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Exceptional points in parity–time-symmetric subwavelength metamaterials

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Abstract

When sources of energy gain and loss are introduced to a wave-scattering system, the underlying mathematical formulation will be non-Hermitian. This paves the way for the existence of exceptional points, where eigenmodes are linearly dependent. The primary goal of this work is to study the existence of exceptional points in high-contrast subwavelength metamaterials. We begin by studying a parity–time-symmetric pair of subwavelength resonators and prove that this system supports asymptotic exceptional points. We then investigate further properties of parity–time-symmetric subwavelength metamaterials. First, we study cavities of many small resonators and use homogenization theory to show that non-Hermitian behaviour can be replicated at the macroscale. Thereafter, we model a metascreen of subwavelength resonators which we prove exhibits asymptotic unidirectional reflectionless transmission at certain frequencies, and demonstrate extraordinary transmission close to these frequencies.

Mathematics Subject Classification (MSC2000): 35J05, 35C20, 35P20.

Keywords: $\mathcal{PT}$ symmetry, exceptional points, subwavelength resonance, metamaterials, unidirectional reflection, extraordinary transmission, homogenization

1 Introduction

Exceptional points are parameter values at which a system's eigenvalues and their associated eigenvectors simultaneously coincide. This phenomenon has been observed in a variety of quantum-mechanical, optical, acoustic and photonic settings. Crucially, exceptional points can only occur when the underlying system is non-Hermitian, as the eigenvectors are linearly independent otherwise. A prominent class of non-Hermitian systems where exceptional points are well known to occur are structures with so-called *parity-time* or $\mathcal{PT}$ *symmetry* [12, 15, 24, 28]. The exceptional points in such systems originate from the fact that the spectrum of a $\mathcal{PT}$-symmetric operator is conjugate symmetric. In this work, we study the occurrence of exceptional points in structures composed of subwavelength resonators. These are material inclusions with parameters that differ greatly from those of the background medium, the large material contrast meaning that they experience resonant behaviour in response to critical wavelengths much greater than their size. Such structures, often known as *subwavelength metamaterials* to highlight their complex microscopic structure, can exhibit exotic scattering properties and appear in a variety of photonic and phononic applications [7, 18, 21, 27].

We begin by studying a pair of high-contrast subwavelength resonators. This two-body system, which is often known as a *dimer*, is known to exhibit two subwavelength resonant modes [8]. We

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examine the case of non-real material parameters, which corresponds to systems with gain and loss. The geometry and material parameters are chosen so that the structure is $\mathcal{PT}$-symmetric, which means that the structure is symmetric and that the gain and loss are balanced. We will prove that the resonant modes can be approximated by the eigenstates of a 2×2-matrix, known as the *weighted capacitance matrix*. Then, we show that if these parameters are suitably tuned then the two eigenvalues and eigenvectors of the weighted capacitance matrix coincide, giving what we will refer to as an *asymptotic exceptional point*.

Structures that are poised at an exceptional point have applications in enhanced sensors. Typically, a small perturbation in the vicinity of a sensor induces a measurable effect that is proportional to the strength of the perturbation. However, in the case of a sensor that is poised at an exceptional point, the higher-order nature of the singularity means that the output will be greatly enhanced. In particular, an N^{th}-order exceptional point (one where N eigenmodes coincide) will generally lead to an output that scales with the N^{th} root of the strength of the perturbation, and thus is greatly enhanced for small perturbations [2, 10, 16, 22, 30, 31].

We will analyse the macroscopic properties of bounded metamaterials composed of a large number of subwavelength resonators with complex material coefficients. In particular, we consider cavities filled with large numbers of small resonators and use homogenization theory to derive effective material properties as the resonators become infinitesimally small. We show that a cavity of resonators with 'fixed sign' (*i.e.* all gain or all loss) converges to an effective system whose material parameters retain this property. We also observe that a structure that is $\mathcal{PT}$-symmetric at the microscale will have real-valued material parameters at the macroscale, after homogenization [26].

The subwavelength resonators we study here have broken Hermiticity due to the gain and loss. In particular, this implies that standard energy conservation relations no longer apply, which can result in exotic scattering behaviour [13]. While being impossible in Hermitian systems, $\mathcal{PT}$-symmetric structures can have frequencies at which the reflection is zero when the wave is impinging from one side, but non-zero when the wave is impinging from the opposite side [20, 23, 34]. We will refer to such case as *unidirectional reflectionless transmission*, or *unidirectional reflection* for short. Also, since energy conservation no longer applies, the scattering coefficients are not bounded by unity, and could possibly be very large. We refer to this as *extraordinary transmission*, which has been demonstrated to occur in both optical and acoustic systems [32, 33, 35].

We study unidirectional reflection and extraordinary transmission in an unbounded, $\mathcal{PT}$-symmetric structure at subwavelength frequencies. This structure is composed of periodically repeating $\mathcal{PT}$-symmetric dimers in a thin sheet, a *metascreen*. We will show, in particular, that the reflection coefficients approximately vanish for frequencies close to the second band function. Moreover, as the magnitude of the gain and loss increases, there is a shift in these approximate zeros: the zero of one of the reflection coefficients will be shifted upwards and the other will be shifted downwards. Additionally, for a certain magnitude of the gain/loss, extraordinary transmission will occur at the middle point between the zeros. We emphasize that, unlike previous work based on coupled-mode approximations [20, 29] or perturbation theory [34] which are more formal, the methods presented here provide a mathematically rigorous framework for unidirectional reflectionless transmission. Furthermore, the obtained results are valid even in regimes with large gain and loss.

2 Exceptional points of two resonators

We will, first, study a structure composed of two resonators $D_1, D_2 \subset \mathbb{R}^3$ which are connected domains such that $\partial D_i \in C^{1,s}, 0 < s < 1$. The dimer D is defined as $D = D_1 \cup D_2$. We assume that the wave speed v_i inside the i^{th} resonator D_i is complex while the wave speed v in the surrounding material is real. Denoting the frequency of the waves by ω, we define the wave numbers, for $i = 1, 2$, as

$$k = \frac{\omega}{v}, \quad k_i = \frac{\omega}{v_i}.$$

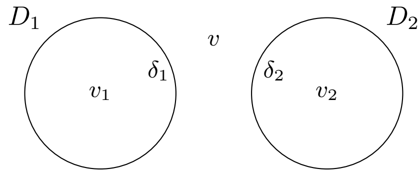

Figure 1: Two subwavelength resonators D_1 and D_2 with wave speeds v_1, v_2, and wave speed v in the surrounding material. The contrast between the i^{th} resonator and the surrounding material is described by δ_i. This system is $\mathcal{PT}$-symmetric if $D_1 = -D_2$ and $v_1^2\delta_1 = \overline{v_2^2\delta_2}$.

We denote the material contrast parameters of the two resonators by $\delta_i,\ i = 1, 2$, which are also complex-valued. For $\omega \in \mathbb{C}$, we study the scattering problem

$$\begin{cases} \Delta u + k^2 u = 0 & \text{in } \mathbb{R}^3 \setminus \overline{D}, \\ \Delta u + k_i^2 u = 0 & \text{in } D_i,\ i = 1, 2, \\ u|_+ - u|_- = 0 & \text{on } \partial D, \\ \delta_i \left.\dfrac{\partial u}{\partial \nu}\right|_+ - \left.\dfrac{\partial u}{\partial \nu}\right|_- = 0 & \text{on } \partial D_i,\ i = 1, 2, \\ u(x) - u^{in}(x) & \text{satisfies the Sommerfeld radiation} \\ & \text{condition as } |x| \to \infty, \end{cases} \tag{2.1}$$

where $|_+$ and $|_-$ denote the limits from the outside and inside of D. Here, u^{in} is the incident field which we assume satisfies $\Delta u^{in} + k^2 u^{in} = 0$ in $\mathbb{R}^3$ and $\nabla u^{in}\big|_D = O(\omega)$. We restrict to frequencies such that $\mathrm{Re}(k), \mathrm{Re}(k_i) > 0$, whereby the Sommerfeld radiation condition is given by

$$\lim_{|x| \to \infty} |x| \left(\frac{\partial}{\partial |x|} - \mathrm{i}k \right) u = 0, \tag{2.2}$$

which corresponds to the case where u radiates energy outwards (and not inwards).

Next, we describe the $\mathcal{PT}$-symmetry of the problem. The parity operator $\mathcal{P} : \mathbb{R}^3 \to \mathbb{R}^3$ and the time-reversal operator $\mathcal{T} : \mathbb{C} \to \mathbb{C}$ are given, respectively, by

$$\mathcal{P}(x) = -x, \qquad \mathcal{T}(z) = \overline{z}.$$

We assume that the dimer D is $\mathcal{PT}$-symmetric, by which we mean that

$$D_1 = \mathcal{P}D_2, \quad \text{and} \quad v_1^2\delta_1 = \mathcal{T}(v_2^2\delta_2).$$

We will see shortly that this indeed is the assumption required to ensure that the system is $\mathcal{PT}$-symmetric, at leading order. We define $\delta := |\delta_1|$, and assume that

$$\delta \ll 1, \quad \delta_2 = O(\delta), \quad v_i = O(1).$$

The assumption that δ is small means that we are studying high-contrast resonators. We introduce the notation

$$v_1^2\delta_1 := a + \mathrm{i}b, \qquad v_2^2\delta_2 := a - \mathrm{i}b,$$

for real-valued parameters a and b. The parameter b can be interpreted as the magnitude of the gain and the loss.

We say that a frequency ω is a *resonant frequency* if the real part of ω is positive and there is a non-zero solution to the problem (2.1) with $u^{in} = 0$. Moreover, we say that the resonant frequency ω is a subwavelength resonant frequency if $\omega \to 0$ as $\delta \to 0$.

The scattering problem (2.1) is a model problem for subwavelength resonators with high-contrast materials. It can be used as a model for studying $\mathcal{PT}$-symmetric systems in both photonics and phononics (see *e.g.* [14]).

2.1 Layer potential theory on bounded domains

The solutions to the Helmholtz problem (2.1) can be effectively studied using representations in terms of integral operators. In particular, let $\mathcal{S}_D^k$ be the single layer potential, defined by

$$\mathcal{S}_D^k[\phi](x) := \int_{\partial D} G^k(x-y)\phi(y)\,\mathrm{d}\sigma(y), \quad x \in \mathbb{R}^3, \tag{2.3}$$

where $G^k(x)$ is the outgoing Helmholtz Green's function, given by

$$G^k(x) := -\frac{e^{\mathrm{i}k|x|}}{4\pi|x|}, \quad x \in \mathbb{R}^3,\ \mathrm{Re}(k) \geq 0.$$

Here, "outgoing" refers to the fact that G^k satisfies the Sommerfeld radiation condition (2.2).

For the single layer potential corresponding to the Laplace equation, $\mathcal{S}_D^0$, we will omit the superscript and write $\mathcal{S}_D$. It is well known that the trace operator $\mathcal{S}_D : L^2(\partial D) \to H^1(\partial D)$ is invertible, where $H^1(\partial D)$ is the space of functions that are square integrable on ∂D and have a weak first derivative that is also square integrable.

The Neumann-Poincaré operator $\mathcal{K}_D^{k,*} : L^2(\partial D) \to L^2(\partial D)$ is defined by

$$\mathcal{K}_D^{k,*}[\phi](x) := \int_{\partial D} \frac{\partial}{\partial \nu_x} G^k(x-y)\phi(y)\,\mathrm{d}\sigma(y), \quad x \in \partial D,$$

where $\partial/\partial\nu_x$ denotes the outward normal derivative at $x \in \partial D$.

The behaviour of $\mathcal{S}_D^k$ on the boundary ∂D is described by the following relations, often known as *jump relations*,

$$\mathcal{S}_D^k[\phi]\big|_+ = \mathcal{S}_D^k[\phi]\big|_-, \tag{2.4}$$

and

$$\frac{\partial}{\partial \nu}\mathcal{S}_D^k[\phi]\Big|_\pm = \left(\pm\frac{1}{2}I + \mathcal{K}_D^{k,*}\right)[\phi], \tag{2.5}$$

where $|_\pm$ denote the limits from outside and inside D. When k is small, the single layer potential satisfies

$$\mathcal{S}_D^k = \mathcal{S}_D + k\mathcal{S}_{D,1} + O(k^2), \tag{2.6}$$

where the error term is with respect to the operator norm $\|.\|_{\mathcal{L}(L^2(\partial D),H^1(\partial D))}$, and the operator $\mathcal{S}_{D,1} : L^2(\partial D) \to H^1(\partial D)$ is given by

$$\mathcal{S}_{D,1}[\phi](x) = \frac{1}{4\pi\mathrm{i}}\int_{\partial D} \phi\,\mathrm{d}\sigma, \qquad x \in \partial D.$$

Moreover, we have

$$\mathcal{K}_D^{k,*} = \mathcal{K}_D^{0,*} + k^2\mathcal{K}_{D,2} + k^3\mathcal{K}_{D,3} + O(k^4), \tag{2.7}$$

where the error term is with respect to the operator norm $\|.\|_{\mathcal{L}(L^2(\partial D),L^2(\partial D))}$ and where

$$\mathcal{K}_{D,2}[\phi](x) = \frac{1}{8\pi}\int_{\partial D} \frac{(x-y)\cdot\nu_x}{|x-y|}\phi(y)\,\mathrm{d}\sigma(y), \quad \mathcal{K}_{D,3}[\phi](x) = \frac{\mathrm{i}}{12\pi}\int_{\partial D}(x-y)\cdot\nu_x\phi(y)\,\mathrm{d}\sigma(y).$$

We have the following lemma from [8].

Lemma 2.1. *For any $\varphi \in L^2(\partial D)$ we have, for $i = 1,2$,*

$$\begin{aligned}
&\int_{\partial D_i}\left(-\frac{1}{2}I + \mathcal{K}_D^*\right)[\varphi]\,\mathrm{d}\sigma = 0, &&\int_{\partial D_i}\left(\frac{1}{2}I + \mathcal{K}_D^*\right)[\varphi]\,\mathrm{d}\sigma = \int_{\partial D_i}\varphi\,\mathrm{d}\sigma,\\
&\int_{\partial D_i}\mathcal{K}_{D,2}[\varphi]\,\mathrm{d}\sigma = -\int_{D_i}\mathcal{S}_D[\varphi]\,\mathrm{d}x, &&\int_{\partial D_i}\mathcal{K}_{D,3}[\varphi]\,\mathrm{d}\sigma = \frac{\mathrm{i}|D_i|}{4\pi}\int_{\partial D}\varphi\,\mathrm{d}\sigma.
\end{aligned} \tag{2.8}$$

A thorough presentation of other properties of layer potential operator and their use in wave-scattering problems can be found in *e.g.* [7].

2.2 Capacitance matrix analysis

Our approach to solving (2.1) is to study the *weighted capacitance matrix*. We will see that the eigenstates of this 2×2-matrix characterize, at leading order in δ, the resonant modes of the system. This approach offers a rigorous discrete approximation to the differential problem.

In order to introduce the notion of capacitance, we define the functions ψ_j, for $j = 1, 2$, as

$$\psi_j = \mathcal{S}_D^{-1}[\chi_{\partial D_j}],$$

where $\chi_A : \mathbb{R}^3 \to \{0, 1\}$ is used to denote the characteristic function of a set $A \subset \mathbb{R}^3$. It is well-known that ψ_1 and ψ_2 form a basis for $\ker\left(-\frac{1}{2}I + \mathcal{K}_D^*\right)$. The capacitance coefficients C_{ij}, for $i, j = 1, 2$, are then defined as

$$C_{ij} = -\int_{\partial D_i} \psi_j \, \mathrm{d}\sigma,$$

and the capacitance matrix is the matrix $C = (C_{ij})$. Finally, we define the *weighted* capacitance matrix $C^v = (C_{ij}^v)$ as

$$C^v := VC = \begin{pmatrix} v_1^2\delta_1 C_{11} & v_1^2\delta_1 C_{12} \\ v_2^2\delta_2 C_{21} & v_2^2\delta_2 C_{22} \end{pmatrix}, \qquad V := \begin{pmatrix} v_1^2\delta_1 & 0 \\ 0 & v_2^2\delta_2 \end{pmatrix}. \tag{2.9}$$

This has been weighted to account for the different material parameters inside the different resonators, see *e.g.* [4, 8] for other variants in slightly different settings. It is well known that $C_{21} = C_{12}$, $C_{12} < 0$ and $C_{11} > -C_{12}$, while the symmetry assumption $D_1 = \mathcal{P}D_2$ implies that $C_{11} = C_{22}$ (see *e.g.* [8, 11, 19]).

We define the functions S_1^ω, S_2^ω as

$$S_1^\omega(x) = \begin{cases} \mathcal{S}_D^k[\psi_1](x), & x \in \mathbb{R}^3 \setminus \overline{D}, \\ \mathcal{S}_D^{k_i}[\psi_1](x), & x \in D_i, \ i = 1, 2, \end{cases} \qquad S_2^\omega(x) = \begin{cases} \mathcal{S}_D^k[\psi_2](x), & x \in \mathbb{R}^3 \setminus \overline{D}, \\ \mathcal{S}_D^{k_i}[\psi_2](x), & x \in D_i, \ i = 1, 2. \end{cases}$$

Lemma 2.2. *As $\omega \to 0$, the solution to the scattering problem (2.1) can be written as*

$$u - u^{in} = q_1 S_1^\omega + q_2 S_2^\omega - \mathcal{S}_D^k\left[\mathcal{S}_D^{-1}[u^{in}]\right] + O(\omega),$$

for constants q_1 and q_2 which satisfy, up to an error of order $O(\delta\omega + \omega^3)$, the problem

$$\left(C^v - \omega^2|D_1|I\right)\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = -\begin{pmatrix} v_1^2\delta_1 \int_{\partial D_1} \mathcal{S}_D^{-1}[u^{in}]\,\mathrm{d}\sigma \\ v_2^2\delta_2 \int_{\partial D_2} \mathcal{S}_D^{-1}[u^{in}]\,\mathrm{d}\sigma \end{pmatrix}. \tag{2.10}$$

Proof. The solutions can be represented as

$$u = \begin{cases} u^{in}(x) + \mathcal{S}_D^k[\psi](x), & x \in \mathbb{R}^3 \setminus \overline{D}, \\ \mathcal{S}_D^{k_i}[\phi](x), & x \in D_i, \ i = 1, 2, \end{cases} \tag{2.11}$$

for some surface potentials $(\phi, \psi) \in L^2(\partial D) \times L^2(\partial D)$, which must be chosen so that u satisfies the transmission conditions across ∂D. Using the jump conditions (2.4) and (2.5), we see that in order to satisfy the transmission conditions, the layer densities ϕ and ψ must satisfy

$$\begin{aligned} \mathcal{S}_D^{k_i}[\phi] - \mathcal{S}_D^k[\psi] &= u^{in} \quad \text{on } \partial D_i, \\ \left(-\frac{1}{2}I + \mathcal{K}_D^{k_i,*}\right)[\phi] - \delta_i\left(\frac{1}{2}I + \mathcal{K}_D^{k,*}\right)[\psi] &= \delta_i \frac{\partial u^{in}}{\partial \nu} \quad \text{on } \partial D_i, \end{aligned}$$

for $i = 1, 2$, where I is the identity operator on $L^2(\partial D)$. From the asymptotic expansions (2.6) and (2.7) and the assumption that $\nabla u^{in} = O(\omega)$ we have that

$$\mathcal{S}_D[\phi - \psi] = u^{in} + O(\omega) \quad \text{on } \partial D_1 \cup \partial D_2, \tag{2.12}$$

$$\left(-\frac{1}{2}I + \mathcal{K}_D^* + \frac{\omega^2}{v_i^2}\mathcal{K}_{D,2}\right)[\phi] - \delta_i\left(\frac{1}{2}I + \mathcal{K}_D^*\right)[\psi] = O(\delta\omega + \omega^3) \quad \text{on } \partial D_i.$$

From (2.12) and the fact that $\mathcal{S}_D$ is invertible we can see that

$$\psi = \phi - \mathcal{S}_D^{-1}[u^{in}] + O(\omega). \tag{2.13}$$

Thus, we are left with the equations

$$\left(-\frac{1}{2}I + \mathcal{K}_D^* + \frac{\omega^2}{v_i^2}\mathcal{K}_{D,2} - \delta_i\left(\frac{1}{2}I + \mathcal{K}_D^*\right)\right)[\phi] = -\delta_i\left(\frac{1}{2}I + \mathcal{K}_D^*\right)\mathcal{S}_D^{-1}[u^{in}] + O(\delta\omega + \omega^3), \tag{2.14}$$

on $\partial D_i, i = 1, 2$. Integrating (2.14) over ∂D_i, and using Lemma 2.1 gives us that

$$-\omega^2\int_{D_i}\mathcal{S}_D[\phi]\,\mathrm{d}x - v_i^2\delta_i\int_{\partial D_i}\phi\,\mathrm{d}\sigma = -v_i^2\delta_i\int_{\partial D_i}\mathcal{S}_D^{-1}[u^{in}]\,\mathrm{d}\sigma + O(\delta\omega + \omega^3).$$

At leading order, (2.14) says that $\left(-\frac{1}{2}I + \mathcal{K}_D^*\right)[\phi] = 0$ so, since ψ_1 and ψ_2 form a basis for $\ker\left(-\frac{1}{2}I + \mathcal{K}_D^*\right)$, the solution can be written as

$$\phi = q_1\psi_1 + q_2\psi_2 + O(\omega^2 + \delta), \tag{2.15}$$

for constants $q_1, q_2 = O(1)$. Making this substitution we reach, up to an error of order $O(\delta\omega + \omega^3)$, the problem

$$\left(C^v - \omega^2|D_1|I\right)\begin{pmatrix}q_1\\ q_2\end{pmatrix} = -\begin{pmatrix}v_1^2\delta_1\int_{\partial D_1}\mathcal{S}_D^{-1}[u^{in}]\,\mathrm{d}\sigma\\ v_2^2\delta_2\int_{\partial D_2}\mathcal{S}_D^{-1}[u^{in}]\,\mathrm{d}\sigma\end{pmatrix}. \tag{2.16}$$

The result now follows from (2.11) combined with the expressions for ϕ, ψ in (2.13), (2.15) and (2.16). □

Theorem 2.3. *As $\delta \to 0$, the subwavelength resonant frequencies satisfy the asymptotic formula*

$$\omega_i = \sqrt{\frac{\lambda_i}{|D_1|}} + O(\delta), \quad i = 1, 2,$$

where $|D_1|$ is the volume of a single resonator and the branch of the square root is chosen with positive real part. Here, λ_i are the eigenvalues of the weighted capacitance matrix C^v.

Proof. If $u^{in} = 0$, we find from Lemma 2.2 that there is a non-zero solution q_1, q_2 to the eigenvalue problem (2.10) precisely when $\omega^2|D_1|$ is an eigenvalue of C^v. □

The eigenvalues of the matrix C^v are given by

$$\lambda_i = aC_{11} + (-1)^i\sqrt{a^2C_{12}^2 - b^2(C_{11}^2 - C_{12}^2)}. \tag{2.17}$$

The following theorem describes the asymptotic exceptional point of the resonator dimer, which occurs when $\lambda_1 = \lambda_2$.

Theorem 2.4. *There is a magnitude $b_0 = b_0(a) > 0$ of the gain/loss such that the resonator dimer has an asymptotic exceptional point: the frequencies ω_1 and ω_2, and corresponding eigenmodes, coincide to leading order in δ. Moreover, to leading order in δ, we have*

Case $b < b_0$: ω_1 *and* ω_2 *are real, and* $\omega_1 < \omega_2$,
Case $b > b_0$: ω_1 *and* ω_2 *are non-real, and* $\omega_1 = \overline{\omega_2}$.

Proof. Combining Theorem 2.3 and (2.17), we find that b_0 is given by

$$b_0 = \frac{aC_{12}}{\sqrt{C_{11}^2 - C_{12}^2}},$$

which corresponds to the point where C^v has a double eigenvalue corresponding to a one-dimensional eigenspace. From (2.15), it follows that the eigenmodes are linearly dependent. The remaining statements are straightforward to check. □

Remark 2.5. *Theorem 2.4 states that the exceptional point occurs only at leading order in δ. This is not due to a limitation of the method and we do not, in fact, expect the system to exhibit an exact exceptional point. This is a consequence of the radiation condition, which means the differential operator corresponding to the problem* (2.1) *is not $\mathcal{PT}$-symmetric (even in the case $b = 0$ the resonant frequencies have small but non-zero imaginary parts [8]). However, the discrete approximation given by the weighted capacitance matrix is indeed $\mathcal{PT}$-symmetric. The approximate nature of the exceptional point can be observed from the simulations presented in Figure 2.*

Lemma 2.6. *If $b \neq b_0$, the eigenmodes u_i corresponding to the resonant frequencies $\omega_i, i = 1, 2$ are given by*

$$u_i = \mathbf{v}_i^1 S_1^\omega + \mathbf{v}_i^2 S_2^\omega + O(\delta^{1/2}),$$

where $\mathbf{v}_i = \begin{pmatrix} \mathbf{v}_i^1 & \mathbf{v}_i^2 \end{pmatrix}^{\mathrm{T}}$ (using superscript T *to denote the matrix transpose) are the eigenvectors of C^v given by*

$$\mathbf{v}_i = \begin{pmatrix} -C_{12} \\ C_{11} - \mu_i \end{pmatrix}, \qquad \mu_i = \frac{\lambda_i}{(a + ib)}.$$

2.3 Numerical computations

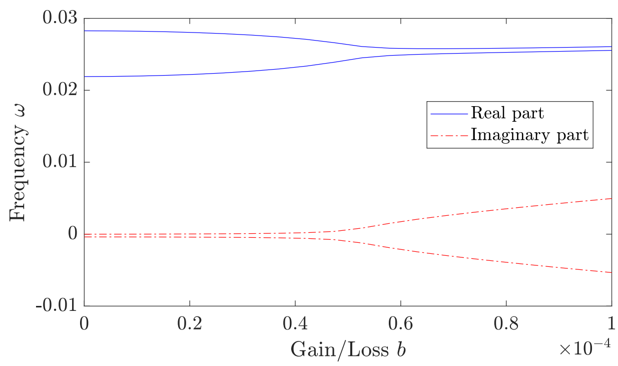

Figure 2: Plot of the real part (blue) and imaginary part (red) of the resonant frequencies of the dimer as the gain/loss parameter b increases. The asymptotic exceptional point occurs at $b_0 \approx 0.5 \times 10^{-4}$, at which point the frequencies coincide to leading order. For b smaller than b_0, the frequencies are real, while for b larger than b_0 the frequencies are conjugate to each other, again to leading order. Here, we simulate spherical resonators with unit radius, separation distance 2 and material parameters $a = 2 \times 10^{-4}$ and $v = 1$.

Figure 2 shows the two resonant frequencies ω_1 and ω_2 as functions of b. For $b = b_0$, the resonant frequencies coincide at leading order in δ. The leading order terms are real for $b < b_0$ and complex conjugates with zero real part for larger b. These numerical simulations were performed on spherical resonators using the multipole expansion method, which is outlined in [3, Appendix A].

3 Resonator cavities

In this section, we examine the properties of finite metamaterials taking the form of cavities filled with a large number of small subwavelength resonators with non-real material parameters. While the pair of high-contrast resonators in Section 2 interacts with wavelengths much larger than their size, we would like to design these cavities so that they might exhibit similar exceptional behaviour in response to wavelengths of the same order as their dimensions. We study this system using a homogenization approach, deriving the effective equations as the size of the resonators becomes small and the number of resonators becomes large.

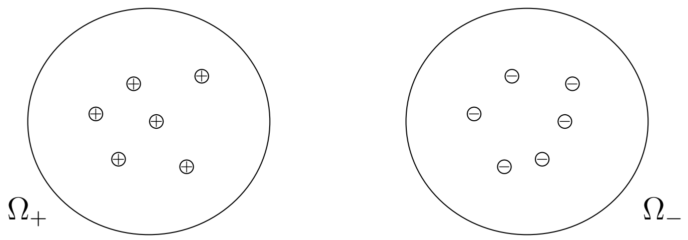

Figure 3: A pair of $\mathcal{PT}$-symmetric cavities of many small resonators. Here, $+$ and $-$ denote opposite signs of the imaginary part of the material coefficients.

3.1 Non-Hermitian cavities

We first derive a version of Lemma 2.2 which describes how an asymptotically small resonator $D_0^r = rD_0 + z$ (where D_0 is some fixed, connected domain) scatters an incoming field. So that the resonant frequencies are of order 1, we will assume that if the size of the resonator $r \to 0$ then the material parameters of its interior are given by

$$v_0^2\delta_0 := r^2 a + \mathrm{i}r^{2+\varepsilon_1}b, \tag{3.1}$$

for some fixed $0 < \varepsilon_1 < 1$ and real-valued constants $a, b = O(1)$. We will fix $a > 0$ and consider the cases $b > 0$ and $b < 0$ separately. We study the scattering problem

$$\begin{cases} \Delta u + k^2 u = 0 & \text{in } \mathbb{R}^3 \setminus \overline{D_0^r}, \\ \Delta u + k_0^2 u = 0 & \text{in } D_0^r, \\ u|_+ - u|_- = 0 & \text{on } \partial D_0^r, \\ \delta_0 \left.\dfrac{\partial u}{\partial \nu}\right|_+ - \left.\dfrac{\partial u}{\partial \nu}\right|_- = 0 & \text{on } \partial D_0^r, \\ u(x) - u^{in}(x) & \text{satisfies the Sommerfeld radiation} \\ & \text{condition as } |x| \to \infty, \end{cases} \tag{3.2}$$

where $\delta_0 \ll 1$ and $k_0 = \omega/v_0$ with $\mathrm{Re}(k), \mathrm{Re}(k_0) \geq 0$.

Lemma 3.1. *Let $D_0 \subset \mathbb{R}^3$ be some fixed resonator (whose boundary satisfies $\partial D_0 \in C^{1,s}$ for some $0 < s < 1$) and define the small resonator D_0^r, for some small $r > 0$, as*

$$D_0^r = rD_0 + z,$$

where $z \in \mathbb{R}^3$ is the new centre of D_0^r. Assume that the material parameters within D_0^r satisfy (3.1) and that $\omega^2 - (\omega^*)^2 = Cr^{\varepsilon_1}$ for some fixed $C \in \mathbb{C}$, where

$$(\omega^*)^2 = \frac{(a + \mathrm{i}r^{\varepsilon_1}b)\mathrm{Cap}_{D_0}}{|D_0|}.$$

As $r \to 0$, the solution to the Helmholtz problem (3.2) for scattering by D_0^r can be written as

$$u(x) - u^{in}(x) = r\mathrm{Cap}_{D_0} \frac{\omega^2}{\omega^2 - (\omega^*)^2} G^k(x - z) u^{in}(z) + O(r^{2-\varepsilon_1}).$$

Proof. The solutions to the scattering problem can be represented as

$$u = \begin{cases} u^{in}(x) + \mathcal{S}_{D_0^r}^k[\psi](x), & x \in \mathbb{R}^3 \setminus \overline{D_0^r}, \\ \mathcal{S}_{D_0^r}^{k_1}[\phi](x), & x \in D_0^r, \end{cases}$$

where $k_1 = \omega/v_1$, for some surface potentials $(\phi, \psi) \in L^2(\partial D_0^r) \times L^2(\partial D_0^r)$, which must be chosen so that u satisfies the transmission conditions across ∂D_0^r.

We wish to replicate Lemma 2.2 in the present setting, using asymptotic expansions in terms of $r \ll 1$ (and $\delta = O(r^2)$), while $\omega = O(1)$. We have, as $r \to 0$, that

$$\mathcal{S}_{D_0^r}[\phi - \psi] = u^{in} + O(r) \quad \text{on } \partial D_0^r,$$
$$\left(-\frac{1}{2}I + \mathcal{K}^*_{D_0^r} + \frac{\omega^2}{v_1^2}\mathcal{K}_{D_0^r,2}\right)[\phi] - \delta_0 \left(\frac{1}{2}I + \mathcal{K}^*_{D_0^r}\right)[\psi] = O(r^2) \quad \text{on } \partial D_0^r.$$

Repeating the arguments of Lemma 2.2, we find that the solution to the scattering problem can be written as

$$u - u^{in} = qS^\omega_{D_0^r} - \mathcal{S}^k_{D_0^r}\left[\mathcal{S}^{-1}_{D_0^r}[u^{in}]\right] + O(r),$$

where

$$S^\omega_{D_0^r}(x) = \begin{cases} \mathcal{S}^k_{D_0^r}\left[\mathcal{S}^{-1}_{D_0^r}[\chi_{\partial D_0^r}]\right](x), & x \in \mathbb{R}^3 \setminus \overline{D_0^r}, \\ \mathcal{S}^{k_1}_{D_0^r}\left[\mathcal{S}^{-1}_{D_0^r}[\chi_{\partial D_0^r}]\right](x), & x \in D_0^r, \end{cases}$$

and $q = q(\omega)$ satisfies

$$\left(-\omega^2|D_0^r| - v_0^2\delta_0 \int_{\partial D_0^r} \mathcal{S}^{-1}_{D_0^r}[\chi_{\partial D_0^r}] \,\mathrm{d}\sigma\right) q = -v_0^2\delta_0 \int_{\partial D_0^r} \mathcal{S}^{-1}_{D_0^r}[u^{in}] \,\mathrm{d}\sigma + O(r^4).$$

Let

$$\mathrm{Cap}_{D_0} := -\int_{\partial D_0} \mathcal{S}^{-1}_{D_0}[\chi_{\partial D_0}] \,\mathrm{d}\sigma,$$

then we have that

$$\int_{\partial D_0^r} \mathcal{S}^{-1}_{D_0^r}[\chi_{\partial D_0^r}] \,\mathrm{d}\sigma = -r\mathrm{Cap}_{D_0}, \qquad \int_{\partial D_0^r} \mathcal{S}^{-1}_{D_0^r}[u^{in}] \,\mathrm{d}\sigma = -r\mathrm{Cap}_{D_0} u^{in}(z) + O(r^2),$$
$$S^\omega_{D_0^r} = -r\mathrm{Cap}_{D_0} G^k(x - z) + O(r^2),$$
$$\mathcal{S}^k_{D_0^r}\left[\mathcal{S}^{-1}_{D_0^r}[u^{in}]\right] = -r\mathrm{Cap}_{D_0} u^{in}(z) G^k(x - z) + O(r^2),$$

from which the result follows. □

We now wish to consider a spherical domain Ω which contains a (large) number of small, identical resonators (*e.g.* Ω_+ or Ω_- in Figure 3). If D_0 is a fixed domain, then for some $r > 0$ the N resonators are given, for $1 \leq j \leq N$, by

$$D_{0,j}^{r,N} = rD_0 + z_j^N,$$

for positions z_j^N. We will always assume that r is sufficiently small such that the resonators are not overlapping and that $D_0^{r,N} = \bigcup_{j=1}^N D_{0,j}^{r,N} \Subset \Omega$. We choose the number of resonators N so that there exists some positive number Λ such that

$$r^{1-\varepsilon_1} N = \Lambda. \tag{3.3}$$

The choice of Λ will be an important subtlety in the major theorem of this section.

We will find the effective equation in the specific case that the frequency $\omega = O(1)$ satisfies

$$\omega^2 = \frac{a\mathrm{Cap}_{D_0}}{|D_0|}. \tag{3.4}$$

In this case, we are able to use a result from [9] which says that, since the resonators are small, we can use the point-scatter approximation from Lemma 3.1 to describe how they interact with incoming waves. To do so, we must make some extra assumptions on the regularity of the distribution $\{z_j^N : 1 \leq j \leq N\}$ so that the system is well behaved as $N \to \infty$ (under the assumption

(3.3)). In particular, we assume that there exists some constant η such that for any N it holds that

$$\min_{i\neq j} |z_i^N - z_j^N| \geq \frac{\eta}{N^{1/3}}, \tag{3.5}$$

and, further, there exists some $0 < \varepsilon_0 < 1$ and constants $C_1, C_2 > 0$ such that for all $h \geq 2\eta N^{-1/3}$,

$$\sum_{|x - z_j^N| \geq h} \frac{1}{|x - y_j^N|^2} \leq C_1 N |h|^{-\varepsilon_0}, \qquad \text{uniformly for all } x \in \Omega, \tag{3.6}$$

$$\sum_{2\eta N^{-1/3} \leq |x - z_j^N| \leq 3h} \frac{1}{|x - y_j^N|} \leq C_2 N |h|, \qquad \text{uniformly for all } x \in \Omega. \tag{3.7}$$

Finally, we will also need that

$$\varepsilon_2 := \frac{\varepsilon_1}{1 - \varepsilon_1} - \frac{\varepsilon_0}{3} > 0. \tag{3.8}$$

If we represent the field that is scattered by the collection of resonators $D_0^{r,N} = \bigcup_{j=1}^N D_{0,j}^{r,N}$ as

$$u^N(x) = \begin{cases} u^{in}(x) + \mathcal{S}^k_{D_0^{r,N}}[\psi^N](x), & x \in \mathbb{R}^3 \setminus \overline{D_0^{r,N}}, \\ \mathcal{S}^{k_0}_{D_0^{r,N}}[\phi^N](x), & x \in D_0^{r,N}, \end{cases}$$

for some $\psi^N, \phi^N \in L^2(\partial D_0^{r,N})$, then we have the following lemma, which follows from [9, Proposition 3.1]. This justifies using a point-scatter approximation to describe the total incident field acting on the resonator $D_{0,j}^{r,N}$ and the scattered field due to $D_{0,j}^{r,N}$, defined respectively as

$$u_j^{in,N} = u^{in} + \sum_{i \neq j} \mathcal{S}^k_{D_{0,i}^{r,N}}[\psi^N] \qquad \text{and} \qquad u_j^{s,N} = \mathcal{S}^k_{D_{0,j}^{r,N}}[\psi^N].$$

Lemma 3.2. *Under the assumptions* (3.4)–(3.8)*, it holds that the total incident field acting on the resonator $D_{0,j}^{r,N}$ is given, at z_j^N, by*

$$u_j^{in,N}(z_j^N) = u^{in}(z_j^N) + \sum_{i \neq j} r \mathrm{Cap}_{D_0} \frac{\omega^2}{\omega^2 - (\omega^*)^2} G^k(z_j^N - z_i^N) u^{in}(z_j^N),$$

up to an error of order $O(N^{-\varepsilon_2})$. Similarly, it holds that the scattered field due to the resonator $D_{0,j}^{r,N}$ is given, at x such that $|x - z_j^N| \gg r$, by

$$u_j^{s,N}(x) = r \mathrm{Cap}_D \frac{\omega^2}{\omega^2 - (\omega^*)^2} G^k(x - z_j^N) u_j^{in,N}(z_j^N),$$

up to an error of order $O(N^{-\varepsilon_2} + r|x - z_j^N|^{-1})$.

In order for the sums in Lemma 3.2 to be well behaved as $N \to \infty$, we make one additional assumption on the regularity of the distribution: that there exists a real-valued function $\widetilde{V} \in C^1(\overline{\Omega})$ such that for any $f \in C^{0,\alpha}(\Omega)$, with $0 < \alpha \leq 1$, there is a constant C_3 such that

$$\max_{1 \leq j \leq N} \left| \frac{1}{N} \sum_{i \neq j} G^k(z_j^N - z_i^N) f(z_i^N) - \int_\Omega G^k(z_j^N - y) \widetilde{V}(y) f(y) \, \mathrm{d}y \right| \leq C_3 \frac{1}{N^{\alpha/3}} \|f\|_{C^{0,\alpha}(\Omega)}. \tag{3.9}$$

Remark 3.3. *It will hold that $\widetilde{V} \geq 0$. If the resonators' centres $\{z_j^N : j = 1, \dots, N\}$ are uniformly distributed, then $\widetilde{V}$ will be a positive constant, $\widetilde{V} = \frac{1}{|\Omega|}$.*

Under all these assumptions, we are able to derive effective equations for the system with an arbitrarily large number of small resonators. If we let $\varepsilon_3 \in (0, \frac{1}{3})$, then we will seek effective equations on the set given by

$$Y_{\varepsilon_3}^N := \left\{ x \in \mathbb{R}^3 : |x - z_j^N| \geq N^{\varepsilon_3 - 1} \text{ for all } 1 \leq j \leq N \right\},$$

which is the set of points that are sufficiently far from the resonators, so avoid the singularities of the Green's function.

Theorem 3.4. *Under the assumptions* (3.3)–(3.9)*, the solution u^N to the scattering problem* (3.2) *with the system of resonators $D_0^{r,N} = \bigcup_{j=1}^N D_{0,j}^{r,N}$ converges to the solution of*

$$\begin{cases} \left(\Delta + k^2 - \frac{\mathrm{i}\Lambda a \mathrm{Cap}_D}{b} \widetilde{V}(x)\right) u(x) = 0, & x \in \Omega, \\ \left(\Delta + k^2\right) u(x) = 0, & x \in \mathbb{R}^3 \setminus \Omega, \end{cases}$$

as $N \to \infty$, together with a radiation condition governing the behaviour in the far field, which says that uniformly for all $x \in Y_{\varepsilon_3}^N$ it holds that

$$|u^N(x) - u(x)| \leq C N^{-\min\left\{\frac{1-\varepsilon_0}{6}, \varepsilon_2, \varepsilon_3, \frac{1-\varepsilon_3}{3}\right\}}.$$

If $a > 0$ and $b < 0$, then this convergence holds regardless of the choice of Λ. If $b > 0$, then there exists at least one $\Lambda \in \mathbb{R}$ for which the solution converges.

Proof. This follows by modifying the results of [9]. Much of this is straightforward, the important subtlety being to show that the operator

$$\mathcal{T}[f](x) := \frac{\mathrm{i}\Lambda a \mathrm{Cap}_{D_0}}{b} \int_\Omega G^k(x-y) \widetilde{V}(y) f(y)\, \mathrm{d}y,$$

is such that $I - \mathcal{T}$ is invertible. Since $\mathcal{T}$ is compact, $I - \mathcal{T}$ is of Fredholm type so is invertible if and only if it is injective. Consider, first, the case that $a > 0$ and $b < 0$ and suppose $f \in C^{0,\alpha}(\Omega)$ is such that $(I - \mathcal{T})[f] = 0$. Applying $\Delta + k^2$, we see that

$$\Delta f = -k^2 f + \frac{\mathrm{i}\Lambda a \mathrm{Cap}_{D_0}}{b} \widetilde{V} f \quad \text{in } \Omega,$$

from which we see that

$$-\int_\Omega |\nabla f|^2\, \mathrm{d}x + \int_{\partial\Omega} \frac{\partial f}{\partial \nu} \overline{f}\, \mathrm{d}\sigma = -k^2 \int_\Omega |f|^2\, \mathrm{d}x + \frac{\mathrm{i}\Lambda a \mathrm{Cap}_{D_0}}{b} \int_\Omega \widetilde{V} |f|^2\, \mathrm{d}x. \tag{3.10}$$

From [25] we know that

$$\mathrm{Im} \int_{\partial\Omega} \frac{\partial f}{\partial \nu} \overline{f}\, \mathrm{d}\sigma \geq 0, \tag{3.11}$$

with equality only if $f = 0$. Since $\widetilde{V} \geq 0$ we have also that $\int_\Omega \widetilde{V} |f|^2\, \mathrm{d}x \geq 0$ so taking the imaginary part of (3.10) gives us that

$$0 \leq \mathrm{Im} \int_{\partial\Omega} \frac{\partial f}{\partial \nu} \overline{f}\, \mathrm{d}\sigma = \frac{\Lambda a \mathrm{Cap}_{D_0}}{b} \int_\Omega \widetilde{V} |f|^2\, \mathrm{d}x \leq 0,$$

hence $f = 0$.

Conversely, if $b > 0$ then we must take more care to choose the constant Λ to guarantee invertibility. Assume, for contradiction, that we cannot choose Λ such that $I - \mathcal{T}$ is invertible. Then, we can choose a sequence of real numbers $\{\Lambda_n : n \in \mathbb{N}\}$ such that $\Lambda_n \to 0$ and for each n there exists $0 \neq f_n \in H^1(\Omega)$ such that $(I - \mathcal{T}) f_n = 0$. Hence, it holds that $g_n := f_n / \|f_n\|_{H^1(\Omega)}$ satisfies

$$\begin{cases} \Delta g_n + k^2 g_n - \frac{\mathrm{i}\Lambda_n a \mathrm{Cap}_{D_0}}{b} \widetilde{V} g_n = 0 & \text{in } \Omega, \\ \frac{\partial g_n}{\partial \nu} = \mathcal{N}_k(g_n) & \text{on } \partial\Omega, \end{cases} \tag{3.12}$$

where $\mathcal{N}_k$ is the Dirichlet-to-Neumann map on the exterior of Ω, defined as $\mathcal{N}_k[\varphi] := \frac{\partial v}{\partial \nu}\big|_{\partial\Omega}$ where v solves $(\Delta + k^2)v = 0$ on $\mathbb{R}^3 \setminus \overline{\Omega}$ with $v = \varphi$ on $\partial\Omega$ and the Sommerfeld radiation condition at infinity. Since $\{g_n : n \in \mathbb{N}\}$ is bounded in $H^1(\Omega)$, which is compactly embedded into $L^2(\Omega)$, there exists some $g \in H^1(\Omega)$ such that (passing to a subsequence) $g_n \to g$ in $L^2(\Omega)$.

We want to show that, in fact, g_n converges strongly to g in $H^1(\Omega)$ and that $g = 0$, which will contradict the fact that $\|g_n\|_{H^1\Omega} = 1$ for all n. Studying the limiting form of (3.12), we see that the limit g is the restriction of w to Ω, where w is the solution to $(\Delta + k^2)w = 0$ on $\mathbb{R}^3$ with the

Sommerfeld radiation condition at infinity. This is well known to have a unique solution given by $w = 0$, hence $g = w|_\Omega = 0$. Analogous to (3.10), it holds for each n that

$$-\int_\Omega |\nabla g_n|^2 \,\mathrm{d}x + \int_{\partial\Omega} \frac{\partial g_n}{\partial \nu}\overline{g_n}\,\mathrm{d}\sigma = -k^2\int_\Omega |g_n|^2\,\mathrm{d}x + \frac{\mathrm{i}\Lambda_n a \mathrm{Cap}_{D_0}}{b}\int_\Omega \widetilde{V}|g_n|^2\,\mathrm{d}x,$$

and we know from [25] that

$$\mathrm{Re}\int_{\partial\Omega} \frac{\partial g_n}{\partial \nu}\overline{g_n}\,\mathrm{d}\sigma \le 0, \tag{3.13}$$

so we see that

$$\int_\Omega |\nabla g_n|^2\,\mathrm{d}x \le k^2\int_\Omega |g_n|^2\,\mathrm{d}x.$$

Therefore, $\nabla g_n \to 0$ in $L^2(\Omega)$ so we have that $g_n \to 0$ in $H^1(\Omega)$, which gives the desired contradiction.

Once we know that $I - \mathcal{T}$ is invertible, we can see that the limiting system is well posed and the rest of the argument (in particular, proving that the field given by Lemma 3.2 converges to the limiting system) follows from [9]. □

Remark 3.5. *The assumption* (3.4) *is important so that the frequency ω is close to the resonant frequency ω^*. In particular, the difference is such that $\omega^2 - (\omega^*)^2 = O(r^{\varepsilon_1})$. This means that the behaviour will be dominated by the monopole resonant modes of each small resonator. If we relaxed this assumption, then other coupled modes might be excited, invalidating the use of the point-interaction approximation from Lemma 3.2.*

Remark 3.6. *The assumption that Ω is spherical is needed so that we are able to infer* (3.11) *and* (3.13) *from the results of [25].*

3.2 Homogenization of $\mathcal{PT}$-symmetric pairs

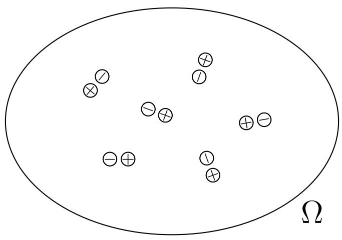

Figure 4: A cavity containing many small $\mathcal{PT}$-symmetric pairs of resonators. Here, $+$ and $-$ denote opposite signs of the imaginary part of the material coefficients. Microscopic $\mathcal{PT}$-symmetry is lost under homogenization.

It is interesting to consider how a cavity filled with a large collection of small $\mathcal{PT}$-symmetric pairs of resonators would behave, as depicted in Figure 4. In particular, interesting behaviour is seen when each pair is poised at an asymptotic exceptional point (*cf.* similar analysis of the real-valued case in [8]).

Recall the $\mathcal{PT}$-symmetric resonator pair $D = D_1 \cup D_2$ from Section 2. We will define the small dimer $D^r = D_1^r \cup D_2^r$, for some small $r > 0$, as

$$D^r = rD + z,$$

where $z \in \mathbb{R}^3$ is the new centre of D^r. We re-use the notation for the material parameters from Section 2 but, in order for resonance to occur at $O(1)$ frequencies, scale the material parameters so that

$$v_1^2\delta_1 := r^2 a + \mathrm{i}r^2 b, \qquad v_2^2\delta_2 := r^2 a - \mathrm{i}r^2 b, \tag{3.14}$$

for real-valued constants $a, b = O(1)$. In this case, we have chosen both the real and imaginary parts of $v_i^2 \delta_i$ to be $O(r^2)$ since they need to have the same asymptotic behaviour in order for the resonator pair to support an asymptotic exceptional point, as predicted by Theorem 2.4.

We must first replicate Lemma 2.2 in the present setting, using asymptotic expansions in terms of $r \ll 1$ (and $\delta = O(r^2)$), while $\omega = O(1)$. We have, as $r \to 0$, that the solution to the problem (2.1) for scattering by D^r can be represented in the form (2.11) with densities $\phi, \psi \in L^2(\partial D^r) \times L^2(\partial D^r)$ which satisfy

$$\mathcal{S}_{D^r}[\phi - \psi] = u^{in} + O(r), \quad \text{on } \partial D_1^r \cup \partial D_2^r,$$
$$\left(-\frac{1}{2} I + \mathcal{K}_{D^r}^* + \frac{\omega^2}{v_j^2} \mathcal{K}_{D^r,2}\right)[\phi] - \delta_j \left(\frac{1}{2} I + \mathcal{K}_{D^r}^*\right)[\psi] = O(r^2), \quad \text{on } \partial D_j^r,\ j = 1, 2.$$

Repeating the arguments of Lemma 2.2, we find that the solution to the scattering problem can be written as

$$u - u^{in} = q_1 S_{D^r,1}^{\omega} + q_2 S_{D^r,2}^{\omega} - \mathcal{S}_{D^r}^{\omega}\left[\mathcal{S}_{D^r}^{-1}[u^{in}]\right] + O(r), \tag{3.15}$$

where

$$S_{D^r,j}^{\omega}(x) = \begin{cases} \mathcal{S}_{D^r}^{k}\left[\mathcal{S}_{D^r}^{-1}[\chi_{\partial D_j^r}]\right](x), & x \in \mathbb{R}^3 \setminus \overline{D^r}, \\ \mathcal{S}_{D^r}^{k_i}\left[\mathcal{S}_{D^r}^{-1}[\chi_{\partial D_j^r}]\right](x), & x \in D_i^r,\ i = 1, 2, \end{cases}$$

and the constants q_1 and q_2 satisfy

$$\left(C_{D^r}^v - \omega^2 |D_1^r| I\right)\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = -\begin{pmatrix} r^2(a + \mathrm{i}b)\int_{\partial D_1^r} \mathcal{S}_{D^r}^{-1}[u^{in}]\,\mathrm{d}\sigma \\ r^2(a - \mathrm{i}b)\int_{\partial D_2^r} \mathcal{S}_{D^r}^{-1}[u^{in}]\,\mathrm{d}\sigma \end{pmatrix} + O(r^4). \tag{3.16}$$

We now wish to compute expressions for q_1 and q_2 in the case that we are at the asymptotic exceptional point, meaning that $b = b_0$ as specified by Theorem 2.4. In this case, $C_{D^r}^v$ is non-Hermitian and has one eigenvalue with a one-dimensional eigenspace. We will use the Jordan decomposition for $C_{D^r}^v$. Using the notation C_{ij} to denote the capacitance coefficients of the original fixed dimer D, as defined in Section 2, the eigenvalue of $C_{D^r}^v$ is given by $r^3\lambda_1$ where $\lambda_1 = aC_{11}$. We have that

$$C_{D^r}^v = SJS^{-1}, \tag{3.17}$$

where

$$J = \begin{pmatrix} r^3\lambda_1 & 1 \\ 0 & r^3\lambda_1 \end{pmatrix}, \quad S = \begin{pmatrix} -rC_{12} & \frac{\mathrm{i}C_{12}}{r^2 b_0 C_{11}} \\ \frac{\mathrm{i}rb_0C_{11}}{a+ib_0} & 0 \end{pmatrix}, \quad S^{-1} = -\begin{pmatrix} 0 & \frac{\mathrm{i}(a+\mathrm{i}b_0)}{rb_0C_{11}} \\ \frac{\mathrm{i}r^2b_0C_{11}}{C_{12}} & r^2(a+ib_0) \end{pmatrix}.$$

Using (3.17) and writing $\lambda = r^{-3}\omega^2|D_1^r| = \omega^2|D_1|$, the formula (3.16) gives us that

$$\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = -S\begin{pmatrix} r^{-3}(\lambda_1 - \lambda)^{-1} & -r^{-6}(\lambda_1 - \lambda)^{-2} \\ 0 & r^{-3}(\lambda_1 - \lambda)^{-1} \end{pmatrix} S^{-1}\begin{pmatrix} r^2(a + \mathrm{i}b)\int_{\partial D_1^r} \mathcal{S}_{D^r}^{-1}[u^{in}]\,\mathrm{d}\sigma \\ r^2(a - \mathrm{i}b)\int_{\partial D_2^r} \mathcal{S}_{D^r}^{-1}[u^{in}]\,\mathrm{d}\sigma \end{pmatrix} + O(r),$$

i.e.

$$\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = r^{-1}\begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix}\begin{pmatrix} (a + \mathrm{i}b)\int_{\partial D_1^r} \mathcal{S}_{D^r}^{-1}[u^{in}]\,\mathrm{d}\sigma \\ (a - \mathrm{i}b)\int_{\partial D_2^r} \mathcal{S}_{D^r}^{-1}[u^{in}]\,\mathrm{d}\sigma \end{pmatrix} + O(r), \tag{3.18}$$

where

$$Q_{11} = \mathrm{i}b_0C_{11}\frac{1}{(\lambda - \lambda_1)^2} + \frac{1}{\lambda - \lambda_1}, \qquad Q_{12} = C_{12}(a + \mathrm{i}b_0)\frac{1}{(\lambda - \lambda_1)^2},$$
$$Q_{21} = \frac{b_0^2C_{11}^2}{(a + \mathrm{i}b_0)C_{12}}\frac{1}{(\lambda - \lambda_1)^2}, \qquad Q_{22} = -\mathrm{i}b_0C_{11}\frac{1}{(\lambda - \lambda_1)^2} + \frac{1}{\lambda - \lambda_1}.$$

Lemma 3.7. *As $r \to 0$, the solution to the Helmholtz problem* (2.1) *for scattering by the small $\mathcal{PT}$-symmetric dimer $D^r = rD + z$ with fixed frequency $\omega = O(1)$ can be written as*

$$u(x) - u^{in}(x) = r\, m(\omega) G^k(x) u^{in}(0) + O(r^2),$$

where, if $\omega_1 = \sqrt{aC_{11}|D_1|^{-1}}$,

$$m(\omega) = \mathrm{Cap}_D \left(\frac{a^2 C_{11} C_{12}}{|D_1|^2} \frac{1}{(\omega^2 - \omega_1^2)^2} + \frac{a \mathrm{Cap}_D}{2|D_1|} \frac{1}{\omega^2 - \omega_1^2} + 1 \right).$$

Proof. The terms in (3.15) and (3.18) can be further simplified using scaling properties analogous to (3.1). Note that, thanks to the assumed symmetry $\mathcal{P}D = D$, it holds that $\mathrm{Cap}_D = 2(C_{11}+C_{12})$. Then, we have that

$$\int_{\partial D_j^r} \mathcal{S}_{D^r}^{-1}[u^{in}] \,\mathrm{d}\sigma = -r\tfrac{1}{2}\mathrm{Cap}_D u^{in}(0) + O(r^2),$$

$$S_{D^r,j}^{\omega}(x) = -r\tfrac{1}{2}\mathrm{Cap}_D G^k(x) + O(r^2),$$

$$\mathcal{S}_{D^r}^k \left[\mathcal{S}_{D^r}^{-1}[u^{in}]\right](x) = -r\mathrm{Cap}_D u^{in}(0) G^k(x) + O(r^2). \qquad \square$$

Remark 3.8. *It is interesting to consider using Lemma 3.7 as the starting point for a similar homogenization argument to the one we applied to cavities of single resonators in the previous section. Define N small resonator pairs as $D_j^N = rD + z_j^N$. Allowing a formal argument (and assuming all the required conditions to guarantee* e.g. *the validity of the point-scatter approximation and the convergence of the microfield to the effective one), we observe that as $N \to \infty$ we should obtain the homogenized equation*

$$\begin{cases} \left(\Delta + k^2 - \Lambda m(k/v) V(x)\right) u(x) = 0, & x \in \Omega, \\ \left(\Delta + k^2\right) u(x) = 0, & x \in \mathbb{R}^3 \setminus \Omega, \end{cases}$$

where m is specified in Lemma 3.7 and V is a function that depends on the resonators' positions. Both m and V are real valued, meaning this effective equation has purely real parameters.

4 $\mathcal{PT}$-symmetric metascreens

Here, we study a metascreen consisting of periodically repeated $\mathcal{PT}$-symmetric dimers. There are multiple goals. First, we will derive results analogous to those in Section 2, which characterize the band structure and exceptional points of the metascreen. Thereafter, we will solve the plane-wave scattering problem for the metascreen. Using this, we will prove that the metascreen exhibits asymptotic unidirectional reflectionless transmission. In other words, there are frequencies at which an incoming wave from one side will have zero reflection at leading order, while an incoming wave from the opposite side has non-zero reflection. Moreover, we will demonstrate that at a specific magnitude of the gain/loss, the peak transmittance will be extraordinarily large.

4.1 Scattering problem for the metascreen

We consider a structure composed of $\mathcal{PT}$-symmetric dimers in a two dimensional square lattice with period $L > 0$. The lattice is given by $\Lambda := L\mathbb{Z}^2$ and we assume that the structure is periodic with unit cell $Y = [-L/2, L/2] \times [-L/2, L/2] \times \mathbb{R}$. We adopt the notation from Section 2 where D is a pair of unscaled resonators D_i with material parameters $v_i^2 \delta_i$, for $i = 1, 2$:

$$D = D_1 \cup D_2, \quad v_1^2 \delta_1 = a + \mathrm{i}b, \quad v_2^2 \delta_2 = a - \mathrm{i}b.$$

Additionally, we now assume that D is contained inside Y. We define the periodically repeated resonators as

$$\mathcal{C}_i = \bigcup_{(m_1,m_2)\in\Lambda} D_i + (m_1, m_2, 0), \ i = 1, 2, \qquad \mathcal{C} = \mathcal{C}_1 \cup \mathcal{C}_2.$$

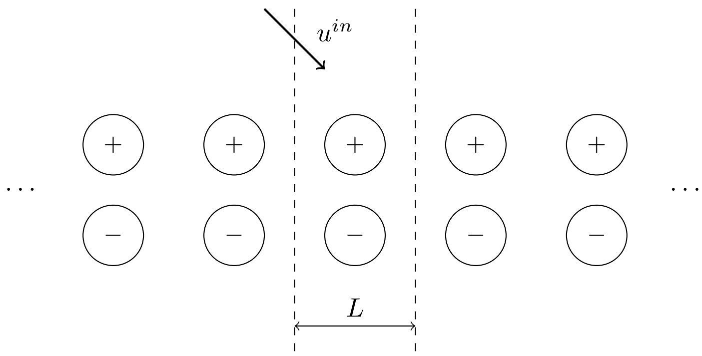

Figure 5: A $\mathcal{PT}$-symmetric metascreen with an incident plane wave u^{in}. Here, $+$ and $-$ denote opposite signs of the imaginary part of the material coefficients.

The dual lattice Λ^* of Λ is defined as $\Lambda^* = (2\pi/L)\Lambda$. The torus $Y^* := \mathbb{R}^2/\Lambda^*$ is known as the *Brillouin zone*. A function $f(y)$, $y \in \mathbb{R}^2$, is said to be α-quasiperiodic, with *quasiperiodicity* $\alpha \in Y^*$, if $e^{-\mathrm{i}\alpha\cdot y} f(y)$ is periodic as a function of y.

We study the scattering problem

$$\begin{cases} \Delta u + k^2 u = 0 & \text{in } \mathbb{R}^3 \setminus \mathcal{C}, \\ \Delta u + k_i^2 u = 0 & \text{in } \mathcal{C}_i, \ i = 1,2, \\ u|_+ - u|_- = 0 & \text{on } \partial\mathcal{C}, \\ \delta_i \dfrac{\partial u}{\partial \nu}\Big|_+ - \dfrac{\partial u}{\partial \nu}\Big|_- = 0 & \text{on } \partial\mathcal{C}_i, \ i = 1,2, \\ u(x) - u^{in}(x) & \text{satisfies the outgoing quasiperiodic} \\ & \text{radiation condition as } |x_3| \to \infty. \end{cases} \tag{4.1}$$

Here, u^{in} is the incident field and the outgoing quasiperiodic radiation condition states that $u(x) - u^{in}(x)$ behaves as a superposition of outgoing plane waves as $|x_3| \to \infty$. We seek solutions u which are α-quasiperiodic in (x_1, x_2) for some α, *i.e.*

$$u(x + (m_1, m_2, 0)) = e^{\mathrm{i}\alpha\cdot(m_1,m_2)} u(x), \quad (m_1, m_2) \in \Lambda.$$

If $u^{in} = 0$, these α-quasiperiodic solutions are the Bloch modes of the metascreen, while if u^{in} is a plane wave, we will seek solutions at α specified by the wave vector of u^{in} (see *e.g.* [7]).

We will study the scattering problem (4.1) using a layer potential formulation analogously as in Section 2. For $\alpha \in Y^*$, the quasiperiodic Green's function $G^{\alpha,k}(x)$ is defined as the solution to

$$\Delta G^{\alpha,k}(x) + k^2 G^{\alpha,k}(x) = \sum_{(m_1,m_2)\in\Lambda} \delta(x - (m_1, m_2, 0)) e^{\mathrm{i}\alpha\cdot(m_1,m_2)},$$

along with the outgoing quasiperiodic radiation condition, where $\delta(x)$ denotes the Dirac delta distribution. $G^{\alpha,k}$ can be written as

$$G^{\alpha,k}(x, y) := -\sum_{(m_1,m_2)\in\Lambda} \frac{e^{\mathrm{i}k|x-(m_1,m_2,0)|}}{4\pi|x - (m_1, m_2, 0)|} e^{\mathrm{i}\alpha\cdot(m_1,m_2)}, \tag{4.2}$$

where the series in the spatial representation (4.2) converges uniformly for x in compact sets of $\mathbb{R}^3$, $x \neq 0$, and $k \neq |\alpha + q|$ for all $q \in \Lambda^*$ (see *e.g* [7, Section 2.12]). We define the quasiperiodic single layer potential $\mathcal{S}_D^{\alpha,k}$ by

$$\mathcal{S}_D^{\alpha,k}[\phi](x) := \int_{\partial D} G^{\alpha,k}(x - y)\phi(y)\,\mathrm{d}\sigma(y), \quad x \in \mathbb{R}^3.$$

On the boundary of D, it satisfies the jump relations

$$\mathcal{S}_D^{\alpha,k}[\phi]\big|_+ = \mathcal{S}_D^{\alpha,k}[\phi]\big|_- \quad \text{on } \partial D, \tag{4.3}$$

and

$$\frac{\partial}{\partial \nu}\mathcal{S}_D^{\alpha,k}[\phi]\Big|_\pm = \left(\pm\frac{1}{2}I + (\mathcal{K}_D^{-\alpha,k})^*\right)[\phi] \quad \text{on } \partial D, \tag{4.4}$$

where $(\mathcal{K}_D^{-\alpha,k})^*$ is the quasiperiodic Neumann-Poincaré operator, given by

$$(\mathcal{K}_D^{-\alpha,k})^*[\phi](x) := \int_{\partial D} \frac{\partial}{\partial \nu_x} G^{\alpha,k}(x-y)\phi(y)\,\mathrm{d}\sigma(y).$$

Lemma 4.1. *The quasiperiodic single layer potential $\mathcal{S}_D^{\alpha,k} : L^2(\partial D) \to H^1(\partial D)$ is invertible if k is small enough and $k \neq |\alpha + q|$ for all $q \in \Lambda^*$.*

Proof. If $\varphi \in L^2(\partial D)$ satisfies $\mathcal{S}_D^{\alpha,\omega}[\varphi] = 0$ on ∂D, then $u := \mathcal{S}_D^{\alpha,\omega}[\varphi]$ satisfies $\Delta u + k^2 u = 0$ in $Y \setminus \partial D$. Since 0 is not a Dirichlet eigenvalue of $-\Delta$ in D, and neither a Dirichlet eigenvalue of $-\Delta$ on $Y \setminus D$ with quasiperiodic conditions on ∂Y, it follows that $u = 0$ for small enough k. Then, from the jump condition (4.3) we have $\varphi = \partial u/\partial \nu|_+ - \partial u/\partial \nu|_- = 0$, which proves the claim. $\square$

Remark 4.2. *Throughout Section 4, we study the problem in three spatial dimensions. However, all the arguments carry over to the case of two spatial dimensions with a one-dimensional screen of resonators, producing similar results. Indeed, the numerical simulations used to create Figures 6 and 7 are performed on an arrays of circular resonators that are the two-dimensional analogues of those which are analysed here.*

4.2 Band structure and exceptional points

In this section, we study the resonance problem, or in other words, the problem (4.1) with $u^{in} = 0$. Moreover, we study the regime when $\omega \to 0$ while $|\alpha| > c > 0$ for some c independent on ω. In this regime, we have the asymptotic expansions [7]

$$\mathcal{S}_D^{\alpha,k} = \mathcal{S}_D^{\alpha,0} + O(k^2), \tag{4.5}$$

and

$$(\mathcal{K}_D^{-\alpha,k})^* = (\mathcal{K}_D^{-\alpha,0})^* + O(k^2). \tag{4.6}$$

Here, the error terms are with respect to the operator norms, and are uniform for $|\alpha| > c > 0$. As in Section 2, we define the quasiperiodic capacitance coefficients C_{ij}^α, for $i,j = 1,2$, as

$$C_{ij}^\alpha = -\int_{\partial D_i} \psi_j^\alpha \,\mathrm{d}\sigma, \qquad \psi_j^\alpha = (\mathcal{S}_D^{\alpha,0})^{-1}[\chi_{\partial D_j}]. \tag{4.7}$$

The *quasiperiodic capacitance matrix* C^α is defined as the matrix $C^\alpha = (C_{ij}^\alpha)$, while the *weighted* quasiperiodic capacitance matrix $C^{v,\alpha}$ is defined as

$$C^{v,\alpha} = VC^\alpha,$$

with V as in (2.9). As we shall see, the capacitance matrix gives the leading order approximation of the solution to the resonance problem (4.1). We have the following lemma from [3, Lemma 3.1].

Lemma 4.3. *We have*

$$C_{11}^\alpha = C_{22}^\alpha \in \mathbb{R}, \qquad C_{12}^\alpha = \overline{C_{21}^\alpha}.$$

Directly following the arguments of Section 2, but instead using the jump conditions (4.3), (4.4) and the asymptotic expansions (4.5), (4.6), we can show the following theorem on the band structure of the metascreen, which is the analogue of Theorem 2.3.

Theorem 4.4. *As $\delta \to 0$, the quasiperiodic resonant frequencies satisfy the asymptotic formula*

$$\omega_i^\alpha = \sqrt{\frac{\lambda_i^\alpha}{|D_1|}} + O(\delta), \quad i = 1, 2,$$

where $|D_1|$ is the volume of a single resonator. Here, λ_i^α are the eigenvalues of the weighted quasiperiodic capacitance matrix $C^{v,\alpha}$.

Analogously to the case of a single dimer studied in Section 2, the eigenvalues of the weighted quasiperiodic capacitance matrix are given by

$$\lambda_i^\alpha = aC_{11}^\alpha \pm \sqrt{a^2|C_{12}^\alpha|^2 - b^2\big((C_{11}^\alpha)^2 - |C_{12}^\alpha|^2\big)}, \tag{4.8}$$

meaning the asymptotic exceptional point occurs when $b = b_0(\alpha)$, given by

$$b_0(\alpha) = \frac{a|C_{12}^\alpha|}{\sqrt{(C_{11}^\alpha)^2 - |C_{12}^\alpha|^2}}.$$

The exceptional point now depends both on the geometry and on α, and will therefore correspond to a point in the band structure. This is illustrated in Figure 6, which shows the band structure of a $\mathcal{PT}$-symmetric metascreen. The computations were performed using the multipole discretization (see *e.g.* [7]). Close to the origin of the Brillouin zone the system is always below the exceptional point. For larger α and for large enough b, there will be a point where $b = b_0(\alpha)$. For α above this point, the band structure of the system has a non-zero imaginary part and the two bands are complex-conjugated.

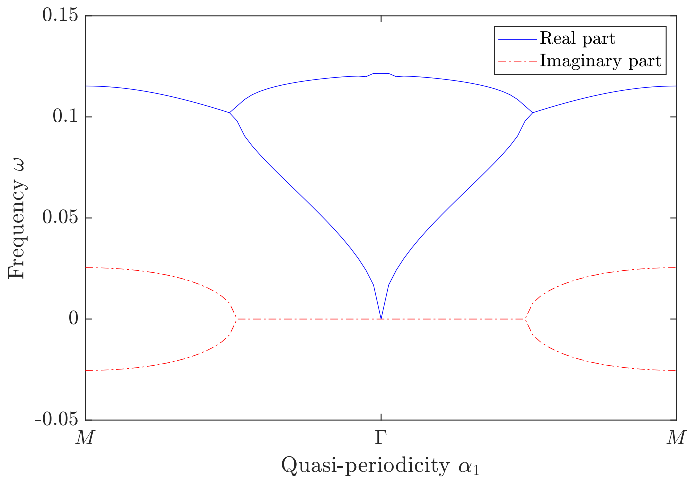

Figure 6: Plot of the real parts (blue) and imaginary parts (red) of the band structure of the metascreen. The exceptional point is a point (α, ω), at which the frequencies coincide to leading order. Here, we simulate a two-dimensional problem using circular resonators with period $L = 1$, separation distance $0.5L$, radius $0.15L$ and material parameters $a = 2 \times 10^{-4}, b = 1 \times 10^{-4}$ and $v = 1$.

4.3 Periodic Green's functions and capacitance matrix

We will now study the layer potentials and capacitance coefficients when both ω and α approach zero. We consider $k \in \mathbb{R}$ and study the regime when $|\alpha| < k < \inf_{q \in \Lambda^* \setminus \{0\}} |\alpha + q|$, which is not encompassed by the analysis in Section 4.2. In this case, it was shown in [5] that the quasiperiodic Green's function admits the spectral representation

$$G^{\alpha,k}(x) = \frac{e^{\mathrm{i}\alpha\cdot(x_1,x_2)}e^{\mathrm{i}k_3|x_3|}}{2\mathrm{i}k_3L^2} - \sum_{q \in \Lambda^* \setminus \{0\}} \frac{e^{\mathrm{i}(\alpha+q)\cdot(x_1,x_2)}e^{-\sqrt{|\alpha+q|^2-k^2}|x_3|}}{2L^2\sqrt{|\alpha+q|^2-k^2}}, \tag{4.9}$$

where $k_3 = \sqrt{k^2 - |\alpha|^2}$. The series in (4.9) converges uniformly for x in compact sets of $\mathbb{R}^3$, $x \neq 0$, and $k \neq |\alpha + q|$ for all $q \in \Lambda^*$ (again, see *e.g.* [7]).

In the case when $k = \alpha = 0$, we call $G^{0,0}$ the *periodic* Green's function and we have [5]

$$G^{0,0}(x) = \frac{|x_3|}{2L^2} - \sum_{q \in \Lambda^* \setminus \{0\}} \frac{e^{\mathrm{i}q\cdot(x_1,x_2)} e^{-|q||x_3|}}{2L^2|q|}. \tag{4.10}$$

In the subsequent sections, we are interested in the case when the incident wave has a fixed direction of incidence and a frequency ω in the subwavelength regime. We therefore set $k = \omega, \alpha = \omega\alpha_0$ and $w_3 = \sqrt{1 - |\alpha_0|^2}$ for some α_0 independent of ω (here, α_0 represents the incident direction). When $\omega \to 0$, we have

$$G^{\omega\alpha_0,\omega}(x) = \frac{1}{2\mathrm{i}\omega w_3 L^2} + G^{0,0}(x) + \frac{\alpha_0 \cdot (x_1, x_2)}{2w_3 L^2} + \omega G_1^{\alpha_0}(x) + O(\omega^2). \tag{4.11}$$

Here, $G_1^{\alpha_0}$ is a function independent of ω, which can be written [5]

$$G_1^{\alpha_0}(x) = \frac{\mathrm{i}\left(w_3|x_3| + \alpha_0 \cdot (x_1, x_2)\right)^2}{4w_3 L^2} + \alpha_0 \cdot g_1(x),$$

where $g_1(x)$ is a vector-valued function independent of α and ω, satisfying

$$g_1(x_1, x_2, x_3) = g_1(x_1, x_2, -x_3), \qquad g_1(x_1, x_2, x_3) = -g_1(-x_1, -x_2, x_3).$$

From (4.11) we in particular observe that the Green's function has a singularity of order ω^{-1}. This fact makes the subsequent analysis qualitatively similar to the case of finite resonator systems in two dimensions, studied for example in [1, 6].

We define the operators $\hat{\mathcal{S}}_D^{\alpha,k} : L^2(\partial D) \to H^1(\partial D)$ and $(\hat{\mathcal{K}}_D^{-\alpha,k})^* : L^2(\partial D) \to L^2(\partial D)$ as

$$\hat{\mathcal{S}}_D^{\alpha,k}[\varphi](x) = \mathcal{S}_D^{0,0}[\varphi](x) - \frac{\mathrm{i} + \alpha \cdot (x_1, x_2)}{2k_3 L^2} \int_{\partial D} \varphi \,\mathrm{d}\sigma + \int_{\partial D} \frac{\alpha \cdot (y_1, y_2)}{2k_3 L^2} \varphi(y) \,\mathrm{d}\sigma(y), \tag{4.12}$$

and

$$(\hat{\mathcal{K}}_D^{-\alpha,k})^*[\varphi](x) = (\mathcal{K}_D^{0,0})^*[\varphi](x) - \frac{\alpha \cdot (\nu_{x,1}, \nu_{x,2})}{2k_3 L^2} \int_{\partial D} \varphi \,\mathrm{d}\sigma.$$

Here, $\nu_x = (\nu_{x,1}, \nu_{x,2}, \nu_{x,3})$ denotes the outwards pointing normal of D at x. Moreover, we define the operators $\mathcal{S}_1^{\alpha_0} : L^2(\partial D) \to H^1(\partial D)$ and $(\mathcal{K}_{D,1}^{-\alpha_0})^* : L^2(\partial D) \to L^2(\partial D)$ as

$$\mathcal{S}_1^{\alpha_0}[\phi](x) := \int_{\partial D} G_1^{\alpha_0}(x - y)\phi(y) \,\mathrm{d}\sigma(y), \qquad (\mathcal{K}_{D,1}^{-\alpha_0})^*[\phi](x) := \int_{\partial D} \frac{\partial}{\partial \nu_x} G_1^{\alpha_0}(x - y)\phi(y) \,\mathrm{d}\sigma(y).$$

In view of (4.11) we have the following asymptotic expansions

$$\mathcal{S}_D^{\omega\alpha_0,\omega} = \hat{\mathcal{S}}_D^{\omega\alpha_0,\omega} + \omega \mathcal{S}_1^{\alpha_0} + O(\omega^2), \qquad (\mathcal{K}_D^{-\omega\alpha_0,\omega})^* = (\hat{\mathcal{K}}_D^{-\omega\alpha_0,\omega})^* + \omega(\mathcal{K}_{D,1}^{-\alpha_0})^* + O(\omega^2), \tag{4.13}$$

as $\omega \to 0$, where the error terms are with respect to corresponding operator norms. Similarly to Lemma 2.1, we have the following lemma.

Lemma 4.5. *For any $\varphi \in L^2(\partial D)$ we have, for $i = 1, 2$,*

$$\int_{\partial D_i} \left(-\frac{1}{2}I + (\hat{\mathcal{K}}_D^{-\alpha,k})^*\right)[\varphi] \,\mathrm{d}\sigma = 0, \qquad \int_{\partial D_i} (\mathcal{K}_{D,1}^{-\alpha_0})^*[\varphi] = \frac{\mathrm{i}|D_1|}{2w_3 L^2} \int_{\partial D} \varphi \,\mathrm{d}\sigma.$$

Proof. For any $\varphi \in L^2(\partial D)$ we have [7]

$$\int_{\partial D_i} \left(-\frac{1}{2}I + (\mathcal{K}_D^{0,0})^*\right)[\varphi] \,\mathrm{d}\sigma = 0,$$

and since $\int_{\partial D} \nu_x \, \mathrm{d}\sigma(x) = 0$, the first equation follows. To prove the second equation, we use the first equation to conclude that, as $\omega \to 0$,

$$\int_{\partial D_i} \left(-\frac{1}{2} I + (\mathcal{K}_D^{-\omega\alpha_0,\omega})^* \right) [\varphi] \, \mathrm{d}\sigma = \omega \int_{D_i} (\mathcal{K}_{D,1}^{-\alpha_0})^* [\varphi] + O(\omega^2). \tag{4.14}$$

On the other hand, using the jump condition and integration by parts we have that

$$\begin{aligned}\int_{\partial D_i} \left(-\frac{1}{2} I + (\mathcal{K}_D^{-\omega\alpha_0,\omega})^* \right) [\varphi] \, \mathrm{d}\sigma &= \int_{D_i} \Delta \mathcal{S}_D^{\omega\alpha_0,\omega}[\varphi] \, \mathrm{d}x = -\omega^2 \int_{D_i} \mathcal{S}_D^{\omega\alpha_0,\omega}[\varphi] \, \mathrm{d}x \\ &= \omega \frac{\mathrm{i}|D_1|}{2w_3 L^2} \int_{\partial D} \varphi \, \mathrm{d}\sigma + O(\omega^2). \end{aligned} \tag{4.15}$$

Since (4.14) and (4.15) hold for any small ω, we obtain the second equation. $\square$

The periodic single-layer potential could fail to be invertible and its kernel is described in the next lemma.

Lemma 4.6. *The dimension of* $\ker \mathcal{S}_D^{0,0}$ *is at most one. Moreover, if* $\varphi \in \ker \mathcal{S}_D^{0,0}$ *satisfies* $\int_{\partial D} \varphi \, \mathrm{d}\sigma = 0$, *then* $\varphi = 0$.

Proof. For small but non-zero k we know from Lemma 4.1 that $\mathcal{S}_D^{0,k}$ is invertible, and therefore, by (4.13), $\hat{\mathcal{S}}_D^{0,k}$ is also invertible for small k. We can write $\mathcal{S}_D^{0,0}$ as

$$\mathcal{S}_D^{0,0}[\varphi] = \hat{\mathcal{S}}_D^{0,k}[\varphi] + \frac{\mathrm{i}}{2k_3 L^2} \int_{\partial D} \varphi \, \mathrm{d}\sigma,$$

or, in other words, $\mathcal{S}_D^{0,0}$ is a rank-1 perturbation of the invertible operator $\hat{\mathcal{S}}_D^{0,k}$. This shows that $\dim \ker \mathcal{S}_D^{0,0} \leq 1$ and, moreover, that any non-zero $\varphi \in \ker \mathcal{S}_D^{0,0}$ satisfies $\int_{\partial D} \varphi \, \mathrm{d}\sigma \neq 0$. $\square$

Lemma 4.7. *If* $\mathcal{S}_D^{0,0}[\varphi] = K\chi_{\partial D}$ *for some constant* K *and some* $\varphi \in L^2(\partial D)$ *satisfying* $\int_{\partial D} \varphi \mathrm{d}\sigma = 0$, *then* $\varphi = 0$.

Proof. For $x \in \mathbb{R}^3 \setminus \mathcal{C}$, define $V(x) := \mathcal{S}_D^{0,0}[\varphi](x)$. Then V solves the following differential problem,

$$\begin{cases} \Delta V = 0 & \text{in } \mathbb{R}^3 \setminus \mathcal{C}, \\ V|_+ = K & \text{on } \partial \mathcal{C}, \\ V(x + (m_1, m_2, 0)) = V(x) & \text{for all } (m_1, m_2) \in \Lambda, \\ V(x) \to \pm V_\infty & \text{as } x_3 \to \pm\infty, \end{cases} \tag{4.16}$$

for some constant V_∞. Moreover, using the jump relations and integration by parts, we have that

$$\int_{\partial D} \varphi \, \mathrm{d}\sigma = K \int_{Y \setminus D} |\nabla V|^2 \, \mathrm{d}x = 0.$$

If $K \neq 0$, it follows from (4.16) that $\int_{Y \setminus D} |\nabla V|^2 \, \mathrm{d}x \neq 0$. In other words we must have $K = 0$ and, since $\int_{\partial D} \varphi \, \mathrm{d}\sigma = 0$, it follows from Lemma 4.6 that $\varphi = 0$. $\square$

Let $L_0^2(\partial D)$ be the mean-zero space defined as

$$L_0^2(\partial D) = \left\{ f \in L^2(\partial D) \;\middle|\; \int_{\partial D} f \, \mathrm{d}\sigma = 0 \right\}.$$

By Lemma 4.6 and Lemma 4.7, $\mathcal{S}_D^{0,0}$ is invertible from $L_0^2(\partial D)$ onto its image, which does not contain the constant functions.

We will now define the analogous capacitance coefficients in the periodic setting. We begin with the following lemma.

Lemma 4.8. *For any $\alpha_0 \in Y^*$ with $|\alpha_0| < 1$, $\left(\hat{\mathcal{S}}_D^{\omega\alpha_0,\omega}\right)^{-1}$ is a holomorphic operator-valued function of ω in a neighbourhood of $\omega = 0$.*

Proof. We know that $\hat{\mathcal{S}}_D^{\omega\alpha_0,\omega}$ is a meromorphic operator-valued function of ω with a pole at $\omega = 0$. From [7, Corollary 1.10], we find that $\left(\hat{\mathcal{S}}_D^{\omega\alpha_0,\omega}\right)^{-1}$ is also meromorphic for ω in a neighbourhood of 0. It remains to show that the principal part vanishes.

To reach a contradiction, we assume that $\left(\hat{\mathcal{S}}_D^{\omega\alpha_0,\omega}\right)^{-1}$ is singular as $\omega \to 0$, which means that there is some ϕ, depending on ω, such that $\|\phi\|_{L^2(\partial D)} = O(1)$ while $\|\hat{\mathcal{S}}_D^{\omega\alpha_0,\omega}[\phi]\|_{H^1(\partial D)} = O(\omega)$. We can rewrite ϕ as $\phi = \phi_0 + \phi_1$ where ϕ_0 is non-zero and independent of ω, while $\phi_1 = O(\omega)$. Then the singular part of $\hat{\mathcal{S}}_D^{\alpha,k}$ must vanish on ϕ_0, *i.e.*,

$$\int_{\partial D} \phi_0 \, \mathrm{d}\sigma = 0.$$

Substituting into (4.12) we find that, for some constant K, we have $\mathcal{S}_D^{0,0}[\phi_0] = K\chi_{\partial D}$. It then follows from Lemma 4.7 that $\phi_0 = 0$, which contradicts the fact that $\|\phi\| = O(1)$. □

We can now define the periodic capacitance coefficients C_{ij}^0. For $\alpha \in Y^*$, we let

$$\psi_i^{\alpha,\omega} = \left(\hat{\mathcal{S}}_D^{\alpha,\omega}\right)^{-1}[\chi_{\partial D_i}].$$

Then, if $\alpha = \omega\alpha_0$ for some fixed α_0 with $|\alpha_0| < 1$, we have the following expansion from Lemma 4.8,

$$\psi_i^{\omega\alpha_0,\omega} = \psi_i^0 + \omega\hat{\psi}_i^{1,\alpha_0} + O(\omega^2), \tag{4.17}$$

as $\omega \to 0$, for some $\psi_i^0, \hat{\psi}_i^{1,\alpha_0} \in L^2(\partial D)$ independent of ω. We then define

$$C_{ij}^0 = -\int_{\partial D_i} \psi_j^0 \, \mathrm{d}\sigma. \tag{4.18}$$

We call the matrix $C^0 = (C_{ij}^0)$ the *periodic capacitance matrix* (not to be confused with the *quasi*periodic capacitance matrix, studied in Section 4.2). The periodic capacitance matrix might *a priori* depend on α_0, but we will later see that, under an extra symmetry condition, ψ_j^0 and C^0 are independent of α_0.

Lemma 4.9. *The periodic capacitance matrix C^0 is a real matrix given by*

$$C^0 = C_{11}^0 \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

Proof. Since $\hat{\mathcal{S}}_D^{\omega\alpha_0,\omega}[\psi_i^{\omega\alpha_0,\omega}]$ is bounded as $\omega \to 0$, the singular part of $\hat{\mathcal{S}}_D^{\omega\alpha_0,\omega}$ must vanish on ψ_i^0, or in other words

$$\int_{\partial D} \psi_i^0 \, \mathrm{d}\sigma = 0.$$

From this it follows that $C_{i1}^0 = -C_{i2}^0$ for $i = 1,2$. From the condition $\hat{\mathcal{S}}_D^{\omega\alpha_0,\omega}[\psi_i^{\omega\alpha_0,\omega}] = \chi_{\partial D_i}$, we have that

$$\chi_{\partial D_i} = \mathcal{S}_D^{0,0}[\psi_i^0] + \frac{1}{2\mathrm{i}w_3L^2}\int_{\partial D} \hat{\psi}_i^{1,\alpha_0} \, \mathrm{d}\sigma + \int_{\partial D} \frac{\alpha_0 \cdot (y_1, y_2)}{2w_3L^2}\psi_i^0(y) \, \mathrm{d}\sigma(y), \tag{4.19}$$

or, in other words, that $\mathcal{S}_D^{0,0}[\psi_i^0] = \chi_{\partial D_i} + K\chi_{\partial D}$ for some constant K. Summing over the resonators, we find that $\mathcal{S}_D^{0,0}[\psi_1^0 + \psi_2^0] = \widetilde{K}\chi_{\partial D}$. By Lemma 4.7 we find that $\widetilde{K} = 0$ and that

$$\psi_1^0 = -\psi_2^0. \tag{4.20}$$

It follows that $C_{1j}^0 = -C_{2j}^0$ for $j = 1,2$, which proves the expression of C^0. It remains to prove that C_{11}^0 is real. Taking the complex conjugate of (4.19) we find that $\mathcal{S}_D^{0,0}[\psi_i^0 - \overline{\psi_i^0}] = K\chi_{\partial D}$ for some new constant K. From Lemma 4.7 we find that $\psi_i^0 = \overline{\psi_i^0}$, and hence $C_{11}^0 = \overline{C_{11}^0}$. □

Lemma 4.10. *As $\omega \to 0$, we have*

$$(\mathcal{S}_D^{\omega\alpha_0,\omega})^{-1}[\chi_{\partial D_j}] = \psi_j^0 + \omega\psi_j^{1,\alpha_0} + O(\omega^2),$$

where

$$\psi_j^{1,\alpha_0} = \hat{\psi}_j^{1,\alpha_0} - \left(\hat{\mathcal{S}}_D^{\omega\alpha_0,\omega}\right)^{-1} \mathcal{S}_1^{\alpha_0}\psi_j^0.$$

Proof. From (4.13), and using the Neumann series, we have

$$\begin{aligned}(\mathcal{S}_D^{\omega\alpha_0,\omega})^{-1}[\chi_{\partial D_j}] &= \left(\hat{\mathcal{S}}_D^{\omega\alpha_0,\omega}\right)^{-1}[\chi_{\partial D_j}] - \omega\left(\hat{\mathcal{S}}_D^{\omega\alpha_0,\omega}\right)^{-1}\mathcal{S}_1^{\alpha_0}\left(\hat{\mathcal{S}}_D^{\omega\alpha_0,\omega}\right)^{-1}[\chi_{\partial D_j}] + O(\omega^2),\\ &= \psi_j^0 + \omega\psi_j^{1,\alpha_0} + O(\omega^2),\end{aligned}$$

which proves the claim. □

Analogously to before, we define the weighted periodic capacitance matrix as

$$C^{v,0} = VC^0.$$

From Lemma 4.9, we find that the eigenvalues λ_1^0, λ_2^0 and corresponding eigenvectors $\mathbf{v}_1^0, \mathbf{v}_2^0$ of $C^{v,0}$ are given by

$$\lambda_1^0 = 0, \quad \lambda_2^0 = 2aC_{11}^0, \qquad \mathbf{v}_1^0 = \begin{pmatrix}1\\1\end{pmatrix}, \quad \mathbf{v}_2^0 = \begin{pmatrix}-(a+\mathrm{i}b)\\ a-\mathrm{i}b\end{pmatrix}.$$

As we shall see, the weighted periodic capacitance matrix asymptotically describes the resonant frequencies and the scattered field to leading order. In addition, we will need to consider two sources of higher-order effects. Firstly, we define the vector-valued coefficients $\mathbf{c}_i$ as

$$\mathbf{c}_i = \int_{\partial D} y\psi_i^0(y)\,\mathrm{d}\sigma(y), \quad i = 1,2. \tag{4.21}$$

From (4.20) we have that $\mathbf{c}_1 = -\mathbf{c}_2$. Secondly, we define the matrix $C^{1,\alpha_0} = (C_{ij}^{1,\alpha_0})$ as

$$C_{ij}^{1,\alpha_0} = -\int_{\partial D_i} \psi_j^{1,\alpha_0}\,\mathrm{d}\sigma,$$

for $i,j = 1,2$. Corresponding weighted matrix $C^{v,1,\alpha_0} = (C_{ij}^{v,1,\alpha_0})$ is defined as

$$C^{v,1,\alpha_0} = VC^{1,\alpha_0}.$$

The next lemma describes some of the structure of C^{1,α_0}.

Lemma 4.11. *We have*

$$\int_{\partial D}\psi_j^{1,\alpha_0}\,\mathrm{d}\sigma = \int_{\partial D}\hat{\psi}_j^{1,\alpha_0}\,\mathrm{d}\sigma + O(\omega) \quad \textit{and} \quad \int_{\partial D}\psi_1^{1,\alpha_0} + \psi_2^{1,\alpha_0}\,\mathrm{d}\sigma = 2\mathrm{i}w_3L^2.$$

Proof. Using the fact that the $L^2(\partial D)$-dual of $\hat{\mathcal{S}}_D^{\alpha,k}$ is $\overline{\hat{\mathcal{S}}_D^{-\alpha,k}}$, we have

$$\int_{\partial D}\left(\hat{\mathcal{S}}_D^{\omega\alpha_0,\omega}\right)^{-1}\mathcal{S}_1^{\alpha_0}[\psi_j^0] = \int_{\partial D}\mathcal{S}_1^{\alpha_0}[\psi_j^0]\left(\hat{\mathcal{S}}_D^{-\omega\alpha_0,\omega}\right)^{-1}[\chi_{\partial D}]\,\mathrm{d}\sigma = O(\omega).$$

Moreover, since $\psi_1^0 = -\psi_2^0$ we have

$$\int_{\partial D}\psi_1^{1,\alpha_0} + \psi_2^{1,\alpha_0}\,\mathrm{d}\sigma = \int_{\partial D}\hat{\psi}_1^{1,\alpha_0} + \hat{\psi}_2^{1,\alpha_0}\,\mathrm{d}\sigma = 2\mathrm{i}w_3L^2,$$

where the last step follows from (4.19) together with (4.20). This proves the claim. □

Remark 4.12. *It is straightforward to generalise Lemma 4.9 to a general number N of resonators inside the unit cell. The weighted periodic capacitance matrix $C^{v,0}$ will always have one vanishing eigenvalue. This corresponds to the well-known fact that the first band function ω_1^α satisfies $\omega_1^0 = 0$ corresponding to monopole modes $\mathbf{v}_1^0 = (1,...,1)^{\mathrm{T}} \in \mathbb{R}^N$. The other eigenvalues of $C^{v,0}$ describe the values of the other band functions $\omega_2^\alpha, \omega_3^\alpha, ..., \omega_N^\alpha$ around $\alpha = 0$.*

4.4 Plane wave scattering problem

We assume that the incident field u^{in} is a plane wave with frequency $\omega \in \mathbb{R}$ and wave vector $\mathbf{k} = \begin{pmatrix} k_1 & k_2 & k_3 \end{pmatrix}^{\mathrm{T}}$. Again, superscript T denotes the transpose operator. In other words,

$$u^{in}(x) = e^{\mathrm{i}\mathbf{k}\cdot x}, \qquad |\mathbf{k}| = k = \frac{\omega}{v},$$

where $|\mathbf{k}|$ denotes the Euclidean norm of $\mathbf{k}$. For simplicity, we assume that the units are chosen such that $v = 1$. We will consider the subwavelength regime, *i.e.* when $\delta \to 0$ and $\omega = O(\delta^{1/2})$. In this limit, we assume that the incident direction $\mathbf{w}$ of $\mathbf{k}$ is fixed, *i.e.* that $\mathbf{k}$ scales as

$$\mathbf{k} = \omega \mathbf{w}, \quad \mathbf{w} = \begin{pmatrix} w_1 \\ w_2 \\ s w_3 \end{pmatrix}, \quad w_3 > 0, \quad s = \pm 1,$$

where $\mathbf{w}$ is independent of ω. We define

$$\alpha = \begin{pmatrix} k_1 \\ k_2 \end{pmatrix} = \omega \alpha_0 \in Y^*.$$

We define the functions $S_j^{\alpha,\omega}$, for $j = 1, 2$, as

$$S_j^{\alpha,\omega}(x) = \begin{cases} \mathcal{S}_D^{\alpha,k}[\psi_j^0 + \omega \psi_j^{1,\alpha_0}](x), & x \in \mathbb{R}^3 \setminus \overline{\mathcal{C}}, \\ \mathcal{S}_D^{\alpha,k_i}[\psi_j^0 + \omega \psi_j^{1,\alpha_0}](x), & x \in \mathcal{C}_i, \ i = 1, 2. \end{cases}$$

Proposition 4.13. *Let $\lambda_2^0, \mathbf{v}_2^0$ be the second eigenpair of $C^{v,0}$, and let $\lambda = \omega^2 |D_1|$. Assume that $\mathrm{Im}(d^{\mathrm{T}} C^{v,1,\alpha_0} \mathbf{v}_2^0) \neq 0$, where $d = \left(\begin{smallmatrix} 1 \\ -1 \end{smallmatrix}\right)$. Then, for $\omega \in \mathbb{R}$ in the subwavelength regime such that $\lambda = \lambda_2^0 + \lambda^*$, where $\lambda^* = O(\omega^3)$, the solution to the scattering problem (4.1) can be written as*

$$u - u^{in} = -(a + \mathrm{i}b)\mu S_1^{\alpha,\omega} + (a - \mathrm{i}b)\mu S_2^{\alpha,\omega} - \mathcal{S}_D^{\alpha,k}\left(\mathcal{S}_D^{\alpha,k}\right)^{-1}[u^{in}] + O(\omega^2),$$

where μ is given by

$$\mu = \frac{d^{\mathrm{T}} p}{d^{\mathrm{T}}\left(\omega C^{v,1,\alpha_0} - \lambda^* I\right)\mathbf{v}_2^0} + O(\omega), \qquad p = -\begin{pmatrix} v_1^2 \delta_1 \int_{\partial D_1} \left(\mathcal{S}_D^{\alpha,k}\right)^{-1}[u^{in}]\,\mathrm{d}\sigma \\ v_2^2 \delta_2 \int_{\partial D_2} \left(\mathcal{S}_D^{\alpha,k}\right)^{-1}[u^{in}]\,\mathrm{d}\sigma \end{pmatrix}.$$

Here, the error terms are uniform with respect to λ^* in a neighbourhood of 0.

Proof. The solutions to (4.1) can be represented as

$$u = \begin{cases} u^{in}(x) + \mathcal{S}_D^{\alpha,k}[\psi](x), & x \in \mathbb{R}^3 \setminus \overline{\mathcal{C}}, \\ \mathcal{S}_D^{k_i}[\phi](x), & x \in \mathcal{C}_i, \ i = 1, 2, \end{cases} \tag{4.22}$$

for some surface densities $(\phi, \psi) \in L^2(\partial D) \times L^2(\partial D)$, which must be chosen so that u satisfies the transmission conditions across ∂D. Using the jump conditions (4.3) and (4.4), we see that this implies that the layer densities ϕ and ψ satisfies

$$\mathcal{S}_D^{k_i}[\phi] - \mathcal{S}_D^{\alpha,k}[\psi] = u^{in} \quad \text{on } \partial D_i, \tag{4.23}$$

$$\left(-\frac{1}{2}I + \mathcal{K}_D^{k_i,*}\right)[\phi] - \delta_i\left(\frac{1}{2}I + (\mathcal{K}_D^{-\alpha,k})^*\right)[\psi] = \delta_i \frac{\partial u^{in}}{\partial \nu} \quad \text{on } \partial D_i, \tag{4.24}$$

for $i = 1, 2$. Using the asymptotic expansions (4.13) and (2.7) we have from (4.24) that, on ∂D_i,

$$\left(-\frac{1}{2}I + \mathcal{K}_D^* + \frac{\omega^2}{v_i^2}\mathcal{K}_{D,2} + \frac{\omega^3}{v_i^3}\mathcal{K}_{D,3}\right)[\phi] - \delta_i\left(\frac{1}{2}I + (\hat{\mathcal{K}}_D^{-\alpha,k})^* + \omega(\mathcal{K}_{D,1}^{-\alpha,k})^*\right)[\psi] = O(\delta\omega^2 + \omega^4). \tag{4.25}$$

Integrating over ∂D_i, using Lemmas 2.1 and 4.5 along with (2.8), gives us that

$$-\frac{\omega^2}{v_i^2}\int_{D_i}\mathcal{S}_D[\phi]\,\mathrm{d}x+\frac{\omega^3}{v_i^3}\frac{\mathrm{i}|D_i|}{4\pi}\int_{\partial D}\phi\,\mathrm{d}\sigma-\delta_i\int_{\partial D_i}\psi\,\mathrm{d}\sigma-\delta_i\frac{\mathrm{i}\omega|D_1|}{2w_3L^2}\int_{\partial D}\psi\,\mathrm{d}\sigma=O(\delta\omega^2+\omega^4). \quad (4.26)$$

At leading order, (4.25) says that $\left(-\frac{1}{2}I+\mathcal{K}_D^*\right)[\phi]=0$ so, in light of the fact that ψ_1 and ψ_2 form a basis for ker $\left(-\frac{1}{2}I+\mathcal{K}_D^*\right)$, ϕ can be written as

$$\phi=q_1\psi_1+q_2\psi_2+O(\omega^2+\delta), \quad (4.27)$$

for constants $q_1,q_2=O(1)$. Using (2.6), we can expand $\mathcal{S}_D^{k_i}[\psi_j]$ as

$$\mathcal{S}_D^{k_i}[\psi_j]=\chi_{\partial D_i}-\frac{\omega\mathrm{Cap}_D}{8\pi\mathrm{i}v_i}\chi_{\partial D}+O(\omega^2),$$

where $\mathrm{Cap}_D=2(C_{11}+C_{12})$. From (4.23), we then find that

$$\mathcal{S}_D^{\alpha,k}[\psi]=\chi_{\partial D_1}\left(q_1-(q_1+q_2)\frac{\omega\mathrm{Cap}_D}{8\pi\mathrm{i}v_1}\right)+\chi_{\partial D_2}\left(q_2-(q_1+q_2)\frac{\omega\mathrm{Cap}_D}{8\pi\mathrm{i}v_2}\right)+O(\omega^2+\delta),$$

and then from Lemma 4.10 that

$$\begin{aligned}\psi=q_1&\left(\psi_1^0+\omega\psi_1^{1,\alpha_0}-\frac{\omega\mathrm{Cap}_D}{8\pi\mathrm{i}}\left(\frac{\psi_1^0}{v_1}+\frac{\psi_2^0}{v_2}\right)\right)\\&+q_2\left(\psi_2^0+\omega\psi_2^{1,\alpha_0}-\frac{\omega\mathrm{Cap}_D}{8\pi\mathrm{i}}\left(\frac{\psi_1^0}{v_1}+\frac{\psi_2^0}{v_2}\right)\right)-\left(\mathcal{S}_D^{\alpha,k}\right)^{-1}[u^{in}]+O(\omega^2+\delta). \quad (4.28)\end{aligned}$$

Substituting (4.27) and (4.28) into (4.26), and using the fact that $\int_{\partial D}\left(\mathcal{S}_D^{\alpha,k}\right)^{-1}[u^{in}]\,\mathrm{d}\sigma=O(\omega)$, we reach, up to an error of order $O(\delta\omega^2+\omega^4)$, the problem

$$\left(C^{v,0}-\lambda I+E\right)\begin{pmatrix}q_1\\q_2\end{pmatrix}=-\begin{pmatrix}v_1^2\delta_1\int_{\partial D_1}\left(\mathcal{S}_D^{\alpha,k}\right)^{-1}[u^{in}]\,\mathrm{d}\sigma\\ v_2^2\delta_2\int_{\partial D_2}\left(\mathcal{S}_D^{\alpha,k}\right)^{-1}[u^{in}]\,\mathrm{d}\sigma\end{pmatrix}, \quad (4.29)$$

where $\lambda=\omega^2|D_1|$, while $E=(E_{i,j})=O(\delta\omega+\omega^3),\ i,j=1,2$ is the matrix given by

$$E_{i,j}=\frac{\omega\mathrm{Cap}_D}{8\pi\mathrm{i}}\left(\frac{|D_1|\omega^2}{v_i}-\frac{C_{i1}^{v,0}}{v_1}-\frac{C_{i2}^{v,0}}{v_2}\right)-v_i^2\delta_i\omega\int_{\partial D_i}\psi_j^{1,\alpha_0}\,\mathrm{d}\sigma.$$

We write $q=\left(\begin{smallmatrix}q_1\\q_2\end{smallmatrix}\right)$ and denote the right-hand side of (4.29) by p. Recall that we are working in the subwavelength regime $\omega=O(\delta^{1/2})$. Assuming $\lambda=\lambda_2^0+\lambda^*$, where $\lambda^*=O(\omega^3)$, we can rewrite (4.29) into

$$\left(C^{v,0}-\lambda_2^0I+E-\lambda^*I\right)q=p. \quad (4.30)$$

Using the second eigenvector $\mathbf{v}_2^0$ of $C^{v,0}$, we can find a constant μ such that

$$q=\mu\mathbf{v}_2^0+q_0,$$

for some q_0 satisfying $\mathbf{v}_2^0\cdot q_0=0$.

Next, we compute p. Since u^{in} is a plane wave with wave vector $\mathbf{k}=\omega\mathbf{w}$, we have

$$u^{in}(x)=1+\omega\mathrm{i}\mathbf{w}\cdot x+O(\omega^2),\quad x\in\partial D.$$

Using duality, we have that

$$\int_{\partial D_i}\left(\mathcal{S}_D^{\alpha,k}\right)^{-1}[u^{in}]\,\mathrm{d}\sigma=\int_{\partial D}u^{in}\left(\mathcal{S}_D^{-\alpha,k}\right)^{-1}[\chi_{\partial D_i}]\,\mathrm{d}\sigma=O(\omega).$$

We conclude that $q = O(\omega^3)$. Therefore, the leading order of (4.30) shows that $q_0 = O(\omega)$. We are now able to compute μ. Letting $d = \left(\begin{smallmatrix} 1 \\ -1 \end{smallmatrix}\right)$, it is straightforward to compute

$$\mu d^{\mathrm{T}}(E - \lambda^* I)\mathbf{v}_2^0 = d^{\mathrm{T}} p + O(\omega^4).$$

We can simplify

$$E\mathbf{v}_2^0 = -\frac{\omega b \mathrm{Cap}_D C_{11}^0}{4\pi}\left(\frac{a - \mathrm{i}b}{v_1} + \frac{a + \mathrm{i}b}{v_2}\right)\begin{pmatrix} 1 \\ 1 \end{pmatrix} + \omega C^{v,1,\alpha_0}\mathbf{v}_2^0.$$

Then

$$d^{\mathrm{T}}(E - \lambda^* I)\mathbf{v}_2^0 = d^{\mathrm{T}}\left(\omega C^{1,v,\alpha_0} - \lambda^* I\right)\mathbf{v}_2^0.$$

From the assumption $\mathrm{Im}(d^{\mathrm{T}} C^{1,v,\alpha_0}\mathbf{v}_2^0) \neq 0$, and since λ^* is real, we find that $\left|d^{\mathrm{T}}\left(\omega C^{1,v,\alpha_0} - \lambda^* I\right)\mathbf{v}_2^0\right| > \omega^3 K > 0$ for some constant K, for all λ^* in a neighbourhood of 0. We then have

$$\mu = \frac{d^{\mathrm{T}} p}{d^{\mathrm{T}}\left(\omega C^{v,1,\alpha_0} - \lambda^* I\right)\mathbf{v}_2^0} + O(\omega),$$

uniformly for λ^* in a neighbourhood of 0. Then, combining (4.22) and (4.28), we find that for $x \in \mathbb{R}^3$,

$$u(x) - u^{in}(x) = -\mu(a + \mathrm{i}b)S_1^{\alpha,\omega}(x) + \mu(a - \mathrm{i}b)S_2^{\alpha,\omega}(x) - \mathcal{S}_D^{\alpha,k}\left(\mathcal{S}_D^{\alpha,k}\right)^{-1}[u^{in}](x) + O(\omega^2),$$

(we emphasise that there is no cancellation in the last term for $x \notin \partial D$). This proves the claim. $\square$

Remark 4.14. *If ω is instead close to the first resonant frequency $\omega_1^0 = 0$, the solution q to* (4.30) *will be approximated by the first eigenvector $\mathbf{v}_1^0$. Consequently, it can be shown that ψ vanishes to high order. In other words, the incoming wave is largely unaffected by the metascreen and the scattered field is small.*

4.5 Unidirectional reflection and extraordinary transmission

In this section, we prove that there is a frequency such that the metascreen has zero reflection when the incident wave is from one side and non-zero reflection when the incident wave is from the other side of the screen. We will also demonstrate the occurrence of extraordinary transmission. The main results are stated in Theorem 4.17.

We begin by studying the radiative behaviour of the basis functions $S_1^{\alpha,\omega}$ and $S_2^{\alpha,\omega}$, in terms of which the scattered field is expressed. The quasiperiodic radiation condition implies that the single layer potential behaves as a superposition of outgoing plane waves as $|x_3| \to \infty$. Throughout this section, we will use $\sim$ to denote equality up to exponentially decaying factors, *i.e.* for functions $f, g \in C(\mathbb{R})$ we have $f(x) \sim g(x), x \to \infty$ if and only if

$$|f(x) - g(x)| = O(e^{-Kx}) \text{ as } x \to \infty,$$

for some constant $K > 0$. The following result describes the radiative behaviour of the single layer potential in the case of a single propagating mode, and is a direct consequence of the expansion of the Green's function in (4.9).

Proposition 4.15. *Assume that $|\alpha| < k < \inf_{q\in\Lambda^*\setminus\{0\}}|\alpha + q|$. Then, as $|x_3| \to \infty$, the quasiperiodic single layer potential satisfies*

$$\mathcal{S}_D^{\alpha,k}[\phi] \sim \begin{cases} \dfrac{e^{\mathrm{i}\mathbf{k}_+\cdot x}}{2\mathrm{i}k_3 L^2}\displaystyle\int_{\partial D} e^{-\mathrm{i}\mathbf{k}_+\cdot y}\phi(y)\,\mathrm{d}\sigma(y), & x_3 \to \infty, \\[2ex] \dfrac{e^{\mathrm{i}\mathbf{k}_-\cdot x}}{2\mathrm{i}k_3 L^2}\displaystyle\int_{\partial D} e^{-\mathrm{i}\mathbf{k}_-\cdot y}\phi(y)\,\mathrm{d}\sigma(y), & x_3 \to -\infty. \end{cases}$$

Here, $k_3 = \sqrt{k^2 - |\alpha|^2}$ while $\mathbf{k}_+ = (\alpha, k_3)$ and $\mathbf{k}_- = (\alpha, -k_3)$.

We define the coefficients

$$R_{j,\pm} = \frac{1}{2\mathrm{i}k_3L^2}\int_{\partial D} e^{-\mathrm{i}\mathbf{k}_\pm\cdot y}\left(\psi_j^0(y) + \omega\psi_j^{1,\alpha_0}(y)\right)\,\mathrm{d}\sigma(y), \quad i = 1,2.$$

By Proposition 4.15, the basis functions $S_1^{\omega,\alpha}, S_2^{\omega,\alpha}$ for the scattered field satisfies the radiative behaviour

$$S_j^{\alpha,\omega} \sim R_{j,\pm}e^{\mathrm{i}\mathbf{k}_\pm\cdot x}, \quad x_3 \to \pm\infty. \tag{4.31}$$

4.5.1 Scattering matrix and unidirectional reflectionless transmission

Recall that we are considering the limit when $\delta \to 0$ and supposing that $\omega = O(\sqrt{\delta})$. The condition $|\alpha| < k < \inf_{l\in\mathbb{Z}^2\setminus\{0\}}|2\pi lL - \alpha|$ will be satisfied for small enough ω, so the scattered wave will behave as a single plane wave as $|x_3| \to \infty$. If the incident field is given by

$$u^{in}(x) = c_1e^{\mathrm{i}\mathbf{k}_-\cdot x} + c_2e^{\mathrm{i}\mathbf{k}_+\cdot x},$$

the total field will behave as

$$u \sim \begin{cases} c_1e^{\mathrm{i}\mathbf{k}_-\cdot x} + d_1e^{\mathrm{i}\mathbf{k}_+\cdot x}, & x_3 \to \infty,\\ c_2e^{\mathrm{i}\mathbf{k}_+\cdot x} + d_2e^{\mathrm{i}\mathbf{k}_-\cdot x}, & x_3 \to -\infty,\end{cases} \tag{4.32}$$

where

$$\begin{pmatrix} d_1\\ d_2\end{pmatrix} = S\begin{pmatrix} c_1\\ c_2\end{pmatrix}, \qquad S = \begin{pmatrix} r_+ & t_-\\ t_+ & r_-\end{pmatrix}. \tag{4.33}$$

S is known as the scattering matrix. The reflection and transmission coefficients r_+, t_+ are the coefficients of the outgoing part of the field in the case $u^{in}(x) = e^{\mathrm{i}\mathbf{k}_-\cdot x}$, *i.e.* when the incident field is a plane wave from the positive x_3 direction (and reversely for r_-, t_-). Next, we will compute the scattering matrix in the asymptotic limit specified in Section 4.4.

For simplicity, we set $u^{in} = e^{\mathrm{i}\mathbf{k}\cdot x}$ with $\mathbf{k} = \mathbf{k}_+$ or $\mathbf{k} = \mathbf{k}_-$, and then use linearity to obtain the full scattering matrix. From Proposition 4.13, we know that the scattered field is given by

$$u - u^{in} = -(a + \mathrm{i}b)\mu S_1^{\alpha,\omega} + (a - \mathrm{i}b)\mu S_2^{\alpha,\omega} - \mathcal{S}_D^{\alpha,k}\left(\mathcal{S}_D^{\alpha,k}\right)^{-1}[u^{in}] + O(\omega^2). \tag{4.34}$$

As $\omega \to 0$, we have the following asymptotic behaviour of

$$\begin{aligned} R_{j,\pm} &= \frac{1}{2\mathrm{i}k_3L^2}\int_{\partial D}\psi_j^0(y)\,\mathrm{d}\sigma(y) - \frac{1}{2\mathrm{i}k_3L^2}\int_{\partial D}\mathrm{i}\mathbf{k}_\pm\cdot y\psi_j^0(y)\,\mathrm{d}\sigma(y) + \frac{\omega}{2\mathrm{i}k_3L^2}\int_{\partial D}\psi_j^{1,\alpha_0}\,\mathrm{d}\sigma + O(\omega)\\ &= -\frac{\mathbf{k}_\pm\cdot\mathbf{c}_j}{2k_3L^2} + \frac{1}{2\mathrm{i}w_3L^2}\int_{\partial D}\psi_j^{1,\alpha_0}\,\mathrm{d}\sigma + O(\omega).\end{aligned}$$

Moreover,

$$\frac{1}{2\mathrm{i}k_3L^2}\int_{\partial D} e^{-\mathrm{i}\mathbf{k}_\pm\cdot y}\left(\mathcal{S}_D^{\alpha,\omega}\right)^{-1}[u^{in}]\,\mathrm{d}\sigma(y) = \frac{\omega}{2\mathrm{i}k_3L^2}\int_{\partial D}\left(\psi_1^{1,\alpha_0} + \psi_2^{1,\alpha_0}\right)\,\mathrm{d}\sigma + O(\omega) = 1 + O(\omega).$$

Therefore, from Proposition 4.15, (4.31) and (4.34), the scattered field satisfies

$$u - u^{in} \sim \left(\frac{\mu a\mathbf{k}_\pm\cdot\mathbf{c}_1}{k_3L^2} - \mathrm{i}\mu b - 1 + O(\omega)\right)e^{\mathrm{i}\mathbf{k}_\pm\cdot x}, \tag{4.35}$$

$$=: \big(G_{s\pm}(\lambda^*) + O(\omega)\big)e^{\mathrm{i}\mathbf{k}_\pm\cdot x}, \tag{4.36}$$

as $x_3 \to \pm\infty$. Here s denotes the sign of the third component of $\mathbf{k}$ (recall that μ depends on $\mathbf{k}$). From (4.32) and (4.35), it follows that the scattering matrix, defined in (4.33), can be written as

$$S = \begin{pmatrix} G_{-+}(\lambda^*) & 1 + G_{++}(\lambda^*)\\ 1 + G_{--}(\lambda^*) & G_{+-}(\lambda^*)\end{pmatrix} + O(\omega). \tag{4.37}$$

Up to this point, the only assumption we have made on the resonators' geometry is that they are symmetric under the parity operator $\mathcal{P}$. In order to simplify the above expressions, we will additionally assume that the resonators have an in-plane parity symmetry $\mathcal{P}_2$, *i.e.* that

$$\mathcal{P}_2 D_i = D_i, \; i = 1,2, \qquad \text{where} \qquad \mathcal{P}_2(x_1,x_2,x_3) = (-x_1,-x_2,x_3).$$

We then have the following result on the capacitance coefficients.

Lemma 4.16. *Assume that $\mathcal{P}_2 D_i = D_i, \; i = 1,2$.*

(i) ψ_j^0, and consequently C_{ij}^0 and $\mathbf{c}_j$, are independent of α_0.

(ii) For some $c \in \mathbb{R}$ we have

$$\mathbf{c}_1 = \begin{pmatrix} 0 \\ 0 \\ c \end{pmatrix}, \quad \mathbf{c}_2 = \begin{pmatrix} 0 \\ 0 \\ -c \end{pmatrix},$$

and

$$C^{1,\alpha_0} = -\frac{\mathrm{i}w_3 L^2}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} - \frac{\mathrm{i}w_3 c^2}{2L^2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} + O(\omega).$$

Proof of (i). Using the symmetries described by $\mathcal{P}$ and by $\mathcal{P}_2$, and using the fact that $\psi_1^0 = -\psi_2^0$ we have

$$\psi_j^0(y) = -\psi_j^0(\mathcal{P}\mathcal{P}_2 y), \qquad \hat{\psi}_1^{1,\alpha_0}(y) = \hat{\psi}_2^{1,\alpha_0}(\mathcal{P}\mathcal{P}_2 y), \tag{4.38}$$

for $j = 1,2$. Using the first identity, we have for $i = 1,2$,

$$\mathbf{e}_i \cdot \mathbf{c}_j = \int_{\partial D} \mathcal{P}\mathcal{P}_2(y_i)\psi_j^0(\mathcal{P}\mathcal{P}_2 y)\,\mathrm{d}\sigma(y) = -\int_{\partial D} y_i \psi_j^0\,\mathrm{d}\sigma = -\mathbf{e}_i \cdot \mathbf{c}_j, \tag{4.39}$$

where $\mathbf{e}_i$ is the i^{th} standard vector. Using the second identity of (4.38), we have

$$\int_{\partial D} \hat{\psi}_1^{1,\alpha_0}\,\mathrm{d}\sigma = \int_{\partial D} \hat{\psi}_2^{1,\alpha_0}\,\mathrm{d}\sigma. \tag{4.40}$$

Using (4.39) and (4.40), we find from (4.19) that

$$\mathcal{S}_D^{0,0}[\psi_1^0] = \frac{1}{2}\chi_{\partial D_1} - \frac{1}{2}\chi_{\partial D_2}, \qquad \mathcal{S}_D^{0,0}[\psi_2^0] = -\frac{1}{2}\chi_{\partial D_1} + \frac{1}{2}\chi_{\partial D_2}.$$

Since $\mathcal{S}_D^{0,0}$ is injective on $L_0^2(\partial D)$, and $\mathcal{S}_D^{0,0}$ does not depend on α_0, we conclude that ψ_j^0 does not depend on α_0. ☐

Proof of (ii). In the proof of Lemma 4.9 it was proved that ψ_j^0, and hence $\mathbf{c}_j$, is real-valued. The first statement of *(ii)* now follows from (4.39) and the fact that $\mathbf{c}_1 = -\mathbf{c}_2$.

To prove the second statement of *(ii)*, we use (4.40) to conclude that

$$\begin{aligned}\mathcal{S}_D^{0,0}[\hat{\psi}_1^{1,\alpha_0} - \hat{\psi}_2^{1,\alpha_0}] &= K\chi_{\partial D} + \frac{\alpha\cdot(x_1,x_2)}{2k_3L^2}\int_{\partial D}\left(\hat{\psi}_1^{1,\alpha_0} - \hat{\psi}_2^{1,\alpha_0}\right)\mathrm{d}\sigma \\ &= K\chi_{\partial D},\end{aligned}$$

for some constant K. From Lemma 4.7 it follows that

$$\hat{\psi}_1^{1,\alpha_0} = \hat{\psi}_2^{1,\alpha_0}.$$

Then, using Lemma 4.11, we can write the matrix C^{1,α_0} as

$$C^{1,\alpha_0} = -\frac{\mathrm{i}w_3 L^2}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + h\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} + O(\omega),$$

where

$$h = \int_{\partial D} \mathcal{S}_1^{\alpha_0}[\psi_1^0]\psi_1^0\,\mathrm{d}\sigma.$$

The only remaining task is to explicitly compute h. To this end, we write the kernel function $G_1^{\alpha_0}$ of $\mathcal{S}_1^{\alpha_0}$ as

$$G_1^{\alpha_0}(x) = K_1(x) + K_2^{\alpha_0}(x) + K_3^{\alpha_0}(x),$$

and hence

$$h = \int_{\partial D}\int_{\partial D} \left(K_1(x-y) + K_2^{\alpha_0}(x-y) + K_3^{\alpha_0}(x-y)\right)\psi_1^0(x)\psi_1^0(y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y),$$

where

$$K_1(x) = \frac{\mathrm{i}w_3x_3^2}{4L^2}, \quad K_2^{\alpha_0}(x) = \alpha_0\cdot\left(\frac{\mathrm{i}|x_3|(x_1,x_2)}{2L^2} + g_1(x)\right), \quad K_3^{\alpha_0}(x) = \frac{\mathrm{i}\left(\alpha_0\cdot(x_1,x_2)\right)^2}{4w_3L^2}.$$

Next, we will show that only K_1 gives a non-zero contribution to h. Firstly, we observe that $K_2^{\alpha_0}(\mathcal{P}_2x) = -K_2^{\alpha_0}(x)$ while $\psi_1^0(\mathcal{P}_2x) = \psi_1^0(x)$. Therefore

$$\int_{\partial D}\int_{\partial D} K_2^{\alpha_0}(x-y)\psi_1^0(x)\psi_1^0(y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) = 0.$$

Secondly, we study the contribution of K_3. We have

$$K_3^{\alpha_0}(x-y) = \frac{\mathrm{i}}{4w_3L^2}\left(\left(\alpha_0\cdot(x_1,x_2)\right)^2 - 2\left(\alpha_0\cdot(x_1,x_2)\right)\left(\alpha_0\cdot(y_1,y_2)\right) + \left(\alpha_0\cdot(y_1,y_2)\right)^2\right),$$

and hence

$$\begin{aligned}&\int_{\partial D}\int_{\partial D} K_3^{\alpha_0}(x-y)\psi_1^0(x)\psi_1^0(y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) = \\ &\frac{\mathrm{i}}{4w_3L^2}\Bigg(\int_{\partial D}\left(\alpha_0\cdot(x_1,x_2)\right)^2\psi_1^0(x)\,\mathrm{d}\sigma(x)\int_{\partial D}\psi_1^0\,\mathrm{d}\sigma + \int_{\partial D}\left(\alpha_0\cdot(y_1,y_2)\right)^2\psi_1^0(y)\,\mathrm{d}\sigma(y)\int_{\partial D}\psi_1^0\,\mathrm{d}\sigma \\ &\qquad - 2\int_{\partial D}\alpha_0\cdot(x_1,x_2)\psi_1^0(x)\,\mathrm{d}\sigma(x)\int_{\partial D}\alpha_0\cdot(y_1,y_2)\psi_1^0(y)\,\mathrm{d}\sigma(y)\Bigg).\end{aligned}$$

The first two terms in the right-hand side vanish since $\int_{\partial D}\psi_1^0\,\mathrm{d}\sigma = 0$, while the last term vanishes since $\mathbf{e}_i\cdot\mathbf{c}_1 = 0$ for $i=1,2$. We conclude that only K_1 has a non-zero contribution to h. We have

$$K_1(x-y) = \frac{\mathrm{i}w_3}{4L^2}\left(x_3^2 - 2x_3y_3 + y_3^2\right),$$

so analogously to K_3, we can use the fact that $\int_{\partial D}\psi_1^0\,\mathrm{d}\sigma = 0$ to conclude that

$$\begin{aligned}h = \int_{\partial D}\int_{\partial D} K_1(x-y)\psi_1^0(x)\psi_1^0(y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) &= -\frac{\mathrm{i}w_3}{2L^2}\int_{\partial D}x_3\psi_1^0(x)\,\mathrm{d}\sigma(x)\int_{\partial D}y_3\psi_1^0(y)\,\mathrm{d}\sigma(y) \\ &= -\frac{\mathrm{i}w_3c^2}{2L^2}.\end{aligned}$$

This proves the claim. □

Theorem 4.17. *Assume that $\mathcal{P}_2D_i = D_i$, $i=1,2$ and that $|bL^2| \neq |ac|$. Let $\lambda = \omega^2|D_1|$, and assume that ω is in the subwavelength regime such that $\lambda = \lambda_2^0 + \lambda^*$ for $\lambda^* = O(\omega^3)$. We then have the following asymptotic expansion of the scattering matrix:*

$$S = \frac{1}{\mathrm{i}k_3\left(\frac{b^2L^2}{a} - \frac{ac^2}{L^2}\right) - \lambda^*}\begin{pmatrix}\lambda^* - 2k_3bc & \mathrm{i}k_3\left(\frac{b^2L^2}{a} + \frac{ac^2}{L^2}\right) \\ \mathrm{i}k_3\left(\frac{b^2L^2}{a} + \frac{ac^2}{L^2}\right) & \lambda^* + 2k_3bc\end{pmatrix} + O(\omega),$$

where the error term is uniform with respect to λ^* in a neighbourhood of 0. In particular, we have $r_+ \neq r_-$, and to leading order r_+ and r_- vanish, respectively, at $\lambda^* = \lambda_+$ and $\lambda^* = \lambda_-$ given by

$$\lambda_+ = 2k_3bc, \quad \lambda_- = -2k_3bc.$$

Proof. We begin by computing p. We have

$$\int_{\partial D_i} \left(\mathcal{S}_D^{\alpha,k}\right)^{-1}[u^{in}]\,\mathrm{d}\sigma = \int_{\partial D} u^{in}\left(\mathcal{S}_D^{-\alpha,k}\right)^{-1}[\chi_{\partial D_i}]\,\mathrm{d}\sigma = \int_{\partial D} \mathrm{i}\mathbf{k}\cdot x\psi_i^0\,\mathrm{d}\sigma + \omega\int_{\partial D}\psi_i^{1,-\alpha_0}\,\mathrm{d}\sigma + O(\omega^2)$$
$$= \mathrm{i}k_3 c + \mathrm{i}k_3 L^2 + O(\omega^2).$$

Then we find that

$$d^{\mathrm{T}}p = -2\mathrm{i}k_3\left(sac + \mathrm{i}bL^2\right) + O(\omega^4).$$

Moreover, writing $f(\lambda^*) = d^{\mathrm{T}}\left(\omega C^{1,v,\alpha_0} - \lambda^* I\right)\mathbf{v}_2^0$ we have

$$f(\lambda^*) = -2\mathrm{i}k_3\left(b^2L^2 - \frac{a^2c^2}{L^2}\right) + 2a\lambda^* + O(\omega^6).$$

We can then compute G as

$$G_{s\sigma}(\lambda^*) = -\frac{2k_3}{f(\lambda^*)L^2}\left(sac + \mathrm{i}bL^2\right)\left(\sigma ac - \mathrm{i}bL^2\right) - 1 + O(\omega).$$

Then, to leading order we have

$$G_{++}(\lambda^*) = G_{--}(\lambda^*), \qquad G_{+-}(\lambda^*) - G_{-+}(\lambda^*) = -\frac{8k_3abc}{f(\lambda^*)}.$$

If $b \neq 0$, it is clear that $r_+ \neq r_-$. Simplifying these expressions, we have

$$G_{\pm\mp}(\lambda^*) = \frac{-2a}{f(\lambda^*)}\left(\lambda^* \pm 2k_3bc\right) + O(\omega).$$

To leading order, we then have the following expressions for $t_\pm$ and $r_\pm$:

$$r_+ = \frac{\lambda^* - 2k_3bc}{\mathrm{i}k_3\left(\frac{b^2L^2}{a} - \frac{ac^2}{L^2}\right) - \lambda^*}, \qquad t_- = \frac{\mathrm{i}k_3\left(\frac{b^2L^2}{a} + \frac{ac^2}{L^2}\right)}{\mathrm{i}k_3\left(\frac{b^2L^2}{a} - \frac{ac^2}{L^2}\right) - \lambda^*},$$
$$t_+ = \frac{\mathrm{i}k_3\left(\frac{b^2L^2}{a} + \frac{ac^2}{L^2}\right)}{\mathrm{i}k_3\left(\frac{b^2L^2}{a} - \frac{ac^2}{L^2}\right) - \lambda^*}, \qquad r_- = \frac{\lambda^* + 2k_3bc}{\mathrm{i}k_3\left(\frac{b^2L^2}{a} - \frac{ac^2}{L^2}\right) - \lambda^*}.$$

The expression for S and the zeros of $r_\pm$ follow directly from this. □

Remark 4.18. *There are two subwavelength frequency regimes not covered in Theorem 4.17: when ω is close to the first band function $\omega_1^0 = 0$ or when ω is well-separated from the two band functions. When ω is close to ω_1^0, Remark 4.14 tells us that $t_+ = t_- = 1$ and $r_+ = r_- = 0$. When ω is well-separated from ω_1^0 and ω_2^α, the solution q to* (4.30) *will be small. Consequently, it is easy to show that t_+ and t_- will be small, while r_+ and r_- have magnitude close to 1. These regimes are demonstrated in Figure 7.*

Remark 4.19. *The assumption $|bL^2| \neq |ac|$ comes from the condition* $\mathrm{Im}(d^{\mathrm{T}}C^{v,1,\alpha_0}\mathbf{v}_2^0) \neq 0$ *in Proposition 4.13. At the critical point $b = \pm\frac{ac}{L^2}$, the denominator of S will vanish at $\lambda^* = 0$. Around this point, we therefore expect the transmittance and reflectance to be very large, corresponding to extraordinary transmission. This is numerically demonstrated in Figure 8.*

Remark 4.20. *Throughout this section, we use the classical convention for the scattering matrix S, defined in* (4.33)*. If we instead define $S = S(\lambda^*)$ by*

$$S = \begin{pmatrix} t_+ & r_- \\ r_+ & t_- \end{pmatrix}.$$

we see that the points $\lambda^* = \lambda_+$ and $\lambda^* = \lambda_-$ represent exceptional points of S (see, for example, [17] for further elaborations on the connection between unidirectional reflection and exceptional points).

Remark 4.21. *In the case that $b = 0$, i.e. without gain and loss, it is well-known that $r_+ = r_-$ and $t_+ = t_-$, which is consistent with the fact that $G_{+-} = G_{-+}$ and $G_{++} = G_{--}$ in this case.*

4.5.2 Numerical illustration

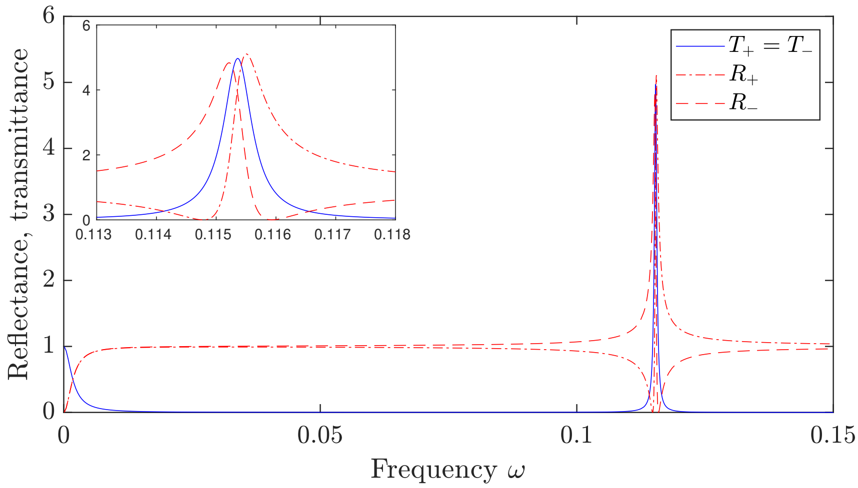

Figure 7: Plot of the transmittance $T_\pm = |t_\pm|^2$ (blue) and reflectance $R_\pm = |r_\pm|^2$ (red) as functions of the frequency. The inlay shows the behaviour around the critical frequency range and demonstrates both unidirectional reflection and extraordinary transmission. Here, we simulate a two-dimensional problem with the same parameters and the same frequency range as Figure 6, with incident direction $\mathbf{w} = \frac{1}{2}\left(-\sqrt{3},\ \pm 1\right)^{\mathrm{T}}$.

Figure 7 shows the transmittance $T_\pm = |t_\pm|^2$ and reflectance $R_\pm = |r_\pm|^2$ as functions of the frequency. The computations were performed using the multipole discretization (see, for example, [7]), independently of the asymptotic analysis in the previous sections. As is well known for $\mathcal{PT}$-symmetric structures (see *e.g.* [34]), the two transmission coefficients t_+ and t_- coincide. The figure clearly shows the shifted zeros of the reflectances close to the second resonant frequency. For a frequency at one of these zeros, the system will exhibit unidirectional reflectionless transmission.

Due to the gain and loss, the reflectance and transmittance satisfy the “generalized” energy conservation relation [13]

$$R_+R_- + 2\sqrt{T_+T_-} - T_+T_- = 1,$$

which, in particular, allows the scattering matrix to be non-unitary and allows the reflectance or transmittance to exceed 1. In Figure 8, the peak transmittance is plotted as a function of the gain/loss parameter b, which clearly demonstrates the extraordinary transmission.

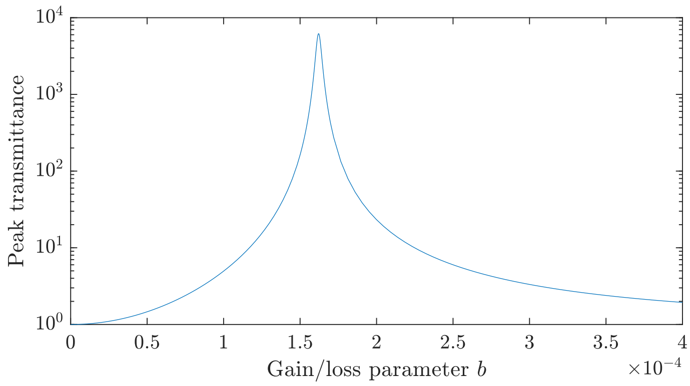

Figure 8: Plot of the peak transmittance as a function of the gain/loss parameter. The extraordinarily high transmittance at $b = \left|\frac{ac}{L^2}\right|$ is clearly demonstrated. Here, we simulate a two-dimensional problem with the same parameters as Figure 6 and Figure 7.

5 Concluding remarks

In this work, we have studied non-Hermitian systems of high-contrast subwavelength resonators with parity–time symmetry. We have proved the existence of asymptotic exceptional points in a system of two resonators. More precisely, we have proved that there is a value of the gain/loss parameter such that the resonant frequencies and eigenmodes coincide at leading order (in terms of the material contrast). Moreover, we have proved that large ensembles of non-Hermitian resonators collectively behave as non-Hermitian systems, meaning they might, for example, support exceptional points on a macroscopic scale. Finally, we have studied a metascreen of $\mathcal{PT}$-symmetric resonators. We proved that the two reflection coefficients asymptotically vanish at distinct frequencies, which allows for unidirectional reflectionless transmission, and also showed that, for a specific magnitude of the gain/loss, extraordinarily high transmittance can occur for frequencies close to the second band function.

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