \cdot E^i(0)\right](\widetilde{\mathbf{x}}) & \text{in } B \end{cases}$$

satisfies the boundary conditions and the far-field condition in (4.25) and indeed solves (4.25). Furthermore, it is easy to check that the right-hand side of (4.27) is the gradient of u.

Next, we show that $\nabla \times \mathcal{A}_{\mathrm{m}}^0[\widetilde{\phi}_{0,0}]$ can also be written as a gradient of some solution to (4.25). In fact, by the continuity of its normal trace and the jump formula of its tangential trace (cf. (3.24) with $\mathbf{k} = 0$), we find

$$\left[\nu \cdot \nabla \times \mathcal{A}_{\mathrm{m}}^0[\widetilde{\phi}_{0,0}]\right] = 0\,, \quad \left[\mu\left(\nu \times \nabla \times \mathcal{A}_{\mathrm{m}}^0[\widetilde{\phi}_{0,0}]\right)\right] = \nu \times E^i(0)\,.$$

However, noticing that $\nabla_{\partial B} \cdot \widetilde{\phi}_{0,0} = 0$, we get

$$\nabla \times \nabla \times \mathcal{A}_{\mathrm{m}}^0[\widetilde{\phi}_{0,0}] = \nabla \mathcal{S}_{\mathrm{m}}^0[\nabla_{\partial B} \cdot \widetilde{\phi}_{0,0}] = 0 \quad \text{in } \Omega\backslash\partial B\,,$$

which implies (cf. [45, Theorem 3.37])

$$\nabla \times \mathcal{A}_{\mathrm{m}}^0[\widetilde{\phi}_{0,0}] = \nabla p \quad \text{for some } p \in H^1(\mathcal{B}) \text{ or } H^1_{loc}(\mathbb{R}^3_+\backslash\bar{\mathcal{B}})\,. \tag{B.1}$$

Moreover, we can assume that $p = 0$ on Γ by noting the fact that $\mathbf{e}_3 \times \nabla \times \mathcal{A}_{\mathrm{m}}^0[\widetilde{\phi}_{0,0}] = \mathbf{e}_3 \times \nabla p = 0$ on Γ. To see that p is indeed a solution to (4.25), it remains to show that p, up to a constant, satisfies

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(i) p is periodic with respect to Λ.
(ii) there exists a complex constant c_p such that $p - c_p$ decays exponentially as $x_3 \to \infty$.

For the above two claims, let us first define the translation operator $\mathcal{T}_i : L^2_{loc}(\mathbb{R}^3_+) \longmapsto L^2_{loc}(\mathbb{R}^3_+)$ associated with $\mathbf{a}_i$ (i = 1, 2):

$$\mathcal{T}_i u(x', x_3) = u(x' + \mathbf{a}_i, x_3).$$

We note that $\mathcal{T}_i$ commutes with the gradient, namely, $\mathcal{T}_i \nabla = \nabla T_i$, in the distribution sense. Since $\mathcal{T}_i \nabla p = \nabla p$ by (B.1), we have $\nabla(\mathcal{T}_i p - p) = 0$, which implies that there exist two constants C_1 and C_2 such that $\mathcal{T}_i p = p + C_i$ in $\Omega \backslash \bar{B}$. We now choose vectors $\mathbf{b}_i$ such that $\mathbf{a}_i \cdot \mathbf{b}_j = \delta_{ij}$ and define an auxiliary function $\widetilde{p} = p - (C_1 \mathbf{b}_1 + C_2 \mathbf{b}_2) \cdot x'$. Then we can directly check that $\widetilde{p}$ is periodic with respect to Λ, i.e.,

$$\widetilde{p}(x' + \mathbf{a}_i, x_3) = p(x' + \mathbf{a}_i, x_3) - (C_1 \mathbf{b}_1 + C_2 \mathbf{b}_2) \cdot (x' + \mathbf{a}_i) = \widetilde{p}(x', x_3)\,.$$

In the case of far fields, noting that $\Delta \widetilde{p} = 0$, we can expand $\widetilde{p}$ by Fourier series (cf. [19]),

$$\widetilde{p} = \sum_{\xi \in \Lambda^*} p_\xi e^{i\xi \cdot x' - |\xi| x_3}, \quad p_\xi \in \mathbb{C}\,. \tag{B.2}$$

It is easy to see from the formulas (3.38) and (3.39) that $\nabla \times \mathcal{A}^0_{\mathrm{m}}[\widetilde{\phi}_{0,0}]$ decays exponentially as $x_3 \to \infty$. Recalling (B.1) and (B.2) and the definition of $\widetilde{p}$, we can show that $C_1 = 0$ and $C_2 = 0$, by matching the far-field modes of ∇p and $\nabla \times \mathcal{A}^0_{\mathrm{m}}[\widetilde{\phi}_{0,0}]$. Hence we can conclude $\widetilde{p} = p$, and our two claims follow.

Finally, we prove ∇u and ∇p defined above can be uniquely determined by the system (4.25). For doing so, it suffices to show that the gradient of any solution u^e to (4.25) is zero in $\Omega \backslash \partial B$ if we replace the jump data $\nu \times E^i(0)$ in (4.25) by 0. Then the jump condition $\mu_c(\nu \times \nabla u^e)|_- = (\nu \times \nabla u^e)|_+$, together with the formula (2.5), implies that

$$\nabla_{\partial B} \left[(\mu u^e)|_- - (\mu u^e)|_+ \right] = 0\,,$$

equivalently, $(\mu u^e)|_- = (\mu u^e)|_+ + C$ for some constant C. Without loss of generality, we assume $C = 0$; otherwise we may consider $u^e - \frac{C}{\mu_c} \chi_B$. By integration by parts and interface conditions, we get

$$\int_\Omega \mu |\nabla u^e|^2 (\widetilde{\mathbf{x}}) d\widetilde{\mathbf{x}} = 0\,. \tag{B.3}$$

If $\mathfrak{Re}\mu_c > 0$, or if $\mathfrak{Re}\mu_c \leq 0$ and $\mathfrak{Im}\mu_c \neq 0$, we can deduce $\nabla u^e = 0$ in B and $\nabla u^e = 0$ in $\Omega \backslash \bar{B}$. For the case $\mu_c \leq 0$ ($\lambda_\mu \notin \sigma\big(\mathcal{K}^{0,*}_{\mathrm{e}}\big)$), we can consider it as a limiting case of $\mu + i\eta$ as $\eta \to 0$, and then the same argument as the proof of [32, Theorem 3.1] helps us to complete the proof.

Appendix C. Proof of Lemma 4.6. We shall only show how to compute the quantities involving $\widetilde{\psi}$, as the same can be done for the terms related to $\widetilde{\phi}$. To do so, we first consider $\int_{\partial B} \widetilde{\mathbf{y}}^\alpha \widetilde{\psi}_{\beta,0}(\widetilde{\mathbf{y}}) d\sigma$ for $|\alpha| \leq 1$. Using the formula (4.19) and the decomposition for any proper f,

$$f = \left(1 - \varepsilon_c\right) \left(\lambda_\varepsilon - \mathcal{M}_{\mathrm{e}} + \frac{1}{2} + \mathcal{M}_{\mathrm{e}} \right) [f]\,,$$

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we can compute

$$\begin{aligned}\int_{\partial B}\widetilde{\mathbf{y}}^{\alpha}\widetilde{\psi}_{\beta,0}(\widetilde{\mathbf{y}})d\sigma &= \int_{\partial B}\widetilde{\mathbf{y}}^{\alpha}\Big(1-\varepsilon_c\Big)\Big(\lambda_\varepsilon-\mathcal{M}_{\rm e}+\frac{1}{2}+\mathcal{M}_{\rm e}\Big)\Big[\widetilde{\psi}_{\beta,0}\Big](\widetilde{\mathbf{y}})d\sigma\\ &= \int_{\partial B}\widetilde{\mathbf{y}}^{\alpha}\Big(1-\varepsilon_c\Big)\Big(\frac{i\nu(\widetilde{\mathbf{y}})\times\widetilde{\mathbf{y}}^{\beta}\partial^{\beta}H^i(0)}{k(1-\varepsilon_c)}+g_\beta\Big)d\sigma\\ &\quad+\int_{\partial B}\widetilde{\mathbf{y}}^{\alpha}\Big(1-\varepsilon_c\Big)\nu\times\nabla\times\mathcal{A}_{\rm e}\Big[\widetilde{\psi}_{\beta,0}\Big]d\sigma\\ &= \frac{i}{k}\int_B\nabla\times\Big(\widetilde{\mathbf{y}}^{\alpha}\widetilde{\mathbf{y}}^{\beta}\partial^{\beta}H^i(0)\Big)d\widetilde{\mathbf{y}}+(1-\varepsilon_c)\int_{\partial B}\widetilde{\mathbf{y}}^{\alpha}g_\beta d\sigma\\ &\quad+(1-\varepsilon_c)\int_B\nabla\times\Big(\widetilde{\mathbf{y}}^{\alpha}\nabla\times\mathcal{A}_{\rm e}\Big[\widetilde{\psi}_{\beta,0}\Big]\Big)d\widetilde{\mathbf{y}}\,.\end{aligned}$$

In particular, we get for $|\alpha|=1\,,|\beta|=0$ that

$$\int_{\partial B}\widetilde{y}_j\widetilde{\psi}_{0,0}d\sigma=\frac{i}{k}\mathbf{e}_j\times H^i(0)|B|+(1-\varepsilon_c)\int_B\nabla\times\Big(\widetilde{y}_j\nabla\times\mathcal{A}_e\left[\widetilde{\psi}_{0,0}\right]\Big)\,d\widetilde{\mathbf{y}}\,,$$

where we have used the Stokes's theorem and the fact that $g_\beta=0$ for $\beta=0$. Then formula (4.31) follows directly from the relation

$$\nabla\times\Big(\widetilde{y}_j\nabla\times\mathcal{A}_{\rm e}\left[\widetilde{\psi}_{\beta,0}\right]\Big)=\mathbf{e}_j\times\nabla\times\mathcal{A}_{\rm e}\left[\widetilde{\psi}_{0,0}\right]+\nabla\mathcal{S}^0_{\rm e}\left[\nabla_{\partial B}\cdot\widetilde{\psi}_{j,0}\right]$$

and the formula

$$\begin{aligned}&\int_B\nabla\times\mathcal{A}_{\rm e}\Big[\widetilde{\psi}_{0,0}\Big]d\widetilde{\mathbf{y}}=\int_{\partial B}(\nu\times\mathcal{A}_{\rm e})|_-\Big[\widetilde{\psi}_{0,0}\Big]d\sigma\\ &=\int_{\partial B}\left(\frac{1}{2}+\mathcal{M}_{\rm e}\right)\Big[\widetilde{\psi}_{0,0}\Big]d\sigma=-\int_{\partial B}\widetilde{\mathbf{y}}\nabla_{\partial B}\cdot\left(\frac{1}{2}+\mathcal{M}_{\rm e}\right)\Big[\widetilde{\psi}_{0,0}\Big]d\sigma\\ &=-\int_{\partial B}\widetilde{\mathbf{y}}\left(\frac{1}{2}-\mathcal{K}^*_{\rm e}\right)\Big[\nabla_{\partial B}\cdot\widetilde{\psi}_{0,0}\Big]d\sigma=0\,,\end{aligned}$$

where we have used (4.22) again. For $|\alpha|=0,|\beta|=1$, we note that

$$\int_{\partial B}g_\beta d\sigma=0\quad\text{for }|\beta|=1\,,$$

then a similar derivation leads to (4.33).

REFERENCES

[1] T. Abboud and H. Ammari, *Diffraction at a biperiodic curved structure-homogenization*, C. R. Acad. Sci. Ser. I Math., 320 (1995), pp. 301–306.

[2] T. Abboud and H. Ammari, *Diffraction at a curved grating: TM and TE cases, homogenization*, J. Math. Anal. Appl., 202 (1996), pp. 995–1026.

[3] Y. Achdou, O. Pironneau, and F. Valentin, *Effective boundary conditions for laminar flows over periodic rough boundaries*, J. Comput. Phys., 147 (1998), pp. 187–218.

[4] G. Allaire and M. Amar, *Boundary layer tails in periodic homogenization*, ESAIM Control Optim. Cal. Var., 4 (1999), pp. 209–243.

[5] H. Ammari, Y. Deng, and P. Millien, *Surface plasmon resonance of nanoparticles and applications in imaging*, Arch. Ration. Mech. Anal., 220 (2016), pp. 109–153.

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[6] H. Ammari, B. Fitzpatrick, D. Gontier, H. Lee, and H. Zhang, *A mathematical and numerical framework for bubble meta-screens*, SIAM J. Appl. Math., 77 (2017), pp. 1827–1850.
[7] H. Ammari, B. Fitzpatrick, H. Kang, M. Ruiz, S. Yu, and H. Zhang, *Mathematical and Computational Methods in Photonics and Phononics*, Math. Surveys Monogr. 235, AMS, Providence, RI, 2018.
[8] H. Ammari and H. Kang, *Polarization and Moment Tensors: With Applications to Inverse Problems and Effective Medium Theory*, Appl. Math. Sci. 162, Springer, New York, 2007.
[9] H. Ammari, H. Kang, and H. Lee, *Layer Potential Techniques in Spectral Analysis*, Math. Surveys Monogr. 153, AMS, Providence, RI, 2009.
[10] H. Ammari, P. Millien, M. Ruiz, and H. Zhang, *Mathematical analysis of plasmonic nanoparticles: The scalar case*, Arch. Ration. Mech. Anal., 224 (2017), pp. 597–658.
[11] H. Ammari, M. Ruiz, W. Wu, S. Yu, and H. Zhang, *Mathematical and numerical framework for metasurfaces using thin layers of periodically distributed plasmonic nanoparticles*, Proc. A, 472 (2016), 20160445.
[12] H. Ammari, M. Ruiz, S. Yu, and H. Zhang, *Mathematical analysis of plasmonic resonances for nanoparticles: The full Maxwell equations*, J. Differential Equations, 261 (2016), pp. 3615–3669.
[13] K. Ando and H. Kang, *Analysis of plasmon resonance on smooth domains using spectral properties of the Neumann–Poincaré operator*, J. Math. Anal. Appl., 435 (2016), pp. 162–178.
[14] A. Arbabi and A. Faraon, *Fundamental limits of ultrathin metasurfaces*, Scientific Reports, 7 (2017), 43722.
[15] A. Bensoussan, J. Lions, and G. Papanicolaou, *Asymptotic Analysis for Periodic Structures*, AMS, Providence, RI, 2011.
[16] E. Bonnetier and F. Triki, *Asymptotic of the green function for the diffraction by a perfectly conducting plane perturbed by a sub-wavelength rectangular cavity*, Math. Methods Appl. Sci., 33 (2010), pp. 772–798.
[17] G. Bouchitté, C. Bourel, and D. Felbacq, *Homogenization near resonances and artificial magnetism in three dimensional dielectric metamaterials*, Arch. Ration. Mech. Anal., 225 (2017), pp. 1233–1277.
[18] A. Buffa, M. Costabel, and D. Sheen, *On traces for H(curl, Ω) in Lipschitz domains*, J. Math. Anal. Appl, 276 (2002), pp. 845–867.
[19] M. Cessenat, *Mathematical Methods in Electromagnetism: Linear Theory and Applications*, World Scientific, Singapore, 1996.
[20] H. Chen, A. J. Taylor, and N. Yu, *A review of metasurfaces: Physics and applications*, Rep. Progr. Phys., 79 (2016), 076401.
[21] Y. Chen and R. Lipton, *Resonance and double negative behavior in metamaterials*, Arch. Ration. Mech. Anal., 209 (2013), pp. 835–868.
[22] D. Colton and R. Kress, *Inverse Acoustic and Electromagnetic Scattering Theory*, Appl. Math. Sci. 93, Springer, New York, 2012.
[23] B. Delourme, *Asymptotic Models for Thin Periodic Layers in Electromagnetism*, theses, Université Pierre et Marie Curie, Paris VI, 2010, https://tel.archives-ouvertes.fr/tel-00650354.
[24] B. Delourme, *High-order asymptotics for the electromagnetic scattering by thin periodic layers*, Math. Methods Appl. Sci., 38 (2015), pp. 811–833.
[25] B. Delourme, H. Haddar, and P. Joly, *On the well-posedness, stability and accuracy of an asymptotic model for thin periodic interfaces in electromagnetic scattering problems*, Math. Models Methods Appl. Sci., 23 (2013), pp. 2433–2464.
[26] D. Felbacq, *Layer homogenization of a 2D periodic array of scatterers*, Photonics Nanostructures-Fundamentals Appl., 11 (2013), pp. 436–441.
[27] D. Felbacq, *Impedance operator description of a metasurface with electric and magnetic dipoles*, Math. Probl. Eng., 2015 (2015).
[28] G. B. Folland, *Introduction to Partial Differential Equations*, Princeton University Press, Princeton, NJ, 1995.
[29] R. Griesmaier, *An asymptotic factorization method for inverse electromagnetic scattering in layered media*, SIAM J. Appl. Math., 68 (2008), pp. 1378–1403.
[30] P. A. Huidobro, S. A. Maier, and J. B. Pendry, *Tunable plasmonic metasurface for perfect absorption*, EPJ Appl. Metamaterials, 4 (2017), 6.
[31] A. Ishikawa, T. Tanaka, and S. Kawata, *Negative magnetic permeability in the visible light region*, Phys. Rev. Lett., 95 (2005), 237401.
[32] H. Kang, K. Kim, H. Lee, J. Shin, and S. Yu, *Spectral properties of the Neumann–Poincaré operator and uniformity of estimates for the conductivity equation with complex coefficients*, J. London Math. Soc., 93 (2016), pp. 519–545.

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[33] A. V. Kildishev, A. Boltasseva, and V. M. Shalaev, *Planar photonics with metasurfaces*, Science, 339 (2013), 1232009.
[34] M. Kraft, A. Braun, Y. Luo, S. A. Maier, and J. B. Pendry, *Bianisotropy and magnetism in plasmonic gratings*, ACS Photonics, 3 (2016), pp. 764–769.
[35] M. Kraft, Y. Luo, S. Maier, and J. Pendry, *Designing plasmonic gratings with transformation optics*, Phys. Rev. X, 5 (2015), 031029.
[36] V. Leroy, A. Strybulevych, M. Lanoy, F. Lemoult, A. Tourin, and J. H. Page, *Superabsorption of acoustic waves with bubble metascreens*, Phys. Rev. B, 91 (2015), 020301.
[37] J. Lin, S. P. Shipman, and H. Zhang, *Fano Resonance for a Periodic Array of Perfectly Conducting Narrow Slits*, preprint, arXiv:1904.11019, 2019.
[38] J. Lin and H. Zhang, *Scattering and field enhancement of a perfect conducting narrow slit*, SIAM J. Appl. Math., 77 (2017), pp. 951–976.
[39] J. Lin and H. Zhang, *Scattering by a periodic array of subwavelength slits* I: *Field enhancement in the diffraction regime*, Multiscale Model. Simul., 16 (2018), pp. 922–953.
[40] J. Lin and H. Zhang, *Scattering by a periodic array of subwavelength slits* II: *Surface bound states, total transmission, and field enhancement in homogenization regimes*, Multiscale Model. Simul., 16 (2018), pp. 954–990.
[41] J. Lin and H. Zhang, *An integral equation method for numerical computation of scattering resonances in a narrow metallic slit*, J. Comput. Phy., 385 (2019), pp. 75–105.
[42] C. M. Linton, *Lattice sums for the Helmholtz equation*, SIAM Rev., 52 (2010), pp. 630–674.
[43] R. Lipton, A. Polizzi, and L. Thakur, *Novel metamaterial surfaces from perfectly conducting subwavelength corrugations*, SIAM J. Appl. Math., 77 (2017), pp. 1269–1291.
[44] S. A. Maier, *Plasmonics: Fundamentals and Applications*, Springer, New York, 2007.
[45] P. Monk, *Finite Element Methods for Maxwell's Equations*, Oxford University Press, New York, 2003.
[46] J. Nédélec, *Acoustic and Electromagnetic Equations: Integral Representations for Harmonic Problems*, Appl. Math. Sci. 144, Springer, New York, 2001.
[47] D. R. Smith, W. J. Padilla, D. Vier, S. C. Nemat-Nasser, and S. Schultz, *Composite medium with simultaneously negative permeability and permittivity*, Physi. Rev. Lett., 84 (2000), pp. 4184–4187.
[48] S. Sun, Q. He, J. Hao, S. Xiao, and L. Zhou, *Electromagnetic metasurfaces: Physics and applications*, Adv. Optics Photonics, 11 (2019), pp. 380–479.
[49] S. Tretyakov, *Metasurfaces for general transformations of electromagnetic fields*, Phil. Trans. R. Soc. A, 373 (2015), 20140362.
[50] L. Zhang, S. Mei, K. Huang, and C. Qiu, *Advances in full control of electromagnetic waves with metasurfaces*, Adv. Optical Materials, 4 (2016), pp. 818–833.

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