Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Seminar for Applied Mathematics

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Research Report No. 2020-17
March 2020

Seminar für Angewandte Mathematik
Eidgenössische Technische Hochschule
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Switzerland

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, whereby eigenmodes are linearly dependent. The main goal of this work is to study the existence and consequences of exceptional points in the setting of high-contrast subwavelength metamaterials. We begin by studying a system of two parity–time-symmetric subwavelength resonators and prove that this system supports exceptional points. Using homogenization theory, we study a large ensemble of resonators and show that this behaviour can be replicated at the macroscale. Finally, we study a metascreen of subwavelength resonators and prove that there are frequencies at which this system exhibits unidirectional reflectionless transmission.

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

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

1 Introduction

Exceptional points are parameter values at which eigenvalues, and their associated eigenvectors, simultaneously coincide, and have been observed in a variety of quantum mechanical, optical and photonic settings. Crucially, exceptional points can only occur when the underlying system is non-Hermitian, as the eigenvectors are linearly independent otherwise. An important class of non-Hermitian systems, where exceptional points are well known to occur, are structures with so-called *parity-time-* or *$\mathcal{PT}$-symmetry* [10, 12, 19, 22]. 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 means that they experience resonant behaviour in response to critical wavelengths much greater than their size. Such structures, often known as *metamaterials* to highlight their complex microscopic structure, can exhibit exotic scattering properties and appear in a variety of photonic and phononic applications [16, 21, 14].

We begin by studying a pair of subwavelength resonators. This system is known to exhibit two subwavelength resonant modes [6]. We examine the case of non-real material parameters, which corresponds to introducing gain and loss to the system. The geometry and material parameters are chosen so that the structure is $\mathcal{PT}$-symmetric, which means that the structure is symmetric

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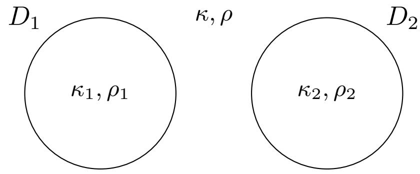

Figure 1: Two subwavelength resonators. This system is $\mathcal{PT}$-symmetric if $\mathcal{P}D = D$, $\kappa_1 = \overline{\kappa_2}$ and $\rho_1 = \overline{\rho_2}$.

and that the gain and loss is balanced. We show that if these parameters are suitably balanced then the two eigenvalues and eigenvectors coincide.

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 [9, 13, 17, 24, 25].

In Section 3 we study 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 pair of cavities, which have conjugate material parameters but neither of which is $\mathcal{PT}$-symmetric at the microscale, can be designed to support an exceptional point. We also verify that a structure that is $\mathcal{PT}$-symmetric at the microscale will not exhibit this symmetry at the macroscale, after homogenization [20].

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 [11]. For example, the scattered wave can now depend on which side the incident wave is impinging from. While being impossible in structures without gain and loss, $\mathcal{PT}$-symmetric structures can have frequencies at which the reflection is zero when the wave is impinging from one side, and non-zero when the wave is impinging from the opposite side [15, 18, 26]. We will refer to such case as *unidirectional reflectionless transmission.* An interesting special case of this is when the transmission is simultaneously unity, leading to a one-sided "invisible" structure that will leave incident waves unaffected.

In Section 4 we study an unbounded, $\mathcal{PT}$-symmetric structure that exhibits unidirectional reflectionless transmission for 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 are zero for frequencies close to a critical frequency. Moreover, as the gain and loss increases, there is a shift in the zeros: the zero of one of the reflection coefficients will be shifted upwards and one will be shifted downwards. We emphasize that, unlike previous work based on coupled-mode approximations (for example [15, 23]) or perturbation theory [26], the methods presented here provide a rigorous explanation for unidirectional reflectionless transmission and are valid even in regimes with large gain and loss.

2 Exceptional point of two resonators

We will study a resonator structure composed of two resonators $D_1, D_2 \subset \mathbb{R}^3$ satisfying $\partial D_i \in C^{1,s}, 0 < s < 1$. We assume that the material inside the ith resonator D_i has complex-valued bulk modulus $\kappa_i \in \mathbb{C}$ and density $\rho_i \in \mathbb{C}$. Corresponding parameters κ, ρ of the surrounding material are assumed to be real. We denote the frequency of the waves by ω and define the parameters, for $i = 1, 2$,

$$v_i = \sqrt{\frac{\kappa_i}{\rho_i}}, \quad v = \sqrt{\frac{\kappa}{\rho}}, \quad \delta_i = \frac{\rho_i}{\rho}, \quad k = \frac{\omega}{v}, \quad k_i = \frac{\omega}{v_i}.$$

In the frequency domain, the time-reversal operator $\mathcal{T}$ is given by complex conjugation, while the parity operator $\mathcal{P}$ is given by $\mathcal{P}: \mathbb{R}^3 \to \mathbb{R}^3$,

$$\mathcal{P}(x) = -x.$$

We assume that the resonator pair $D = D_1 \cup D_2$ is $\mathcal{PT}$-symmetric, which means that

$$\mathcal{P}D = D, \qquad \text{and} \qquad \kappa_1 = \overline{\kappa_2}, \quad \rho_1 = \overline{\rho_2}.$$

With this assumption we have $|\delta_1| = |\delta_2| := \delta$. Then δ correspond to the density contrast, and we assume that

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

We introduce the notation

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

The parameter b can be interpreted as the magnitude of the gain and the loss. We study the scattering problem

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

Here, u^{in} is the incident field, which we assume satisfy $\Delta u^{in} + k^2 u^{in} = 0$ in $\mathbb{R}^3$ and, moreover, $\nabla u^{in}\big|_D = O(\omega)$. The Sommerfeld radiation condition is specified in (A.1) in Appendix A. 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 $u^{in} = 0$.

Let $\mathcal{S}_D^k$ be the single layer potential, defined by

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

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

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

We present some elementary properties of the single layer potential in Appendix A. We use the notation $\mathcal{S}_D$ for $\mathcal{S}_D^0$, *i.e.* for the Laplace single layer potential.

2.1 Capacitance-matrix analysis

Our approach to solving (2.1) in the case that $u^{in} = 0$ 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 $A \subset \mathbb{R}^3$. 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, finally, the weighted capacitance matrix $C^v = (C^v_{ij})$ as

$$C^v = \begin{pmatrix} v_1^2\delta_1 C_{11} & v_1^2\delta_1 C_{12} \\ v_2^2\delta_2 C_{12} & v_2^2\delta_2 C_{11} \end{pmatrix}. \tag{2.2}$$

This has been weighted to account for the different material parameters inside the different resonators, see *e.g.* [6, 2] for other variants in slightly different settings.

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 2.1. *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

$$\left(C^v - \omega^2|D_1|I\right)\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = -\begin{pmatrix} v_1^2\delta_1 \int_{\partial D_1} \mathcal{S}_D^{-1}[u^{in}]\,\mathrm{d}\sigma \\ v_2^2\delta_2 \int_{\partial D_2} \mathcal{S}_D^{-1}[u^{in}]\,\mathrm{d}\sigma \end{pmatrix}. \tag{2.3}$$

Proof. The solutions can be represented as

$$u = \begin{cases} u^{in}(x) + \mathcal{S}_D^k[\psi](x), & x \in \mathbb{R}^3 \setminus \overline{D}, \\ \mathcal{S}_D^{k_i}[\phi](x), & x \in D_i,\ i = 1,2, \end{cases} \tag{2.4}$$

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. Because of the jump conditions (A.2), (A.3), in order to satisfy the transmission conditions, the 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 (A.4), (A.5) and the assumption that $\nabla u^{in} = O(\omega)$ we have that

$$\begin{aligned} \mathcal{S}_D[\phi - \psi] &= u^{in} + O(\omega) \quad \text{on } \partial D_1 \cup \partial D_2, \\ \left(-\frac{1}{2}I + \mathcal{K}_D^* + \frac{\omega^2}{v_i^2}\mathcal{K}_{D,2}\right)[\phi] - \delta_i\left(\frac{1}{2}I + \mathcal{K}_D^*\right)[\psi] &= O(\delta\omega + \omega^3) \quad \text{on } \partial D_i. \end{aligned} \tag{2.5}$$

From the (2.5) and the fact that $\mathcal{S}_D$ is invertible we can see that

$$\psi = \phi - \mathcal{S}_D^{-1}[u^{in}] + O(\omega). \tag{2.6}$$

Thus, we are left with the equation

$$\left(-\frac{1}{2}I + \mathcal{K}_D^* + \frac{\omega^2}{v_i^2}\mathcal{K}_{D,2} - \delta_i\left(\frac{1}{2}I + \mathcal{K}_D^*\right)\right)[\phi] = -\delta_i\left(\frac{1}{2}I + \mathcal{K}_D^*\right)\mathcal{S}_D^{-1}[u^{in}] + O(\delta\omega + \omega^3), \tag{2.7}$$

on $\partial D_i, i = 1,2$. We recall, *e.g.* from [6, Lemma 2.1], that for any $\varphi \in L^2(\partial D)$ we have, for $i = 1,2$,

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

Integrating (2.7) over ∂D_i 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, (2.7) 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 $\left(-\frac{1}{2}I + \mathcal{K}_D^*\right)$, the solution can be written as

$$\phi = q_1\psi_1 + q_2\psi_2 + O(\omega^2 + \delta), \tag{2.8}$$

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

$$\left(C^v - \omega^2|D_1|I\right)\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = -\begin{pmatrix} v_1^2\delta_1 \int_{\partial D_1} \mathcal{S}_D^{-1}[u^{in}] \, \mathrm{d}\sigma \\ v_2^2\delta_2 \int_{\partial D_2} \mathcal{S}_D^{-1}[u^{in}] \, \mathrm{d}\sigma \end{pmatrix}. \tag{2.9}$$

The result now follows from (2.4) combined with the expressions for ϕ, ψ in (2.6), (2.8) and (2.9). □

Theorem 2.2. *As $\delta \to 0$, the 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 2.1 that there is a non-zero solution q_1, q_2 to the eigenvalue problem (2.3) precisely when $\omega^2|D_1|$ is an eigenvalue of C^v. □

The eigenvalues of C^v are given by

$$\lambda_i = aC_{11} + (-1)^i \sqrt{a^2C_{12}^2 - b^2(C_{11}^2 - C_{12}^2)}. \tag{2.10}$$

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

Theorem 2.3. *There is a magnitude $b_0 = b_0(a) > 0$ of the gain/loss such that the resonator dimer has an 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 2.2 and (2.10), 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 (2.8), it follows that the eigenmodes are linearly dependent. The remaining statements are straightforward to check. □

Remark 2.4. *Theorem 2.3 states that the exceptional point occurs to leading order in δ. In fact, we do not expect the system to exhibit an exact exceptional point. This is because differential operator corresponding to the problem (2.1) is not $\mathcal{PT}$-symmetric, due to the radiation condition. However, the discrete approximation given by the weighted capacitance matrix is indeed $\mathcal{PT}$-symmetric, resulting in approximately conjugate-symmetric resonant frequencies. This can be observed in Figure 2. Even in the case without gain and loss ($b = 0$), the system is non-Hermitian, and the imaginary parts of the resonant frequencies are non-zero to higher orders [6].*

Lemma 2.5. *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 $\mathbf{v}_i = \left[\mathbf{v}_i^1, \mathbf{v}_i^2\right]^{\mathrm{T}}, i = 1, 2,$ are the eigenvectors of C^v, given by

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

2.2 Numerical results

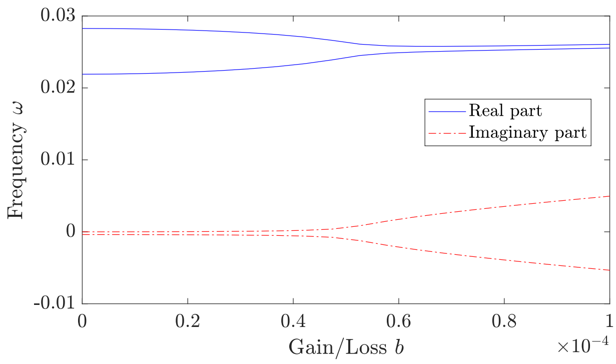

Figure 2: Plot of the real part (blue) and imaginary part (red) of the resonant frequencies of the dimer as the gain/loss parameter b increases. The exceptional point occurs at $b_0 \approx 0.5 \times 10^{-4}$, at which point the frequencies coincide to leading order. For b smaller than b_0, the frequencies 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 resonant frequencies ω_1, ω_2 as functions of b. For $b = b_0$, the resonant frequencies coincide to leading order, and for larger b the two resonant frequencies are complex-conjugated. The numerical simulations in this work were performed on spherical resonators using the multipole expansion method, which is outlined in [1, Appendix A].

3 Resonator cavities

In this section, we examine the properties of bounded metamaterials taking the form of cavities filled with subwavelength resonators with gain and loss. 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 exhibit similar exceptional behaviour in response to wavelengths of the same order as their dimensions.

The non-Hermitian nature of a large collection of $\mathcal{PT}$-symmetric dimers is expected to be lost due to averaging. Instead, in order to create a $\mathcal{PT}$-symmetric pair of cavities that support an exceptional point, we propose filling each individual cavity with resonators of a single sign of the gain/loss parameter. Such cavities are considered in Section 3.1, where we see that the parameters can be chosen such that the macroscopic structure is non-Hermitian after homogenization. In Section 3.2, we verify that the homogenized medium of a single cavity filled with $\mathcal{PT}$-symmetric dimers corresponds to a Hermitian system, and can therefore not exhibit exceptional points.

3.1 $\mathcal{PT}$-symmetric cavities

Consider a cavity $\Omega_\pm$ that is filled with N identical, single resonators that all have the same material parameters. That is, if D is some fixed resonator define the small resonators B_j^N for

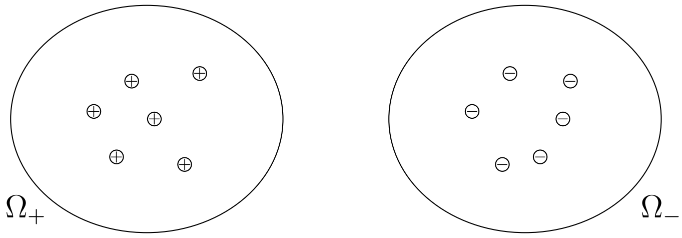

Figure 3: A pair of $\mathcal{PT}$-symmetric cavities which supports a macroscopic exceptional point. Here, + and − denote opposite signs of the imaginary part of the material coefficients.

$1 \leq j \leq N$ as

$$B_j^N = rR_j^N D + z_j^N,$$

for a scale $0 < r \ll 1$, some rotations R_j^N and positions z_j^N.

We assume that the material inside D has complex bulk modulus $\kappa_b \in \mathbb{C}$ and density $\rho_b \in \mathbb{C}$. We define the parameters

$$v_b = \sqrt{\frac{\kappa_b}{\rho_b}}, \quad v = \sqrt{\frac{\kappa}{\rho}}, \quad \delta_b = \frac{\rho_b}{\rho}.$$

As in Section 2, we assume that $v_b = O(1)$ and, in order for the resonant frequency to be $O(1)$, also that

$$v_b^2 \delta_b = \frac{\kappa_b}{\rho} = r^2 a + \mathrm{i} r^2 b,$$

for $a, b = O(1)$.

We can show (in Appendix B.1) that if $rN = \Lambda$ (for some constant Λ) then as $N \to \infty$, assuming the distribution of the resonators is sufficiently regular, the limiting system is described by the homogenized equation

$$\Delta u(x) + M(x)u(x) = 0, \qquad x \in \mathbb{R}^3, \tag{3.1}$$

with an effective compressibility given by

$$M(x) = \begin{cases} \omega^2 v^{-2}, & x \in \mathbb{R}^3 \setminus \Omega_\pm, \\ \omega^2 v^{-2} + (A(\omega, a, b) + \mathrm{i} b B(\omega, a, b))\, V(x), & x \in \Omega_\pm, \end{cases} \tag{3.2}$$

where $V(x)$ is a real-valued function that depends on the resonators' distribution and, if $|D|$ and Cap_D are the volume and capacitance of the (unscaled) resonator D, respectively, and v is the wave speed outside the resonators, A and B are given by

$$A(\omega, a, b) = \frac{\Lambda \omega^2 \mathrm{Cap}_D (\omega^2 - a \mathrm{Cap}_D |D|^{-1})}{(\omega^2 - a \mathrm{Cap}_D |D|^{-1})^2 + b^2 \mathrm{Cap}_D^2 |D|^{-2}},$$
$$B(\omega, a, b) = \frac{\Lambda \omega^2 \mathrm{Cap}_D^2 |D|^{-1}}{(\omega^2 - a \mathrm{Cap}_D |D|^{-1})^2 + b^2 \mathrm{Cap}_D^2 |D|^{-2}}.$$

Since $A(\omega, a, b) = A(\omega, a, -b)$ and $B(\omega, a, b) = B(\omega, a, -b)$, a consequence of (3.2) is that changing the sign of b changes the sign of the imaginary part of the cavity's effective material parameters. This means that a $\mathcal{PT}$-symmetric pair of cavities, Ω_+ and Ω_-, can be constructed by taking $b = \beta$ for the resonators in Ω_+ and $b = -\beta$ in Ω_-, for some $\beta > 0$ (as depicted in Figure 3).

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

It is important to note that a $\mathcal{PT}$-symmetric pair of cavities which support an exceptional point, as designed in Section 3.1, cannot be achieved through homogenization of resonators already possessing $\mathcal{PT}$-symmetry [20]. Suppose that we start with $D = D_1 \cup D_2$ as a fixed pair of $\mathcal{PT}$-symmetric

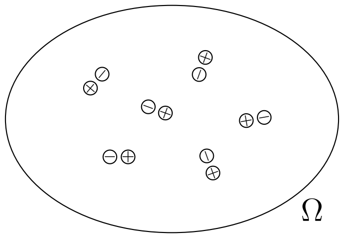

Figure 4: Exceptional behaviour is lost under homogenization. Here, + and − denote opposite signs of the imaginary part of the material coefficients.

resonators, as studied in Section 2. Then, as in Section 3.1, we define a system of small resonators B_j^N for $1 \leq j \leq N$ as

$$B_j^N = rR_j^N D + z_j^N,$$

for a scale $0 < r \ll 1$, some rotations R_j^N and positions z_j^N (depicted in Figure 4). Once again, we scale the material parameters so that

$$v_1^2 \delta_1 = \frac{\kappa_1}{\rho} = r^2 a + \mathrm{i} r^2 b,$$

for $a, b = O(1)$.

If Ω is a cavity filled with the dimers B_j^N, $1 \leq j \leq N$, then homogenization as $N \to \infty$ with $rN = \Lambda$ (see Appendix B.2 for details) yields the equation

$$\Delta u(x) + M(x)u(x) = 0, \qquad x \in \mathbb{R}^3, \tag{3.3}$$

where the effective parameter is given by

$$M(x) = \begin{cases} \omega^2 v^{-2}, & x \in \mathbb{R}^3 \setminus \Omega, \\ \omega^2 v^{-2} - \Lambda \tilde{m}(\omega) V(x), & x \in \Omega, \end{cases} \tag{3.4}$$

where $V(x)$ is a real-valued function that depends on the resonators' distribution and, if $|D_1|$, C_{ij} and Cap_D are the volume, capacitance coefficients and capacitance of the unscaled resonators, respectively, and if $\omega_1 = \sqrt{aC_{11}|D_1|^{-1}}$, we have that

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

We can see that, in this setting, the effective medium parameter (3.4) is always real valued. This means that, via this construction, we cannot hope to create a system of cavities with a non-Hermitian capacitance matrix and the possibility of an exceptional point. Conversely, the existence of a second-order singularity in $\tilde{m}(\omega)$ is notably peculiar and will have a strong influence on the system's behaviour for frequencies in this neighbourhood.

4 Unidirectional reflection in a $\mathcal{PT}$-symmetric metascreen

Here, we study a metascreen consisting of periodically repeated $\mathcal{PT}$-symmetric dimers. There are two main goals. Firstly, we will derive analogous results as in Section 2, thereby characterising the band structure and exceptional points of the metascreen. Moreover, we will prove that the metascreen exhibits unidirectional reflectionless transmission. In other words, the reflection coefficients depend on the side the incident wave comes from, and there are frequencies at which an incoming wave from one side will have zero reflection, while an incoming wave from the opposite side has non-zero reflection.

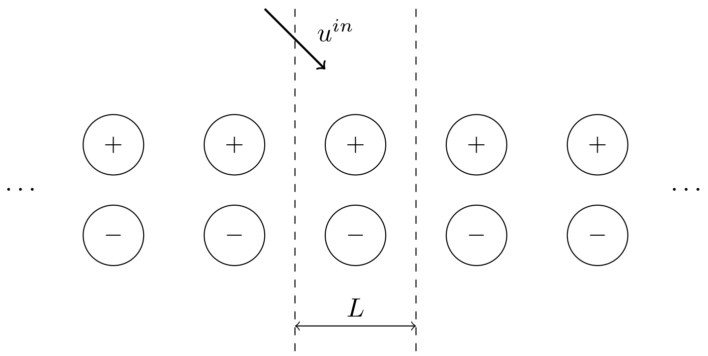

Figure 5: A $\mathcal{PT}$-symmetric metascreen with an incident plane wave u^{in}. Here, $+$ and $-$ denote opposite signs of the imaginary part of the material coefficients.

4.1 Band structure and exceptional points of the metascreen

We consider a structure with $\mathcal{PT}$-symmetric dimers repeated periodically in two dimensions. We let $Y_2 = [-L/2, L/2] \times [-L/2, L/2]$, where $L \in \mathbb{R}$ is the periodicity, and assume that the structure is periodic with unit cell $Y = Y_2 \times \mathbb{R}$. We adopt the notation from Section 2, and now assume that the pair of resonators $D = D_1 \cup D_2$ is contained inside Y. We define the periodically repeated resonators as

$$\mathcal{C}_i = \bigcup_{n \in \mathbb{Z}^2} D_i + nL, \ i = 1, 2, \qquad \mathcal{C} = \mathcal{C}_1 \cup \mathcal{C}_2.$$

We will assume that the incident field u^{in} is a plane wave with frequency ω and wave vector $\mathbf{k} = (k_1, k_2, k_3)^{\mathrm{T}}$,

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

where $|\mathbf{k}|$ denotes the Euclidean norm of $\mathbf{k}$. We will consider the subwavelength limit when $\delta \to 0$ and $\omega = O(\delta^{1/2})$. In this limit, we assume that the incident direction $\mathbf{v}_0$ of $\mathbf{k}$ is fixed, *i.e.* that $\mathbf{k}$ scales as

$$\mathbf{k} = \frac{\omega}{v}\mathbf{v}_0.$$

We define

$$\alpha = \begin{pmatrix} k_1 \\ k_2 \end{pmatrix} \in \mathbb{R}^2/(2\pi/L)\mathbb{Z}^2,$$

and we make the additional assumption that $\alpha \neq 0$, which, for small ω, corresponds to non-normal incidence. Observe that α, known as the *quasiperiodicity*, is defined modulo $2\pi/L$, and $Y^* := \mathbb{R}^2/(2\pi/L)\mathbb{Z}^2$ is known as the *first Brillouin zone*. A function $f(x), x \in \mathbb{R}^2$ is said to be α-quasiperiodic, with quasiperiodicity $\alpha \in \mathbb{R}$, if $e^{-\mathrm{i}\alpha\cdot x} f(x)$ is periodic.

We study the scattering problem

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

The outgoing quasiperiodic radiation condition states that $u(x) - u^{in}(x)$ behaves as a superposition of outgoing plane waves as $|x_3| \to \infty$. It is well known [4] that the solution u to this equation will be quasiperiodic in (x_1, x_2), *i.e.*

$$u(x_1 + n_1 L, x_2 + n_2 L, x_3) = e^{\mathrm{i}\alpha\cdot(n_1,n_2)L} u(x_1, x_2, x_3).$$

Let $\mathcal{S}_D^{k,\alpha}$ be the quasiperiodic single layer potential, defined analogously as $\mathcal{S}_D^k$ in (2) but using the quasiperiodic Green's function

$$G^{\alpha,k}(x,y) := -\sum_{(m_1,m_2)\in\mathbb{Z}^2} \frac{e^{\mathrm{i}k|x-y-L(m_1,m_2,0)|}}{4\pi|x-y-L(m_1,m_2,0)|} e^{\mathrm{i}\alpha\cdot(m_1,m_2)L}.$$

Again, we refer to Appendix A for properties of the quasiperiodic layer potential. Similarly as in Section 2, we define the quasiperiodic capacitance coefficients C_{ij}^α, for $i,j=1,2$, as

$$C_{ij}^\alpha = -\int_{\partial D_i} \psi_j^\alpha \,\mathrm{d}\sigma, \qquad \psi_j^\alpha = (\mathcal{S}_D^{0,\alpha})^{-1}[\chi_{\partial D_j}], \tag{4.2}$$

and then the weighted quasiperiodic capacitance matrix $C^{v,\alpha} = (C_{ij}^v)$ as

$$C^{v,\alpha} = \begin{pmatrix} v_1^2\delta_2 C_{11}^\alpha & v_1^2\delta_1 C_{12}^\alpha \\ v_2^2\delta_2 C_{21}^\alpha & v_2^2\delta_2 C_{22}^\alpha \end{pmatrix}. \tag{4.3}$$

We also define $\mathbf{c}_i \in \mathbb{C}^3$ by

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

As we shall see, the capacitance matrix gives the leading order approximation of the scattering problem (4.1), and $\mathbf{c}_i$ can be thought of as higher-order capacitance coefficients. The following lemma follows from the $\mathcal{P}$-symmetry of the resonators.

Lemma 4.1. *We have*

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

and, moreover, $\mathbf{c}_1 = \overline{\mathbf{c}_2}$.

Proof. The statements on C_{11}^α and C_{12}^α are proved in the same way as in [5]. To prove that $\mathbf{c}_1 = \overline{\mathbf{c}_2}$, we observe that

$$\psi_1^\alpha(\mathcal{P}y) = \psi_2^{-\alpha}(y) = \overline{\psi_2^\alpha(y)}, \quad y\in\partial D,$$

and similarly, $\psi_2^\alpha(\mathcal{P}y) = \overline{\psi_1^\alpha(y)}$. Then

$$\begin{aligned}\mathbf{c}_1 &= \mathrm{i}\int_{\partial D} y\psi_1^\alpha(y)\,\mathrm{d}\sigma(y) = \mathrm{i}\int_{\partial D} \mathcal{P}(y)\psi_1^\alpha(\mathcal{P}y)\,\mathrm{d}\sigma(y) = -\mathrm{i}\int_{\partial D} y\overline{\psi_2^\alpha}(y)\,\mathrm{d}\sigma(y)\\ &= \overline{\mathbf{c}_2}.\end{aligned}$$

This concludes the proof. □

We define the functions $S_1^{\omega,\alpha}, S_2^{\omega,\alpha}$ as

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

Lemma 4.2. *Let $\lambda = \omega^2|D_1|$. For ω such that λ is not an eigenvalue of $C^{v,\alpha}$, the solution to the scattering problem* (4.1) *can be written as*

$$u - u^{in} = q_1 S_1^{\omega,\alpha} + q_2 S_2^{\omega,\alpha} - \mathcal{S}_D^{\omega,\alpha}[\xi^{\mathbf{k}}] + O(\omega^2),$$

where the constants q_1, q_2 are given by

$$\begin{pmatrix} q_1\\ q_2\end{pmatrix} = \frac{1}{(\lambda-\lambda_1)(\lambda-\lambda_2)}\left(\lambda\begin{pmatrix} v_1^2\delta_1 C_{12}^\alpha - v_2^2\delta_2 C_{11}^\alpha + \lambda\\ v_2^2\delta_2\overline{C_{12}^\alpha} - v_1^2\delta_1 C_{11}^\alpha + \lambda\end{pmatrix} + \begin{pmatrix} \mathbf{k}\cdot\Big(\big(C_{11}^\alpha\mathbf{c}_1 - C_{12}^\alpha\mathbf{c}_2\big)|v_1^2\delta|^2 - \lambda v_1^2\delta_1\mathbf{c}_1\Big)\\ \mathbf{k}\cdot\Big(\big(C_{11}^\alpha\mathbf{c}_2 - \overline{C_{12}^\alpha}\mathbf{c}_1\big)|v_1^2\delta|^2 - \lambda v_2^2\delta_2\mathbf{c}_2\Big)\end{pmatrix}\right),$$

and

$$\xi^{\mathbf{k}} = \left(\mathcal{S}_D^{0,\alpha}\right)^{-1}[\mathrm{i}\mathbf{k}\cdot x].$$

Proof. Following the proof of Lemma 2.1, using the jump conditions (A.7), (A.8) and the asymptotic expansions (A.9),(A.10), we can show that

$$u - u^{in} = \widetilde{q}_1 S_1^{\omega,\alpha} + \widetilde{q}_2 S_2^{\omega,\alpha} - \mathcal{S}_D^{\omega,\alpha}\left(\mathcal{S}_D^{0,\alpha}\right)^{-1}[u^{in}] + O(\omega^2), \tag{4.4}$$

for constants $\widetilde{q}_1$ and $\widetilde{q}_2$ which satisfy the problem

$$(C^{v,\alpha} - \lambda I)\begin{pmatrix}\widetilde{q}_1\\ \widetilde{q}_2\end{pmatrix} = -\begin{pmatrix} v_1^2\delta_1 \int_{\partial D_1}\left(\mathcal{S}_D^{0,\alpha}\right)^{-1}[u^{in}]\,\mathrm{d}\sigma \\ v_2^2\delta_2 \int_{\partial D_2}\left(\mathcal{S}_D^{0,\alpha}\right)^{-1}[u^{in}]\,\mathrm{d}\sigma\end{pmatrix}, \tag{4.5}$$

where $\lambda = \omega^2|D_1|$. Since u^{in} is a plane wave with frequency ω we have

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

It follows that

$$\left(\mathcal{S}_D^{0,\alpha}\right)^{-1}[u^{in}] = \psi_1^\alpha + \psi_2^\alpha + \xi^{\mathbf{k}} + O(\omega^2).$$

Using this, we can compute

$$-\begin{pmatrix} v_1^2\delta_1 \int_{\partial D_1}\left(\mathcal{S}_D^{0,\alpha}\right)^{-1}[u^{in}]\,\mathrm{d}\sigma \\ v_2^2\delta_2 \int_{\partial D_2}\left(\mathcal{S}_D^{0,\alpha}\right)^{-1}[u^{in}]\,\mathrm{d}\sigma\end{pmatrix} = \begin{pmatrix} v_1^2\delta_1\left(C_{11}^\alpha + C_{12}^\alpha - \int_{\partial D_1}\xi^{\mathbf{k}}\,\mathrm{d}\sigma\right) \\ v_2^2\delta_2\left(C_{11}^\alpha + \overline{C_{12}^\alpha} - \int_{\partial D_2}\xi^{\mathbf{k}}\,\mathrm{d}\sigma\right)\end{pmatrix} + O(\delta\omega^2). \tag{4.6}$$

Moreover,

$$\mathcal{S}_D^{\omega,\alpha}\left(\mathcal{S}_D^{0,\alpha}\right)^{-1}[u^{in}] = S_1^{\omega,\alpha} + S_2^{\omega,\alpha} + \mathcal{S}_D^{\omega,\alpha}[\xi^{\mathbf{k}}] + O(\omega^2). \tag{4.7}$$

Combining (4.4), (4.5), (4.6) and (4.7), we conclude that

$$u - u^{in} = q_1 S_1^{\omega,\alpha} + q_2 S_2^{\omega,\alpha} - \mathcal{S}_D^{\omega,\alpha}[\xi^{\mathbf{k}}] + O(\omega^2),$$

where the constants q_1, q_2 are given by

$$\begin{pmatrix} q_1\\ q_2\end{pmatrix} = (C^{v,\alpha} - \lambda I)^{-1}\begin{pmatrix} v_1^2\delta_1\left(C_{11}^\alpha + C_{12}^\alpha - \int_{\partial D_1}\xi^{\mathbf{k}}\,\mathrm{d}\sigma\right) \\ v_2^2\delta_2\left(C_{11}^\alpha + \overline{C_{12}^\alpha} - \int_{\partial D_2}\xi^{\mathbf{k}}\,\mathrm{d}\sigma\right)\end{pmatrix} - \begin{pmatrix}1\\1\end{pmatrix} + O(\omega^2). \tag{4.8}$$

Using duality, we have that

$$\int_{\partial D_i}\xi^{\mathbf{k}}(x)\,\mathrm{d}\sigma(x) = \int_{\partial D} i\mathbf{k}\cdot y\left(\mathcal{S}_D^{0,\alpha}\right)^{-1}[\chi_{\partial D_i}](y)\,\mathrm{d}\sigma(y) = \mathbf{k}\cdot\mathbf{c}_i.$$

Using this, and simplifying the matrix inverse in (4.8), we find that

$$\begin{pmatrix} q_1\\ q_2\end{pmatrix} = \frac{1}{(\lambda-\lambda_1)(\lambda-\lambda_2)}\left(\lambda\begin{pmatrix} v_1^2\delta_1 C_{12}^\alpha - v_2^2\delta_2 C_{11}^\alpha + \lambda \\ v_2^2\delta_2\overline{C_{12}^\alpha} - v_1^2\delta_1 C_{11}^\alpha + \lambda\end{pmatrix} + \begin{pmatrix}\mathbf{k}\cdot\left(\left(C_{11}^\alpha\mathbf{c}_1 - C_{12}^\alpha\mathbf{c}_2\right)|v_1^2\delta|^2 - \lambda v_1^2\delta_1\mathbf{c}_1\right) \\ \mathbf{k}\cdot\left(\left(C_{11}^\alpha\mathbf{c}_2 - \overline{C_{12}^\alpha}\mathbf{c}_1\right)|v_1^2\delta|^2 - \lambda v_2^2\delta_2\mathbf{c}_2\right)\end{pmatrix}\right),$$

when λ is not an eigenvalue of $C^{v,\alpha}$. This concludes the proof. □

Analogously to Theorem 2.2, we have the following theorem on the band structure of the metascreen.

Theorem 4.3. *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

$$\lambda_i^\alpha = aC_{11}^\alpha \pm \sqrt{a^2|C_{12}^\alpha|^2 - b^2\big((C_{11}^\alpha)^2 - |C_{12}^\alpha|^2\big)}, \tag{4.9}$$

meaning the exceptional point occurs when $b = b_0(\alpha)$

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

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. As $\alpha \to 0$ we have $b_0(\alpha) \to \infty$, so 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.

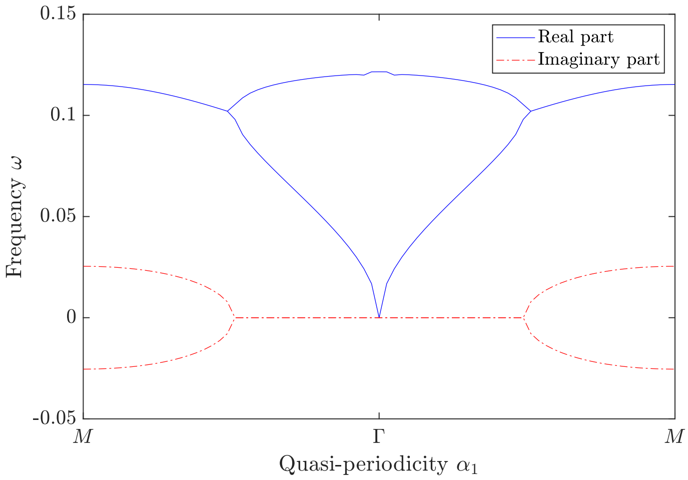

Figure 6: Plot of the real parts (blue) and imaginary parts (red) of the band structure of the metascreen. The exceptional point is a point (α, ω), at which point the frequencies coincide to leading order. Here, for simplicity, we simulate the analogous problem in two dimensions, using circular resonators with $L = 1$, separation distance $0.5L$, radius $0.3D$ and material parameters $a = 2 \times 10^{-4}, b = 1 \times 10^{-4}$ and $v = 1$.

4.2 Unidirectional reflectionless transmission

In this section we prove that there is a frequency such that the metascreen will have zero reflection when the incident wave from one side, and non-zero reflection when the incident wave is from the other side of the screen. The main results are stated in Theorem 4.6 and Remark 4.7.

We begin by studying the radiative behaviour of the basis functions $S_1^{\alpha,\omega}, S_2^{\alpha,\omega}$ of the scattered field. 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. It is worth emphasising that this is a general result, of independent interest.

Proposition 4.4. *Assume that $|\alpha| < k < \inf_{l\in\mathbb{Z}^2\setminus\{0\}} |2\pi l L - \alpha|$. Then, as $|x_3| \to \infty$, the quasiperiodic single layer potential satisfies*

$$\mathcal{S}_D^{\alpha,k}[\phi] \sim \begin{cases} \dfrac{e^{\mathrm{i}\mathbf{k}_+\cdot x}}{2\mathrm{i}k_3L^2}\displaystyle\int_{\partial D} e^{-\mathrm{i}\mathbf{k}_+\cdot y}\phi(y)\,\mathrm{d}\sigma(y), & x_3 \to \infty, \\ \dfrac{e^{\mathrm{i}\mathbf{k}_-\cdot x}}{2\mathrm{i}k_3L^2}\displaystyle\int_{\partial D} e^{-\mathrm{i}\mathbf{k}_-\cdot y}\phi(y)\,\mathrm{d}\sigma(y), & x_3 \to -\infty. \end{cases}$$

Here,

$$k_1 = \alpha_1, \quad k_2 = \alpha_2, \quad k_3 = \sqrt{k^2 - (k_1^2 + k_2^2)},$$

and

$$\mathbf{k}_+ = \begin{pmatrix} k_1 \\ k_2 \\ k_3 \end{pmatrix}, \quad \mathbf{k}_- = \begin{pmatrix} k_1 \\ k_2 \\ -k_3 \end{pmatrix}.$$

Proof. From [3] we have the following expansion of the quasiperiodic Green's function,

$$G^{\alpha,k}(x,y) = \frac{e^{\mathrm{i}\alpha\cdot(x_1,x_2)}e^{\mathrm{i}k_3|x_3|}}{2\mathrm{i}k_3L^2} - \sum_{l\in\mathbb{Z}^2\setminus\{0\}} \frac{e^{\mathrm{i}(\alpha+2\pi lL)\cdot(x_1,x_2)}e^{-\sqrt{|2\pi lL-\alpha|^2-k^2}|x_3|}}{2L^2\sqrt{|2\pi lL-\alpha|^2-k^2}}.$$

As $x_3 \to \infty$, every term inside the summation decays exponentially. Hence

$$\begin{aligned}\mathcal{S}_D^{\alpha,k}[\phi](x) &\sim \int_{\partial D} \frac{e^{\mathrm{i}\mathbf{k}_\pm\cdot(x-y)}}{2\mathrm{i}k_3L^2}\phi(y)\,\mathrm{d}\sigma(y) \\ &= \frac{e^{\mathrm{i}\mathbf{k}_\pm\cdot x}}{2\mathrm{i}k_3L^2}\int_{\partial D} e^{-\mathrm{i}\mathbf{k}_\pm\cdot y}\phi(y)\,\mathrm{d}\sigma(y),\end{aligned}$$

as $x_3 \to \pm\infty$. □

We define the coefficients

$$R_{i,\pm} = \frac{1}{2\mathrm{i}k_3L^2}\int_{\partial D} e^{-\mathrm{i}\mathbf{k}_\pm\cdot y}\psi_i^\alpha(y)\,\mathrm{d}\sigma(y), \quad i = 1,2.$$

By Proposition 4.4, the basis functions $S_1^{\omega,\alpha}, S_2^{\omega,\alpha}$ for the scattered field satisfies the radiation behaviour

$$S_i^{\alpha,\omega} \sim R_{i,\pm}e^{\mathrm{i}\mathbf{k}_\pm\cdot x}, \quad x_3 \to \pm\infty, \tag{4.10}$$

for $i = 1, 2$.

4.2.1 Scattering matrix and unidirectional reflectionless transmission

Recall that we consider the limit when $\delta \to 0$ and $\omega = O(\sqrt{\delta})$. 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

$$u \sim \begin{cases} c_1e^{\mathrm{i}\mathbf{k}_-\cdot x} + d_1e^{\mathrm{i}\mathbf{k}_+\cdot x}, & x_3 \to \infty, \\ c_2e^{\mathrm{i}\mathbf{k}_+\cdot x} + d_2e^{\mathrm{i}\mathbf{k}_-\cdot x}, & x_3 \to -\infty, \end{cases} \tag{4.11}$$

where

$$\begin{pmatrix} d_1 \\ d_2 \end{pmatrix} = S\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}, \qquad S = \begin{pmatrix} r_+ & t_- \\ t_+ & r_- \end{pmatrix}. \tag{4.12}$$

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 similarly for r_-, t_-). Next, we will compute the scattering matrix in the asymptotic limit as $\delta \to 0$ and $\omega = O(\delta^{1/2})$.

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 Lemma 4.2, we know that the scattered field is given by

$$u - u^{in} = q_1 S_1^{\omega,\alpha} + q_2 S_2^{\omega,\alpha} - \mathcal{S}_D^{\omega,\alpha}[\xi^{\mathbf{k}}] + O(\omega^2). \tag{4.13}$$

Letting

$$q^{(0)}(\lambda) = \frac{\lambda}{(\lambda-\lambda_1)(\lambda-\lambda_2)}\left(v_1^2\delta_1 C_{12}^\alpha - v_2^2\delta_2 C_{11}^\alpha + \lambda\right),$$

and

$$q^{(1)}(\lambda,\mathbf{k}) = \frac{v_1^2\delta_1}{(\lambda-\lambda_1)(\lambda-\lambda_2)}\mathbf{k}\cdot\Big(\big(C_{11}^\alpha\mathbf{c}_1 - C_{12}^\alpha\mathbf{c}_2\big)v_2^2\delta_2 - \lambda\mathbf{c}_1\Big),$$

we have, for real λ and for $b < b_0$,

$$\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = \begin{pmatrix} q^{(0)} \\ \overline{q^{(0)}} \end{pmatrix} + \begin{pmatrix} q^{(1)} \\ \overline{q^{(1)}} \end{pmatrix}.$$

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

$$\begin{aligned} R_{i,\pm} &= \frac{1}{2\mathrm{i}k_3L^2}\int_{\partial D}\psi_i^\alpha(y)\,\mathrm{d}\sigma(y) + \frac{1}{2\mathrm{i}k_3L^2}\int_{\partial D}\mathrm{i}\mathbf{k}_\pm\cdot y\psi_i^\alpha(y)\,\mathrm{d}\sigma(y) + O(\omega^2) \\ &= \frac{1}{2\mathrm{i}k_3L^2}\left(C_{1i}^\alpha + C_{2i}^\alpha + \mathbf{k}_\pm\cdot\mathbf{c}_i\right) + O(\omega). \end{aligned}$$

Moreover,

$$\frac{1}{2\mathrm{i}k_3L^2}\int_{\partial D} e^{-\mathrm{i}\mathbf{k}_\pm\cdot y}\xi^{\mathbf{k}}(y)\,\mathrm{d}\sigma(y) = \frac{1}{2\mathrm{i}k_3L^2}\int_{\partial D}\xi^{\mathbf{k}}\,\mathrm{d}\sigma + O(\omega) = \frac{1}{2\mathrm{i}k_3L^2}\mathbf{k}\cdot(\mathbf{c}_1+\mathbf{c}_2) + O(\omega).$$

Therefore, from Proposition 4.4, (4.10) and (4.13) the scattered field satisfies

$$\begin{aligned} u - u^{in} \sim \frac{1}{2\mathrm{i}k_3L^2}\Big(& q_1(C_{11}^\alpha + \overline{C_{12}^\alpha}) + q_2(C_{11}^\alpha + C_{12}^\alpha) \\ & + q_1\mathbf{k}_\pm\cdot\mathbf{c}_1 + q_2\mathbf{k}_\pm\cdot\mathbf{c}_2 - \mathbf{k}\cdot(\mathbf{c}_1+\mathbf{c}_2)\Big)e^{\mathrm{i}\mathbf{k}_\pm\cdot x} + O(\omega), \\ = \big(F(\lambda) + G(&\lambda,\mathbf{k},\mathbf{k}_\pm)\big)e^{\mathrm{i}\mathbf{k}_\pm\cdot x} + O(\omega), \end{aligned} \tag{4.14}$$

as $x_3 \to \pm\infty$. The term $F(\lambda)$, of order $O(\omega^{-1})$, is given by

$$\begin{aligned} F(\lambda) &= \frac{1}{2\mathrm{i}k_3L^2}\left(q^{(0)}(C_{11}^\alpha + \overline{C_{12}^\alpha}) + \overline{q^{(0)}}(C_{11}^\alpha + C_{12}^\alpha)\right) \\ &= \frac{1}{\mathrm{i}k_3L^2}\frac{\lambda\left(C_{11}^\alpha + \mathrm{Re}(C_{12}^\alpha)\right)}{(\lambda-\lambda_1)(\lambda-\lambda_2)}(\lambda-\lambda^*), \end{aligned} \tag{4.15}$$

where

$$\lambda^* = \frac{\mathrm{Re}(v_1^2\delta_1)\left((C_{11}^\alpha)^2 - |C_{12}^\alpha|^2\right)}{C_{11}^\alpha + \mathrm{Re}(C_{12}^\alpha)}.$$

The point $\lambda = \lambda^*$ is a critical point where the leading-order term vanishes. The higher-order term G is given by

$$G(\lambda,\mathbf{k},\mathbf{k}_\pm) = \frac{1}{\mathrm{i}k_3L^2}\left(\mathrm{Re}\left(q^{(1)}(\lambda,\mathbf{k})(C_{11}^\alpha + \overline{C_{12}^\alpha})\right) + \mathrm{Re}\left(q^{(0)}(\lambda)\mathbf{k}_\pm\cdot\mathbf{c}_1\right) - \mathrm{Re}(\mathbf{k}\cdot\mathbf{c}_1)\right).$$

From (4.11) and (4.14), it follows that the scattering matrix, defined in (4.12), can be written as

$$S = \begin{pmatrix} F(\lambda) & F(\lambda)+1 \\ F(\lambda)+1 & F(\lambda) \end{pmatrix} + \begin{pmatrix} G(\lambda,\mathbf{k}_-,\mathbf{k}_+) & G(\lambda,\mathbf{k}_+,\mathbf{k}_+) \\ G(\lambda,\mathbf{k}_-,\mathbf{k}_-) & G(\lambda,\mathbf{k}_+,\mathbf{k}_-) \end{pmatrix} + O(\omega). \tag{4.16}$$

It is worth emphasising that up to this point we have only assumed parity symmetry $\mathcal{P}$ of the geometry of the resonators. In order to simplify above expressions, we will additionally assume that the resonators have an in-plane parity symmetry $\mathcal{P}_2$, *i.e.*

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

We then have the following result on the capacitance coefficients.

Lemma 4.5. *Assume that $\mathcal{P}_2 D_i = D_i,\ i=1,2$. Then $C_{12}^\alpha \in \mathbb{R}$ and for $i = 1,2$,*

$$e_1 \cdot \mathbf{c}_i = e_1 \cdot \overline{\mathbf{c}_i}, \qquad e_2 \cdot \mathbf{c}_i = e_2 \cdot \overline{\mathbf{c}_i}, \qquad e_3 \cdot \mathbf{c}_i = -e_3 \cdot \overline{\mathbf{c}_i}.$$

Here, e_1, e_2, e_3 is the standard basis of $\mathbb{R}^3$.

Proof. By symmetry, we have that

$$\psi_i^\alpha(\mathcal{P}_2 y) = \psi_i^{-\alpha}(y) = \overline{\psi_i^\alpha(y)}, \quad y \in \partial D$$

for $i = 1,2$. Then

$$C_{12}^\alpha = -\int_{\partial D_1} \psi_2^\alpha \,\mathrm{d}\sigma = -\int_{\partial D_1} \overline{\psi_2^\alpha}\,\mathrm{d}\sigma = \overline{C_{12}^\alpha}.$$

The results for $\mathbf{c}_i$ follow similarly. □

Theorem 4.6. *Let $\lambda = \omega^2|D_1|$, assume that $\mathcal{P}_2 D_i = D_i,\ i=1,2$ and that $0 < b < b_0(\alpha)$. As $\delta \to 0$, there is a critical point $\lambda = \lambda^*$ where the reflection coefficients $r_\pm, t_\pm$ vanish at leading order in δ. Close to this point, for $\lambda - \lambda^* = O(\delta^{1/2})$, we have the following asymptotic expansions of the scattering coefficients,*

$$r_+(\lambda) = f(\lambda) - g + O\left(\delta^{1/2}\right), \qquad t_-(\lambda) = f(\lambda) + 1 + O\left(\delta^{1/2}\right),$$

and

$$t_+(\lambda) = f(\lambda) + 1 + O\left(\delta^{1/2}\right), \qquad r_-(\lambda) = f(\lambda) + g + O\left(\delta^{1/2}\right),$$

where

$$f(\lambda) = \frac{a}{\mathrm{i}b^2k_3L^2}\left(\lambda - \lambda^*\right), \qquad g = \frac{2a}{bL^2} e_3 \cdot \mathbf{c}_1.$$

Proof. We will Taylor expand the terms $F(\lambda)$ and $G(\lambda,\mathbf{k},\mathbf{k}_\pm)$ for λ close to λ^*. For F, we have

$$F(\lambda) = \frac{a}{\mathrm{i}b^2k_3L^2}\left(\lambda-\lambda^*\right) + O\left(\omega^{-1}\left(\lambda-\lambda^*\right)^2\right). \tag{4.17}$$

We now turn to G. Under the extra symmetry $\mathcal{P}_2 D_i = D_i,\ i=1,2$, we have from Lemma 4.5,

$$\lambda^* = \mathrm{Re}(v_1^2\delta_1)\left(C_{11}^\alpha - C_{12}^\alpha\right).$$

Using this fact, we can simplify

$$\mathrm{Re}\left(q^{(1)}(\lambda^*,\mathbf{k})(C_{11}^\alpha + \overline{C_{12}^\alpha})\right) = \mathrm{Re}(\mathbf{k}\cdot\mathbf{c}_1) + \frac{a}{b}\mathrm{Im}(\mathbf{k}\cdot\mathbf{c}_1)$$

and

$$\mathrm{Re}\left(q^{(0)}(\lambda^*)\mathbf{k}_\pm\cdot\mathbf{c}_1\right) = -\frac{a}{b}\mathrm{Im}(\mathbf{k}_\pm\cdot\mathbf{c}_1).$$

Hence, for λ close to λ^* we have by Taylor expansion

$$G(\lambda,\mathbf{k},\mathbf{k}_\pm) = \frac{a}{\mathrm{i}bk_3L^2}\big(\mathrm{Im}(\mathbf{k}\cdot\mathbf{c}_1) - \mathrm{Im}(\mathbf{k}_\pm\cdot\mathbf{c}_1)\big) + O(\lambda-\lambda^*). \tag{4.18}$$

Observe that $G(\lambda^*, \mathbf{k}_+, \mathbf{k}_+) = G(\lambda^*, \mathbf{k}_-, \mathbf{k}_-) = 0$ while

$$G(\lambda^*, \mathbf{k}_+, \mathbf{k}_-) = -G(\lambda^*, \mathbf{k}_-, \mathbf{k}_+) = \frac{2a}{bL^2} e_3 \cdot \mathbf{c}_1.$$

If $\lambda - \lambda^* = O(\delta^{1/2})$, we use the expression (4.16) together with (4.17) and (4.18) to conclude the proof. $\square$

Remark 4.7. *For fixed λ, the leading-order terms in the expansions of the reflection coefficients r_+ and r_- (in terms of δ) are given by $F(\lambda)$, and are zero at $\lambda = \lambda^*$. For λ close to λ^*, the higher-order terms will contribute to a shift of this zero. The shifted zeros λ_+^* and λ_-^* of r_+, r_- respectively, are given by*

$$\lambda_+^* = \lambda^* + 2\mathrm{i}k_3 b(e_3 \cdot \mathbf{c}_1) + O(\delta), \qquad \lambda_-^* = \lambda^* - 2\mathrm{i}k_3 b(e_3 \cdot \mathbf{c}_1) + O(\delta).$$

The factor $e_3 \cdot \mathbf{c}_1$ is purely imaginary, so depending on the sign of $\mathrm{i}(e_3 \cdot \mathbf{c}_1)$, one of these zeros will be shifted upwards and one will be shifted downwards.

Remark 4.8. *In the case $b = 0$, we clearly have $r_+ = r_-$ and $t_+ = t_-$. Moreover, in this case, the critical point λ^* coincides with one of the eigenvalues of the weighted capacitance matrix $C^{v,\alpha}$. Thus, according to (4.15), the reflection coefficients will be non-vanishing to leading order.*

4.2.2 Numerical illustration

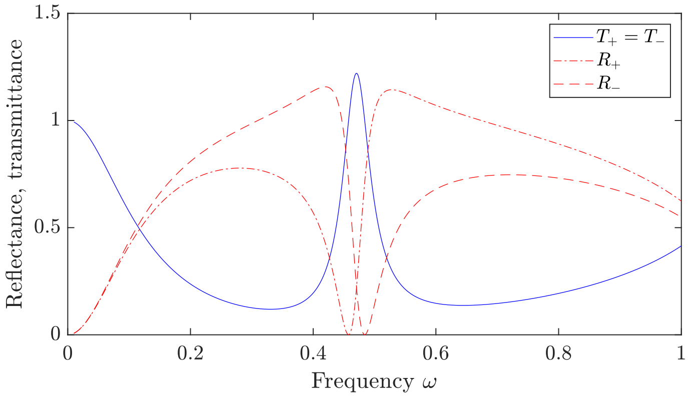

Figure 7: Plot of the transmittance $T_\pm = |t_\pm|^2$ (blue) and reflectance $R_\pm = |r_\pm|^2$ (red) as functions of the frequency. Here, for simplicity, we simulate the analogous problem in two dimensions, using circular resonators with $L = 1$, separation distance $0.5L$, radius $0.3D$ and material parameters $a = 1 \times 10^{-3}, b = 1 \times 10^{-3}$ and $v = 1$.

Figure 7 shows the transmittance $T_\pm = |t_\pm|^2$ and reflectance $R_\pm = |r_\pm|^2$ as functions of the frequency. As is well known (see, for example, [26]) for $\mathcal{PT}$-symmetric structures, the two transmission coefficients t_+ and t_- coincide. The figure clearly shows the shift of the zeros of the reflectance close to the critical point. 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 [11]

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

which, in particular, allows the scattering matrix to be non-unitary and allows the reflectance or transmittance to exceed 1.

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 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 the eigenmodes, coincide up to leading order (in terms of the density contrast). Moreover, we have proved that large ensembles of $\mathcal{PT}$-symmetric resonators can behave as non-Hermitian systems and hence support exceptional points on a macroscopic scale. Finally, we have studied a metascreen of $\mathcal{PT}$-symmetric resonators and proved that both reflection coefficients are zero close to a critical frequency. As the gain/loss parameter increases, these zeros will be shifted apart: the zero of the reflection coefficient from one side will be shifted upwards, and the zero of the reflection coefficient from the other side will be shifted downwards.

A Layer potential theory

Here, we briefly describe the theory of the layer potentials for the Helmholtz equation. A thorough presentation can, for example, be found in [7].

A.1 Bounded domains

As in Section 2 we assume that $D \in \mathbb{R}^3$ is a bounded domain, possibly with multiple connected components. Further, suppose that there exists some $0 < s < 1$ so that ∂D_i is of Hlder class $C^{1,s}$ for each $i = 1, \ldots, N$. The Laplace and outgoing Helmholtz Green's functions, G^0 respectively G^k, are given by

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

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

$$\lim_{|x|\to\infty} |x| \left(\frac{\partial}{\partial|x|} - \mathrm{i}k \right) G^k(x, y) = 0, \tag{A.1}$$

which can be interpreted as G^k corresponding to the case where energy radiates outwards (and not inwards).

The single layer potential is an operator $\mathcal{S}_D^k : L^2(\partial D) \to H^1_{\mathrm{loc}}(\mathbb{R}^3)$ defined by

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

$H^1_{\mathrm{loc}}(\mathbb{R}^3)$ denotes the space of functions that are square integrable, and with square integrable weak derivative, on every compact subset of $\mathbb{R}^3$.

For the single layer potential corresponding to the Laplace equation, 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*

$$\mathcal{S}_D^k[\phi]\big|_+ = \mathcal{S}_D^k[\phi]\big|_-, \tag{A.2}$$

and

$$\frac{\partial}{\partial\nu} \mathcal{S}_D^k[\phi]\Big|_\pm = \left(\pm\frac{1}{2} I + \mathcal{K}_D^{k,*} \right) [\phi], \tag{A.3}$$

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

$$\mathcal{S}_D^k = \mathcal{S}_D + O(k), \tag{A.4}$$

where the error term is with respect to the operator norm $\|.\|_{\mathcal{L}(L^2(\partial D),H^1(\partial D))}$. Moreover, we have

$$\mathcal{K}_D^{k,*} = \mathcal{K}_D^{0,*} + k^2\mathcal{K}_{D,2} + O(k^3), \tag{A.5}$$

where

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

A.2 Quasiperiodic layer potentials

We will use the notation for Y, Y^* and D as in Section 4. For $\alpha \in Y^*$, the quasiperiodic Green's function $G^{\alpha,k}(x,y)$ is defined as

$$G^{\alpha,k}(x,y) := -\sum_{(m_1,m_2)\in\mathbb{Z}^2}\frac{e^{\mathrm{i}k|x-y-(Lm,0,0)|}}{4\pi|x-y-L(m_1,m_2,0)|}e^{\mathrm{i}\alpha\cdot(m_1,m_2)L}, \tag{A.6}$$

and satisfies

$$\Delta_x G^{\alpha,k} + k^2 G^{\alpha,k} = \sum_{(m_1,m_2)\in\mathbb{Z}^2}\delta(x-y-L(m_1,m_2,0))e^{\mathrm{i}\alpha\cdot(m_1,m_2)L}.$$

Here $\delta(x)$ denotes the Dirac delta.

We define the quasiperiodic single layer potential $\mathcal{S}_D^{\alpha,k}$ by

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

It is known that $\mathcal{S}_D^{\alpha,0} : L^2(\partial D) \to H^1(\partial D)$ is invertible if $\alpha \neq 0$ [7]. It satisfies the jump relations

$$\mathcal{S}_D^{\alpha,k}[\phi]\big|_+ = \mathcal{S}_D^{\alpha,k}[\phi]\big|_-, \tag{A.7}$$

and

$$\frac{\partial}{\partial\nu}\mathcal{S}_D^{\alpha,k}[\phi]\Big|_\pm = \left(\pm\frac{1}{2}I + (\mathcal{K}_D^{-\alpha,k})^*\right)[\phi] \quad \text{on } \partial D, \tag{A.8}$$

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

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

In view of (A.6), we have expansions

$$\mathcal{S}_D^{\alpha,k} = \mathcal{S}_D^{\alpha,0} + O(k^2), \tag{A.9}$$

and

$$(\mathcal{K}_D^{-\alpha,k})^* = (\mathcal{K}_D^{-\alpha,0})^* + k^2\mathcal{K}_{D,2}^\alpha + O(k^4), \tag{A.10}$$

for some bounded operator $\mathcal{K}_{D,2}^\alpha : L^2(\partial D) \to L^2(\partial D)$ which can be explicitly computed.

B Homogenization theory

Here, we compute the effective material properties of cavities filled with large numbers of small resonators. This homogenisation is done in a formal way, see [8] for a rigorous justification of a closely related problem (*cf.* [6]).

B.1 Cavities of single resonators

Let D be some fixed resonator. We will define the small resonator B^r, for some small $r > 0$, as

$$B^r = rRD + z,$$

where $R : \mathbb{R}^3 \to \mathbb{R}^3$ is some rotation and $z \in \mathbb{R}^3$ is the new centre of mass of B^r. In order for resonance to occur at $O(1)$ frequencies we also scale the material parameters so that

$$v_b^2\delta_b := r^2 a + \mathrm{i} r^2 b,$$

for $a, b = O(1)$. The solutions to the scattering problem can be represented as

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

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

We wish to replicate Lemma 2.1 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

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

Repeating the arguments of Lemma 2.1, we find that the solution to the scattering problem can be written as

$$u - u^{in} = qS_{B^r}^{\omega} - S_{B^r}^{\omega}\left[\mathcal{S}_{B^r}^{-1}[u^{in}]\right] + O(r),$$

where

$$S_{B^r}^{\omega}(x) = \begin{cases} \mathcal{S}_{B^r}^{k}\left[\mathcal{S}_{B^r}^{-1}[\chi_{\partial B^r}]\right](x), & x \in \mathbb{R}^3 \setminus \overline{B^r}, \\ \mathcal{S}_{B^r}^{k_b}\left[\mathcal{S}_{B^r}^{-1}[\chi_{\partial B^r}]\right](x), & x \in B^r, \end{cases}$$

and $q = q(\omega)$ satisfies

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

Let

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

then we have that

$$\int_{\partial B^r}\mathcal{S}_{B^r}^{-1}[\chi_{\partial B^r}]\,\mathrm{d}\sigma = -r\mathrm{Cap}_D, \qquad \int_{\partial B^r}\mathcal{S}_{B^r}^{-1}[u^{in}]\,\mathrm{d}\sigma = -r\mathrm{Cap}_D u^{in}(0) + O(r^2),$$
$$S_{B^r}^{\omega} = -r\mathrm{Cap}_D G(x,k) + O(r^2), \tag{B.1}$$
$$\mathcal{S}_{B^r}^{k}\left[\mathcal{S}_{B^r}^{-1}[u^{in}]\right] = -r\mathrm{Cap}_D u^{in}(0)G(x,k) + O(r^2).$$

Thus, we find that

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

where

$$m(\omega) = \frac{\omega^2\mathrm{Cap}_D}{\omega^2 - \omega_M^2} \quad \text{and} \quad \omega_M = \frac{(a + \mathrm{i}b)\mathrm{Cap}_D}{|D|}.$$

We now wish to consider a domain Ω which contains a (large) number of small, identical resonators (*e.g.* Ω_+ or Ω_- in Figure 3). We choose the number of resonators N so that there exists some positive number Λ such that

$$rN = \Lambda.$$

The N resonators are given, for $1 \le j \le N$, by

$$B_j^N = rR_j^N D + z_j^N,$$

for rotations R_j^N and positions z_j^N. We assume that the resonators are not overlapping and that $\cup_{j=1}^N B_j^N \Subset \Omega$ for all N. Define the set Ω^N as

$$\Omega^N := \Omega \setminus \cup_{j=1}^N B_j^N.$$

Note that the volume of $\cup_{j=1}^N B_j^N$ is given by

$$\left| \bigcup_{j=1}^N B_j^N \right| = \sum_{j=1}^N |B_j^N| = Nr^3|D| = \Lambda r^2 |D| = O(r^2).$$

Since the resonators are small, we will use the point-scatter approximation (B.2) to describe how they interact with incoming waves. For $1 \le j \le N$, denote by $u_j^{in,N}$ the total incident field that impinges on the resonator B_j^N and by $u_j^{sc,N}$ the corresponding scattered field. We have that the total field, in the presence of N bubbles, is given, for $x \in \Omega^N$, by

$$u^N(x) = u^{in}(x) + \sum_{j=1}^N u_j^{sc,N}(x). \tag{B.3}$$

Using (B.2) we have that, for $x \in \Omega^N$,

$$u_j^{sc,N}(x) = \frac{1}{N}\Lambda m(\omega) u_j^{in,N}(z_j^N) G(x - z_j^N, k) + O(N^{-2}). \tag{B.4}$$

We must make some further assumptions to understand the convergence of (B.3), even under the approximation (B.4). We assume that the distribution $\{z_j^N : 1 \le j \le N\}$ is such that there exists some constant η such that for any N it holds that

$$\min_{i \ne j} |z_i^N - z_j^N| \ge \frac{\eta}{N^{1/3}}. \tag{B.5}$$

We, further, assume the distribution is sufficiently regular that there exists a real-valued function $V \in C^1(\overline{\Omega})$ such that for any $f \in C^{0,\alpha}(\Omega)$, $0 < \alpha \le 1$, there is a constant C such that

$$\max_{1 \le j \le N} \left| \frac{1}{N} \sum_{i \ne j} G(z_j^N - z_i^N, k) f(z_i^N) - \int_\Omega G(z_j^N - z, k) V(y) f(y) \,\mathrm{d}y \right| \le C \frac{1}{N^{\alpha/3}} \|f\|_{C^{0,\alpha}(\Omega)}. \tag{B.6}$$

Finally, we assume that there exists some macroscopic field $u \in C^{1,\alpha}(\Omega)$, for some $0 < \alpha \le 1$, such that

$$u^N \to u, \tag{B.7}$$

in the sense that for any $\varepsilon > 0$ there exists N_0 such that for all $N > N_0$

$$\|u^N - u\|_{C^{1,\alpha}(\Omega)} \le \varepsilon.$$

From (B.3) and (B.4), we have that

$$u^N(x) = u^{in}(x) + \sum_{j=1}^N \frac{1}{N} \Lambda m(\omega) u_j^{in,N}(z_j^N) G(x - z_j^N, k) + O(N^{-1}).$$

Letting $N \to \infty$, and using the assumptions (B.5), (B.6) and (B.7), we have that for $x \in \Omega$

$$u(x) = u^{in}(x) + \int_\Omega \Lambda m(\omega) V(y) u(y) G(x - y, k) \,\mathrm{d}y. \tag{B.8}$$

Applying the operator $\Delta + k^2$ to (B.8) gives, for $x \in \mathbb{R}^3$,

$$\Delta u(x) + M(x) u(x) = 0,$$

where

$$M(x) = \begin{cases} k^2, & x \in \mathbb{R}^3 \setminus \Omega, \\ k^2 - \Lambda m(k/v) V(x), & x \in \Omega. \end{cases}$$

B.2 Cavities of exceptional pairs of resonators

Recall the resonator pair $D = D_1 \cup D_2$ from Section 2. We will define the small dimer $B^r = B_1^r \cup B_2^r$, for some small $r > 0$, as

$$B^r = rRD + z,$$

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

$$v_1^2 \delta_1 := r^2 a + \mathrm{i} r^2 b,$$

for $a, b = O(1)$.

We must first replicate Lemma 2.1 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

$$\mathcal{S}_{B^r}[\phi - \psi] = u^{in} + O(r), \quad \text{on } \partial B_1^r \cup \partial B_2^r,$$
$$\left(-\frac{1}{2} I + \mathcal{K}_{B^r}^* + \frac{\omega^2}{v_j^2} \mathcal{K}_{B^r,2} \right)[\phi] - \delta_j \left(\frac{1}{2} I + \mathcal{K}_{B^r}^* \right)[\psi] = O(r^2), \quad \text{on } \partial B_j^r,\ j = 1, 2.$$

Repeating the arguments of Lemma 2.1, we find that the solution to the scattering problem can be written as

$$u - u^{in} = q_1 S_{B^r,1}^{\omega} + q_2 S_{B^r,2}^{\omega} - \mathcal{S}_{B^r}^{\omega}\left[\mathcal{S}_{B^r}^{-1}[u^{in}] \right] + O(r), \tag{B.9}$$

where

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

and the constants q_1 and q_2 satisfy

$$\left(C_{B^r}^{v} - \omega^2 |B_1^r| I \right) \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = - \begin{pmatrix} v_1^2 \delta_1 \int_{\partial B_1^r} \mathcal{S}_{B^r}^{-1}[u^{in}] \, \mathrm{d}\sigma \\ v_2^2 \delta_2 \int_{\partial B_2^r} \mathcal{S}_{B^r}^{-1}[u^{in}] \, \mathrm{d}\sigma \end{pmatrix} + O(r^4). \tag{B.10}$$

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

$$C_{B^r}^{v} = S J S^{-1}, \tag{B.11}$$

where

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

Using (B.11) and writing $\lambda^r = \omega^2 |B_1^r| = r^3 \omega^2 |D_1|$, the formula (B.10) gives us that

$$\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = -S \begin{pmatrix} (\lambda_1^r - \lambda^r)^{-1} & -(\lambda_1^r - \lambda^r)^{-2} \\ 0 & (\lambda_1^r - \lambda^r)^{-1} \end{pmatrix} S^{-1} \begin{pmatrix} v_1^2 \delta_1 \int_{\partial B_1^r} \mathcal{S}_{B^r}^{-1}[u^{in}] \, \mathrm{d}\sigma \\ v_2^2 \delta_2 \int_{\partial B_2^r} \mathcal{S}_{B^r}^{-1}[u^{in}] \, \mathrm{d}\sigma \end{pmatrix} + O(r),$$

i.e.

$$\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix} \begin{pmatrix} v_1^2 \delta_1 \int_{\partial B_1^r} \mathcal{S}_{B^r}^{-1}[u^{in}] \, \mathrm{d}\sigma \\ v_2^2 \delta_2 \int_{\partial B_2^r} \mathcal{S}_{B^r}^{-1}[u^{in}] \, \mathrm{d}\sigma \end{pmatrix} + O(r), \tag{B.12}$$

where

$$Q_{11} = \mathrm{i} r^3 b_0 C_{11} \frac{1}{(\lambda^r - \lambda_1^r)^2} + \frac{1}{\lambda^r - \lambda_1^r}, \qquad Q_{12} = r^3 C_{12} (a + \mathrm{i} b_0) \frac{1}{(\lambda^r - \lambda_1^r)^2},$$
$$Q_{21} = \frac{r^3 b_0^2 C_{11}^2}{(a + \mathrm{i} b_0) C_{12}} \frac{1}{(\lambda^r - \lambda_1^r)^2}, \qquad Q_{22} = -\mathrm{i} r^3 b_0 C_{11} \frac{1}{(\lambda^r - \lambda_1^r)^2} + \frac{1}{\lambda^r - \lambda_1^r}.$$

Remark B.1. *Note that since* λ^r, $\lambda_1^r = O(r^3)$ *we have that* $M_{ij} = O(r^{-3})$*, meaning that* $q_i = O(1)$.

The terms in (B.9) and (B.12) can be further simplified using scaling properties analogous to (B.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

$$\int_{\partial B_j^r} \mathcal{S}_{B^r}^{-1}[u^{in}]\,\mathrm{d}\sigma = -r\tfrac{1}{2}\mathrm{Cap}_D u^{in}(0) + O(r^2),$$
$$S_{B^r,j}^{\omega} = -r\tfrac{1}{2}\mathrm{Cap}_D G(x,k) + O(r^2),$$
$$\mathcal{S}_{B^r}^{k}\left[\mathcal{S}_{B^r}^{-1}[u^{in}]\right] = -r\mathrm{Cap}_D u^{in}(0)G(x,k) + O(r^2).$$

Thus, we find that

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

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

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

The point-scatter approximation can be used in the same way as in Appendix B.1, above. That is, define N small dimers

$$B_j^N = rR_j^N D + z_j^N,$$

in terms of the rotations R_j^N and positions z_j^N. Then, letting $N \to \infty$ under the assumptions (B.5), (B.6) and (B.7), we have the homogenized equation

$$\Delta u(x) + M(x)u(x) = 0, \qquad x \in \mathbb{R}^3,$$

where

$$M(x) = \begin{cases} k^2, & x \in \mathbb{R}^3 \setminus \Omega, \\ k^2 - \Lambda\tilde{m}(k/v)V(x), & x \in \Omega. \end{cases}$$

References

[1] H. Ammari, B. Davies, E. O. Hiltunen, and S. Yu. Topologically protected edge modes in one-dimensional chains of subwavelength resonators. *arXiv preprint arXiv:1906.10688*, 2019.

[2] H. Ammari, B. Davies, and S. Yu. Close-to-touching acoustic subwavelength resonators: eigenfrequency separation and gradient blow-up. *preprint arXiv:2001.04888*, 2020.

[3] H. Ammari, B. Fitzpatrick, D. Gontier, H. Lee, and H. Zhang. A mathematical and numerical framework for bubble meta-screens. *SIAM J. Appl. Math.*, 77(5):1827–1850, 2017.

[4] H. Ammari, B. Fitzpatrick, H. Kang, M. Ruiz, S. Yu, and H. Zhang. *Mathematical and computational methods in photonics and phononics*, volume 235 of *Mathematical Surveys and Monographs*. American Mathematical Society, Providence, 2018.

[5] H. Ammari, B. Fitzpatrick, H. Lee, E. O. Hiltunen, and S. Yu. Honeycomb-lattice Minnaert bubbles. *arXiv:1811.03905*, 2018.

[6] H. Ammari, B. Fitzpatrick, H. Lee, S. Yu, and H. Zhang. Double-negative acoustic metamaterials. *Q. Appl. Math.*, 77(4):767–791, 2019.

[7] H. Ammari and H. Zhang. A mathematical theory of super-resolution by using a system of sub-wavelength Helmholtz resonators. *Commun. Math. Phys.*, 337(1):379–428, 2015.

[8] H. Ammari and H. Zhang. Effective medium theory for acoustic waves in bubbly fluids near Minnaert resonant frequency. *SIAM J. Math. Anal.*, 49(4):3252–3276, 2017.

[9] W. Chen, Ş. K. Özdemir, G. Zhao, J. Wiersig, and L. Yang. Exceptional points enhance sensing in an optical microcavity. *Nature*, 548(7666):192–196, 2017.

[10] L. Feng, R. El-Ganainy, and L. Ge. Non-hermitian photonics based on parity–time symmetry. *Nat. Photonics*, 11(12):752–762, 2017.

[11] L. Ge, Y. D. Chong, and A. D. Stone. Conservation relations and anisotropic transmission resonances in one-dimensional $\mathcal{PT}$-symmetric photonic heterostructures. *Phys. Rev. A*, 85:023802, Feb 2012.

[12] W. Heiss. The physics of exceptional points. *J. Phys. A: Math. Theor.*, 45(44):444016, 2012.

[13] H. Hodaei, A. U. Hassan, S. Wittek, H. Garcia-Gracia, R. El-Ganainy, D. N. Christodoulides, and M. Khajavikhan. Enhanced sensitivity at higher-order exceptional points. *Nature*, 548(7666):187–191, 2017.

[14] N. Kaina, F. Lemoult, M. Fink, and G. Lerosey. Negative refractive index and acoustic superlens from multiple scattering in single negative metamaterials. *Nature*, 525(7567):77–81, 2015.

[15] Z. Lin, H. Ramezani, T. Eichelkraut, T. Kottos, H. Cao, and D. N. Christodoulides. Unidirectional invisibility induced by $\mathcal{PT}$-symmetric periodic structures. *Phys. Rev. Lett.*, 106:213901, May 2011.

[16] Z. Liu, X. Zhang, Y. Mao, Y. Zhu, Z. Yang, C. T. Chan, and P. Sheng. Locally resonant sonic materials. *science*, 289(5485):1734–1736, 2000.

[17] Z.-P. Liu, J. Zhang, Ş. K. Özdemir, B. Peng, H. Jing, X.-Y. Lü, C.-W. Li, L. Yang, F. Nori, and Y.-x. Liu. Metrology with $\mathcal{PT}$-symmetric cavities: enhanced sensitivity near the $\mathcal{PT}$-phase transition. *Phys. Rev. Lett.*, 117(11):110802, 2016.

[18] S. Longhi. Invisibility in $\mathcal{PT}$-symmetric complex crystals. *J. Phys. A: Math. Theor.*, 44(48):485302, nov 2011.

[19] M.-A. Miri and A. Alù. Exceptional points in optics and photonics. *Science*, 363(6422):eaar7709, 2019.

[20] D. V. Novitsky, A. S. Shalin, and A. Novitsky. Nonlocal homogenization of PT-symmetric multilayered structures. *Phys. Rev. A*, 99(4):043812, 2019.

[21] E. Ozbay. Plasmonics: merging photonics and electronics at nanoscale dimensions. *Science*, 311(5758):189–193, 2006.

[22] Ş. Özdemir, S. Rotter, F. Nori, and L. Yang. Parity–time symmetry and exceptional points in photonics. *Nat. Mater.*, 18(8):783–798, 2019.

[23] N. X. A. Rivolta and B. Maes. Side-coupled resonators with parity-time symmetry for broadband unidirectional invisibility. *Phys. Rev. A*, 94:053854, Nov 2016.

[24] J. Wiersig. Enhancing the sensitivity of frequency and energy splitting detection by using exceptional points: application to microcavity sensors for single-particle detection. *Phys. Rev. Lett.*, 112(20):203901, 2014.

[25] J. Wiersig. Sensors operating at exceptional points: general theory. *Phys. Rev. A*, 93(3):033809, 2016.

[26] L. Yuan and Y. Y. Lu. Unidirectional reflectionless transmission for two-dimensional $\mathcal{PT}$-symmetric periodic structures. *Phys. Rev. A*, 100:053805, Nov 2019.