Robust edge modes in dislocated systems of subwavelength resonators

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Robust edge modes in dislocated systems of subwavelength resonators

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Abstract

Robustly manipulating waves on subwavelength scales can be achieved by, firstly, designing a structure with a subwavelength band gap and, secondly, introducing a defect so that eigenfrequencies fall within the band gap. Such frequencies are well known to correspond to localized modes. We study a one-dimensional array of subwavelength resonators, proving that there is a subwavelength band gap, and showing that by introducing a dislocation we can place localized modes at any point within the band gap. We complement this analysis by studying the stability properties of the corresponding finite array of resonators, demonstrating the value of being able to customize the position of eigenvalues within the band gap.

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

Keywords: subwavelength resonance, subwavelength phononic and photonic crystals, topological metamaterials, protected edge states, dislocation.

1 Introduction

Recent breakthroughs in the field of wave manipulation have led to the creation of structures that can guide, localize, and trap waves at *subwavelength* scales (*i.e.* at spatial scales that are significantly smaller than the operating wavelength) [2, 4, 6, 11, 37, 44–47, 49, 54, 55]. The building blocks of these structures are subwavelength resonators: objects exhibiting resonant phenomena in response to wavelengths much greater than their size. Examples include plasmonic particles, Minnaert bubbles, and high-index dielectric particles. The highly contrasting material parameters (relative to the background medium) of these objects are the crucial mechanism responsible for their subwavelength response (see *e.g.* [5]). The goal for researchers, now, is to develop *robust* versions of these designs, that retain their wave-manipulation properties even in the presence of structural imperfections [3, 38, 39, 58, 59].

An approach to creating materials with low-frequency localized modes is to start with an array of subwavelength resonators that exhibits a *subwavelength band gap*, that is, a range of frequencies within the subwavelength regime that cannot propagate through the material. We then introduce a *defect* to the structure. If done correctly, this perturbation creates subwavelength resonant frequencies that are inside the band gap and correspond to resonant modes whose amplitude decays exponentially away from the defect [6, 11, 16, 45, 51]. We will refer to these resonant frequencies as *mid-gap frequencies* and the associated modes as *localized modes*.

It is widely understood that both the rate at which the localized mode decays and the stability of the mid-gap frequency depend on the location of the frequency within the band gap [18, 43]. Typically, the localization is stronger if the frequency is closer to the middle of the band gap. Moreover, eigenvalues in the middle of the band gap are more robust to imperfections of the material, particularly since a small perturbation is likely to keep the eigenvalue inside the band gap. With this in mind, our aim is to introduce defects in such a way that we are able to place a mid-gap frequency at any given point in the subwavelength band gap, enabling controllable and robust wave guiding at subwavelength scales.

In this work, we will begin with a one-dimensional array of pairs of subwavelength resonators which, we prove, exhibits a band gap within the subwavelength regime. We will then introduce a defect by adding a dislocation within one of the resonator pairs (see Figure 1). We will see that, as a result of this

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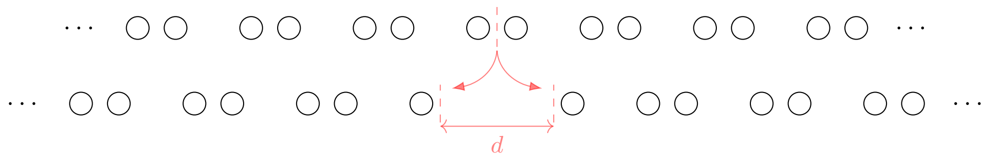


Figure 1: We start with an array of pairs of subwavelength resonators, known to have a subwavelength band gap. A dislocation (with size $d > 0$) is introduced to create mid-gap frequencies.

dislocation, mid-gap frequencies enter the band gap from either side and converge to a single frequency, within the band gap, as the dislocation becomes arbitrarily large (see Figure 2).

The localized modes studied in this work are, in particular, *edge modes*. Localized modes are known as edge modes when the defect responsible for their existence is the interface between two materials with different *bulk indexes*. Edge modes will propagate along the interface without entering the bulk of the material. The bulk index of a material is a topological quantity associated with a periodic structure and it is well known that the interface of two such materials supports robust edge modes [3, 14, 30–32, 48, 50, 53, 57, 60]. A typical example of an edge mode is that occurring at the edge of a material with nonzero bulk index (which is the interface with the absence of material, which has a bulk index of zero). It is in this sense that the two localized modes studied here are edge modes, since it was proved in [3] that the corresponding array of resonator pairs has nonzero bulk index.

There are a plethora of different ways to introduce an interface capable of supporting edge modes. An example from the setting of the Schrödinger operator, which is the quantum mechanical analogue of the structure analysed here, is to introduce dislocations to periodic potentials. This has been widely studied in both one [19, 22, 40, 41] and two dimensions [33–36]. There are some important differences between the dislocation of an array of resonators (as studied here) and the dislocation of a periodic potential. Most notably, when a periodic potential is dislocated the original configuration will be recovered periodically. Then, a quantity of interest is the *edge index*, which can be defined as the net number of eigenvalues which cross a band gap over a period of dislocation (see for example [15, 19]) If the edge index is nonzero, it means that a mid-gap frequency can be placed at any given position within the band gap (which, we said, is our goal). Moreover, according to the *bulk-edge correspondence* [19–21, 26–28], the edge index coincides with the bulk index of the structure without dislocation.

In our setting we will not periodically recover the original structure as we increase the dislocation and will, instead, produce two coupled half-space arrays. As the dislocation is increased, the coupling between the two halves will diminish and both mid-gap frequencies will converge to a single frequency. This single frequency corresponds to the edge mode of a half-space array, the existence of which is predicted by the bulk-edge correspondence. There are two main results of our analysis of the dislocated infinite structure. Firstly, we will show that when a dislocation is introduced, a mid-gap frequency enters the band gap from each edge (Theorem 3.17). Following this, we prove that there are two mid-gap frequencies which converge to a single frequency within the band gap as the dislocation becomes large (Theorem 3.35). These two frequencies correspond to the hybridized modes of two semi-infinite arrays.

Physical realizations of the infinite structures studied here are arrays of finitely many resonators, corresponding to truncated versions of the infinite structures. To complement the aforementioned analysis, we also study a finite array of resonator pairs to which a dislocation is introduced (Section 4). We show that, similar to the infinite structure, the finite array decouples into two half-systems as the dislocation increases which hybridize for intermediate dislocations. We also conduct a stability analysis to demonstrate that the edge-mode frequencies are the most stable (with respect to physical imperfections) and achieve optimal stability when the frequency is in the middle of the band gap.

2 Preliminaries

In this section, we briefly review the layer potential operators and Floquet-Bloch theory that will be used in the subsequent analysis. More details on this material can, for example, be found in [7].

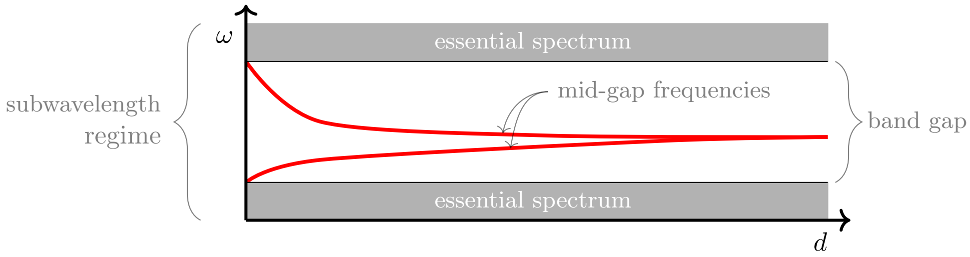


Figure 2: As the dislocation size d increases from zero, a mid-gap frequency appears from each edge of the subwavelength band gap. These two frequencies converge to a single value within the subwavelength band gap as $d \to \infty$.

2.1 Layer potential techniques

Let $\Omega \in \mathbb{R}^3$ be a bounded domain such that $\partial\Omega$ is of class $\mathcal{C}^{1,s}$ for some $0 < s < 1$. Let G^0 and G^k be the Laplace and outgoing Helmholtz Green's functions, respectively, defined by

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

We define the single layer potential $\mathcal{S}_\Omega^k : L^2(\partial\Omega) \to H^1_{\text{loc}}(\mathbb{R}^3)$ by

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

Here, the space $H^1_{\text{loc}}(\mathbb{R}^3)$ consists of functions that are square integrable on every compact subset of $\mathbb{R}^3$ and have a weak first derivative that is also square integrable. It is well known that the trace $\mathcal{S}_\Omega^0 : L^2(\partial\Omega) \to H^1(\partial\Omega)$ is an invertible operator. Here $H^1(\partial\Omega)$ denotes the set of functions that are square integrable on $\partial\Omega$ and have a weak first derivative that is also square integrable.

We also define the Neumann-Poincaré operator $\mathcal{K}_\Omega^{k,*} : L^2(\partial\Omega) \to L^2(\partial\Omega)$ by

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

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

The following so-called *jump relations* describe the behaviour of the trace of $\mathcal{S}_\Omega^k$ on the boundary $\partial\Omega$ (see, for example, [7]):

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

and

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

where $|_+$ and $|_-$ are used to denote the limits from outside and inside Ω, respectively, and I is the identity.

2.2 Floquet-Bloch theory and quasiperiodic layer potentials

A function $f(x) \in L^2(\mathbb{R})$ is said to be α-quasiperiodic, with quasiperiodicity $\alpha \in \mathbb{R}$, if $e^{-i\alpha x}f(x)$ is periodic. If the period is $L \in \mathbb{R}^+$, the quasiperiodicity α is an element of the torus $Y^* := \mathbb{R}/\frac{2\pi}{L}\mathbb{Z} \simeq (-\pi/L, \pi/L]$, known as the *Brillouin zone*. Given a function $f \in L^2(\mathbb{R})$, the Floquet transform of f is defined as

$$\mathcal{F}[f](x,\alpha) := \sum_{m\in\mathbb{Z}} f(x - Lm)e^{iL\alpha m}.$$

$\mathcal{F}[f]$ is always α-quasiperiodic in x and periodic in α. Let $Y_0 = [-L/2, L/2)$ be the unit cell for the α-quasiperiodicity in x. The Floquet transform is an invertible map $\mathcal{F} : L^2(\mathbb{R}) \to L^2(Y_0 \times Y^*)$, with inverse (see, for instance, [7, 42])

$$\mathcal{F}^{-1}[g](x) = \frac{1}{2\pi}\int_{Y^*} g(x,\alpha) \,\mathrm{d}\alpha, \quad x \in \mathbb{R},$$

where $g(x,\alpha)$ is the quasiperiodic extension of g for x outside of the unit cell Y_0.

We will consider a three-dimensional problem which is periodic in one dimension. Define the unit cell Y as $Y := Y_0 \times \mathbb{R}^2$. The quasiperiodic Green's function $G^{\alpha,k}(x,y)$, for $x, y \in \mathbb{R}^3$, is defined as the Floquet transform of $G^k(x,y)$ in the x_1 direction with fixed y, *i.e.*,

$$G^{\alpha,k}(x,y) := -\sum_{m\in\mathbb{Z}} \frac{e^{ik|x-y-(Lm,0,0)|}}{4\pi|x-y-(Lm,0,0)|} e^{i\alpha Lm}.$$

Let Ω be as above but with the additional assumption that $\Omega \Subset Y$. The quasiperiodic single layer potential $\mathcal{S}_\Omega^{\alpha,k}$ is defined analogously to $\mathcal{S}_\Omega^\omega$, by

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

It is known that $\mathcal{S}_\Omega^{\alpha,0} : L^2(\partial\Omega) \to H^1(\partial\Omega)$ is invertible if $\alpha \neq 0$ [7]. There are also jump relations for the quasiperiodic single layer potential, given by

$$\mathcal{S}_\Omega^{\alpha,k}[\phi]\big|_+ = \mathcal{S}_\Omega^{\alpha,k}[\phi]\big|_-, \tag{2.1}$$

and

$$\frac{\partial}{\partial\nu}\mathcal{S}_\Omega^{\alpha,k}[\phi]\Big|_\pm = \left(\pm\frac{1}{2}I + (\mathcal{K}_\Omega^{-\alpha,k})^*\right)[\phi] \quad \text{on } \partial\Omega, \tag{2.2}$$

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

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

The quasiperiodic single layer potential satisfies the following low-frequency expansion [7]:

$$\mathcal{S}_\Omega^{\alpha,k} = \mathcal{S}_\Omega^{\alpha,0} + O(k^2). \tag{2.3}$$

3 Infinite dislocated system

We will now study the problem of the dislocation of an infinite array of resonators. We will show that, in the case corresponding to nonzero bulk index, there are two mid-gap frequencies. These cover an interval in the middle of the band gap as the dislocation is varied. In Section 3.1 we study the periodic system, *i.e.* the system without dislocation, and prove that it has a subwavelength band gap. In Section 3.2 we study the dislocated system in the asymptotic case when the dislocation d is arbitrarily small. We show that as the dislocation increases from zero, two mid-gap frequencies appear, one from each edge of the band gap. In Section 3.3 we study the case when the dislocation size is an integer number of unit cell lengths, using the fact that this special case is equivalent to removing a finite number of resonators from the periodic structure. Here, we prove the existence of two mid-gap frequencies in the simplest case $d = L$, which corresponds to removing two resonators. We also show that as $d \to \infty$, the two mid-gap frequencies must converge to a single value. Finally, in Section 3.4, we study the dislocated system for a general dislocation that is larger than the width of one resonator. These values of d include those in Section 3.3, but the corresponding integral operator is much harder to analyse. The main goal of this section is to prove that for these dislocations all mid-gap frequencies will be bounded away from the edges of the band gap, meaning that the mid-gap frequencies found in Section 3.3 will remain within the band gap. Moreover, these frequencies, as functions of d, will fill an interval in the middle of the band gap.

We first describe the geometry of the periodic structure, *i.e.* the case without dislocation, depicted in Figure 3. Let $Y = [-L, L] \times \mathbb{R}^2$ be the unit cell, $Y_1 = [-L, 0] \times \mathbb{R}^2$, and $Y_2 = [0, L] \times \mathbb{R}^2$. For $j = 1, 2$, we assume that Y_j contains a resonator D_j such that $\partial D_j \in \mathcal{C}^{1,s}$ for some $0 < s < 1$. We denote a pair of resonators, a so-called dimer, by $D = D_1 \cup D_2$. We assume that the resonators in each dimer are separated by distance l, and that each individual resonator has reflection symmetry. More precisely, we assume that

$$R_1 D_1 = D_1, \qquad R_0 D = D, \tag{3.1}$$

where R_1 is the reflection in the plane $\{-l/2\} \times \mathbb{R}^2$ and R_0 is the reflection in the plane $\{0\} \times \mathbb{R}^2$. Observe that $R_2 := R_0 R_1 R_0$ describes reflection in the plane $\{l/2\} \times \mathbb{R}^2$, and therefore the assumptions (3.1) also imply that

$$R_2 D_2 = D_2.$$

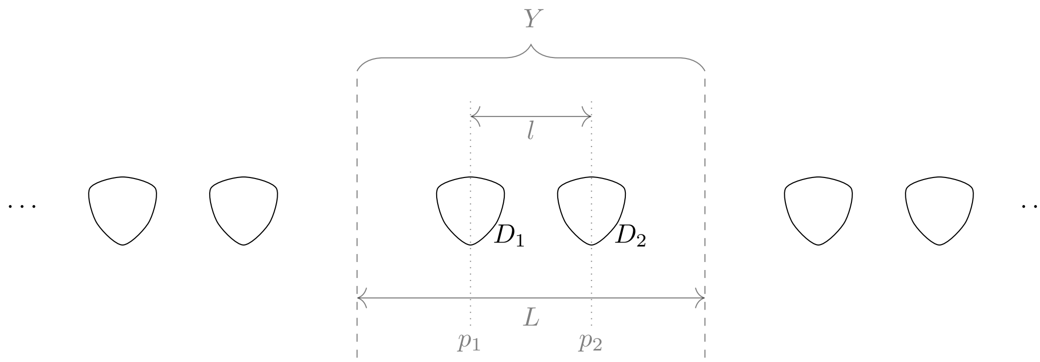


Figure 3: Example of the array in the case d = 0. The resonators are drawn to illustrate the symmetry assumptions.

Starting from the periodic system, we assume that half of this structure is dislocated along the x_1-axis. Let $\mathbf{v} = (1, 0, 0)$ and let d denote the dislocation size. We then define the periodic and dislocated systems, respectively, as

$$\mathcal{C}_0 = \bigcup_{\substack{m\in\mathbb{Z}\\ j=1,2}} D_j^m, \qquad \mathcal{C}_d = \Bigg(\bigcup_{\substack{m\in\mathbb{Z}^-\\ j=1,2}} D_j^m\Bigg) \cup \Bigg(\bigcup_{\substack{m\in\mathbb{N}\\ j=1,2}} D_j^m + d\mathbf{v}\Bigg).$$

Here, we use the notation

$$D_j^m = D_j + mL\mathbf{v}, \quad j = 1, 2, \ m \in \mathbb{Z},$$

for the resonators in the m^{th} unit cell. We introduce the notation $l_0 = l/L$, *i.e.* l_0 is the ratio of the separation of the resonators to the unit cell length. There are two fundamentally different cases: $l_0 < 1/2$ and $l_0 > 1/2$. In the first case, the dislocation occurs between dimers of resonators, keeping each pair of resonators intact. The second case corresponds to the dislocation occurring within a dimer, splitting one pair of resonators into two "edge" resonators. The case $l_0 > 1/2$ was illustrated in Figure 1, and we will show that this is the only case with mid-gap frequencies.

Wave propagation inside the infinite dislocated system is modelled by the Helmholtz problem

$$\begin{cases} \Delta u + \omega^2 u = 0 & \text{in } \mathbb{R}^3 \setminus \partial\mathcal{C}_d, \\ u|_+ - u|_- = 0 & \text{on } \partial\mathcal{C}_d, \\ \delta \dfrac{\partial u}{\partial \nu}\Big|_+ - \dfrac{\partial u}{\partial \nu}\Big|_- = 0 & \text{on } \partial\mathcal{C}_d, \\ u(x_1, x_2, x_3) & \text{satisfies the outgoing radiation condition as } \sqrt{x_2^2 + x_3^2} \to \infty. \end{cases} \tag{3.2}$$

Here, $\partial/\partial\nu$ denotes the outward normal derivative and $|_\pm$ indicates the limits from outside and inside D, respectively. Moreover, ω is the frequency of the incident waves which is assumed to be small, such that we are in a subwavelength regime. We refer to [1, 29] for the definition of the outgoing radiation condition for the scattering from compactly perturbed periodic structures. The material parameter δ represents the material contrast between the resonators and the background.

In order for subwavelength resonant modes to exist, we assume that δ satisfies the high-contrast condition

$$\delta \ll 1.$$

We say that a resonant frequency ω is *subwavelength* if ω scales as $O(\sqrt{\delta})$ as $\delta \to 0$.

We denote the spectrum corresponding to the problem (3.2) by $\Lambda(d)$. By a *mid-gap frequency*, we mean a value $\omega > 0$ that is in the subwavelength regime and is such that $\omega \in \Lambda(d)$ but $\omega \notin \Lambda(0)$. Here, the condition $\omega \notin \Lambda(0)$ means that ω is within the band gap of the periodic system. It is worth emphasizing that, due to radiation in x_2- and x_3-directions, the resonant frequencies are complex with negative imaginary parts. Nevertheless, as we will see in Theorem 3.2, the resonant frequencies are real at leading order so we consider only their real parts in this work.

3.1 Periodic system

This section concerns the infinite system in the case of no dislocation. We first state some preliminary results from [3] concerning the capacitance matrix. In Section 3.1.2 we prove the existence of a band gap between the first and the second band, which is a strengthening of a result from [3]. Moreover, we derive the asymptotic behaviour of the integral operator corresponding to the periodic problem as the frequency ω approaches the first or the second band.

Taking the Floquet transform of the solution u to (3.2), the α-quasiperiodic component u^α satisfies the Helmholtz problem

$$\begin{cases} \Delta u^\alpha + \omega^2 u = 0 & \text{in } Y \setminus \partial D, \\ u^\alpha|_+ - u^\alpha|_- = 0 & \text{on } \partial D, \\ \delta \dfrac{\partial u^\alpha}{\partial \nu}\Big|_+ - \dfrac{\partial u^\alpha}{\partial \nu}\Big|_- = 0 & \text{on } \partial D, \\ e^{-i\alpha_1 x_1} u^\alpha(x_1,x_2,x_3) & \text{is periodic in } x_1, \\ u^\alpha(x_1,x_2,x_3) & \text{satisfies the } \alpha\text{-quasiperiodic outgoing radiation condition} \\ & \quad \text{as } \sqrt{x_2^2+x_3^2} \to \infty. \end{cases} \tag{3.3}$$

We refer to [7] for the definition of the α-quasiperiodic outgoing radiation condition. Next, we formulate the quasiperiodic resonance problem (3.3) as an integral equation. The solution u^α of (3.3) can be represented as

$$u^\alpha(x) = \begin{cases} \mathcal{S}_{D_1}^\omega[\phi_1^{\alpha,i}](x), & x \in D_1, \\ \mathcal{S}_{D_2}^\omega[\phi_2^{\alpha,i}](x), & x \in D_2, \\ \mathcal{S}_D^{\alpha,\omega}[\phi^{\alpha,o}](x), & x \in Y \setminus D, \end{cases}$$

for some densities $\phi_1^{\alpha,i} \in L^2(\partial D_1)$, $\phi_2^{\alpha,i} \in L^2(\partial D_2)$ and $\phi^{\alpha,o} \in L^2(\partial D)$ (here, the superscripts i and o indicate *inside* and *outside*, respectively). Throughout, we will identify $L^2(\partial D) = L^2(\partial D_1) \times L^2(\partial D_2)$. With this identification, we write $\phi^{\alpha,i} = (\phi_1^{\alpha,i}, \phi_2^{\alpha,i})$.

Using the jump relations (2.1) and (2.2), it can be shown that (3.3) is equivalent to the boundary integral equation

$$\mathcal{A}^\alpha(\omega,\delta)[\Phi^\alpha] = 0,$$

where

$$\mathcal{A}^\alpha(\omega,\delta) = \begin{pmatrix} \hat{\mathcal{S}}_D^\omega & -\mathcal{S}_D^{\alpha,\omega} \\ -\frac{1}{2}I + \hat{\mathcal{K}}_D^{\omega,*} & -\delta\left(\frac{1}{2}I + (\mathcal{K}_D^{-\alpha,\omega})^*\right) \end{pmatrix}, \qquad \Phi^\alpha = \begin{pmatrix} \phi^{\alpha,i} \\ \phi^{\alpha,o} \end{pmatrix}, \tag{3.4}$$

and

$$\hat{\mathcal{S}}_D^\omega = \begin{pmatrix} \mathcal{S}_{D_1}^\omega & 0 \\ 0 & \mathcal{S}_{D_2}^\omega \end{pmatrix}, \qquad \hat{\mathcal{K}}_D^{\omega,*} = \begin{pmatrix} \mathcal{K}_{D_1}^{\omega,*} & 0 \\ 0 & \mathcal{K}_{D_2}^{\omega,*} \end{pmatrix}. \tag{3.5}$$

Remark 3.1. Here, we use the standard single-layer potential to represent the solution inside the resonators. This leads to a block 2×2 integral equation, which might seem more complicated than the scalar integral equation studied in [3]. However, this representation will, in fact, simplify the analysis of the fictitious sources used later in this paper. Another advantage of this representation is that it easily generalizes to the case of different wave speeds inside and outside the resonators.

3.1.1 Quasiperiodic capacitance matrix

In this section, we state some results from [3] on the quasiperiodic capacitance matrix. Let V_j^α be the solution to

$$\begin{cases} \Delta V_j^\alpha = 0 & \text{in } \quad Y \setminus D, \\ V_j^\alpha = \delta_{ij} & \text{on } \quad \partial D_i, \\ e^{-i\alpha_1 x_1} V_j^\alpha(x_1,x_2,x_3) & \text{is periodic in } x_1, \\ V_j^\alpha(x_1,x_2,x_3) = O\left(\frac{1}{\sqrt{x_2^2+x_3^2}}\right) & \text{as } \sqrt{x_2^2+x_2^2} \to \infty, \text{ uniformly in } x_1, \end{cases}$$

where δ_{ij} is the Kronecker delta. We then define the quasiperiodic capacitance matrix $C^\alpha = (C_{ij}^\alpha)$ by

$$C_{ij}^\alpha := \int_{Y \setminus D} \overline{\nabla V_i^\alpha} \cdot \nabla V_j^\alpha \, \mathrm{d}x, \quad i,j = 1,2.$$

The main motivation for studying the capacitance matrix is given in the following theorem, proved in [8, 10, 12].

Theorem 3.2. *The characteristic values $\omega_j^\alpha = \omega_j^\alpha(\delta)$, $j = 1, 2$, of the operator $\mathcal{A}^\alpha(\omega, \delta)$, defined in* (3.4)*, can be approximated as*

$$\omega_j^\alpha = \sqrt{\frac{\delta \lambda_j^\alpha}{|D_1|}} + O(\delta),$$

where λ_j^α, $j = 1, 2$, are eigenvalues of the quasiperiodic capacitance matrix C^α.

In other words, this theorem says that the continuous spectral problem (3.3) can be approximated, to leading order in δ, by the discrete eigenvalue problem for C^α.

Lemma 3.3. *The matrix C^α is Hermitian with constant diagonal, i.e.,*

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

Using the jump conditions, in the case $\alpha \neq 0$, it can be shown that the capacitance coefficients C_{ij}^α are also given by

$$C_{ij}^\alpha = -\int_{\partial D_i} \psi_j^\alpha \, \mathrm{d}\sigma, \quad i, j = 1, 2,$$

where ψ_j^α are defined by

$$\psi_j^\alpha = (\mathcal{S}_D^{\alpha,0})^{-1}[\chi_{\partial D_j}].$$

Since C^α is Hermitian, the following lemma follows directly.

Lemma 3.4. *The eigenvalues and corresponding eigenvectors of the quasiperiodic capacitance matrix are given by*

$$\lambda_1^\alpha = C_{11}^\alpha - |C_{12}^\alpha|, \qquad \begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} -e^{i\theta_\alpha} \\ 1 \end{pmatrix},$$
$$\lambda_2^\alpha = C_{11}^\alpha + |C_{12}^\alpha|, \qquad \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\theta_\alpha} \\ 1 \end{pmatrix},$$

where, for α such that $C_{12}^\alpha \neq 0$, $\theta_\alpha \in [0, 2\pi)$ is defined to be such that

$$e^{i\theta_\alpha} = \frac{C_{12}^\alpha}{|C_{12}^\alpha|}.$$

Using these eigenvectors, we define bases $\{u_1^\alpha, u_2^\alpha\}$, $\{\chi_1^\alpha, \chi_2^\alpha\}$ of $\ker\left(-\frac{1}{2}I + \left(\mathcal{K}_D^{0,-\alpha}\right)^*\right)$ and $\ker\left(-\frac{1}{2}I + \mathcal{K}_D^{0,\alpha}\right)$, respectively, as

$$u_1^\alpha = \frac{1}{\sqrt{2}}\left(-e^{i\theta_\alpha}\psi_1^\alpha + \psi_2^\alpha\right), \qquad u_2^\alpha = \frac{1}{\sqrt{2}}\left(e^{i\theta_\alpha}\psi_1^\alpha + \psi_2^\alpha\right),$$
$$\chi_1^\alpha = \frac{1}{\sqrt{2}}\left(-e^{i\theta_\alpha}\chi_{\partial D_1} + \chi_{\partial D_2}\right), \qquad \chi_2^\alpha = \frac{1}{\sqrt{2}}\left(e^{i\theta_\alpha}\chi_{\partial D_1} + \chi_{\partial D_2}\right).$$

Observe that $\langle \chi_i^\alpha, u_j^\alpha \rangle = -\delta_{i,j}\lambda_i^\alpha$ for $i, j = 1, 2$. Here, $\langle \cdot, \cdot \rangle$ denotes the $L^2(\partial D)$ inner product

$$\langle u, v \rangle = \int_{\partial D} \overline{u(y)} v(y) \, \mathrm{d}\sigma(y).$$

In the dilute regime, the capacitance coefficients can be computed explicitly. In this regime, we assume that the two resonators can be expressed as a rescaling of the two fixed domains B_1 and B_2:

$$D_1 = \varepsilon B_1 - \frac{l}{2}\mathbf{v}, \quad D_2 = \varepsilon B_2 + \frac{l}{2}\mathbf{v}, \tag{3.6}$$

for some small parameter $\varepsilon > 0$.

We define the capacitance Cap_{B_i} of the fixed domains as

$$\mathrm{Cap}_{B_i} := -\int_{\partial B_i} \psi_{B_i} \, \mathrm{d}\sigma,$$

where $\psi_{B_i} := (\mathcal{S}_{B_i}^0)^{-1}[\chi_{\partial B_i}]$. Due to symmetry, the capacitance is the same for the two cases $i = 1, 2$, and therefore will simply be denoted by Cap_B. Rescaling the domain, we have that

$$\mathrm{Cap}_{\varepsilon B_i} = \varepsilon \mathrm{Cap}_B \quad i = 1, 2.$$

Similarly, by rescaling, we find that the capacitance coefficients satisfy

$$|C_{i,j}^\alpha| \leq \varepsilon C \quad i, j = 1, 2, \tag{3.7}$$

for some constant C independent of $\alpha \in Y^*$.

Lemma 3.5. *We assume that the resonators are in the dilute regime specified by* (3.6)*. Then, for every $\varepsilon_0 > 0$ and $p \in \mathbb{N}$ there exists a constant A_p such that we have the following asymptotics of the capacitance matrix C_{ij}^α for $\varepsilon < \varepsilon_0$:*

$$C_{11}^\alpha = \varepsilon \mathrm{Cap}_B - \frac{(\varepsilon \mathrm{Cap}_B)^2}{4\pi} \sum_{m \neq 0} \frac{e^{im\alpha L}}{|mL|} + o(\varepsilon^2),$$
$$C_{12}^\alpha = -\frac{(\varepsilon \mathrm{Cap}_B)^2}{4\pi} \sum_{m=-\infty}^{\infty} \frac{e^{im\alpha L}}{|mL + l|} + o(\varepsilon^2),$$

uniformly in α for $|\alpha| \geq A_p \varepsilon^p$.

Lemma 3.5 is a slight generalisation of a result from [3], and shows, essentially, that for smaller ε, the asymptotic formulas are valid for α closer to 0. Lemma 3.5 can be proved by following the steps in [3] under the additional observation that the sums have a logarithmic behaviour as $\alpha \to 0$:

$$\sum_{m \neq 0} \frac{e^{im\alpha L}}{|m|} = -\log\big(2 - 2\cos(\alpha L)\big).$$

3.1.2 Bandgap opening and singularity of $\mathcal{A}^\alpha$

The next theorem describes the subwavelength band gap opening and the edge points of the bands.

Theorem 3.6. *In the dilute regime, we have*

$$\max_{\alpha \in Y^*} \lambda_1^\alpha = \lambda_1^{\pi/L}, \qquad \min_{\alpha \in Y^*} \lambda_2^\alpha = \lambda_2^{\pi/L},$$

for ε small enough.

Proof. Observe first that if $l_0 > 1/2$, we can redefine the unit cell so that $l_0 < 1/2$, without changing the band structure. Therefore, it is enough to consider the case $l_0 \leq 1/2$. We have

$$\begin{aligned} \lambda_1^\alpha &= C_{11}^\alpha - |C_{12}^\alpha| \\ &\leq C_{11}^\alpha + \mathrm{Re}\,(C_{12}^\alpha) \\ &= \frac{1}{2} \mathrm{Cap}_D^\alpha, \end{aligned}$$

where Cap_D^α is the capacitance of D defined by

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

Using the variational characterization of Cap_D^α, in the same way as in [12], it is shown that the maximum of Cap_D^α is attained at $\alpha = \pi/L$. Moreover, in the dilute regime, $C_{12}^{\pi/L}$ is a non-positive real number [3]. We therefore have

$$\lambda_1^{\pi/L} = \frac{1}{2} \mathrm{Cap}_D^{\pi/L},$$

so the maximum of λ_1^α is attained at $\alpha = \pi/L$.

We now turn to the second eigenvalue λ_2^α. Similarly, we have

$$\begin{aligned} \lambda_2^\alpha &= C_{11}^\alpha + |C_{12}^\alpha| \\ &\geq C_{11}^\alpha - \mathrm{Re}\,(C_{12}^\alpha). \end{aligned} \tag{3.8}$$

We can formulate a variational characterization for $C_{11}^\alpha - \mathrm{Re}\,(C_{12}^\alpha)$ in terms of the Dirichlet energy. Let $\mathcal{C}_\alpha^\infty$ be the set of functions in $\mathcal{C}^\infty(Y)$ that can be extended to α-quasiperiodic functions in $\mathcal{C}^\infty(\mathbb{R}^3)$ decaying as $O\left((x_2^2+x_3^2)^{-1/2}\right)$ as $\sqrt{x_2^2+x_3^2} \to \infty$. Let

$$\mathcal{H} = \left\{ v \in H^1_{\mathrm{loc}}(Y) \;\middle|\; v(x_1,x_2,x_3) = O\left(\frac{1}{\sqrt{x_2^2+x_3^2}}\right) \text{ as } \sqrt{x_2^2+x_3^2} \to \infty \right\}$$

and let $\mathcal{H}_\alpha$ be the closure of $\mathcal{C}_\alpha^\infty$ in $\mathcal{H}$. Then define (see, for instance, [52])

$$\mathcal{V}_\alpha = \left\{ v \in \mathcal{H}_\alpha \;\middle|\; v = -\frac{1}{\sqrt{2}} \text{ on } \partial D_1, v = \frac{1}{\sqrt{2}} \text{ on } \partial D_2 \right\}.$$

We then have the variational characterization

$$C_{11}^\alpha - \mathrm{Re}\,(C_{12}^\alpha) = \min_{v \in \mathcal{V}_\alpha} \int_{Y \setminus D} |\nabla v|^2 \,\mathrm{d}x. \tag{3.9}$$

Indeed, the minimizer v_0 satisfies $\Delta v_0 = 0$ in $Y \setminus D$, and therefore $v_0 = \frac{1}{\sqrt{2}}\left(-V_1^\alpha + V_2^\alpha\right)$. Equation (3.9) then follows by expanding the integral.

Define $\mathcal{V} = \cup_{\alpha \in Y^*} \mathcal{V}_\alpha$. From (3.9) we find

$$\min_{\alpha \in Y^*} \left[C_{11}^\alpha - \mathrm{Re}\,(C_{12}^\alpha) \right] = \min_{v \in \mathcal{V}} \int_{Y \setminus D} |\nabla v|^2 \,\mathrm{d}x.$$

Because of the symmetry of D, the corresponding minimizer v_1 is an odd function in x_1. In other words, v_1 is a π/L-quasiperiodic function, and so

$$\min_{\alpha \in Y^*} \left[C_{11}^\alpha - \mathrm{Re}\,(C_{12}^\alpha) \right] = C_{11}^{\pi/L} - \mathrm{Re}\left(C_{12}^{\pi/L}\right). \tag{3.10}$$

At $\alpha = \pi/L$, (3.8) is an equality. This, together with (3.10), proves that the minimum of λ_2^α is attained at $\alpha = \pi/L$. □

Corollary 3.7. *In the dilute regime and with δ is sufficiently small, there exists a subwavelength band gap between the first two bands if $l_0 \neq 1/2$, i.e.*

$$\max_{\alpha \in Y^*} \omega_1^\alpha < \min_{\alpha \in Y^*} \omega_2^\alpha,$$

for ε and δ small enough.

Proof. From [3], we know that if $l_0 \neq 1/2$ then $\lambda_1^{\pi/L} < \lambda_2^{\pi/L}$. Hence, Theorem 3.6 gives us that

$$\max_{\alpha \in Y^*} \lambda_1^\alpha < \min_{\alpha \in Y^*} \lambda_2^\alpha.$$

The result then follows from Theorem 3.2, provided that δ is sufficiently small. □

Next, we will explicitly describe the behaviour of $\left(\mathcal{A}^\alpha(\omega,\delta)\right)^{-1}$ as ω approaches the edge of the first or the second band. The results are similar to Lemmas 4.1 and 4.2 of [11], but generalized to the case when D consists of two connected domains of general shape. Throughout the remainder of this section, we assume that $|\alpha| > \alpha_0 > 0$ for some α_0.

Using $u_1^\alpha, u_2^\alpha, \chi_1^\alpha$, and χ_2^α as defined in Section 3.1.1, we decompose the operator $\frac{1}{2}I + (\mathcal{K}_D^{-\alpha,0})^*$ as

$$\frac{1}{2}I + (\mathcal{K}_D^{-\alpha,0})^* = P_\alpha + Q_\alpha,$$

where

$$P_\alpha = -\frac{\langle \chi_1^\alpha, \cdot \rangle}{\lambda_1^\alpha} u_1^\alpha - \frac{\langle \chi_2^\alpha, \cdot \rangle}{\lambda_2^\alpha} u_2^\alpha, \qquad Q_\alpha = \frac{1}{2} + (\mathcal{K}_D^{-\alpha,0})^* - P_\alpha.$$

Then it follows that $Q_\alpha[u_i^\alpha] = 0$ and $Q_\alpha^*[\chi_i^\alpha] = 0$ for $i = 1,2$. Here, * denotes the adjoint operator. As we will see, the reason for using this decomposition is that Q_α will only contribute to higher-order terms when computing the inverse $\left(\mathcal{A}^\alpha(\omega,\delta)\right)^{-1}$.

We consider the limit as δ goes to zero. Recall that for ω inside the corresponding band gap, we have $\omega = O(\sqrt{\delta})$. Then we can decompose the operator $\mathcal{A}^\alpha(\omega,\delta)$ as

$$\mathcal{A}^\alpha(\omega,\delta) = \begin{pmatrix} \hat{\mathcal{S}}_D^\omega & -\mathcal{S}_D^{\alpha,\omega} \\ -\frac{1}{2}I + \hat{\mathcal{K}}_D^{\omega,*} & 0 \end{pmatrix} - \delta \begin{pmatrix} 0 & 0 \\ 0 & P_\alpha \end{pmatrix} - \delta \begin{pmatrix} 0 & 0 \\ 0 & Q_\alpha \end{pmatrix} + O(\delta^3).$$

We define

$$A_0(\omega) = \begin{pmatrix} \hat{\mathcal{S}}_D^\omega & -\mathcal{S}_D^{\alpha,\omega} \\ -\frac{1}{2}I + \hat{\mathcal{K}}_D^{\omega,*} & 0 \end{pmatrix}, \qquad A_1(\omega,\delta) = I - \delta A_0^{-1} \begin{pmatrix} 0 & 0 \\ 0 & P_\alpha \end{pmatrix}.$$

Analogously to u_1^α and u_2^α, we introduce the basis $\{u_1, u_2\}$ of ker $\left(-\frac{1}{2}I + \hat{\mathcal{K}}_D^{\omega,*}\right)$ as follows

$$u_1 = \frac{1}{\sqrt{2}}\left(-e^{i\theta_\alpha}\psi_1 + \psi_2\right), \qquad u_2 = \frac{1}{\sqrt{2}}\left(e^{i\theta_\alpha}\psi_1 + \psi_2\right),$$

where ψ_j are defined by

$$\psi_j = (\mathcal{S}_{D_j}^0)^{-1}[\chi_{\partial D_j}].$$

We then have the following result.

Lemma 3.8. *(i) For $\omega \neq 0$, $A_0 : \left(L^2(\partial D)\right)^2 \to \left(L^2(\partial D)\right)^2$ is invertible, and as $\omega \to 0$,*

$$A_0^{-1} = \begin{pmatrix} 0 & -\dfrac{\langle \chi_{\partial D_1}, \cdot\rangle \psi_1 + \langle \chi_{\partial D_2}, \cdot\rangle\psi_2}{\omega^2|D_1|} + O\left(\dfrac{1}{\omega}\right) \\ -\left(\mathcal{S}_D^{\alpha,0}\right)^{-1} + O(\omega^2) & -\dfrac{\langle \chi_{\partial D_1}, \cdot\rangle \psi_1^\alpha + \langle \chi_{\partial D_2}, \cdot\rangle\psi_2^\alpha}{\omega^2|D_1|} + O\left(\dfrac{1}{\omega}\right) \end{pmatrix},$$

where $|D_1|$ denotes the volume of D_1.

(ii) For $\omega \neq \omega^\alpha$, $A_1 : L^2(\partial D) \to L^2(\partial D)$ is invertible, and as $\omega \to 0$ and $\delta \to 0$,

$$A_1^{-1} = \begin{pmatrix} I & -P\left(P_\alpha^\perp\right)^{-1} \\ 0 & \left(P_\alpha^\perp\right)^{-1} \end{pmatrix} + O(\omega),$$

where

$$P = \frac{\delta}{\omega^2|D_1|}\left(\langle \chi_1^\alpha, \cdot\rangle u_1 + \langle \chi_2^\alpha, \cdot\rangle u_2\right), \qquad P_\alpha^\perp = I + \frac{\delta}{\omega^2|D_1|}\left(\langle \chi_1^\alpha, \cdot\rangle u_1^\alpha + \langle \chi_2^\alpha, \cdot\rangle u_2^\alpha\right).$$

Proof of (i). Using block matrix inversion, we find that

$$A_0^{-1} = \begin{pmatrix} 0 & \left(-\dfrac{1}{2}I + \hat{\mathcal{K}}_D^{\omega,*}\right)^{-1} \\ -\left(\mathcal{S}_D^{\alpha,\omega}\right)^{-1} & \left(\mathcal{S}_D^{\alpha,\omega}\right)^{-1}\hat{\mathcal{S}}_D^\omega\left(-\dfrac{1}{2}I + \hat{\mathcal{K}}_D^{\omega,*}\right)^{-1} \end{pmatrix}, \tag{3.11}$$

which is well-defined since $-\frac{1}{2}I + \mathcal{K}_{D_i}^{\omega,*} : L^2(\partial D) \to L^2(\partial D)$ is invertible for $\omega \neq 0$ for both $i = 1, 2$, see, for instance, [7]. Here, $\hat{\mathcal{S}}_D^\omega$ and $\hat{\mathcal{K}}_D^{\omega,*}$ are defined in (3.5).

From the low-frequency expansion (2.3) of $\mathcal{S}_D^{\alpha,\omega}$ we have

$$\left(\mathcal{S}_D^{\alpha,\omega}\right)^{-1} = \left(\mathcal{S}_D^{\alpha,0}\right)^{-1} + O(\omega^2). \tag{3.12}$$

The operator $\left(-\frac{1}{2}I + \mathcal{K}_{D_i}^{\omega,*}\right)^{-1}$ is known to be singular as $\omega \to 0$, see [7]. Explicitly, we have

$$\left(-\frac{1}{2}I + \mathcal{K}_{D_i}^{\omega,*}\right)^{-1} = -\frac{\langle \chi_{\partial D_i}, \cdot\rangle}{\omega^2|D_i|}\psi_i + R_i(\omega),$$

where $R_i(\omega) = O(1)$ as $\omega \to 0$. Since $|D_1| = |D_2|$, we have

$$\left(-\frac{1}{2}I + \hat{\mathcal{K}}_D^{\omega,*}\right)^{-1} = -\frac{\langle \chi_{\partial D_1}, \cdot\rangle \psi_1 + \langle \chi_{\partial D_2}, \cdot\rangle\psi_2}{\omega^2|D_1|} + O(1), \tag{3.13}$$

where we identify $L^2(\partial D) = L^2(\partial D_1) \times L^2(\partial D_2)$. Moreover, we know that $\mathcal{S}_{D_i}^{\omega}[\psi_i] = \chi_{\partial D_i} + O(\omega)$, and so

$$\left(\mathcal{S}_D^{\alpha,\omega}\right)^{-1} \hat{\mathcal{S}}_D^{\omega} \left(-\frac{1}{2}I + \hat{\mathcal{K}}_D^{\omega,*}\right)^{-1} = -\frac{\langle \chi_{\partial D_1}, \cdot\rangle \psi_1^\alpha + \langle \chi_{\partial D_2}, \cdot\rangle \psi_2^\alpha}{\omega^2 |D_1|} + O\left(\frac{1}{\omega}\right). \tag{3.14}$$

Combining equations (3.11), (3.12), (3.13) and (3.14) proves *(i)*. □

Proof of (ii). We can compute

$$\left(-\frac{1}{2}I + \hat{\mathcal{K}}_D^{\omega,*}\right)^{-1} P_\alpha = -\frac{\langle \chi_1^\alpha, \cdot\rangle u_1 + \langle \chi_2^\alpha, \cdot\rangle u_2}{\omega^2 |D_1|} + O\left(\frac{1}{\omega}\right).$$

Similarly, we have

$$\left(\mathcal{S}_D^{\alpha,\omega}\right)^{-1} \hat{\mathcal{S}}_D^{\omega} \left(-\frac{1}{2}I + \hat{\mathcal{K}}_D^{\omega,*}\right)^{-1} P_\alpha = -\frac{\langle \chi_1^\alpha, \cdot\rangle u_1^\alpha + \langle \chi_2^\alpha, \cdot\rangle u_2^\alpha}{\omega^2 |D_1|} + O\left(\frac{1}{\omega}\right).$$

We then find that

$$A_1 = \begin{pmatrix} I & \dfrac{\delta}{\omega^2 |D_1|}\big(\langle \chi_1^\alpha, \cdot\rangle u_1 + \langle \chi_2^\alpha, \cdot\rangle u_2\big) \\ 0 & I + \dfrac{\delta}{\omega^2 |D_1|}\big(\langle \chi_1^\alpha, \cdot\rangle u_1^\alpha + \langle \chi_2^\alpha, \cdot\rangle u_2^\alpha\big) \end{pmatrix} + O(\omega).$$

Define

$$P = \frac{\delta}{\omega^2 |D_1|}\big(\langle \chi_1^\alpha, \cdot\rangle u_1 + \langle \chi_2^\alpha, \cdot\rangle u_2\big),$$

and

$$P_\alpha^\perp = I + \frac{\delta}{\omega^2 |D_1|}\big(\langle \chi_1^\alpha, \cdot\rangle u_1^\alpha + \langle \chi_2^\alpha, \cdot\rangle u_2^\alpha\big).$$

The leading order of A_1 is invertible precisely when $P_\alpha^\perp$ is invertible. This occurs precisely when $P_\alpha^\perp u_i^\alpha \neq 0$ for $i = 1, 2$, *i.e.* when

$$\omega \neq \sqrt{\frac{\delta \lambda_i^\alpha}{|D_1|}} = \omega_i^\alpha \quad \text{for } i = 1, 2.$$

Moreover, we have

$$A_1^{-1} = \begin{pmatrix} I & -P\left(P_\alpha^\perp\right)^{-1} \\ 0 & \left(P_\alpha^\perp\right)^{-1} \end{pmatrix} + O(\omega).$$

This shows *(ii)*. □

The following result can be proved by using the same arguments as those in [11].

Lemma 3.9. *For $\omega \neq \omega^\alpha$, and as $\omega \to 0$ and $\delta \to 0$, we have*

$$\left(\mathcal{A}^\alpha(\omega, \delta)\right)^{-1} = A_1^{-1} A_0^{-1}\big(I + O(\delta)\big).$$

Explicitly, we have

$$\begin{aligned}
&\left(\mathcal{A}^\alpha(\omega, \delta)\right)^{-1} = A_1^{-1} A_0^{-1}\big(I + O(\delta)\big) \\
&= \begin{pmatrix} I & -P\left(P_\alpha^\perp\right)^{-1} \\ 0 & \left(P_\alpha^\perp\right)^{-1} \end{pmatrix} \begin{pmatrix} 0 & -\dfrac{\langle \chi_{\partial D_1}, \cdot\rangle \psi_1 + \langle \chi_{\partial D_2}, \cdot\rangle \psi_2}{\omega^2 |D_1|} + O\left(\dfrac{1}{\omega}\right) \\ -\left(\mathcal{S}_D^{\alpha,0}\right)^{-1} + O(\omega^2) & -\dfrac{\langle \chi_{\partial D_1}, \cdot\rangle \psi_1^\alpha + \langle \chi_{\partial D_2}, \cdot\rangle \psi_2^\alpha}{\omega^2 |D_1|} + O\left(\dfrac{1}{\omega}\right) \end{pmatrix} \\
&= \begin{pmatrix} P\left(P_\alpha^\perp\right)^{-1}\left(\mathcal{S}_D^{\alpha,0}\right)^{-1} + O(\omega) & -\dfrac{\langle \chi_{\partial D_1}, \cdot\rangle \psi_1 + \langle \chi_{\partial D_2}, \cdot\rangle \psi_2}{\omega^2 |D_1|} + P\left(P_\alpha^\perp\right)^{-1} \dfrac{\langle \chi_{\partial D_1}, \cdot\rangle \psi_1^\alpha + \langle \chi_{\partial D_2}, \cdot\rangle \psi_2^\alpha}{\omega^2 |D_1|} + O\left(\dfrac{1}{\omega}\right) \\ -\left(P_\alpha^\perp\right)^{-1}\left(\mathcal{S}_D^{\alpha,0}\right)^{-1} + O(\omega) & -\left(P_\alpha^\perp\right)^{-1} \dfrac{\langle \chi_{\partial D_1}, \cdot\rangle \psi_1^\alpha + \langle \chi_{\partial D_2}, \cdot\rangle \psi_2^\alpha}{\omega^2 |D_1|} + O\left(\dfrac{1}{\omega}\right) \end{pmatrix}.
\end{aligned}$$

We will simplify the upper right element in the above expression, which is the part of $(\mathcal{A}^\alpha)^{-1}$ that is relevant for the rest of the work. Define

$$\left(\mathcal{A}^\alpha(\omega, \delta)\right)^{-1} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}.$$

We can compute

$$\left(P_\alpha^\perp\right)^{-1}\psi_1^\alpha = -\frac{e^{-i\theta_\alpha}}{\sqrt{2}}\left(\frac{\omega^2}{\omega^2-(\omega_1^\alpha)^2}\right)u_1^\alpha + \frac{e^{-i\theta_\alpha}}{\sqrt{2}}\left(\frac{\omega^2}{\omega^2-(\omega_2^\alpha)^2}\right)u_2^\alpha,$$
$$\left(P_\alpha^\perp\right)^{-1}\psi_2^\alpha = \frac{1}{\sqrt{2}}\left(\frac{\omega^2}{\omega^2-(\omega_1^\alpha)^2}\right)u_1^\alpha + \frac{1}{\sqrt{2}}\left(\frac{\omega^2}{\omega^2-(\omega_2^\alpha)^2}\right)u_2^\alpha.$$

Then we obtain

$$Pu_1^\alpha = -\frac{(\omega_1^\alpha)^2}{\omega^2}u_1, \qquad Pu_2^\alpha = -\frac{(\omega_2^\alpha)^2}{\omega^2}u_2.$$

Consequently, we have

$$\begin{aligned} A_{12} &= -\frac{\langle\chi_{\partial D_1},\cdot\rangle\psi_1 + \langle\chi_{\partial D_2},\cdot\rangle\psi_2}{\omega^2|D_1|} + P\left(P_\alpha^\perp\right)^{-1}\frac{\langle\cdot,\chi_{\partial D_1}\rangle\psi_1^\alpha + \langle\chi_{\partial D_2},\cdot\rangle\psi_2^\alpha}{\omega^2|D_1|} + O\left(\frac{1}{\omega}\right) \\ &= -\frac{\langle\chi_{\partial D_1},\cdot\rangle\psi_1 + \langle\chi_{\partial D_2},\cdot\rangle\psi_2}{\omega^2|D_1|} - \frac{\langle\chi_1^\alpha,\cdot\rangle u_1}{\omega^2|D_1|}\left(\frac{(\omega_1^\alpha)^2}{\omega^2-(\omega_1^\alpha)^2}\right) - \frac{\langle\chi_2^\alpha,\cdot\rangle u_2}{\omega^2|D_1|}\left(\frac{(\omega_2^\alpha)^2}{\omega^2-(\omega_2^\alpha)^2}\right) \\ &\quad + O\left(\frac{1}{\omega}\right), \end{aligned} \tag{3.15}$$

and

$$\begin{aligned} A_{22} &= -\left(P_\alpha^\perp\right)^{-1}\frac{\langle\chi_{\partial D_1},\cdot\rangle\psi_1^\alpha + \langle\chi_{\partial D_2},\cdot\rangle\psi_2^\alpha}{\omega^2|D_1|} + O\left(\frac{1}{\omega}\right) \\ &= -\frac{\langle\chi_1^\alpha,\cdot\rangle u_1^\alpha}{\omega^2|D_1|}\left(\frac{\omega^2}{\omega^2-(\omega_1^\alpha)^2}\right) - \frac{\langle\chi_2^\alpha,\cdot\rangle u_2^\alpha}{\omega^2|D_1|}\left(\frac{\omega^2}{\omega^2-(\omega_2^\alpha)^2}\right) \\ &\quad + O\left(\frac{1}{\omega}\right). \end{aligned}$$

The singularity of $\mathcal{A}^\alpha$ as $\omega\to\omega_1^\alpha$ or $\omega\to\omega_2^\alpha$ is, to leading order, described by the operator $P_\alpha^\perp$. Defining

$$\Psi_j^\alpha = \begin{pmatrix} u_j \\ u_j^\alpha \end{pmatrix} \qquad \Phi_j^\alpha = \begin{pmatrix} -\delta u_j^\alpha \\ \chi_j^\alpha \end{pmatrix},$$

the above computations imply the following result.

Proposition 3.10. *As $\omega\to\omega_j^\alpha, j=1,2$, we have*

$$\left(\mathcal{A}^\alpha(\omega,\delta)\right)^{-1} = -\frac{1}{2\omega_j^\alpha|D_1|}\frac{\langle\Phi_j^\alpha,\cdot\rangle\Psi_j^\alpha}{\omega-\omega_j^\alpha} + \mathcal{R}_j^\alpha(\omega),$$

where $\mathcal{R}_j^\alpha(\omega)$ is holomorphic for ω in a neighbourhood of ω_j^α.

3.2 Dislocated system for small dislocation

In this section, we study the problem when a dislocation is introduced so that half of the array of resonators is translated in the x_1-direction. We will model the defect problem using the fictitious source superposition method [6].

3.2.1 Fictitious sources for dislocated resonator with a small dislocation

Here, we briefly describe the method of fictitious sources for a single translated resonator, in the asymptotic limit when the translation $d\to 0$. This will be developed for use on a dislocated array in Section 3.2.2. Throughout this subsection, Ω denotes a bounded domain such that $\partial\Omega\in\mathcal{C}^{1,s}$, $\Omega_d := \Omega + d\mathbf{v}$, and U is a neighbourhood of $\Omega\cup\Omega_d$. Although this subsection is phrased for a general domain Ω, we think of Ω as a pair of resonators in the dislocated array.

We define the map $p:\partial\Omega\to\partial\Omega_d, x\mapsto x+d\mathbf{v}$ and the map $q: L^2(\partial\Omega)\to L^2(\partial\Omega_d), q(\phi)(y) = \phi(p^{-1}(y))$.

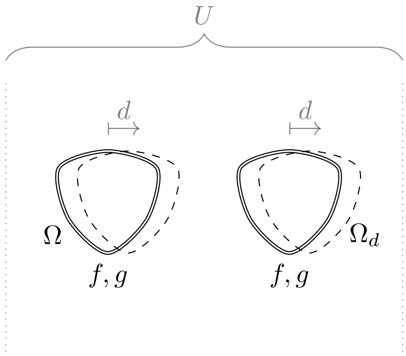


Figure 4: A dislocated pair of resonators in the case of a small dislocation d. Legend: ═ *resonator with fictitious sources,* - - - *dislocated resonator.*

Lemma 3.11. *Let $x \in \partial\Omega$, let ν_x be the outward unit normal to $\partial\Omega$ at x and let p, q be defined as above. For $\phi \in L^2(\partial\Omega)$, we have*

(i) If $\nu_x \cdot \mathbf{v} \geq 0$, then
$$\mathcal{S}_\Omega^\omega[\phi](p(x)) = \mathcal{S}_\Omega^\omega[\phi](x) + d\mathbf{v}\cdot\nabla\mathcal{S}_\Omega^\omega[\phi]\big|_+(x) + O(d^2).$$

(ii) If $\nu_x \cdot \mathbf{v} < 0$, then
$$\mathcal{S}_\Omega^\omega[\phi](p(x)) = \mathcal{S}_\Omega^\omega[\phi](x) + d\mathbf{v}\cdot\nabla\mathcal{S}_\Omega^\omega[\phi]\big|_-(x) + O(d^2).$$

These estimates are valid uniformly in $x \in \partial\Omega$ in the following sense: There is a constant C, independent of d, such that
$$\left\|\mathcal{S}_\Omega^\omega[\phi]\circ p - \left(\mathcal{S}_\Omega^\omega[\phi] + d\mathbf{v}\cdot\nabla\mathcal{S}_\Omega^\omega[\phi]\big|_\pm\right)\right\|_{L^2(\partial\Omega)} \leq Cd^2$$
for d small enough.

Proof. The cases $\nu_x\cdot\mathbf{v} > 0$ or $\nu_x\cdot\mathbf{v} < 0$ correspond, respectively, to the cases when $p(x)$ is inside or outside Ω for small enough d. In these cases, pointwise in x, the estimates follow by Taylor series expansions. If $x \in \partial\Omega$ is such that $\nu_x \cdot \mathbf{v} = 0$ we have [17]
$$\mathbf{v}\cdot\nabla\mathcal{S}_\Omega^\omega[\phi]\big|_+(x) = \mathbf{v}\cdot\nabla\mathcal{S}_\Omega^\omega\big|_-[\phi](x).$$
For a fixed d, we define $U \subset \partial\Omega$ as the set of points x such that $p(x) \notin \Omega$ but $\nu_x \cdot \mathbf{v} < 0$, and $V \subset \partial\Omega$ as the set of points x such that $p(x) \in \Omega$ but $\nu_x \cdot \mathbf{v} > 0$ for some $d_0 < d$. Since $\partial\Omega \in \mathcal{C}^1$, we have $\nu_x \cdot \mathbf{v} = O(d)$ uniformly for $x \in U \cup V$, and so
$$\mathbf{v}\cdot\nabla\mathcal{S}_\Omega^\omega[\phi]\big|_+(x) = \mathbf{v}\cdot\nabla\mathcal{S}_\Omega^\omega[\phi]\big|_-(x) + O(d),$$
uniformly for $x \in U \cup V$. This proves the claim. □

We now assume $\Omega = \Omega_1 \cup \Omega_2$ for two connected domains $\Omega_i, i = 1, 2$. To study the problem for the dislocated resonator, we consider the problem when the resonator Ω has its original position, along with fictitious sources f, g on the boundary. Explicitly, we consider the problem
$$\begin{cases} \Delta\widetilde{u} + \omega^2\widetilde{u} = 0 & \text{in } U\setminus\partial\Omega, \\ \widetilde{u}|_+ - \widetilde{u}|_- = f & \text{on } \partial\Omega, \\ \delta\dfrac{\partial\widetilde{u}}{\partial\nu}\bigg|_+ - \dfrac{\partial\widetilde{u}}{\partial\nu}\bigg|_- = g & \text{on } \partial\Omega. \end{cases} \tag{3.16}$$
We assume we have a reference solution u satisfying
$$\begin{cases} \Delta u + \omega^2 u = 0 & \text{in } U\setminus\partial\Omega_d, \\ u|_+ - u|_- = 0 & \text{on } \partial\Omega_d, \\ \delta\dfrac{\partial u}{\partial\nu}\bigg|_+ - \dfrac{\partial u}{\partial\nu}\bigg|_- = 0 & \text{on } \partial\Omega_d. \end{cases} \tag{3.17}$$

We want to determine the fictitious sources f, g such that

$$u = \widetilde{u} \quad \text{in } U \setminus (\Omega \cup \Omega_d)\,, \tag{3.18}$$
$$u = \widetilde{u} \quad \text{in } \Omega \cap \Omega_d. \tag{3.19}$$

Inside U, the two solutions u and $\widetilde{u}$ can be respectively represented as

$$u = \begin{cases} \hat{\mathcal{S}}_{\Omega_d}^{\omega}[\phi^{i,d}] & \text{in } \Omega_d, \\ \mathcal{S}_{\Omega_d}^{\omega}[\phi^{o,d}] + H & \text{in } U \setminus \Omega_d, \end{cases} \tag{3.20}$$

and

$$\widetilde{u} = \begin{cases} \hat{\mathcal{S}}_{\Omega}^{\omega}[\phi^{i}] & \text{in } \Omega, \\ \mathcal{S}_{\Omega}^{\omega}[\phi^{o}] + \widetilde{H} & \text{in } U \setminus \Omega, \end{cases} \tag{3.21}$$

for some functions H and $\widetilde{H}$ satisfying $\Delta H + \omega^2 H = 0$ and $\Delta \widetilde{H} + \omega^2 \widetilde{H} = 0$ in U. H and $\widetilde{H}$ can be thought of as background solutions, while the single layer potentials account for the local effect of the resonators. From (3.18) it follows that $H = \widetilde{H}$. Using the jump relations and the boundary conditions in (3.17) and (3.16) we find that

$$\mathcal{A}_d(\omega, \delta)\Phi_d = \begin{pmatrix} H\big|_{\partial\Omega_d} \\ \delta \partial_\nu H\big|_{\partial\Omega_d} \end{pmatrix}, \qquad \mathcal{A}(\omega, \delta)\Phi = \begin{pmatrix} H\big|_{\partial\Omega} \\ \delta \partial_\nu H\big|_{\partial\Omega} \end{pmatrix} - \begin{pmatrix} f \\ g \end{pmatrix}, \tag{3.22}$$

where

$$\mathcal{A}_d(\omega, \delta) = \begin{pmatrix} \hat{\mathcal{S}}_{\Omega_d}^{\omega} & -\mathcal{S}_{\Omega_d}^{\omega} \\ -\frac{1}{2}I + \hat{\mathcal{K}}_{\Omega_d}^{\omega,*} & -\delta\left(\frac{1}{2}I + \mathcal{K}_{\Omega_d}^{\omega})^*\right) \end{pmatrix}, \quad \mathcal{A}(\omega, \delta) = \begin{pmatrix} \hat{\mathcal{S}}_{\Omega}^{\omega} & -\mathcal{S}_{\Omega}^{\omega} \\ -\frac{1}{2}I + \hat{\mathcal{K}}_{\Omega}^{\omega,*} & -\delta\left(\frac{1}{2}I + (\mathcal{K}_{\Omega}^{\omega})^*\right) \end{pmatrix},$$

and

$$\Phi_d = \begin{pmatrix} \phi^{i,d} \\ \phi^{o,d} \end{pmatrix}, \quad \Phi = \begin{pmatrix} \phi^{i} \\ \phi^{o} \end{pmatrix}.$$

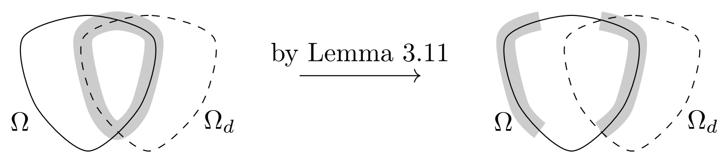


Figure 5: In the fictitious sources approach, for the case of a small dislocation, we seek solutions that match on the shaded region. In (3.23) and (3.24), equality is imposed on the region highlighted in the left image. Using Lemma 3.11 this is mapped to a subset of $\partial\Omega$. After this transformation, the length of the part of $\partial\Omega$ not included will be $O(d)$, where d is the size of the dislocation. Legend: —— original resonator, - - - dislocated resonator, region of enforced equality.

By equations (3.18) and (3.19), we have

$$\hat{\mathcal{S}}_{\Omega_d}^{\omega}[\phi^{i,d}](\widetilde{x}) = \hat{\mathcal{S}}_{\Omega}^{\omega}[\phi^{i}](\widetilde{x}), \quad \widetilde{x} \in \partial\Omega_d \cap \Omega, \tag{3.23}$$
$$\hat{\mathcal{S}}_{\Omega_d}^{\omega}[\phi^{i,d}](x) = \hat{\mathcal{S}}_{\Omega}^{\omega}[\phi^{i}](x), \quad x \in \partial\Omega \cap \Omega_d. \tag{3.24}$$

We decompose the boundaries of the resonators as $\partial\Omega_d^i = \partial\Omega_d \cap \Omega$ and $\partial\Omega_d^o = \partial\Omega_d \setminus \partial\Omega_d^i$, and define $\partial\Omega^i = \partial\Omega_d^i - d\mathbf{v}$ and $\partial\Omega^o = \partial\Omega_d^o - d\mathbf{v}$. Because of translation invariance, we have $\hat{\mathcal{S}}_{\Omega_d}^{\omega}\left[\phi^{i,d}\right](\widetilde{x}) = \hat{\mathcal{S}}_{\Omega}^{\omega}\left[q^{-1}(\phi^{i,d})\right](x)$, where $\widetilde{x} = p(x)$. Therefore, using Lemma 3.11, we obtain

$$\begin{cases} \hat{\mathcal{S}}_{\Omega}^{\omega}\left[q^{-1}(\phi^{i,d})\right] = \hat{\mathcal{S}}_{\Omega}^{\omega}[\phi^{i}] + d\mathbf{v} \cdot \nabla \hat{\mathcal{S}}_{\Omega}^{\omega}[\phi^{i}]\big|_{-} + O(d^2) & \text{on } \partial\Omega^i, \\ \hat{\mathcal{S}}_{\Omega}^{\omega}\left[q^{-1}(\phi^{i,d})\right] - d\mathbf{v} \cdot \nabla \hat{\mathcal{S}}_{\Omega}^{\omega}\left[q^{-1}(\phi^{i,d})\right]\big|_{-} = \hat{\mathcal{S}}_{\Omega}^{\omega}\left[\phi^{i}\right] + O(d^2) & \text{on } \partial\Omega \cap \Omega_d. \end{cases}$$

This transformation is depicted in Figure 5. The boundary $\partial\Omega$ is decomposed into disjoint parts $\partial\Omega^i$ and $\partial\Omega^o$, and the length of the "missing" part of the boundary, $\partial\Omega^o \setminus (\partial\Omega \cap \Omega_d)$, scales as $O(d)$. Moreover, on this part (3.24) holds to order $O(d)$. Using the Neumann series, we can invert the second equation to obtain

$$q^{-1}(\phi^{i,d}) = \phi^i + d\left(\hat{\mathcal{S}}_{\Omega}^{\omega}\right)^{-1} \mathbf{v} \cdot \nabla \hat{\mathcal{S}}_{\Omega}^{\omega}[\phi^{i}]\big|_{-} + O(d^2) \quad \text{on } \partial\Omega.$$

We define $Q : L^2(\partial\Omega)^2 \to L^2(\partial\Omega_d)^2$ by

$$Q(u,v) = \begin{pmatrix} q(u) \\ q(v) \end{pmatrix}.$$

By analogous computations for $\mathcal{S}_\Omega^\omega[\phi^{o,d}](x)$ as those for $\hat{\mathcal{S}}_\Omega^\omega[\phi^{i,d}](x)$, we find that

$$Q^{-1}\Phi_d = \mathcal{P}_1\Phi, \qquad \mathcal{P}_1 = I + d\begin{pmatrix} \left(\hat{\mathcal{S}}_\Omega^\omega\right)^{-1}\mathbf{v}\cdot\nabla\hat{\mathcal{S}}_\Omega^\omega\big|_- & 0 \\ 0 & \left(\mathcal{S}_\Omega^\omega\right)^{-1}\mathbf{v}\cdot\nabla\mathcal{S}_\Omega^\omega\big|_+ \end{pmatrix} + O(d^2), \tag{3.25}$$

where $\mathcal{P}_1 : L^2(\partial\Omega) \to L^2(\partial\Omega)$. We denote the linear term in d by $\mathcal{P}_1^{(1)}$, *i.e.*, $\mathcal{P}_1 = I + d\mathcal{P}_1^{(1)} + O(d^2)$.

We now use Taylor series expansions to relate $H|_{\partial\Omega}$ and $H|_{\partial\Omega_d}$. We have that

$$\begin{aligned} H|_{\partial\Omega} &= H|_{\partial\Omega_d} - d\mathbf{v}\cdot\nabla H|_{\partial\Omega_d} + O(d^2) \\ &= H|_{\partial\Omega_d} - d\left((\mathbf{v}\cdot\nu)\frac{\partial}{\partial\nu}H|_{\partial\Omega_d} + \frac{\partial}{\partial T}H|_{\partial\Omega_d}\right) + O(d^2), \end{aligned}$$

where $\frac{\partial}{\partial T} := (\mathbf{v} - (\mathbf{v}\cdot\nu)\nu)\cdot\nabla$ is the tangential derivative in the direction specified by $\mathbf{v}$. Moreover,

$$\frac{\partial}{\partial\nu}H|_{\partial\Omega} = \frac{\partial}{\partial\nu}H|_{\partial\Omega_d} - d\left((\mathbf{v}\cdot\nu)\frac{\partial^2}{\partial\nu^2}H|_{\partial\Omega_d} + \frac{\partial^2}{\partial T\partial\nu}H|_{\partial\Omega_d}\right) + O(d^2).$$

The Laplacian in local coordinates defined by the normal and tangential directions of $\partial\Omega_d$ can be written as

$$\Delta = \frac{\partial^2}{\partial\nu^2} + 2\tau(\widetilde{x})\frac{\partial}{\partial\nu} + \Delta_{\partial\Omega_d},$$

where τ denotes the mean curvature of $\partial\Omega_d$ and $\Delta_{\partial\Omega_d}$ denotes the Laplace-Beltrami operator on $\partial\Omega_d$. Since H satisfies the Helmholtz equation $(\Delta + \omega^2)H = 0$, we get

$$\frac{\partial^2}{\partial\nu^2}H|_{\partial\Omega_d} = -\left(\omega^2 + \Delta_{\partial\Omega_d}\right)H|_{\partial\Omega_d} - 2\tau\frac{\partial}{\partial\nu}H|_{\partial\Omega_d}.$$

Hence, we have

$$\begin{pmatrix} H\big|_{\partial\Omega} \\ \delta\partial_\nu H\big|_{\partial\Omega} \end{pmatrix} = \mathcal{P}_2 Q^{-1}\begin{pmatrix} H\big|_{\partial\Omega_d} \\ \delta\partial_\nu H\big|_{\partial\Omega_d} \end{pmatrix}, \tag{3.26}$$

where the operator $\mathcal{P}_2 : L^2(\partial\Omega)^2 \to L^2(\partial\Omega)^2$ is given by

$$\mathcal{P}_2 = I + d\mathcal{P}_2^{(1)} + O(d^2), \qquad \mathcal{P}_2^{(1)} = \begin{pmatrix} -\partial_T & -\frac{(\mathbf{v}\cdot\nu)}{\delta} \\ \delta(\mathbf{v}\cdot\nu)\left(\omega^2 + \Delta_{\partial\Omega}\right) & 2\tau - \partial_T \end{pmatrix}.$$

Since Ω_d and Ω only differ by a translation, we have that

$$\mathcal{A}_d = Q\mathcal{A}Q^{-1}. \tag{3.27}$$

Combining (3.22), (3.25), (3.26) and (3.27), we arrive at the following result.

Proposition 3.12. *The layer densities ϕ^i and ϕ^o and the fictitious sources f and g satisfy*

$$\begin{pmatrix} f \\ g \end{pmatrix} = B(\omega,\delta,d)\begin{pmatrix} \phi^i \\ \phi^o \end{pmatrix}, \qquad B(\omega,\delta,d) = \mathcal{P}_2\mathcal{A}\mathcal{P}_1 - \mathcal{A}.$$

3.2.2 Integral equation for the dislocated system

In this section, we use Proposition 3.12 to derive an integral equation for the dislocated system when the dislocation size is small.

To study the dislocated problem (3.2), we consider the problem with periodic geometry, along with fictitious sources f_m, g_m placed on the boundary of $D^m = D_1^m \cup D_2^m$. Explicitly, we consider the problem

$$\begin{cases} \Delta\widetilde{u} + \omega^2\widetilde{u} = 0 & \text{in } \mathbb{R}^3 \setminus \partial\mathcal{C}, \\ \widetilde{u}|_+ - \widetilde{u}|_- = f_m & \text{on } \partial D^m, m \in \mathbb{N}, \\ \delta\frac{\partial\widetilde{u}}{\partial\nu}\bigg|_+ - \frac{\partial\widetilde{u}}{\partial\nu}\bigg|_- = g_m & \text{on } \partial D^m, m \in \mathbb{N}, \\ \widetilde{u}(x_1,x_2,x_3) & \text{satisfies the outgoing radiation condition as } \sqrt{x_2^2 + x_3^2} \to \infty. \end{cases} \tag{3.28}$$

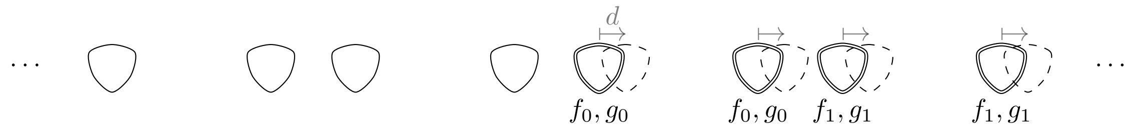


Figure 6: The dislocated system is equivalent to the original array with the addition of so-called fictitious sources f_m, g_m, on the boundary of D^m for $m \in \mathbb{N}$. Legend: —— untouched resonator, ═══ resonator with fictitious sources, - - - dislocated resonator.

Assume we have a nonzero solution u to (3.2). Inside $Y^m := Y + md\mathbf{v}$, we can represent the solution as in (3.20) with the choices $\Omega = D^m$ and $U = Y^m$. In this way, we define the layer densities $\phi^{i,d}$ and $\phi^{o,d}$. Since $\mathcal{P}_1$ is invertible for small enough d, we can define the layer densities ϕ^i_m and ϕ^o_m as

$$\begin{pmatrix} \phi^i_m \\ \phi^o_m \end{pmatrix} = (\mathcal{P}_1)^{-1} Q^{-1} \begin{pmatrix} \phi^{i,d} \\ \phi^{o,d} \end{pmatrix}.$$

We then set the fictitious sources as

$$\begin{pmatrix} f_m \\ g_m \end{pmatrix} = \begin{cases} 0, & m < 0, \\ B^m \begin{pmatrix} \phi^i_m \\ \phi^o_m \end{pmatrix}, & m \geq 0, \end{cases} \tag{3.29}$$

where B^m is defined as in Proposition 3.12 with the choice $\Omega = D^m$. We then define the solution $\widetilde{u}$ by (3.21) with $\widetilde{H} = H$, and because of (3.29) this coincides with u in $\Big(Y^m \setminus \big(D^m \cup (D^m + d\mathbf{v})\big)\Big) \cup \big(D^m \cap (D^m + d\mathbf{v})\big)$.

Conversely, if we have a nonzero solution $\widetilde{u}$ to (3.28), represented as (3.21) in Y^m and with sources satisfying (3.29), we can define $\phi^{i,d}$ and $\phi^{o,d}$ to get a nonzero solution u to (3.2) coinciding with $\widetilde{u}$ in $\Big(Y^m \setminus \big(D^m \cup (D^m + d\mathbf{v})\big)\Big) \cup \big(D^m \cap (D^m + d\mathbf{v})\big)$.

From the above arguments, it follows that the spectral problem (3.2) is equivalent to (3.28). So, in the remainder of this subsection we will only study the latter problem. For simplicity, since the solutions coincide, we will omit the superscript $\widetilde{\ }$ and simply write u for $\widetilde{u}$.

We define u^α as the Floquet transform of u, *i.e.*,

$$u^\alpha = \sum_{m \in \mathbb{Z}} u(x - mL\mathbf{v}) e^{i\alpha m}.$$

The transformed solution u^α satisfies

$$\begin{cases} \Delta u^\alpha + \omega^2 u^\alpha = 0 & \text{in } \mathbb{R}^3 \setminus \partial D, \\ u^\alpha|_+ - u^\alpha|_- = f^\alpha & \text{on } \partial D, \\ \delta \dfrac{\partial u^\alpha}{\partial \nu}\Big|_+ - \dfrac{\partial u^\alpha}{\partial \nu}\Big|_- = g^\alpha & \text{on } \partial D, \\ e^{-i\alpha x_1} u^\alpha(x_1, x_2, x_3) & \text{is periodic in } x_1, \\ u^\alpha(x_1, x_2, x_3) & \text{satisfies the } \alpha\text{-quasiperiodic outgoing radiation condition} \\ & \quad \text{as } \sqrt{x_2^2 + x_3^2} \to \infty, \end{cases} \tag{3.30}$$

where

$$f^\alpha = \sum_{m \in \mathbb{Z}} f_m e^{-i\alpha m}, \qquad g^\alpha = \sum_{m \in \mathbb{Z}} g_m e^{-i\alpha m}. \tag{3.31}$$

From now on, we identify functions $u_m \in L^2(\partial D^m)$, for any m, with $u_0 \in L^2(\partial D)$ by translating the argument, *i.e.*, by $u_0(x) = u_m(x + mL\mathbf{v})$. Observe that under this identification, all operators $B^m, m \in \mathbb{N}$ coincide and will be denoted by $\mathcal{B}_0$.

The solution u^α can be represented using quasiperiodic layer potentials as

$$u^\alpha = \begin{cases} \hat{\mathcal{S}}^\omega_D[\psi^\alpha] & \text{in } D, \\ \mathcal{S}^{\alpha,\omega}_D[\phi^\alpha] & \text{in } Y \setminus \overline{D}, \end{cases}$$

where the pair $(\phi^{\alpha,i}, \phi^{\alpha,o}) \in L^2(\partial D)^2$ is the solution to

$$\mathcal{A}^\alpha(\omega,\delta)\begin{pmatrix}\psi^\alpha\\ \phi^\alpha\end{pmatrix} = \begin{pmatrix}\hat{\mathcal{S}}_D^\omega & -\mathcal{S}_D^{\alpha,\omega}\\ -\frac{1}{2}I+\hat{\mathcal{K}}_D^{\omega,*} & -\delta\left(\frac{1}{2}I+\left(\mathcal{K}_D^{-\alpha,\omega}\right)^*\right)\end{pmatrix}\begin{pmatrix}\phi^{\alpha,i}\\ \phi^{\alpha,o}\end{pmatrix} = \begin{pmatrix}-f^\alpha\\ -g^\alpha\end{pmatrix}. \tag{3.32}$$

Then the original solution u can be recovered by the inverse Floquet transform,

$$u(x) = \frac{1}{2\pi}\int_{Y^*} u^\alpha(x)\,\mathrm{d}\alpha.$$

Because of the quasiperiodicity of u^α, the solution u inside the region D^m satisfies

$$u = \hat{\mathcal{S}}_{D^m}^\omega\left[\frac{1}{2\pi}\int_{Y^*} e^{i\alpha m}\phi^{\alpha,i}\,\mathrm{d}\alpha\right]. \tag{3.33}$$

Similarly, inside the region $Y^m \setminus \overline{D^m}$, we have

$$\begin{aligned} u &= \frac{1}{2\pi}\int_{Y^*} \mathcal{S}_D^{\alpha,\omega}[\phi^{\alpha,o}]\,\mathrm{d}\alpha \\ &= \mathcal{S}_{D^m}^\omega\left[\frac{1}{2\pi}\int_{Y^*} e^{i\alpha m}\phi^{\alpha,o}\,\mathrm{d}\alpha\right] + \frac{1}{2\pi}\int_{Y^*}\sum_{n\in\mathbb{Z},n\neq m}\mathcal{S}_D^\omega[\phi^{\alpha,o}](\,\cdot - nL\mathbf{v})e^{in\alpha}\,\mathrm{d}\alpha. \end{aligned} \tag{3.34}$$

The last term in the right-hand side of (3.34) satisfies the homogeneous Helmholtz equation $(\Delta+\omega^2)u = 0$ in Y^m. Therefore, combining (3.33) and (3.34) together with (3.21), we can identify ϕ^m, ψ^m and $\widetilde{H}$ as follows:

$$\phi_m^{\alpha,i} = \frac{1}{2\pi}\int_{Y^*} e^{i\alpha m}\phi^{\alpha,i}\,\mathrm{d}\alpha, \quad \phi_m^{\alpha,o} = \frac{1}{2\pi}\int_{Y^*} e^{i\alpha m}\phi^{\alpha,o}\,\mathrm{d}\alpha, \tag{3.35}$$

and

$$\widetilde{H} = \frac{1}{2\pi}\int_{Y^*}\sum_{n\in\mathbb{Z},n\neq m}\mathcal{S}_D^\omega[\phi^{\alpha,o}](\,\cdot - nL\mathbf{v})e^{in\alpha}\,\mathrm{d}\alpha.$$

We define the operator $I_m : L^2(\partial D\times Y^*) \to L^2(\partial D)$, by

$$I_m[\varphi](x) = \frac{1}{2\pi}\int_{Y^*}\varphi(x,\alpha)e^{i\alpha m}\,\mathrm{d}\alpha.$$

Since the operator $\mathcal{A}_\alpha$ is invertible for ω in the band gap, we have from (3.32) that

$$\begin{pmatrix}\phi^{\alpha,i}\\ \phi^{\alpha,o}\end{pmatrix} = \mathcal{A}^\alpha(\omega,\delta)^{-1}\begin{pmatrix}-f^\alpha\\ -g^\alpha\end{pmatrix}.$$

Combining this together with (3.35) and (3.31), we obtain the following result.

Proposition 3.13. *As $d\to 0$, the mid-gap frequencies of (3.2) are precisely the values ω such that there is a nonzero solution $\phi^{\alpha,i}, \phi^{\alpha,o} \in L^2(\partial D\times Y^*)$ to the equation*

$$\begin{pmatrix}\phi^{\alpha,i}\\ \phi^{\alpha,o}\end{pmatrix} = -\left(\mathcal{A}^\alpha(\omega,\delta)\right)^{-1}\left(\sum_{m=0}^{\infty} e^{-im\alpha}\mathcal{B}_0 I_m\right)\begin{pmatrix}\phi^{\alpha,i}\\ \phi^{\alpha,o}\end{pmatrix}. \tag{3.36}$$

It is clear that $\mathcal{B}_0 = O(d)$. As $d\to 0$, it follows from Proposition 3.10 that any characteristic value $\omega = \omega(d)$ satisfies $\omega(d)\to\omega_j^\alpha$ for some ω_j^α. Denote

$$\omega_1^\diamond = \max_{\alpha\in Y^*}\omega_1^\alpha, \qquad \omega_2^\diamond = \min_{\alpha\in Y^*}\omega_2^\alpha.$$

The following lemma follows from Theorem 3.6.

Lemma 3.14. *To leading order in δ, the critical values $\omega_1^\diamond$ and $\omega_2^\diamond$ are attained at $\alpha^\diamond = \pi/L$, and for α close to $\alpha^\diamond$ we have*

$$\omega_1^\alpha = \omega_1^\diamond - c_1(\alpha-\alpha^\diamond)^2 + O\left(|\alpha-\alpha^\diamond|^3+\delta\right), \qquad \omega_2^\alpha = \omega_2^\diamond - c_2(\alpha-\alpha^\diamond)^2 + O\left(|\alpha-\alpha^\diamond|^3+\delta\right),$$

for some constants c_1, c_2.

In what follows, we will consistently use the superscript $^\diamond$ to denote corresponding quantity evaluated at the critical point $\alpha^\diamond = \pi/L$, to leading order in δ.

Lemma 3.15. *Assume that D_1 and D_2 are strictly convex. Then, in the dilute regime, we have the following:*

$$\begin{aligned} &\textit{Case } l_0 < 1/2: \qquad \langle \Phi_1^\diamond, \mathcal{B}_0 \Psi_1^\diamond \rangle < 0 \quad \textit{and} \quad \langle \Phi_2^\diamond, \mathcal{B}_0 \Psi_2^\diamond \rangle > 0, \\ &\textit{Case } l_0 > 1/2: \qquad \langle \Phi_1^\diamond, \mathcal{B}_0 \Psi_1^\diamond \rangle > 0 \quad \textit{and} \quad \langle \Phi_2^\diamond, \mathcal{B}_0 \Psi_2^\diamond \rangle < 0, \end{aligned}$$

for small enough ε, δ and d.

We refer to Appendix A.1 for the proof of Lemma 3.15. We will also need the following lemma.

Lemma 3.16. *We have*

$$\mathrm{Re}\left(\frac{1}{2\pi}\sum_{m=0}^{\infty} e^{-im\alpha}\int_0^{2\pi} \frac{e^{im\alpha'}}{1+c^2(\alpha'-\pi)^2}\,\mathrm{d}\alpha'\right) = \frac{1}{2}\left(\frac{1}{1+c^2(\alpha-\pi)^2} + \frac{1}{\pi c}\arctan(\pi c)\right).$$

Proof. Define $I(\alpha)$ as

$$I(\alpha) = \frac{1}{2\pi}\sum_{m=0}^{\infty} e^{-im\alpha}\int_0^{2\pi} \frac{e^{im\alpha'}}{1+c^2(\alpha'-\pi)^2}\,\mathrm{d}\alpha'.$$

Completing the Fourier series, we have

$$I(\alpha) + \overline{I(\alpha)} - \frac{1}{2\pi}\int_0^{2\pi} \frac{1}{1+c^2(\alpha'-\pi)^2}\,\mathrm{d}\alpha' = \frac{1}{1+c^2(\alpha-\pi)^2}.$$

Since $I(\alpha) + \overline{I(\alpha)} = 2\mathrm{Re}(I(\alpha))$, and since

$$\frac{1}{2\pi}\int_0^{2\pi} \frac{1}{1+c^2(\alpha'-\pi)^2}\,\mathrm{d}\alpha' = \frac{1}{\pi c}\arctan(\pi c),$$

the lemma follows. ☐

From Lemma 3.16 we find that

$$\frac{1}{2\pi}\sum_{m=0}^{\infty}(-1)^m\int_0^{2\pi} \frac{e^{im\alpha'}}{1+c^2(\alpha'-\pi)^2}\,\mathrm{d}\alpha' = \frac{1}{2} + \frac{1}{2\pi c}\arctan(\pi c). \tag{3.37}$$

The next theorem, which is the main result of this section, describes how the mid-gap frequencies emerge from the edges of the band gap.

Theorem 3.17. *Assume that D_1 and D_2 are strictly convex. For small enough d and δ, and in the case $l_0 > 1/2$, there are two mid-gap frequencies $\omega_1(d), \omega_2(d)$ such that $\omega_j(d) \to \omega_j^\diamond, j = 1,2$ as $d \to 0$. In the case $l_0 < 1/2$, there are no mid-gap frequencies as $d, \delta \to 0$.*

Proof. We seek solutions to (3.36) as $d \to 0$, corresponding to solutions ω in a small neighbourhood of $\omega_j^\diamond$ for $j = 1$ or $j = 2$. By Proposition 3.10 and Lemma 3.14, $(\mathcal{A}^\alpha)^{-1}$ has a pole at $\omega^\diamond$. Recall that we seek solutions $\omega = O(\sqrt{\delta})$ as $\delta \to 0$. At $\delta = 0$ and $\omega = 0$, the problem (3.2) decouples into a Neumann problem on each resonator, with constant solution inside each resonator. Since $\hat{\mathcal{S}}_D^0[u_j]$ is constant inside D, we find that

$$\phi^{\alpha,i} = c_1(\alpha)u_1 + c_2(\alpha)u_2$$

for some coefficients $c_1(\alpha)$ and $c_2(\alpha)$. It follows that the root function is such that the singularity of $(\mathcal{A}^\alpha)^{-1}$ does not vanish. Hence, from Proposition 3.10 and Lemma 3.14, the solution can be written, for α close to $\alpha^\diamond$, as

$$\begin{pmatrix}\phi^{\alpha,i}\\ \phi^{\alpha,o}\end{pmatrix} = \frac{\Psi_j^\diamond}{\omega - \omega_j^\diamond + c_j|\alpha-\alpha^\diamond|^2}h(\omega,\delta,d) + K_1(\omega,\alpha,\delta,d),$$

where $K_1(\omega,\alpha)$ is bounded uniformly in d for (ω,α) in a neighbourhood of $(\omega_j^\diamond, \alpha^\diamond)$ and h is constant in α. Applying (3.37), we then find that

$$\sum_{m=0}^{\infty} e^{-i\alpha m}\mathcal{B}_0 I_m \begin{pmatrix}\phi^{\alpha,i}\\ \phi^{\alpha,o}\end{pmatrix} = \frac{\mathcal{B}_0\Psi_j^\diamond}{2(\omega-\omega_j^\diamond)}h(\omega,\delta,d) + K_2$$

for some K_2 with norm of order $O(d)$ in a neighbourhood of $(\omega_j^\diamond, \alpha^\diamond)$. We then have

$$-\left(\mathcal{A}^\alpha(\omega,\delta)\right)^{-1}\sum_{m=0}^{\infty} e^{i\alpha m}\mathcal{B}_0 I_m \begin{pmatrix}\phi^{\alpha,i}\\ \phi^{\alpha,o}\end{pmatrix} = \frac{\Psi_j^\diamond}{\omega-\omega_j^\diamond + c_j|\alpha-\alpha^\diamond|^2}\frac{\langle \Phi_j^\diamond, \mathcal{B}_0\Psi_j^\diamond\rangle}{4\omega_j^\diamond|D_1|(\omega-\omega_j^\diamond)}h(\omega,\delta,d) + K_3.$$

Equation (3.36) then reads

$$\frac{\langle \Phi_j^\diamond, \mathcal{B}_0\Psi_j^\diamond\rangle}{4\omega_j^\diamond|D_1|(\omega-\omega_j^\diamond)} = 1 + O\left(\frac{d}{\sqrt{\omega-\omega_j^\diamond}}\right),$$

which has precisely one solution $\omega = \omega_1(d)$, expanded as

$$\omega_j(d) = \omega_j^\diamond + \frac{\langle \Phi_j^\diamond, \mathcal{B}_0\Psi_j^\diamond\rangle}{4\omega_j^\diamond|D_1|} + O(d^{3/2}).$$

From Lemma 3.15 it follows that $\omega_j(d)$ is inside the band gap precisely in the case $l_0 > 1/2$. □

Remark 3.18. It should be noted that the assumptions of convexity made in this section are not an intrinsic part of the method. This was only needed to simplify the arguments in the proof of Lemma 3.15. Indeed, the fictitious source method is repeatedly used in the rest of this work without any assumptions of convexity.

3.3 Integer unit length dislocation

In this section, we study the problem when the dislocation is an integer number of unit cell lengths. This is equivalent to the case when an integer multiple of dimers are removed from the original, periodic structure, thus creating a cavity. We will model this defect cavity problem using the fictitious source superposition method [6].

3.3.1 Fictitious sources for a removed resonator

Here, we describe the method of fictitious sources when a single resonator is removed. Throughout this subsection, Ω denotes a connected, bounded domain such that $\partial\Omega \in \mathcal{C}^{1,s}$, and U denotes a neighbourhood of Ω. Although the argument can be made for general Ω, we assume that Ω consists of two connected components $\Omega = \Omega_1 \cup \Omega_2$.

To study this problem, we consider the problem when the removed resonator Ω is reintroduced, along with fictitious dipole sources g on the boundary. We assume we have a reference solution u satisfying

$$\Delta u + \omega^2 u = 0 \qquad \text{in } U.$$

Let $\widetilde{u}$ satisfy the fictitious source problem

$$\begin{cases} \Delta\widetilde{u} + \omega^2\widetilde{u} = 0 & \text{in } U\setminus\partial\Omega,\\ \widetilde{u}|_+ - \widetilde{u}|_- = 0 & \text{on } \partial\Omega,\\ \delta\dfrac{\partial\widetilde{u}}{\partial\nu}\Big|_+ - \dfrac{\partial\widetilde{u}}{\partial\nu}\Big|_- = g & \text{on } \partial\Omega.\end{cases}$$

We want to determine the fictitious sources g such that $u = \widetilde{u}$ inside U. Any solution $\widetilde{u}$ can be represented as

$$\widetilde{u} = \begin{cases}\hat{\mathcal{S}}_\Omega^\omega[\phi^i] & \text{in } \Omega,\\ \hat{\mathcal{S}}_\Omega^\omega[\phi^o] + H & \text{in } U\setminus\Omega,\end{cases} \tag{3.38}$$

for some H satisfying $\Delta H + \omega^2 H = 0$ in U. Imposing $\widetilde{u} = u$ in U is equivalent to

$$\phi^i = \left(\hat{\mathcal{S}}_\Omega^\omega\right)^{-1}[u|_{\partial\Omega}], \qquad \phi^o = 0, \qquad H = u.$$

Moreover, using the jump conditions, we find the following expression of g.

Proposition 3.19. *The fictitious sources g and the layer density ϕ^i satisfy*

$$g = B(\omega,\delta)\phi^i, \quad B(\omega,\delta) = (\delta-1)\left(-\frac{1}{2}I + \hat{\mathcal{K}}_\Omega^{\omega,*}\right).$$

Conversely, by the unique continuation property of the Helmholtz equation, if g satisfies Proposition 3.19, then $\widetilde{u} = u$ in U.

3.3.2 Integral equation for the dislocated system

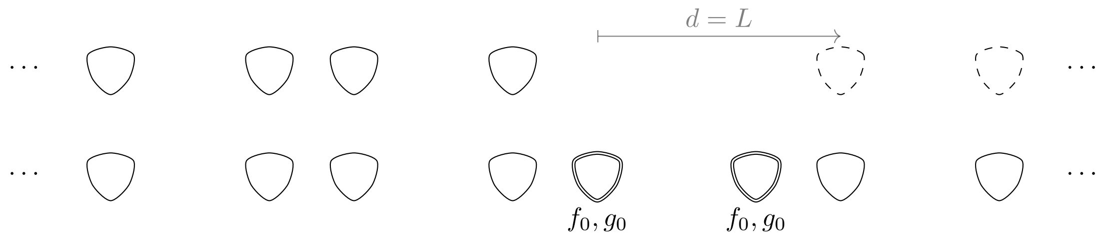


Figure 7: The dislocated system with dislocation equals to a multiple of the length of the unit cell (i.e. $d = NL$) is equivalent to the original array with the addition of so-called fictitious sources f_m, g_m, on the boundary of D^m for $m = 0, \ldots, N-1$. The case $N = 1$ is depicted here. Legend: —— untouched resonator, ═══ resonator with fictitious sources, - - - dislocated resonator.

We now assume that $2N$ resonators are removed, so that u satisfies (3.2) with

$$\mathcal{C}_d = \mathcal{C}_0 \setminus \left(\bigcup_{m=0}^{N-1} D^m \right). \tag{3.39}$$

Again, we model this using the fictitious source method as in (3.28), following the approach of Section 3.2.2. We put $f_m = 0$ for all m. Moreover, g_m will be defined as in Proposition 3.19 for all the removed resonators.

Assume we have a nonzero solution u to (3.2). Inside $Y^m, m = 0, 1, \cdots, N-1$, we can define the layer density ϕ_m^i as

$$\phi_m^i = \left(\hat{\mathcal{S}}_\Omega^\omega\right)^{-1} \left[u|_{\partial D^m}\right].$$

We then set the fictitious sources as

$$g_m = B_D \phi_m^i, \quad 0 < m < N-1, \tag{3.40}$$

and $g_m = 0$ otherwise. Here, B_D are the operators defined in Proposition 3.12 with the choice $\Omega = D$. Then, putting $\phi^o = 0$ and $H = u$, we obtain a solution $\widetilde{u}$ defined by (3.38), which coincides with u on $Y^m \setminus D^m$.

Conversely, if we have a nonzero solution $\widetilde{u}$ to (3.28), represented as (3.38) in Y^m and with sources satisfying (3.40), then we can define a nonzero solution $u = \widetilde{u}$ to (3.2) coinciding with $\widetilde{u}$ on $Y^m \setminus D^m$.

We introduce the extended operator on $\left(L^2(\partial D)\right)^2$,

$$B = \begin{pmatrix} 0 & 0 \\ B_D & 0 \end{pmatrix}.$$

For $\alpha \in Y^*$, define $\mathcal{B}^\alpha : \left(L^2(\partial D)\right)^{2N} \to \left(L^2(\partial D)\right)^2$ block-wise as

$$\mathcal{B}^\alpha = \begin{pmatrix} B & e^{-i\alpha} B & \cdots & e^{-(N-1)i\alpha} B \end{pmatrix},$$

and define $E^\alpha : \left(L^2(\partial D)\right)^2 \to \left(L^2(\partial D)\right)^{2N}$ block-wise as

$$E^\alpha = \begin{pmatrix} I \\ e^{i\alpha} I \\ e^{2i\alpha} I \\ \vdots \\ e^{(N-1)i\alpha} I \end{pmatrix}.$$

Next, we follow the approach of Section 3.2.2 to derive the integral equation for the dislocated system. By taking the Fourier transform, we obtain (3.30) together with the relation (3.35) for ϕ_m^i and ϕ_m^o. Putting

$$\Phi_N = \begin{pmatrix} \phi_0^i \\ \phi_0^o \\ \vdots \\ \phi_{N-1}^i \\ \phi_{N-1}^o \end{pmatrix},$$

we then obtain the following result.

Proposition 3.20. *For $\mathcal{C}_d$ as in* (3.39)*, the mid-gap frequencies of* (3.2) *are precisely the values ω such that there is a nonzero solution $\Phi_N \in \left(L^2(\partial D)\right)^{2N}$ to the equation*

$$\Phi_N = -\frac{1}{2\pi}\left(\int_{Y^*} E^\alpha \big(\mathcal{A}^\alpha(\omega,\delta)\big)^{-1}\mathcal{B}^\alpha \,\mathrm{d}\alpha\right)\Phi_N. \tag{3.41}$$

In order to analyse (3.41), we will need the following lemma, which is an immediate consequence of the structure of B.

Lemma 3.21. *We have*

$$\big(\mathcal{A}^\alpha(\omega,\delta)\big)^{-1}B = \begin{pmatrix} A_{12}B_D & 0 \\ A_{22}B_D & 0\end{pmatrix}. \tag{3.42}$$

As $\delta \to 0$ and $\omega = O(\sqrt{\delta})$, the operator A_{12} can be approximated by (3.15).

Although A_{22} can be computed explicitly, this will not enter into the remaining arguments and is therefore omitted. Due to the zero column in (3.42), it is clear that (3.41) reduces to an equation for $\phi_m^i, \cdots, \phi_{N-1}^i$ only. In fact, from (3.41), it follows that

$$\Phi_N^i = -\frac{1}{2\pi}\int_{Y^*}\begin{pmatrix} 1 & e^{i\alpha} & \cdots & e^{-(N-1)i\alpha} \\ e^{i\alpha} & 1 & \cdots & e^{-(N-2)i\alpha} \\ \vdots & \vdots & \ddots & \vdots \\ e^{(N-1)i\alpha} & e^{(N-2)i\alpha} & \cdots & 1\end{pmatrix}\begin{pmatrix} A_{12}B_D & 0 & \cdots & 0 \\ 0 & A_{12}B_D & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & A_{12}B_D\end{pmatrix}\Phi_N^i \,\mathrm{d}\alpha, \tag{3.43}$$

where

$$\Phi_N^i = \begin{pmatrix}\phi_0^i \\ \phi_1^i \\ \vdots \\ \phi_{N-1}^i\end{pmatrix}.$$

From Lemma 3.21, we obtain that, to leading order, ϕ_m^i is a linear combination of ψ_1 and ψ_2,

$$\phi_m^i = c_m\psi_1 + d_m\psi_2 + O(\omega).$$

Define, for $j = 1, 2$,

$$t_{i,j}^m = \frac{1}{2\pi}\int_{Y^*} e^{im\alpha}\left\langle \chi_{\partial D_i}, (I + A_{12}B_D)[\psi_j]\right\rangle \,\mathrm{d}\alpha.$$

Then, taking inner products $\langle \chi_{\partial D_i}, \cdot\rangle$ in equation (3.43) we find

$$\frac{1}{2\pi}\int_{Y^*} e^{im\alpha}\begin{pmatrix}\left\langle \chi_{\partial D_1}, I + A_{12}B_D[\phi_n^i]\right\rangle \\ \left\langle \chi_{\partial D_2}, I + A_{12}B_D[\phi_n^i]\right\rangle\end{pmatrix}\mathrm{d}\alpha = T_m\begin{pmatrix} c_n \\ d_n\end{pmatrix},$$

where T_m denotes the 2×2 matrix $\left(t_{i,j}^m\right)$. We thus have

$$\mathcal{T}_N(\omega)C_N = 0, \tag{3.44}$$

where we have defined

$$\mathcal{T}_N(\omega) = \begin{pmatrix} T_0 & T_{-1} & \cdots & T_{-(N-1)} \\ T_1 & T_0 & \cdots & T_{-(N-2)} \\ \vdots & \vdots & \ddots & \vdots \\ T_{N-1} & T_{N-2} & \cdots & T_0\end{pmatrix}, \qquad C_N = \begin{pmatrix} c_0 \\ d_0 \\ c_1 \\ \vdots \\ d_{N-1}\end{pmatrix}.$$

Observe that $\mathcal{T}_N$ is a block Toeplitz matrix generated by the symbol φ,

$$\varphi = \varphi(\alpha) = \begin{pmatrix}\varphi_{1,1} & \varphi_{1,2} \\ \varphi_{2,1} & \varphi_{2,2}\end{pmatrix}, \qquad \varphi_{i,j} = \left\langle \chi_{\partial D_i}, (I + A_{12}B_D)[\psi_j]\right\rangle, \quad i, j = 1, 2.$$

In the following lemma, we compute φ.

Lemma 3.22. *We have*

$$\varphi(\alpha) = -\frac{\mathrm{Cap}_{D_1}}{2} \begin{pmatrix} \Omega_1+\Omega_2 & -e^{i\theta_\alpha}\left(\Omega_1-\Omega_2\right) \\ -e^{-i\theta_\alpha}\left(\Omega_1-\Omega_2\right) & \Omega_1+\Omega_2 \end{pmatrix}, \qquad \det\varphi = \left(\mathrm{Cap}_{D_1}\right)^2\Omega_1\Omega_2,$$

where

$$\Omega_j = \frac{\left(\omega_j^\alpha\right)^2}{\omega^2-\left(\omega_j^\alpha\right)^2}, \quad j=1,2.$$

Proof. As computed in [5], we have

$$\left\langle \chi_{\partial D_j}, \left(-\frac{1}{2}I+\mathcal{K}_{D_j}^{\omega,*}\right)\psi_j\right\rangle = -\omega^2|D_1| + O(\omega^3),$$

and therefore,

$$\langle \chi_{\partial D_i}, B_D\psi_j\rangle = \omega^2|D_1|\delta_{i,j} + O(\omega^3),\ i,j=1,2.$$

From this, using Lemma 3.21 and (3.15) we find that

$$\begin{aligned} A_{12}B_D[\psi_1] &= \left(-1+\frac{\Omega_1+\Omega_2}{2}\right)\psi_1 - e^{-i\theta_\alpha}\frac{\Omega_1-\Omega_2}{2}\psi_2 + O(\omega), \\ A_{12}B_D[\psi_2] &= -e^{i\theta_\alpha}\frac{\Omega_1-\Omega_2}{2}\psi_1 + \left(-1+\frac{\Omega_1+\Omega_2}{2}\right)\psi_2 + O(\omega). \end{aligned}$$

The result now follows from the facts that $\langle \chi_{\partial D_i}, \psi_j\rangle = -\mathrm{Cap}_{D_i}\delta_{i,j}$ and $\mathrm{Cap}_{D_1} = \mathrm{Cap}_{D_2}$. □

Observe, in particular, that φ is a Hermitian matrix, and therefore the Toeplitz matrices $\mathcal{T}_N$ are also Hermitian. We define the "exchange" matrix $J_m \in \mathbb{R}^{2m}, m\in\mathbb{N}$, as

$$J_m = \begin{pmatrix} 0 & \cdots & 0 & 1 \\ 0 & \cdots & 1 & 0 \\ \vdots & \iddots & \vdots & \vdots \\ 1 & \cdots & 0 & 0 \end{pmatrix}.$$

The following lemma describes the centrosymmetry property of Hermitian Toeplitz matrices.

Lemma 3.23. *We have*

$$T_m = J_1\overline{T}_{-m}J_1, \qquad \mathcal{T}_N = J_N\overline{\mathcal{T}_N}J_N.$$

Proof. We have $J_1\varphi J_1 = \overline{\varphi}$, and therefore

$$\begin{aligned} T_m &= \frac{1}{2\pi}\int_{Y^*} e^{im\alpha}\varphi(\alpha)\,\mathrm{d}\alpha \\ &= \frac{1}{2\pi}\int_{Y^*} J_1\overline{e^{-im\alpha}\varphi(\alpha)}J_1\,\mathrm{d}\alpha \\ &= J_1\overline{T}_{-m}J_1. \end{aligned}$$

The second equality of the statement follows from the first one together with the Toeplitz structure of $\mathcal{T}_N$. □

We will study the solutions to (3.44) in the two cases $N=1$ and $N\to\infty$. The following proposition characterizes the solutions in the case $N=1$, corresponding to two removed resonators.

Proposition 3.24. *If $N=1$, the equation (3.44) has a nonzero solution if and only if ω is a solution to one of the two equations*

$$\frac{1}{2\pi}\int_{Y^*}\Big(\Omega_1\left(1\pm e^{i\theta_\alpha}\right) + \Omega_2\left(1\mp e^{i\theta_\alpha}\right)\Big)\,\mathrm{d}\alpha = 0. \tag{3.45}$$

If $l_0 < 1/2$, there are no solution to the equations (3.45), while if $l_0 > 1/2$, each equation has exactly one solution.

Proof. In the case $N = 1$, equation (3.44) reads

$$T_0 \begin{pmatrix} c_0 \\ d_0 \end{pmatrix} = 0,$$

which has a nonzero solution if and only if $\det T_0 = 0$. We have

$$\det T_0 = \frac{\left(\mathrm{Cap}_{D_1}\right)^2}{4} \left((I_1)^2 - |I_2|^2 \right),$$

where

$$I_1 = \frac{1}{2\pi} \int_{Y^*} (\Omega_1 + \Omega_2) \, \mathrm{d}\alpha, \qquad I_2 = \frac{1}{2\pi} \int_{Y^*} e^{i\theta_\alpha} (\Omega_1 - \Omega_2) \, \mathrm{d}\alpha.$$

By time-reversal symmetry, we have $\omega_j^{-\alpha} = \omega_j^{\alpha}, j = 1, 2$, which implies $I_2 \in \mathbb{R}$. Hence $\det T_0 = 0$ is equivalent to

$$I_1 - I_2 = 0, \text{ or } I_1 + I_2 = 0.$$

The remaining part of the proof is given in Appendix B. It is shown that that each of these equations has a unique solution in the case $l_0 > 1/2$, while no solutions in the case $l_0 > 1/2$. □

Denote by $\mathcal{T}(\omega)$ the infinite Toeplitz matrix corresponding to $\mathcal{T}_N(\omega)$, *i.e.*,

$$\mathcal{T}(\omega) = \begin{pmatrix} T_0 & T_{-1} & T_{-2} & \cdots \\ T_1 & T_0 & T_{-1} & \cdots \\ T_2 & T_1 & T_0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

which defines a bounded operator on the space l_2^2 of sequences of two-dimensional vectors. More precisely, l_2^2 consists of sequences $\{x_n\}_{n=0}^{\infty} \in l_2^2$ of vectors $x_n \in \mathbb{R}^2$ such that

$$\left(\sum_{n=0}^{\infty} \|x_n\|^2 \right)^{1/2} < \infty,$$

where $\|\cdot\|$ denotes the Euclidean norm.

Proposition 3.25. *Given ω_∞ inside the band gap such that $\mathcal{T}(\omega_\infty)$ has eigenvalue 0, there are two frequencies $\omega_1(N), \omega_2(N) \to \omega_\infty$ as $N \to \infty$, such that $\mathcal{T}_N$ is not invertible at $\omega_1(N), \omega_2(N)$.*

Proof. Let $X = \{x_n\}_{n=0}^{\infty} \in l_2^2$ be an eigenvector with $\mathcal{T}(\omega_\infty)X = 0$, and let $x \in \mathbb{R}^{2N}$ be a truncation of X. Since $\mathcal{T}(\omega_\infty)X = 0$, we have

$$\sum_{n=0}^{\infty} T_{k-n} x_n = 0 \tag{3.46}$$

for all $k \in \mathbb{N}$. Define $z_1, z_2 \in \mathbb{R}^{4N}$,

$$z_1 = \begin{pmatrix} x \\ J_N \overline{x} \end{pmatrix}, \qquad z_2 = \begin{pmatrix} x \\ -J_N \overline{x} \end{pmatrix}.$$

Then, using Lemma 3.23 we have

$$\mathcal{T}_{2N}(\omega_\infty) z_1 = \begin{pmatrix} \vdots \\ \sum_{n=0}^{N-1} T_{k-n} x_n + \sum_{n=0}^{N-1} T_{k-N-n} J_N \overline{x}_{N-1-n} \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ \sum_{n=0}^{N-1} T_{k-n} x_n + J_N \overline{\sum_{n=0}^{N-1} T_{2N-1-k-n} x_n} \\ \vdots \end{pmatrix}$$

for $k = 0, \cdots, 2N - 1$.

In view of (3.46), given $\varepsilon > 0$ we can choose N such that

$$\|\mathcal{T}_{2N} z_1\| < \varepsilon,$$

which implies that 0 is in the ε-pseudospectrum of $\mathcal{T}_{2N}(\omega_\infty)$ (see, for example, [56] for a thorough discussion on the definition and properties of pseudospectra). Since $\mathcal{T}_{2N}(\omega_\infty)$ is Hermitian, it follows that there is an eigenvalue μ_1 of $\mathcal{T}_{2N}(\omega_\infty)$ with $|\mu_1| < \varepsilon$. From this, it follows that there is a characteristic value ω_1 of $\mathcal{T}_{2N}(\omega)$ with $|\omega_1 - \omega_\infty| < K\varepsilon$ for some K independent on ε [7].

In the same way, we can show that given $\varepsilon > 0$ we can choose N such that

$$\|\mathcal{T}_{2N} z_2\| < \varepsilon,$$

and therefore there is a characteristic value ω_2 of $\mathcal{T}_{2N}(\omega)$ with $|\omega_2 - \omega_\infty| < K\varepsilon$ for some K independent on ε.

The above argument shows that $\omega_i(2N) \to \omega_\infty$ as $N \to \infty$. The case of the sequence $\omega_i(2N-1)$, corresponding to odd indices, follows similarly by choosing the truncation $x \in \mathbb{R}^{2N-1}$ and constructing z_1, z_2 analogously. □

Remark 3.26. The values of the nonzero solutions C_N to (3.44) correspond to the values of the mid-gap modes inside the dislocation region. The two pseudomodes z_1 and z_2 can be interpreted as approximations of the monopole and dipole modes, respectively, arising from the hybridization of the two semi-infinite half-structures. As the dislocation increases, *i.e.*, as $N \to \infty$, the strength of the hybridization decreases and the frequencies corresponding to these modes converge to the same value ω_∞.

Remark 3.27. The work in the present section shows the intimate connection between localized edge modes, and the fact that Toeplitz matrices have eigenvectors which are exponentially localized to the edges of the vector for sufficiently smooth symbols [56].

3.4 Dislocation larger than resonator width

In this section, we assume that the size of the dislocation is at least the width of one resonator. In other words, this means that each dislocated resonator does not overlap with the original resonator.

We begin by stating some facts from [13] on the eigenfunctions of the Neumann-Poincaré operator $\mathcal{K}_\Omega^{0,*}$ for a domain Ω with $\partial\Omega \in \mathcal{C}^{1,s}, 0 < s < 1$. We additionally assume that Ω is connected, which means that Ω can be thought of as a single resonator $\mathcal{D}_j^m$ in the dislocated array. The operator $\mathcal{K}_\Omega^{0,*}$ is known to be self-adjoint in the inner product $\langle\cdot,\cdot\rangle_{-1/2}$ on $H^{-1/2}(\partial\Omega)$ defined by

$$\langle u, v\rangle_{-1/2} = -\left\langle u, \mathcal{S}_\Omega^0[v]\right\rangle_{-1/2,1/2},$$

where $\langle\cdot,\cdot\rangle_{-1/2,1/2}$ denotes the duality pairing of $H^{-1/2}(\partial\Omega)$ and $H^{1/2}(\partial\Omega)$. Then, by the spectral theorem, the eigenfunctions $\psi_\Omega^j, j = 1, 2, 3, \cdots$, of $\mathcal{K}_\Omega^{0,*}$ form a basis of $H^{-1/2}(\partial\Omega)$ that is orthonormal with respect to $\langle\cdot,\cdot\rangle_{-1/2}$, while the functions $\mathcal{S}_\Omega^0[\psi_\Omega^j]$ form a basis of $H^{1/2}(\partial\Omega)$ that is orthogonal with respect to the inner product $\langle\cdot,\cdot\rangle_{1/2}$ defined by

$$\langle u, v\rangle_{1/2} = -\left\langle \left(\mathcal{S}_\Omega^0\right)^{-1}[u], v\right\rangle_{-1/2,1/2}.$$

The following addition theorem gives an expansion of Green's function $G^\omega(x,z)$, with the origin shifted by $z \notin \partial\Omega$, in terms of $\mathcal{S}_\Omega^\omega[\psi_\Omega^j](x)$.

Proposition 3.28. *For $x \in \partial\Omega$, $z \notin \partial\Omega$ and ω small enough, we have*

$$G^\omega(x,z) = -\sum_{i=1}^{\infty} \mathcal{S}_\Omega^\omega[\xi_\Omega^i](z)\mathcal{S}_\Omega^\omega[\psi_\Omega^i](x),$$

where $\xi_\Omega^i = \left(\mathcal{S}_\Omega^\omega\right)^{-1}\mathcal{S}_\Omega^0[\psi_\Omega^i]$.

Proof. The proof follows the same arguments as those in [13], where an analogous result was proven for Laplace Green's function G^0. We include the proof for the sake of completeness.

Since $\mathcal{S}_\Omega^0[\psi_\Omega^i]$ is a basis of $H^{1/2}(\partial\Omega)$, and since $\mathcal{S}_\Omega^\omega : H^{-1/2}(\partial\Omega) \to H^{1/2}(\partial\Omega)$ is invertible for ω small enough, we can expand G^ω for fixed z as follows,

$$G^\omega(\cdot,z) = \sum_{i=1}^{\infty} c_i(z)\mathcal{S}_\Omega^\omega[\psi_\Omega^i], \tag{3.47}$$

for some coefficients c_i with

$$\sum_{i=1}^{\infty} |c_i(z)|^2 < \infty, \quad z \notin \partial\Omega.$$

Moreover, ψ_i are orthonormal in $H^{-1/2}(\partial\Omega)$ equipped with $\langle\cdot,\cdot\rangle_{-1/2}$. From $(\mathcal{S}_\Omega^\omega)^* = \overline{\mathcal{S}_\Omega^\omega}$, we have

$$\begin{aligned} -\left\langle \overline{\xi_\Omega^i}, \mathcal{S}_\Omega^\omega[\psi_\Omega^j] \right\rangle_{-1/2,1/2} &= -\left\langle \left(\overline{\mathcal{S}_\Omega^\omega}\right)^{-1} \mathcal{S}_\Omega^0[\psi_\Omega^i], \mathcal{S}_\Omega^\omega[\psi_\Omega^j] \right\rangle_{-1/2,1/2} \\ &= \delta_{i,j}. \end{aligned} \tag{3.48}$$

Therefore,

$$\left\langle \overline{\xi_\Omega^i}, G^\omega(\cdot, z) \right\rangle_{-1/2,1/2} = \mathcal{S}_\Omega^\omega[\xi_\Omega^i](z). \tag{3.49}$$

Combining (3.47) together with (3.48) and (3.49) shows the claim. □

We denote $\Omega_d = \Omega + d\mathbf{v}$. We then have the following proposition.

Proposition 3.29. *Assume that $\overline{\Omega} \cap \overline{\Omega}_d = \emptyset$. Then, for $\phi \in H^{-1/2}(\partial\Omega_d)$, we have*

$$\mathcal{S}_{\Omega_d}^\omega[\phi](x - d\mathbf{v}) = \mathcal{S}_{\Omega_d}^\omega[V\phi](x), \quad x \in \partial\Omega_d,$$

where $V : H^{-1/2}(\partial\Omega_d) \to H^{-1/2}(\partial\Omega_d)$ is given by

$$V[\psi_{\Omega_d}^j] = \sum_{i=1}^{\infty} V_{i,j}\psi_{\Omega_d}^i, \qquad V_{i,j} = -\int_{\partial\Omega_d} \mathcal{S}_{\Omega_d}^\omega[\xi_{\Omega_d}^i](y - d\mathbf{v})\psi_{\Omega_d}^j(y)\,\mathrm{d}\sigma(y), \quad i,j \geq 1.$$

Proof. Since

$$\mathcal{S}_{\Omega_d}^\omega[\phi](x - d\mathbf{v}) = \int_{\partial\Omega_d} G^\omega(x, y + d\mathbf{v})\phi(y)\,\mathrm{d}\sigma(y),$$

and since $y + d\mathbf{v} \notin \partial\Omega_d$, the proposition follows from Proposition 3.28. □

We will also need the following addition theorem for the normal derivative of the single-layer potential. We let $\mathcal{D}_\Omega^\omega$ denote the double-layer potential (for details on this operator we refer, for example, to [7]).

Proposition 3.30. *Assume that $\overline{\Omega} \cap \overline{\Omega}_d = \emptyset$. Then, for $\phi \in H^{-1/2}(\partial\Omega_d)$, we have*

$$\frac{\partial \mathcal{S}_{\Omega_d}^\omega}{\partial \nu_{x-d\mathbf{v}}}[\phi](x - d\mathbf{v}) = W \left.\frac{\partial \mathcal{S}_{\Omega_d}^\omega}{\partial \nu_x}\right|_+ [\phi](x), \quad x \in \partial\Omega_d,$$

where $W : H^{-1/2}(\partial\Omega_d) \to H^{-1/2}(\partial\Omega_d)$ is given by

$$W\left(\frac{1}{2} + \mathcal{K}_{\Omega_d}^{\omega,*}\right)^{-1}[\psi_{\Omega_d}^j] = \sum_{i=1}^{\infty} W_{i,j}\psi_{\Omega_d}^i, \qquad W_{i,j} = \int_{\partial\Omega_d} \mathcal{D}_{\Omega_d}^\omega \mathcal{S}_{\Omega_d}^0[\psi_{\Omega_d}^i](y + d\mathbf{v})\psi_{\Omega_d}^j(y)\,\mathrm{d}\sigma(y), \quad i,j \geq 1.$$

Here, $\partial/\partial_{\nu_{x-d\mathbf{v}}}$ denotes the normal derivative with respect to Ω.

Proof. Analogously to the proof of Proposition 3.28, we can show that

$$\frac{\partial G^\omega}{\partial \nu_x}(x, y) = \sum_{i=1}^{\infty} \mathcal{D}_\Omega^\omega \mathcal{S}_\Omega^0[\psi_\Omega^i](y)\psi_\Omega^i(x), \qquad x \in \partial\Omega,\ y \notin \partial\Omega.$$

The result now follows by the same argument as the one in the proof of Proposition 3.29, using the jump relation

$$\left.\frac{\partial \mathcal{S}_{\Omega_d}^\omega}{\partial \nu_x}\right|_+ [\phi] = \left(\frac{1}{2} + \mathcal{K}_{\Omega_d}^{\omega,*}\right)[\phi].$$

□

3.4.1 Fictitious sources for the non-overlapping resonators

Here we describe the method of fictitious sources when a single resonator Ω is dislocated by d such that $\overline{\Omega}\cap\overline{\Omega}_d=\emptyset$, where $\Omega_d=\Omega+d\mathbf{v}$.

The arguments follow closely those of Section 3.2.1. Again, we consider the two problems (3.16) and (3.17) corresponding, respectively, to the original geometry with sources and to the dislocated geometry without sources. Representing the solutions as (3.20) and (3.21), we again arrive at the equations given in (3.22). Next, we will use Proposition 3.29 to study these equations.

Let U_0 be a neighbourhood of Ω not containing Ω_d. Imposing $u=\widetilde{u}$ in $U_0\setminus\Omega$ we find from Proposition 3.29 that

$$\Phi_d=\mathcal{P}_1\Phi,\qquad \text{where}\quad \mathcal{P}_1:=\begin{pmatrix}V^{-1} & 0\\ 0 & V^{-1}\end{pmatrix}Q.$$

As before, since Ω_d and Ω only differ by a translation, we can easily see that

$$\mathcal{A}_d=Q\mathcal{A}Q^{-1}.$$

In U_0, we can represent H as

$$H(x)=\sum_{i=1}^{\infty}c_i\mathcal{S}_{\Omega_d}^{\omega}(x),\quad x\in U_0.$$

This gives

$$\begin{pmatrix}H\big|_{\partial\Omega}\\ \delta\partial_\nu H\big|_{\partial\Omega}\end{pmatrix}=\mathcal{P}_2\begin{pmatrix}H\big|_{\partial\Omega_d}\\ \delta\partial_\nu H\big|_{\partial\Omega_d}\end{pmatrix},\qquad \text{where}\quad \mathcal{P}_2:=Q\begin{pmatrix}V^* & 0\\ 0 & W\end{pmatrix}.$$

Here, $V^*:H^{1/2}(\partial\Omega_d)\to H^{1/2}(\partial\Omega_d)$ is defined by

$$V^*\left[\mathcal{S}_{\Omega_d}^{\omega}[\psi_{\Omega_d}^j]\right]=\sum_{i=1}^{\infty}V_{i,j}\mathcal{S}_{\Omega_d}^{\omega}[\psi_{\Omega_d}^i].$$

Combining this together with (3.22) gives the following result.

Proposition 3.31. *The layer densities ϕ^i and ϕ^o and the fictitious sources f and g satisfy*

$$\begin{pmatrix}f\\ g\end{pmatrix}=B(\omega,\delta,d)\begin{pmatrix}\phi^i\\ \phi^o\end{pmatrix},\qquad B(\omega,\delta,d)=\mathcal{P}_2\mathcal{A}\mathcal{P}_1-\mathcal{A}.$$

3.4.2 Integral equation for dislocations larger than the resonator width

We define d_0 as the width of one resonator in the x_1-direction, *i.e.*,

$$d_0=\inf\left\{d\in\mathbb{R}^+\mid \overline{D_1}\cap\overline{D_1+d\mathbf{v}}=\emptyset\right\}.$$

We define

$$\mathcal{B}_d=\hat{\mathcal{P}}_2\hat{\mathcal{A}}\hat{\mathcal{P}}_1-\hat{\mathcal{A}},$$

where

$$\hat{\mathcal{A}}=\begin{pmatrix}\hat{\mathcal{S}}_D^{\omega} & -\hat{\mathcal{S}}_D^{\omega}\\ -\frac{1}{2}I+\hat{\mathcal{K}}_D^{\omega,*} & -\delta\left(\frac{1}{2}I+(\hat{\mathcal{K}}_D^{\omega})^*\right)\end{pmatrix},\quad \hat{\mathcal{P}}_1=\begin{pmatrix}\hat{V}^{-1} & 0\\ 0 & \hat{V}^{-1}\end{pmatrix},\quad \hat{\mathcal{P}}_2=\begin{pmatrix}\hat{V}^* & 0\\ 0 & \hat{W}\end{pmatrix},$$

with

$$\hat{V}=\begin{pmatrix}V_1 & 0\\ 0 & V_2\end{pmatrix},\quad \hat{V}^*=\begin{pmatrix}V_1^* & 0\\ 0 & V_2^*\end{pmatrix},\quad \hat{W}=\begin{pmatrix}W_1 & 0\\ 0 & W_2\end{pmatrix},$$

where V_j,V_j^*,W_j are defined as in Section 3.4.1 with $\Omega=D_j$, $j=1,2$. Then $\mathcal{B}_d$ describes the fictitious sources for the dimer. Following the same arguments as those in Section 3.2.2, we obtain the following result.

Proposition 3.32. *For $d>d_0$, the mid-gap frequencies of* (3.2) *are precisely the values ω such that there is a nonzero solution $\phi^{\alpha,i},\phi^{\alpha,o}\in L^2(\partial D\times Y^*)$ to the equation*

$$\begin{pmatrix}\phi^{\alpha,i}\\ \phi^{\alpha,o}\end{pmatrix}=-\left(\mathcal{A}^{\alpha}(\omega,\delta)\right)^{-1}\left(\sum_{m=0}^{\infty}e^{-im\alpha}\mathcal{B}_dI_m\right)\begin{pmatrix}\phi^{\alpha,i}\\ \phi^{\alpha,o}\end{pmatrix}.\tag{3.50}$$

Our next goal is to show that as d increases, any mid-gap frequency will remain inside the band gap. We begin by stating the following lemma, which is the analogue of Lemma 3.15.

Lemma 3.33. *Assume that the resonators are in the dilute regime specified by (3.6). Then, for $d \in (d_0, \infty)$ and for small enough ε and δ*

$$|\langle \Phi_j^\diamond, \mathcal{B}_d \Psi_j^\diamond \rangle| > K > 0, \qquad j = 1, 2,$$

for some constant K independent of d.

The proof of this result is given in Appendix A.2. We are now ready to state and prove the main result of this section. Recall that we denote the edges of the band gap by

$$\omega_1^\diamond = \max_{\alpha \in Y^*} \omega_1^\alpha, \qquad \omega_2^\diamond = \min_{\alpha \in Y^*} \omega_2^\alpha.$$

We then have the following proposition.

Proposition 3.34. *For $d > d_0$ and δ small enough, any mid-gap frequency $\omega(d)$ is bounded away from the edges of the band gap, i.e.*

$$|\omega(d) - \omega_j^\diamond| > c, \qquad j = 1, 2,$$

for all $d > d_0$ and for some positive constant c independent of d.

Proof. We want to show that there are no solutions to (3.50) that approaches the edges of the band gap. Assume the contrary, *i.e.* that we have a solution $\omega \to \omega_j^\diamond$. Following the proof of Theorem 3.17, we obtain

$$\frac{\langle \Phi_j^\diamond, \mathcal{B}_d \Psi_j^\diamond \rangle}{4\omega_j^\diamond |D_1| (\omega - \omega_j^\diamond)} = 1 + o(1),$$

as $\omega \to \omega_j^\diamond$. But since $|\langle \Phi_1^\diamond, B \Psi_1^\diamond \rangle| > K > 0$ for all d, this equation has no solution. □

3.5 Theorem on mid-gap frequencies

We now combine the results of the two previous sections, namely Proposition 3.24, Proposition 3.25 and Proposition 3.34, into the following theorem.

Theorem 3.35. *Assume that the resonators are in the dilute regime specified by* (3.6)*. Then, for small enough δ and ε, there exists some $d_0 = O(\varepsilon)$ such that there are two mid-gap frequencies $\omega_1(d)$ and $\omega_2(d)$ for all $d \in [d_0, \infty)$, both of which converge to the same value ω_∞ as $d \to \infty$.*

Corollary 3.36. *Assume that the resonators are in the dilute regime specified by* (3.6)*. Then, for small enough δ and ε, there is an interval $\mathcal{I} = [\omega_1(d_0), \omega_2(d_0)]$ within the band gap such that if $\omega \in \mathcal{I} \setminus \{\omega_\infty\}$, then there exists some $d > d_0$ such that $\omega \in \{\omega_1(d), \omega_2(d)\}$.*

Corollary 3.36 says that any frequency $\omega \in \mathcal{I} \setminus \{\omega_\infty\}$ is a mid-gap frequency of the structure for some dislocation d. From Proposition 3.24, we have an explicit way to compute the interval $\mathcal{I}$, and as we will see from the numerical computations, this interval contains the middle region of the band gap. What we have shown is that we can choose a frequency in the middle of the band gap and create a structure having this as a resonant frequency, thus corresponding to exponentially localized edge modes that are stable under perturbations.

Proposition 3.25 and Theorem 3.17 hint to the physical origin of the two mid-gap frequencies. For infinitely large dislocations, the system corresponds to two identical semi-infinite systems which each support edge modes with frequency ω_∞. As these two semi-infinite systems approach each other, they hybridize and ω_∞ splits into two frequencies, corresponding to monopole and dipole modes.

Seen from the other direction, $d = 0$ corresponds to the periodic structure, which is known to have a band gap and no mid-gap frequencies. As d increases from 0, two mid-gap frequencies will emerge, one from each edge of the band gap.

Remark 3.37. The requirement that $d > d_0$ in Theorem 3.35 was used in Section 3.4. We assumed that the dislocation was sufficiently large that the translated resonators do not overlap with the originals. Since we are assuming that the structure is dilute and the size of each resonator is $O(\varepsilon)$, $d_0 = O(\varepsilon)$. The non-overlapping assumption was made purely to simplify the analysis and not for any physical reason. Based on this, we conjecture that Theorem 3.35 is true for all $d \in (0, \infty)$, which is in accordance with our numerical experiments. In this case, the interval $\mathcal{I}$ in Corollary 3.36 would include all of the band gap.

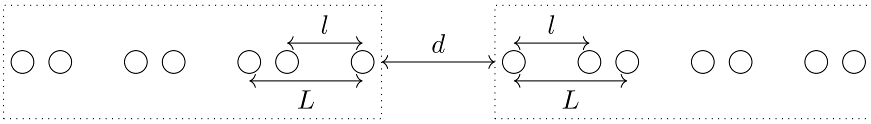


Figure 8: An array of 14 spherical resonators formed by separating an array of 7 dimers in the centre by a dislocation distance $d > 0$.

4 Finite arrays of resonators

In this section, we will study the finite array of resonators which is a truncation of the system studied in Section 3. We will see that this structure, which represents the physical manifestation of our above analysis, shares the important properties of the infinite system. We will also conduct a stability analysis of the structure.

Consider the structure D that is a truncation of the infinite, dislocated array $\mathcal{C}_d$ studied in Section 3. Let $M = 4K + 2$ for some $K \in \mathbb{Z}_+$, and assume

$$D = D_2^{-K-1} \cup \left(\bigcup_{m=-1}^{-K} D_1^m \cup D_2^m \right) \cup \left(\bigcup_{m=0}^{K-1} (D_1^m \cup D_2^m) + d\mathbf{v} \right) \cup \left(D_1^K + d\mathbf{v} \right), \tag{4.1}$$

where D_1^m, D_2^m are as in Section 3, so that the symmetry assumptions (3.1) are satisfied. Moreover, we assume $l_0 > 1/2$ (recall that $l_0 = l/L$), corresponding to the case where the array supports edge modes.

We model wave scattering by D with the Helmholtz problem

$$\begin{cases} \Delta u + \omega^2 u = 0 & \text{in } \mathbb{R}^3 \setminus \partial D, \\ u|_+ - u|_- = 0 & \text{on } \partial D, \\ \delta \dfrac{\partial u}{\partial \nu}\Big|_+ - \dfrac{\partial u}{\partial \nu}\Big|_- = 0 & \text{on } \partial D, \\ |x| \left(\frac{\partial}{\partial |x|} - ik \right) u \to 0 & \text{as } |x| \to \infty. \end{cases}$$

The resonant frequencies and eigenmodes of this finite system of resonators can be expressed in terms of the eigenpairs of the associated *capacitance matrix*. Let $V_j, j = 1, \cdots, M$, be the solution to

$$\begin{cases} \Delta V_j = 0 & \text{in } R^3 \setminus D, \\ V_j = \delta_{ij} & \text{on } \partial D_i, \\ V_j(x) = O\left(\frac{1}{|x|}\right) & \text{as } |x| \to \infty. \end{cases}$$

We then define the capacitance matrix $C = (C_{i,j})$

$$C_{i,j} := - \int_{\partial D_i} \frac{\partial V_j}{\partial \nu}\Big|_+ \mathrm{d}\sigma, \quad i, j = 1, \cdots, M.$$

The following theorem, first proved in [9], shows that the eigenvalues of C determine the resonant frequencies of the finite structure.

Theorem 4.1. *The characteristic values $\omega_j = \omega_j(\delta)$, $j = 1, \cdots, M$, of $\mathcal{A}(\omega, \delta)$ can be approximated as*

$$\omega_j = \sqrt{\frac{\delta \lambda_j}{|D_1|}} + O(\delta),$$

where λ_j, $j = 1, \cdots, M$, are the eigenvalues of the capacitance matrix C and $|D_1|$ is the volume of each individual resonator.

4.1 Behaviour for large dislocations

As the separation distance d becomes large, the capacitance matrix converges to a block diagonal form. This is because, for large d, we have two systems of $M/2$ resonators whose interactions diminish with increasing d. This is made precise by the following lemma.

Lemma 4.2. *As the dislocation size $d \to \infty$, the capacitance matrix has the form*

$$C = \begin{pmatrix} \widetilde{C} & 0 \\ 0 & \widetilde{C}^\star \end{pmatrix} + O(d^{-1}),$$

where $\widetilde{C}$ is the capacitance matrix of the $M/2$-resonator system $D_1 \cup \cdots \cup D_{M/2}$, and $\widetilde{C}^\star$ is the rearranged matrix

$$\widetilde{C}^\star_{i,j} := C_{M+1-i,M+1-j}.$$

Proof. We can use the jump conditions to show that the capacitance coefficients $C_{i,j}$ are given by

$$C_{i,j} = -\int_{\partial D_i} \psi_j \,\mathrm{d}\sigma, \quad i,j = 1, \cdots, M,$$

where the functions ψ_j are defined as

$$\psi_j = (\mathcal{S}_D^0)^{-1}[\chi_{\partial D_j}].$$

We make the identification $\partial D = \partial D_1 \times \cdots \times \partial D_M$ and use this to write the single layer potential $\mathcal{S}_D^0$ in a decomposed matrix form, as

$$\mathcal{S}_D^0 = S_I + S_{II}, \tag{4.2}$$

where S_I and S_{II} are block matrices defined as

$$[S_I]_{ij} := \begin{cases} \mathcal{S}_{D_i}^0|_{\partial D_j}, & \text{if } i,j \le M/2 \text{ or } i,j \ge M/2+1, \\ 0, & \text{otherwise,} \end{cases}$$

$$[S_{II}]_{ij} := \begin{cases} 0, & \text{if } i,j \le M/2 \text{ or } i,j \ge M/2+1, \\ \mathcal{S}_{D_i}^0|_{\partial D_j}, & \text{otherwise.} \end{cases}$$

The decomposition (4.2) has been chosen so that S_I contains precisely the parts of $\mathcal{S}_D^0$ that are unaffected by varying the parameter d. Conversely, based on the decay of Green's function G^0 we can see that, if $i \le M/2$ and $j \ge M/2+1$ or vice versa, it holds that

$$\|\mathcal{S}_{D_j}^0|_{\partial D_i}\|_{\mathcal{B}(L^2(\partial D_j), H^1(\partial D_i))} = O(d^{-1}),$$

as $d \to \infty$, hence

$$\|S_{II}\|_{\mathcal{B}(L^2(\partial D), H^1(\partial D))} = O(d^{-1}).$$

Therefore, $\|S_I^{-1} S_{II}\| = O(d^{-1})$ so we may use a Neumann series to see that

$$\begin{aligned} (\mathcal{S}_D^0)^{-1}[\chi_{\partial D_j}] &= (S_I + S_{II})^{-1}[\chi_{\partial D_j}] \\ &= (I + S_I^{-1} S_{II})^{-1} S_I^{-1}[\chi_{\partial D_j}] \\ &= (I - S_I^{-1} S_{II})[\phi_j] + O(d^{-1}), \end{aligned}$$

where $\phi_j := S_I^{-1}[\chi_{\partial D_j}]$. Therefore,

$$C_{i,j} = -\int_{\partial D_i} (\mathcal{S}_D^0)^{-1}[\chi_{\partial D_j}] \,\mathrm{d}\sigma = -\int_{\partial D_i} (I - S_I^{-1} S_{II})[\phi_j] \,\mathrm{d}\sigma + O(d^{-1}).$$

Suppose that $i \le M/2$ and $j \ge M/2+1$ or vice versa. Then since $(S_I)^{-1}$ is also block diagonal we can see that $\phi_j|_{\partial D_i} = 0$ so $\int_{\partial D_i} \phi_j \,\mathrm{d}\sigma = 0$. Thus, $C_{i,j} = O(d^{-1})$. Conversely, if $i,j \le M/2$ then $(S_I^{-1} S_{II})[\phi_j]|_{\partial D_i} = 0$ so we find that

$$\begin{aligned} C_{i,j} &= -\int_{\partial D_i} \phi_j \,\mathrm{d}\sigma + O(d^{-1}) \\ &= \widetilde{C}_{i,j} + O(d^{-1}). \end{aligned}$$

In the case that $i,j \ge M/2+1$ the result with $\widetilde{C}^\star$ follows similarly. □

Remark 4.3. At its heart, Lemma 4.2 is a consequence of the decay of the Helmholtz Green's function in free space and not a particular property of the system studied here. The dislocation of any general collection of (finitely many) resonators would yield a similar result (albeit without such elegant notation for the two blocks, which is a consequence of the structure's symmetry).

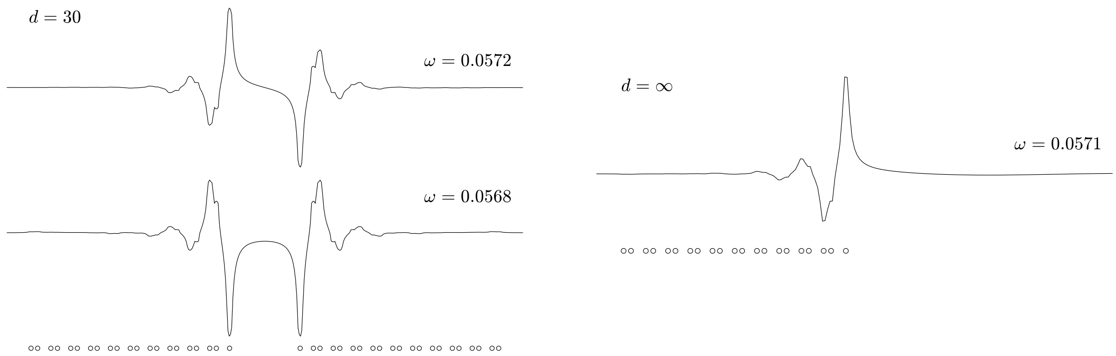


Figure 9: Left: The two edge modes for an array of 42 spherical resonators of radius 1*. Here, we simulate an array with parameters* $L = 9$*,* $l = 6$*,* $d = 30$ *and* $\delta = 1/7000$*. Right: For comparison, the edge mode of the corresponding 'half system' is shown, which can be thought of as the* $d = \infty$ *case. In both cases, the eigenmodes are shown directly above the corresponding system of resonators*

Remark 4.4. $\widetilde{C}^\star$ corresponds to the capacitance matrix of the $M/2$-resonator system $D_{M/2+1} \cup \cdots \cup D_M$. This is the same system as that for which $\widetilde{C}$ is the capacitance matrix, but with the resonators labelled in the reverse order. That they have the same eigenvalues is easy to see from the fact that $\widetilde{C}^\star = J\widetilde{C}J$, where J is the exchange matrix (1 on the off-diagonal and 0 elsewhere). Thus, in the limit as $d \to \infty$ the eigenvalues of C converge to $M/2$ pairs of values.

The behaviour for large d can be understood by examining the eigenmodes, examples of which are given in Figure 9. The dislocation splits the structure into two "half structures" which interact with one another. This coupling leads to the creation of two resonant modes, with monopole- and dipole-like characteristics (*cf.* [9]), which are the two edge modes.

4.2 Stability analysis

We consider the simplest example of a resonator array of the form (4.1), which has just six resonators arranged as three pairs. The geometry of this structure is parametrised by l and L (Figure 8). We wish to study how robust the system is with respect to variations in

We know from Lemma 4.2 that as $d \to \infty$ this system will behave like two separate three-resonator systems. Even in the case of a three-resonator system, finding explicit representations for the entries of the capacitance matrix (with a view to *e.g.* calculating its eigenvalues) is a challenging problem. Consider the case of a *dilute* array of resonators: that is, a structure where the distances between the resonators (l and L) are much larger than the size of each individual resonator. In this case, we can recall the following representation of the capacitance matrix, proved in [3].

Lemma 4.5. *Consider a dilute system of* M *identical subwavelength resonators with size of order* ε*, given by*

$$D = \bigcup_{j=1}^{M} (\varepsilon B + z_j),$$

where $0 < \varepsilon \ll 1$*,* B *is a fixed domain of unit size and* z_j *represents the translated position of each resonator. In the limit as* $\varepsilon \to 0$*, the capacitance matrix is given by*

$$C_{i,j} = \begin{cases} \varepsilon \mathrm{Cap}_B + O(\varepsilon^3), & i = j, \\ -\dfrac{\varepsilon^2 (\mathrm{Cap}_B)^2}{4\pi |z_i - z_j|} + O(\varepsilon^3), & i \neq j, \end{cases} \tag{4.3}$$

where $\mathrm{Cap}_B := -\int_{\partial B} (\mathcal{S}_B^0)^{-1}[\chi_B] \, \mathrm{d}\sigma$.

In the case of a three-resonator system with $|z_1 - z_2| = l$ and $|z_1 - z_3| = L$, we can use the expansion (4.3) to show that the eigenvalues of the capacitance matrix are given, as $\varepsilon \to 0$, by

$$\lambda_k = \varepsilon \mathrm{Cap}_B + \varepsilon^2 \frac{(\mathrm{Cap}_B)^2 \gamma}{2\sqrt{3}\pi} \cos\left[\frac{1}{3}\left(\arccos\left(\frac{-3\sqrt{3}}{lL(L-l)\gamma^3}\right) + 2k\pi\right)\right] + O(\varepsilon^3), \tag{4.4}$$

for $k = 1,2,3$, where $\gamma = \gamma(l,L) := \sqrt{l^{-2}+L^{-2}+(L-l)^{-2}}$. The convergence of the six resonant frequencies of the six-resonator system to these three values is demonstrated in Figure 10a.

We know that, in order for the undislocated structure ($d = 0$) to have a subwavelength band gap it must be asymmetric, *i.e.* $l/L \neq 1/2$ (see *e.g.* [3]). In the case of a sufficiently asymmetric structure, we can show that the middle eigenvalue is more stable with respect to changes in the resonator positions. This is achieved by Lemma 4.6, which describes the extent to which the eigenvalues (4.4) are affected by variations in the parameters l and L. In particular, it says that if $l' := L - l$ is sufficiently small then

$$\left|\frac{\partial \lambda_2}{\partial l}\right| \ll \left|\frac{\partial \lambda_1}{\partial l}\right|, \quad \left|\frac{\partial \lambda_2}{\partial l}\right| \ll \left|\frac{\partial \lambda_3}{\partial l}\right|,$$

and that the dependence of all three eigenvalues on L is comparatively negligible.

Lemma 4.6. *Let $l' := L - l$. As $l' \to 0^+$, it holds that*

$$\left|\frac{\partial \lambda_1}{\partial l}\right| \to \infty, \quad \left|\frac{\partial \lambda_2}{\partial l}\right| = O(1), \quad \left|\frac{\partial \lambda_3}{\partial l}\right| \to \infty.$$

Meanwhile, for $k = 1,2,3$,

$$\left|\frac{\partial \lambda_k}{\partial L}\right| = O(l').$$

Proof. Define the functions

$$c(l',L,k) := \cos\left[\frac{1}{3}\left(\arccos\left(\frac{-3\sqrt{3}}{l'L(L-l')\gamma(l',L)^3}\right) + 2k\pi\right)\right], \quad 0 < l' < L,\ k = 1,2,3,$$

and

$$s(l',L,k) := \sin\left[\frac{1}{3}\left(\arccos\left(\frac{-3\sqrt{3}}{l'L(L-l')\gamma(l',L)^3}\right) + 2k\pi\right)\right], \quad 0 < l' < L,\ k = 1,2,3.$$

As $l' \to 0^+$ it holds that

$$\begin{aligned} &c(l',L,1) \to -\frac{\sqrt{3}}{2}, \quad &&c(l',L,2) \to 0, \quad &&c(l',L,3) \to \frac{\sqrt{3}}{2},\\ &s(l',L,1) \to \frac{1}{2}, &&s(l',L,2) \to -1, &&s(l',L,3) \to \frac{1}{2}. \end{aligned} \tag{4.5}$$

In addition to this, for fixed L and k we see that, as $l' \to 0^+$,

$$\frac{\partial \lambda_k}{\partial l'} \sim \frac{\varepsilon^2(\mathrm{Cap}_B)^2}{2\sqrt{3}\pi}\left[-\frac{1}{(l')^2}c(l',L,k) - \frac{2\sqrt{3}}{L^2}s(l',L,k)\right],$$

where the notation $\sim$ is used to mean that $f \sim g$ if and only if $\lim f/g = 1$. From this and (4.5) we can see that, as $l' \to 0^+$,

$$\frac{\mathrm{d}\lambda_1}{\mathrm{d}l'} \to \infty, \quad \frac{\mathrm{d}\lambda_3}{\mathrm{d}l'} \to -\infty.$$

Conversely, using Taylor series expansions we can see that, as $l' \to 0^+$,

$$c(l',L,2) = \frac{\sqrt{3}}{L^2}(l')^2 + O\left((l')^3\right),$$

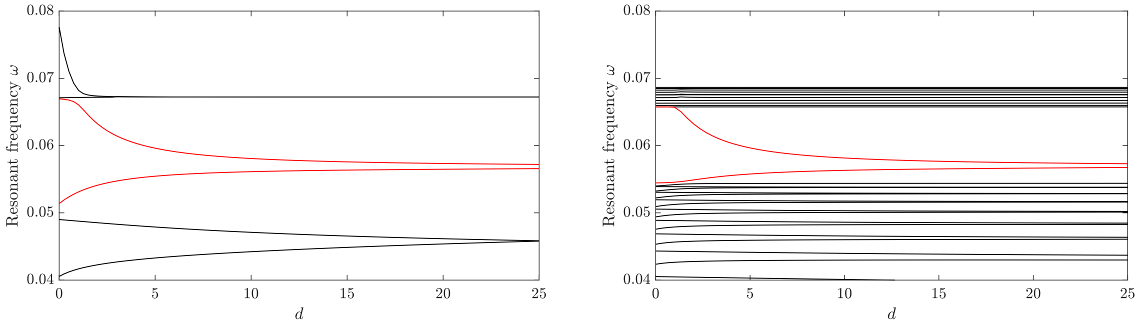
hence as $l' \to 0^+$ it holds that

$$\frac{\partial \lambda_2}{\partial l'} \to \frac{\varepsilon^2(\mathrm{Cap}_B)^2}{2\pi L^2}.$$

Likewise, the result for $\mathrm{d}\lambda_k/\mathrm{d}L$ follows from the fact that, as $l' \to 0^+$,

$$\frac{\mathrm{d}\lambda_k}{\mathrm{d}L} \sim \frac{\varepsilon^2(\mathrm{Cap}_B)^2}{2\sqrt{3}\pi}\left[-\frac{2l'}{L^3}c(l',L,k) - \frac{2\sqrt{3}l'}{L^3}s(l',L,k)\right],$$

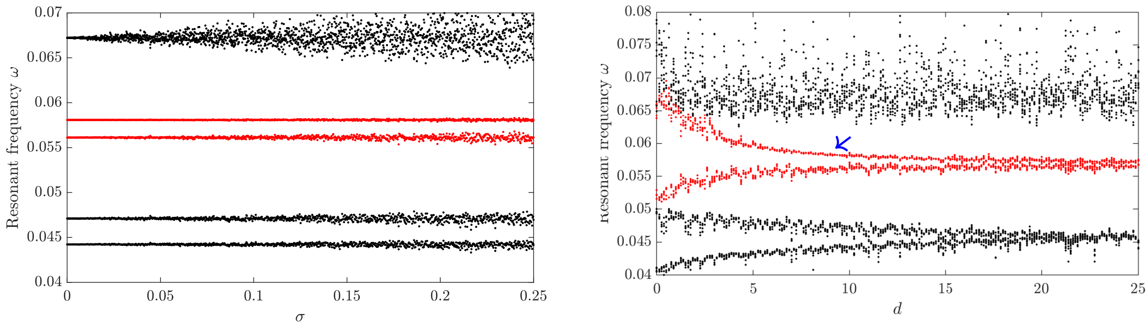
for $k = 1,2,3$. □



(a) Resonator array with 6 resonators.

(b) Resonator array with 42 resonators.

Figure 10: Simulation of the resonant frequencies of different subwavelength resonator arrays as the dislocation d is increased.



(a) Increasing imperfection deviation σ, for $d = 10$.

(b) Increasing dislocation d, for $\sigma = 0.2$.

Figure 11: Analysis of the stability of the resonant frequencies of a system of six resonators. An array of six resonators with dislocation size d is repeatedly simulated after random imperfections, drawn from the distribution $\mathcal{N}(0, \sigma^2)$, are introduced to the resonator positions. An arrow indicates the position of minimum variance.

In Figures 10 and 11, simulations were performed on spherical resonators with radius 1 arranged with distances $L = 9$ and $l = 6$ (as depicted in Figure 8), and with $\delta = 1/7000$. The multipole expansion method was used to find the characteristic values of $\mathcal{A}$ (see the appendix of [3] for details).

The stability that is predicted by Lemma 4.6 can be investigated numerically by repeatedly introducing random imperfections to the structure (see Figure 11). It can, firstly, be observed that the middle eigenvalues (which both converge to λ_2, as defined in (4.4), as $d \to \infty$) are more stable, as expected. It is also interesting to observe how the stability varies as a function of the dislocation d. The minimal variance of any resonant frequency is observed for ω_4 when $d \approx 8$, as indicated by the arrow in Figure 11b. At this point, ω_4 is in the centre of the band gap so it is as far as possible from the other (unlocalized) modes, consistent with *e.g.* [18, 43]. This demonstrates the value of being able to control the position of mid-gap frequencies within the band gap.

5 Concluding remarks

In this paper, we have studied a one-dimensional array of subwavelength resonators capable of robustly manipulating waves on subwavelength scales. This is based on the principle that eigenmodes corresponding to mid-gap frequencies that are far from the edges of that band gap will be strongly localized in space and robust to structural imperfections. Thus, the goal was to design a structure that could be manipulated so as to place a mid-gap frequency at any given point within the band gap. This can be achieved by introducing a dislocation to an array of subwavelength resonator pairs. In this paper we have proved that the mid-gap frequencies emerge from the edges of the band gap, and span an interval in the middle of the band gap.

Our study of the periodic structure was complemented by an analysis of the corresponding finite array of resonators. Created by truncating the infinite array, this physically-realizable structure shared the spectral behaviour of the infinite array. Further, a stability analysis confirmed the value of being able to fine-tune the structure in order to optimise robustness.

In the setting of the Schrödinger operator, two-dimensional structures exhibiting edge modes have been studied via the bulk-edge correspondence. It is well known that materials with nonzero bulk index can be achieved, for example, by perturbing honeycomb-like materials exhibiting *Dirac cones* [20, 24, 25]. Dirac cones have also been shown to exist in two-dimensional honeycomb structures of subwavelength resonators [10], suggesting the potential for analogous results in this setting.

A Proofs of Lemma 3.15 and Lemma 3.33

Here we give proofs of Lemma 3.15 and Lemma 3.33. Qualitatively, these results describe the strength of the fictitious source interactions in the two cases studied in Section 3.2 and Section 3.4, respectively.

A.1 Proof of Lemma 3.15

We will expand $\mathcal{S}_D^\omega$ and $\mathcal{K}_D^{\omega,*}$ in the dilute regime specified by (3.6). Recall the matrix form of $\mathcal{S}_D^\omega$:

$$\mathcal{S}_D^\omega = \begin{pmatrix} \mathcal{S}_{D_1}^\omega & \mathcal{S}_{D_2}^\omega\big|_{\partial D_1} \\ \mathcal{S}_{D_1}^\omega\big|_{\partial D_2} & \mathcal{S}_{D_2}^\omega \end{pmatrix} = \hat{\mathcal{S}}_D^\omega + \begin{pmatrix} 0 & \mathcal{S}_{D_2}^\omega\big|_{\partial D_1} \\ \mathcal{S}_{D_1}^\omega\big|_{\partial D_2} & 0 \end{pmatrix}.$$

We define the centres z_1, z_2 of the resonators in the dilute regime specified by (3.6):

$$z_1 = -\frac{l}{2}\mathbf{v}, \qquad z_2 = \frac{l}{2}\mathbf{v}.$$

Then, as $\varepsilon \to 0$, we have for $i \neq j$,

$$\begin{aligned}
\mathcal{S}_{D_j}^0\big|_{\partial D_i}[\phi](x) &= \int_{\partial D_j} \Big(G^0(x, z_j) + (y - z_j) \cdot \nabla_y G^0(x, y_0) \Big) \phi(y) \, \mathrm{d}\sigma(y) \\
&= -\frac{\chi_{\partial D_i}(x)}{4\pi l} \int_{\partial D_j} \phi(y) \, \mathrm{d}\sigma(y) + O\left(\varepsilon \int_{\partial D_j} |\phi(y)| \, \mathrm{d}\sigma(y) \right).
\end{aligned}$$

Here, y_0 means a point on the line segment joining y and z_j. Hence we have

$$\begin{aligned}
\mathcal{S}_D^0 &= \hat{\mathcal{S}}_D^0 - \frac{1}{4\pi l} \begin{pmatrix} 0 & \langle \chi_{\partial D_2}, \cdot \rangle \chi_{\partial D_1} \\ \langle \chi_{\partial D_1}, \cdot \rangle \chi_{\partial D_2} & 0 \end{pmatrix} + O(\varepsilon^3) \\
&= \hat{\mathcal{S}}_D^0 + \mathcal{S}_D^{(1)} + O(\varepsilon^3).
\end{aligned}$$

In the same way, we can compute

$$\begin{aligned}
\mathcal{K}_D^{0,*} &= \hat{\mathcal{K}}_D^{0,*} + \frac{\mathbf{v} \cdot \nu}{4\pi l} \begin{pmatrix} 0 & -\langle \chi_{\partial D_2}, \cdot \rangle \\ \langle \chi_{\partial D_1}, \cdot \rangle & 0 \end{pmatrix} + O(\varepsilon^3) \\
&= \hat{\mathcal{K}}_D^{0,*} + \mathcal{K}_D^{(1)} + O(\varepsilon^3).
\end{aligned}$$

Following the computations in the proof of Lemma 3.3 of [3], we have for $\alpha \neq 0$

$$\begin{aligned}
\psi_1^\alpha &= \psi_1 + \varepsilon \mathrm{Cap}_B \sum_{m \neq 0} \frac{e^{im\alpha L}}{4\pi |m| L} \psi_1 + \varepsilon \mathrm{Cap}_B \sum_{m \in \mathbb{Z}} \frac{e^{im\alpha L}}{4\pi |l - mL|} \psi_2 + O(\varepsilon), \\
\psi_2^\alpha &= \psi_2 + \varepsilon \mathrm{Cap}_B \sum_{m \in \mathbb{Z}} \frac{e^{im\alpha L}}{4\pi |l + mL|} \psi_1 + \varepsilon \mathrm{Cap}_B \sum_{m \neq 0} \frac{e^{im\alpha L}}{4\pi |mL|} \psi_2 + O(\varepsilon).
\end{aligned}$$

In these equations, observe that $\|\psi_i\|_{L^2(\partial D_i)} = O(\varepsilon^{-1})$. At $\alpha = \pi/L$, $u_j^\diamond$ and u_j correspond to either monopole or dipole modes:

$$u_j^\diamond = \frac{1}{\sqrt{2}} \left(\pm \psi_1^\diamond + \psi_2^\diamond \right), \qquad u_j = \frac{1}{\sqrt{2}} \left(\pm \psi_1 + \psi_2 \right).$$

The sign is positive, corresponding to a monopole mode, if $l_0 < 1/2$ and $j = 1$ or $l_0 > 1/2$ and $j = 2$, and negative if $l_0 < 1/2$ and $j = 2$ or $l_0 > 1/2$ and $j = 1$. Hence, from the expansions of ψ_1^α and ψ_2^α it follows that

$$u_j^\diamond = u_j + \varepsilon u_j^{(1)} u_j + O(\varepsilon),$$

where

$$u_j^{(1)} = \begin{cases} \mathrm{Cap}_B \left(\sum_{m\in\mathbb{Z}} \dfrac{(-1)^m}{4\pi|l+mL|} - \dfrac{\log(2)}{4\pi L} \right) & l_0 < 1/2, j=1 \quad \text{or} \quad l_0 > 1/2, j=2, \\ \mathrm{Cap}_B \left(-\sum_{m\in\mathbb{Z}} \dfrac{(-1)^m}{4\pi|l+mL|} - \dfrac{\log(2)}{4\pi L} \right) & l_0 < 1/2, j=2 \quad \text{or} \quad l_0 > 1/2, j=1. \end{cases}$$

From [3] we have that

$$\begin{cases} u_j^{(1)} < 0, & l_0 < 1/2, j=1 \quad \text{or} \quad l_0 < 1/2, j=2, \\ u_j^{(1)} > 0, & l_0 < 1/2, j=2 \quad \text{or} \quad l_0 > 1/2, j=1. \end{cases}$$

We are now ready to compute $B\Psi_j^\diamond$. Recall that $B = \mathcal{P}_2\mathcal{A}\mathcal{P}_1 - \mathcal{A}$. Since

$$\mathcal{P}_i = I + d\mathcal{P}_i^{(1)} + O(d^2),$$

we have

$$B = d\left(\mathcal{P}_2^{(1)}\mathcal{A} + \mathcal{A}\mathcal{P}_1^{(1)}\right) + O(d^2).$$

Moreover, we compute

$$\mathcal{A}\mathcal{P}_1^{(1)} \begin{pmatrix} u_j \\ u_j^\diamond \end{pmatrix} = \begin{pmatrix} \mathbf{v}\cdot\left(\nabla\hat{\mathcal{S}}_D^\omega\big|_-[u_j] - \nabla\mathcal{S}_D^\omega\big|_+[u_j^\diamond]\right) \\ \left(-\frac{1}{2} + \hat{\mathcal{K}}_D^{\omega,*}\right)[\xi_1] - \delta\left(\frac{1}{2} + \mathcal{K}_D^{\omega,*}\right)[\xi_2] \end{pmatrix},$$

where

$$\xi_1 = \left(\hat{\mathcal{S}}_D^\omega\right)^{-1} \mathbf{v}\cdot\nabla\hat{\mathcal{S}}_D^\omega\big|_-[u_j], \qquad \xi_2 = \left(\mathcal{S}_D^\omega\right)^{-1} \mathbf{v}\cdot\nabla\mathcal{S}_D^\omega\big|_+[u_j^\diamond].$$

Hence

$$\begin{aligned} \langle \Phi_j^\diamond, \mathcal{A}\mathcal{P}_1^{(1)}\Psi_j^\diamond\rangle &= -\delta\left\langle u_j^\diamond, \mathbf{v}\cdot\left(\nabla\hat{\mathcal{S}}_D^0\big|_-[u_j] - \nabla\mathcal{S}_D^0\big|_+[u_j^\diamond]\right)\right\rangle + \left\langle\left(-\frac{1}{2} + \hat{\mathcal{K}}_D^\omega\right)[\chi_j^\diamond], \xi_1\right\rangle \\ &\quad - \delta\left\langle\left(\frac{1}{2} + \mathcal{K}_D^0\right)[\chi_j^\diamond], \xi_2\right\rangle \\ &= \delta\left\langle u_j^\diamond, \mathbf{v}\cdot\nabla\mathcal{S}_D^0\big|_+[u_j^\diamond]\right\rangle + \omega^2\left\langle\hat{\mathcal{K}}_{D,2}[\chi_j^\diamond], \left(\hat{\mathcal{S}}_D^0\right)^{-1}\partial_T\hat{\mathcal{S}}_D^0\big|_-[u_j]\right\rangle \\ &\qquad - \delta\left\langle\left(\mathcal{S}_D^0\right)^{-1}[\chi_j^\diamond], \mathbf{v}\cdot\nabla\mathcal{S}_D^0\big|_+[u_j^\diamond]\right\rangle + O(\omega^3) \\ &= \delta\left\langle u_j^\diamond, \mathbf{v}\cdot\nabla\mathcal{S}_D^0\big|_+[u_j^\diamond]\right\rangle - \delta\left\langle\left(\mathcal{S}_D^0\right)^{-1}[\chi_j^\diamond], \mathbf{v}\cdot\nabla\mathcal{S}_D^0\big|_+[u_j^\diamond]\right\rangle + O(\omega^3). \end{aligned}$$

Using the expansions in the dilute regime, we have to leading order in ε,

$$\begin{aligned} \langle \Phi_j^\diamond, \mathcal{A}\mathcal{P}_1^{(1)}\Psi_j^\diamond\rangle &= \delta\left\langle u_j, \mathbf{v}\cdot\nabla\hat{\mathcal{S}}_D^0\big|_+[u_j]\right\rangle - \delta\left\langle\left(\hat{\mathcal{S}}_D^0\right)^{-1}[\chi_j^\diamond], \mathbf{v}\cdot\nabla\hat{\mathcal{S}}_D^0\big|_+[u_j]\right\rangle + O(\omega^3 + \omega^2\varepsilon) \\ &= \delta\langle u_j, (\mathbf{v}\cdot\nu)u_j\rangle - \delta\langle u_j, (\mathbf{v}\cdot\nu)u_j\rangle + O(\omega^3 + \omega^2\varepsilon) \\ &= O(\omega^3 + \omega^2\varepsilon). \end{aligned}$$

Passing to higher orders in ε we have, after simplifications,

$$\begin{aligned} \langle \Phi_j^\diamond, \mathcal{A}\mathcal{P}_1^{(1)}\Psi_j^\diamond\rangle &= \delta\varepsilon u_j^{(1)}\langle u_j, (\mathbf{v}\cdot\nu)u_j\rangle + \delta\left\langle\left(\hat{\mathcal{S}}_D^0\right)^{-1}\mathcal{S}_D^{(1)}[u_j], (\mathbf{v}\cdot\nu)u_j\right\rangle + O(\omega^3 + \omega^2\varepsilon^2) \\ &= \delta\varepsilon\left(u_j^{(1)} \pm \frac{\mathrm{Cap}_B}{4\pi l}\right)\langle u_j, (\mathbf{v}\cdot\nu)u_j\rangle + O(\omega^3 + \omega^2\varepsilon^2), \end{aligned}$$

where $\pm$ is chosen as positive if u_j is a monopole mode, and negative if u_j is a dipole mode. Due to the reflection symmetry of D_1 and D_2, we have $\langle u_j, (\mathbf{v}\cdot\nu)u_j\rangle = 0$, and hence

$$\langle \Phi_j^\diamond, \mathcal{A}\mathcal{P}_1^{(1)}\Psi_j^\diamond\rangle = O(\omega^3+\omega^2\varepsilon^2).$$

Next, we compute $\langle \Phi_j^\diamond, \mathcal{P}_2^{(1)}\mathcal{A}\Psi_j^\diamond\rangle$. Using the dilute expansions, we can write

$$\mathcal{A} = \mathcal{A}^{(0)} + \mathcal{A}^{(1)} + O(\varepsilon^3), \qquad \Psi_j^\diamond = \Psi^{(0)} + \Psi^{(1)} + O(\varepsilon),$$

where $\mathcal{A}^{(0)}$ and $\Psi^{(0)}$ are the leading order terms. At $\omega = \omega_j^\diamond$, we have $\mathcal{A}^{(0)}\Psi^{(0)} = O(\omega^3)$, and hence

$$\mathcal{A}\Psi_j^\diamond = \mathcal{A}^{(1)}\Psi^{(0)} + \mathcal{A}^{(0)}\Psi_1^{(1)} + O(\omega^3).$$

We can see that

$$\mathcal{A}^{(1)}\Psi^{(0)} = -\begin{pmatrix} \mathcal{S}_D^{(1)}[u_j] \\ \delta\mathcal{K}_D^{(1)}[u_j]\end{pmatrix}, \qquad \mathcal{A}^{(0)}\Psi^{(1)} = -\varepsilon u_j^{(1)}\begin{pmatrix} \hat{\mathcal{S}}_D^\omega[u_j] \\ \delta\left(\frac{1}{2}+\hat{\mathcal{K}}_D^{\omega,*}\right)[u_j]\end{pmatrix}.$$

Observe that $\mathcal{S}_D^{(1)}[u_j]$ and $\hat{\mathcal{S}}_D^\omega[u_j]$ are constant on ∂D. Combining these results, we arrive at

$$\begin{aligned}\langle \Phi_j^\diamond, \mathcal{P}_2^{(1)}\mathcal{A}\Psi_j^\diamond\rangle &= -\delta\left\langle u_j, \mathcal{K}_D^{(1)}[u_j]\right\rangle - \delta\left\langle \chi_j^\diamond, (2\tau-\partial_T)\mathcal{K}_D^{(1)}[u_j]\right\rangle - \delta\varepsilon u_j^{(1)}\left\langle \chi_j^\diamond, (2\tau-\partial_T)u_j\right\rangle + O(\omega^3+\varepsilon\omega^2)\\ &= -\delta\varepsilon u_j^{(1)}\left\langle \chi_j^\diamond, (2\tau-\partial_T)u_j\right\rangle + O(\omega^3+\varepsilon\omega^2)\\ &= -\delta\varepsilon u_j^{(1)}\left\langle \chi_j^\diamond, 2\tau u_j\right\rangle + O(\omega^3+\varepsilon\omega^2).\end{aligned}$$

Consequently, we obtain that

$$\langle \Phi_j^\diamond, \mathcal{B}_0\Psi_j^\diamond\rangle = -\delta\varepsilon u_j^{(1)}\left\langle \chi_j^\diamond, 2\tau u_j\right\rangle + O(\omega^3+\varepsilon\omega^2).$$

Observe that $\left\langle \chi_j^\diamond, u_j\right\rangle < 0$, and in the case D_1 and D_2 are strictly convex we have $\tau(x) > \tau_0 > 0$ for all $x \in D$, hence $\left\langle \chi_j^\diamond, 2\tau u_j\right\rangle < 0$. Combining this with the sign of $u_j^{(1)}$, the result follows. □

A.2 Proof of Lemma 3.33

We begin by computing the expansion of $\hat{V}$ in the dilute regime. Using ψ_j as in the previous sections, that is, $\psi_j = (\hat{\mathcal{S}}_D^0)^{-1}[\chi_{D_j}]$, we have

$$\psi_j = \sqrt{\varepsilon\mathrm{Cap}_B}\,\psi_{D_j}^1, \quad j = 1, 2.$$

Then

$$\begin{aligned}(V_j)_{m,n} &= -\int_{\partial D_j}\int_{\partial D_j} G^\omega(x-d\mathbf{v}, y)\xi_{D_j}^m(y)\psi_{D_j}^n(x)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y)\\ &= -\int_{\partial D_j}\int_{\partial D_j}\big(G^\omega(d\mathbf{v},0) + (x-y)\cdot\nabla_x G^\omega(d\mathbf{v},0)\big)\xi_{D_j}^m(z)\psi_{D_j}^n(y)\,\mathrm{d}\sigma(z)\,\mathrm{d}\sigma(y) + O(\varepsilon^3)\\ &= -\sqrt{\varepsilon\mathrm{Cap}_B}G^\omega(d\mathbf{v},0)\delta_{n,1}\int_{\partial D_j}\xi_{D_j}^m\,\mathrm{d}\sigma + O(\varepsilon^3)\\ &= \frac{\varepsilon\mathrm{Cap}_B}{4\pi d}\delta_{m,1}\delta_{n,1} + O(\varepsilon^3+\omega\varepsilon), \end{aligned} \tag{A.1}$$

where we have used symmetry in the integration together the orthogonality relation

$$\int_{\partial D_j}\psi_{D_j}^m\,\mathrm{d}\sigma = \sqrt{\varepsilon\mathrm{Cap}_B}\,\delta_{m,1}.$$

Observe that at $m=1$ we have $\mathcal{D}_{D_j}^0[\chi_{D_j}] = 0$ outside D_j, and so

$$(W_j)_{1,n} = O(\omega^2) \tag{A.2}$$

for all n. Recall the expansion, from the proof of Lemma 3.15,

$$\Psi_j^\diamond = \Psi^{(0)} + \Psi^{(1)} + O(\varepsilon), \qquad \Psi^{(0)} = \begin{pmatrix} u_j \\ u_j \end{pmatrix}, \qquad \Psi^{(1)} = \begin{pmatrix} 0 \\ \varepsilon u_j^{(1)} u_j \end{pmatrix},$$

where, at $\omega = \omega_j^\diamond$, $\hat{\mathcal{A}}\Psi^{(0)} = O(\omega^3)$. Also, recall that

$$\Phi_j^\diamond = \begin{pmatrix} -\delta u_j^\diamond \\ \chi_j^\diamond \end{pmatrix}.$$

Then we can compute

$$\left\langle \Phi_j^\diamond, \hat{\mathcal{P}}_2 \hat{\mathcal{A}} \hat{\mathcal{P}}_1 \Psi^{(0)} \right\rangle = O(\omega^3).$$

Turning to higher orders of $\Psi_j^\diamond$, we have

$$\left\langle \Phi_j^\diamond, \left(\hat{\mathcal{P}}_2 \hat{\mathcal{A}} \hat{\mathcal{P}}_1 - \hat{\mathcal{A}}\right) \Psi^{(1)} \right\rangle = -\delta\varepsilon u_j^{(1)} \Bigg(\left\langle \chi_j^\diamond, W\left(\frac{1}{2} + \hat{\mathcal{K}}_D^{0,*}\right)[V^{-1}u_j] \right\rangle - \left\langle \chi_j^\diamond, \left(\frac{1}{2} + \hat{\mathcal{K}}_D^{0,*}\right)[u_j] \right\rangle + \left\langle u_j^\diamond, V^* \mathcal{S}_D^0[V^{-1}u_j] \right\rangle - \left\langle u_j, \mathcal{S}_D^0[u_j] \right\rangle \Bigg) + O(\omega^3).$$

From (A.2), it holds that

$$\left\langle \chi_j^\diamond, W\left(\frac{1}{2} + \hat{\mathcal{K}}_D^{0,*}\right)[V^{-1}u_j] \right\rangle = O(\omega^2).$$

Moreover, (A.1) yields

$$\left\langle u_j^\diamond, V^* \mathcal{S}_D^0[V^{-1}u_j] \right\rangle - \left\langle u_j, \mathcal{S}_D^0[u_j] \right\rangle = O(\varepsilon^2 + \omega^2).$$

Finally, since $\left\langle \chi_j^\diamond, \left(\frac{1}{2} + \hat{\mathcal{K}}_D^{0,*}\right)[u_j] \right\rangle = \left\langle \chi_j^\diamond, u_j \right\rangle = \varepsilon \mathrm{Cap}_B$, we have

$$\left\langle \Phi_j^\diamond, \mathcal{B}_d \Psi_j^\diamond \right\rangle = \delta\varepsilon^2 \mathrm{Cap}_B u_j^{(1)} + O(\omega^3 + \varepsilon^3\omega^2).$$

Since the leading order is independent of d, the conclusion follows. □

B Proof of Proposition 3.24

We will restrict the analysis to the equation

$$\frac{1}{2\pi} \int_{Y^*} \left(\Omega_1 \left(1 - e^{i\theta_\alpha}\right) + \Omega_2 \left(1 + e^{i\theta_\alpha}\right) \right) \mathrm{d}\alpha = 0, \tag{B.1}$$

since the proof of the equation in (3.45) with the other sign is similar. Define

$$\lambda = \frac{\omega^2 |D_1|}{\delta}, \qquad \lambda_1^\alpha = C_{11}^\alpha - |C_{12}^\alpha|, \qquad \lambda_2^\alpha = C_{11}^\alpha + |C_{12}^\alpha|.$$

Then, as $\delta \to 0$,

$$\frac{1}{2\pi} \int_{Y^*} \left(\Omega_1 \left(1 - e^{i\theta_\alpha}\right) + \Omega_2 \left(1 + e^{i\theta_\alpha}\right) \right) \mathrm{d}\alpha = \frac{1}{\pi} \int_{Y^*} \frac{\lambda\left(C_{11}^\alpha + \mathrm{Re}(C_{12}^\alpha)\right) - \lambda_1^\alpha \lambda_2^\alpha}{(\lambda - \lambda_1^\alpha)(\lambda - \lambda_2^\alpha)} \mathrm{d}\alpha + O(\delta^{1/2}), \tag{B.2}$$

where the imaginary part vanishes due to symmetry. Observe that for ω inside the band gap, we have $\lambda - \lambda_1^\alpha > 0$ and $\lambda - \lambda_2^\alpha < 0$. Define

$$f(\alpha) = \lambda\left(C_{11}^\alpha + \mathrm{Re}(C_{12}^\alpha)\right) - \lambda_1^\alpha \lambda_2^\alpha.$$

We will now study the two cases $l_0 < 1/2$ and $l_0 > 1/2$ separately. We will show that the right-hand side of (B.1) is always positive in the first case, while in the second case it has a sign depending on λ. We will do so by splitting the integral into two parts, one with α close to 0 and one with α bounded away from 0, and show that the first part is negligible.

B.1 Case $l_0 < 1/2$

In the dilute regime, as $\varepsilon \to 0$, it follows from Lemma 3.5 that the width of the band gap scales as $O(\varepsilon^2)$. Moreover, if ω is inside the band gap then we are able to write that

$$\lambda = \varepsilon \mathrm{Cap}_B + \varepsilon^2 (\mathrm{Cap}_B)^2 \lambda_0 + O(\varepsilon^3)$$

for some $\lambda_0 \in \mathbb{R}$. From the expansions of the capacitance coefficients in Lemma 3.5, and the fact that λ_1^α (resp. λ_2^α) attains its maximum (resp. minimum) at $\alpha = \pi/L$, we have the following bounds on λ_0:

$$-\frac{1}{4\pi L}\sum_{m\neq 0}\frac{e^{i\alpha mL}}{|m|} - \frac{1}{4\pi L}\sum_{m=-\infty}^{\infty}\frac{e^{i\alpha mL}}{|m+l_0|} < \lambda_0 < -\frac{1}{4\pi L}\sum_{m\neq 0}\frac{e^{i\alpha mL}}{|m|} + \frac{1}{4\pi L}\sum_{m=-\infty}^{\infty}\frac{e^{i\alpha mL}}{|m+l_0|}. \tag{B.3}$$

We fix constants $C > 0$, $p \in \mathbb{N}$. Then, for α such that $|\alpha| > C\varepsilon^p$, $f(\alpha)$ can be expanded in the dilute regime as

$$\begin{aligned} f(\alpha) =& \varepsilon^3(\mathrm{Cap}_B)^3\left(\lambda_0 - \frac{1}{4\pi l} + \frac{1}{4\pi L}\sum_{m\neq 0}\frac{\cos(m\alpha L)}{|m|} - \frac{1}{4\pi L}\sum_{m\neq 0}\frac{\cos(m\alpha L)}{|m+l_0|}\right) + o(\varepsilon^3) \\ =& \varepsilon^3(\mathrm{Cap}_B)^3\left(\lambda_0 - \frac{1}{4\pi l} + \frac{1}{4\pi L}\sum_{m=1}^{\infty}\cos(m\alpha L)\left(\frac{2}{m} - \frac{1}{m+l_0} - \frac{1}{m-l_0}\right)\right) + o(\varepsilon^3). \end{aligned} \tag{B.4}$$

Define $g(\alpha)$ as

$$g(\alpha) = \sum_{m=1}^{\infty} e^{im\alpha L}\left(\frac{2}{m} - \frac{1}{m+l_0} - \frac{1}{m-l_0}\right).$$

We can rewrite g as

$$\begin{aligned} g(\alpha) &= e^{i\alpha L}\sum_{m=0}^{\infty} e^{im\alpha L}\left(\frac{2}{m+1} - \frac{1}{m+1+l_0} - \frac{1}{m+1-l_0}\right) \\ &= e^{i\alpha L}\big(2\Phi(e^{i\alpha L},1,1) - \Phi(e^{i\alpha L},1,1+l_0) - \Phi(e^{i\alpha L},1,1-l_0)\big). \end{aligned}$$

Here, $\Phi(z,s,a)$ denotes Lerch's transcendent function, defined by the power series

$$\Phi(z,s,a) = \sum_{m=0}^{\infty}\frac{z^m}{(a+m)^s},$$

for $z \in \mathbb{C}$ where this series converges, and is extended by analytic continuation (for details on this function we refer, for example, to [23]). For arguments in the regime $\mathrm{Re}(s) > 0, \mathrm{Re}(a) > 0$ and $z \in \mathbb{C}\setminus[1,\infty)$, this function admits an integral representation as

$$\Phi(z,s,a) = \frac{1}{\Gamma(s)}\int_0^\infty \frac{t^{s-1}e^{-at}}{1-ze^{-t}}\,\mathrm{d}t,$$

where Γ is the Gamma function. From this, we have a representation of $g(\alpha), \alpha \neq 0$, as

$$\begin{aligned} g(\alpha) &= \int_0^\infty \frac{2e^{-t} - e^{-(1+l_0)t} - e^{-(1-l_0)t}}{1 - e^{i\alpha L}e^{-t}}\,\mathrm{d}t \\ &= \int_0^\infty \frac{(\cosh(l_0 t) - 1)\left(e^{-t} - \cos(\alpha L)\right)}{\cosh(t) - \cos(\alpha L)}\,\mathrm{d}t. \end{aligned}$$

From (B.4), using the bounds on λ_0 from (B.3) and for α such that $|\alpha| > C\varepsilon^p$, we have

$$\begin{aligned} f(\alpha) &< \frac{\varepsilon^3(\mathrm{Cap}_B)^3}{4\pi L}\left(\sum_{m=1}^{\infty}\left(\cos(m\alpha L) - (-1)^m\right)\left(\frac{2}{m} - \frac{1}{m+l_0} - \frac{1}{m-l_0}\right)\right) + o(\varepsilon^3) \\ &= \frac{\varepsilon^3(\mathrm{Cap}_B)^3}{4\pi L}\left(\mathrm{Re}\big(g(\alpha)\big) - g(\pi/L)\right) + o(\varepsilon^3) \\ &= \frac{\varepsilon^3(\mathrm{Cap}_B)^3}{4\pi L}\int_0^\infty (\cosh(l_0 t) - 1)\sinh(t)\left(\frac{1}{\cosh(t)+1} - \frac{1}{\cosh(t) - \cos(\alpha L)}\right) + o(\varepsilon^3) \\ &= A_1(\alpha)\varepsilon^3 + o(\varepsilon^3) \end{aligned}$$

for some $A_1(\alpha) \leq 0$ independent of ε, with $A_1(\alpha) = 0$ precisely when $\alpha = \pi/L$. It follows that

$$\frac{1}{\pi}\int_{Y^*\setminus[-C\varepsilon^p,C\varepsilon^p]} \frac{\lambda\left(C_{11}^\alpha + \mathrm{Re}(C_{12}^\alpha)\right) - \lambda_1^\alpha\lambda_2^\alpha}{(\lambda-\lambda_1^\alpha)(\lambda-\lambda_2^\alpha)}\,\mathrm{d}\alpha = \frac{A_2}{\varepsilon} + o(\varepsilon^{-1}) \tag{B.5}$$

for some constant $A_2 > 0$. From the scaling property (3.7), we know that $|f(\alpha)| < \varepsilon^2 K_1$ for some $K_1 > 0$ independent on α. The minimum of $\left|(\lambda-\lambda_1^\alpha)(\lambda-\lambda_2^\alpha)\right|$ is attained at π/L, and from Lemma 3.5, we have $\left|(\lambda-\lambda_1^\alpha)(\lambda-\lambda_2^\alpha)\right| > K_2\varepsilon^4$. Therefore, we have

$$\left|\frac{1}{\pi}\int_{[-C\varepsilon^p,C\varepsilon^p]} \frac{\lambda\left(C_{11}^\alpha + \mathrm{Re}(C_{12}^\alpha)\right) - \lambda_1^\alpha\lambda_2^\alpha}{(\lambda-\lambda_1^\alpha)(\lambda-\lambda_2^\alpha)}\,\mathrm{d}\alpha\right| < A_3\varepsilon^{p-2},$$

for some constant A_3. Choosing $p > 2$, and combining this with (B.5), we find that

$$\frac{1}{\pi}\int_{Y^*} \frac{\lambda\left(C_{11}^\alpha + \mathrm{Re}(C_{12}^\alpha)\right) - \lambda_1^\alpha\lambda_2^\alpha}{(\lambda-\lambda_1^\alpha)(\lambda-\lambda_2^\alpha)}\,\mathrm{d}\alpha > 0$$

for ε small enough. Therefore, when $l_0 < 1/2$, by (B.2) we find that, for λ sufficiently close to $\lambda_1^{\pi/L}$, we have

$$\frac{1}{2\pi}\int_{Y^*} \Big(\Omega_1\left(1-e^{i\theta_\alpha}\right) + \Omega_2\left(1+e^{i\theta_\alpha}\right)\Big)\,\mathrm{d}\alpha > 0,$$

when ε and δ are small enough.

B.2 Case $l_0 > 1/2$

We will show that (B.1) has a solution. We denote the left-hand side by

$$I(\lambda) := \frac{1}{2\pi}\int_{Y^*} \Big(\Omega_1\left(1-e^{i\theta_\alpha}\right) + \Omega_2\left(1+e^{i\theta_\alpha}\right)\Big)\,\mathrm{d}\alpha.$$

From Lemma 3.5, we find that for ε small enough, $C_{12}^{\pi/L} > 0$ in the case $l_0 > 1/2$. Hence $e^{i\theta_{\pi/L}} = 1$, so $I(\lambda) \to -\infty$ as $\lambda \to \lambda_2^{\pi/L}$. Next, we will show that $I(\lambda)$ is positive for λ sufficiently close to $\lambda_1^{\pi/L}$.

Since $C_{12}^{\pi/L}$ is positive, we now have the following bounds for λ_0:

$$-\frac{1}{4\pi L}\sum_{m\neq 0}\frac{e^{i\alpha mL}}{|m|} + \frac{1}{4\pi L}\sum_{m=-\infty}^{\infty}\frac{e^{i\alpha mL}}{|m+l_0|} < \lambda_0 < -\frac{1}{4\pi L}\sum_{m\neq 0}\frac{e^{i\alpha mL}}{|m|} - \frac{1}{4\pi L}\sum_{m=-\infty}^{\infty}\frac{e^{i\alpha mL}}{|m+l_0|}.$$

Fix some small $\kappa > 0$, and choose λ_0 as

$$\lambda_0 = \kappa - \frac{1}{4\pi L}\sum_{m\neq 0}\frac{e^{i\alpha mL}}{|m|} + \frac{1}{4\pi L}\sum_{m=-\infty}^{\infty}\frac{e^{i\alpha mL}}{|m+l_0|}.$$

Observe that $\kappa \to 0$ corresponds to $\lambda \to \lambda_1^{\pi/L}$. Using (B.4) and following the same subsequent steps, we find that

$$f(\alpha) = \varepsilon^3\left(\left(\mathrm{Cap}_B\right)^3\kappa + A_1(\alpha)\right) + o(\varepsilon^3).$$

Then, analogously to (B.5), we have

$$\frac{1}{\pi}\int_{Y^*\setminus[-C\varepsilon^p,C\varepsilon^p]} \frac{\lambda\left(C_{11}^\alpha + \mathrm{Re}(C_{12}^\alpha)\right) - \lambda_1^\alpha\lambda_2^\alpha}{(\lambda-\lambda_1^\alpha)(\lambda-\lambda_2^\alpha)}\,\mathrm{d}\alpha = \frac{A_2 + A_4\kappa}{\varepsilon} + o(\varepsilon^{-1}),$$

where, again, A_2 is a constant $A_2 > 0$, and A_4 is a constant $A_4 < 0$. Thus, for κ small enough, we have $A_2 + A_4\kappa > 0$, and then we can proceed as in Section B.1 to show that

$$I(\lambda) > 0,$$

for λ sufficiently close to $\lambda_1^{\pi/L}$, and for small enough ε and δ. This, combined with the fact that $I(\lambda) < 0$ for λ sufficiently close to $\lambda_2^{\pi/L}$, allows us to conclude that $I(\hat\lambda) = 0$ for some $\lambda_1^{\pi/L} < \hat\lambda < \lambda_2^{\pi/L}$.

In order to show that this solution $\hat{\lambda}$ is unique, we show that $I(\lambda)$ is strictly monotonic for $\lambda_1^{\pi/L} < \lambda < \lambda_2^{\pi/L}$. Differentiating (B.2) gives

$$I'(\lambda) = \frac{1}{\pi} \int_{Y^*} \frac{(C_{11}^\alpha + \mathrm{Re}(C_{12}^\alpha))\,(\lambda - \lambda_1^\alpha)(\lambda - \lambda_2^\alpha) - (\lambda\,(C_{11}^\alpha + \mathrm{Re}(C_{12}^\alpha)) - \lambda_1^\alpha\lambda_2^\alpha)\,(2\lambda - \lambda_1^\alpha - \lambda_2^\alpha)}{(\lambda - \lambda_1^\alpha)^2(\lambda - \lambda_2^\alpha)^2} \mathrm{d}\alpha + O(\delta^{1/2}).$$

Define

$$\begin{aligned}
h(\alpha) &= (C_{11}^\alpha + \mathrm{Re}(C_{12}^\alpha))\,(\lambda - \lambda_1^\alpha)(\lambda - \lambda_2^\alpha) - (\lambda\,(C_{11}^\alpha + \mathrm{Re}(C_{12}^\alpha)) - \lambda_1^\alpha\lambda_2^\alpha)\,(2\lambda - \lambda_1^\alpha - \lambda_2^\alpha) \\
&= (C_{11}^\alpha + \mathrm{Re}(C_{12}^\alpha))\,(-\lambda^2 + \lambda_1^\alpha\lambda_2^\alpha) + \lambda_1^\alpha\lambda_2^\alpha\,(2\lambda - \lambda_1^\alpha - \lambda_2^\alpha) \\
&\leq \begin{cases} \lambda_2^\alpha\left(-\lambda^2 + \lambda_1^\alpha\lambda_2^\alpha + \lambda_1^\alpha\,(2\lambda - \lambda_1^\alpha - \lambda_2^\alpha)\right), & \text{if } \lambda^2 \leq \lambda_1^\alpha - \lambda_2^\alpha, \\ \lambda_1^\alpha\left(-\lambda^2 + \lambda_1^\alpha\lambda_2^\alpha + \lambda_2^\alpha\,(2\lambda - \lambda_1^\alpha - \lambda_2^\alpha)\right), & \text{if } \lambda^2 > \lambda_1^\alpha - \lambda_2^\alpha, \end{cases} \\
&= \begin{cases} -\lambda_2^\alpha\,(\lambda - \lambda_1^\alpha)^2, & \text{if } \lambda^2 \leq \lambda_1^\alpha - \lambda_2^\alpha, \\ -\lambda_1^\alpha\,(\lambda - \lambda_2^\alpha)^2, & \text{if } \lambda^2 > \lambda_1^\alpha - \lambda_2^\alpha. \end{cases}
\end{aligned} \tag{B.6}$$

Using the bounds (B.6) we have that if $\lambda_1^{\pi/L} < \lambda < \lambda_2^{\pi/L}$ then $I'(\lambda) < 0$, provided δ is sufficiently small. Therefore, if $l_0 > 1/2$ then (B.1) has a unique solution, when ε and δ are small enough.

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