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Fano resonances in all-dielectric electromagnetic metasurfaces

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Abstract

We are interested in the resonant electromagnetic (EM) scattering by all-dielectric metasurfaces made of a two-dimensional lattice of nanoparticles with high refractive indices. In [Ammari et al., *Trans. AMS*, 376 (2023), 39-90], it has been shown that a single high-index nanoresonator can couple with the incident wave and exhibit a strong magnetic dipole response. Recent physics experiments reveal that when the particles are arranged in certain periodic configurations, they may have different anomalous scattering effects in the macroscopic scale, compared to the single particle case. In this work, we shall develop a rigorous mathematical framework for analyzing the resonant behaviors of all-dielectric metasurfaces. We start with the characterization of subwavelength scattering resonances in this periodic setting and their asymptotic expansions in terms of the refractive index of the nanoparticles. Then we show that real resonances always exist below the essential spectrum of the periodic Maxwell operator, and that they are the simple poles of the scattering resolvent with the exponentially decaying resonant modes. By using group theory, we also discuss the implications of the symmetry of the metasurface on the subwavelength band functions and their associated eigenfunctions. For the symmetric metasurfaces with the normal incidence, we use a variational method to show the existence of embedded eigenvalues (i.e., real subwavelength resonances embedded in the continuous radiation spectrum). Furthermore, we break the configuration symmetry by a small deformation field on the particles and consider a slightly non-normal incidence to prove that in this case Fano-type reflection and transmission anomalies could occur.

1 Introduction

The study of electromagnetic metamaterials has been a very topical subject in the field of nanophotonics over the last few years, due to their great potentials in wave front control, field concentration, and light focusing at subwavelength scales [21, 56, 89]. The plasmonic nanoresonators (e.g., metallic nanoparticles) is one of the widely used building blocks for novel optical metamaterials [68]; see the monograph [6] and the references therein for a mathematical treatment. However, the practical applications of the plasmonic metamaterials are severely limited by the heat dissipation induced by the imaginary part of the electric permittivity in the visible light range. This motivates physicists and engineers to search for alternatives to the plasmonic elements. Recently, the dielectric nanoresonators (e.g., silicon nanoparticles) have received considerable attention for their low intrinsic losses and high electric permittivity. It was experimentally demonstrated in [30, 32, 54, 63] that a single silicon nanoparticle can resonate in the optical realm with a high Q-factor (i.e., the so-called dielectric resonances), and the excited electric and magnetic dipole moments can have comparable order of magnitudes. Such properties are desirable and attractive in many applications in imaging science, material science and wireless communications, and lead to a superior performance of the all-dielectric metamaterials over the lossy plasmonic devices [8, 44, 50, 54, 80]. For the case of spherical nanoparticles, the dielectric resonance can be well understood by the Mie scattering theory [85], while for the TM or TE polarization case, the quasi-static dielectric resonance is equivalent to the eigenvalue problem for the Newtonian potential [2]; see also [64] for the discussion on the nonlinear Kerr-type material. The complete mathematical theories for the cases of a single dielectric nanoparticle and a cluster of dielectric nanoparticles with the full Maxwell's equations have been achieved in [9] and [20], respectively.

Metasurfaces are two-dimensional composite materials with thicknesses much smaller than the operating wavelength, which enable the complete control of the phase, amplitude, and polarization of the scattered wave [43, 55, 82]. We refer the readers to [1, 5, 7, 57] for recent mathematical results on plasmonic metasurfaces and bubble meta-screens. Thanks to the unique optical properties of the resonant dielectric nanoparticles, great effort has also been made to develop the all-dielectric metasurfaces for realizing the high-efficiency light manipulation. The current work is mainly motivated by [49, 58], where the authors designed a class of dielectric metasurfaces with broken in-plane symmetry

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that can support the bound states in the continuum and allow the Fano-type transmission and reflection. Fano resonance is a special resonant scattering phenomenon corresponding to the asymmetric resonance peaks in transmission spectra, which was initially investigated by Ugo Fano [31] in quantum mechanics. Such phenomenon has been extensively explored for various photonic periodic structures since the 1990s [59, 70]. The basic physical origin of the Fano resonance lies in the interference between the continuous state in the background and the discrete resonant state from the scattering system, as pointed out by Fano in his original work [31]. Mathematically, it is closely related to the resonances embedded in the continuous spectrum of the underlying operators of the interested models and the associated bound states in the continuum (BICs), which are generally nonrobust with respect to the perturbations. In more detail, for the ideal system where the embedded eigenvalues exist, the BICs are the resonant states localized to the nanoresonators and decoupled from the far field. When the system is slightly perturbed, the embedded eigenvalue will be shifted into the lower complex half plane with a small imaginary part, and the bound states become leaky and will interact with the broad background radiation, which gives rise to the sharp transmission peaks and dips. This mechanism has been utilized in many nanophotonic materials, e.g., the metallic slab with arrays of subwavelength holes [42, 90], the plasmonic metasurface [62], and the arrays of dielectric spheres and rods [17, 19, 75].

The existence of embedded eigenvalues (equivalently, BICs) for the EM grating of periodic conductors was first rigorously proved by Bonnet-Bendhia and Starling [14] under some symmetry assumptions. Their arguments are based on a variational formulation of the problem with some ideas borrowed from the earlier work by Nédélec and Starling [66]. Later, Shipman and Volkov [71] characterized the robust and nonrobust bound states for the homogeneous periodic slabs and gave sufficient conditions for the nonexistence of guided modes. Moreover, in [70, 72–74], Shipman et al. considered the asymptotics of the embedded eigenvalues with respect to the perturbation of the Bloch wave vector (which breaks the symmetry of the grating), and analyzed the Fano-type transmission anomalies by the analytic perturbation theory. Recently, Lin et al. [60] quantitatively investigated the Fano resonance phenomenon and the field enhancement in the setting of a metallic grating with subwavelength slits by using layer potential techniques. In their subsequent work [61], they focused on the case of the perfectly conducting grating with strongly coupled slits and analyzed the BICs and the corresponding Fano resonances. A similar configuration for the bubble meta-screen was discussed in [3], where Ammari et al. used the capacitance matrix to explicitly approximate the scattering matrix and justify the Fano-type anomalies. In all of these works [3, 60, 61], the authors showed that there exist two classes of subwavelength resonances, where one of them has a much smaller imaginary part than the other one. The discrete resonant state corresponds to the resonance with the larger imaginary part and gives a broad resonance peak, while the continuum state with the smaller imaginary part is perturbed from the bound state and has a narrow resonance peak. It is exactly the hybridization of these two states that gives rise to a Fano transmission phenomenon. However, the rigorous analysis for the full Maxwell system has not been well developed yet. We are aiming to fill this gap.

In this work, we will establish a unified mathematical framework for the EM resonant scattering by asymmetric dielectric metasurfaces of nanoparticles with high refractive indices. For such structures, the BICs and the Fano resonances have been experimentally reported in [49]. Our analysis is based on both the variational method and the Lippmann-Schwinger equation for the full Maxwell’s equations. As in the case of the single dielectric nanoparticles [9], the dielectric resonances are defined as the complex poles of the scattering resolvent of the Maxwell operator, which are located in the lower complex plane $\{\omega \in \mathbb{C}; \Im \omega \leq 0\}$. We shall be particularly interested in the real subwavelength dielectric resonances, and, for convenience, we will use the words *real resonances* and *eigenvalues* interchangeably in what follows, if there is no confusion. In Section 2, we start with the notion of the subwavelength scattering resonances in the periodic setting. We prove that the real resonances are the simple poles of the resolvent of the volume integral operator for the EM scattering problem, and that the associated resonant mode exponentially decays in the far field and is decoupled from the incoming wave; see Propositions 2.5 and 2.6. Hence, we can relate the real scattering resonances to the eigenvalue problem of the unbounded Maxwell operator on the L^2 -space. We proceed to characterize the essential spectrum of the periodic Maxwell operator, which turns out to be the continuous radiation spectrum, and show that there is always a discrete eigenvalue below the infimum of the essential spectrum; see Theorem 2.8. However, the resonant states for the eigenvalue below the essential spectrum do not interact with the background radiation, and thus would not induce any Fano-type resonance phenomenon.

As discussed above, the desired bound states in the continuum correspond to the real scattering resonances embedded in the continuous essential spectrum, the existence of which is a difficult task and usually depends on the additional structure of the configuration, e.g., the symmetry assumption. In this work, we mainly focus on the in-plane inversion symmetry (3.1) motivated by the physical setup [49, 58]. In Section 2.2, we discuss the general symmetry properties of the dielectric metasurfaces by using the representation theory of the symmetry group and its consequences on the resonances and the resonant modes. With these preparations, in Section 3, we manage to show the existence of the real subwavelength resonances which are embedded in the continuous spectrum in the high contrast regime (i.e., the refractive indices of the nanoparticles are large enough), under the normal incidence and a mild assumption on the limiting problem; see Theorem 3.8. In doing so, we adopt the regularized variational formulation for the EM scattering problem [12, 13] and follow the analysis framework of [14, 70] for the acoustic case. It is worth emphasizing that our arguments are much more involved with the main difficulty coming from the infinite-dimensional kernel of the curl

operator. In addition, to justify that the real resonance is in the subwavelength regime for the large contrast, it is necessary to investigate the limiting eigenvalue problem, for which we exploit the techniques from [37, 77] on the convergence of the monotone sesquilinear form.

It is known that the bound states associated with such embedded eigenvalues are unstable with respect to the perturbation of the metasurface that destroys the symmetry (3.1). In Section 4, we slightly perturb the normal incidence and the symmetric dielectric metasurface by a deformation field as in [49, 58]. In this case, the BICs become the quasi-modes with finite Q-factors. We shall show that for the perturbed asymmetric metasurface, the reflection energy could present a sharp asymmetric shape of Fano-type. For this, we first derive the asymptotic expansions of the subwavelength resonances with respect to the high contrast in Theorem 4.2. Then, we calculate the shape derivative of the leading-order approximation of the subwavelength resonance; see Proposition 4.4. This allows us to find the asymptotics of the resonances for the perturbed metasurface in Corollary 4.5, where we assume that the eigenspace of the leading-order operator is spanned by a symmetric field and an antisymmetric one for simplicity. To quantify the expected Fano resonance phenomenon, we calculate the quasi-static approximation of the scattered polarization vectors that uniformly holds for the incident frequencies near the resonances, which readily implies the asymptotic expansion of the reflection and transmission energy; see Corollary 4.7. Thanks to the energy conservation property, we only focus on the reflection energy and demonstrate that it can be effectively described by the classical Fano formula [49, 70], meaning that there is a sharp asymmetric line shape in the reflection spectrum.

We close the introduction with a list of notations used in this work.

- We write (x', x_3) for $x = (x_1, x_2, x_3) \in \mathbb{R}^3$ with $x' = (x_1, x_2) \in \mathbb{R}^2$ and $x_3 \in \mathbb{R}$.
- We use the standard asymptotic notations: for f in a normed vector space, we denote $f = O(\epsilon)$ if $\|f\| \leq C|\epsilon|$ holds for constant $C > 0$ independent of ϵ , and $f = o(\epsilon)$ if $\|f\|/|\epsilon| \rightarrow 0$ as $\epsilon \rightarrow 0$. Moreover, for real $a, b > 0$, we write $a \ll b$ if $a \leq Cb$ for small enough C independent of a, b , and $a \gg b$ if $a \geq Cb$ for large enough C independent of a, b .
- Let Λ be a two-dimensional lattice generated by the vectors $v_1, v_2 \in \mathbb{R}^2$:

$$\Lambda := \{\gamma \in \mathbb{R}^2; \gamma = n_1 v_1 + n_2 v_2, n_i \in \mathbb{Z}\},$$

with the fundamental cell Y :

$$Y := \{\gamma \in \mathbb{R}^2; \gamma = c_1 v_1 + c_2 v_2, c_i \in [-1/2, 1/2]\}.$$

For simplicity, the area of Y is assumed to be one, i.e., $|Y| = 1$. We also define some fundamental cells in \mathbb{R}^3 by

$$Y_\infty := Y \times \mathbb{R}, \quad Y_h := Y \times [-h, h], \quad \text{for } h > 0,$$

for later use. Moreover, we introduce the reciprocal lattice Λ^* by

$$\Lambda^* := \{q \in \mathbb{R}^2; q \cdot \gamma \in 2\pi\mathbb{Z} \text{ for any } \gamma \in \Lambda\}, \quad (1.1)$$

and the first Brillouin zone of Λ^* by

$$\mathcal{B} := \{\alpha \in \mathbb{R}^2; |\alpha| \leq |\alpha - q| \quad \forall q \in \Lambda^*\}. \quad (1.2)$$

- A function (or vector field) f on \mathbb{R}^3 is α -quasi-periodic in the variables x_1 and x_2 if there holds

$$f(x + (\gamma, 0)) = e^{i\alpha \cdot \gamma} f(x), \quad \gamma \in \Lambda. \quad (1.3)$$

- We use the standard Sobolev spaces on a three-dimensional domain $D \subset \mathbb{R}^3$ or a two-dimensional surface $\Sigma \subset \mathbb{R}^3$. The bold typeface is used to indicate the spaces of vector fields, e.g., $\mathbf{L}^2(D)$ is the space of L^2 -integrable vector fields on D . We use the subscript *loc* to denote the spaces of locally integrable functions (fields), and the subscript α to denote the Sobolev spaces of α -quasi-periodic functions (fields), for instance,

$$\mathbf{H}_{\alpha, loc}(\text{curl}, Y_\infty) := \{\varphi \in \mathbf{L}_{loc}^2(Y_\infty); \text{curl}\varphi \in \mathbf{L}_{loc}^2(Y_\infty), \varphi \text{ satisfies (1.3)}\}.$$

In the case of $\alpha = 0$, we have the spaces of periodic functions and shall use the subscript p to avoid confusion, e.g., the space $\mathbf{H}_p^1(Y_h)$ consists of periodic H^1 -fields. Moreover, we use the subscript T to denote the tangential vector fields on the surface Σ , e.g., $\mathbf{H}_T^{-1/2}(\text{curl}, \Sigma) := \{\varphi \in \mathbf{H}_T^{-1/2}(\Sigma); \text{curl}_\Sigma \varphi \in H^{-1/2}(\Sigma)\}$, where curl_Σ is the surface curl operator. We refer the readers to [65] for the definition of the surface differential operators. In particular, for the reader's convenience, we recall the space of divergence-free vector fields $\mathbf{H}(\text{div}0, D) = \{\varphi \in \mathbf{L}^2(D); \text{div}\varphi = 0\}$ and its subspace

$$\mathbf{H}_0(\text{div}0, D) = \{\varphi \in \mathbf{H}(\text{div}0, D); \nu \cdot \varphi = 0 \text{ on } \partial D\}.$$

We also need the weighted L^2 -space: for a nonnegative function $\varepsilon \in L^\infty(Y_\infty)$,

$$\mathbf{L}_{\alpha,\varepsilon}^2(Y_\infty) := \{f; f \text{ is a measurable vector field satisfying (1.3) and } \varepsilon|f|^2 \in L^1(Y_\infty)\}.$$

Similarly, we define

$$\mathbf{H}_\alpha(\varepsilon; \text{div}0, Y_\infty) := \{f \in \mathbf{L}_{\alpha,\varepsilon}^2(Y_\infty); \text{div}(\varepsilon f) = 0\}. \quad (1.4)$$

The tangential component trace for a $H(\text{curl})$ -vector field is defined by

$$\pi_t(u) := (\nu \times u) \times \nu. \quad (1.5)$$

- For two Banach spaces X and Y , we denote by $\mathcal{L}(X, Y)$ the bounded linear operators from X to Y , or simply by $\mathcal{L}(X)$ if $Y = X$. We write $\|\cdot\|_X$ for the norm on the space X , or simply, write $\|\cdot\|$, when no confusion is caused. In particular, for notation simplicity, we denote by $(\cdot, \cdot)_D$ the L^2 -inner product on D , and by $(\cdot, \cdot)_{\varepsilon, D}$ the weighted L^2 -inner product on D , i.e., $(f, g)_{\varepsilon, D} = \int_D \varepsilon \bar{f} g \, dx$, while the standard complex dual pairing on the surface Σ is denoted by $\langle \cdot, \cdot \rangle_\Sigma$.

2 Scattering resonances of all-dielectric metasurfaces

In this section, we consider the resonant electromagnetic (EM) scattering by periodically distributed dielectric nanoparticles with high refractive indices. We will first define the scattering resonances as the poles of the associated scattering resolvent and introduce the band dispersion functions. Then in Section 2.1, we show that the real resonances are the simple poles of the resolvent and the corresponding resonant modes are exponentially decaying in the far field. We also prove that the real resonances always exist below the light line when the refractive index of the nanoparticle is larger than the background. In Section 2.2, we will provide some general results on the symmetry properties of the band function and the multiplicity of the scattering resonance based on the symmetry group of the metasurface.

We begin with the formulation of the periodic electromagnetic scattering problem. Suppose that the nanoparticles D are contained inside Y_h for some $h > 0$, where D is a bounded open set with the smooth boundary ∂D and a characteristic size of order one. The all-dielectric metasurface is defined as the collection of nanoparticles that are periodically distributed on the lattice Λ , which is denoted by

$$\mathcal{D} := \bigcup_{\gamma \in \Lambda} (D + (\gamma, 0)). \quad (2.1)$$

Moreover, we assume that the nanoparticles are non-magnetic (i.e., the magnetic permeability $\mu = 1$ on \mathbb{R}^3) and have the electric permittivity of the form:

$$\varepsilon := 1 + \tau \chi_{\mathcal{D}}, \quad \tau \gg 1, \quad \text{on } \mathbb{R}^3, \quad (2.2)$$

where $\chi_{\mathcal{D}}$ is the characteristic function of the set \mathcal{D} , and $\tau \in \mathbb{R}$ is the contrast parameter. Let (E^i, H^i) be the incident EM field satisfying the homogeneous Maxwell's equations. It follows from the standard Floquet-Bloch theory [47, 51, 53] that the EM scattering problem by the lattice of the nanoresonators \mathcal{D} can be modelled by the following family of α -quasi-periodic scattering problems:

$$\begin{cases} \nabla \times E = i\omega H & \text{in } \mathbb{R}^3 \setminus \partial \mathcal{D}, \\ \nabla \times H = -i\omega \varepsilon E & \text{in } \mathbb{R}^3 \setminus \partial \mathcal{D}, \\ [\nu \times E] = [\nu \times H] = 0 & \text{on } \partial \mathcal{D}, \\ (E - E^i, H - H^i) & \text{satisfies the outgoing radiation condition as } x_3 \rightarrow \pm\infty. \end{cases} \quad (2.3)$$

We are interested in the α -quasi-periodic solutions (E, H) to (2.3). The outgoing radiation condition in (2.3) is given by the Rayleigh-Bloch expansion [14, 47]:

$$E(x', x_3) = \begin{cases} \sum_{q \in \Lambda^*} E_q(h, \alpha) e^{i(\alpha+q) \cdot x'} e^{i\beta_q(x_3-h)}, & \text{for } x_3 > h, \\ \sum_{q \in \Lambda^*} E_q(-h, \alpha) e^{i(\alpha+q) \cdot x'} e^{-i\beta_q(x_3+h)}, & \text{for } x_3 < -h, \end{cases} \quad (2.4)$$

where for $q \in \Lambda^*$,

$$\beta_q := \sqrt{\omega^2 - |\alpha + q|^2}, \quad (2.5)$$

and $E_q(\pm h, \alpha)$ is the Fourier coefficient of $e^{-i\alpha \cdot x'} E$ on $x_3 = \pm h$:

$$E_q(\pm h, \alpha) := \frac{1}{(2\pi)^2} \int_Y e^{-i\alpha \cdot x'} E(x', \pm h) e^{-iq \cdot x'} dx'. \quad (2.6)$$

Here and in what follows, the square root $\sqrt{\cdot}$ is chosen with the positive real part or with the positive imaginary part, and we always assume that for a fixed $\alpha \in \mathcal{B}$, there holds

$$\omega^2 \notin Z(\alpha) := \{|\alpha + q|^2; q \in \Lambda^*\},$$

which guarantees that $\beta_q \neq 0$ is well defined.

For our analysis of the scattering problem (2.3), let us first introduce the quasi-periodic Green's function by

$$G^{\alpha, \omega}(\mathbf{x}) = \frac{1}{2} \sum_{q \in \Lambda^*} i\beta_q^{-1} e^{i(\alpha+q) \cdot x'} e^{i\beta_q |x_3|}, \quad (2.7)$$

which is the fundamental solution to the equation:

$$-(\Delta + \omega^2)G^{\alpha, \omega}(x) = \sum_{\gamma \in \Lambda} \delta(x - (\gamma, 0))e^{i\gamma \cdot \alpha}, \quad (2.8)$$

satisfying the outgoing condition (2.4). Then, we define the vector potentials:

$$\mathcal{K}_D^{\alpha, \omega}[\varphi] = \int_D G^{\alpha, \omega}(x, y)\varphi(y) dy : \mathbf{L}^2(D) \rightarrow \mathbf{H}_{\alpha, loc}^2(Y_\infty), \quad (2.9)$$

and

$$\mathcal{T}_D^{\alpha, \omega}[\varphi] = (\omega^2 + \nabla \operatorname{div})\mathcal{K}_D^{\alpha, \omega}[\varphi] : \mathbf{L}^2(D) \rightarrow \mathbf{H}_{\alpha, loc}(\operatorname{curl}, Y_\infty). \quad (2.10)$$

By definition, it is easy to check that $\mathcal{T}_D^{\alpha, \omega}[\varphi]$ is α -quasi-periodic and satisfies the equation:

$$(\nabla \times \nabla \times - \omega^2)\mathcal{T}_D^{\alpha, \omega}[\varphi] = \omega^2 \varphi \chi_D \quad \text{on } \mathbb{R}^3, \quad (2.11)$$

and the Rayleigh-Bloch expansion (2.4). Then the Lippmann-Schwinger equation for (2.3) readily follows:

$$E^s := E - E^i = \tau \mathcal{T}_D^{\alpha, \omega}[E] \quad \text{on } \mathbb{R}^3. \quad (2.12)$$

We recall the Helmholtz decomposition for L^2 -vector fields [10, 33]:

$$\mathbf{L}^2(D) = \nabla H_0^1(D) \oplus \mathbf{H}(\operatorname{div}0, D) = \nabla H_0^1(D) \oplus \mathbf{H}_0(\operatorname{div}0, D) \oplus W, \quad (2.13)$$

where W is the space of the gradients of harmonic H^1 -functions. It is known [9, 24, 25] that for $\alpha, \omega \in \mathbb{C}$ with $\omega^2 \notin Z(\alpha)$, $\nabla H_0^1(D)$ and $\mathbf{H}(\operatorname{div}0, D)$ are invariant subspaces of $\mathcal{T}_D^{\alpha, \omega}$ with $\mathcal{T}_D^{\alpha, \omega}[\nabla \phi] = -\nabla[\phi \chi_D]$ for $\phi \in H_0^1(D)$. Moreover, the spectrum $\sigma(\mathcal{T}_D^{\alpha, \omega})$ is a disjoint union of the essential spectrum $\sigma_{ess}(\mathcal{T}_D^{\alpha, \omega}) = \{-1, 0, -\frac{1}{2}\}$ and the discrete spectrum $\sigma_{disc}(\mathcal{T}_D^{\alpha, \omega})$. We then define

$$\mathcal{A}_\tau(\alpha, \omega) := \tau^{-1} - \mathcal{T}_D^{\alpha, \omega} : \mathbf{H}(\operatorname{div}0, D) \rightarrow \mathbf{H}(\operatorname{div}0, D), \quad (2.14)$$

which is an operator-valued analytic function on the set $\{(\tau, \alpha, \omega) \in \mathbb{C}^3; |\tau| \gg 1, \omega^2 \notin Z(\alpha)\}$. By the multidimensional analytic Fredholm theorem [52, 81, 83], we have the following basic lemma.

Lemma 2.1. *The set of poles of the resolvent $(\mathcal{A}_\tau(\alpha, \omega))^{-1}$:*

$$\Omega(\mathcal{A}_\tau(\alpha, \omega)) := \{(\tau, \alpha, \omega) \in \mathbb{C}^3; |\tau| \gg 1, \omega^2 \notin Z(\alpha), \mathcal{A}_\tau(\alpha, \omega) \text{ is not invertible}\}, \quad (2.15)$$

is either empty, or an analytic subset of \mathbb{C}^3 of codimension 1 (that is, it is locally given by the zeros of an analytic function in the variables τ, α , and ω).

It is straightforward to follow [9, Section 2] to introduce the scattering resolvent for the problem (2.3) and show that its poles are the same as those of $\mathcal{A}_\tau(\alpha, \cdot)^{-1}$, which we call the *scattering resonances* of the dielectric metasurface. Then by Lemma 2.1, it is easy to see that the slice of the set $\Omega(\mathcal{A}_\tau(\alpha, \omega))$ at (α, τ) , denoted by $\Omega(\mathcal{A}_\tau(\alpha, \omega))|_{(\alpha, \tau)}$, gives the discrete set of resonant frequencies ω_j for the problem (2.3):

$$\{\omega_j(\alpha, \tau)\}_j = \Omega(\mathcal{A}_\tau(\alpha, \omega))|_{(\alpha, \tau)}.$$

For each j , the resonance $\omega_j(\alpha, \tau)$, as a function in $\alpha \in \mathcal{B}$, is Lipschitz continuous and known as the band dispersion function [53]. In this work, we are mainly interested in the resonances in the subwavelength regime, i.e., those $\omega_j \ll 1$. In analogy with the analysis in [9, Section 3], we have the following asymptotic result for the subwavelength band function $\omega_j(\alpha, \tau)$. Let \mathbb{P}_d and \mathbb{P}_w be the orthogonal projections for the decomposition (2.13):

$$\mathbb{P}_d : \mathbf{L}^2(D) \rightarrow \mathbf{H}_0(\operatorname{div}0, D), \quad \mathbb{P}_w : \mathbf{L}^2(D) \rightarrow W. \quad (2.16)$$

Theorem 2.2. *In the high contrast regime (2.2), the subwavelength resonances for the scattering problem (2.3) exist with the asymptotic form: as $\tau \rightarrow \infty$,*

$$\omega_j(\alpha, \tau) = \frac{1}{\sqrt{\tau \lambda_j^\alpha}} + O(\tau^{-1}),$$

where the remainder term is complex, and $\{\lambda_j^\alpha\}$ are the eigenvalues of the compact self-adjoint operator $\mathbb{P}_d \mathcal{K}_D^{\alpha,0} \mathbb{P}_d$.

2.1 Real resonances and Bound states

It is clear that for a fixed $\alpha \in \mathcal{B}$, at each resonance $\omega_j(\alpha, \tau)$, there are nonzero solutions (E, H) to (2.3) with $(E^i, H^i) = 0$, which are called *Bloch modes*. We will first prove in Proposition 2.5 that when the resonant frequency is real, the associated Bloch modes exponentially decay and hence do not couple to the far field. It follows that in this case, the resonant modes are bounded with respect to the L^2 -norm and usually referred to as the *bound states*. The argument is standard and based on the variational method.

We start with the definition of the EM Dirichlet to Neumann (DtN) operators \mathcal{T} . We introduce the notations:

$$\Sigma_{\pm h} := Y \times \{\pm h\} = \{x \in \mathbb{R}^3; x' \in Y, x_3 = \pm h\}, \quad \text{for } h > 0.$$

and

$$\Sigma = \Sigma_h \cup \Sigma_{-h}.$$

Definition 2.3. Let $\varphi \in H_{\alpha, T}^{-1/2}(\text{curl}, \Sigma_{\pm h})$ be an α -quasi-periodic tangent field on $\Sigma_{\pm h}$ with the Fourier expansion:

$$\varphi(x', \pm h) := \sum_{q \in \Lambda^*} (\varphi_q, 0) e^{i(\alpha+q) \cdot x'}, \quad \varphi_q := (\varphi_{1,q}, \varphi_{2,q}) \in \mathbb{R}^2.$$

The DtN operator $\mathcal{T} : H_{\alpha, T}^{-1/2}(\text{curl}, \Sigma_{\pm h}) \rightarrow H_{\alpha, T}^{-1/2}(\text{div}, \Sigma_{\pm h})$ is defined by

$$\mathcal{T}\varphi = \sum_{q \in \Lambda^*} ((\mathcal{T}\varphi)_q, 0) e^{i(\alpha+q) \cdot x'}, \quad (2.17)$$

where the coefficients $(\mathcal{T}\varphi)_q \in \mathbb{R}^2$, $q \in \Lambda^*$, are given by

$$(\mathcal{T}\varphi)_q := \frac{1}{\omega \beta_q} \{ \beta_q^2 \varphi_q + ((\alpha + q) \cdot \varphi_q)(\alpha + q) \}.$$

With the help of the operator \mathcal{T} , one can readily obtain the variational formulation for the resonance problem: find $(\omega, E) \in \mathbb{C} \times \mathbf{H}_\alpha(\text{curl}, Y_h)$ with $\omega^2 \notin Z(\alpha)$ such that

$$B_{\alpha, \tau, \omega}(\varphi, E) := (\text{curl} \varphi, \text{curl} E)_{Y_h} - \omega^2 (\varphi, \varepsilon E)_{Y_h} - i\omega \langle \pi_t(\varphi), \mathcal{T} \pi_t(E) \rangle_\Sigma = 0, \quad \forall \varphi \in \mathbf{H}_\alpha(\text{curl}, Y_h), \quad (2.18)$$

where $\langle \cdot, \cdot \rangle_\Sigma = \langle \cdot, \cdot \rangle_{\Sigma_h} + \langle \cdot, \cdot \rangle_{\Sigma_{-h}}$ and the trace $\pi_t(\cdot)$ is given in (1.5). We note from Definition 2.3 that

$$\langle \varphi, \mathcal{T}\psi \rangle_{\Sigma_{\pm h}} = \sum_{q \in \Lambda^*} \frac{1}{\omega \beta_q} \{ \beta_q^2 \psi_q \cdot \overline{\varphi_q} + ((\alpha + q) \cdot \psi_q)(\alpha + q) \cdot \overline{\varphi_q} \}, \quad \forall \psi, \varphi \in H_{\alpha, T}^{-1/2}(\text{curl}, \Sigma_{\pm h}), \quad (2.19)$$

which implies

$$\langle \psi, \mathcal{T}_\pm \psi \rangle_{\Sigma_{\pm h}} = \sum_{q \in \Lambda^*} \frac{1}{\omega \beta_q} \{ \beta_q^2 |\psi_q|^2 + |(\alpha + q) \cdot \psi_q|^2 \}. \quad (2.20)$$

For $\omega \in \mathbb{R}$, we introduce the following subsets of the reciprocal lattice Λ^* :

$$\Lambda_{\mathcal{P}}^* := \{q \in \Lambda^*; \omega^2 > |\alpha + q|^2\}, \quad \Lambda_{\mathcal{E}}^* := \{q \in \Lambda^*; \omega^2 < |\alpha + q|^2\}, \quad (2.21)$$

and define the associated operators $\mathcal{T}^{\mathcal{P}}$ and $\mathcal{T}^{\mathcal{E}}$ as in (2.17) but with the sum over $\Lambda_{\mathcal{P}}^*$ and $\Lambda_{\mathcal{E}}^*$, respectively. By definition, we have that $\Lambda_{\mathcal{P}}^*$ is a finite set with $\beta_q > 0$ for $q \in \Lambda_{\mathcal{P}}^*$, while for $q \in \Lambda_{\mathcal{E}}^*$, β_q is purely imaginary. Then, recalling the Rayleigh-Bloch expansion, it is clear that $\Lambda_{\mathcal{P}}^*$ corresponds to the indices of propagating modes, and $\Lambda_{\mathcal{E}}^*$ is the indices for the exponentially decaying modes. Note that $\omega = |\alpha + q|$ separates the (ω, α) plane into the regions where the wave has different radiation behaviours as $|x_3| \rightarrow \infty$. For $\alpha \in \mathcal{B}$, by definition (1.2), we have that the minimal $|\alpha + q|$ is given by $|\alpha|$, i.e.,

$$|\alpha| = \inf_{q \in \Lambda^*} |\alpha + q|, \quad (2.22)$$

which is the so-called *light line* [15, 18]. The following lemma is a simple consequence of (2.19) and (2.20).

Lemma 2.4. Let $\omega \neq 0 \in \mathbb{R}$ and $\alpha \in \mathcal{B}$ with $\omega^2 \notin Z(\alpha)$. For $\psi, \varphi \in H_{\alpha, T}^{-1/2}(\text{curl}, \Sigma_{\pm h})$, it holds that

$$\langle \varphi, -i\mathcal{I}^{\mathcal{E}}\psi \rangle_{\Sigma_{\pm h}} = \langle -i\mathcal{I}^{\mathcal{E}}\varphi, \psi \rangle_{\Sigma_{\pm h}}, \quad \langle \mathcal{I}^{\mathcal{P}}\varphi, \psi \rangle_{\Sigma_{\pm h}} = \langle \varphi, \mathcal{I}^{\mathcal{P}}\psi \rangle_{\Sigma_{\pm h}}.$$

Moreover, we have

$$\langle \psi, \mathcal{I}^{\mathcal{P}}\psi \rangle_{\Sigma_{\pm h}} \geq 0.$$

Proposition 2.5. Let ω be a resonant frequency for $\alpha \in \mathcal{B}$ with $\omega^2 \notin Z(\alpha)$, and $E \in \mathbf{H}_{\alpha, \text{loc}}(\text{curl}, Y_{\infty})$ be the associated Bloch mode with the expansion (2.4). Then ω is real if and only if E exponentially decays as $x_3 \rightarrow \infty$. In this case, we have $E \in \mathbf{H}_{\alpha}(\text{curl}, Y_{\infty})$.

Proof. Suppose that (ω, E) solves the variational problem (2.18). It implies

$$\Im B_{\alpha, \tau, \omega}(E, E) = -\Im i\omega \langle \pi_t(E), \mathcal{I}^{\mathcal{P}}\pi_t(E) \rangle_{\Sigma} = -\Re \omega \langle \pi_t(E), \mathcal{I}^{\mathcal{P}}\pi_t(E) \rangle_{\Sigma} = 0.$$

We hence have $\Re \langle \pi_t(E), \mathcal{I}^{\mathcal{P}}\pi_t(E) \rangle_{\Sigma} = \langle \pi_t(E), \mathcal{I}^{\mathcal{P}}\pi_t(E) \rangle_{\Sigma} = 0$ by formulas (2.5) and (2.20) and the definition of $\mathcal{I}^{\mathcal{P}}$. Then it follows from Lemma 2.4 that the coefficients $(\pi_t(E))_q$ for $q \in \Lambda_{\mathcal{P}}^*$ on $\Sigma_{\pm h}$ vanish. Recalling the Rayleigh-Bloch expansion (2.4) and $\text{div}E = 0$ on $Y_{\infty} \setminus Y_h$, we obtain the exponential decay of the resonant mode E when $x_3 \rightarrow \infty$. Conversely, suppose that the Bloch mode E exponentially decays in the far field. Then, we have that for any suitably large h , the restriction of E to Y_h satisfies (2.18) with $\langle \pi_t(E), \mathcal{I}^{\mathcal{P}}\pi_t(E) \rangle_{\Sigma} \rightarrow 0$ as $h \rightarrow \infty$, by formulas (2.6) and (2.20), and the exponential decay of E . Thus, there holds $\langle \text{curl}E, \text{curl}E \rangle_{Y_{\infty}} - \omega^2 \langle E, \varepsilon E \rangle_{Y_{\infty}} = 0$, which readily gives $E \in \mathbf{H}_{\alpha}(\text{curl}, Y_{\infty})$ and $\omega \in \mathbb{R}$. \square

We proceed to prove that the real resonances are the simple poles of the scattering resolvent, which means that for a real resonance, its algebraic multiplicity equals to its geometric multiplicity [29, 34, 35]. For the reader's convenience, let us first recall some preliminaries about the related concepts, following [35]. Suppose that $\mathcal{A}(\lambda)$ is an operator-valued analytic function from a neighbourhood $N_{\varepsilon}(\lambda_0)$ of $\lambda_0 \in \mathbb{C}$ to $\mathcal{L}(\mathcal{H})$, where \mathcal{H} is a Banach space. λ_0 is a pole of $\mathcal{A}(\lambda)^{-1}$ means that there exists an analytic function $\phi(\lambda) : N_{\varepsilon}(\lambda_0) \rightarrow \mathcal{H}$, called a root function for $\mathcal{A}(\lambda)$ at λ_0 , such that $\phi(\lambda_0) \neq 0$ and $\mathcal{A}(\lambda_0)\phi(\lambda_0) = 0$. It is clear that $\phi(\lambda_0)$ is an eigenvector of $\mathcal{A}(\lambda_0)$, and we define the geometric multiplicity of λ_0 by $\dim \ker(\mathcal{A}(\lambda_0))$. By analyticity, we have $\mathcal{A}(\lambda)\phi(\lambda) = (\lambda - \lambda_0)^m \psi(\lambda)$ for some $m > 0$ with $\psi(\lambda_0) \neq 0$ and call the number m the multiplicity of the root function $\phi(\lambda)$. We define the rank of an eigenvector ϕ_0 by $\text{rank}(\phi_0) := \{m(\phi); \phi(\lambda) \text{ is a root function with } \phi(\lambda_0) = \phi_0\}$. Let $\{\phi_0^j\}$ be an orthogonal set of eigenvectors that span $\ker(\mathcal{A}(\lambda_0))$ with the property: $\text{rank}(\phi_0^j)$ is the maximum of the ranks of all ϕ in the orthogonal complement of $\text{span}\{\phi_0^1, \dots, \phi_0^{j-1}\}$ in $\ker(\mathcal{A}(\lambda_0))$. We then define the algebraic multiplicity of λ_0 by $\sum_j \text{rank}(\phi_0^j)$.

Proposition 2.6. For a fixed $\alpha \in \mathcal{B}$, the real resonances are the simple poles of $\mathcal{A}_{\tau}(\alpha, \omega)^{-1}$.

Proof. Let ω_0 be a real resonance, i.e., a real pole of $\mathcal{A}_{\tau}(\alpha, \omega)^{-1}$. By definition, it suffices to prove that for any eigenfunction $E_0 \in \ker(\mathcal{A}_{\tau}(\alpha, \omega_0))$, its rank equals to one. For this, without loss of generality, we assume that E_0 is well defined on Y_{∞} and exponentially decays as $x_3 \rightarrow \infty$, by considering $\mathcal{T}_D^{\alpha, \omega}[E_0]$ and Proposition 2.5. Let $E(\omega)$ be an associated root function with $E_0 = E(\omega_0)$. We write

$$\mathcal{A}_{\tau}(\alpha, \omega)[E(\omega)] = (\omega - \omega_0)\psi(\omega). \quad (2.23)$$

We will show that $\psi(\omega_0) \neq 0$, which gives $\text{rank}(E_0) = 1$ and thus completes the proof of the proposition. Noting that $E_0 \in \mathbf{H}_{\alpha}(\text{curl}, Y_{\infty})$ exponentially decays, by integration by parts, it holds that, for $\omega \in \mathbb{C}$ near ω_0 ,

$$\begin{aligned} 0 &= (\mathcal{T}_D^{\alpha, \omega}[\varphi], \nabla \times \nabla \times E_0 - \omega_0^2 E_0)_{Y_{\infty}} \\ &= (\nabla \times \nabla \times \mathcal{T}_D^{\alpha, \omega}[\varphi], E_0)_{Y_{\infty}} - \omega_0^2 (\mathcal{T}_D^{\alpha, \omega}[\varphi], \varepsilon E_0)_{Y_{\infty}} \\ &= (\omega^2 \mathcal{T}_D^{\alpha, \omega}[\varphi] + \omega^2 \varphi \chi_D, E_0)_{Y_{\infty}} - \omega_0^2 (\mathcal{T}_D^{\alpha, \omega}[\varphi], (1 + \tau \chi_D) E_0)_{Y_{\infty}}, \quad \forall \varphi \in \mathbf{H}(\text{div}0, D), \end{aligned}$$

where the last step follows from (2.11). Then we obtain

$$(\omega^2 \varphi \chi_D, E_0)_{Y_{\infty}} - \tau \omega_0^2 (\mathcal{T}_D^{\alpha, \omega}[\varphi], \chi_D E_0)_{Y_{\infty}} = ((\omega_0^2 - \omega^2) \mathcal{T}_D^{\alpha, \omega}[\varphi], E_0)_{Y_{\infty}}. \quad (2.24)$$

Taking $\varphi = E(\omega)$ in the above formula (2.24) and using (2.23) gives

$$((\omega^2 - \omega_0^2)E(\omega), E_0)_D + \tau \omega_0^2 ((\omega - \omega_0)\psi(\omega), E_0)_D = ((\omega_0^2 - \omega^2) \mathcal{T}_D^{\alpha, \omega}[E(\omega)], E_0)_{Y_{\infty}},$$

which further implies, by eliminating the factor $\omega - \omega_0$ and letting $\omega = \omega_0$,

$$\begin{aligned} 2\omega_0 (E(\omega_0), E_0)_D + \tau \omega_0^2 (\psi(\omega_0), E_0)_D &= -2\omega_0 (\mathcal{T}_D^{\alpha, \omega_0}[E(\omega_0)], E_0)_{Y_{\infty}} \\ &= -2\tau^{-1} \omega_0 (E(\omega_0), E_0)_{Y_{\infty}}. \end{aligned} \quad (2.25)$$

If $\psi(\omega_0) = 0$, we obtain from (2.25) that $\tau \|E_0\|_D^2 = -\|E_0\|_{Y_{\infty}}^2$. It follows that $E_0 = 0$, which is a contradiction. Hence, $\psi(\omega_0) \neq 0$ and the proof is complete. \square

An immediate and important following-up question is the existence of real resonances, which would be the main focus of the remaining section and Section 3. Next, we will prove that there always exist real resonances below the light line $|\alpha|$, by extending Theorem 4.1 and Theorem 4.4 of [14] for the scalar case. For this purpose, we define the Maxwell operator by $\mathcal{M}_\varepsilon(\alpha) := \varepsilon^{-1}(\nabla \times)^2$ with the domain $\text{dom}(\mathcal{M}_\varepsilon(\alpha))$ given by the space $\mathbf{C}_{c,\alpha}^\infty(Y_\infty)$ of quasi-periodic smooth fields with compact support, which is a densely defined positive unbounded operator on $\mathbf{L}_{\alpha,\varepsilon}^2(Y_\infty)$. We claim that by Friedrichs extension [76], the operator \mathcal{M}_ε admits a self-adjoint extension. Indeed, we consider the following sesquilinear unbounded form on $\mathbf{L}_{\alpha,\varepsilon}^2(Y_\infty)$:

$$\begin{aligned} a_{\alpha,\varepsilon}(\varphi, E) &:= (\varphi, \mathcal{M}_\varepsilon(\alpha)E)_{\varepsilon, Y_\infty} + (\varphi, E)_{\varepsilon, Y_\infty} \\ &= (\nabla \times \varphi, \nabla \times E)_{Y_\infty} + (\varphi, \varepsilon E)_{Y_\infty}, \quad \forall E, \varphi \in \mathbf{C}_{c,\alpha}^\infty(Y_\infty). \end{aligned}$$

Clearly, $a_{\alpha,\varepsilon}(\cdot, \cdot)$ also defines an inner product on $\text{dom}(\mathcal{M}_\varepsilon(\alpha))$. It then follows that the completed space $\overline{\text{dom}(\mathcal{M}_\varepsilon(\alpha))}^{a_{\alpha,\varepsilon}}$ is nothing else than $\mathbf{H}_\alpha(\text{curl}, Y_\infty)$, and hence $a_{\alpha,\varepsilon}(\cdot, \cdot)$ is $\mathbf{H}_\alpha(\text{curl}, Y_\infty)$ -elliptic. Then, by Riesz representation, we define the operator $\mathcal{N}_{\alpha,\varepsilon} : \text{dom}(\mathcal{N}_{\alpha,\varepsilon}) \rightarrow \mathbf{L}_{\alpha,\varepsilon}^2(Y_\infty)$ satisfying that for $E \in \text{dom}(\mathcal{N}_{\alpha,\varepsilon})$ and $\varphi \in \mathbf{H}_\alpha(\text{curl}, Y_\infty)$,

$$a_{\alpha,\varepsilon}(\varphi, E) = (\varphi, \mathcal{N}_{\alpha,\varepsilon}(E))_{Y_\infty}, \quad (2.26)$$

where the domain of $\mathcal{N}_{\alpha,\varepsilon}$ is given by

$$\text{dom}(\mathcal{N}_{\alpha,\varepsilon}) := \{E \in \mathbf{H}_\alpha(\text{curl}, Y_\infty); \varphi \rightarrow a_{\alpha,\varepsilon}(\varphi, E) \text{ is continuous on } \mathbf{H}_\alpha(\text{curl}, Y_\infty) \text{ w.r.t. } \mathbf{L}_\alpha^2\text{-topology}\}.$$

Note that $(\nabla \times \varphi, \nabla \times E)_{Y_\infty}$ is continuous in $\varphi \in \mathbf{H}_\alpha(\text{curl}, Y_\infty)$ w.r.t. \mathbf{L}_α^2 -topology if and only if there exists $\psi \in \mathbf{L}_\alpha^2(Y_\infty)$ such that $(\nabla \times \varphi, \nabla \times E)_{Y_\infty} = (\varphi, \psi)_{Y_\infty}$. We hence have

$$\text{dom}(\mathcal{N}_{\alpha,\varepsilon}) = \{E \in \mathbf{L}_\alpha^2(Y_\infty); \text{curl } E \in \mathbf{L}_\alpha^2(Y_\infty), \text{curlcurl } E \in \mathbf{L}_\alpha^2(Y_\infty)\}, \quad (2.27)$$

and the Friedrichs extension allows us to conclude the following lemma.

Lemma 2.7. *The operator $\mathcal{N}_{\alpha,\varepsilon} : \text{dom}(\mathcal{N}_{\alpha,\varepsilon}) \rightarrow \mathbf{L}_{\alpha,\varepsilon}^2(Y_\infty)$ defined in (2.26) is bijective, positive, and self-adjoint on $\mathbf{L}_{\alpha,\varepsilon}^2(Y_\infty)$ with $\mathcal{N}_{\alpha,\varepsilon}^{-1} \in \mathcal{L}(\mathbf{L}_{\alpha,\varepsilon}^2(Y_\infty))$. In particular, the positive operator $\mathcal{N}_{\alpha,\varepsilon} - 1$ is the self-adjoint extension of the Maxwell operator $\mathcal{M}_\varepsilon(\alpha)$.*

Recalling Proposition 2.5 above, it is easy to see that $\omega \neq 0$ is a real resonance if and only if ω^2 is an eigenvalue of $\mathcal{M}_\varepsilon(\alpha)$ with eigenfunctions in $\mathbf{H}_\alpha(\varepsilon; \text{div}0, Y_\infty)$ (cf. (1.4)). Therefore, for the existence of real resonances, it suffices to investigate the spectral properties of the self-adjoint operator $\mathcal{M}_\varepsilon(\alpha)$ on $\mathbf{H}_\alpha(\varepsilon; \text{div}0, Y_\infty)$:

$$\mathcal{M}_\varepsilon(\alpha) : \text{dom}(\mathcal{M}_\varepsilon(\alpha)) \rightarrow \mathbf{H}_\alpha(\varepsilon; \text{div}0, Y_\infty), \quad \text{with } \text{dom}(\mathcal{M}_\varepsilon(\alpha)) := \text{dom}(\mathcal{N}_{\alpha,\varepsilon}) \cap \mathbf{H}_\alpha(\varepsilon; \text{div}0, Y_\infty). \quad (2.28)$$

We define

$$\begin{aligned} \mu_n(\tau) &:= \sup_{\{\varphi_i\}_{i=1}^{n-1} \subset \text{dom}(\mathcal{M}_\varepsilon(\alpha))} \inf_{\substack{\varphi \in \text{dom}(\mathcal{M}_\varepsilon(\alpha)) \\ \|\varphi\|_{\varepsilon, Y_\infty} = 1, \varphi \perp \varphi_i}} (\varphi, \mathcal{M}_\varepsilon(\alpha)\varphi)_{\varepsilon, Y_\infty} \\ &= \sup_{\varphi_i} \inf_{\varphi} \left\{ \frac{(\nabla \times \varphi, \nabla \times \varphi)_{Y_\infty}}{((1 + \tau\chi_D)\varphi, \varphi)_{Y_\infty}}; \varphi, \varphi_i \in \text{dom}(\mathcal{M}_\varepsilon(\alpha)), \varphi \perp \varphi_i, 1 \leq i \leq n-1 \right\}, \end{aligned} \quad (2.29)$$

which is a decreasing function in $\tau > 0$. By the min-max principle for self-adjoint operators [78, Theorem XIII.1], we have that for each n , either $\mu_n = \inf\{\lambda; \lambda \in \sigma_{\text{ess}}(\mathcal{M}_\varepsilon(\alpha))\}$ and in this case $\mu_m = \mu_n$ for any $m \geq n$, or μ_n is the n th eigenvalue of $\mathcal{M}_\varepsilon(\alpha)$ counting multiplicity with $\mu_n < \inf\{\lambda; \lambda \in \sigma_{\text{ess}}(\mathcal{M}_\varepsilon(\alpha))\}$.

In Theorem 2.8 below, we characterize the essential spectrum of the Maxwell operator $\sigma_{\text{ess}}(\mathcal{M}_\varepsilon(\alpha))$ and show the existence of discrete eigenvalues of $\mathcal{M}_\varepsilon(\alpha)$ below $|\alpha|^2$, equivalently, the real resonances exist below the light line $|\alpha|$. For ease of exposition, we recall the Weyl's criterion for the essential spectrum [41, Theorem 7.2]: $\lambda \in \sigma_{\text{ess}}(\mathcal{M}_\varepsilon(\alpha))$ if and only if there exists a so-called *Weyl sequence* $\varphi_k \in \text{dom}(\mathcal{M}_\varepsilon(\alpha))$ associated with λ in the sense that $\|\varphi_k\|_{\varepsilon, Y_\infty} = 1$, $\varphi_k \rightarrow 0$ weakly and $\|(\mathcal{M}_\varepsilon(\alpha) - \lambda)\varphi_k\|_{\varepsilon, Y_\infty} \rightarrow 0$, when $k \rightarrow \infty$.

Theorem 2.8. *Let $\mathcal{M}_\varepsilon(\alpha)$, $\alpha \in \mathcal{B}$, be the self-adjoint positive operator defined in (2.28). Then it holds that*

1. $\sigma_{\text{ess}}(\mathcal{M}_\varepsilon(\alpha)) = [|\alpha|^2, +\infty)$.
2. *There exists a discrete eigenvalue of $\mathcal{M}_\varepsilon(\alpha)$ below $|\alpha|^2$ for any $\tau > 0$, i.e., $\mu_1(\tau) < |\alpha|^2$.*

Proof. For our first statement, let $\lambda \geq |\alpha|^2$ and ψ be a C^∞ -compactly supported function on Y_∞ satisfying $\psi(x_3) = 0$ for $|x_3| \leq h$ and $\int_{\mathbb{R}} \psi(x_3)^2 dx_3 = 1$, where h is suitably large such that D is included in Y_h . We consider the following sequence of vector fields:

$$\tilde{E}_n = \frac{1}{\sqrt{n}} \psi\left(\frac{x_3}{n}\right) p e^{id \cdot x} \quad \text{with } p, d = (\alpha, \sqrt{\lambda - |\alpha|^2}) \in \mathbb{R}^3, \quad |p| = 1 \text{ and } p \cdot d = 0.$$

It is easy to see that $\|\tilde{E}_n\|_{Y_\infty} = 1$ and \tilde{E}_n weakly converge to zero in $\mathbf{L}_{\alpha, \varepsilon}^2(Y_\infty)$. Moreover, by a direct computation and vector calculus identities, we find

$$\begin{aligned} (\mathcal{M}_\varepsilon - \lambda)[\tilde{E}_n] &= \nabla(\operatorname{div} \tilde{E}_n) - \Delta \tilde{E}_n - \lambda \tilde{E}_n \\ &= \nabla\left(\frac{1}{n\sqrt{n}} \psi'\left(\frac{x_3}{n}\right) p_3 e^{id \cdot x}\right) - \frac{1}{\sqrt{n}} p \left(\frac{1}{n^2} \psi''\left(\frac{x_3}{n}\right) e^{id \cdot x} + 2 \frac{id_3}{n} \psi'\left(\frac{x_3}{n}\right) e^{id \cdot x}\right), \end{aligned}$$

which tends to zero as $n \rightarrow \infty$. To obtain a Weyl sequence, we add to \tilde{E}_n a corrective gradient field $\nabla p_n \in \mathbf{L}_\alpha^2(Y_\infty)$ such that $\operatorname{div}(\tilde{E}_n + \varepsilon \nabla p_n) = 0$, which is equivalent to solving the elliptic equation $-\operatorname{div}(\varepsilon \nabla p_n) = \operatorname{div} \tilde{E}_n$. By Lemma A.1, it is uniquely solvable in the weighted Sobolev space $H_\alpha^{1,-1}(Y_\infty)/\mathbb{R}$ and there holds

$$\|\nabla p_n\|_{Y_\infty} \lesssim \|\operatorname{div} \tilde{E}_n\|_{Y_\infty} = \frac{|p_3|}{n} \left(\int_{\mathbb{R}} |\psi'|^2 dx\right)^{1/2} \rightarrow 0, \quad \text{as } n \rightarrow \infty.$$

We then define $E_n := (\tilde{E}_n + \nabla p_n) / \|\tilde{E}_n + \nabla p_n\|_{Y_\infty}$. It is straightforward to check that $\{E_n\} \subset \operatorname{dom}(\mathcal{M}_\varepsilon(\alpha))$ is a Weyl sequence for λ , which implies $[|\alpha|^2, +\infty) \subset \sigma_{ess}(\mathcal{M}_\varepsilon(\alpha))$.

To show the reverse direction, we will prove the following two claims:

$$\sigma_{ess}(\mathcal{M}) \subset [|\alpha|^2, +\infty) \quad \text{and} \quad \sigma_{ess}(\mathcal{M}_\varepsilon) \subset \sigma_{ess}(\mathcal{M}), \quad (2.30)$$

where \mathcal{M} is defined as \mathcal{M}_ε with $\varepsilon = 1$ (i.e., $\tau = 0$). For the first one, suppose that $\{E_n\}$ is a Weyl sequence associated with $\lambda \in \sigma_{ess}(\mathcal{M})$, which readily implies

$$((\mathcal{M} - \lambda)[E_n], E_n)_{Y_\infty} = \|\nabla \times E_n\|_{Y_\infty}^2 - \lambda \rightarrow 0, \quad \text{as } n \rightarrow \infty. \quad (2.31)$$

Note that $\operatorname{div} E_n = 0$ and E_n , as a quasi-periodic function, admits the expansion: $E_n(x) = \sum_{q \in \Lambda^*} E_{n,q}(x_3) e^{i(\alpha+q) \cdot x}$. We can estimate, thanks to (2.22),

$$\int_{Y_\infty} |\nabla \times E_n|^2 + |\operatorname{div} E_n|^2 dx = \int_{Y_\infty} |\nabla E_n|^2 dx \geq |\alpha|^2,$$

which, by (2.31), gives $\lambda \geq |\alpha|^2$.

We next show the second claim. Letting $\lambda \in \sigma_{ess}(\mathcal{M}_\varepsilon)$, it suffices to construct a Weyl sequence associated with λ but for the operator \mathcal{M} . By abuse of notation, suppose that $\{\tilde{E}_n\}$ is a Weyl sequence corresponding to $\lambda \in \sigma_{ess}(\mathcal{M}_\varepsilon)$. We define a smooth cutoff function θ on \mathbb{R} such that $\theta(x_3) = 0$ on $(-h, h)$ and $\theta(x_3) = 1$ on $\mathbb{R} \setminus (-2h, 2h)$. It is clear that the sequence $\theta \tilde{E}_n$ weakly converges to zero in $\mathbf{L}_\alpha^2(Y_\infty)$ and so does $(1 - \theta) \tilde{E}_n$. Noting that $1 - \theta$ is a C^∞ function compactly supported in Y_{2h} , we can check that $(1 - \theta) \tilde{E}_n$ is a bounded sequence in the space:

$$V = \{\psi \in \mathbf{L}_\alpha^2(Y_{2h}); \operatorname{curl} \psi \in \mathbf{L}_\alpha^2(Y_{2h}), \operatorname{div}(\varepsilon \psi) \in \mathbf{L}_\alpha^2(Y_{2h}), \nu \times \psi = 0 \text{ on } \Sigma_{\pm 2h}\},$$

which is compactly embedded into the space $\mathbf{L}_\alpha^2(Y_{2h})$, by the classical result of Weber [86] (see also [36, Appendix B]). As a consequence, we have, by the weak convergence of $(1 - \theta) \tilde{E}_n$,

$$\|(1 - \theta) \tilde{E}_n\|_{\varepsilon, Y_\infty} \rightarrow 0, \quad \text{as } n \rightarrow \infty.$$

It follows from $\|\tilde{E}_n\|_{\varepsilon, Y_\infty} = 1$ that $\|\theta \tilde{E}_n\|_{\varepsilon, Y_\infty} \rightarrow 1$. We next check

$$(\mathcal{M} - \lambda)[\theta \tilde{E}_n] \rightarrow 0, \quad \text{when } n \rightarrow \infty. \quad (2.32)$$

Indeed, $\partial_j \theta$, for $j = 1, 2, 3$, is C^∞ -smooth on \mathbb{R} and compactly supported in the closure of $Y_{2h} \setminus Y_h$. Then, a direct computation gives

$$\begin{aligned} \nabla \times \nabla \times (\theta \tilde{E}_n) &= \nabla \times (\nabla \theta \times \tilde{E}_n + \theta \nabla \times \tilde{E}_n) \\ &= \nabla \theta \operatorname{div} \tilde{E}_n - \tilde{E}_n \Delta \theta + (\tilde{E}_n \cdot \nabla)(\nabla \theta) - (\nabla \theta \cdot \nabla) \tilde{E}_n + \nabla \theta \times (\nabla \times \tilde{E}_n) + \theta \nabla \times \nabla \times \tilde{E}_n. \end{aligned} \quad (2.33)$$

Since \tilde{E}_n is a Weyl sequence for \mathcal{M}_ε , we have $\nabla\theta\operatorname{div}\tilde{E}_n = 0$ and, as $n \rightarrow \infty$,

$$\|\theta\nabla \times \nabla \times \tilde{E}_n - \lambda\theta\tilde{E}_n\|_{Y_\infty} = \|\theta(\mathcal{M}_\varepsilon - \lambda)[\tilde{E}_n]\|_{Y_\infty} \rightarrow 0. \quad (2.34)$$

Moreover, by the standard interior regularity for the Maxwell's equation, we see that \tilde{E}_n is bounded in $\mathbf{H}_\alpha^2(Y_{2h}\setminus Y_h)$. Therefore, it follows that

$$\|-\tilde{E}_n\Delta\theta + (\tilde{E}_n \cdot \nabla)(\nabla\theta) - (\nabla\theta \cdot \nabla)\tilde{E}_n + \nabla\theta \times (\nabla \times \tilde{E}_n)\|_{Y_\infty} \rightarrow 0, \quad \text{as } n \rightarrow \infty, \quad (2.35)$$

thanks to the compact embedding from $\mathbf{H}_\alpha^1(Y_{2h}\setminus Y_h)$ to $\mathbf{L}_\alpha^2(Y_{2h}\setminus Y_h)$. Collecting (2.33)–(2.35) gives (2.32). Again, to obtain the desired Weyl sequence, we need to consider a corrective L^2 -field ∇p_n defined by the equation

$$-\Delta p_n = \operatorname{div}(\theta\tilde{E}_n).$$

We compute $\operatorname{div}(\theta\tilde{E}_n) = \nabla\theta \cdot \tilde{E}_n$ and find $\|\operatorname{div}(\theta\tilde{E}_n)\|_{Y_\infty} \rightarrow 0$, similarly to (2.35), which, by Lemma A.1, also implies $\|\nabla p_n\|_{Y_\infty} \rightarrow 0$. Then, it is easy to see that $\lambda \in \sigma_{\text{ess}}(\mathcal{M})$ and $E_n := (\theta\tilde{E}_n + \nabla p_n)/\|\theta\tilde{E}_n + \nabla p_n\|_{Y_\infty}$ is an associated Weyl sequence. We hence have proved (2.30) and showed $\sigma_{\text{ess}}(\mathcal{M}_\varepsilon(\alpha)) = [|\alpha|^2, +\infty)$.

For the second statement, we consider $\tilde{E} := f(x_3)pe^{i\alpha \cdot x}$ with $p := (\alpha_2, -\alpha_1, 0)$ and

$$f(x_3) := \begin{cases} 1, & \text{if } |x_3| < h, \\ 2 - h^{-1}|x_3|, & \text{if } h < |x_3| < 2h, \\ 0, & \text{if } |x_3| > 2h, \end{cases}$$

where $h > 0$ is large enough so that $D \subset Y_h$. Clearly, there holds $\operatorname{div}\tilde{E} = 0$. We then define $p \in H_\alpha^{1,-1}(Y_\infty)/\mathbb{R}$, for a given ε of the form (2.2), by $\operatorname{div}(\varepsilon(\nabla p + \tilde{E})) = 0$, and let $E := \tilde{E} + \nabla p$, which belongs to the domain $\operatorname{dom}(\mathcal{M}_\varepsilon(\alpha))$. We note that $\operatorname{div}(\varepsilon\tilde{E}) = \tau\operatorname{div}(\chi_D\tilde{E})$ is independent of h , hence so is the function p . We proceed to compute

$$\nabla \times \tilde{E} = (f'(x_3)\alpha_1, f'(x_3)\alpha_2, -i|\alpha|^2 f(x_3))e^{i\alpha \cdot x}$$

and

$$\frac{(\nabla \times E, \nabla \times E)_{Y_\infty}}{(\varepsilon E, E)_{Y_\infty}} = \frac{(\nabla \times \tilde{E}, \nabla \times \tilde{E})_{Y_\infty}}{(\varepsilon E, E)_{Y_\infty}} = \frac{(\nabla \times \tilde{E}, \nabla \times \tilde{E})_{Y_\infty} - |\alpha|^2(\varepsilon E, E)_{Y_\infty}}{(\varepsilon E, E)_{Y_\infty}} + |\alpha|^2,$$

which yields

$$\begin{aligned} & (\nabla \times \tilde{E}, \nabla \times \tilde{E}) - |\alpha|^2(\varepsilon E, E) \\ &= \int_{\mathbb{R}} |\alpha|^2 (f'(x_3)^2 + |\alpha|^2 f(x_3)^2) dx_3 - |\alpha|^2 \|E\|_{\varepsilon, Y_\infty}^2 \\ &= 2|\alpha|^2 h^{-1} - |\alpha|^2 (\|E\|_{\varepsilon, Y_\infty}^2 - \|\tilde{E}\|_{Y_\infty}^2). \end{aligned} \quad (2.36)$$

By Lemma A.2, we have that the difference $\|E\|_{\varepsilon, Y_\infty}^2 - \|\tilde{E}\|_{Y_\infty}^2$ is strictly positive and independent of h , and

$$\|E\|_{\varepsilon, Y_\infty}^2 - \|\tilde{E}\|_{Y_\infty}^2 \geq \|\nabla p\|_{Y_\infty} \|\tilde{E}\|_D.$$

Therefore, for large enough h , we conclude from (2.36) that

$$(\nabla \times E, \nabla \times E)_{Y_\infty} - |\alpha|^2(\varepsilon E, E)_{Y_\infty} < 0,$$

which, by the min-max representation (2.29), means $\mu_1(\tau) < |\alpha|^2$. \square

2.2 Symmetry of band functions and multiplicity

In this section, we consider dielectric metasurfaces with certain symmetries, and derive some consequences on the symmetry properties of the band functions $\omega_j(\alpha)$ and Bloch modes, and the multiplicity of scattering resonances. These results will be useful in Section 3.

We first note from (2.2) and (2.3) that the symmetry of the scattering problem is completely determined by the symmetry group of the metasurface \mathcal{D} (i.e., the set of isometries that carry \mathcal{D} to itself). Here, an isometry of \mathbb{R}^d is a distance-preserving map from \mathbb{R}^d to itself, which can be uniquely written as the composition of a translation and an orthogonal linear map; see [11, Corollary 6.2.7]. We denote by M_d the set of all isometries of \mathbb{R}^d . Since this work only considers a single layer of dielectric nanoparticles, for the sake of simplicity, we will not discuss the symmetry

of \mathcal{D} along the z -direction. Thus, the symmetry group of \mathcal{D} reduces to the well-investigated plane symmetry group. To be precise, let g be a two-dimensional isometry. By abuse of notation, we still denote by g its three-dimensional extension: $gx = (gx', x_3)$ for $x \in \mathbb{R}^3$. Then we define the symmetry group of \mathcal{D} as follows:

$$\mathcal{G} := \{g; g \text{ is a two-dimensional isometry and } g(\mathcal{D}) = \mathcal{D}\},$$

which is a discrete group, according to [11, Definition 6.5.1] and the structure (2.1) of \mathcal{D} . Moreover, there are two important subgroups associated with \mathcal{G} : the translation group \mathcal{L} and the point group $\bar{\mathcal{G}}$. The group \mathcal{L} is simply defined as the subgroup of \mathcal{G} of the translations. Recalling that an isometry g of \mathbb{R}^2 is uniquely decomposed as $g = t_a \bar{g}$, where $\bar{g} \in O_2$ and t_a is a translation: $t_a x = x + a$ for $x \in \mathbb{R}^2$, we can introduce a homomorphism $\pi : M_2 \rightarrow O_2$ by $\pi(g) = \bar{g}$. Here O_d denotes the group of orthogonal matrices on \mathbb{R}^d .

The point group $\bar{\mathcal{G}}$ is then defined as the image of \mathcal{G} under the map π , which, by [11, Proposition 6.5.10], is a finite group. We remark that the point group $\bar{\mathcal{G}}$ is generally not a subgroup of \mathcal{G} . In what follows, we consider the following mild assumption on the translation group \mathcal{L} , for ease of analysis,

$$\text{the lattice } \Lambda \text{ gives all the translation vectors in } \mathcal{L}. \quad (2.37)$$

By [11, Proposition 6.5.11], along with the assumption (2.37) and the definition (1.1), we have

$$\bar{g}(\Lambda) = \Lambda \quad \text{and} \quad \bar{g}(\Lambda^*) = \Lambda^*, \quad (2.38)$$

that is, the group $\bar{\mathcal{G}}$ is contained in the symmetry group of Λ and Λ^* . One may also observe that the symmetry group \mathcal{G} implicitly enforces some symmetry conditions on the shape of D in the sense that up to a translation, there holds $\bar{g} \in \bar{\mathcal{G}}$ maps D to D , i.e., $\bar{g}(D) = D + (b, 0)$ for some $b \in \mathbb{R}^2$.

We next consider the invariance of the operator $\mathcal{T}_D^{\alpha, \omega}$ under the action of the symmetry group \mathcal{G} of \mathcal{D} . We introduce the quasi-periodic extension of the function space $\mathbf{L}^2(D)$:

$$\mathbf{L}_\alpha^2(D) := \left\{ \sum_{\gamma \in \Lambda} (f \chi_D)(x - \gamma) e^{i\alpha \cdot \gamma}, f \in \mathbf{L}^2(D) \right\} \subset \mathbf{L}_\alpha^2(Y_\infty).$$

By definition of $\mathcal{T}_D^{\alpha, \omega}$ and $\mathbf{L}_\alpha^2(D)$, we readily see

$$\mathcal{T}_D^{\alpha, \omega}[\varphi|_D] = \mathcal{T}_{D+\gamma}^{\alpha, \omega}[\varphi|_{D+\gamma}], \quad \forall \gamma \in \Lambda, \varphi \in \mathbf{L}_\alpha^2(D). \quad (2.39)$$

Then, we define the group action \mathcal{O} of \mathcal{G} on the vector fields φ by

$$\mathcal{O}_g[\varphi] := \bar{g}\varphi(g^{-1}x), \quad \text{for } g \in \mathcal{G}. \quad (2.40)$$

Note that $g^{-1}(x + \gamma) = g^{-1}x + \bar{g}^{-1}\gamma$ for any $x, \gamma \in \mathbb{R}^2$, as g is an invertible affine map. Thus, by the relation (2.38), it holds that, for vector fields φ with the quasi-periodicity $\alpha \in \mathcal{B}$,

$$\mathcal{O}_g[\varphi](x + \gamma) = \bar{g}\varphi(g^{-1}x + \bar{g}^{-1}\gamma) = \mathcal{O}_g[\varphi](x) e^{i\alpha \cdot \bar{g}^{-1}\gamma} = \mathcal{O}_g[\varphi](x) e^{i\bar{g}[\alpha] \cdot \gamma}. \quad (2.41)$$

This means that \mathcal{O}_g is an isometric isomorphism from $\mathbf{L}_\alpha^2(Y_\infty)$ to $\mathbf{L}_{\bar{g}[\alpha]}^2(Y_\infty)$. With the above preparation, we have the following result.

Lemma 2.9. *For $\varphi \in \mathbf{L}_\alpha^2(D)$, it holds that*

$$\mathcal{T}_D^{\bar{g}[\alpha], \omega}[\mathcal{O}_g \varphi] = \mathcal{O}_g \mathcal{T}_D^{\alpha, \omega}[\varphi]. \quad (2.42)$$

Proof. By definition, we first have

$$\begin{aligned} \mathcal{T}_D^{\bar{g}[\alpha], \omega}[\mathcal{O}_g \varphi] &= (\omega^2 + \nabla \operatorname{div}) \int_D G^{\bar{g}[\alpha], \omega}(x, y) \bar{g}\varphi(g^{-1}y) dy \\ &= (\omega^2 + \nabla \operatorname{div}) \bar{g} \int_{g^{-1}(D)} G^{\bar{g}[\alpha], \omega}(x, gy) \varphi(y) dy. \end{aligned}$$

We then calculate, by writing $g = t_a \bar{g}$ and noting that \bar{g} maps Λ^* to itself (cf. (2.38)),

$$\begin{aligned} G^{\bar{g}[\alpha], \omega}(x, gy) &= \frac{1}{2} \sum_{q \in \Lambda^*} i\beta_q^{-1} e^{i(\bar{g}[\alpha+q]) \cdot (x' - gy')} e^{i\beta_q |x_3 - y_3|} \\ &= \frac{1}{2} \sum_{q \in \Lambda^*} i\beta_q^{-1} e^{i(\alpha+q) \cdot (\bar{g}^{-1}(x' - a) - y')} e^{i\beta_q |x_3 - y_3|} \\ &= G^{\alpha, \omega}(g^{-1}x, y). \end{aligned}$$

We also find, by a direct computation, for a smooth vector field φ ,

$$\nabla \operatorname{div} \mathcal{O}_g \varphi = \nabla(\operatorname{div} \varphi)(g^{-1}x) = \bar{g}(\nabla \operatorname{div} \varphi)(g^{-1}x) = \mathcal{O}_g[\nabla \operatorname{div} \varphi].$$

Hence, we can conclude from the above formulas,

$$\begin{aligned} \mathcal{T}_D^{\bar{g}[\alpha], \omega}[\mathcal{O}_g \varphi] &= (\omega^2 + \nabla \operatorname{div} \bar{g}) \int_{g^{-1}(D)} G^{\alpha, \omega}(g^{-1}x, y) \varphi(y) dy \\ &= \mathcal{O}_g \mathcal{T}_{g^{-1}(D)}^{\alpha, \omega}[\varphi] = \mathcal{O}_g \mathcal{T}_D^{\alpha, \omega}[\varphi], \end{aligned}$$

where the last equality follows from $g^{-1}(D) = D + (\gamma, 0)$ for some $\gamma \in \Lambda$ and (2.39). \square

As a consequence of Lemma 2.9, if $(\omega_*, \varphi_*) \in \mathbb{C} \times \mathbf{L}_{\alpha}^2(D)$ is an eigenpair of $\mathcal{A}(\alpha, \omega)$, then we have

$$\mathcal{A}(\bar{g}[\alpha], \omega_*)[\mathcal{O}_g \varphi_*] = \mathcal{O}_g \mathcal{A}(\alpha, \omega_*)[\varphi_*] = 0, \quad (2.43)$$

and equivalently, the following corollary holds (note from the definition (1.2) that \bar{g} maps \mathcal{B} to itself for any $\bar{g} \in \bar{\mathcal{G}}$).

Corollary 2.10. *The band dispersion function $\omega_j(\alpha)$ for each j has the following symmetry:*

$$\omega_j(\bar{g}\alpha) = \omega_j(\alpha), \quad \forall \bar{g} \in \bar{\mathcal{G}}, \alpha \in \mathcal{B}.$$

Moreover, suppose that $\varphi \in \mathbf{L}_{\alpha}^2(D)$ is an eigenfunction of $\mathcal{A}(\alpha, \omega)$ for some resonance ω with the quasi-periodicity α . Then $\mathcal{O}_g \varphi$ is an eigenfunction for the same resonance but with the quasi-periodicity $\bar{g}\alpha$.

This motivates us to introduce the notion of high symmetry points in the Brillouin zone \mathcal{B} [46].

Definition 2.11. We say that $\alpha \in \mathcal{B}$ is a high symmetry point, if the subgroup $\bar{\mathcal{G}}_{\alpha} = \{\bar{g} \in \bar{\mathcal{G}}; \bar{g}\alpha - \alpha \in \Lambda^*\}$ of the point group $\bar{\mathcal{G}}$ is nontrivial.

We shall discuss the geometric multiplicity of a resonance $\omega(\alpha)$ at the high symmetry points $\alpha_* \in \mathcal{B}$ by using the group representation theory. To do so, we first recall some preliminaries following [40]. It has been seen that $\bar{\mathcal{G}}_{\alpha_*}$ is a finite compact subgroup of O_2 . We define its representation on a Hilbert space \mathcal{H} by a group homomorphism $\pi : \bar{\mathcal{G}}_{\alpha_*} \rightarrow GL(\mathcal{H})$, where $GL(\mathcal{H})$ is the group of invertible continuous linear operators on \mathcal{H} . The representation π is unitary, if π_g is a unitary operator for each g . Moreover, we say that π is finite dimensional if \mathcal{H} is finite dimensional, and that a subspace $\mathcal{H}' \subset \mathcal{H}$ is invariant for π if $\pi_g(\mathcal{H}') \subset \mathcal{H}'$ for any $g \in \bar{\mathcal{G}}_{\alpha_*}$. It is natural to define the associated subrepresentation $\pi|_{\mathcal{H}'} : \bar{\mathcal{G}}_{\alpha_*} \rightarrow GL(\mathcal{H}')$ by $(\pi|_{\mathcal{H}'})_g := \pi_g|_{\mathcal{H}'}$. If the only invariant subspaces are $\{0\}$ and \mathcal{H} , then the representation π is said to be irreducible.

To proceed, we note from (2.41) that the map \mathcal{O}_g in (2.40) actually defines a unitary representation of $\bar{\mathcal{G}}_{\alpha_*}$ on $\mathbf{L}_{\alpha_*}^2(D)$ at a high symmetry point α_* . Let $\hat{\mathcal{G}}_{\alpha_*}$ be the set of (equivalent classes of) irreducible representations of $\bar{\mathcal{G}}_{\alpha_*}$. It is known that any irreducible representation of a compact group is finite-dimensional [48]. Hence, we can denote by d_{σ} the dimension of a representation $\sigma \in \hat{\mathcal{G}}_{\alpha_*}$ and define its character χ_{σ} by $\chi_{\sigma}(g) = \operatorname{tr} \pi_g$. Then for each $\sigma \in \hat{\mathcal{G}}_{\alpha_*}$, we introduce the projection $P_{\sigma} : \mathbf{L}_{\alpha_*}^2(D) \rightarrow \mathbf{L}_{\alpha_*}^2(D)$ by

$$P_{\sigma}[\varphi] = \frac{1}{|\bar{\mathcal{G}}_{\alpha_*}|} \sum_{g \in \bar{\mathcal{G}}_{\alpha_*}} d_{\sigma} \overline{\chi_{\sigma}(g)} \mathcal{O}_g[\varphi], \quad (2.44)$$

where $|\bar{\mathcal{G}}_{\alpha_*}|$ is the order of the finite group $\bar{\mathcal{G}}_{\alpha_*}$. The following lemma is from [40, Theorem (27.44)].

Lemma 2.12. *The projections P_{σ} in (2.44) are orthogonal and give an orthogonal decomposition of $\mathbf{L}_{\alpha_*}^2(D)$:*

$$\mathbf{L}_{\alpha_*}^2(D) = \bigoplus_{\sigma \in \hat{\mathcal{G}}_{\alpha_*}} M_{\sigma}, \quad M_{\sigma} := P_{\sigma} \mathbf{L}_{\alpha_*}^2(D). \quad (2.45)$$

For each σ , M_{σ} is either zero or a direct orthogonal sum of invariant subspaces $M_{j, \sigma}$ ($1 \leq j \leq m_{\sigma} \leq \infty$) of dimension d_{σ} with $\mathcal{O}|_{M_{j, \sigma}} \in \sigma$. Moreover, M_{σ} is the smallest closed subspace of $\mathbf{L}_{\alpha_*}^2(D)$ containing all the invariant subspaces of $\mathbf{L}_{\alpha_*}^2(D)$ on which \mathcal{O} is in the equivalent class of the irreducible representation σ .

We are now ready to give some results on the multiplicity of resonances at α_* . By Lemma 2.9 and (2.44), we see that the projection P_{σ} commutes with the operator $\mathcal{A}(\alpha_*, \omega)$ for any ω . It follows that M_{σ} is an invariant subspace for $\mathcal{A}(\alpha_*, \omega)$, and the following result holds.

Proposition 2.13. *Let $\alpha_* \in \mathcal{B}$ be a high symmetry point and let M_{σ} be defined in (2.45). For any resonance $\omega(\alpha_*)$ of the operator $\mathcal{A}(\alpha_*, \omega)$ restricted on the subspace M_{σ} , its geometric multiplicity is a multiple of the dimension d_{σ} of the reducible representation σ , i.e., $\dim \mathcal{A}(\alpha_*, \omega)|_{M_{\sigma}} = cd_{\sigma}$ for some positive integer c .*

Proof. We consider the eigenspace $V^{\omega(\alpha_*)} := \{E \in M_{\sigma}; \mathcal{A}(\alpha_*, \omega)|_{M_{\sigma}}[E] = 0\}$ associated with the resonance $\omega(\alpha_*)$, which is of finite dimension. Note from (2.43) that the subspace $V^{\omega(\alpha_*)}$ is invariant for the representation \mathcal{O} . Then, by Lemma 2.12 above, we have the decomposition: $V^{\omega(\alpha_*)} = \bigoplus_{j=1}^c V_j^{\omega(\alpha_*)}$ for a positive integer c , where each space $V_j^{\omega(\alpha_*)}$ satisfies $\mathcal{O}|_{V_j^{\omega(\alpha_*)}} \in \sigma$. It readily yields $\dim \mathcal{A}(\alpha_*, \omega)|_{M_{\sigma}} = cd_{\sigma}$ and completes the proof. \square

3 Existence of embedded eigenvalues

We have seen in Theorem 2.8 that the square of the light line $|\alpha| = \inf_{q \in \Lambda^*} |\alpha + q|$ is nothing else than the infimum of the essential spectrum, and there exists a real scattering resonance below $|\alpha|$. In this section, we consider the high symmetry point $\alpha = 0$ with $\tilde{\mathcal{G}}_0 = \tilde{\mathcal{G}}$ by Definition 2.11, which corresponds to the case of the normal incident wave. We further assume that the dielectric permittivity ε in (2.2) has the following symmetry:

$$\varepsilon(x, y, z)|_{Y_h} = \varepsilon(-x, y, z)|_{Y_h}, \quad \varepsilon(x, y, z)|_{Y_h} = \varepsilon(x, -y, z)|_{Y_h}. \quad (3.1)$$

It follows that the dihedral group D_2 is a subgroup of both the symmetry group \mathcal{G} and the point group $\tilde{\mathcal{G}}$ of the metasurface. We shall show that in this scenario, the real subwavelength scattering resonances for dielectric metasurfaces can exist above the light line, which are the eigenvalues of the Maxwell operator $\mathcal{M}_\varepsilon(0)$ embedded in the continuous spectrum $[0, \infty)$ and hence named as *embedded eigenvalues*. The associated Bloch modes are the so-called *bound states in the continuum* [49, 88, 90].

Our argument is based on a regularized variational formulation in terms of the magnetic fields. We follow the discussions in [12, 13, 36] and note that $\omega > 0$ is a real scattering resonance if and only if there is a divergence-free periodic magnetic field H solving the equation:

$$\nabla \times (\varepsilon^{-1} \nabla \times H) - \nabla(\varepsilon^{-1} \operatorname{div} H) - \omega^2 H = 0, \quad (3.2)$$

with the Rayleigh-Bloch expansion (2.4). Here $-\nabla(\varepsilon^{-1} \operatorname{div} H)$ is a regularization term added for the coercivity of the associated sesquilinear form. As we have assumed that the magnetic permeability μ is constant on the whole space, the magnetic field H is expected to have the H^1 -regularity. Similar to (2.18), to include the outgoing radiation condition into the variational form, we need the following DtN operator,

$$\mathcal{T}f := \sum_{q \in \Lambda^*} i\beta_q f_q e^{iq \cdot x} : H_p^{1/2}(\Sigma_{\pm h}) \rightarrow H_p^{-1/2}(\Sigma_{\pm h}), \quad (3.3)$$

where $f_q, q \in \Lambda^*$, are the Fourier coefficients of f , i.e., $f = \sum_{q \in \Lambda^*} f_q e^{iq \cdot x}$, and β_q are defined in (2.5) with $\alpha = 0$. For a vector field $f \in \mathbf{H}_p^{1/2}(\Sigma_{\pm h})$, we define $\mathcal{T}f$ by acting \mathcal{T} on each component of f . Then the outgoing condition for H can be modelled by the transparent boundary condition:

$$\frac{\partial}{\partial \nu} H = \mathcal{T}H \quad \text{on } \Sigma = \Sigma_h \cup \Sigma_{-h}. \quad (3.4)$$

We also introduce the following pseudo-differential operator:

$$\mathcal{R} = (\partial_1, \partial_2, \mathcal{T}) : H_p^{1/2}(\Sigma_{\pm h}) \rightarrow \mathbf{H}_p^{-1/2}(\Sigma_{\pm h}). \quad (3.5)$$

For convenience, we shall simply write ∇_T for (∂_1, ∂_2) in what follows. By a standard integration by parts with the boundary condition (3.4), we obtain the variational problem for (3.2): find $(\omega, H) \in \mathbb{R} \setminus \{0\} \times \mathbf{H}_p^1(Y_h)$ such that

$$A_{\tau, \omega}(\varphi, H) = \omega^2(\varphi, H)_{Y_h} \quad \forall \varphi \in \mathbf{H}_p^1(Y_h), \quad (3.6)$$

where

$$A_{\tau, \omega}(\varphi, H) := (\nabla \times \varphi, \varepsilon^{-1} \nabla \times H)_{Y_h} + (\operatorname{div} \varphi, \varepsilon^{-1} \operatorname{div} H)_{Y_h} + \langle \varphi, \nu \times (\mathcal{R} \times H) \rangle_\Sigma - \langle \nu \cdot \varphi, \mathcal{R} \cdot H \rangle_\Sigma. \quad (3.7)$$

Moreover, a direct computation gives

$$\langle \varphi, \nu \times (\mathcal{R} \times H) \rangle_\Sigma - \langle \nu \cdot \varphi, \mathcal{R} \cdot H \rangle_\Sigma = -\langle \varphi, \mathcal{T}H \rangle_\Sigma - \langle \nu \cdot \varphi, \nabla_T \cdot H \rangle_\Sigma - \langle \nabla_T \cdot \varphi, \nu \cdot H \rangle_\Sigma. \quad (3.8)$$

Therefore, to show existence of embedded eigenvalues, it suffices to prove that there exists a real subwavelength eigenfrequency ω for (3.6) with a divergence-free eigenfunction.

Let us now focus on the eigenvalue problem (3.6). Motivated by the analysis in [14], we introduce the operators $\mathcal{T}^{\mathcal{P}}$ and $\mathcal{T}^{\mathcal{E}}$ by considering the sum in (3.3) over $\Lambda_{\mathcal{P}}^*$ and $\Lambda_{\mathcal{E}}^*$, respectively. Then the operators $\mathcal{R}^{\mathcal{P}}$ and $\mathcal{R}^{\mathcal{E}}$ can be defined as in (3.5) correspondingly. By using $\mathcal{R}^{\mathcal{E}}$ and the identity (3.8), we define the sesquilinear form on $\mathbf{H}_p^1(Y_h)$:

$$A_{\tau, \omega}^{\mathcal{E}}(\varphi, H) := (\nabla \times \varphi, \varepsilon^{-1} \nabla \times H)_{Y_h} + (\operatorname{div} \varphi, \varepsilon^{-1} \operatorname{div} H)_{Y_h} - \langle \varphi, \mathcal{T}^{\mathcal{E}} H \rangle_\Sigma - \langle \nu \cdot \varphi, \nabla_T \cdot H \rangle_\Sigma - \langle \nabla_T \cdot \varphi, \nu \cdot H \rangle_\Sigma, \quad (3.9)$$

which is actually the real part of $A_{\tau, \omega}$ in the sense that $\Re \mathcal{A}_{\tau, \omega}(H, H) = A_{\tau, \omega}^{\mathcal{E}}(H, H)$. By a similar argument as in the proof of Proposition 2.5, we see that the eigenfunction H for (3.6) associated with a real resonant frequency satisfies $H_q = 0$ on Σ for $q \in \Lambda_{\mathcal{P}}^*$ and hence exponentially decays as $x_3 \rightarrow \infty$. Moreover, we have the following lemma.

Lemma 3.1. *The magnetic field $H \in \mathbf{H}_p^1(Y_h)$ solves (3.6) for some $\omega > 0$ if and only if it satisfies*

$$A_{\tau,\omega}^{\mathcal{E}}(\varphi, H) = \omega^2(\varphi, H)_{Y_h}, \quad \forall \varphi \in \mathbf{H}_p^1(Y_h), \quad (3.10)$$

with

$$H_q = 0 \quad \text{on } \Sigma_{\pm h} \quad \text{for } q \in \Lambda_*^{\mathcal{P}}. \quad (3.11)$$

Remark 3.2. In the above lemma, the variational problem (3.10) is equivalent to the equation (3.2) with the transparent boundary condition $\partial_\nu H = \mathcal{T}^{\mathcal{E}} H$ on Σ , which only allows the exponentially decaying modes of the field H passing through the boundary Σ and going into the far field. The second condition (3.11) means that if the eigenpair of (3.10) is also an eigenpair of (3.6), then the propagating part of H indeed vanishes.

As suggested by Lemma 3.1, we shall prove the existence of real resonances for problem (3.6) in the subwavelength regime by the following two steps. We will first consider the eigenvalue problem (3.10) and show that the real subwavelength resonant frequency does exist when the contrast τ is large enough. Then, with the help of the tools developed in Section 2.2, we show that under the symmetry assumption (3.1), we can find an associated eigenfunction of (3.10) satisfying the condition (3.11).

To analyze the eigenvalue problem (3.10), we first note that the sesquilinear form $A_{\tau,\omega}^{\mathcal{E}}(\cdot, \cdot)$ is conjugate-symmetric, i.e., $A_{\tau,\omega}^{\mathcal{E}}(H, \varphi) = \overline{A_{\tau,\omega}^{\mathcal{E}}(\varphi, H)}$. We next investigate its coercivity and dependence on the parameters τ and ω in detail. We compute, by (3.9), for $H \in \mathbf{H}_p^1(Y_h)$,

$$A_{\tau,\omega}^{\mathcal{E}}(H, H) = \int_{Y_h} \varepsilon^{-1} |\nabla \times H|^2 + \varepsilon^{-1} |\operatorname{div} H|^2 dx - \langle H, \mathcal{T}^{\mathcal{E}} H \rangle_{\Sigma} - 2 \Re \langle \nu \cdot H, \nabla_T \cdot H \rangle_{\Sigma}, \quad (3.12)$$

which, along with the following identity,

$$\int_{Y_h} |\nabla \times H|^2 + |\operatorname{div} H|^2 dx = \int_{Y_h} |\nabla H|^2 dx + 2 \Re \langle \nu \cdot H, \nabla_T \cdot H \rangle_{\Sigma}, \quad (3.13)$$

readily gives

$$\begin{aligned} A_{\tau,\omega}^{\mathcal{E}}(H, H) &= \int_{Y_h} \left(\frac{1}{\varepsilon} - \frac{1}{1+\tau} \right) |\nabla \times H|^2 + \left(\frac{1}{\varepsilon} - \frac{1}{1+\tau} \right) |\operatorname{div} H|^2 dx - \langle H, \mathcal{T}^{\mathcal{E}} H \rangle_{\Sigma} - 2 \Re \langle \nu \cdot H, \nabla_T \cdot H \rangle_{\Sigma} \\ &\quad + \frac{1}{1+\tau} \int_{Y_h} |\nabla H|^2 dx + \frac{2}{1+\tau} \Re \langle \nu \cdot H, \nabla_T \cdot H \rangle_{\Sigma}. \end{aligned} \quad (3.14)$$

Recall that we are mainly interested in the high contrast and subwavelength regime. We follow [9] to introduce a new real variable:

$$\hat{\omega} = \sqrt{\tau} \omega, \quad (3.15)$$

and assume that $\hat{\omega}$ is in some compact set, so that ω is in the subwavelength regime and there holds

$$\Lambda_{\hat{\omega}}^* = \Lambda^* \setminus \{0\}. \quad (3.16)$$

By definition of $\mathcal{T}^{\mathcal{E}}$, we have, for $\omega > 0$,

$$-\langle H, \mathcal{T}^{\mathcal{E}} H \rangle_{\Sigma_{\pm h}} = \sum_{q \in \Lambda_{\hat{\omega}}^*} \sqrt{|q|^2 - \omega^2} |H_q|^2 \geq 0. \quad (3.17)$$

Then, thanks to (3.15), we can derive, for τ large enough and $\hat{\omega}$ in a compact set K of \mathbb{R} ,

$$\begin{aligned} & -\langle H, \mathcal{T}^{\mathcal{E}} H \rangle_{\Sigma_{\pm h}} - 2 \Re \langle \nu \cdot H, \nabla_T \cdot H \rangle_{\Sigma} + \frac{2}{1+\tau} \Re \langle \nu \cdot H, \nabla_T \cdot H \rangle_{\Sigma} \\ & \geq \sum_{q \in \Lambda_{\hat{\omega}}^*} (\sqrt{|q|^2 - \tau^{-1} \hat{\omega}^2} - |q|) |H_q|^2 + \frac{1}{1+\tau} |q| |H_q|^2 \\ & \geq \sum_{q \in \Lambda_{\hat{\omega}}^*} -c_0 \frac{\hat{\omega}^2}{\tau} \frac{1}{|q|} |H_q|^2 + \frac{1}{1+\tau} |q| |H_q|^2 \\ & \geq \sum_{q \in \Lambda_{\hat{\omega}}^*} \frac{1}{1+\tau} |q| |H_q|^2 - c_0 \frac{\hat{\omega}^2}{\tau} \frac{1}{\min_{q \in \Lambda_{\hat{\omega}}^*} |q|} \|H\|_{\Sigma}, \end{aligned} \quad (3.18)$$

where the first inequality follows from (3.17) and the following estimate:

$$2 |\Re \langle \nu \cdot H, \nabla_T \cdot H \rangle_{\Sigma_{\pm h}}| \leq \sum_{q \in \Lambda_{\mathcal{E}}^*} |q| |H_q|^2,$$

and the second inequality is from the following asymptotics uniformly in $q \in \Lambda_{\mathcal{E}}^*$ and $\hat{\omega} \in K$, as $\tau \rightarrow \infty$,

$$|q| - \sqrt{|q|^2 - \tau^{-1} \hat{\omega}^2} = |q| - |q| \sqrt{1 - |q|^{-2} \tau^{-1} \hat{\omega}^2} = O(|q|^{-1} \tau^{-1} \hat{\omega}^2).$$

Here the generic constant c_0 in (3.18) is independent of $\tau \gg 1$, $q \in \Lambda_{\mathcal{E}}^*$ and $\hat{\omega} \in K$. We recall the weighted trace inequality: for any given $\eta > 0$, there holds

$$\|u\|_{\Sigma} \leq \eta \|\nabla u\|_{Y_h} + C(\eta) \|u\|_{Y_h}, \quad \forall u \in \mathbf{H}_p^1(Y_h), \quad (3.19)$$

with a constant $C(\eta)$ satisfying $C(\eta) = O(1)$ as $\eta \rightarrow \infty$ and $C(\eta) = O(\eta^{-1})$ as $\eta \rightarrow 0$. Then it readily follows from the formula (3.14), the estimate (3.18), and the inequality (3.19) with

$$\eta = \frac{1}{2} \frac{\tau}{1 + \tau} \frac{\min_{q \in \Lambda_{\mathcal{E}}^*} |q|}{c_0 \hat{\omega}^2}$$

that there exists a constant C independent of $\tau \gg 1$ and $\hat{\omega} \in K$ such that

$$A_{\tau, \sqrt{\tau}^{-1} \hat{\omega}}^{\mathcal{E}}(H, H) \geq \frac{1}{2} \frac{1}{1 + \tau} \int_{Y_h} |\nabla H|^2 dx - C \frac{\hat{\omega}^2}{\tau} \int_{Y_h} |H|^2 dx, \quad \forall H \in \mathbf{H}_p^1(Y_h). \quad (3.20)$$

We define a new form on $\mathbf{H}_p^1(Y_h)$:

$$\tilde{A}_{\tau, \hat{\omega}}^{\mathcal{E}}(\varphi, H) = \tau A_{\tau, \sqrt{\tau}^{-1} \hat{\omega}}^{\mathcal{E}}(\varphi, H), \quad (3.21)$$

and consider the following eigenvalue problem equivalent to (3.10):

$$\tau A_{\tau, \sqrt{\tau}^{-1} \hat{\omega}}^{\mathcal{E}}(\varphi, H) = \hat{\omega}^2(\varphi, H)_{Y_h}, \quad \forall \varphi \in \mathbf{H}_p^1(Y_h). \quad (3.22)$$

In view of Garding's inequality (3.20) and the compact embedding from $\mathbf{H}_p^1(Y_h)$ to $\mathbf{L}_p^2(Y_h)$, we have the following min-max principle: for $j = 0, 1, 2, \dots$,

$$\lambda_j(\tau, \hat{\omega}) = \min_{\substack{V \subset \mathbf{H}_p^1(Y_h) \\ \dim V = j}} \max_{\substack{H \in V \\ \|H\|_{Y_h} = 1}} \tilde{A}_{\tau, \hat{\omega}}^{\mathcal{E}}(H, H), \quad (3.23)$$

recalling that $\tilde{A}_{\tau, \hat{\omega}}^{\mathcal{E}}$ is a symmetric form. Then $\hat{\omega}$ is an eigenfrequency for (3.22) if and only if for some j , there holds

$$\lambda_j(\tau, \hat{\omega}) = \hat{\omega}^2. \quad (3.24)$$

We now summarize some basic important properties of the form $\tilde{A}_{\tau, \hat{\omega}}^{\mathcal{E}}$ and its eigenvalues $\lambda_j(\tau, \hat{\omega})$, according to what we have discussed above.

Proposition 3.3. *Let $\hat{\omega}$ be in a compact set K of \mathbb{R} . For large enough $\tau > 0$, we have*

1. *The sesquilinear form $\tilde{A}_{\tau, \hat{\omega}}^{\mathcal{E}}$ on $\mathbf{H}_p^1(Y_h)$ defined in (3.21) is conjugate-symmetric and bounded from below:*

$$\tilde{A}_{\tau, \hat{\omega}}^{\mathcal{E}}(H, H) \geq \frac{1}{4} \|\nabla H\|_{Y_h}^2 - C \hat{\omega}^2 \|H\|_{Y_h}^2, \quad \forall H \in \mathbf{H}_p^1(Y_h), \quad (3.25)$$

for a constant C independent of $\tau \gg 1$ and $\hat{\omega} \in K$.

2. *For each $j \geq 0$, the eigenvalue $\lambda_j(\tau, \hat{\omega})$ in (3.23) is decreasing in $\hat{\omega}$, and continuously depends on τ and $\hat{\omega}$.*

In particular, if $\hat{\omega} = 0$, the form $\tilde{A}_{\tau, 0}^{\mathcal{E}}$ is symmetric and positive for any $\tau > 0$. Moreover, $\lambda_0(\tau, 0) = 0$ holds with the eigenfunctions being constant vector fields, while for $j \geq 1$, there holds $\lambda_j(\tau, 0) > 0$.

Proof. The estimate (3.25) follows from (3.20) directly. The continuous dependence of $\lambda_j(\tau, \hat{\omega})$ on τ and $\hat{\omega}$ is a consequence of the continuity of the form $\tilde{A}_{\tau, \hat{\omega}}^{\mathcal{E}}$ in τ and $\hat{\omega}$ and the standard perturbation theory. Note from (3.12) and (3.17) that only the term $-\tau \langle H, \mathcal{T}^{\mathcal{E}} H \rangle_{\Sigma}$ in $\tilde{A}_{\tau, \hat{\omega}}^{\mathcal{E}}$ depends on the parameter $\hat{\omega}$ and it is decreasing in $\hat{\omega}$ for a fixed $H \in \mathbf{H}_p^1(Y_h)$. It then follows from the representation (3.23) that the eigenvalue $\lambda_j(\tau, \hat{\omega})$ is decreasing in $\hat{\omega}$. We now consider the last statement. By the same estimates as in (3.18) and (3.20), we see that for any $\tau > 0$, there holds

$$\tilde{A}_{\tau, 0}^{\mathcal{E}}(H, H) \geq \frac{1}{2} \frac{\tau}{1 + \tau} \|\nabla H\|_{Y_h}^2,$$

which readily gives $\lambda_j \geq 0$ for any j , and $\tilde{A}_{\tau, 0}^{\mathcal{E}}(H, H) = 0$ if and only if H is a constant vector field. This means that $\lambda_0(\tau, 0) = 0$ with constant eigenfunctions. The proof is complete. \square

By Proposition 3.3 above, we see that for any given compact set K of \mathbb{R} , there exists a large enough τ_0 such that for each j , $\lambda_j(\tau, \hat{\omega})$ in (3.23) is well defined for $\tau \geq \tau_0$ and $\hat{\omega} \in K$. Moreover, since $\lambda_j(\tau, \hat{\omega})$ is a decreasing and continuous curve in $\hat{\omega} \in K$ with $\lambda_j(\tau, 0) \geq 0$, one may expect that the equation (3.24) admits a unique solution that immediately gives a desired eigenvalue to the problem (3.22). However, to rigorously show the existence of a solution to (3.24) in some given compact set K , we need to investigate the limiting behavior of the eigenvalues $\lambda_j(\tau, \hat{\omega})$ as $\tau \rightarrow \infty$.

For this purpose, we first show that if $\hat{\omega}$ is suitably small, then $\tilde{A}_{\tau, \hat{\omega}}^{\mathcal{E}}(H, H)$ is increasing in τ . By (3.14), we have

$$\begin{aligned} \tilde{A}_{\tau, \hat{\omega}}^{\mathcal{E}}(H, H) &= \int_{Y_h \setminus D} \frac{\tau^2}{1+\tau} \left(|\nabla \times H|^2 + |\operatorname{div} H|^2 \right) dx + \frac{\tau}{1+\tau} \int_{Y_h} |\nabla H|^2 dx \\ &\quad - \tau \langle H, \mathcal{T}^{\mathcal{E}} H \rangle_{\Sigma} - 2\tau \Re \langle \nu \cdot H, \nabla_T \cdot H \rangle_{\Sigma} + \frac{2\tau}{1+\tau} \Re \langle \nu \cdot H, \nabla_T \cdot H \rangle_{\Sigma}. \end{aligned} \quad (3.26)$$

Since both $\tau^2/(1+\tau)$ and $\tau/(1+\tau)$ are increasing functions in τ , we only need to consider the boundary integrals in (3.26) for the monotonicity of $\tilde{A}_{\tau, \hat{\omega}}^{\mathcal{E}}$. We compute, by the Fourier expansion of $H = (H', H_3)$ on Σ ,

$$\begin{aligned} & -\tau \langle H, \mathcal{T}^{\mathcal{E}} H \rangle_{\Sigma_{\pm h}} - 2\tau \Re \langle \nu \cdot H, \nabla_T \cdot H \rangle_{\Sigma_{\pm h}} + \frac{2\tau}{1+\tau} \Re \langle \nu \cdot H, \nabla_T \cdot H \rangle_{\Sigma_{\pm h}} \\ &= \sum_{q \in \Lambda_{\mathcal{E}}^*} \tau \sqrt{|q|^2 - \tau^{-1} \hat{\omega}^2} |H_q|^2 - 2\left(\tau - \frac{\tau}{1+\tau}\right) \Re \langle i\bar{H}_{3,q} q \cdot H'_q \rangle. \end{aligned} \quad (3.27)$$

Consequently, by a simple Cauchy's inequality: $2\Re \langle i\bar{H}_{3,q} q \cdot H'_q \rangle \leq |q| |H_q|^2$, it suffices to show that, for any $q \in \Lambda_{\mathcal{E}}^*$,

$$\tilde{\tau} \sqrt{|q|^2 - \tilde{\tau}^{-1} \hat{\omega}^2} - \tau \sqrt{|q|^2 - \tau^{-1} \hat{\omega}^2} \geq \left(\tilde{\tau} - \frac{\tilde{\tau}}{1+\tilde{\tau}} - \left(\tau - \frac{\tau}{1+\tau} \right) \right) |q|, \quad \forall \tilde{\tau} > \tau \gg 1. \quad (3.28)$$

For this, a direct computation gives

$$\tilde{\tau} \sqrt{|q|^2 - \tilde{\tau}^{-1} \hat{\omega}^2} - \tau \sqrt{|q|^2 - \tau^{-1} \hat{\omega}^2} = \frac{(\tilde{\tau}^2 - \tau^2) |q|^2 - (\tilde{\tau} - \tau) \hat{\omega}^2}{\tilde{\tau} \sqrt{|q|^2 - \tilde{\tau}^{-1} \hat{\omega}^2} + \tau \sqrt{|q|^2 - \tau^{-1} \hat{\omega}^2}}, \quad (3.29)$$

and

$$\left(\tilde{\tau} - \frac{\tilde{\tau}}{1+\tilde{\tau}} \right) - \left(\tau - \frac{\tau}{1+\tau} \right) = (\tilde{\tau} - \tau) - \frac{\tilde{\tau} - \tau}{(1+\tilde{\tau})(1+\tau)}. \quad (3.30)$$

With the above formulas (3.29) and (3.30), by Taylor expansion:

$$\begin{aligned} & \tilde{\tau} \sqrt{1 - \tilde{\tau}^{-1} |q|^{-2} \hat{\omega}^2} + \tau \sqrt{1 - \tau^{-1} |q|^{-2} \hat{\omega}^2} \\ &= \tilde{\tau} \left(1 - \frac{1}{2} \tilde{\tau}^{-1} |q|^{-2} \hat{\omega}^2 + O(\tilde{\tau}^{-2} |q|^{-4} \hat{\omega}^4) \right) + \tau \left(1 - \frac{1}{2} \tau^{-1} |q|^{-2} \hat{\omega}^2 + O(\tau^{-2} |q|^{-4} \hat{\omega}^4) \right) \\ &= \tilde{\tau} + \tau - |q|^{-2} \hat{\omega}^2 + O(\tilde{\tau}^{-1} |q|^{-4} \hat{\omega}^4) + O(\tau^{-1} |q|^{-4} \hat{\omega}^4), \end{aligned}$$

we estimate, as $\tilde{\tau} > \tau \rightarrow \infty$,

$$\begin{aligned} \frac{\tilde{\tau} \sqrt{|q|^2 - \tilde{\tau}^{-1} \hat{\omega}^2} - \tau \sqrt{|q|^2 - \tau^{-1} \hat{\omega}^2}}{\left(\tilde{\tau} - \frac{\tilde{\tau}}{1+\tilde{\tau}} \right) - \left(\tau - \frac{\tau}{1+\tau} \right)} &\geq \frac{(\tilde{\tau} + \tau) |q|^2 - \hat{\omega}^2}{\tilde{\tau} \sqrt{|q|^2 - \tilde{\tau}^{-1} \hat{\omega}^2} + \tau \sqrt{|q|^2 - \tau^{-1} \hat{\omega}^2}} \left(1 + \frac{1}{(1+\tilde{\tau})(1+\tau)} \right) \\ &\geq \frac{(\tilde{\tau} + \tau) |q| - |q|^{-1} \hat{\omega}^2}{\tilde{\tau} \sqrt{1 - \tilde{\tau}^{-1} |q|^{-2} \hat{\omega}^2} + \tau \sqrt{1 - \tau^{-1} |q|^{-2} \hat{\omega}^2}} \left(1 + \frac{1}{(1+\tilde{\tau})(1+\tau)} \right) \\ &\geq |q| \frac{(\tilde{\tau} + \tau) - |q|^{-2} \hat{\omega}^2}{\tilde{\tau} + \tau - |q|^{-2} \hat{\omega}^2 + O(\tilde{\tau}^{-1} |q|^{-4} \hat{\omega}^4) + O(\tau^{-1} |q|^{-4} \hat{\omega}^4)} \left(1 + \frac{1}{(1+\tilde{\tau})(1+\tau)} \right) \\ &\geq |q| \frac{1}{1 + O(\tilde{\tau}^{-2} |q|^{-4} \hat{\omega}^4) + O((\tau \tilde{\tau})^{-1} |q|^{-4} \hat{\omega}^4)} \left(1 + O((\tau \tilde{\tau})^{-1}) \right), \end{aligned} \quad (3.31)$$

where the generic constants involved in the big O -terms are independent of $\tau \gg 1$, $q \in \Lambda_{\mathcal{E}}^*$, and $\hat{\omega}$ in a compact set K . Therefore, it is clear that if K is suitably small, there holds

$$\frac{1}{1 + O(\tilde{\tau}^{-2} |q|^{-4} \hat{\omega}^4) + O((\tau \tilde{\tau})^{-1} |q|^{-4} \hat{\omega}^4)} \left(1 + O((\tau \tilde{\tau})^{-1}) \right) > 1, \quad \text{as } \tilde{\tau} > \tau \rightarrow \infty,$$

and then the inequality (3.28) follows. Moreover, we can conclude that the following lemma holds.

Lemma 3.4. *There exists a compact subset K_* of \mathbb{R} such that for any $\hat{\omega} \in K_*$ and $H \in \mathbf{H}_p^1(Y_h)$, $\tilde{A}_{\tau, \hat{\omega}}^\varepsilon(H, H)$ is increasing in τ when τ is large enough.*

We next follow the arguments in [37, 77] to define a limiting form of $\tilde{A}_{\tau, \hat{\omega}}^\varepsilon$ with $\hat{\omega} \in K_*$ as $\tau \rightarrow \infty$, by using the monotonicity of $\tilde{A}_{\tau, \hat{\omega}}^\varepsilon$ in τ . We regard the sesquilinear form $\tilde{A}_{\tau, \hat{\omega}}^\varepsilon$ as a densely defined and closed unbounded form on $\mathbf{L}_p^2(Y_h)$ with domain $\text{dom}(\tilde{A}_{\tau, \hat{\omega}}^\varepsilon) = \mathbf{H}_p^1(Y_h)$, which is bounded from below by (3.25). By the first representation theorem [45, Theorem VI-2.1], there is a unique self-adjoint operator $\mathbb{A}_{\tau, \hat{\omega}}^\varepsilon$ on $\mathbf{L}_p^2(Y_h)$ such that

$$\tilde{A}_{\tau, \hat{\omega}}^\varepsilon(\varphi, H) = (\varphi, \mathbb{A}_{\tau, \hat{\omega}}^\varepsilon H)_{Y_h}, \quad H \in \text{dom}(\mathbb{A}_{\tau, \hat{\omega}}^\varepsilon), \quad \varphi \in \text{dom}(\tilde{A}_{\tau, \hat{\omega}}^\varepsilon),$$

with $\text{dom}(\mathbb{A}_{\tau, \hat{\omega}}^\varepsilon)$ dense in $\text{dom}(\tilde{A}_{\tau, \hat{\omega}}^\varepsilon)$ with respect to the $\|\cdot\|_{\mathbf{H}^1(Y_h)}$ -norm. Thanks to Lemma 3.4, we now define a closed limiting quadratic form on $\mathbf{L}_p^2(Y_h)$ by

$$\tilde{A}_{\infty, \hat{\omega}}^\varepsilon(H, H) = \sup_{\tau > 0} \tilde{A}_{\tau, \hat{\omega}}^\varepsilon(H, H) = \lim_{\tau \rightarrow +\infty} \tilde{A}_{\tau, \hat{\omega}}^\varepsilon(H, H), \quad (3.32)$$

with the domain:

$$\text{dom}(\tilde{A}_{\infty, \hat{\omega}}^\varepsilon) := \{H \in \mathbf{H}_p^1(Y_h); \sup_{\tau > 0} \tilde{A}_{\tau, \hat{\omega}}^\varepsilon(H, H) < \infty\};$$

see [45, Theorem VIII-3.13a]. Similarly, there exists a unique self-adjoint operator $\mathbb{A}_{\infty, \hat{\omega}}^\varepsilon$ on $\mathbf{L}_p^2(Y_h)$, corresponding to the form $\tilde{A}_{\infty, \hat{\omega}}^\varepsilon$. It is clear that both the operators $\mathbb{A}_{\tau, \hat{\omega}}^\varepsilon$ and $\mathbb{A}_{\infty, \hat{\omega}}^\varepsilon$ have compact resolvents and thus have purely discrete spectrum. We denote by $\{\mu_j(\hat{\omega})\}_{j=0}^\infty$ the eigenvalues of the operator $\mathbb{A}_{\infty, \hat{\omega}}^\varepsilon$, recalling that the eigenvalues of $\mathbb{A}_{\tau, \hat{\omega}}^\varepsilon$ have been characterized by (3.23). The following result is a corollary of [45, Theorem VIII-3.15], and helps us to estimate the solution of (3.24) (see Corollary 3.6 below).

Proposition 3.5. *Let K_* be the compact set given in Lemma 3.4. It holds that for $j \geq 0$,*

$$\lambda_j(\tau, \hat{\omega}) \nearrow \mu_j(\hat{\omega}), \quad \text{as } \tau \rightarrow \infty, \quad (3.33)$$

pointwisely for $\hat{\omega} \in K_*$, and $\mu_j(\hat{\omega})$ is a decreasing function on K_* .

Proof. The monotonicity of the functions $\lambda_j(\tau, \hat{\omega})$ in τ follows from Lemma 3.4 and the min-max formula (3.23), while [45, Theorem VIII-3.15] guarantees the pointwise convergence of $\lambda_j(\tau, \hat{\omega})$ to $\mu_j(\hat{\omega})$ as $\tau \rightarrow \infty$, which, by definition, also gives that μ_j is decreasing in $\hat{\omega}$. \square

Corollary 3.6. *Let $\{\mu_j\}$ be the eigenvalues of the form $\tilde{A}_{\infty, 0}^\varepsilon$ defined in (3.32). For each $j \geq 0$, when τ is large enough, the equation (3.24) has a unique solution $0 \leq \hat{\omega}_j(\tau) \leq \sqrt{\mu_j}$ and $\sqrt{\tau}^{-1} \hat{\omega}_j$ gives a eigenfrequency for (3.10).*

Proof. It suffices to note that the curve $\hat{\omega}^2$ intersects with the constant curve μ_j at the point $\sqrt{\mu_j}$, and that for τ large enough, by Proposition 3.3 and Corollary 3.6, the curve $\lambda_j(\tau, \hat{\omega})$ is well defined on $\hat{\omega} \in [0, \sqrt{\mu_j}]$ and it is decreasing and continuous with respect to $\hat{\omega}$ for $\lambda_j(\tau, \hat{\omega}) \leq \mu_j$ and $\lambda_j(\tau, 0) \geq 0$. \square

By Corollary 3.6 with (3.21) and (3.22), we have proved the existence of the subwavelength eigenfrequencies for problem (3.10) in the high contrast regime. We proceed to show that there exists associated eigenfunctions H such that the condition (3.11) holds. Recalling Lemma 3.1, this will complete the proof of the existence of subwavelength resonances for the eigenvalue problem (3.6). We first note that in the subwavelength regime, there holds $\Lambda_{\mathcal{P}}^* = \{0\}$, and hence the condition (3.11) reduces to

$$\int_{\Sigma_{\pm h}} H \, dx = 0. \quad (3.34)$$

We recall that the symmetry assumption (3.1) implies that the dihedral group D_2 is a subgroup of the symmetry group \mathcal{G} and the point group $\tilde{\mathcal{G}}$ of the configuration \mathcal{D} . It is also easy to see that \mathcal{O}_g with $g \in D_2$, defined in (2.40), gives a unitary representation of D_2 on $\mathbf{L}_p^2(Y_h)$. It is well known that D_2 is an abelian group with 4 one-dimensional irreducible representations that are completely determined by its characteristic table. Similarly to (2.44) and (2.45), by the projections P_σ corresponding to the group D_2 , the space $\mathbf{L}_p^2(Y_h)$ can be written as the orthogonal sum of the following four subspaces: for $i, j = 0, 1$,

$$\begin{aligned} M_{i,j} = \{f \in \mathbf{L}_p^2(Y_h); & f_1(-x_1, x_2, x_3) = (-1)^{1+i} f_1(x_1, x_2, x_3), \quad f_1(x_1, -x_2, x_3) = (-1)^j f_1(x_1, x_2, x_3), \\ & f_2(-x_1, x_2, x_3) = (-1)^i f_2(x_1, x_2, x_3), \quad f_2(x_1, -x_2, x_3) = (-1)^{1+j} f_2(x_1, x_2, x_3), \\ & f_3(-x_1, x_2, x_3) = (-1)^i f_3(x_1, x_2, x_3), \quad f_3(x_1, -x_2, x_3) = (-1)^j f_3(x_1, x_2, x_3)\}. \end{aligned} \quad (3.35)$$

Theorem 3.7. *For the large enough contrast τ , the eigenvalue problem (3.6) admits subwavelength eigenfrequencies $\omega = O(\sqrt{\tau}^{-1})$ as $\tau \rightarrow \infty$.*

Proof. We consider the subspaces $\mathbf{H}_{p,0}^1(Y_h) := (M_{0,0} \oplus M_{0,1} \oplus M_{1,0}) \cap \mathbf{H}_p^1(Y_h)$ and $\mathbf{H}_{p,1}^1(Y_h) := M_{1,1} \cap \mathbf{H}_p^1(Y_h)$. By a lengthy but direct computation, one can check that these two function spaces are orthogonal with respect to the sesquilinear form $A_{\tau,\omega}$ in (3.7) and the \mathbf{H}_p^1 -inner product. Therefore, if the field $H \in \mathbf{H}_{p,1}^1(Y_h)$ satisfies the variational equation (3.6) for all $\varphi \in \mathbf{H}_{p,1}^1(Y_h)$, then (3.6) holds for all $\varphi \in \mathbf{H}_p^1(Y_h)$. It suffices to consider the eigenvalue problem (3.6) on the subspace $\mathbf{H}_{p,1}^1(Y_h)$. We denote by $\lambda_j^{(1)}(\tau, \omega)$ the eigenvalues of the form $A_{\tau,\omega}^\mathcal{E}$ restricted on $\mathbf{H}_{p,1}^1(Y_h)$. By similar arguments as above, we can conclude that for each j , when τ is large enough, there exists $\omega_j^{(1)}(\tau)$ satisfying $\lambda_j(\tau, \omega_j^{(1)}) = (\omega_j^{(1)})^2$ and $\omega_j(\tau) = O(\sqrt{\tau}^{-1})$ as $\tau \rightarrow \infty$, and that there holds, for some $H \in \mathbf{H}_{p,1}^1(Y_h)$, the equation (3.10) holds for any $\varphi \in \mathbf{H}_{p,1}^1(Y_h)$; see Corollary 3.6. The proof is completed by noting that the condition (3.34) holds for any $H \in \mathbf{H}_{p,1}^1(Y_h)$ due to the symmetry, and that Lemma 3.1 still holds if we restrict the space to $\mathbf{H}_{p,1}^1(Y_h)$. \square

It is clear that the set of eigenfrequencies of (3.6) is a subset of the eigenfrequencies of (3.10). For the sake of simplicity, in the remaining of this section, we focus on the first nonzero positive eigenfrequency for the eigenvalue problem (3.6):

$$\omega_*(\tau) := \sqrt{\tau}^{-1} \hat{\omega}_{j_0}(\tau), \quad \text{for some } j_0 > 0, \quad (3.36)$$

where $\hat{\omega}_{j_0}$ is given as in Corollary 3.6. To show that $\omega_*(\tau)$ is a desired real scattering resonance embedded in the continuous spectrum for the problem (2.3), we only need to prove that there exists an associated divergence-free eigenfunction H_{j_0} of (3.6). For this, we define $u = \varepsilon^{-1} \operatorname{div} H$ for $H \in \mathbf{H}_p^1(Y_h)$ satisfying the equation (3.2) with (3.4). It was shown in [12, Theorem 4.3] that u satisfies

$$\Delta u + \omega^2 \varepsilon u = 0 \quad \text{on } Y_h, \quad \frac{\partial}{\partial \nu} u = \mathcal{T} u \quad \text{on } \Sigma = \Sigma_h \cup \Sigma_{-h}. \quad (3.37)$$

If $\operatorname{div} H \neq 0$, then (ω, u) is clearly an eigen-pair for the above eigenvalue problem (3.37). In Appendix B, we characterize the limiting behavior of the resonances of (3.37) following the analysis in [2, 9], which readily provides a sufficient condition for the existence of the embedded eigenvalue of the Maxwell operator $\mathcal{M}_\varepsilon(0)$.

Theorem 3.8. *Let $\omega_*(\tau) = \sqrt{\tau}^{-1} \hat{\omega}_{j_0}(\tau)$ be the lowest real resonance (3.36) of (3.6). If there holds*

$$\sqrt{\mu_{j_0}} < c_0 := \max\{\sqrt{\eta_0}^{-1}, \sqrt{\gamma_0}\}, \quad (3.38)$$

then, for large enough τ , $\omega_(\tau)$ is a subwavelength embedded eigenvalue for the scattering problem (2.3), where the constant μ_{j_0} is the j_0 th eigenvalue of the form $\tilde{A}_{\infty,0}^\mathcal{E}$ in (3.32), η_0 is the largest eigenvalue of the operator \mathcal{K}_D in (B.4), and the constant γ_0 is given in (B.11).*

Proof. We note from Proposition B.1 and Proposition B.2 that for any small $\delta > 0$, when the contrast τ is large enough, the equation (3.37) admits only trivial solution for any $\omega \in (0, \sqrt{\tau}^{-1}(c_0 - \delta))$. By Corollary 3.6, we also have $\omega_*(\tau) \leq \sqrt{\tau}^{-1} \sqrt{\mu_{j_0}}$. Then it follows from the assumption $\sqrt{\mu_{j_0}} < c_0$ that for sufficiently large τ , the problem (3.37) is well-posed at $\omega_*(\tau)$ and hence has only zero solution $u = 0$, which means that the associated H is divergence-free. \square

Remark 3.9. Since the set of real resonances is clearly a subset of all scattering resonances that satisfy the asymptotics (B.6) in the subwavelength regime, a straightforward way to relax the assumption (3.38) in the above result is to consider the constant $c_0 := \min\{\sqrt{\eta_j}^{-1}; \omega = \sqrt{\tau} \eta_j^{-1} + O(\tau^{-1}) \text{ is a real subwavelength resonance}\}$. However, to show that (3.38) can indeed hold in some scenarios, we need to quantitatively estimate the resonances of (3.6) and (3.37), which is beyond the scope of this work.

4 Fano-type reflection anomaly

This section is devoted to the investigation of the Fano-type reflection anomaly for the dielectric metasurface with broken symmetry. To this end, we first note from the symmetry assumption (3.1) that $\varepsilon(x, y, z)|_{Y_h} = \varepsilon(-x, -y, z)|_{Y_h}$. We define the symmetric and the antisymmetric vector fields for the inversion operation $(x', x_3) \rightarrow (-x', x_3)$ via the projections (2.44):

$$\mathbf{L}_{sym}^2(D) := \{f \in \mathbf{L}^2(D); f_1(x', x_3) = f_1(-x', x_3), f_2(x', x_3) = f_2(-x', x_3), f_3(x', x_3) = -f_3(-x', x_3)\}, \quad (4.1)$$

and

$$\mathbf{L}_{ant}^2(D) := \{f \in \mathbf{L}^2(D); f_1(x', x_3) = -f_1(-x', x_3), f_2(x', x_3) = -f_2(-x', x_3), f_3(x', x_3) = f_3(-x', x_3)\}. \quad (4.2)$$

One may observe that $\mathbf{L}_{sym}^2(D) := \mathbf{L}^2(D) \cap (M_{0,1} \cup M_{1,0})$ and $\mathbf{L}_{ant}^2(D) := \mathbf{L}^2(D) \cap (M_{0,0} \cup M_{1,1})$, where $M_{i,j}$ are given in (3.35). We write $\mathbf{H}_{ant}(\text{div}0, D) := \mathbf{L}_{ant}^2(D) \cap \mathbf{H}(\text{div}0, D)$ and $\mathbf{H}_{sym}(\text{div}0, D) := \mathbf{L}_{sym}^2(D) \cap \mathbf{H}(\text{div}0, D)$. Similarly, we denote by $\mathbf{H}_{0,ant}(\text{div}0, D)$ and $\mathbf{H}_{0,sym}(\text{div}0, D)$ the antisymmetric and symmetric parts of the space $\mathbf{H}_0(\text{div}0, D)$.

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

$$E^i = \mathbf{p}^i e^{i\omega \mathbf{d} \cdot x}, \quad H^i = \frac{1}{i\omega} \nabla \times E^i = \mathbf{d} \times \mathbf{p}^i e^{i\omega \mathbf{d} \cdot x}, \quad \omega > 0, \quad (4.3)$$

where $\mathbf{d} \in \mathbb{S}$ is the incident direction with $d_3 > 0$, and $\mathbf{p}^i \in \mathbb{S}$ is the polarization vector with $\mathbf{p}^i \cdot \mathbf{d} = 0$. By Fredholm alternative, the scattering problem (2.3) with $\alpha = \omega d'$ is solvable for any incident plane wave with $\omega > 0$ [69], although the solution may not be unique. Note that the subwavelength incident frequency, i.e., $\omega \ll 1$, is located in the first radiation continuum $|\alpha| < \omega < \inf_{q \in \Lambda^* \setminus \{0\}} |\alpha + q|$, so that the scattered wave E^s consists of a single propagating mode in the far field. In what follows, we write $f \sim g$ for two continuous functions (vector fields) on \mathbb{R} if there holds $|f(x) - g(x)| = O(e^{-K|x_3|})$ as $x_3 \rightarrow \pm\infty$. Then the total electric field E is of the form:

$$E \sim \begin{cases} \mathbf{p}^t e^{i\omega \mathbf{d}_+ \cdot x} & x_3 \rightarrow \infty, \\ \mathbf{p}^i e^{i\omega \mathbf{d}_+ \cdot x} + \mathbf{p}^r e^{i\omega \mathbf{d}_- \cdot x} & x_3 \rightarrow -\infty, \end{cases} \quad (4.4)$$

where $\mathbf{d}_\pm = (d', \pm d_3)$, and \mathbf{p}^t and \mathbf{p}^r are the reflection and transmission polarization vectors, respectively. Moreover, the energy conservation gives [28]

$$|\mathbf{p}^t|^2 + |\mathbf{p}^r|^2 = |\mathbf{p}^i|^2 = 1.$$

We next derive the volume integral representations for \mathbf{p}^t and \mathbf{p}^r . We recall the quasi-periodic Green's function (2.7) with $\alpha = \omega d'$:

$$G^{\omega d', \omega}(x) = \frac{i}{2} \frac{e^{i\omega d' \cdot x'} e^{i\omega d_3 |x_3|}}{\omega d_3} + \frac{1}{2} \sum_{q \in \Lambda^* \setminus \{0\}} \frac{e^{i(\omega d' + q) \cdot x'} e^{-\sqrt{|\omega d' + q|^2 - \omega^2} |x_3|}}{\sqrt{|\omega d' + q|^2 - \omega^2}}. \quad (4.5)$$

which implies, as $|x_3| \rightarrow \infty$,

$$G^{\omega d', \omega}(x) \sim \frac{i}{2} \frac{e^{i\omega d' \cdot x'} e^{i\omega d_3 |x_3|}}{\omega d_3}.$$

Then it follows from the Lippmann-Schwinger equation (2.12) that as $x_3 \rightarrow \pm\infty$,

$$E \sim \mathbf{p}^i e^{i\omega \mathbf{d}_+ \cdot x} + \mathbf{p}_\pm(\mathbf{d}, D) e^{i\omega \mathbf{d}_\pm \cdot x}, \quad (4.6)$$

where $E = (1 - \tau \mathcal{T}_D^{\omega d', \omega})^{-1} [E^i] = \tau^{-1} \mathcal{A}_\tau(\omega d', \omega)^{-1} [E^i]$ (cf. (2.14)) and

$$\mathbf{p}_\pm(\mathbf{d}, D) = \tau \frac{i\omega}{2d_3} (\mathbf{I} - \mathbf{d}_\pm \otimes \mathbf{d}_\pm) \int_D e^{-i\omega \mathbf{d}_\pm \cdot y} E(y) dy. \quad (4.7)$$

Combining (4.4) and (4.6) readily gives $\mathbf{p}^t = \mathbf{p}^i + \mathbf{p}_+$ and $\mathbf{p}^r = \mathbf{p}_-$.

In Section 3, we have considered the case of the normal incident wave (i.e., $\mathbf{d} = (0, 0, 1)$) and discussed the existence of embedded eigenvalues under the symmetry assumption for the metasurface (3.1). In this case, we have the bound states in the continuum with the energy confined near the metasurface. When the symmetry is broken, the real resonance may be shifted into the complex plane and the resonant modes can propagate into the far field, which leads to the anomalous Fano scattering phenomena near the resonances. Inspired by recent physical advances [16, 49, 90], we break the symmetry (3.1) by perturbing the domain D by a symmetric field V , i.e.,

$$V(x) \in \mathbf{L}_{sym}^2(\Omega) \cap \mathbf{C}^\infty(\Omega) \quad (4.8)$$

with $\mathbf{L}_{sym}^2(\Omega)$ defined as in (4.1), where Ω is an open neighborhood of \bar{D} , and considering the incident direction $\mathbf{d} \in \mathbb{S}$ perturbed from the normal incidence:

$$\mathbf{d} = (\epsilon \alpha_0, d_3), \quad \text{with } \epsilon \ll 1 \text{ and } |\alpha_0| = 1. \quad (4.9)$$

We denote the perturbed domain by

$$D_t := (I + tV)(D), \quad |t| \ll 1. \quad (4.10)$$

The main aim of this section is to approximate the scattered polarization $\mathbf{p}_\pm(\mathbf{d}, D_t)$ for such symmetry-broken configuration uniformly in the incident frequency ω near the real resonance, and analyze the reflection and transmission energy $|\mathbf{p}^r|^2$ and $|\mathbf{p}^t|^2$.

For the sake of simplicity and clarity, we introduce the following assumptions:

C.1 In view of Theorems 3.7 and 3.8, we assume that ω_* is a subwavelength embedded eigenvalue of (2.3) for the normal incidence with an antisymmetric eigenfunction $E \in \mathbf{H}_{ant}(\text{div}0, D)$ satisfying $\mathcal{A}_\tau(0, \omega_*)[E] = 0$.

C.2 By Theorem 2.2, without loss of generality, we let $\omega_* = \sqrt{\tau\lambda_0}^{-1} + O(\tau^{-1})$ with λ_0 being the largest eigenvalue of the operator $\mathbb{P}_d \mathcal{K}_D^{0,0} \mathbb{P}_d$. We assume that the eigenspace of $\mathbb{P}_d \mathcal{K}_D^{0,0} \mathbb{P}_d$ for λ_0 is spanned by a real antisymmetric field $\varphi_1 \in \mathbf{H}_{0,ant}(\text{div}0, D)$ and a real symmetric field $\varphi_2 \in \mathbf{H}_{0,sym}(\text{div}0, D)$.

C.3 Let $\hat{\omega} = \sqrt{\tau}\omega > 0$ be the scaled incident frequency. We assume that $\hat{\omega} - \sqrt{\tau}\omega_*$ is in a small compact neighbourhood U of the origin. We always write $\hat{\omega}_0 = \sqrt{\lambda_0}^{-1}$ in what follows.

To justify the reasonability of the assumption (C.2), we first note that since the kernel $G^{0,0}$ of the operator $\mathcal{K}_D^{0,0}$ is real, it suffices to consider the real eigenfunctions of $\mathbb{P}_d \mathcal{K}_D^{0,0} \mathbb{P}_d$. Moreover, it is easy to check that for $\varphi \in \mathbf{H}_0(\text{div}0, D)$, we can decompose it as $\varphi = \varphi_{sym} + \varphi_{ant}$ with $\varphi_{sym} \in \mathbf{H}_{0,sym}(\text{div}0, D)$ and $\varphi_{ant} \in \mathbf{H}_{0,ant}(\text{div}0, D)$, where both $\mathbf{H}_{0,ant}(\text{div}0, D)$ and $\mathbf{H}_{0,sym}(\text{div}0, D)$ are invariant subspaces of $\mathbb{P}_d \mathcal{K}_D^{0,0} \mathbb{P}_d$. It follows that if φ is an eigenfunction for $\mathbb{P}_d \mathcal{K}_D^{0,0} \mathbb{P}_d$ associated with the eigenvalue λ_0 , which is neither antisymmetric or symmetric, then φ_{sym} and φ_{ant} are linearly independent eigenfunctions for λ_0 . However, it is a difficult task to characterize the conditions when the eigenspace is of dimension two and exactly spanned by φ_{sym} and φ_{ant} . From the generic simplicity [23, 84], we expect that such result holds generically, at least in the dilute regime. But here we leave the detailed investigation for a future work. We remark that this fact can be proved for the acoustic Minnaert resonance in terms of the capacitance matrix [3, 4]. But in our case, due to the infinite-dimensional kernel of the leading-order operator of $\mathcal{T}_D^{\alpha,\omega}$ consisting of magnetostatic fields, there is essentially an infinite number of scattering resonances hybridizing with each other so that the capacitance-matrix characterization is not available. We also would like to mention that an alternative approach to analyze the Fano anomaly is to regard the reflection energy $|\mathbf{p}^r|^2$ as an analytic function in ω and investigate its behavior near the embedded eigenvalue by the asymptotic analysis as in [70, Sections 5.2 and 5.3]. In this way, the assumption (C.2) can be removed (but some additional assumptions may be involved).

We shall design a structure in terms of the parameters $\alpha_0, V, \tau, \epsilon$ and τ , under the assumptions (C.1)-(C.3), such that the reflection energy $|\mathbf{p}^r|^2$ presents a Fano-resonance shape near ω_* . The analysis for the transmission energy is similar. Before we proceed, we collect some asymptotic formulas from [3, 9] for the Green's functions and the integral operators, which apply to the general domain D without any symmetry assumption.

We start with the Taylor expansion of $G^{\omega d', \omega}$ in (4.5): as $\omega \rightarrow 0$,

$$G^{\omega d', \omega}(x) = -\frac{1}{2i\omega d_3} + G_0^{d'}(x) + \omega G_1^{d'}(x) + \sum_{n=2}^{\infty} \omega^n G_n^{d'}(x), \quad (4.11)$$

where the function $G_0^{d'}$ is defined by

$$G_0^{d'}(x) := G^{0,0}(x) - \frac{d' \cdot x'}{2d_3}, \quad (4.12)$$

with $G^{0,0}(\mathbf{x})$ being the periodic Green's function (i.e., $G^{\alpha,\omega}$ with $\alpha = 0$ and $\omega = 0$), and $G_1^{d'}$ is given by

$$G_1^{d'} := -\frac{i(d_3|x_3| + d' \cdot x')^2}{4d_3} - d' \cdot g_1(x), \quad (4.13)$$

with g_1 being a purely imaginary vector-valued function independent of d' and ω and satisfying

$$g_1(x', x_3) = g_1(x', -x_3) = -g_1(-x', x_3). \quad (4.14)$$

Then, by (4.11), we have the asymptotics for the operators $\mathcal{K}_D^{\omega d', \omega}$ and $\mathcal{T}_D^{\omega d', \omega}$ in (2.9) and (2.10): for $\varphi \in \mathbf{L}^2(D)$,

$$\mathcal{K}_D^{\omega d', \omega}[\varphi] = -\frac{1}{2i\omega d_3} \langle 1, \varphi \rangle_D + \sum_{n=0}^{\infty} \omega^n \mathcal{K}_{D,n}^{d'}[\varphi],$$

and

$$\mathcal{T}_D^{\omega d', \omega} = \sum_{n=0}^{\infty} \omega^n \mathcal{T}_{D,n}^{d'}, \quad (4.15)$$

where the series converge in the operator norm for $\omega \ll 1$. Here the operators $\mathcal{K}_{D,n}^{d'}$, $n \geq 0$, are defined by

$$\mathcal{K}_{D,n}^{d'}[\varphi] := \int_D G_n^{d'}(x-y) \varphi(y) dy, \quad (4.16)$$

with $G_n^{d'}$ given in (4.11), while the operators $\mathcal{T}_{D,n}^{d'}, n \geq 0$, are defined by

$$\mathcal{T}_{D,0}^{d'}[\varphi] = \nabla \operatorname{div} \mathcal{K}_{D,0}^{d'}[\varphi], \quad \mathcal{T}_{D,1}^{d'}[\varphi] = -\frac{1}{2id_3} \langle 1, \varphi \rangle_D + \nabla \operatorname{div} \mathcal{K}_{D,1}^{d'}[\varphi],$$

and

$$\mathcal{T}_{D,n}^{d'}[\varphi] := \mathcal{K}_{D,n-2}^{d'}[\varphi] + \nabla \operatorname{div} \mathcal{K}_{D,n}^{d'}[\varphi], \quad n \geq 2. \quad (4.17)$$

In particular, we can derive, by (4.12) and (4.16),

$$\mathcal{K}_{D,0}^{d'}[\varphi] = \mathcal{K}_D^{0,0}[\varphi] - \frac{d' \cdot x'}{2d_3} \langle 1, \varphi \rangle + \frac{1}{2d_3} \int_D d' \cdot y' \varphi(y) dy,$$

which gives

$$\mathbb{P}_d \mathcal{K}_{D,0}^{d'} \mathbb{P}_d = \mathbb{P}_d \mathcal{K}_D^{0,0} \mathbb{P}_d, \quad (4.18)$$

and

$$\mathcal{T}_{D,0}^{d'}[\varphi] = \nabla \operatorname{div} \mathcal{K}_{D,0}^{d'}[\varphi] = \nabla \operatorname{div} \mathcal{K}_D^{0,0}[\varphi] = \mathcal{T}_D^{0,0}[\varphi]. \quad (4.19)$$

The following result on the basic properties of the operator $\mathcal{T}_D^{0,0}$ is adapted from [9, Lemma 3.6].

Lemma 4.1. *Both W and $\mathbf{H}_0(\operatorname{div}0, D)$ are the invariant subspaces of the operator $\mathcal{T}_D^{0,0} : \mathbf{H}(\operatorname{div}0, D) \rightarrow \mathbf{H}(\operatorname{div}0, D)$ with $\ker \mathcal{T}_D^{0,0} = \mathbf{H}_0(\operatorname{div}0, D)$. Moreover, we have $\sigma(\mathcal{T}_D^{0,0}|_W) \subset [-1, 0)$ and $\sigma(\mathcal{T}_D^{0,0}) = \sigma(\mathcal{T}_D^{0,0}|_W) \cup \{0\}$.*

By integration by parts, it is easy to see that

$$(\phi, \mathcal{T}_{D,n}^{d'}[\varphi])_D = (\phi, (\mathcal{K}_{D,n-2}^{d'} + \nabla \operatorname{div} \mathcal{K}_{D,n}^{d'})[\varphi])_D = (\phi, \mathcal{K}_{D,n-2}^{d'}[\varphi])_D, \quad (4.20)$$

for any $\phi \in \mathbf{L}^2(D)$, $\varphi \in \mathbf{H}_0(\operatorname{div}0, D)$, or $\varphi \in \mathbf{L}^2(D)$, $\phi \in \mathbf{H}_0(\operatorname{div}0, D)$. It readily gives

$$\mathbb{P}_s \mathcal{K}_{D,n-2}^{d'} \mathbb{P}_t = \mathbb{P}_s \mathcal{T}_{D,n}^{d'} \mathbb{P}_t, \quad \text{for } s, t = d, w \text{ except the case } s, t = w. \quad (4.21)$$

It follows from (4.15) and (4.21) that

$$\mathbb{P}_s \mathcal{T}_D^{\omega d', \omega} \mathbb{P}_t = \sum_{n=2}^{\infty} \omega^n \mathbb{P}_s \mathcal{K}_{D,n-2}^{d'} \mathbb{P}_t, \quad \text{for } s, t = d, w \text{ except the case } s, t = w, \quad (4.22)$$

and

$$\mathbb{P}_w \mathcal{T}_D^{\omega d', \omega} \mathbb{P}_w = \sum_{n=0}^{\infty} \omega^n \mathbb{P}_w \mathcal{T}_{D,n}^{d'} \mathbb{P}_w. \quad (4.23)$$

We are now ready to give the first-order approximation for the subwavelength resonances ω (i.e., the poles of the meromorphic function $\mathcal{A}_\tau(\omega d', \omega)^{-1}$ near the origin) in terms of the high contrast τ . For convenience, we define

$$\mathbb{K}_D := \mathbb{P}_d \mathcal{K}_D^{0,0} \mathbb{P}_d : \mathbf{H}_0(\operatorname{div}0, D) \rightarrow \mathbf{H}_0(\operatorname{div}0, D). \quad (4.24)$$

Theorem 4.2. *Let D be a general smooth domain. When the contrast τ is large enough, the scattering resonances for the problem (2.3) with the plane wave incidence (4.3) exist in the subwavelength regime. Moreover, for any subwavelength resonance ω , as $\tau \rightarrow \infty$, there exists some eigenvalue λ_i of the operator \mathbb{K}_D with the orthogonal eigenfunctions $\{\varphi_j\}_{j=1}^{n_i} \in \mathbf{H}_0(\operatorname{div}0, D)$ such that the following asymptotics holds,*

$$\omega = \frac{1}{\sqrt{\tau} \lambda_i} - \frac{c_{i,j}}{2\tau \lambda_i^2} + O(\tau^{-\frac{3}{2}}), \quad (4.25)$$

where $c_{i,j}$, $1 \leq j \leq n_i$ are the eigenvalues of the matrix C defined by

$$C_{kl} = (\varphi_k, \mathbb{P}_d \mathcal{K}_{D,1}^{d'} \mathbb{P}_d[\varphi_l])_D, \quad \text{for } 1 \leq k, l \leq n_i. \quad (4.26)$$

Proof. By the generalized Rouché theorem [34, 35] and a similar argument as in [9, Section 3.3], we have the existence of the subwavelength resonances $\omega = O(\sqrt{\tau}^{-1})$ in the high contrast regime. To derive the asymptotic formula for a subwavelength resonance ω , we consider the equation

$$\mathcal{A}_\tau(\omega d', \omega)[E] = 0 \quad \text{with } E \in \mathbf{H}(\text{div}0, D) \text{ and } \|E\|_D = 1. \quad (4.27)$$

Acting the projection \mathbb{P}_w on the above equation gives, by (4.19), (4.22), and (4.23),

$$\left(\mathcal{T}_D^{0,0} + O(\sqrt{\tau}^{-1})\right)[\mathbb{P}_w E] = O(\tau^{-1}),$$

which, by the invertibility of $\mathcal{T}_D^{0,0}$ on W in Lemma 4.1, implies $\mathbb{P}_w E = O(\tau^{-1})$. We then act the projection \mathbb{P}_d on the equation (4.27) and find, by (4.18) and (4.22),

$$(1 - \hat{\omega}^2 \mathbb{K}_D - \sqrt{\tau}^{-1} \hat{\omega}^3 \mathbb{P}_d \mathcal{K}_{D,1}^{d'} \mathbb{P}_d + O(\tau^{-1}))[E] = O(\tau^{-1}), \quad (4.28)$$

where $\hat{\omega} = \sqrt{\tau}\omega$ is the scaled resonance. It is easy to observe from (4.28) that the leading-order approximation for $\hat{\omega}$ is given by $\hat{\omega} = \sqrt{\lambda_i}^{-1} + O(\sqrt{\tau}^{-1})$ for some eigenvalue λ_i of \mathbb{K}_D . For the higher-order approximation, letting $\{\varphi_j\}_{j=1}^{n_i}$ be the orthogonal eigenfunctions of \mathbb{K}_D for λ_i , by the standard perturbation theory with the Lyapunov–Schmidt reduction, we need to consider the zeros of the following determinant near $\hat{\omega}_i := \sqrt{\lambda_i}^{-1}$:

$$\det(I - \hat{\omega}^2 \lambda_i I - \sqrt{\tau}^{-1} \hat{\omega}^3 C) = 0, \quad (4.29)$$

with the $n_i \times n_i$ matrix C given in (4.26). It is easy to see that linearizing the above equation (4.29) at $\hat{\omega}_i$ gives

$$\det(-2(\hat{\omega} - \hat{\omega}_i)\hat{\omega}_i^{-1}I - \sqrt{\tau}^{-1}\hat{\omega}_i^3 C) = 0.$$

Then, the desired approximation (4.25) for the resonance follows. \square

4.1 Shape derivatives and asymptotics

In order to analyze the scattering effect by the symmetry-broken metasurface, it is necessary to understand the dependence of the subwavelength resonance ω on the domain D . For this, in view of (4.25), we will compute the shape derivatives of the eigenvalues λ_i of the operator \mathbb{K}_D , which is also of independent interest.

Suppose that Ω is a smooth convex bounded domain such that $\bar{D} \subset \Omega$ and let $V \in \mathbf{C}^\infty(\Omega)$ be the feasible deformation fields. For a given field V , we define the map $\Phi_t := I + tV$ for $t \geq 0$. Then $\Phi_0(D) = D$ and Φ_t gives a family of C^∞ -diffeomorphisms for small enough $|t|$. As in (4.10), we denote by $D_t = \Phi_t(D)$ the deformed domain. Moreover, for any diffeomorphism Φ on D , we introduce the pullback of a function f on $\Phi(D)$: $\Phi^* f = f \circ \Phi$, and the pushforward of a function g on D : $\Phi_* g = g \circ \Phi^{-1}$. Note that Φ_* is a smooth bijective map between $\mathbf{L}^2(D_t)$ and $\mathbf{L}^2(D)$. With these notions, the eigenvalue problem on the deformed domain D_t :

$$\mathbb{K}_{D_t}[E] = \lambda E, \quad \text{on } \mathbf{L}^2(D_t),$$

can be equivalently transformed into a family of eigenvalue problems on the reference domain D :

$$\tilde{\mathbb{K}}_{D,t}[E] = \lambda E, \quad \text{on } \mathbf{L}^2(D), \quad \text{with } \tilde{\mathbb{K}}_{D,t} := \Phi_t^* \mathbb{K}_{D_t} \Phi_{t,*}. \quad (4.30)$$

It is clear that the operator $\tilde{\mathbb{K}}_{D,t}$ is the composition of

$$\mathbb{P}_D^t := \Phi_t^* \mathbb{P}_{d,D_t} \Phi_{t,*} \quad \text{and} \quad \tilde{\mathcal{K}}_D^t := \Phi_t^* \mathcal{K}_{D_t}^{0,0} \Phi_{t,*}, \quad (4.31)$$

namely, $\tilde{\mathbb{K}}_{D,t} = \mathbb{P}_D^t \tilde{\mathcal{K}}_D^t \mathbb{P}_D^t$, where $\mathbb{P}_{d,D_t} : \mathbf{L}^2(D_t) \rightarrow \mathbf{H}_0(\text{div}0, D_t)$ is the projection defined as in (2.16) (we add the subscript to emphasize its dependence on the domain). The main results of this section are as follows. We postpone their proofs to Appendix C for the sake of clarity.

Lemma 4.3. *The operators $\mathbb{P}_D^t, \tilde{\mathcal{K}}_D^t : \mathbf{L}^2(D) \rightarrow \mathbf{L}^2(D)$, defined in (4.31), are differentiable at $t = 0$ with the derivatives:*

$$\left. \frac{d}{dt} \right|_{t=0} \mathbb{P}_D^t[E] = (\nabla V)^T \mathbb{P}_{d,D}^\perp E - \nabla w, \quad (4.32)$$

with $w \in H^1(D)$ being a solution to

$$(\nabla w, \nabla \varphi)_D = ((-\nabla V + \text{div}V)\mathbb{P}_{d,D} E + (\nabla V)^T \mathbb{P}_{d,D}^\perp E, \nabla \varphi)_D, \quad \forall \varphi \in H^1(D), \quad (4.33)$$

and

$$\left. \frac{d}{dt} \right|_{t=0} \tilde{\mathcal{K}}_D^t[E] = \int_D -\text{div}_y [G^{0,0}(x, y)(V(x) - V(y))] E(y) dy. \quad (4.34)$$

Here, the projection $\mathbb{P}_{d,D}^\perp$ is the orthogonal complement of $\mathbb{P}_{d,D}$.

Proposition 4.4. *Suppose that λ_0 is an eigenvalue of the operator \mathbb{K}_D with eigenfunctions $\{\varphi_j\}_{j=1}^m \subset \mathbf{L}^2(D)$. Then, given a deformation field $V \in \mathbf{C}^\infty(\Omega)$, there exists $0 < t_0 \ll 1$ such that for any $|t| \leq t_0$, the operator \mathbb{K}_{D_t} on the perturbed domain $D_t = \Phi_t(D)$ has exactly m eigenvalues near λ_0 , denoted by $\{\lambda_{0,j}(t)\}_{j=1}^m$, that are continuously differentiable in t with the derivatives $\dot{\lambda}_{0,j}(0)$ being eigenvalues of the $m \times m$ Hermitian matrix \hat{K} defined by*

$$\hat{K}_{ij} := \left. \frac{d}{dt} \right|_{t=0} K_{ij}(t) = \lambda_0(\nu \cdot V\varphi_i, \varphi_j)_{\partial D}, \quad (4.35)$$

where

$$K_{ij}(t) := (\varphi_i, \tilde{\mathbb{K}}_{D,t}\varphi_j)_D.$$

With Theorem 4.2 and Proposition 4.4 above, we can easily derive the asymptotic expansions of the subwavelength resonances for the symmetry-broken geometry, which will be useful in the next section. For ease of exposition, we first introduce the following matrices under the assumptions (C.1)-(C.3) with the incident direction \mathbf{d} given in (4.9). Let the fields $\varphi_1 \in \mathbf{H}_{0,ant}(\text{div}0, D)$ and $\varphi_2 \in \mathbf{H}_{0,sym}(\text{div}0, D)$ be given in the assumption (C.2), and V be a deformation field (4.8). By a slight abuse of notation, we define the 2×2 symmetric matrix C^0 by

$$C_{ij}^0 := (\nu \cdot V\varphi_i, \varphi_j)_{\partial D}, \quad (4.36)$$

and the 2×2 matrix C^{1,α_0} as in (4.26) by

$$C_{ij}^{1,\alpha_0} := (\varphi_i, \mathbb{P}_d \mathcal{K}_{D,1}^{\epsilon\alpha_0} \mathbb{P}_d[\varphi_j])_D. \quad (4.37)$$

Note from (3.1) that the unit outer normal vector ν to ∂D is antisymmetric in the sense of (4.2). Thanks to the symmetry properties of V and φ_i , we have

$$C^0 = \begin{bmatrix} 0 & c_0 \\ c_0 & 0 \end{bmatrix}, \quad \text{with } c_0 := (\nu \cdot V\varphi_1, \varphi_2)_{\partial D}. \quad (4.38)$$

Moreover, recalling the kernel $G_1^{\epsilon\alpha_0}$ (4.13) for the operator $\mathbb{P}_d \mathcal{K}_{D,1}^{\epsilon\alpha_0} \mathbb{P}_d$, we write it as

$$G_1^{\epsilon\alpha_0}(x) = iK_1(x) + i\epsilon^2 K_2(x) + i\epsilon K_3(x),$$

with

$$K_1(x) = -\frac{d_3|x_3|^2}{4}, \quad K_2(x) = -\frac{(\alpha_0 \cdot x')^2}{4d_3}, \quad K_3(x) = -\alpha_0 \cdot \left(\frac{|x_3|x'}{2} - ig_1(x) \right).$$

We remark that all K_i are real functions, since g_1 is purely imaginary. Again, by the symmetry of φ_i and g_1 in (4.14), it follows that

$$C^{1,\alpha_0} = i \begin{bmatrix} c_{1,1} & 0 \\ 0 & c_{1,2} \end{bmatrix} + i\epsilon^2 \begin{bmatrix} c_{2,1} & 0 \\ 0 & c_{2,2} \end{bmatrix} + i\epsilon \begin{bmatrix} 0 & c_3 \\ -c_3 & 0 \end{bmatrix}, \quad (4.39)$$

with real numbers:

$$c_{s,l} = \int_D \int_D K_s(x-y) \varphi_l(x) \cdot \varphi_l(y) \, dx dy, \quad s = 1, 2, \quad l = 1, 2, \quad (4.40)$$

and

$$c_3 = \int_D \int_D K_3(x-y) \varphi_2(x) \cdot \varphi_1(y) \, dx dy. \quad (4.41)$$

We claim that $c_{1,1}$ is zero and $c_{1,2} \geq 0$. Indeed, if the assumptions (C.1) and (C.2) hold, Theorem 4.2 for the case of the normal incidence and the symmetric domain D shows that there are two characteristic values ω_1 and ω_2 of $\mathcal{A}_\tau(0, \omega)$ near $\sqrt{\tau\lambda_0}^{-1}$ with asymptotics: for $j = 1, 2$, as $\tau \rightarrow \infty$,

$$\omega_j = \frac{1}{\sqrt{\tau\lambda_0}} - \frac{ic_{1,j}}{2\tau\lambda_0^2} + O(\tau^{-\frac{3}{2}}), \quad (4.42)$$

where $c_{1,j}$, $j = 1, 2$, is defined in (4.40). Noting that the resonance $\omega_1 = \omega_*$ corresponds to the antisymmetric function, the assumption (C.1) enforces the vanishing of the imaginary part of ω_1 , that is, $c_{1,1} = 0$ and

$$\omega_* = \frac{1}{\sqrt{\tau\lambda_0}} + O(\tau^{-\frac{3}{2}}). \quad (4.43)$$

Moreover, it is well known that the scattering resonances exist in the lower half plane [9, 29], which implies $c_{1,2} \geq 0$.

Corollary 4.5. *Given a deformation field V in (4.8), let \mathbf{d} and D_t be the perturbed incident direction and domain defined in (4.9) and (4.10). Under the assumptions (C.1) and (C.2), there exist two subwavelength resonances ω_1 and ω_2 near $\sqrt{\tau\lambda_0}^{-1}$ for the scattering problem (2.3) with $\alpha = \epsilon\alpha_0$, which satisfy the asymptotic expansions: for $j = 1, 2$,*

$$\omega_j = \frac{1}{\sqrt{\tau}} \left(\frac{1}{\sqrt{\lambda_0}} - \frac{\mu_{0,j}}{2} \right) + O(\tau^{-\frac{3}{2}} + |t|^2\tau^{-\frac{1}{2}}), \quad \text{as } \tau \rightarrow \infty, |t| \rightarrow 0,$$

with $\mu_{0,j}$ being the eigenvalues of the following matrix:

$$\mathbf{M} = t\lambda_0^{-\frac{1}{2}} \begin{bmatrix} 0 & c_0 \\ c_0 & 0 \end{bmatrix} + \tau^{-\frac{1}{2}}\lambda_0^{-2} \left(i \begin{bmatrix} 0 & 0 \\ 0 & c_{1,2} \end{bmatrix} + i\epsilon \begin{bmatrix} 0 & c_3 \\ -c_3 & 0 \end{bmatrix} \right) + O(\epsilon^2\tau^{-\frac{1}{2}}), \quad (4.44)$$

where $c_{1,2} \geq 0$ and $c_0, c_3 \in \mathbb{R}$ are given in (4.38), (4.40) and (4.41).

Proof. We only provide a sketch of the proof, as it is almost the same as those of Theorem 4.2 and Proposition 4.4. Let $\hat{\omega} = \sqrt{\tau}\omega$ be the scaled resonance. We consider the characteristic values of $(1 - \tau\mathcal{T}_{D_t}^{\omega d', \omega})[E] = 0$ near $\sqrt{\tau}^{-1}\hat{\omega}_0$ with $\|E\|_D = 1$ and $\hat{\omega}_0 = \sqrt{\lambda_0}^{-1}$. Similarly to the proof of Theorem 4.2, there holds $\mathbb{P}_w E = O(\tau^{-1})$, and it suffices to solve, after mapping the problem to the reference domain D as in (4.30),

$$(1 - \hat{\omega}^2 \tilde{\mathbb{K}}_{D,t} - \sqrt{\tau}^{-1} \hat{\omega}^3 \mathbb{P}_D^t \Phi_t^* \mathcal{K}_{D,1}^{d'} \Phi_{t,*} \mathbb{P}_D^t)[\Phi_t^* E] = O(\tau^{-1}). \quad (4.45)$$

We linearize the above equation (4.45) at $\hat{\omega} = \hat{\omega}_0$ and $t = 0$, and find that, up to an error term of $O(\tau^{-1}) + O(|t|^2)$, the scaled resonance $\hat{\omega}$ near $\hat{\omega}_0$ satisfies

$$\det \left(-2(\hat{\omega} - \hat{\omega}_0)\hat{\omega}_0^{-1}\mathbf{I} - t\mathbf{C}^0 - \sqrt{\tau}^{-1}\hat{\omega}_0^3\mathbf{C}^{1,\alpha_0} \right) = 0,$$

which readily completes the proof, by a direct computation. \square

4.2 Analysis of the reflection energy

In this section, we investigate the Fano-type transmission and reflection anomalies. For this, we will first derive the leading-order approximation for the scattered polarization vectors \mathbf{p}_{\pm} defined in (4.7). Let φ_1 and φ_2 be the antisymmetric and symmetric functions in the assumption (C.2), respectively. We introduce the following two 3×3 real matrices for later use:

$$\mathbf{A}^{ant} = \int_D x \otimes \varphi_1 dx, \quad \mathbf{A}^{sym} = \int_D x \otimes \varphi_2 dx. \quad (4.46)$$

By symmetry, it is easy to see that \mathbf{A}^{ant} and \mathbf{A}^{sym} are of the block form:

$$\mathbf{A}^{ant} = \begin{bmatrix} \mathbf{A}_1 & 0 \\ 0 & a_2 \end{bmatrix}, \quad \mathbf{A}^{sym} = \begin{bmatrix} 0 & \mathbf{b}_1 \\ \mathbf{b}_2^T & 0 \end{bmatrix},$$

where $\mathbf{b}_1, \mathbf{b}_2 \in \mathbb{R}^2$ and \mathbf{A}_1 is the 2×2 matrix. The following proposition characterizes the solution of the volume integral equation for the incident frequency ω near the embedded eigenvalue ω_* :

$$(1 - \tau\mathcal{T}_{D_t}^{\omega d', \omega})[E] = E^i. \quad (4.47)$$

Theorem 4.6. *Suppose that the assumptions (C.1)-(C.3) hold. Define $\hat{\omega}_{0,j} := \hat{\omega}_0 - \mu_{0,j}/2$ for $j = 1, 2$ with $\mu_{0,j}$ given in Corollary 4.5. There exists a constant $C_A > 0$ such that when $|t| + \tau^{-\frac{1}{2}} \leq C_A|\hat{\omega} - \hat{\omega}_0|$, the solution $E \in \mathbf{H}(\text{div}0, D_t)$ to the equation (4.47) has the asymptotic expansion uniformly in $\hat{\omega}$ near $\hat{\omega}_0$:*

$$\begin{cases} \Phi_t^* \mathbb{P}_{w, D_t} E = -\tau^{-1}(\mathcal{T}_D^{0,0})^{-1}[\mathbf{p}^i] + O\left(\tau^{-1}|t| + \frac{\tau^{-\frac{3}{2}}}{|\hat{\omega} - \hat{\omega}_0|}\right), \\ \Phi_t^* \mathbb{P}_{d, D_t} E = q_1\varphi_1 + q_2\varphi_2 + O\left(\tau^{-\frac{1}{2}} + \frac{\tau^{-\frac{1}{2}}|t| + \tau^{-1}}{|\hat{\omega} - \hat{\omega}_0|}\right), \end{cases} \quad \text{as } \tau \rightarrow \infty, |t| \rightarrow 0, \quad (4.48)$$

with $q_1, q_2 \in \mathbb{C}$ given by

$$\begin{bmatrix} q_1 \\ q_2 \end{bmatrix} = \frac{1 - \hat{\omega}^2\lambda_0}{h} \left(i\tau^{-\frac{1}{2}}\hat{\omega} \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} + O\left(\tau^{-1} + \tau^{-\frac{1}{2}}|t| + \frac{\tau^{-\frac{1}{2}}(|t|^2 + \tau^{-1})}{|\hat{\omega} - \hat{\omega}_0|}\right) \right), \quad (4.49)$$

where h is an analytic function in $\hat{\omega}$ defined by

$$h(\hat{\omega}) = r(\hat{\omega})(\hat{\omega} - \hat{\omega}_{0,1} + O(\tau^{-1} + |t|^2))(\hat{\omega} - \hat{\omega}_{0,2} + O(\tau^{-1} + |t|^2)), \quad (4.50)$$

with $r(\hat{\omega})$ being invertible and analytic in $\hat{\omega}$ with $|r(\hat{\omega})| = 1$, and the real numbers f_1 and f_2 are given by

$$f_1 := \mathbf{d} \cdot A^{ant} \mathbf{p}^i, \quad f_2 := \mathbf{d} \cdot A^{sym} \mathbf{p}^i. \quad (4.51)$$

Proof. Noting the incident frequency $\omega = O(\sqrt{\tau^{-1}})$ and that $\int_{D_t} \varphi \, dx = 0$ holds for any $\varphi \in \mathbf{H}_0(\text{div}0, D_t)$, we have the following asymptotic expansions for the incident wave:

$$\mathbb{P}_{w,D_t} E^i = \mathbf{p}^i + O(\tau^{-\frac{1}{2}}), \quad \mathbb{P}_{d,D_t} E^i = i\omega \mathbb{P}_{d,D_t} [\mathbf{p}^i \mathbf{d} \cdot x] + O(\tau^{-1}), \quad (4.52)$$

which implies, by the pullback Φ_t^* ,

$$\Phi_t^* \mathbb{P}_{d,D_t} E^i = i\omega \mathbb{P}_{d,D} [\mathbf{p}^i \mathbf{d} \cdot x] + O(\tau^{-\frac{1}{2}}|t| + \tau^{-1}).$$

It follows that, by (4.46) and (4.51),

$$\begin{aligned} (\varphi_j, \Phi_t^* \mathbb{P}_{d,D_t} E^i)_D &= i\omega (\varphi_j, \mathbf{p}^i \mathbf{d} \cdot x)_D + O(\tau^{-\frac{1}{2}}|t| + \tau^{-1}) \\ &= i\omega f_j + O(\tau^{-\frac{1}{2}}|t| + \tau^{-1}). \end{aligned} \quad (4.53)$$

Following the analysis in [9, Section 4], we reformulate the equation (4.47) on the reference domain D with a matrix form, by the projections and the pullback Φ_t^* :

$$\mathbb{A}(t, \tau, \omega) \begin{bmatrix} \Phi_t^* \mathbb{P}_{d,D_t} E \\ \Phi_t^* \mathbb{P}_{w,D_t} E \end{bmatrix} = \begin{bmatrix} \Phi_t^* \mathbb{P}_{d,D_t} E^i \\ \tau^{-1} \Phi_t^* \mathbb{P}_{w,D_t} E^i \end{bmatrix}, \quad (4.54)$$

with

$$\mathbb{A}(t, \tau, \omega) := \begin{bmatrix} 1 - \tau \Phi_t^* \mathbb{P}_{d,D_t} \mathcal{T}_{D_t}^{\omega d', \omega} \mathbb{P}_{d,D_t} \Phi_{t,*} & -\tau \Phi_t^* \mathbb{P}_{d,D_t} \mathcal{T}_{D_t}^{\omega d', \omega} \mathbb{P}_{w,D_t} \Phi_{t,*} \\ -\Phi_t^* \mathbb{P}_{w,D_t} \mathcal{T}_{D_t}^{\omega d', \omega} \mathbb{P}_{d,D_t} \Phi_{t,*} & \tau^{-1} - \Phi_t^* \mathbb{P}_{w,D_t} \mathcal{T}_{D_t}^{\omega d', \omega} \mathbb{P}_{w,D_t} \Phi_{t,*} \end{bmatrix}.$$

Similarly to Lemma 4.3, for $n \geq 1$ and $s, t = d, w$, the operator $\Phi_t^* \mathbb{P}_{s,D_t} \mathcal{T}_{D_t,n}^{d'} \mathbb{P}_{t,D_t} \Phi_{t,*}$ is differentiable at $t = 0$, and there holds

$$\Phi_t^* \mathbb{P}_{s,D_t} \mathcal{T}_{D_t,n}^{d'} \mathbb{P}_{t,D_t} \Phi_{t,*} = \mathbb{P}_{s,D} \mathcal{T}_{D_t,n}^{d'} \mathbb{P}_{t,D} + O(|t|),$$

where the error term is measured in the operator norm. Then, by expansions (4.22) and (4.23), we find

$$\mathbb{A}(t, \tau, \omega) = \begin{bmatrix} 1 - \hat{\omega}^2 \mathbb{K}_D & -\hat{\omega}^2 \mathbb{P}_d \mathcal{K}_{D,0}^{d'} \mathbb{P}_w \\ 0 & -\mathcal{T}_D^{0,0} \end{bmatrix} + \begin{bmatrix} O(|t| + \tau^{-\frac{1}{2}}) & O(|t| + \tau^{-\frac{1}{2}}) \\ O(\tau^{-1}) & O(|t| + \tau^{-\frac{1}{2}}) \end{bmatrix}. \quad (4.55)$$

Hence, for $\hat{\omega}$ near $\hat{\omega}_0$, the Neumann series expansion shows that when $|t| + \tau^{-\frac{1}{2}} = O(|\hat{\omega} - \hat{\omega}_0|)$ is suitably small, there holds $\|\mathbb{A}(t, \tau, \omega)\| \lesssim |\hat{\omega} - \hat{\omega}_0|^{-1}$. We also see from (4.52) that $[\mathbb{P}_{d,D_t} E^i, \tau^{-1} \mathbb{P}_{w,D_t} E^i] = O(\sqrt{\tau^{-1}})$. It follows that the solution $E \in \mathbf{H}_0(\text{div}0, D_t)$ to (4.47) satisfies

$$E = O(|\hat{\omega} - \hat{\omega}_0|^{-1} \tau^{-\frac{1}{2}}). \quad (4.56)$$

To obtain (4.48), we consider the second component of the equation (4.54). By estimates (4.52), (4.55) and (4.56), we have

$$\Phi_t^* \mathbb{P}_{w,D_t} E = -\tau^{-1} (\mathcal{T}_D^{0,0})^{-1} [\mathbf{p}^i] + O\left(\tau^{-1}|t| + \frac{\tau^{-\frac{3}{2}}}{|\hat{\omega} - \hat{\omega}_0|}\right). \quad (4.57)$$

Then, we consider the first component of (4.54). By the assumption (C.2), without loss of generality, let the field $\Phi_t^* \mathbb{P}_{d,D_t} E \in \mathbf{L}^2(D)$ have the following ansatz:

$$\Phi_t^* \mathbb{P}_{w,D_t} E = q_1 \varphi_1 + q_2 \varphi_2 + \phi, \quad \text{with } \phi \perp \varphi_i, \quad (4.58)$$

where $\phi \in \mathbf{L}^2(D)$ and $q_1, q_2 \in \mathbb{C}$. Substituting (4.58) into (4.54), and using the asymptotic expansions (4.22) and (4.52) and the estimate (4.57), we can derive

$$\begin{aligned} &\left(1 - \hat{\omega}^2 \tilde{\mathbb{K}}_{D,t} - \tau^{-\frac{1}{2}} \hat{\omega}^3 \mathbb{P}_D^t \Phi_t^* \mathcal{K}_{D,1}^{d'} \Phi_{t,*} \mathbb{P}_D^t + O(\tau^{-1})\right) [q_1 \varphi_1 + q_2 \varphi_2 + \phi] \\ &= i\omega \mathbb{P}_{d,D} [\mathbf{p}^i \mathbf{d} \cdot x] + O(\tau^{-\frac{1}{2}}|t| + \tau^{-1}) + O\left(\frac{\tau^{-\frac{3}{2}}}{|\hat{\omega} - \hat{\omega}_0|}\right). \end{aligned} \quad (4.59)$$

We take the inner product between the above equation (4.59) and ϕ , and obtain

$$\left| \left(\phi, (1 - \hat{\omega}^2 \mathbb{K}_D + O(|t|) + O(\tau^{-\frac{1}{2}}))[q_1 \varphi_1 + q_2 \varphi_2 + \phi] \right)_D \right| \lesssim \left(\tau^{-\frac{1}{2}} + \frac{\tau^{-\frac{3}{2}}}{|\hat{\omega} - \hat{\omega}_0|} \right) \|\phi\|_D. \quad (4.60)$$

Noting from (4.56) that $\|q_1 \varphi_1 + q_2 \varphi_2 + \phi\|_D = O(|\hat{\omega} - \hat{\omega}_0|^{-1} \tau^{-\frac{1}{2}})$, and from the ansatz (4.58) and the assumption (C.2) that, for $\hat{\omega}$ near $\sqrt{\lambda_0^{-1}}$,

$$\|\phi\|_D^2 \lesssim \left| \left(\phi, (1 - \hat{\omega}^2 \mathbb{K}_D)[q_1 \varphi_1 + q_2 \varphi_2 + \phi] \right)_D \right|,$$

we estimate

$$0 < \|\phi\|_D^2 - O\left(\frac{\tau^{-\frac{1}{2}}(|t| + \tau^{-\frac{1}{2}})}{|\hat{\omega} - \hat{\omega}_0|}\right) \|\phi\|_D \lesssim \left| \left(\phi, (1 - \hat{\omega}^2 \mathbb{K}_D + O(|t| + \tau^{-\frac{1}{2}}))[q_1 \varphi_1 + q_2 \varphi_2 + \phi] \right)_D \right|,$$

which, along with (4.60), gives

$$\phi = O\left(\tau^{-\frac{1}{2}} + \frac{\tau^{-\frac{1}{2}}|t| + \tau^{-1}}{|\hat{\omega} - \hat{\omega}_0|}\right). \quad (4.61)$$

We proceed to take the inner product between (4.59) and φ_i . We first have, by Proposition 4.4,

$$\left(\varphi_i, (1 - \hat{\omega}^2 \tilde{\mathbb{K}}_{D,t})[\varphi_j] \right)_D = (I - \hat{\omega}^2 \lambda_0 (I + tC^0))_{ij} + O(|t|^2).$$

Recalling the definition of C^{1,α_0} in (4.37), there holds

$$\left(\varphi_i, \tau^{-\frac{1}{2}} \hat{\omega}^3 \mathbb{P}_D^t \Phi_t^* \mathcal{K}_{D,1}^{d'} \Phi_{t,*} \mathbb{P}_D^t [\varphi_j] \right)_D = \tau^{-\frac{1}{2}} \hat{\omega}^3 C_{ij}^{1,\alpha_0} + O(\tau^{-\frac{1}{2}}|t|).$$

It is also easy to see, by (4.61),

$$\begin{aligned} & \left(\varphi_i, (1 - \hat{\omega}^2 \tilde{\mathbb{K}}_{D,t} - \tau^{-\frac{1}{2}} \hat{\omega}^3 \mathbb{P}_D^t \Phi_t^* \mathcal{K}_{D,1}^{d'} \Phi_{t,*} \mathbb{P}_D^t + O(\tau^{-1}))[\phi] \right)_D \\ &= O\left(\tau^{-1} + \tau^{-\frac{1}{2}}|t| + \frac{\tau^{-\frac{1}{2}}(|t|^2 + \tau^{-1})}{|\hat{\omega} - \hat{\omega}_0|}\right). \end{aligned} \quad (4.62)$$

Combining these facts together, it follows that $[q_1, q_2]$ satisfies the following matrix equation:

$$\begin{aligned} & \left(I - \hat{\omega}^2 \lambda_0 (I + tC^0) - \tau^{-\frac{1}{2}} \hat{\omega}^3 C^{1,\alpha_0} + O(\tau^{-1} + |t|^2) \right) \begin{bmatrix} q_1 \\ q_2 \end{bmatrix} \\ &= i\tau^{-\frac{1}{2}} \hat{\omega} \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} + O\left(\tau^{-1} + \tau^{-\frac{1}{2}}|t| + \frac{\tau^{-\frac{1}{2}}(|t|^2 + \tau^{-1})}{|\hat{\omega} - \hat{\omega}_0|}\right), \end{aligned} \quad (4.63)$$

where the right side is from (4.53) and (4.62).

We write $Z(\hat{\omega})$ for the coefficient matrix of the equation (4.63). By Rouché's theorem, we know that there are two zeros of the analytic function $\det(Z)$ near $\hat{\omega}_0$. We denote them by $z_1, z_2 \in \mathbb{C}$ and have, for $\hat{\omega} \in \mathbb{C}$ near $\hat{\omega}_0$,

$$\det(Z(\hat{\omega})) = r(\hat{\omega})(\hat{\omega} - z_1)(\hat{\omega} - z_2),$$

where $r(\hat{\omega})$ is an invertible analytic function near $\hat{\omega}_0$ with modulus of order one. Then, it follows from the analysis in Corollary 4.5 that z_i can be approximated by $z_i = \hat{\omega}_0 - \mu_{0,j}/2 + O(\tau^{-1} + |t|^2)$. Therefore, the formula (4.49) holds by the inverse formula for 2×2 matrices. The proof is complete by estimates (4.57), (4.58), and (4.61). \square

With the help of Theorem 4.6 above, we are now ready to derive the asymptotic expansion for the scattered polarization vectors (4.7). The estimate (4.48) has shown that, for the solution E to (4.47),

$$\mathbb{P}_{\mathbf{w}, D_t} E = O\left(\tau^{-1} + \frac{\tau^{-\frac{3}{2}}}{|\hat{\omega} - \hat{\omega}_0|}\right), \quad \mathbb{P}_{\mathbf{d}, D_t} E = O\left(\frac{\tau^{-\frac{1}{2}}}{|\hat{\omega} - \hat{\omega}_0|}\right).$$

By the above estimate and Taylor expansion with $\omega = \sqrt{\tau^{-1}} \hat{\omega}$, we find

$$\begin{aligned} \mathbf{p}_{\pm}(\mathbf{d}, D_t) &= \tau^{\frac{1}{2}} \frac{i\hat{\omega}}{2d_3} (I - \mathbf{d}_{\pm} \otimes \mathbf{d}_{\pm}) \int_{D_t} \left(\mathbb{P}_{\mathbf{w}, D_t} E - i\tau^{-\frac{1}{2}} \hat{\omega} \mathbf{d}_{\pm} \cdot y \mathbb{P}_{\mathbf{d}, D_t} E \right) dy + O\left(\frac{\tau^{-1}}{|\hat{\omega} - \hat{\omega}_0|}\right) \\ &= \frac{\hat{\omega}^2}{2d_3} (I - \mathbf{d}_{\pm} \otimes \mathbf{d}_{\pm}) \int_{D_t} \mathbf{d}_{\pm} \cdot y \mathbb{P}_{\mathbf{d}, D_t} E dy + O\left(\tau^{-\frac{1}{2}} + \frac{\tau^{-1}}{|\hat{\omega} - \hat{\omega}_0|}\right). \end{aligned}$$

Then, by a change of variables and (4.48), as well as (4.46), we further calculate

$$\begin{aligned}
\mathbf{p}_\pm(\mathbf{d}, D_t) &= \frac{\hat{\omega}^2}{2d_3} (\mathbf{I} - \mathbf{d}_\pm \otimes \mathbf{d}_\pm) \int_D (\mathbf{d}_\pm \cdot \Phi_t) (\Phi_t^* \mathbb{P}_{\mathbf{d}, D_t} E) d\Phi_t + O\left(\tau^{-\frac{1}{2}} + \frac{\tau^{-1}}{|\hat{\omega} - \hat{\omega}_0|}\right) \\
&= \frac{\hat{\omega}^2}{2d_3} (\mathbf{I} - \mathbf{d}_\pm \otimes \mathbf{d}_\pm) \int_D \mathbf{d}_\pm \cdot y (q_1 \varphi_1 + q_2 \varphi_2) dy + O\left(\tau^{-\frac{1}{2}} + \frac{\tau^{-\frac{1}{2}}(\tau^{-\frac{1}{2}} + |t|)}{|\hat{\omega} - \hat{\omega}_0|}\right) \\
&= \frac{\hat{\omega}^2}{2d_3} (q_1 \mathbf{g}_1^\pm + q_2 \mathbf{g}_2^\pm) + O\left(\tau^{-\frac{1}{2}} + \frac{\tau^{-\frac{1}{2}}(\tau^{-\frac{1}{2}} + |t|)}{|\hat{\omega} - \hat{\omega}_0|}\right), \tag{4.64}
\end{aligned}$$

where

$$\mathbf{g}_1^\pm = (\mathbf{A}^{ant})^T \mathbf{d}_\pm - \langle \mathbf{d}_\pm, \mathbf{A}^{ant} \mathbf{d}_\pm \rangle \mathbf{d}_\pm,$$

and

$$\mathbf{g}_2^\pm = (\mathbf{A}^{sym})^T \mathbf{d}_\pm - \langle \mathbf{d}_\pm, \mathbf{A}^{sym} \mathbf{d}_\pm \rangle \mathbf{d}_\pm.$$

Recall that the perturbed incident direction \mathbf{d} is of the form (4.9). A direct computation gives

$$\mathbf{g}_1^\pm = \epsilon \begin{bmatrix} (\mathbf{A}_1^T - a_2) \alpha_0 \\ 0 \end{bmatrix} + O(\epsilon^2), \quad \mathbf{g}_2^\pm = \begin{bmatrix} \pm \mathbf{b}_2 \\ -\epsilon \mathbf{b}_2 \cdot \alpha_0 \end{bmatrix} + O(\epsilon^2), \quad \text{as } \epsilon \rightarrow 0. \tag{4.65}$$

Similarly, thanks to $\mathbf{p} \cdot \mathbf{d} = 0$, we have

$$f_1 = O(\epsilon), \quad f_2 = O(1). \tag{4.66}$$

For simplicity, we introduce the small parameter:

$$\delta = |t| + \tau^{-\frac{1}{2}},$$

and consider the regime:

$$\delta = o(|\hat{\omega} - \hat{\omega}_0|), \quad \text{as } \hat{\omega} \rightarrow \hat{\omega}_0. \tag{4.67}$$

By the estimate (4.48) and the expansions (4.64), (4.65) and (4.66), we readily have

$$\mathbf{p}_\pm(\mathbf{d}, D_t) = \frac{i\tau^{-\frac{1}{2}} \hat{\omega}^3}{2d_3} \frac{1 - \hat{\omega}^2 \lambda_0}{h} f_2 \begin{bmatrix} \pm \mathbf{b}_2 \\ -\epsilon \mathbf{b}_2 \cdot \alpha_0 \end{bmatrix} + O(\delta + \epsilon^2), \tag{4.68}$$

since $(1 - \hat{\omega}^2 \lambda_0)/h = O(|\hat{\omega} - \hat{\omega}_0|^{-1})$ holds for $\hat{\omega}$ near $\hat{\omega}_0$. As a corollary, we can approximate the reflection energy $|\mathbf{p}^r|^2$ as follows.

Corollary 4.7. *Suppose that the assumptions in Theorem 4.6 hold. In the regime (4.67), the reflection energy $|\mathbf{p}^r|^2$ has the following asymptotics: for $\hat{\omega} \in \mathbb{R}$ near $\hat{\omega}_0$,*

$$|\mathbf{p}^r|^2 = \tau^{-1} \frac{|1 - \hat{\omega}^2 \lambda_0|^2}{|h|^2} p_0 + o(\delta + \epsilon^2), \quad \text{as } \delta, \epsilon \rightarrow 0,$$

with the real function p_0 in $\hat{\omega}$:

$$p_0(\hat{\omega}) := \frac{|\hat{\omega}|^6}{4(1 - \epsilon^2)} f_2^2 (|\mathbf{b}_2|^2 + \epsilon^2 |\mathbf{b}_2 \cdot \alpha_0|^2),$$

where h and f_2 are given in (4.50) and (4.51), respectively.

We next show our main claim that for certain parameters, the Fano-type resonance can happen for the symmetry-broken metasurface when the incident frequency ω is near the embedded eigenvalue ω_* . Recalling the definition of the classical Fano formula [70] and the scaling $\omega = \sqrt{\tau}^{-1} \hat{\omega}$, it suffices to prove that, for fixed large τ and small t, ϵ ,

$$\tau^{-1} \frac{|1 - \hat{\omega}^2 \lambda_0|^2}{|h|^2} \approx C \frac{|\theta + (\omega - \omega_*)|^2}{\gamma + |\omega - \omega_*|^2}, \quad \text{as } \omega \rightarrow \omega_*, \tag{4.69}$$

for some constant C and parameters $\theta \in \mathbb{R}$ and $\gamma > 0$. We first observe from Corollary 4.5 that, for $j = 1, 2$,

$$\hat{\omega}_{0,j} = \frac{1}{\sqrt{\lambda_0}} - i\eta_j, \tag{4.70}$$

where $\eta_j \geq 0$ are given by

$$\eta_1 = \frac{i\tau^{-\frac{1}{2}}\lambda_0^{-2}c_{1,2} - \sqrt{-\tau^{-1}\lambda_0^{-4}c_{1,2}^2 + 4(t^2\lambda_0^{-1}c_0^2 + \tau^{-1}\lambda_0^{-4}\epsilon^2c_3^2)}}{4} + O(\epsilon^2\tau^{-\frac{1}{2}}),$$

and

$$\eta_2 = \frac{i\tau^{-\frac{1}{2}}\lambda_0^{-2}c_{1,2} + \sqrt{-\tau^{-1}\lambda_0^{-4}c_{1,2}^2 + 4(t^2\lambda_0^{-1}c_0^2 + \tau^{-1}\lambda_0^{-4}\epsilon^2c_3^2)}}{4} + O(\epsilon^2\tau^{-\frac{1}{2}}).$$

Hence, for $t = \tau^{-1}\epsilon^2$, there holds

$$\eta_1 = O(\tau^{-\frac{1}{2}}\epsilon^2), \quad \eta_2 = O(\tau^{-\frac{1}{2}}), \quad (4.71)$$

that is, $\hat{\omega}_{0,1}$ has a much smaller imaginary part than the one of $\hat{\omega}_{0,2}$. By definition (4.50) of h , we can compute

$$\tau^{-1} \frac{|1 - \hat{\omega}^2\lambda_0|^2}{|h|^2} = \frac{\lambda_0^2 |(\hat{\omega}_0 + \hat{\omega})|^2}{|r(\hat{\omega})|^2} \frac{|(\omega - \omega_*) + (\omega_* - \tau^{-\frac{1}{2}}\hat{\omega}_0)|^2}{|\hat{\omega} - \hat{\omega}_{0,1} + O(\tau^{-1})|^2 |\hat{\omega} - \hat{\omega}_{0,2} + O(\tau^{-1})|^2}. \quad (4.72)$$

Then, by estimates (4.43) and (4.70), we see

$$\tau^{-\frac{1}{2}} |\hat{\omega} - \hat{\omega}_{0,i} + O(\tau^{-1})| = |\omega - \omega_* + i\tau^{-\frac{1}{2}}\eta_i + O(\tau^{-\frac{3}{2}})|,$$

which implies, by $\eta_2 = O(\tau^{-\frac{1}{2}})$ in (4.71),

$$\begin{aligned} & \frac{1}{|\hat{\omega} - \hat{\omega}_{0,1} + O(\tau^{-1})|^2 |\hat{\omega} - \hat{\omega}_{0,2} + O(\tau^{-1})|^2} \\ &= \frac{\tau^{-2}}{|\omega - \omega_* + i\tau^{-\frac{1}{2}}\eta_1 + O(\tau^{-\frac{3}{2}})|^2 |\omega - \omega_* + i\tau^{-\frac{1}{2}}\eta_2 + O(\tau^{-\frac{3}{2}})|^2} \\ &= \frac{1}{|\omega - \omega_* + i\tau^{-\frac{1}{2}}\eta_1 + O(\tau^{-\frac{3}{2}})|^2 |\tau(\omega - \omega_*) + i\tau^{\frac{1}{2}}\eta_2 + O(\tau^{-\frac{1}{2}})|^2} \\ &= O(1) \frac{1}{|\omega - \omega_* + i\tau^{-\frac{1}{2}}\eta_1 + O(\tau^{-\frac{3}{2}})|^2} \quad \text{as } \omega \rightarrow \omega_*. \end{aligned} \quad (4.73)$$

Therefore, it follows from (4.72) and (4.73) that, for real ω approximating ω_* ,

$$\begin{aligned} \tau^{-1} \frac{|1 - \hat{\omega}^2\lambda_0|^2}{|h|^2} &= O(1) \frac{|(\omega - \omega_*) + (\omega_* - \tau^{-\frac{1}{2}}\hat{\omega}_0)|^2}{|\omega - \omega_* + i\tau^{-\frac{1}{2}}\eta_1 + O(\tau^{-\frac{3}{2}})|^2} \\ &\approx O(1) \frac{|(\omega - \omega_*) + (\omega_* - \tau^{-\frac{1}{2}}\hat{\omega}_0)|^2}{|\omega - \omega_*|^2 + \tau^{-1}\eta_1^2}, \end{aligned} \quad (4.74)$$

if $\tau^{-\frac{1}{2}} = o(\epsilon^2)$ holds (so that $O(\tau^{-\frac{3}{2}})$ is a higher-order term with respect to $\tau^{-\frac{1}{2}}\eta_1$). The formula (4.74) exactly matches the Fano ansatz in (4.69), and hence justifies the predicted Fano-type scattering anomalies.

5 Concluding remarks and discussions

In this work, we have given a comprehensive investigation for the resonant scattering by all-dielectric metasurfaces of periodically distributed nanoparticles with high refractive indices. We have characterized the essential spectrum of the Maxwell operator associated with the periodic scattering problem. We have showed that the interested real scattering resonances are the simple poles of the EM scattering resolvent with the corresponding resonant modes being the bound states exponentially decaying away from the metasurface. We have found that the real scattering resonances always exist below the essential spectrum of the Maxwell operator. We have also revealed some important relations between the resonances and the symmetry of the metasurface, which helps us to prove that in the high contrast regime, under the normal incidence, the subwavelength embedded eigenvalues exist for the symmetric dielectric metasurfaces. The resonant states corresponding to the embedded eigenvalues are the desired bound states in the continuum. To connect the BICs and the Fano resonances, we break the in-plane symmetry of the metasurface by perturbing the geometry of the dielectric nanoparticles and the incident directions (i.e., the Bloch wave vectors). We have derived the asymptotic expansions of the subwavelength resonances with respect to the high contrast and the

shape perturbation. Furthermore, we have quantitatively approximated the reflection and transmission polarization vectors near the resonances, and characterized the Fano-type asymmetric line shape in terms of the well-known Fano formula. Therefore, this work has provided a solid mathematical theory for the Fano resonance phenomenon physically observed in [49, 58].

There has also been increasing interest in understanding the topological properties of the BICs and the associated Fano resonances. In particular, we can define the topological charge by the winding number of the scattered polarization vectors, and the BICs are noting than the vortex centers of the polarization vectors in the momentum space [90]. We also note that the BICs have a natural connection with the polarization singularities, which is a fundamental concept in the field of singular optics [22, 27, 79, 87]. It would be interesting to explore these concepts in our framework and further investigate the robustness of BICs and the Fano-type resonances.

Appendix A. Auxiliary lemmas

In this section, we establish some useful lemmas for proving Theorem 2.8. Letting $\varepsilon = 1 + \tau\chi_D$ with $\tau > 0$, we consider the following elliptic equation on the unbounded domain Y_∞ :

$$-\operatorname{div}(\varepsilon\nabla p) = f, \quad (\text{A.1})$$

with the quasi-periodic boundary condition. For the well-posedness of (A.1), we need the weighted Sobolev space:

$$H_\alpha^{1,-1}(Y_\infty) := \{u; (1 + |x_3|^2)^{-1/2}u \in L_\alpha^2(Y_\infty), \nabla u \in L_\alpha^2(Y_\infty)\}.$$

It is easy to see that $H_\alpha^{1,-1}(Y_\infty)$ with $\alpha = 0$ (i.e., a periodic boundary condition) contains the constant functions.

Lemma A.1. *For any $f \in (H_\alpha^{1,-1}(Y_\infty))^*$, the equation (A.1) has a unique solution in $H_\alpha^{1,-1}(Y_\infty)/\mathbb{R}$, continuously depending on the data f .*

The proof of the above lemma easily follows from [65, Theorem 2.5.14]. We next discuss how the solution of (A.1) depends on the contrast τ . In fact, the following lemma holds.

Lemma A.2. *Suppose that $E \in \mathbf{L}_\alpha^2(Y_\infty)$ satisfies $\operatorname{div}(\varepsilon E) = 0$ and $\operatorname{div}(\chi_D E) \neq 0$. Define the coefficient $\varepsilon' = \varepsilon + \eta\chi_D$ for $\eta > 0$, and let $p \in H_\alpha^{1,-1}(Y_\infty)/\mathbb{R}$ be the unique solution to*

$$\operatorname{div}(\varepsilon'(E + \nabla p)) = 0. \quad (\text{A.2})$$

Then there holds

$$\|E\|_{\varepsilon, Y_\infty}^2 + \|\nabla p\|_{\varepsilon, Y_\infty}^2 \|E\|_D / \|\nabla p\|_D \leq \|E + \nabla p\|_{\varepsilon', Y_\infty}^2.$$

Proof. By the equation (A.2) and $\operatorname{div}\varepsilon E = 0$, it is clear that

$$-\operatorname{div}(\varepsilon'\nabla p) = \eta\operatorname{div}(\chi_D E),$$

which implies $\nabla p \neq 0$ and

$$\|\nabla p\|_{\varepsilon', Y_\infty}^2 = -\eta(\nabla p, E)_D = -\eta(E, \nabla p)_D. \quad (\text{A.3})$$

Then, a simple use of Cauchy's inequality gives

$$\|\nabla p\|_{\varepsilon, Y_\infty}^2 \leq \eta(\|E\|_D - \|\nabla p\|_D)\|\nabla p\|_D. \quad (\text{A.4})$$

We can directly estimate, with the help of (A.3),

$$\begin{aligned} \|E + \nabla p\|_{\varepsilon', Y_\infty}^2 - \|E\|_{\varepsilon, Y_\infty}^2 &= \eta\|E\|_D^2 + \|\nabla p\|_{\varepsilon', Y_\infty}^2 + \eta(E, \nabla p)_D + \eta(\nabla p, E)_D \\ &= \eta\|E\|_D^2 - \|\nabla p\|_{\varepsilon', Y_\infty}^2 \\ &\geq \eta\|E\|_D(\|E\|_D - \|\nabla p\|_D). \end{aligned} \quad (\text{A.5})$$

The proof is complete by (A.4) and (A.5):

$$\|E + \nabla p\|_{\varepsilon', Y_\infty}^2 - \|E\|_{\varepsilon, Y_\infty}^2 \geq \|\nabla p\|_{\varepsilon, Y_\infty}^2 \|E\|_D / \|\nabla p\|_D \geq 0. \quad \square$$

Appendix B. Analysis of the scalar eigenvalue problem (3.37)

In this section, we will formally discuss the high-contrast limits of the subwavelength resonances and the associated resonant modes of (3.37), and show the existence of real subwavelength resonances with a lower bound under the symmetry assumption of the coefficient:

$$\varepsilon(x, y, z)|_{Y_h} = \varepsilon(-x, -y, z)|_{Y_h}.$$

The rigorous analysis can be performed in the same manner as in [70] and [9]. We recall the periodic Green's function $G^{0,\omega}$ defined in (2.7), which clearly satisfies the transparent boundary condition $\frac{\partial}{\partial \nu} G^{0,\omega} = \mathcal{T}G^{0,\omega}$ on Σ , and the associated volume integral operator $\mathcal{K}_D^{0,\omega}$ in (2.9). By the asymptotic expansion (4.11) of $G^{0,\omega}$:

$$G^{0,\omega} = \hat{G} + O(\omega), \quad \text{with } \hat{G} := \frac{i}{2\omega} + G^{0,0},$$

we have $\mathcal{K}_D^{0,\omega}[\varphi] = \hat{\mathcal{K}}_D[\varphi] + O(\omega)$, where the operator $\hat{\mathcal{K}}_D$ is defined by

$$\hat{\mathcal{K}}_D[\varphi] = \frac{i}{2\omega} \langle 1, \varphi \rangle_D + \mathcal{K}_D^{0,0}[\varphi]. \quad (\text{B.1})$$

It is well known that by the integral operator $\mathcal{K}_D^{0,\omega}$, the eigenvalue problem (3.37) can be reformulated as

$$u = \omega^2 \tau \mathcal{K}_D^{0,\omega}[u]. \quad (\text{B.2})$$

To deal with the $O(\omega^{-1})$ singularity in (B.1), we define the space $L_0^2(D) = \{u \in L^2(D); \langle 1, u \rangle_D = 0\}$ and write the functions $u \in L^2(D)$ as $u = \langle 1_D, u \rangle_D + \bar{u}$, where $1_D := 1/|D|$ and $\bar{u} \in L_0^2(D)$. Such decomposition is unique and orthogonal. Then the problem (B.2) is equivalent to

$$\begin{bmatrix} \langle 1_D, u \rangle_D \\ \bar{u} \end{bmatrix} - \omega^2 \tau \begin{bmatrix} \langle 1_D, \mathcal{K}_D^{0,\omega}[1] \rangle_D & \langle 1_D, \mathcal{K}_D^{0,\omega}[\cdot] \rangle_D \\ \mathcal{K}_D^{0,\omega}[1] - \langle 1_D, \mathcal{K}_D^{0,\omega}[1] \rangle_D & \mathcal{K}_D^{0,\omega}[\cdot] - \langle 1_D, \mathcal{K}_D^{0,\omega}[\cdot] \rangle_D \end{bmatrix} \begin{bmatrix} \langle 1_D, u \rangle_D \\ \bar{u} \end{bmatrix} = 0.$$

By the asymptotic expansion (B.1) and $\hat{\mathcal{K}}_D[1] = \frac{i|D|}{2\omega} + \mathcal{K}_D^{0,0}[1]$, we have

$$\begin{bmatrix} 1 - \omega\tau \frac{i|D|}{2} + O(\omega^2\tau) & O(\omega^2\tau) \\ -\omega^2\tau\phi_1 + O(\omega^3\tau) & 1 - \omega^2\tau\mathcal{K}_D + O(\omega^3\tau) \end{bmatrix} \begin{bmatrix} \langle 1_D, u \rangle_D \\ \bar{u} \end{bmatrix} = 0, \quad (\text{B.3})$$

where $\phi_1 := \mathcal{K}_D^{0,0}[1] - \langle 1_D, \mathcal{K}_D^{0,0}[1] \rangle_D$ and

$$\mathcal{K}_D[\cdot] := \mathcal{K}_D^{0,0}[\cdot] - \langle 1_D, \mathcal{K}_D^{0,0}[\cdot] \rangle_D : L_0^2(D) \rightarrow L_0^2(D). \quad (\text{B.4})$$

Note from the coefficient matrix in (B.3) that in the high contrast regime, the subwavelength resonances of (3.37) can happen in two cases: $\omega = O(\tau^{-1})$ and $\omega = O(\sqrt{\tau^{-1}})$. In the first case, we have the asymptotics:

$$\begin{bmatrix} 1 - \omega\tau \frac{i|D|}{2} + O(\omega^2\tau) & O(\omega^2\tau) \\ -\omega^2\tau\phi_1 + O(\omega^3\tau) & 1 - \omega^2\tau\mathcal{K}_D + O(\omega^3\tau) \end{bmatrix} = \begin{bmatrix} 1 - \omega\tau \frac{i|D|}{2} & 0 \\ 0 & 1 \end{bmatrix} + O(\tau^{-1}),$$

which readily gives a subwavelength resonance $\omega = \frac{2}{i\tau|D|} + O(\tau^{-2})$ with the associated resonant mode being almost constant: $u = 1 + O(\tau^{-1})$ on D . In the other case: $\omega = O(\sqrt{\tau^{-1}})$, we first divide the first row of (B.3) by $\sqrt{\tau^{-1}}$ and then find

$$\begin{bmatrix} 1 - \omega\sqrt{\tau} \frac{i|D|}{2} + O(\omega^2\sqrt{\tau}) & O(\omega^2\sqrt{\tau}) \\ -\omega^2\tau\phi_1 + O(\omega^3\tau) & 1 - \omega^2\tau\mathcal{K}_D + O(\omega^3\tau) \end{bmatrix} = \begin{bmatrix} 1 - \omega\sqrt{\tau} \frac{i|D|}{2} & 0 \\ -\omega^2\tau\phi_1 & 1 - \omega^2\tau\mathcal{K}_D \end{bmatrix} + O(\sqrt{\tau^{-1}}). \quad (\text{B.5})$$

Suppose that the compact self-adjoint operator \mathcal{K}_D admits the eigen-decomposition:

$$\mathcal{K}_D[u] = \sum_{j=1}^{\infty} \eta_j (v_j, u)_D v_j, \quad \text{for } u \in L_0^2(D).$$

Then, by the asymptotics (B.5), we can have another class of subwavelength resonances $\omega_j = \sqrt{\eta_j} \tau^{-1} + O(\tau^{-1})$ for each j , with the resonant modes $u_j = v_j + O(\sqrt{\tau^{-1}})$ on D . We now summarize the above discussion as follows.

Proposition B.1. *The subwavelength resonances exist for the problem (3.37) in the high contrast regime. Moreover, for any subwavelength resonance ω , there holds either*

$$\omega = \frac{2}{i\tau|D|} + O(\tau^{-2}), \quad \text{or} \quad \omega = \frac{1}{\sqrt{\eta_j\tau}} + O(\tau^{-1}) \quad \text{for some } j \geq 0, \quad (\text{B.6})$$

where η_j is an eigenvalue of the operator \mathcal{K}_D on $L_0^2(D)$.

We proceed to consider the existence of real subwavelength resonances, which has been discussed in [14, 71]. We provide a sketch of arguments below for completeness. With the help of the DtN operator (3.3), the variational formulation of (3.37) reads as follows: find $(\omega, u) \in \mathbb{R} \setminus \{0\} \times H_p^1(Y_h)$ such that

$$b_\omega(\varphi, u) = \omega^2(\varphi, \varepsilon u)_{Y_h}, \quad \forall \varphi \in H_p^1(Y_h), \quad (\text{B.7})$$

where $b_\omega(\cdot, \cdot)$ is the sesquilinear form on $H_p^1(Y_h)$:

$$b_\omega(\varphi, u) = (\nabla \varphi, \nabla u)_{Y_h} - \langle \varphi, \mathcal{T}u \rangle_\Sigma. \quad (\text{B.8})$$

Let \mathcal{T}^p and \mathcal{T}^ε be defined as in Section 3 and $b_\omega^\varepsilon(\cdot, \cdot)$ be defined by (B.7) with \mathcal{T} replaced by \mathcal{T}^ε . Moreover, we introduce the symmetric and antisymmetric functions:

$$H_{p,\text{sym}}^1(Y_h) = \{\varphi \in H_p^1(Y_h); \varphi(-x', x_3) = \varphi(x', x_3)\},$$

and

$$H_{p,\text{ant}}^1(Y_h) = \{\varphi \in H_p^1(Y_h); \varphi(-x', x_3) = -\varphi(x', x_3)\},$$

which are orthogonal with respect to $b_\omega^\varepsilon(\cdot, \cdot)$. Similarly to Proposition 3.3, we can prove that $b_\omega^\varepsilon(\cdot, \cdot)$ is a symmetric positive form on $H_{p,\text{ant}}^1(Y_h)$ with eigenvalues $\lambda_j^{\text{ant}}(\tau, \omega)$ decreasing in ω , where λ_j^{ant} is given by the min-max principle:

$$\lambda_j^{\text{ant}}(\tau, \omega) = \min_{\substack{V \subset H_{p,\text{ant}}^1(Y_h) \\ \dim V = j}} \max_{H \in V} \frac{b_\omega^\varepsilon(u, u)}{(u, \varepsilon u)_{Y_h}}. \quad (\text{B.9})$$

It follows that for each j , the equation $\lambda_j^{\text{ant}}(\tau, \omega) = \omega^2$ admits a unique solution $\omega_j > 0$, and we can find $u_j \in H_{p,\text{ant}}^1(Y_h)$ such that

$$b_{\omega_j}^\varepsilon(\varphi, u_j) = \omega_j^2(\varphi, \varepsilon u)_{Y_h}, \quad \forall \varphi \in H_{p,\text{ant}}^1(Y_h). \quad (\text{B.10})$$

We claim that for the large enough contrast τ , ω_j would be in the subwavelength regime. Indeed, by (B.9), we have

$$\lambda_j^{\text{ant}}(\tau, \omega) \leq \min_{\substack{V \subset H_{p,\text{ant}}^1(Y_h) \\ \dim V = j}} \max_{H \in V} \frac{b_\omega^\varepsilon(u, u)}{\tau(u, u)_D} = O(\tau^{-1}),$$

with $H_{0,\text{ant}}^1(Y_h) := \{u \in H_{p,\text{ant}}^1(Y_h); u = 0 \text{ on } \overline{Y_h} \setminus \overline{D}\}$, which readily gives $\omega_j = O(\sqrt{\tau^{-1}})$. By the orthogonality between $H_{p,\text{sym}}^1(Y_h)$ and $H_{p,\text{ant}}^1(Y_h)$, the equation (B.10) holds for any $\varphi \in H_p^1(Y_h)$. In addition, thanks to $\omega_j \ll 1$ and $u_j \in H_{p,\text{ant}}^1(Y_h)$, we have $(u_j)_q = 0$ for $q \in \Lambda_p^* = \{0\}$ by symmetry, which gives $b_{\omega_j}^\varepsilon(\varphi, u_j) = b_{\omega_j}(\varphi, u_j)$. Therefore, ω_j is the desired real subwavelength resonance for (3.37). The following result that gives a lower bound for real subwavelength resonances is a variant of [71, Theorem 4.1]. Let X be the subspace of $H_p^1(Y_h)$ defined by

$$X := \{u \in H_p^1(Y_h); u_q = 0 \text{ for } q \in \Lambda_p^*\}.$$

Proposition B.2. *Suppose that ω is a real subwavelength resonance of (3.37) satisfying $\omega = O(\sqrt{\tau^{-1}})$ for large enough τ . Then it holds that*

$$\omega \geq \sqrt{\frac{\gamma_0}{\tau}} + O\left(\frac{1}{\tau^{3/4}}\right),$$

where $\gamma_0 > 0$ is given by

$$\gamma_0 = \inf_{u \in H_p^1(Y_h)} \frac{b_0(u, u)}{(u, u)_{Y_h}}, \quad (\text{B.11})$$

with $b_0(\cdot, \cdot)$ given in (B.8) with $\omega = 0$.

Proof. Let u be a resonant mode associated with the real resonance $\omega = O(\sqrt{\tau}^{-1})$. Then $u \in X$ satisfies

$$b_\omega(\varphi, u) = \omega^2(\varphi, \varepsilon u)_{Y_h}, \quad \forall \varphi \in X.$$

We now consider the following variational eigenvalue problem on X :

$$b_\omega(\varphi, u) = \gamma(\varphi, u)_{Y_h}, \quad \forall \varphi \in X. \quad (\text{B.12})$$

Since $b_\omega(\cdot, \cdot)$ is a positive symmetric form on X , we let $\gamma_j(\omega) \geq 0$ be the eigenvalues of (B.12), which has the asymptotics: $\gamma_j(\omega) = \gamma_j(0) + O(\sqrt{\tau}^{-1})$, by the standard perturbation theory. Hence, we can observe

$$\omega^2 = \frac{b_\omega(u, u)}{(u, \varepsilon u)_{Y_h}} \geq \frac{1}{\tau} \inf_{u \in H_p^1(Y_h)} \frac{b_\omega(u, u)}{(u, u)_{Y_h}} \geq \frac{1}{\tau} \gamma_0(0) + O\left(\frac{1}{\tau^{3/2}}\right).$$

The proof is complete by noting that $\gamma_0(0)$ is strictly positive. Indeed, if $\gamma_0(0) = 0$, then the eigenfunction must be constant which does not belong to the space X . \square

Appendix C. Proofs in Section 4.1

C.1. Proof of Lemma 4.3

Let us first compute the derivative of \mathbb{P}_D^t at $t = 0$. By the construction of the Helmholtz decomposition in [10], we have, for $E \in \mathbf{L}^2(D)$,

$$\mathbb{P}_D^t E = E - \Phi_t^* \nabla u,$$

where, up to constants, $u \in H^1(D_t)$ satisfies the variational equation:

$$(\Phi_{t,*} E, \nabla \varphi)_{\Phi_t(D)} = (\nabla u, \nabla \varphi)_{\Phi_t(D)}, \quad \forall \varphi \in H^1(D_t). \quad (\text{C.1})$$

Then, we define $Q_t = (\nabla \Phi_t)^{-1}$, and find, by chain rule,

$$\mathbb{P}_D^t E = E - \Phi_t^* \nabla u = E - Q_t^T \nabla \Phi_t^* u, \quad (\text{C.2})$$

and

$$\frac{d}{dt} \mathbb{P}_D^t E = -\frac{d}{dt} Q_t^T \nabla \Phi_t^* u - Q_t^T \nabla \frac{d}{dt} \Phi_t^* u. \quad (\text{C.3})$$

It is direct to compute

$$\frac{d}{dt} Q_t^T = \frac{d}{dt} (I + t \nabla V)^{-T} = -(\nabla V)^T. \quad (\text{C.4})$$

Moreover, by change of variables, we can see from (C.1) that $\Phi_t^* u$ is the solution to

$$(E, Q_t^T \nabla \varphi J(\Phi_t))_D = (Q_t Q_t^T \nabla w, \nabla \varphi J(\Phi_t))_D, \quad \forall \varphi \in H^1(D), \quad (\text{C.5})$$

where $J(\Phi_t) := \det((I + t \nabla V))$ is the Jacobian determinant. It is known that [26, 38]

$$\frac{d}{dt} \Big|_{t=0} J(\Phi_t) = \frac{d}{dt} \Big|_{t=0} \det(I + t \nabla V) = \text{div} V. \quad (\text{C.6})$$

We denote by u^0 the solution to (C.1) at $t = 0$, i.e.,

$$(E, \nabla \varphi)_D = (\nabla u^0, \nabla \varphi)_D, \quad \forall \varphi \in H^1(D), \quad (\text{C.7})$$

and take the derivative of the variational equation (C.5) at $t = 0$ with (C.4) and (C.6),

$$(E, (-(\nabla V)^T + \text{div} V) \nabla \varphi)_D = -((\nabla V + (\nabla V)^T - \text{div} V) \nabla u^0, \nabla \varphi)_D + \left(\nabla \frac{d}{dt} \Big|_{t=0} \Phi_t^* u, \nabla \varphi \right)_D.$$

Then, by (C.3), (C.4) and (C.7) with $\nabla u^0 = \mathbb{P}_{d,D}^\perp E$, we can conclude the desired formula (4.32).

We next compute the derivative of $\tilde{\mathcal{K}}_D^t$, which essentially follows from [67, Proposition 3.2]. We sketch the computation below. By definition and change of variables, we have

$$\begin{aligned}\tilde{\mathcal{K}}_D^t[E] &= \Phi_t^* \mathcal{K}_D^{0,0} \Phi_{t,*} [E] = \int_{\Phi_t(D)} G^{0,0}(\Phi_t(x), y) E(\Phi_t^{-1}(y)) dy \\ &= \int_D G^{0,0}(\Phi_t(x), \Phi_t(y)) E(y) J(\Phi_t) dy.\end{aligned}$$

Then, a direct calculation gives

$$\begin{aligned}\frac{d}{dt} \Big|_{t=0} \tilde{\mathcal{K}}_D^t[E] &= \int_D -\nabla_y G^{0,0}(x, y) \cdot (V(x) - V(y)) E(y) dy - \int_D G^{0,0}(x, y) \operatorname{div}_y (V(x) - V(y)) E(y) dy \\ &= \int_D -\operatorname{div}_y [G^{0,0}(x, y) (V(x) - V(y))] E(y) dy.\end{aligned}$$

C.2. Proof of Proposition 4.4

Similarly to Theorem 4.2, the proposition is a direct consequence of the standard perturbation theory with the Lyapunov-Schmidt reduction; see also the monograph [39]. It suffices to compute the Hermitian matrix \hat{K} . We start with the definition, by chain rule,

$$\frac{d}{dt} \Big|_{t=0} K_{ij} = \left(\varphi_i, \frac{d}{dt} \Big|_{t=0} \mathbb{P}_D^t \mathcal{K}_D^{0,0} [\varphi_j] \right)_D + \left(\varphi_i, \mathcal{K}_D^{0,0} \frac{d}{dt} \Big|_{t=0} \mathbb{P}_D^t [\varphi_j] \right)_D + \left(\varphi_i, \frac{d}{dt} \Big|_{t=0} \tilde{\mathcal{K}}_D^t [\varphi_j] \right)_D. \quad (\text{C.8})$$

We observe from [9, Proposition 5.1] that the eigenfunction of \mathbb{K}_D is of H^1 -regularity, which allows us to use the integration by parts for (4.34): for $E \in \mathbf{H}^1(D)$,

$$\frac{d}{dt} \Big|_{t=0} \tilde{\mathcal{K}}_D^t[E] = \int_D G^{0,0}(x, y) \nabla E(y) (V(x) - V(y)) dy - \int_{\partial D} G^{0,0}(x, y) (V(x) - V(y)) \cdot \nu(y) E(y) dy.$$

It follows that the last term in (C.8) can be calculated as

$$\begin{aligned}\left(\varphi_i, \frac{d}{dt} \Big|_{t=0} \tilde{\mathcal{K}}_D^t [\varphi_j] \right)_D &= -(\mathcal{K}_D^{0,0} [\varphi_i], \nabla \varphi_j V)_D + (\mathcal{K}_D^{0,0} [\varphi_i \otimes V], \nabla \varphi_j)_D \\ &\quad + (\mathcal{K}_D^{0,0} [\varphi_i], \nu \cdot V \varphi_j)_{\partial D} - (\mathcal{K}_D^{0,0} [\varphi_i \otimes V], \varphi_j \otimes \nu)_{\partial D}.\end{aligned} \quad (\text{C.9})$$

Thanks to $\mathbb{K}_D[\varphi_i] = \lambda_0 \varphi_i$, for the first and third term in (C.9), there hold

$$-(\mathcal{K}_D^{0,0} [\varphi_i], \nabla \varphi_j V)_D = -(\lambda_0 \varphi_i, \nabla \varphi_j V)_D - (\mathbb{P}_{d,D}^\perp \mathcal{K}_D^{0,0} [\varphi_i], \nabla \varphi_j V)_D, \quad (\text{C.10})$$

and

$$(\mathcal{K}_D^{0,0} [\varphi_i], \nu \cdot V \varphi_j)_{\partial D} = (\lambda_0 \varphi_i, \nu \cdot V \varphi_j)_{\partial D} + (\mathbb{P}_{d,D}^\perp \mathcal{K}_D^{0,0} [\varphi_i], \nu \cdot V \varphi_j)_{\partial D}. \quad (\text{C.11})$$

For the second term in (C.9), a simple computation gives, by changing the order of differentiation and integration,

$$(\mathcal{K}_D^{0,0} [\varphi_i \otimes V], \nabla \varphi_j)_D = (\varphi_i \otimes V, \nabla \mathcal{K}_D^{0,0} [\varphi_j])_D + (\mathcal{K}_D^{0,0} [\varphi_i \otimes V], \varphi_j \otimes \nu)_{\partial D}. \quad (\text{C.12})$$

Then, applying the integration by parts to the first term in the right-hand side of (C.12), we find

$$\begin{aligned}(\varphi_i \otimes V, \nabla \mathcal{K}_D^{0,0} [\varphi_j])_D &= -(\operatorname{div} V \varphi_i + \nabla \varphi_i V, (\mathbb{P}_{d,D} + \mathbb{P}_{d,D}^\perp) \mathcal{K}_D^{0,0} [\varphi_j])_D + (\nu \cdot V \varphi_i, \mathcal{K}_D^{0,0} [\varphi_j])_{\partial D} \\ &= -(\operatorname{div}(\varphi_i \otimes V), \lambda_0 \varphi_j)_D - (\operatorname{div} V \varphi_i + \nabla \varphi_i V, \mathbb{P}_{d,D}^\perp \mathcal{K}_D^{0,0} [\varphi_j])_D + (\nu \cdot V \varphi_i, \mathcal{K}_D^{0,0} [\varphi_j])_{\partial D} \\ &= -(\operatorname{div} V \varphi_i + \nabla \varphi_i V, \mathbb{P}_{d,D}^\perp \mathcal{K}_D^{0,0} [\varphi_j])_D + (\nu \cdot V \varphi_i, \mathcal{K}_D^{0,0} [\varphi_j])_{\partial D} \\ &\quad + (\varphi_i, \lambda_0 \nabla \varphi_j V)_D - (\varphi_i, \lambda_0 \varphi_j \nu \cdot V)_{\partial D}.\end{aligned} \quad (\text{C.13})$$

Combining the above calculations (C.9)-(C.13), we arrive at

$$\begin{aligned}\left(\varphi_i, \frac{d}{dt} \Big|_{t=0} \tilde{\mathcal{K}}_D^t [\varphi_j] \right)_D &= -(\mathbb{P}_{d,D}^\perp \mathcal{K}_D^{0,0} [\varphi_i], \nabla \varphi_j V)_D + (\mathbb{P}_{d,D}^\perp \mathcal{K}_D^{0,0} [\varphi_i], \nu \cdot V \varphi_j)_{\partial D} + \lambda_0 (\nu \cdot V \varphi_i, \varphi_j)_{\partial D} \\ &\quad - (\operatorname{div} V \varphi_i + \nabla \varphi_i V, \mathbb{P}_{d,D}^\perp \mathcal{K}_D^{0,0} [\varphi_j])_D + (\nu \cdot V \varphi_i, \mathbb{P}_{d,D}^\perp \mathcal{K}_D^{0,0} [\varphi_j])_{\partial D}.\end{aligned} \quad (\text{C.14})$$

We next compute the first two terms in (C.8). It is easy to see from (4.32) that

$$\mathbb{P}_{d,D}^\perp \nabla w = \mathbb{P}_{d,D}^\perp (-\nabla V + \operatorname{div} V) \mathbb{P}_{d,D} E + \mathbb{P}_{d,D}^\perp (\nabla V)^T \mathbb{P}_{d,D}^\perp E,$$

which implies

$$\mathbb{P}_{d,D}^\perp \frac{d}{dt} \Big|_{t=0} \mathbb{P}_D^t [E] = \mathbb{P}_{d,D}^\perp (\nabla V - \operatorname{div} V) \mathbb{P}_{d,D} E. \quad (\text{C.15})$$

It is also clear from (4.32) that

$$\mathbb{P}_{d,D} \frac{d}{dt} \Big|_{t=0} \mathbb{P}_D^t = \mathbb{P}_{d,D} (\nabla V)^T \mathbb{P}_{d,D}^\perp. \quad (\text{C.16})$$

By (C.15), we readily have

$$\begin{aligned} \left(\varphi_i, \mathcal{K}_D^{0,0} \frac{d}{dt} \Big|_{t=0} \mathbb{P}_D^t [\varphi_j] \right)_D &= \left(\varphi_i, \mathcal{K}_D^{0,0} (\mathbb{P}_{d,D} + \mathbb{P}_{d,D}^\perp) \frac{d}{dt} \Big|_{t=0} \mathbb{P}_D^t [\varphi_j] \right)_D \\ &= \left(\lambda_0 \varphi_i, \frac{d}{dt} \Big|_{t=0} \mathbb{P}_D^t \varphi_j \right)_D + \left(\mathbb{P}_{d,D}^\perp \mathcal{K}_D^{0,0} \varphi_i, (\nabla V - \operatorname{div} V) \varphi_j \right)_D \\ &= \left(\mathbb{P}_{d,D}^\perp \mathcal{K}_D^{0,0} \varphi_i, (\nabla V - \operatorname{div} V) \varphi_j \right)_D, \end{aligned} \quad (\text{C.17})$$

where the first term in the second equality vanishes due to (C.16). Similarly, we derive

$$\left(\varphi_i, \frac{d}{dt} \Big|_{t=0} \mathbb{P}_D^t \mathcal{K}_D^{0,0} [\varphi_j] \right)_D = \left(\varphi_i, (\nabla V)^T \mathbb{P}_{d,D}^\perp \mathcal{K}_D^{0,0} \varphi_j \right)_D. \quad (\text{C.18})$$

Collecting (C.14), (C.17) and (C.18), we obtain

$$\begin{aligned} \frac{d}{dt} \Big|_{t=0} K_{ij} &= (\mathbb{P}_{d,D}^\perp \mathcal{K}_D^{0,0} \varphi_i, (\nabla V - \operatorname{div} V) \varphi_j - \nabla \varphi_j V)_D + (\mathbb{P}_{d,D}^\perp \mathcal{K}_D^{0,0} [\varphi_i], \nu \cdot V \varphi_j)_{\partial D} \\ &\quad + ((\nabla V - \operatorname{div} V) \varphi_i - \nabla \varphi_i V, \mathbb{P}_{d,D}^\perp \mathcal{K}_D^{0,0} [\varphi_j])_D + (\nu \cdot V \varphi_i, \mathbb{P}_{d,D}^\perp \mathcal{K}_D^{0,0} [\varphi_j])_{\partial D} \\ &\quad + \lambda_0 (\nu \cdot V \varphi_i, \varphi_j)_{\partial D}. \end{aligned} \quad (\text{C.19})$$

To simplify the above formula, we write $\nabla p_i \in \mathbf{L}^2(D)$ for $\mathbb{P}_{d,D}^\perp \mathcal{K}_D^{0,0} \varphi_i$ and then have

$$\begin{aligned} &(\mathbb{P}_{d,D}^\perp \mathcal{K}_D^{0,0} \varphi_i, (\nabla V - \operatorname{div} V) \varphi_j - \nabla \varphi_j V)_D \\ &= (\nabla p_i, \nabla \times (V \times \varphi_j))_D \\ &= (\nabla_{\partial D} p_i, \nu \times (V \times \varphi_j))_{\partial D} \\ &= (\nabla_{\partial D} p_i, -\nu \cdot V \varphi_j)_{\partial D}, \end{aligned}$$

by integration by parts with $\nu \cdot \varphi_j = 0$ on ∂D . It follows that

$$(\mathbb{P}_{d,D}^\perp \mathcal{K}_D^{0,0} \varphi_i, (\nabla V - \operatorname{div} V) \varphi_j - \nabla \varphi_j V)_D + (\mathbb{P}_{d,D}^\perp \mathcal{K}_D^{0,0} [\varphi_i], \nu \cdot V \varphi_j)_{\partial D} = 0.$$

Similar calculation yields the vanishing of the term $((\nabla V - \operatorname{div} V) \varphi_i - \nabla \varphi_i V, \mathbb{P}_{d,D}^\perp \mathcal{K}_D^{0,0} [\varphi_j])_D + (\nu \cdot V \varphi_i, \mathbb{P}_{d,D}^\perp \mathcal{K}_D^{0,0} [\varphi_j])_{\partial D}$. The proof is complete by (C.19).

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