

CREATING BAND GAPS IN PERIODIC MEDIA*

ROBERT LIPTON[†] AND ROBERT VIATOR JR.[‡]

Abstract. We identify explicit conditions on geometry and material contrast for creating band gaps in two-dimensional photonic and three-dimensional acoustic crystals. This approach is novel and makes use of the electrostatic and quasi-periodic source free resonances of the crystal. The source free modes deliver a spectral representation for solution operators associated with propagation of electromagnetic and acoustic waves inside periodic high contrast media. An accurate characterization of the quasi-periodic and electrostatic resonance spectrum in terms of the shape and geometry of the scatters is possible. This information together with the Dirichlet and a Neumann-like spectra associated with the inclusions deliver conditions sufficient for opening band gaps at finite contrast. The theory provides a systematic means for the identification of photonic and phononic band gaps within a specified frequency range.

Key words. spectral theory, band gaps, photonics, periodic media

AMS subject classifications. 35P15, 35Q60, 78A48, 78A45

DOI. 10.1137/16M1083396

1. Introduction. High contrast periodic media are known to exhibit unique optical, acoustic, and elastic properties [16, 35]. In this paper we identify new explicit conditions on geometry and material contrast for creating band gaps in two-dimensional photonic and three-dimensional acoustic crystals. We consider wave propagation through a periodic medium in \mathbb{R}^d , $d = 2, 3$, made from two materials. One of the materials is in the form of disjoint inclusions. The inclusions are completely surrounded by the second material and do not touch the boundary of the period cell. The material coefficient is taken to be 1 inside the inclusions and takes the value $k > 1$ in the surrounding material. The union of all the inclusions D_1, D_2, \dots, D_N inside each period is denoted by D ; see Figure 1. The crystal occupies \mathbb{R}^d and is described by the periodic array of inclusions $\Omega = \cup_{m \in \mathbb{Z}^d} (D + m)$, with fundamental period cell $Y = (0, 1]^d$. The material coefficient for the medium is written $a(x) = k(1 - \chi_\Omega(x)) + \chi_\Omega(x)$, where χ_Ω is the indicator function for Ω taking the value 1 inside Ω and zero outside.

Wave propagation inside the crystal at frequency ω is described by the spectral problem

$$(1.1) \quad -\nabla \cdot (k(1 - \chi_\Omega(x)) + \chi_\Omega(x)) \nabla u(x) = \omega^2 u(x), \quad x \in \mathbb{R}^d, \quad d = 2, 3$$

Here the self-adjoint divergence form operator $L_k = -\nabla \cdot (k(1 - \chi_\Omega) + \chi_\Omega) \nabla$ is defined by the quadratic form in $L^2(\mathbb{R}^d)$, $d = 2, 3$:

*Received by the editors July 6, 2016; accepted for publication (in revised form) June 2, 2017; published electronically November 14, 2017.

<http://www.siam.org/journals/mms/15-4/M108339.html>

Funding: This material is based upon work supported by the Air Force Office of Scientific Research under award FA9550-12-1-0489, NSF grant DMS-1211066, and NSF EPSCOR Cooperative Agreement EPS-1003897 with additional support from the Louisiana Board of Regents.

[†]Department of Mathematics, Louisiana State University, Baton Rouge, LA 70803 (lipton@math.lsu.edu).

[‡]Institute for Mathematics and Its Applications, University of Minnesota, Minneapolis, MN 55455 (rviator@ima.umn.edu).

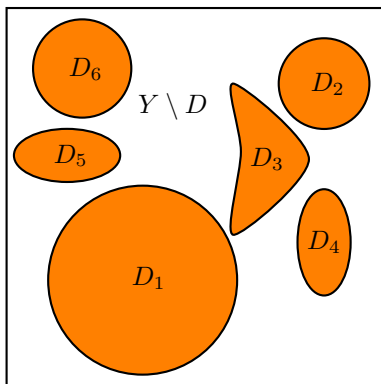


FIG. 1. Period cell.

$$(1.2) \quad \int_{\mathbb{R}^d} a(x)|\nabla u(x)|^2 dx$$

with domain $W^{1,2}(\mathbb{R}^d)$, $d = 2, 3$.

This mathematical formulation describes wave propagation in both two- and three-dimensional acoustic crystals and electromagnetic wave propagation through two-dimensional photonic crystals. For acoustic wave propagation the material coefficient $a^{-1}(x) = \rho(x)$ describes the mass density $\rho(x)$ of the periodic medium. For a two-dimensional photonic crystal $a^{-1}(x) = \epsilon(x)$ describes the dielectric constant of a nonmagnetic medium given by a lattice of infinitely long parallel rods periodically arranged in the plane transverse to the long axis of the rods. The electromagnetic wave travels along the transverse plane with magnetic field directed along the rods and the electric field in the plane.

Floquet theory [30, 24, 34, 29] shows that the spectrum $\sigma(L_k)$ has the band structure

$$(1.3) \quad \sigma(L_k) = \cup_{j \in \mathbb{N}} S_j,$$

where S_j are the spectral bands associated with Bloch waves propagating inside the crystal. The Bloch waves $h(x)$ satisfy

$$(1.4) \quad -\nabla \cdot (k(1 - \chi_\Omega(x)) + \chi_\Omega(x))\nabla h(x) = \omega^2 h(x), \quad x \in \mathbb{R}^d, \quad d = 2, 3$$

together with the α quasi-periodicity condition $h(x + p) = h(x)e^{i\alpha \cdot p}$. Here the wave vector α lies in the first Brillouin zone of the reciprocal lattice given by $Y^* = (-\pi, \pi]^d$. For each $\alpha \in Y^*$ the Bloch eigenvalues ω^2 are of finite multiplicity and are denoted by $\lambda_j(k, \alpha)$ with $\lambda_j(k, \alpha) \leq \lambda_{j+1}(k, \alpha)$, $j \in \mathbb{N}$.

The band structure for the crystal is described by the family of dispersion relations

$$(1.5) \quad \omega^2 = \lambda_j(k, \alpha), \quad j \in \mathbb{N}, \quad \alpha \in Y^*$$

and the spectral bands are given by the intervals

$$(1.6) \quad S_j = \left[\min_{\alpha \in Y^*} \lambda_j(k, \alpha), \max_{\alpha \in Y^*} \lambda_j(k, \alpha) \right].$$

The upper and lower band edges of S_j are denoted by

$$(1.7) \quad b_j = \max_{\alpha \in Y^*} \lambda_j(k, \alpha) \quad \text{and} \quad a_j = \min_{\alpha \in Y^*} \lambda_j(k, \alpha),$$

respectively. The band gaps are frequency intervals $\omega_- < \omega < \omega_+$ for which no waves propagate inside the crystal, i.e.,

$$(1.8) \quad b_j < \omega_-^2 < \omega_+^2 < a_{j+1}.$$

Over the past decades new theoretical insights into the nature of the frequency spectrum for high contrast periodic media have been made [9, 10, 11]. These efforts provide an asymptotic analysis that rigorously establishes the existence of band gaps for photonic and acoustic crystals made from thin walled cubic lattices containing cubes of material with $a = 1$ surrounded by walls with $a = k$. Band gaps are shown to appear in the limit as walls become vanishingly thin as $k \searrow 0$. More recently it has been shown that band gaps appear as one passes to the limit $k \nearrow \infty$ [15]. These gaps open in the vicinity of eigenvalues associated with the Dirichlet spectra of the included phase [15, 12, 31, 1]. In this article we depart from previous high contrast asymptotic investigations and describe the location and width of band gaps for finite values of the contrast $k > \bar{k}$, where \bar{k} is given explicitly in terms of the crystal geometry Ω . We provide rigorous criteria that are based on the crystal geometry and material properties for opening band gaps in both two- and three-dimensional periodic materials; see Theorems 1.1, 1.2, 10.2, 10.3, 12.1, and 12.2. These results apply to a wide class of inclusion geometries associated with smooth boundaries. This class of inclusion geometries include dispersions of smooth but not necessarily convex particles separated by a prescribed minimum distance; these are referred to as *buffered dispersions of inclusions* (see section 8). The buffered dispersions are examples of a more general class of dispersions referred to as P_θ that can be characterized in a simple way in terms of energy inequalities described in Definition 8.3.

To illustrate the ideas, we consider a photonic crystal where $D \subset Y$ is a collection of circular rod cross sections in the transverse plane described by N disks of radius a . The disks can be arranged in any configuration inside the period but neighbors can be no closer than a prescribed minimum distance t inside the crystal Ω , and we write $b = a + t$; see Figure 2. We introduce the Dirichlet spectra associated with the Laplace operator $-\Delta$ on the inclusions. For this case the spectra is characterized by the number of disks N and the Dirichlet spectrum associated with a single disk of radius a . We consider the part of the spectra associated with eigenfunctions having nonzero average over the disk. These simple eigenvalues are denoted by

$$(1.9) \quad \delta_{0j}^* = (\eta_{0,j}/a)^2,$$

where η_{0j} are the zeros of the Bessel function of order zero J_0 ; see, e.g., [14]. The associated eigenfunctions are rotationally symmetric and given by the normalized Bessel functions of order zero:

$$(1.10) \quad u_{0k} = J_0(r\eta_{0k}/a)/(a\sqrt{\pi}J_1(\eta_{0k})).$$

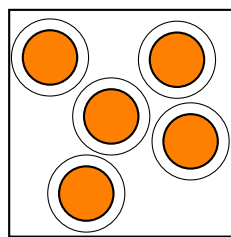


FIG. 2. Shaded regions are inclusions of radius a surrounded by a shell of thickness t .

The Dirichlet eigenvalues associated with mean zero eigenfunctions are of geometric multiplicity two and are denoted by $\nu_{nk} = (\eta_{nk}/a)^2$, where $\eta_{n,k}$ is the k th zero of the n th Bessel function J_n , $1 \leq n$. Next we introduce the roots ν_{0k} of the spectral function

$$(1.11) \quad S(\nu) = N\nu \sum_{k \in \mathbb{N}} \frac{a_{0k}^2}{\nu - \delta_{0k}^*} - 1,$$

where $a_{0k} = \int_D u_{0k} dx$ are the nonzero averages of the rotationally symmetric normalized eigenfunctions u_{0k} .

We write

$$(1.12) \quad \sigma_N = \left\{ \bigcup_{j \in \mathbb{N}} \nu_{0j} \right\} \cup \left\{ \bigcup_{(n,k) \in \mathbb{N}^2} \nu_{nk} \right\}.$$

and the Dirichlet spectrum $\sigma(-\Delta_D)$ given by

$$(1.13) \quad \sigma(-\Delta_D) = \left\{ \bigcup_{j \in \mathbb{N}} \delta_{0j}^* \right\} \cup \left\{ \bigcup_{(n,k) \in \mathbb{N}^2} \nu_{nk} \right\}.$$

We now provide an explicit condition on the contrast k that is sufficient to open a band gap in the vicinity of δ_{0j}^* together with explicit formulas describing its location and bandwidth.

THEOREM 1.1 (Opening a band gap). *Given δ_{0j}^* (see (1.9)) define the set σ_N^+ to be elements $\nu \in \sigma_N$ (see (1.12)) for which $\nu > \delta_{0j}^*$. The element in σ_N^+ closest to δ_{0j}^* is denoted by ν_{j+1} . Set d_j according to*

$$(1.14) \quad d_j = \frac{1}{2} \min \{ |\nu_{j+1}^{-1} - \nu^{-1}|; \nu \in \sigma_N \}.$$

We define \bar{r}_j to be

$$(1.15) \quad \bar{r}_j = \frac{\pi^2 d_j (b^2 - a^2)}{(b^2 + a^2) + \pi^2 d_j (b^2 + 3a^2)}.$$

Then one has the band gap

$$(1.16) \quad \sigma(L_k) \cap \left(\delta_{0j}^*, \nu_{j+1} \left(1 - \frac{\nu_{j+1} d_j}{k \bar{r}_j - 1} \right) \right) = \emptyset$$

if

$$(1.17) \quad k > \bar{k}_j = \bar{r}_j^{-1} \left(1 + \frac{d_j \nu_{j+1}}{1 - \frac{\delta_{0j}^*}{\nu_{j+1}}} \right).$$

Next we provide an explicit condition on k sufficient for the persistence of a spectral band together with explicit formulas describing its location and bandwidth.

THEOREM 1.2 (Persistence of passbands). *Given δ_{0j}^* (see (1.9)) define the the set σ_N^- to be elements $\nu \in \sigma_N$ (see (1.12)) for which $\nu < \delta_{0j}^*$. The element in σ_N^- closest to δ_{0j}^* is denoted by ν_j . Set d_j according to*

$$(1.18) \quad d_j = \frac{1}{2} \min \{ |(\delta_{j0}^*)^{-1} - \delta^{-1}|; \delta \in \sigma(-\Delta_D) \}.$$

Define \underline{r}_j to be

$$(1.19) \quad \underline{r}_j = \frac{2\pi^2 d_j (b^2 - a^2)}{(b^2 + a^2) + 2\pi^2 d_j (b^2 + 3a^2)}.$$

Then one has a passband in the vicinity of δ_{0j}^* and

$$(1.20) \quad \sigma(L_k) \supset \left[\nu_j, \delta_{0j}^* \left(1 - \frac{\delta_{0j}^* d_j}{k \underline{r}_j - 1} \right) \right]$$

if

$$(1.21) \quad k > \underline{k}_j = \underline{r}_j^{-1} \left(1 + \frac{d_j \delta_{0j}^*}{1 - \frac{\nu_j}{\delta_{0j}^*}} \right).$$

Note that both thresholds \bar{k}_j and \underline{k}_j depend explicitly on the crystal geometry through a and b and the Dirichlet spectrum of the disk. Density results on the distribution of zeros of Bessel functions [17, 8] show that the distance between adjacent eigenvalues d_j approaches zero with increasing j . This, together with (1.15) and (1.17), implies that the contrast sufficient to open gaps grows without bound as $j \rightarrow \infty$. Theorems 1.1 and 1.2 are direct applications of Theorems 10.2 and 10.3 to the case of buffered dispersions of equal sized disks with boundaries separated by a prescribed minimum tolerance $t > 0$. Theorems 10.2 and 10.3 show how to construct band gaps and passbands for the more general class of dispersions referred to as P_θ that can be characterized in a simple way in terms of energy inequalities described in Definition 8.3.

In this paper we introduce an approach to quantitatively describe band structure as illustrated in Theorems 1.1 and 1.2. This method is used to establish explicit conditions for band gap opening and persistence of passbands that apply to a wide class of inclusion shapes; see Theorem 10.2 and Theorem 10.3. We begin by introducing the Neumann spectrum defined by the spectral problem on Y given by

$$(1.22) \quad -\nabla \cdot (k(1 - \chi_D(x)) + \chi_D(x)) \nabla h(x) = \omega^2 h(x), \quad x \in Y$$

together with the homogeneous Neumann boundary condition, where h is a function in $H^1(Y)$ with $\int_Y h \, dx = 0$. Here χ_D denotes the indicator function of D in the unit period. The Neumann eigenvalues for (1.22) at fixed $k > 1$ are written $\nu_j(k)$, $j = 1, 2, \dots$ and ordered according to min-max with $0 < \nu_1(k) \leq \nu_2(k) \leq \dots$. The Bloch wave problem can also be restricted to the unit period and is given by the spectral problem

$$(1.23) \quad -\nabla \cdot (k(1 - \chi_D(x)) + \chi_D(x)) \nabla h(x) = \omega^2 h(x), \quad x \in Y$$

together with the α quasi-periodicity condition now expressed as $h(x) = u(x)e^{i\alpha \cdot x}$, where $u(x)$ is a periodic function in $H_{loc}^1(\mathbb{R}^d)$ with unit period Y . For $\alpha = 0$ we require $\int_Y u \, dx = 0$. For future reference we note for $k > 1$ and from the min-max principle that the Neumann spectrum provides a lower bound on the Bloch spectrum given by

$$(1.24) \quad \nu_j(k) \leq \lambda_j(k, \alpha) \quad \text{for } \alpha \in Y^*.$$

Our approach is based upon (1) a representation of the Neumann eigenvalues as convergent series expressed in terms of the contrast k with explicitly defined convergence radii and (2) a representation of the Bloch eigenvalues (1.5) as convergent series expressed in terms of the contrast k with explicitly defined convergence radii. We begin as in [25] by deriving a spectral representation formula for the inverse operator $(-\nabla \cdot (k(1 - \chi_D) + \chi_D)\nabla)^{-1}$ associated with the Neumann spectrum. To proceed we complexify the problem and consider $k \in \mathbb{C}$, noting that the divergence form operator $-\nabla \cdot (k(1 - \chi_D) + \chi_D)\nabla$ is no longer uniformly elliptic. Our approach does not rely on ellipticity and we develop an explicit representation formula for $-\nabla \cdot (k(1 - \chi_D) + \chi_D)\nabla$ that holds for complex values of k .

The spectral representation for $-\nabla \cdot (k(1 - \chi_D) + \chi_D)\nabla$ follows from the existence of a complete orthonormal set of functions associated with the *Neumann electrostatic resonances of the crystal*, i.e., functions v such that $n \cdot \nabla v = 0$ on the boundary of Y and real eigenvalues λ for which

$$(1.25) \quad -\nabla \cdot \chi_D \nabla v = -\lambda \Delta v.$$

These resonances are connected to the spectra of Neumann-Poincaré operators associated with double layer potentials discussed in [18, 23]. They are similar in spirit to the well known electrostatic resonances identified in the composites literature and useful for bounding effective properties [4, 3, 26, 28, 5, 13]. The spectral representation is applied to analytically continue the Neumann spectra for complex values of k ; see Theorem 3.1.

Using this representation formula, we identify the subset $z = 1/k \in \Omega_0$ of \mathbb{C} where this operator is invertible. The explicit formula shows that the solution operator $(-\nabla \cdot (k(1 - \chi_D) + \chi_D)\nabla)^{-1}$ is a meromorphic operator valued function of z for $z \in \Omega_0 = \mathbb{C} \setminus S$; see section 4 and Lemma 4.1. Here the set S is discrete and consists of poles lying on the negative real axis with only one accumulation point at $z = -1$. For the problem treated here we expand about $z = 0$ in the complex plane, and the distance between $z = 0$ and the set S is used to bound the radius of convergence of the series representation of Neumann eigenvalues for real z given by (4.14), (4.15). Next we apply the spectral representation formula for the inverse operator $(-\nabla \cdot (k(1 - \chi_D) + \chi_D)\nabla)^{-1}$ associated with the Bloch spectrum developed in [25]. Here the representation is carried out using the quasi-static resonances associated with the crystal geometry. Applying these ideas to the present context delivers a series representation for the Bloch eigenvalues; see (5.17) and (5.18). Theorems on separation of spectra and convergence of the series are given in Theorems 7.1, 7.2, 7.3, and 7.4. The fundamental theorems on band gaps and passbands, Theorems 10.2 and Theorem 10.3, are shown to follow from Theorems 7.1, 7.2, 7.3 and application of Theorem 7.4 parts 1 and 3 together with the interlacing property of the limit spectrum as $k \rightarrow \infty$, stated in Theorem 10.1.

The same high contrast mechanism can be used to open band gaps when the coefficient satisfies $a(y) = \frac{1}{k} < 1$ inside the array of inclusions and equals 1 outside. This is shown to follow from a *reciprocal relation* satisfied by the spectrum. These aspects are discussed in the concluding section, where a second application to H-polarized modes inside photonic crystals is presented in Theorems 12.1, and 12.2.

The ideas presented here can be used to quickly search for photonic and phononic band gaps within a prescribed frequency range. Once identified, these gaps can be maximized by applying topology optimization or level set methods to find inclusion shapes and lattice geometries that give the largest band gaps; see [7, 33, 27, 19, 2].

The paper is organized as follows: In the next section we introduce the Hilbert space formulation of the Neumann eigenvalue problem and the variational formulation of the Neumann electrostatic resonance problem. The completeness of the eigenfunctions associated with the electrostatic resonance spectrum is established and a spectral representation for the operator $-\nabla \cdot (k(1 - \chi_D) + \chi_D)\nabla$ is obtained. These results are collected and used to continue the Neumann eigenvalues as functions of k , off the real axis onto the complex plane; see Theorem 3.1 of section 3. A self-contained spectral perturbation theory is applied to identify the series representation for Neumann eigenvalues in the neighborhood of ∞ in section 4. The series expansion for the Bloch spectra is developed in section 5. The leading order spectral theory for the Neumann and Bloch spectra is developed in section 6. The main theorems on radius of convergence for the series are presented in section 7 and given by Theorems 7.1, 7.2, 7.3, and 7.4. These theorems apply to the class composite crystals P_θ described in Definition 8.3 provided in section 8. The explicit radii of convergence for distributions of identical disks is presented in section 9. The fundamental theorems on band gaps and passbands are presented and proved in section 10 and are given by Theorems 10.2 and 10.3 for all crystal geometries belonging to P_θ . Theorems 1.1 and 1.2 are direct applications of Theorems 10.2 and 10.3 to the case of dispersions of equal sized disks with boundaries separated by a prescribed minimum tolerance. The explicit formulas for the convergence radii and separation of spectra are all derived directly in a self-contained way in section 11, where Theorems 7.1, 7.2, 7.3, 7.4 are proved. We conclude in section 12 with a reciprocal relation and the identification of spectral gaps for the dual problem $a = \frac{1}{k} < 1$ in Ω and $a = 1$ outside; see Theorems 12.1 and 12.2.

2. Hilbert space setting, Neumann electrostatic resonances, and representation formulas. To begin the study of the spectral problem, we establish the correct Hilbert spaces on which the analysis will be conducted. We will see that the correct choice of Sobolev spaces (which encode the boundary conditions on the unit cell) will play an important role in analyzing the eigenvalue problem 1.1 in the high contrast limit $k \rightarrow \infty$. By choosing the right Sobolev spaces, we will also identify the important electrostatic spectral decomposition of our divergence-form operator with Neumann boundary conditions on Y , which will play a critical role in subsequent analysis. This process will be repeated in later sections for the periodic and quasi-periodic boundary conditions as well.

We denote the space of all square integrable complex valued functions h defined on Y with $\int_Y h \, dx = 0$ by $L_0^2(Y)$, and the L^2 inner product over Y is written

$$(2.1) \quad (u, v) = \int_Y u \bar{v} \, dx.$$

The eigenfunctions h for (1.22) belong to the space

$$(2.2) \quad \mathcal{H} = \{h \in H^1(Y) : \int_Y h \, dx = 0\}.$$

The space \mathcal{H} is a Hilbert space under the inner product

$$(2.3) \quad \langle u, v \rangle = \int_Y \nabla u(x) \cdot \nabla \bar{v}(x) \, dx.$$

The solutions to the Neumann spectral problem (1.22) belong to the subspace $\mathcal{H}_N \subset \mathcal{H}$ defined by

$$(2.4) \quad \mathcal{H}_N = \left\{ h \in \mathcal{H} : \frac{\partial h}{\partial n} = 0 \text{ on } \partial Y \right\}.$$

For any $k \in \mathbb{C}$, the weak formulation of the eigenvalue problem (1.22) for h and ω^2 can be written as

$$(2.5) \quad B_k(h, v) = \omega^2(h, v)$$

for all v in \mathcal{H}_N , where $B_k : \mathcal{H}_N \times \mathcal{H}_N \rightarrow \mathbb{C}$ is the sesquilinear form

$$(2.6) \quad B_k(u, v) = k \int_{Y \setminus D} \nabla u(x) \cdot \nabla \bar{v}(x) dx + \int_D \nabla u(x) \cdot \nabla \bar{v}(x) dx.$$

The linear operator $T_k : \mathcal{H}_N \rightarrow \mathcal{H}_N$ associated with B_k is defined by

$$(2.7) \quad \langle T_k u, v \rangle := B_k(u, v).$$

In what follows we decompose \mathcal{H}_N into invariant subspaces of source free modes and identify the associated Neumann electrostatic resonance spectra. This decomposition will provide an explicit spectral representation for the operator T_k ; see Theorem 2.4. Let $W_1 \subset \mathcal{H}_N$ be the completion in \mathcal{H}_N of the subspace of functions with support away from D . Now let $\tilde{H}_0^1(D)$ denote the subspace of functions $H_0^1(D)$ extended by zero into $Y \setminus D$ and let 1_Y be the indicator function of Y . We define $W_2 \subset \mathcal{H}_N$ to be the subspace of functions given by

$$(2.8) \quad W_2 = \left\{ u = \tilde{u} - \left(\int_D \tilde{u} dx \right) 1_Y \mid \tilde{u} \in \tilde{H}_0^1(D) \right\}.$$

Clearly W_1 and W_2 are orthogonal subspaces of \mathcal{H}_N , so we define $W_3 := (W_1 \oplus W_2)^\perp$. We therefore have

$$(2.9) \quad \mathcal{H}_N = W_1 \oplus W_2 \oplus W_3.$$

The orthogonal decomposition and integration by parts shows that elements $u \in W_3$ are harmonic separately in D and $Y \setminus D$, and

$$(2.10) \quad \frac{\partial u}{\partial n} = 0 \text{ on } \partial Y \text{ and}$$

$$(2.11) \quad \int_{\partial D} \frac{\partial u}{\partial n} \Big|_{\partial D}^+ ds = 0,$$

$$(2.12) \quad \int_{\partial D} \frac{\partial u}{\partial n} \Big|_{\partial D}^- ds = 0,$$

where $\frac{\partial u}{\partial n} \Big|_{\partial D}^-$ and $\frac{\partial u}{\partial n} \Big|_{\partial D}^+$ are traces of the outward directed normal derivative taken from the interior of D and exterior of D , respectively.

To set up the spectral analysis note that elements of W_3 can be represented in terms of single layer potentials supported on ∂D . We introduce the d -dimensional Newtonian potential, $d = 2, 3$, given by

$$(2.13) \quad \Gamma_d(x, y) = \left\{ \frac{1}{2\pi} \ln|x - y| \text{ for } d = 2 \text{ and } -\frac{1}{4\pi} |x - y|^{-1} \text{ for } d = 3 \right\}.$$

Let $\phi(x, y)$ satisfy

$$(2.14) \quad -\Delta_x \phi(x, y) = 0 \quad \text{for } (x, y) \in Y \times Y,$$

with

$$(2.15) \quad \frac{\partial \phi(x, y)}{\partial n(x)} = -\frac{\partial \Gamma_d(x, y)}{\partial n(x)} + \frac{1}{|\partial Y|} \quad \text{for } x \in \partial Y \text{ and } y \in Y,$$

where $|\partial Y|$ denotes the $d - 1$ dimensional Hausdorff measure of ∂Y . The Neumann Green's function is given by

$$(2.16) \quad G(x, y) = \Gamma_d(x, y) + \phi(x, y),$$

and the associated operator $-\Delta_N^{-1} : L_0^2(Y) \rightarrow \mathcal{H}_N$ defined by

$$(2.17) \quad -\Delta_N^{-1} f = \int_Y G(x, y) f(y) dy$$

satisfies

$$(2.18) \quad \langle -\Delta_N^{-1} f, v \rangle = (f, v).$$

The operator $-\Delta_N^{-1}$ is a bounded operator from $L_0^2(Y)$ into \mathcal{H}_N and a bounded compact map of $L_0^2(Y)$ into itself. Let $H^{1/2}(\partial D)$ be the fractional Sobolev space on ∂D defined in the usual way, and denote its dual by $H^{-1/2}(\partial D)$. For $\rho \in H^{-1/2}(\partial D)$ the single layer potential is given by

$$(2.19) \quad S_D \rho(x) = \int_{\partial D} G(x, y) \rho(y) d\sigma(y), \quad x \in Y.$$

The jump in normal derivative across ∂D belongs to $H^{-1/2}(\partial D)$ and is written

$$(2.20) \quad \rho_u = \frac{\partial u}{\partial n} \Big|_{\partial D}^+ - \frac{\partial u}{\partial n} \Big|_{\partial D}^-.$$

For $u \in W_3$ we have the identity

$$(2.21) \quad u = S_D \rho_u,$$

where $\int_{\partial D} \rho_u ds = 0$ follows from (2.11) and (2.12). We introduce $H_0^{-1/2}(\partial D) = \{\rho \in H^{-1/2}(\partial D) : \int_{\partial D} \rho ds = 0\}$, to see that $S_D : H_0^{-1/2}(\partial D) \rightarrow W_3$ maps $H_0^{-1/2}(\partial D)$ onto W^3 . It follows from [6] that for any $\rho \in H^{-1/2}(\partial D)$

$$(2.22) \quad \begin{aligned} \Delta S_D \rho &= 0 \text{ in } D \text{ and } Y \setminus D, \\ S_D \rho \Big|_{\partial D}^+ &= S_D \rho \Big|_{\partial D}^-, \\ \frac{\partial}{\partial n} S_D \rho \Big|_{\partial D}^\pm &= \pm \frac{1}{2} \rho + K_D^* \rho, \end{aligned}$$

where n is the outward directed normal vector on ∂D and K_D^* is the Neumann-Poincaré operator defined by

$$(2.23) \quad K_D^* \rho(x) = \text{p.v.} \int_{\partial D} \frac{\partial G(x, y)}{\partial n(x)} \rho(y) d\sigma(y), \quad x \in \partial D,$$

and K_D is the Neumann–Poincaré operator

$$(2.24) \quad K_D \rho(x) = \text{p.v.} \int_{\partial D} \frac{\partial G(x, y)}{\partial n(y)} \rho(y) d\sigma(y), \quad x \in \partial D.$$

In what follows we assume the boundary ∂D is $C^{1,\gamma}$ for some $\gamma > 0$. Here the layer potentials K_D , and K_D^* are they are continuous linear mappings from $L^2(\partial D)$ to $L^2(\partial D)$ and they are compact, since $\frac{\partial G(x, y)}{\partial n(x)}$ is a continuous kernel of order $d - 2$ in dimensions $d = 2, 3$. The operator S_D is a continuous linear map from $H_0^{-1/2}(\partial D)$ into W_3 and we define $S_{\partial D} \rho = S_D \rho|_{\partial D}$ for all $\rho \in H_0^{-1/2}(\partial D)$. Here $S_{\partial D} : H_0^{-1/2}(\partial D) \rightarrow H^{1/2}(\partial D)$ is continuous and has bounded inverse; see [6].

One readily verifies the symmetry

$$(2.25) \quad G(x, y) = G(y, x),$$

and application delivers the Plemelj symmetry for K_D, K_D^* , and $S_{\partial D}$ as operators on $L^2(\partial D)$ given by

$$(2.26) \quad K_D S_{\partial D} = S_{\partial D} K_D^*.$$

Moreover, as seen in [23], the operator $-S_{\partial D}$ is positive and self-adjoint in $L^2(\partial D)$, and in view of (2.26) K_D^* is a compact operator on $H_0^{-1/2}(\partial D)$.

Let $G : W_3 \rightarrow H^{1/2}(\partial D)$ be the trace operator, which is bounded and onto.

LEMMA 2.1. $S_D : H_0^{-1/2}(\partial D) \rightarrow W_3$ has bounded inverse $S_D^{-1} = S_{\partial D}^{-1} G$.

Proof. Suppose $u \in W_3$, and consider $Gu = u|_{\partial D} \in H^{1/2}(\partial D)$. For all $x \in Y$ define $w(x) = S_D(S_{\partial D}^{-1} Gu)$. Since $u, w \in W_3$, it follows that $w - u \in W_3$ as well. Since $Gu = Gw$, we have that $G(w - u) = 0$, and so $w - u \in (W_1 \oplus W_2)$. But $W_3 = (W_1 \oplus W_2)^\perp$, so $w = u$ as desired. The boundedness follows from the continuity of $S_{\partial D}^{-1}$ and G . \square

We introduce an auxiliary operator $T : W_3 \rightarrow W_3$, given by the sesquilinear form

$$(2.27) \quad \langle Tu, v \rangle = \frac{1}{2} \int_{Y \setminus D} \nabla u(x) \cdot \nabla \bar{v}(x) dx - \frac{1}{2} \int_D \nabla u(x) \cdot \nabla \bar{v}(x) dx.$$

The next theorem will be useful for the spectral decomposition of T_k .

THEOREM 2.2. *The linear map T defined in equation (2.27) is given by*

$$T = S_D K_D^* S_D^{-1}$$

and is compact and self-adjoint.

Proof. For $u, v \in W_3$, consider

$$(2.28) \quad \langle S_D K_D^* S_D^{-1} u, v \rangle = \int_Y \nabla [S_D K_D^* S_D^{-1} u] \cdot \nabla \bar{v}.$$

Since $\Delta S_D \rho = 0$ in D and $Y \setminus D$ for any $\rho \in H_0^{-1/2}(\partial D)$, an integration by parts yields

$$\langle S_D K_D^* S_D^{-1} u, v \rangle = \int_{\partial D} \bar{v} \left(\frac{\partial [S_D K_D^* S_D^{-1} u]}{\partial \nu} \Big|_{\partial D}^- - \frac{\partial [S_D K_D^* S_D^{-1} u]}{\partial \nu} \Big|_{\partial D}^+ \right) d\sigma.$$

Applying the jump conditions from (2.22) yields

$$(2.29) \quad \langle S_D K_D^* S_D^{-1} u, v \rangle = - \int_{\partial D} K_D^* S_D^{-1} u \bar{v} d\sigma.$$

Note that by the same jump conditions

$$(2.30) \quad K_D^* S_D^{-1} u = \frac{1}{2} \left(\frac{\partial u}{\partial \nu} \Big|_{\partial D}^- + \frac{\partial u}{\partial \nu} \Big|_{\partial D}^+ \right).$$

Application of (2.30) to (2.29) and an integration by parts yields the desired result. Compactness follows directly from the properties of S_D and K^* . \square

Rearranging terms in the weak formulation of (1.25) and writing $\mu = 1/2 - \lambda$ delivers the equivalent eigenvalue problem for Neumann electrostatic resonances:

$$\langle Tu, v \rangle = \mu \langle u, v \rangle, \quad u, v \in W_3.$$

Since T is compact and self-adjoint on W_3 , there exists a countable subset $\{\mu_i\}_{i \in \mathbb{N}}$ of the real line with a single accumulation point at 0 and an associated family of orthogonal finite-dimensional projections $\{P_{\mu_i}\}_{i \in \mathbb{N}}$ such that

$$\left\langle \sum_{i=1}^{\infty} P_{\mu_i} u, v \right\rangle = \langle u, v \rangle, \quad u, v \in W_3$$

and

$$\left\langle \sum_{i=1}^{\infty} \mu_i P_{\mu_i} u, v \right\rangle = \langle Tu, v \rangle, \quad u, v \in W_3.$$

Moreover, it is clear by (2.27) that

$$-\frac{1}{2} \leq \mu_i \leq \frac{1}{2}.$$

The upper bound $1/2$ is the eigenvalue associated with the subspace of functions $\Pi \in W_3$, such that functions in Π take constant values c_j on D_j , $j = 1, \dots, N$. Here the N constants c_j lie the $N - 1$ dimensional subspace associated with the mean zero constraint for functions in \mathcal{H} . It is also possible to show that there are no nonzero elements of W_3 that are eigenfunctions associated with eigenvalue $\mu = -1/2$. In section 8 an explicit lower bound μ^- is identified such that the inequality $-1/2 < \mu^- \leq \mu_i$ holds uniformly for a very broad class of geometries.

LEMMA 2.3. *The eigenvalues $\{\mu_i\}_{i \in \mathbb{N}}$ of T are precisely the eigenvalues of the Neumann–Poincaré operator K_D^* associated with quasi-periodic double layer potential restricted to ∂D .*

Proof. If a pair (μ, u) belonging to $(-1/2, 1/2] \times W_3$ satisfies $Tu = \mu u$ then $S_D K_D^* S_D^{-1} u = \mu u$. Multiplication of both sides by S_D^{-1} shows that $S_D^{-1} u$ is an eigenfunction for function for K_D^* associated with μ . Suppose the pair (μ, w) belongs to $(-1/2, 1/2] \times H^{-1/2}(\partial D)$ and satisfies $K_D^* w = \mu w$. Since the trace map from W_3 to $H_0^{1/2}(\partial D)$ is onto then there is a u in W_3 for which $w = S_D^{-1} u$ and $K_D^* S_D^{-1} u = \mu S_D^{-1} u$. Multiplication of this identity by S_D shows that u is an eigenfunction for T associated with μ . \square

Finally, we see that if $u_1 \in W_1$ and $u_2 \in W_2$, then

$$\begin{aligned} \langle Tu_1, v \rangle &= \frac{1}{2} \langle u_1, v \rangle, \\ \langle Tu_2, v \rangle &= -\frac{1}{2} \langle u_2, v \rangle \end{aligned}$$

for all $v \in H_{\#}^1(\alpha, Y)$.

Let P_1, P_2 be the orthogonal projections of \mathcal{H}_N onto $W_1 \oplus \Pi$ and W_2 . Then $\{P_1, P_2\} \cup \{P_{\mu_i}\}_{-\frac{1}{2} < \mu_i < \frac{1}{2}}$ is an orthogonal family of projections, and

$$\left\langle P_1 u + P_2 u + \sum_{-\frac{1}{2} < \mu_i < \frac{1}{2}} P_{\mu_i} u, v \right\rangle = \langle u, v \rangle$$

for all $u, v \in \mathcal{H}_N$.

We now recover the spectral decomposition for T_k associated with the sesquilinear form (2.7).

THEOREM 2.4. *The linear operator $T_k : \mathcal{H}_N \rightarrow \mathcal{H}_N$ associated with the sesquilinear form B_k is given by*

$$\langle T_k u, v \rangle = \left\langle k P_1 u + P_2 u + \sum_{-\frac{1}{2} < \mu_i < \frac{1}{2}} [k(1/2 + \mu_i) + (1/2 - \mu_i)] P_{\mu_i} u, v \right\rangle$$

for all $u, v \in \mathcal{H}_N$.

Proof. For $u, v \in \mathcal{H}_N$ we have

$$B_k(P_{\mu_i} u, v) = k \int_{Y \setminus D} \nabla P_{\mu_i} u \cdot \nabla \bar{v} + \int_D \nabla P_{\mu_i} u \cdot \nabla \bar{v}.$$

Since $P_{\mu_i} u$ is an eigenvector corresponding to $\mu_i \neq \pm \frac{1}{2}$, we have

$$\int_{Y \setminus D} \nabla P_{\mu_i} u \cdot \nabla \bar{v} = \frac{(1/2 + \mu_i)}{(1/2 - \mu_i)} \int_D \nabla P_{\mu_i} u \cdot \nabla \bar{v}$$

and so we calculate

$$B_k(P_{\mu_i} u, v) = \left[k \frac{(1/2 + \mu_i)}{(1/2 - \mu_i)} + 1 \right] \int_D \nabla P_{\mu_i} u \cdot \nabla \bar{v}.$$

But we also know that

$$\int_D \nabla P_{\mu_i} u \cdot \nabla \bar{v} = (1/2 - \mu_i) \int_Y \nabla P_{\mu_i} u \cdot \nabla \bar{v}$$

and so

$$B_k(P_{\mu_i} u, v) = [k(1/2 + \mu_i) + (1/2 - \mu_i)] \int_Y \nabla P_{\mu_i} u \cdot \nabla \bar{v}.$$

Since we clearly have

$$B_k(P_1 u, v) = k \int_{Y \setminus D} \nabla P_1 u \cdot \nabla \bar{v},$$

$$B_k(P_2 u, v) = \int_D \nabla P_2 u \cdot \nabla \bar{v},$$

and the projections P_1, P_2, P_{μ_i} are mutually orthogonal for all $-\frac{1}{2} < \mu_i < \frac{1}{2}$, the proof is complete. \square

It is evident that T_k is invertible whenever

$$(2.31) \quad k \in \mathbb{C} \setminus Z, \quad \text{where } Z = \left\{ \frac{\mu_i - 1/2}{\mu_i + 1/2} \right\}_{\{-\frac{1}{2} \leq \mu_i \leq \frac{1}{2}\}},$$

and, for $z = k^{-1}$,

$$(2.32) \quad (T_k)^{-1} = zP_1u + P_2u + \sum_{-\frac{1}{2} < \mu_i < \frac{1}{2}} z[(1/2 + \mu_i) + z(1/2 - \mu_i)]^{-1}P_{\mu_i}.$$

For future reference we also introduce the set S of $z \in \mathbb{C}$ for which T_k is not invertible, given by

$$(2.33) \quad S = \left\{ \frac{\mu_i + 1/2}{\mu_i - 1/2} \right\}_{\{-\frac{1}{2} < \mu_i < \frac{1}{2}\}},$$

which also lies on the negative real axis. In section 8 we will provide explicit upper bounds on the set S that depend upon the geometry of the inclusions.

3. Neumann spectrum for complex coupling constant. We now characterize the basic properties of the Neumann spectrum corresponding to problem (1.22) for *complex* coupling constants k .

We set $\omega^2 = \nu(k)$ in (1.22) and extend the Neumann eigenvalue problem to complex coefficients k outside the set Z given by (2.31). The Neumann spectral problem (1.22) is written as

$$(3.1) \quad -\nabla \cdot (k(1 - \chi_D) + \chi_D)\nabla u = -\Delta_N T_k u = \nu(k)u,$$

with $u \in \mathcal{H}_N$. Here $-\Delta_N$ is the Laplace operator associated with the bilinear form $\langle \cdot, \cdot \rangle$ defined on \mathcal{H}_N . We characterize the Neumann spectra by analyzing the operator

$$(3.2) \quad B(k) = T_k^{-1}(-\Delta_N^{-1}),$$

where the operator $-\Delta_N^{-1}$ is given by (2.17).

The operator $B(k) : L_0^2(Y) \rightarrow \mathcal{H}_N$ is easily seen to be bounded for $k \notin Z$; see Theorem 11.4. Since $\mathcal{H}_N \subset H^1(Y)$ embeds compactly into $L_0^2(Y)$, we find by virtue of Poincaré's inequality that $B(k)$ is a bounded compact linear operator on $L_0^2(Y)$ and therefore has a discrete spectrum $\{\gamma_i(k)\}_{i \in \mathbb{N}}$ with a possible accumulation point at 0; see Remark 11.5. The corresponding eigenspaces are finite dimensional and the eigenfunctions $p_i \in L_0^2(Y)$ satisfy

$$(3.3) \quad B(k)p_i(x) = \gamma_i(k, \alpha)p_i(x) \quad \text{for } x \text{ in } Y$$

and also belong to \mathcal{H}_N . Note further for $\gamma_i \neq 0$ that (3.3) holds if and only if (3.1) holds with $\nu_i(k) = \gamma_i^{-1}(k)$, and $-\Delta_N T_k u_i = \nu_i(k)u_i$. Collecting results we have the following theorem

THEOREM 3.1. *Let Z denote the set of points on the negative real axis defined by (2.31). Then the Neumann eigenvalue problem (1.22) can be extended for values of the coupling constant k off the positive real axis into $\mathbb{C} \setminus Z$; i.e., the Neumann eigenvalues are of finite multiplicity and are denoted by $\nu_j(k) = \gamma_j^{-1}(k)$, $j \in \mathbb{N}$.*

4. Series representation of Neumann eigenvalues. With the basic band structure of the Neumann eigenvalues of problem (1.22) identified, we now seek a series representation of these eigenvalues in a suitable neighborhood of k near infinity. In later sections, we will demonstrate that the series expansions are in fact uniformly convergent within a certain neighborhood which is defined in terms of the geometry of the crystal. In obtaining series representations for these eigenvalues in terms of k along with a radius of convergence, we will gain access to error estimates on these series which will play a critical role in the proofs of Theorems 1.1 and 1.2, 10.2, 10.3, 12.1, and 12.2.

In what follows we set $\gamma = \nu^{-1}(k)$ and analyze the spectral problem

$$(4.1) \quad B(k)u = \gamma(k)u.$$

Henceforth we will analyze the high contrast limit by developing a power series in $z = \frac{1}{k}$ about $z = 0$ for the spectrum of the family of operators associated with (4.1):

$$(4.2) \quad \begin{aligned} B(k) &:= T_k^{-1}(-\Delta_N)^{-1} \\ &= \left(zP_1 + P_2 + z \sum_{-\frac{1}{2} < \mu_i < \frac{1}{2}} [(1/2 + \mu_i) + z(1/2 - \mu_i)]^{-1} P_{\mu_i} \right) (-\Delta_N)^{-1} \\ &= A(z). \end{aligned}$$

Here we define the operator $A(z)$ such that $A(1/k) = B(k)$ and the associated eigenvalues $\beta_j(1/k) = \gamma_j(k)$, and the spectral problem is $A(z)u = \beta(z)u$ for $u \in L_0^2(Y)$. The Neumann eigenvalues are of finite multiplicity and are described in terms of $\beta_j(z) \in \sigma(A(z))$ by

$$(4.3) \quad \nu_j(k) = \frac{1}{\beta_j(\frac{1}{k})}, \quad j \in \mathbb{N}.$$

The above representation is used to show that $A(z)$ is self-adjoint for $z = 1/k \in \mathbb{R}$ and is a family of bounded operators taking $L_0^2(Y)$ into itself; see Theorem 11.6 and subsequent remarks. We have the following:

LEMMA 4.1. *$A(z)$ is holomorphic on $\Omega_0 := \mathbb{C} \setminus S$, where $S = \bigcup_{i \in \mathbb{N}} z_i$ is the collection of points $z_i = (\mu_i + 1/2)/(\mu_i - 1/2)$ on the negative real axis associated with the eigenvalues $\{\mu_i\}_{i \in \mathbb{N}}$. The set S consists of poles of $A(z)$ with only one accumulation point at $z = -1$.*

In sections 8 and 9 we identify explicit lower bounds $-1/2 < \mu^* \leq \min_i \{\mu_i\}$ that hold for generic classes of inclusion domains D . The corresponding upper bound z^* on S is written

$$(4.4) \quad \max_i \{z_i\} \leq \frac{\mu^* + 1/2}{\mu^* - 1/2} = z^* < 0.$$

Let $\beta_0 \in \sigma(A(0))$ with spectral projection $P(0)$, and let Γ be a closed contour in \mathbb{C} enclosing β_0 but no other $\beta_0 \in \sigma(A(0))$. The spectral projection associated with $\beta(z) \in \sigma(A(z))$ for $\beta(z) \in \text{int}(\Gamma)$ is denoted by $P(z)$. Here we suppose all elements $\beta(z) \in \text{int}(\Gamma)$ converge to β_0 as $z \rightarrow 0$. This collection is known as the eigenvalue group associated with β_0 . We write $M(z) = P(z)L_0^2(Y)$ and suppose for the moment that Γ lies in the resolvent of $A(z)$ and $\dim(M(0)) = \dim(M(z)) = m$, noting that

Theorem 7.3 provides explicit conditions for when this holds true. Since $A(z)$ is analytic in a neighborhood of the origin, we write

$$(4.5) \quad A(z) = A(0) + \sum_{n=1}^{\infty} z^n A_n.$$

Defining the resolvent of $A(z)$ by

$$R(\zeta, z) = (A(z) - \zeta)^{-1},$$

and expanding successively in Neumann series and power series, we have the identity

$$(4.6) \quad \begin{aligned} R(\zeta, z) &= R(\zeta, 0)[I + (A(z) - A(0))R(\zeta, 0)]^{-1} \\ &= R(\zeta, 0) + \sum_{p=1}^{\infty} [-(A(z) - A(0))R(\zeta, 0)]^p \\ &= R(\zeta, 0) + \sum_{n=1}^{\infty} z^n R_n(\zeta), \end{aligned}$$

where

$$R_n(\zeta) = \sum_{k_1 + \dots + k_p = n, k_j \geq 1} (-1)^p R(\zeta, 0) A_{k_1} R(\zeta, 0) A_{k_2} \cdots R(\zeta, 0) A_{k_p}$$

for $n \geq 1$.

Application of the contour integral formula for spectral projections [32, 20, 21] delivers the expansion for the spectral projection,

$$(4.7) \quad \begin{aligned} P(z) &= -\frac{1}{2\pi i} \oint_{\Gamma} R(\zeta, z) d\zeta \\ &= P(0) + \sum_{n=1}^{\infty} z^n P_n, \end{aligned}$$

where $P_n = -\frac{1}{2\pi i} \oint_{\Gamma} R_n(\zeta) d\zeta$. Now we represent the difference $(A(z) - \beta_0)P(z)$ as a contour integral. Start with

$$(4.8) \quad (A(z) - \beta_0)R(\zeta, z) = I + (\zeta - \beta_0)R(\zeta, z)$$

and we have

$$(4.9) \quad (A(z) - \beta_0)P(z) = -\frac{1}{2\pi i} \oint_{\Gamma} (\zeta - \beta_0)R(\zeta, z) d\zeta.$$

Next we develop a series representation for the eigenvalues of $A(z)$ for real $z = 1/k$. We observe that the operator $A(z)$ is self-adjoint and bounded for $z \in \mathbb{R} \setminus S$; see Theorem 11.6. So for $z \in \mathbb{R} \setminus S$ there is a complete orthonormal system of eigenfunctions $\{\varphi_i(z)\}_{i \in \mathbb{N}}$ in $L_0^2(Y)$ and eigenvalues $\{\beta_i(z)\}_{i \in \mathbb{N}}$ such that

$$(4.10) \quad \beta_i(z) = (A(z)\varphi_i(z), \varphi_i(z)) \quad \text{for } z \in \mathbb{R} \setminus S.$$

Now for β_0 such that $\beta_0 = (A(0)\varphi_i(0), \varphi_i(0))$ and $\beta_i(z)$ associated with the eigenvalue group corresponding to β_0 inside Γ we have $P(z)\varphi_i(z) = \varphi_i(z)$, and from (4.9)

$$\begin{aligned}
 \beta_i(z) - \beta_0 &= ((A(z) - \beta_0)P(z)\varphi_i(z), \varphi_i(z)) \\
 (4.11) \qquad &= - \left(\frac{1}{2\pi i} \oint_{\Gamma} (\zeta - \beta_0)R(\zeta, z)d\zeta \varphi_i(z), \varphi_i(z) \right).
 \end{aligned}$$

Next apply (2.32) to write

$$\begin{aligned}
 R(\zeta, z) &= R(\zeta, 0) + \sum_{n=1}^{\infty} [-(A(z) - A(0))R(\zeta, 0)]^n \\
 (4.12) \qquad &= R(\zeta, 0) + \sum_{n=1}^{\infty} z^n \mathcal{N}^n(\zeta, z),
 \end{aligned}$$

where

$$(4.13) \qquad \mathcal{N}(\zeta, z) = \left[\left(P_1 u + \sum_{-\frac{1}{2} < \mu_i < \frac{1}{2}} [(1/2 + \mu_i) + z(1/2 - \mu_i)]^{-1} P_{\mu_i} \right) (-\Delta_N)^{-1} R(\zeta, 0) \right]$$

for $n \geq 1$. Equation (4.11) together with (4.12) deliver a series representation formula for Neumann eigenvalues $\nu_i(k) = (\beta_i(\frac{1}{k}))^{-1}$ for real k in a neighborhood of ∞ . Substituting (4.12) into (4.11) and manipulating yields

$$(4.14) \qquad \beta_i(z) = \beta_0 + \sum_{n=1}^{\infty} z^n \beta_i^n(z),$$

where

$$(4.15) \qquad \beta_i^n(z) = -\frac{1}{2\pi i} \left(\oint_{\Gamma} (\zeta - \beta_0) \mathcal{N}^n(\zeta, z) d\zeta \varphi_i(z), \varphi_i(z) \right), \quad n \geq 1$$

for z in an interval containing $z = 0$.

5. Series representation of Bloch eigenvalues. We now repeat the analysis performed in sections 2, 3, and 4 for the Bloch Eigenvalues of (1.23). Just as before, we begin with the variational description of the Bloch eigenvalue problem (1.23). Denote the spaces of all α quasi-periodic complex valued functions belonging to $L^2_{loc}(\mathbb{R}^d)$ by $L^2_{\#}(\alpha, Y)$. For $\alpha \neq 0$ the eigenfunctions h for (1.23) belong to the space

$$(5.1) \qquad H^1_{\#}(\alpha, Y) = \{h \in H^1_{loc}(\mathbb{R}^d) : h \text{ is } \alpha \text{ quasiperiodic}\}.$$

The space $H^1_{\#}(\alpha, Y)$ is a Hilbert space under the inner product (2.3). When $\alpha = 0$, the pair $h(x) = 1, \omega^2 = 0$ is a solution to (1.23). For this case the remaining eigenfunctions associated with nonzero eigenvalues are orthogonal to 1 in the $L^2(Y)$ inner product. These eigenfunctions belong to the set of square integrable Y periodic functions with zero average denoted by $L^2_{\#}(0, Y)$. They also belong to the space

$$(5.2) \qquad H^1_{\#}(0, Y) = \{h \in H^1_{loc}(\mathbb{R}^d) : h \text{ is periodic, } \int_Y h \, dx = 0\}.$$

The space $H^1_{\#}(0, Y)$ is also Hilbert space with inner product defined by (2.3).

For any $k \in \mathbb{C}$, the variational formulation of the Bloch eigenvalue problem (1.23) for h and ω^2 is given by

$$(5.3) \qquad B_k(h, v) = \omega^2(h, v)$$

for all v in $H_{\#}^1(\alpha, Y)$ and $\alpha \in Y^*$. As before, it is possible to decompose $H_{\#}^1(\alpha, Y)$ into an orthogonal sum of three subspaces W_1 , W_2 , and W_3 to recover an analytic representation for the operator T_k^α associated with the bilinear form $B_k(h, v)$ defined on $H_{\#}^1(\alpha, Y) \times H_{\#}^1(\alpha, Y)$.

We first address the case $\alpha \in Y^* \setminus \{0\}$. Let $W_1 \subset H_{\#}^1(\alpha, Y)$ be the completion in $H_{\#}^1(\alpha, Y)$ of the subspace of functions with support away from D , and let $W_2 \subset H_{\#}^1(\alpha, Y)$ be the subspace of functions in $H_0^1(D)$ extended by zero into Y . Clearly W_1 and W_2 are orthogonal subspaces of $H_{\#}^1(\alpha, Y)$, so we define $W_3 := (W_1 \oplus W_2)^\perp$. We therefore have

$$(5.4) \quad H_{\#}^1(\alpha, Y) = W_1 \oplus W_2 \oplus W_3.$$

The orthogonal decomposition and integration by parts shows that elements $u \in W_3$ are harmonic separately in D and $Y \setminus D$.

Now consider $\alpha = 0$ and decompose $H_{\#}^1(0, Y)$. Let $W_1 \subset H_{\#}^1(0, Y)$ be the completion in $H_{\#}^1(0, Y)$ of the subspace of functions with support away from D . Here let $\tilde{H}_0^1(D)$ denote the subspace of functions $H_0^1(D)$ extended by zero into $Y \setminus D$ and let 1_Y be the indicator function of Y . We define $W_2 \subset H_{\#}^1(0, Y)$ to be the subspace of functions given by

$$(5.5) \quad W_2 = \left\{ u = \tilde{u} - \left(\frac{1}{|Y|} \int_D \tilde{u} dx \right) 1_Y \mid \tilde{u} \in \tilde{H}_0^1(D) \right\}.$$

Clearly W_1 and W_2 are orthogonal subspaces of $H_{\#}^1(0, Y)$, and $W_3 := (W_1 \oplus W_2)^\perp$. As before we have

$$(5.6) \quad H_{\#}^1(0, Y) = W_1 \oplus W_2 \oplus W_3,$$

and W_3 is identified with the subspace of $H_{\#}^1(0, Y)$ functions that are harmonic inside D and $Y \setminus D$, respectively. The orthogonality between W_2 and W_3 follows from the identity $\int_{\partial D} \partial_n w ds = 0$ for $w \in W_3$.

For every $\alpha \in Y^*$ the associated subspace W_3 can be decomposed into finite-dimensional pairwise orthogonal subspaces associated with the eigenvalue problem for quasi-periodic electrostatic resonances given by

$$\langle Tu, v \rangle = \mu \langle u, v \rangle, \quad u, v \in W_3.$$

The operator T defined by the sesquilinear form (2.27) is seen to be compact and self-adjoint on W_3 see, [25]. Since T is compact and self-adjoint on W_3 , there exists a countable subset $\{\mu_i\}_{i \in \mathbb{N}}$ of the real line with a single accumulation point at 0 and an associated family of orthogonal finite-dimensional projections $\{P_{\mu_i}\}_{i \in \mathbb{N}}$ such that

$$\left\langle \sum_{i=1}^{\infty} P_{\mu_i} u, v \right\rangle = \langle u, v \rangle, \quad u, v \in W_3$$

and

$$\left\langle \sum_{i=1}^{\infty} \mu_i P_{\mu_i} u, v \right\rangle = \langle Tu, v \rangle, \quad u, v \in W_3,$$

where

$$-\frac{1}{2} \leq \mu_i \leq \frac{1}{2};$$

see [25]. For $\alpha \neq 0$ the upper bound $1/2$ is the eigenvalue associated with the N -dimensional subspace of functions $\Pi \in W_3$, such that functions in Π take constant values c_j on D_j , $j = 1, \dots, N$. For $\alpha = 0$, the zero average constraint shows that Π is $N - 1$ dimensional. In [25] an explicit lower bound μ^* is identified such that the inequality $-1/2 < \mu^* \leq \mu_i$ holds for a generic class of geometries uniformly with respect to $\alpha \in Y^*$. It is shown that this bound is independent of $\alpha \in Y^*$ (see [25]) and is discussed in sections 8 and 9.

Finally, we see that if $u_1 \in W_1$ and $u_2 \in W_2$, then

$$\begin{aligned} \langle Tu_1, v \rangle &= \frac{1}{2} \langle u_1, v \rangle, \\ \langle Tu_2, v \rangle &= -\frac{1}{2} \langle u_2, v \rangle \end{aligned}$$

for all $v \in H_{\#}^1(\alpha, Y)$.

Let P_1 and P_2 be the projections onto $W_1 \oplus \Pi$ and W_2 . Then $\{P_1, P_2\} \cup \{P_{\mu_i}\}_{-\frac{1}{2} < \mu_i < \frac{1}{2}}$ is an orthogonal family of projections, and

$$\left\langle P_1 u + P_2 u + \sum_{-\frac{1}{2} < \mu_i < \frac{1}{2}} P_{\mu_i} u, v \right\rangle = \langle u, v \rangle$$

for all $u, v \in H_{\#}^1(\alpha, Y)$.

The representation for T_k^α is given by the following lemma

LEMMA 5.1 (Representation of bilinear form [25]). *The linear operator $T_k^\alpha : H_{\#}^1(\alpha, Y) \rightarrow H_{\#}^1(\alpha, Y)$ associated with the bilinear form B_k is given by*

$$\langle T_k^\alpha u, v \rangle = \left\langle kP_1 u + P_2 u + \sum_{-\frac{1}{2} < \mu_i < \frac{1}{2}} [k(1/2 + \mu_i) + (1/2 - \mu_i)] P_{\mu_i} u, v \right\rangle$$

for all $u, v \in H_{\#}^1(\alpha, Y)$.

The Bloch spectral problem can now be written in operator form as

$$(5.7) \quad -\nabla \cdot (k(1 - \chi_D) + \chi_D) \nabla u = -\Delta_\alpha T_k^\alpha u = \nu(k)u,$$

with $u \in H_{\#}(\alpha, \mathbb{R}^d)$. We proceed as in the Neumann case and analyze the Bloch spectra by developing a power series in $z = \frac{1}{k}$ about $z = 0$ for the spectrum of the family of operators given by $A^\alpha(z) = (T_k^\alpha)^{-1}(-\Delta_\alpha)^{-1}$, i.e.,

$$(5.8) \quad A^\alpha(z) = \left(zP_1 + P_2 + z \sum_{-\frac{1}{2} < \mu_i < \frac{1}{2}} [(1/2 + \mu_i) + z(1/2 - \mu_i)]^{-1} P_{\mu_i} \right) (-\Delta_\alpha)^{-1}.$$

Here the operator $(-\Delta_\alpha)^{-1}$ defined for all $\alpha \in Y^*$ is given by

$$(5.9) \quad (-\Delta_\alpha)^{-1} u(x) = - \int_Y G^\alpha(x, y) u(y) dy,$$

where $G^\alpha(x, y)$ is the Green's function for the quasi-periodic Laplace operator.

The operator $A^\alpha(z)$ is self-adjoint for $k \in \mathbb{R}$ and is a family of compact, bounded operators taking $L_{\#}^2(\alpha, Y)$ into itself, and we have [25] the following lemma:

LEMMA 5.2 (Spectrum of $A^\alpha(z)$).

1. $A^\alpha(z)$ is holomorphic on $\Omega_0 := \mathbb{C} \setminus S$, where $S = \bigcup_{i \in \mathbb{N}} z_i$ is the collection of points $z_i = (\mu_i + 1/2)/(\mu_i - 1/2)$ on the negative real axis associated with the eigenvalues $\{\mu_i\}_{i \in \mathbb{N}}$. The set S consists of poles of $A^\alpha(z)$ with only one accumulation point at $z = -1$.
2. For $z \in \Omega_0$ the spectrum of $A^\alpha(z)$ denoted by $\sigma(A^\alpha(z))$ consists of eigenvalues $\beta_j^\alpha(z)$ of finite multiplicity with a possible accumulation point $z = 0$.

We have the following theorem:

THEOREM 5.3 ([25]). *The Bloch eigenvalue problem (1.23) for $-\nabla(k(1 - \chi_D) + \chi_D)\nabla$ defined on $H_{\#}^1(\alpha, Y)$ can be extended for values of the coupling constant k with $k^{-1} \in \mathbb{C} \setminus S$, such that for each $\alpha \in Y^*$ the Bloch eigenvalues are of finite multiplicity and are denoted by $\lambda_j(k, \alpha) = (\beta_j^\alpha(k^{-1}))^{-1}$, $j \in \mathbb{N}$, and the band structure*

$$(5.10) \quad \lambda_j(k, \alpha) = \omega^2, \quad j \in \mathbb{N}$$

extends to complex coupling constants k with $k^{-1} \in \mathbb{C} \setminus S$.

Analysis provided in [25] shows that upper bounds introduced in sections 8 and 9 also apply to the set of quasi-periodic source free resonances, and S is bounded uniformly away from 0 for all $\alpha \in Y^*$, i.e.,

$$(5.11) \quad \max_i \{z_i\} \leq \frac{\mu^* + 1/2}{\mu^* - 1/2} = z^* < 0.$$

Let $\beta_0^\alpha \in \sigma(A^\alpha(0))$ with spectral projection $P(0)$, and let Γ be a closed contour in \mathbb{C} enclosing β_0^α but no other $\beta_0^\alpha \in \sigma(A^\alpha(0))$. The spectral projection associated with $\beta^\alpha(z) \in \sigma(A^\alpha(z))$ for $\beta^\alpha(z) \in \text{int}(\Gamma)$ is denoted by $P(z)$. As before we suppose all elements $\beta^\alpha(z) \in \text{int}(\Gamma)$ converge to β_0^α as $z \rightarrow 0$. This collection is known as the eigenvalue group associated with β_0^α . We write $M(z) = P(z)L_{\#}^2(\alpha, Y)$ and suppose for the moment that Γ lies in the resolvent of $A^\alpha(z)$ and $\dim(M(0)) = \dim(M(z)) = m$, noting that Theorems 7.1 and 7.2 provide explicit conditions for when this holds true. Define the resolvent of $A^\alpha(z)$ by

$$R(\zeta, z) = (A^\alpha(z) - \zeta)^{-1}$$

and proceeding as before, we get

$$(5.12) \quad (A^\alpha(z) - \beta_0^\alpha)P(z) = -\frac{1}{2\pi i} \oint_{\Gamma} (\zeta - \beta_0^\alpha)R(\zeta, z)d\zeta.$$

We now construct a series development suitable for the analysis of band gaps and passbands when $z \in \mathbb{R}$. The operator $A^\alpha(z)$ is self-adjoint and bounded for $z \in \mathbb{R} \notin S$; see [25] or Remark 11.7. So for $z \in \mathbb{R} \setminus S$ there is a complete orthonormal system of eigenfunctions $\{\varphi_i(z)\}_{i \in \mathbb{N}}$ in $L_0^2(Y)$ and eigenvalues $\{\beta_i^\alpha(z)\}_{i \in \mathbb{N}}$ such that

$$(5.13) \quad \beta_i^\alpha(z) = (A^\alpha(z)\varphi_i(z), \varphi_i(z)) \quad \text{for } z \in \mathbb{R} \setminus S.$$

Now for β_0^α such that $\beta_0^\alpha = (A^\alpha(0)\varphi_i(0), \varphi_i(0))$ and $\beta_i^\alpha(z)$ associated with the eigenvalue group corresponding to β_0^α inside Γ we have $P(z)\varphi_i(z) = \varphi_i(z)$, and from (5.12)

$$(5.14) \quad \begin{aligned} \beta_i^\alpha(z) - \beta_0^\alpha &= ((A^\alpha(z) - \beta_0^\alpha)P(z)\varphi_i(z), \varphi_i(z)) \\ &= -\left(\frac{1}{2\pi i} \oint_{\Gamma} (\zeta - \beta_0^\alpha)R(\zeta, z)d\zeta \varphi_i(z), \varphi_i(z)\right). \end{aligned}$$

Expanding the resolvent of $A^\alpha(z)$ in Neumann series and applying (5.8), we write

$$\begin{aligned}
 R(\zeta, z) &= R(\zeta, 0) + \sum_{n=1}^{\infty} [-(A^\alpha(z) - A(0))R(\zeta, 0)]^n \\
 (5.15) \qquad &= R(\zeta, 0) + \sum_{n=1}^{\infty} z^n (\mathcal{N}^\alpha(\zeta, z))^n,
 \end{aligned}$$

where

$$(5.16) \qquad \mathcal{N}^\alpha(\zeta, z) = \left[\left(P_1 u + \sum_{-\frac{1}{2} < \mu_i < \frac{1}{2}} [(1/2 + \mu_i) + z(1/2 - \mu_i)]^{-1} P_{\mu_i} \right) (-\Delta_\alpha)^{-1} R(\zeta, 0) \right]$$

for $n \geq 1$. Equation (5.14) together with (5.15) deliver a series representation formula for Bloch eigenvalues $\lambda_j(k, \alpha) = (\beta_i^\alpha(\frac{1}{k}))^{-1}$ for real k in a neighborhood of ∞ . Substituting (5.15) into (5.14) and manipulating yields

$$(5.17) \qquad \beta_i^\alpha(z) = \beta_0^\alpha + \sum_{n=1}^{\infty} z^n \beta_i^n(z),$$

where

$$(5.18) \qquad \beta_i^n(z) = -\frac{1}{2\pi i} \left(\oint_{\Gamma} (\zeta - \beta_0) (\mathcal{N}^\alpha(\zeta, z))^n d\zeta \varphi_i(z), \varphi_i(z) \right), \quad n \geq 1$$

for z in an interval containing $z = 0$.

6. Neuman and Bloch spectrum in the high contrast limit. In this section, we identify the spectrum of the limiting operators $A(0)$ and $A^\alpha(0)$. Recall that the families of operators $A(z)$ and $A^\alpha(z)$ represent the inverse of the divergence form operator in the spectral problems (1.22) and (1.23), indexed in $z = k^{-1}$, with Neumann and α -quasi-periodic boundary conditions on Y , respectively. The limit spectra of these operators plays a crucial role in establishing the upper and lower bounds of the band gaps and band edges identified in Theorems 1.1 and 1.2.

Using the representation

$$(6.1) \qquad A(z) = \left(zP_1 + P_2 + z \sum_{-\frac{1}{2} < \mu_i < \frac{1}{2}} [(1/2 + \mu_i) + z(1/2 - \mu_i)]^{-1} P_{\mu_i} \right) (-\Delta_N)^{-1},$$

we see that

$$(6.2) \qquad A(0) = P_2(-\Delta_N)^{-1},$$

and denote the spectrum of $A(0)$ by $\sigma(A(0))$.

To begin, consider the Dirichlet eigenvalues of the Laplace operator on D associated with the spectral problem $-\Delta\psi = \delta\psi$, $\psi \in H_0^1(D)$ and denote the spectrum by $\sigma(-\Delta_D)$. The subset of Dirichlet eigenvalues associated with eigenfunctions having zero mean over D is denoted by $\{\delta'_j\}_{j \in \mathbb{N}}$ and the set of Dirichlet eigenvalues associated with eigenfunctions with nonzero mean is denoted by $\{\delta^*_j\}_{j \in \mathbb{N}}$. Next we introduce the

sequence of numbers $\{\nu_j\}_{j \in \mathbb{N}}$ given by the positive roots ν of the spectral function $S(\nu)$ defined by

$$(6.3) \quad S(\nu) = \nu \sum_{i \in \mathbb{N}} \frac{a_i^2}{\nu - \delta_i^*} - 1,$$

where the coefficients $a_j = |\int_D \psi_j dx|$ are integrals of eigenfunctions ψ_j corresponding to the Dirichlet eigenvalues δ_j^* . The explicit characterization of $\sigma(A(0))$ is given by the following theorem.

THEOREM 6.1. $\sigma(A(0)) = \{\delta_j'^{-1}\}_{j \in \mathbb{N}} \cup \{\nu_j^{-1}\}_{j \in \mathbb{N}}$, where the families $\{\delta_j'^{-1}\}_{j \in \mathbb{N}}$ and $\{\nu_j^{-1}\}_{j \in \mathbb{N}}$ are identified in the above paragraph.

To establish the theorem we first show that the eigenvalue problem

$$(6.4) \quad P_2(-\Delta_N)^{-1}u = \lambda u$$

with $\lambda \in \sigma(A^\alpha(0))$ and eigenfunction $u \in L_0^2(Y)$ is equivalent to finding λ and $u \in W_2$ for which

$$(6.5) \quad (u, v) = \lambda \langle u, v \rangle \quad \text{for all } v \in W_2.$$

To see the equivalence note that we have $u = P_2 u$ and, for $v \in \mathcal{H}_N$,

$$(6.6) \quad \langle P_2(-\Delta_N)^{-1}u, v \rangle = \lambda \langle u, v \rangle = \lambda \langle P_2 u, v \rangle,$$

hence

$$(6.7) \quad \langle (-\Delta_N)^{-1}u, P_2 v \rangle = \lambda \langle u, P_2 v \rangle.$$

Since $\langle (-\Delta_N)^{-1}u, v \rangle = (u, v)$ for any $u \in L_0^2(Y)$ and $v \in \mathcal{H}_N$, (6.7) becomes

$$(6.8) \quad (u, P_2 v) = \lambda \langle u, P_2 v \rangle,$$

and the equivalence follows noting that P_2 is the projection of \mathcal{H}_N onto W_2 .

To conclude we show that the set of eigenvalues for (6.4) is given by $\{\delta_j'^{-1}\}_{j \in \mathbb{N}} \cup \{\nu_j^{-1}\}_{j \in \mathbb{N}}$. We see that $u \in W_2$, and from (2.8) we have the dichotomy $\int_D \tilde{u} dx = 0$ and $u = \tilde{u} \in \tilde{H}_0^1(D)$ or $\int_D \tilde{u} dx \neq 0$ and $u = \tilde{u} - \gamma 1_Y$ with $\gamma = \int_D \tilde{u} dx$. It is evident for the first case that the eigenfunction $u \in \tilde{H}_0^1(D)$, and for $v \in W_2$ given by

$$(6.9) \quad v = \tilde{v} - \left(\int_D \tilde{v} dx \right) 1_Y \quad \text{for } \tilde{v} \in \tilde{H}_0^1(D)$$

that problem (6.5) becomes

$$(6.10) \quad \int_D u \tilde{v} = \lambda \int_D \nabla u \cdot \nabla \tilde{v} \quad \text{for all } \tilde{v} \in \tilde{H}_0^1(D),$$

and we conclude that \tilde{u} is a Dirichlet eigenfunction with zero average over D so $\lambda \in \{\delta_j'^{-1}\}_{j \in \mathbb{N}}$. For the second case, we have $u \in W_2$ and again

$$(6.11) \quad \int_D u \tilde{v} = \lambda \int_D \nabla u \cdot \nabla \tilde{v} \quad \text{for all } \tilde{v} \in \tilde{H}_0^1(D).$$

Writing $u = \tilde{u} - \gamma 1_Y$, $\lambda = \nu^{-1}$ and integrating by parts in (6.11) shows that $\tilde{u} \in \tilde{H}_0^1(D)$ is the solution of

$$(6.12) \quad \Delta \tilde{u} + \nu \tilde{u} = \nu \gamma \quad \text{for } x \in D.$$

We normalize \tilde{u} so that $\gamma = \int_D \tilde{u} dx = 1$ and write

$$(6.13) \quad \tilde{u} = \sum_{j=1}^{\infty} c_j \psi_j,$$

where ψ_j are the Dirichlet eigenfunctions of $-\Delta_D$ associated with eigenvalue δ_j extended by zero to Y . Substitution of (6.13) into (6.12) gives

$$(6.14) \quad \sum_{j=1}^{\infty} (-\delta_j + \nu) c_j \psi_j = \nu.$$

Multiplication of both sides of (6.14) by $\overline{\psi_k}$ over Y and orthonormality of $\{\psi_j\}_{j \in \mathbb{N}}$ show that \tilde{u} is given by

$$(6.15) \quad \tilde{u} = \nu \sum_{k \in \mathbb{N}} \frac{\int_D \overline{\psi_k} \psi_k}{\nu - \delta_k^*} \psi_k,$$

where δ_k^* correspond to Dirichlet eigenvalues associated with eigenfunctions for which $\int_D \psi_k dx \neq 0$. To calculate ν , we integrate both sides of (6.15) over D to recover the identity

$$(6.16) \quad \nu \sum_{k \in \mathbb{N}} \frac{a_k^2}{\nu - \delta_k^*} - 1 = 0.$$

It follows from (6.16) that $\lambda \in \{\nu_i^{-1}\}_{i \in \mathbb{N}}$, and the proof of Theorem 6.1 is complete.

We now recover the spectrum of the limiting operator $A^\alpha(0)$ when $\alpha \in Y^*$. Using the representation

$$(6.17) \quad A^\alpha(z) = \left(zP_1 + P_2 + z \sum_{-\frac{1}{2} < \mu_i < \frac{1}{2}} [(1/2 + \mu_i) + z(1/2 - \mu_i)]^{-1} P_{\mu_i} \right) (-\Delta_\alpha)^{-1},$$

we see that

$$(6.18) \quad A^\alpha(0) = P_2(-\Delta_\alpha)^{-1}.$$

The following theorem provides the explicit characterization of the spectrum $\sigma(A^\alpha(0))$ for $\alpha \neq 0$.

THEOREM 6.2 (Limit spectrum for quasi-periodic problem [25]). $\sigma(A^\alpha(0)) = \{\delta_j'^{-1}\}_{j \in \mathbb{N}} \cup \{(\delta_j^*)^{-1}\}_{j \in \mathbb{N}} = \sigma(-\Delta_D^{-1})$, where the families $\{\delta_j'^{-1}\}_{j \in \mathbb{N}}$ and $\{(\delta_j^*)^{-1}\}_{j \in \mathbb{N}}$ are identified in the paragraph above (6.3).

To conclude, we recover the limit spectrum $\sigma(A^0(0))$ for the periodic problem; see [25].

THEOREM 6.3. $\sigma(A^0(0)) = \{\delta_j'^{-1}\}_{j \in \mathbb{N}} \cup \{\nu_j^{-1}\}_{j \in \mathbb{N}}$, where the families $\{\delta_j'^{-1}\}_{j \in \mathbb{N}}$ and $\{\nu_j^{-1}\}_{j \in \mathbb{N}}$ are identified in the paragraph above (6.3).

Theorems 6.1, 6.2, and 6.3 are in accord with Lemma 2.3 parts (b) and (c) of [15].

7. Radius of convergence and separation of spectra. Here we establish the radius of convergence for the series expansions (4.14), (5.17) of the spectra of the operators $A^\alpha(z)$ and $A(z)$. We will see that, for $|z|$ within a radius of convergence dependent explicitly on the geometry of the crystal (and the wave vector $\alpha \in Y^*$ for $A^\alpha(z)$), the analytic representations (4.14), (5.17) are uniformly convergent in the limit $z \rightarrow 0$. As an added result, we obtain separation of spectra results, along with error estimates for the series which will be leveraged to open band gaps presented in Theorems 1.1, 10.2, and 12.1,

Fix an inclusion geometry specified by the domain D . Suppose first $\alpha \in Y^*$ and $\alpha \neq 0$. Recall from Theorem 6.2 that the spectrum of $A^\alpha(0)$ is $\sigma(-\Delta_D^{-1})$. Take Γ to be a closed contour in \mathbb{C} containing an eigenvalue β_0^α in $\sigma(-\Delta_D^{-1})$ but no other element of $\sigma(-\Delta_D^{-1})$; see Figure 3. Define \hat{d} to be the distance between Γ and $\sigma(-\Delta_D^{-1})$, i.e.,

$$(7.1) \quad \hat{d} = \text{dist}(\Gamma, \sigma(-\Delta_D^{-1})) = \inf_{\zeta \in \Gamma} \{\text{dist}(\zeta, \sigma(-\Delta_D^{-1}))\}.$$

The only component of the spectrum of $A^\alpha(0)$ inside Γ is β_0^α , and we denote this by $\Sigma'(0)$. The part of the spectrum of $A^\alpha(0)$ in the domain exterior to Γ is denoted by $\Sigma''(0)$ and $\Sigma''(0) = \sigma(-\Delta_D^{-1}) \setminus \beta_0^\alpha$. The invariant subspace of $A^\alpha(0)$ associated with $\Sigma'(0)$ is denoted by $M'(0)$ with $M'(0) = P(0)L_{\#}^2(\alpha, Y)$.

Let $-1/2 < \mu^*$ denote the lower bound on the quasi-periodic resonance eigenvalues for the domain D . It is noted that in the following a wide class of domains are identified for which there exist lower bounds on both quasi-periodic resonances and electrostatic source free resonances. The corresponding upper bound on the set $z \in S$ for which $A^\alpha(z)$ is not invertible is given by

$$(7.2) \quad z^* = \frac{\mu^* + 1/2}{\mu^* - 1/2} < 0;$$

see (4.4). Now set

$$(7.3) \quad r^* = \frac{|\alpha|^2 \hat{d} |z^*|}{\frac{1}{1/2 - \mu^*} + |\alpha|^2 \hat{d}}.$$

THEOREM 7.1 (Separation of spectra and radius of convergence for $\alpha \in Y^*$, $\alpha \neq 0$). *The following properties hold for inclusions with domains D that satisfy (7.2):*

1. *If $|z| < r^*$ then Γ lies in the resolvent of both $A^\alpha(0)$ and $A^\alpha(z)$ and thus separates the spectrum of $A^\alpha(z)$ into two parts, given by the component of spectrum of $A^\alpha(z)$ inside Γ denoted by $\Sigma'(z)$ and the component exterior to Γ denoted by $\Sigma''(z)$. $\Sigma'(z)$ consists of the eigenvalue group $\beta^\alpha(z)$ associated with β_0^α . The invariant subspace of $A^\alpha(z)$ associated with $\Sigma'(z)$ is denoted by $M'(z)$ with $M'(z) = P(z)L_{\#}^2(\alpha, Y)$.*

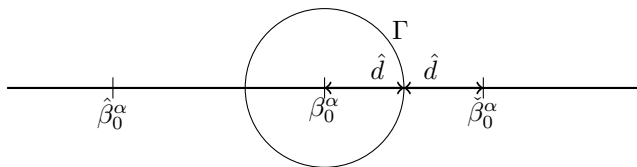


FIG. 3. Γ

2. The projection $P(z)$ is holomorphic for $|z| < r^*$ and $P(z)$ is given by

$$(7.4) \quad P(z) = \frac{-1}{2\pi i} \oint_{\Gamma} R(\zeta, z) d\zeta.$$

3. The spaces $M'(z)$ and $M'(0)$ are isomorphic for $|z| < r^*$.

4. The series (5.17) converges uniformly for $z \in \mathbb{R}$ with $|z| < r^*$.

Suppose now $\alpha = 0$. Recall from Theorem 6.3 that the limit spectrum for $A^0(0)$ is $\sigma(A^0(0)) = \{\delta_j^{-1}\}_{j \in \mathbb{N}} \cup \{\nu_j^{-1}\}_{j \in \mathbb{N}}$. For this case take Γ to be the closed contour in \mathbb{C} containing an eigenvalue β_0^0 in $\sigma(A^0(0))$ but no other element of $\sigma(A^0(0))$, and define

$$(7.5) \quad \hat{d} = \inf_{\zeta \in \Gamma} \{\text{dist}(\zeta, \sigma(A^0(0)))\}.$$

Suppose the lowest periodic resonance eigenvalue for the domain D lies inside $-1/2 < \mu^* < 0$ and the corresponding upper bound on S is given by

$$(7.6) \quad z^* = \frac{\mu^* + 1/2}{\mu^* - 1/2} < 0.$$

Set

$$(7.7) \quad r^* = \frac{4\pi^2 \hat{d} |z^*|}{\frac{1}{1/2 - \mu^*} + 4\pi^2 \hat{d}}.$$

THEOREM 7.2 (Separation of spectra and radius of convergence for $\alpha = 0$). *The following properties hold for inclusions with domains D that satisfy (7.6):*

1. If $|z| < r^*$ then Γ lies in the resolvent of both $A^0(0)$ and $A^0(z)$ and thus separates the spectrum of $A^0(z)$ into two parts, given by the component of spectrum of $A^0(z)$ inside Γ denoted by $\Sigma'(z)$ and the component exterior to Γ denoted by $\Sigma''(z)$. $\Sigma'(z)$ consists of the eigenvalue group $\beta^0(z)$ associated with β_0^0 . The invariant subspace of $A^0(z)$ associated with $\Sigma'(z)$ is denoted by $M'(z)$ with $M'(z) = P(z)L_{\#}^2(0, Y)$.

2. The projection $P(z)$ is holomorphic for $|z| < r^*$ and $P(z)$ is given by

$$(7.8) \quad P(z) = \frac{-1}{2\pi i} \oint_{\Gamma} R(\zeta, z) d\zeta.$$

3. The spaces $M'(z)$ and $M'(0)$ are isomorphic for $|z| < r^*$.

4. The series (5.17) with $\alpha = 0$, converges uniformly for $z \in \mathbb{R}$ with $|z| < r^*$.

It is noted here that parts 1, 2, and 3 of Theorems 7.1, 7.2 are proposed and proven in [25]. Now consider the Neumann spectrum. Recall from Theorem 6.1 that the limit spectrum for $A(0)$ is $\sigma(A(0)) = \{\delta_j^{-1}\}_{j \in \mathbb{N}} \cup \{\nu_j^{-1}\}_{j \in \mathbb{N}}$. For this case take Γ to be the closed contour in \mathbb{C} containing an eigenvalue β_0 in $\sigma(A(0))$ but no other element of $\sigma(A(0))$ and define

$$(7.9) \quad \hat{d} = \inf_{\zeta \in \Gamma} \{\text{dist}(\zeta, \sigma(A(0)))\}.$$

Suppose the lowest Neumann electrostatic resonance eigenvalue for the domain D lies inside $-1/2 < \mu^* < 0$ and the corresponding upper bound on S is given by

$$(7.10) \quad z^* = \frac{\mu^* + 1/2}{\mu^* - 1/2} < 0.$$

Set

$$(7.11) \quad r^* = \frac{\pi^2 \hat{d} |z^*|}{\frac{1}{1/2 - \mu^*} + \pi^2 \hat{d}}.$$

THEOREM 7.3 (Separation of Neumann spectra and radius of convergence). *The following properties hold for inclusions with domains D that satisfy (7.10):*

1. *If $|z| < r^*$ then Γ lies in the resolvent of both $A(0)$ and $A(z)$ and thus separates the spectrum of $A(z)$ into two parts, given by the component of spectrum of $A(z)$ inside Γ denoted by $\Sigma'(z)$ and the component exterior to Γ denoted by $\Sigma''(z)$. $\Sigma'(z)$ consists of the eigenvalue group $\beta(z)$ associated with β_0 . The invariant subspace of $A(z)$ associated with $\Sigma'(z)$ is denoted by $M'(z)$ with $M'(z) = P(z)L_0^2(Y)$.*
2. *The projection $P(z)$ is holomorphic for $|z| < r^*$ and $P(z)$ is given by*

$$(7.12) \quad P(z) = \frac{-1}{2\pi i} \oint_{\Gamma} R(\zeta, z) d\zeta.$$

3. *The spaces $M'(z)$ and $M'(0)$ are isomorphic for $|z| < r^*$.*
4. *The series (4.14) converges uniformly for $z \in \mathbb{R}$ with $|z| < r^*$.*

We have the estimate for the error incurred when only finitely many terms of the series (4.14) and (5.17) are calculated.

THEOREM 7.4 (Error estimates for the eigenvalue expansion).

1. *Let $\alpha \neq 0$, and suppose D , z^* , and r^* are as in Theorem 7.1. Then the following error estimate for the series (5.17) holds for $z \in \mathbb{R}$ and $|z| < r^*$:*

$$(7.13) \quad \left| \beta_i^\alpha(z) - \sum_{n=0}^p z^n \beta_i^n(z) \right| \leq \frac{\hat{d} |z|^{p+1}}{(r^*)^p (r^* - |z|)}.$$

2. *Let $\alpha = 0$, and suppose D , z^* , and r^* are as in Theorem 7.2. Then the following error estimate for the series (5.17) holds for $z \in \mathbb{R}$ and $|z| < r^*$:*

$$(7.14) \quad \left| \beta_i^0(z) - \sum_{n=0}^p z^n \beta_i^n(z) \right| \leq \frac{\hat{d} |z|^{p+1}}{(r^*)^p (r^* - |z|)}.$$

3. *Consider the Neumann spectrum and suppose D , z^* , and r^* are as in Theorem 7.3. Then the following error estimate for the series (4.14) holds for $z \in \mathbb{R}$ and $|z| < r^*$:*

$$(7.15) \quad \left| \beta_i(z) - \sum_{n=0}^p z^n \beta_i^n(z) \right| \leq \frac{\hat{d} |z|^{p+1}}{(r^*)^p (r^* - |z|)}.$$

Remark 7.5. Note that the estimates (7.13) through (7.15) are uniform in the index i for elements in the eigenvalue group for z restricted to the real axis and $|z| < r^*$.

The Theorems 7.1 and 7.2 parts 1 through 3 and explicit convergence radii for the power series representation for the eigenvalue group with $z \in \mathbb{C}$ are proved in [25]. The proofs of part 4 of Theorems 7.1 and 7.2 together with Theorems 7.3 and 7.4 are given in section 11.

8. Radius of convergence and separation of spectra for periodic scatterers of general shape. In the previous section, it was mentioned that a wide class of geometries D existed for which a lower bound (independent of α) on the quasi-static resonances $\mu^* > -\frac{1}{2}$ could be proven to exist. Here we identify precisely those geometries for which this lower bound exists, as well as a characterization of this lower bound in terms of the geometries, guaranteeing all Theorems in section 7 hold.

Consider an inclusion domain $D = \bigcup_{i=1}^N D_i$. Suppose we can surround each D_i by a buffer layer R_i so that each inclusion D_i together with its buffer does not intersect with the any of the other buffered inclusions, i.e., $D_i \cup R_i \cap D_j \cup R_j = \emptyset$, $i \neq j$. The set of such inclusion domains will be called *buffered dispersions of inclusions*; see Figure 2. We denote the operator norm for the Dirichlet to Neumann map for each inclusion by $\|DN_i\|$ and the Poincare constant for each buffer layer by C_{R_i} and we state the following theorem.

THEOREM 8.1 (Convergent power series for the Bloch and Neumann spectra for buffered dispersions of inclusions). *All two-dimensional photonic and d -dimensional acoustic crystals ($d = 2, 3$) made from buffered dispersions with constants C_{R_i} and $\|DN_i\|$ that satisfy*

$$(8.1) \quad \max_i \{(1 + C_{R_i})\|DN_i\|\} < \infty$$

have Bloch and Neumann spectra described by convergent power series for real values of the contrast within a neighborhood of $z = 1/k = 0$. The radii of convergence is controlled by the values $\|DN_i\|$ and C_{R_i} , $i = 1, \dots, N$ and Theorems 7.1 through 7.4 apply to these crystals.

The theorem follows from an explicit condition on the inclusion geometry that guarantees a lower bound μ^* for both Neumann electrostatic resonance spectra and quasi-periodic resonance spectra. The lower bound depends only upon geometry and is uniform in α for the quasi-periodic spectra. This lower bound provides a positive distance between the origin $z = 0$ and the poles of $A^\alpha(z)$ and $A(z)$. The explicit condition is given by the following criterion.

THEOREM 8.2. *Let $D \Subset Y$ be a union of simply connected sets (inclusions) D_i , $i = 1, \dots, N$ with $C^{1,\gamma}$ boundary. Consider the spectrum $\{\mu_i\}_{i \in \mathbb{N}}$ of T restricted to W_3 for $W_3 \subset H_{\#}^1(\alpha, Y)$ or $W_3 \subset \mathcal{H}_N$. For either case if there is a $\theta > 0$ such that for all $u \in W_3$*

$$(8.2) \quad \|\nabla u\|_{L^2(Y \setminus D)}^2 \geq \theta \|\nabla u\|_{L^2(D)}^2,$$

then for $\rho = \min\{\frac{1}{2}, \frac{\theta}{2}\}$ one has the lower bound

$$(8.3) \quad \min_{i \in \mathbb{N}} \{\mu_i\} \geq \mu^* = \rho - \frac{1}{2} > -\frac{1}{2}.$$

This theorem is proved for quasi-periodic resonances in $W_3 = H_{\#}^1(\alpha, Y)$ in [25], and its proof follows identical lines for the Neumann electrostatic resonances in $W_3 = \mathcal{H}_N$.

The parameter θ is a geometric descriptor for D and we define a wide class of crystal geometries to which Theorems 7.1 through 7.4 apply.

DEFINITION 8.3. *The class of crystal geometries characterized by inclusions D such that (8.2) holds for a fixed positive value of θ is denoted by P_θ .*

We have the following corollary:

COROLLARY 8.4. *Theorems 7.1 through 7.4 hold for every inclusion domain D belonging to P_θ .*

The convergent series representation for buffered dispersions of inclusions now follows from the theorem.

THEOREM 8.5. *Suppose there is a $\theta > 0$ for which*

$$(8.4) \quad \theta^{-1} \geq \max_i \{(1 + C_{R_i}) \|DN_i\|\}.$$

Then the buffered geometry lies in P_θ .

This theorem is established in [25] for quasi-periodic spectra and an identical proof can be used to prove it for the Neumann electrostatic spectra discussed here.

9. Radius of convergence and separation of spectra for disks. We now consider both Neumann and Bloch spectra for crystals discussed in the introduction, with each period cell containing an identical distribution of N disks D_i , $i = 1, \dots, N$ of radius a . We suppose that the smallest distance separating the disks is $t_d > 0$. The buffer layers R_i are annuli with inner radii a and outer radii $b = a + t$ where $t \leq t_d/2$ and is chosen so that the collection of buffered disks lie within the period cell. The benefit of the consideration of this specific class of geometries is that the lower bound $\mu^* > -\frac{1}{2}$ on the quasi-static resonances can be explicitly stated, which allows for clear formulas for the radii of convergence (7.3), (7.7) in terms of a , b , and the zeros of Bessel functions.

For this case a suitable constant θ is computed in [5] and is given by

$$(9.1) \quad \theta = \frac{b^2 - a^2}{b^2 + a^2}.$$

Since $a < b$, we have that

$$(9.2) \quad 0 < \theta < 1.$$

We also note that, when D_i are discs of radius $a > 0$, we can recover an explicit formula for d from (7.1), (7.5), and (7.9). In particular, any eigenvalue $\beta_j^\alpha(0) = -\Delta_D^{-1}$, for $\alpha \neq 0$, may be written

$$(9.3) \quad \beta_j^\alpha(0) = \left(\frac{\eta_{n,k}}{a}\right)^{-2},$$

where $\eta_{n,k}$ is the k th zero of the n th Bessel function $J_n(r)$. Let $\tilde{\eta}$ be the minimizer of

$$(9.4) \quad \min_{m,j \in \mathbb{N}} |(\eta_{n,k})^{-2} - (\eta_{m,j})^{-2}|.$$

Then we may choose Γ from section 7 so that

$$(9.5) \quad \hat{d} = \frac{1}{2} \left| \left(\frac{a}{\eta_{n,k}}\right)^2 - \left(\frac{a}{\tilde{\eta}}\right)^2 \right|.$$

We apply the explicit form for θ to obtain a formula for r^* in terms of a, b, d given above, and α . Recall that ρ from Theorem 8.2 is given by $\rho = \min\{\frac{1}{2}, \frac{\theta}{2}\}$. In light of inequality (9.2), we have that

$$(9.6) \quad \rho = \frac{1}{2} \left(\frac{b^2 - a^2}{b^2 + a^2} \right),$$

and we calculate the lower bound μ^* :

$$(9.7) \quad \mu^* = \rho - \frac{1}{2} = -\frac{a^2}{b^2 + a^2}.$$

Recalling that

$$z^* = \frac{\mu^* + 1/2}{1/2 - \mu^*},$$

we obtain an explicit radius of convergence r^* in terms of $a, b, \eta_{n,k}, \tilde{\eta}$, and α for $\alpha \neq 0$:

$$(9.8) \quad r^* = \frac{|\alpha|^2 \left(\left(\frac{a}{\eta_{n,k}} \right)^2 - \left(\frac{a}{\tilde{\eta}} \right)^2 \right) |b^2 - a^2|}{2(b^2 + a^2) + |\alpha|^2 \left(\left(\frac{a}{\eta_{n,k}} \right)^2 - \left(\frac{a}{\tilde{\eta}} \right)^2 \right) |b^2 + 3a^2|}.$$

When $\alpha = 0$ Theorem 6.3 shows that the limit spectrum consists of a component given by the roots ν_{0k} of

$$(9.9) \quad 1 = N\nu \sum_{k \in \mathbb{N}} \frac{a_{0k}^2}{\nu - (\eta_{0k}/a)^2},$$

where $a_{0k} = \int_D u_{0k} dx$ are averages of the rotationally symmetric normalized eigenfunctions u_{0k} given by

$$(9.10) \quad u_{0k} = J_0(r\eta_{0k}/a) / (a\sqrt{\pi}J_1(\eta_{0k})).$$

The other component is composed of the eigenvalues exclusively associated with mean zero eigenfunctions. The collection of these eigenvalues is given by $\{\bigcup_{n \neq 0, k} (\eta_{nk}/a)^2\}$. The elements λ_{nk} of the spectrum $\sigma(A^0(0))$ are given by the set $\{\bigcup_{n \neq 0, k} (\eta_{nk}/a)^2\} \cup \{\bigcup_k \nu_{0k}\}$. Now fix an element λ_{nk} and let $\tilde{\eta}$ be the minimizer of

$$(9.11) \quad \min_{m, j \in \mathbb{N}} |(\lambda_{n,k})^{-1} - (\lambda_{m,j})^{-1}|.$$

Then as before we may choose Γ from section 7 so that

$$(9.12) \quad \hat{d} = \frac{1}{2} |(\lambda_{n,k})^{-1} - \tilde{\eta}^{-1}|$$

and in terms of $a, b, \lambda_{n,k}$, and $\tilde{\eta}$ for $\alpha = 0$,

$$(9.13) \quad r^* = \frac{2\pi^2 |(\lambda_{n,k})^{-1} - \tilde{\eta}^{-1}| (b^2 - a^2)}{(b^2 + a^2) + 2\pi^2 |(\lambda_{n,k})^{-1} - \tilde{\eta}^{-1}| (b^2 + 3a^2)}.$$

Theorem 6.1 shows that the limit spectrum for the Neumann eigenvalue problem also consists of a component given by the roots ν_{0k} of (9.9). The elements λ_{nk} of the spectrum $\sigma(A(0))$ are the same as for the limit periodic case $\sigma(A^0(0))$ and are given by the set $\{\bigcup_{n \neq 0, k} (\eta_{nk}/a)^2\} \cup \{\bigcup_k \nu_{0k}\}$. Proceeding as before, we may choose Γ from section 7 so that

$$(9.14) \quad \hat{d} = \frac{1}{2} |(\lambda_{n,k})^{-1} - \tilde{\eta}^{-1}|$$

and r^* is given by

$$(9.15) \quad r^* = \frac{\pi^2 |(\lambda_{n,k})^{-1} - \tilde{\eta}^{-1}|(b^2 - a^2)}{2(b^2 + a^2) + \pi^2 |(\lambda_{n,k})^{-1} - \tilde{\eta}^{-1}|(b^2 + 3a^2)}.$$

The collection of suspensions of N buffered disks is an example of a class of buffered inclusion geometries, and, collecting results, we have the following:

COROLLARY 9.1. *For every suspension of buffered disks with θ given by (9.1), Theorem 7.1 holds with r^* given by (9.8) for $\alpha \in Y^*$, $\alpha \neq 0$, Theorem 7.2 holds with r^* given by (9.13) for $\alpha = 0$, and Theorem 7.3 holds with r^* given by (9.13). Moreover, Theorem 7.4 part 1 holds with r^* given by (9.8) and parts 2 and 3 hold for r^* given by (9.13) and (9.15), respectively,*

10. Opening band gaps and persistence of pass bands for $k > 1$. We now state and prove the primary results of the paper. We apply the characterization of $\sigma(A(0))$ given by Theorem 6.1 together with (4.3) to recover the high contrast limit of the Neumann spectrum given by

$$(10.1) \quad \sigma_N = \{\delta'_j\}_{j \in \mathbb{N}} \cup \{\nu_j\}_{j \in \mathbb{N}},$$

where δ'_j is the part of the Dirichlet spectra for D associated with mean zero eigenfunctions and ν_j are the roots of the spectral function (6.3). This is precisely the high contrast Neumann spectrum described in [15]. In what follows we do not distinguish between the two component parts of the spectrum, and we write elements of σ_N as ν_j , $j \in \mathbb{N}$. The Dirichlet spectrum is given by $\sigma(-\Delta_D) = \{\delta'_j\}_{j \in \mathbb{N}} \cup \{\delta_j^*\}_{j \in \mathbb{N}}$, where δ_j^* are Dirichlet eigenvalues associated with eigenfunctions with nonzero mean. The relation between σ_N and $\sigma(-\Delta_D)$ is given by the following theorem.

THEOREM 10.1 (Strict interlacing of spectra [15]). *If $\delta_j^* \in \sigma(-\Delta_D)$ is simple, then there exist adjacent elements $\nu_j < \nu_{j+1}$ ordered by min-max belonging to σ_N such that*

$$(10.2) \quad \nu_j < \delta_j^* < \nu_{j+1}.$$

Theorem 10.1 insures the existence of a band gap for sufficiently large contrast k . We give an explicit condition on the contrast k that is sufficient to open a band gap in the vicinity of δ_j^* together with explicit formulas describing its location and bandwidth.

THEOREM 10.2 (Opening a band gap). *Consider any crystal geometry belonging to the class P_θ defined by Definition 8.3. Suppose $\delta_j^* \in \sigma(-\Delta_D)$ is simple, so that $\delta_j^* < \nu_{j+1}$ as in Theorem 10.1. Set*

$$d_j = \frac{1}{2} \text{dist}(\{\nu_{j+1}^{-1}\}, \sigma_N \setminus \{\nu_{j+1}^{-1}\})$$

where σ_N is given by (10.1), and

$$(10.3) \quad \bar{r}_j = \frac{\pi^2 d_j |z^*|}{\frac{1}{1/2 - \mu^*} + \pi^2 d_j}.$$

Then one has the band gap

$$(10.4) \quad \sigma(L_k) \cap \left(\delta_j^*, \nu_{j+1} \left(1 - \frac{\nu_{j+1} d_j}{k \bar{r}_j - 1} \right) \right) = \emptyset$$

if

$$(10.5) \quad k > \bar{k}_j = \bar{r}_j^{-1} \left(1 + \frac{d_j \nu_{j+1}}{1 - \frac{\delta_j^*}{\nu_{j+1}}} \right).$$

Next we provide an explicit condition on k sufficient for the persistence of a spectral band together with explicit formulas describing its location and bandwidth.

THEOREM 10.3 (Persistence of passbands). *Consider any crystal geometry belonging to the class P_θ defined by Definition 8.3. Suppose δ_j^* is simple, so that $\nu_j < \delta_j^*$ as in Theorem 10.1. Set*

$$d_j = \frac{1}{2} \text{dist} (\{(\delta_j^*)^{-1}\}, \sigma(-\Delta_D) \setminus \{(\delta_j^*)^{-1}\})$$

and

$$(10.6) \quad r_j = \frac{d\pi^2 d_j |z^*|}{\frac{1}{1/2 - \mu^*} + d\pi^2 d_j} \quad \text{for } d = 2, 3.$$

Then one has a passband in the vicinity of δ_j^* and

$$(10.7) \quad \sigma(L_k) \supset \left[\nu_j, \delta_j^* \left(1 - \frac{\delta_j^* d_j}{kr_j - 1} \right) \right]$$

if

$$(10.8) \quad k > \underline{k}_j = r_j^{-1} \left(1 + \frac{d_j \delta_j^*}{1 - \frac{\nu_j}{\delta_j^*}} \right).$$

Theorem 1.1 follows from Theorem 10.2 on applying (9.7), (9.13), and (9.14). Theorem 1.2 follows from Theorem 10.3 on applying (9.5), (9.7), and (9.8) with $|\alpha|^2 = d\pi^2$, $d = 2, 3$. (See the proof of Theorem 10.3.)

We now establish Theorem 10.2.

Proof. Consider ν_{j+1} of multiplicity $m < \infty$. Set $\hat{d} = d_j$ with

$$d_j = \frac{1}{2} \text{dist} (\{\nu_{j+1}^{-1}\}, \sigma_N \setminus \{\nu_{j+1}^{-1}\})$$

and $r^* = \bar{r}_j$ and apply Theorem 7.3 so that any element $\beta_i(z)$ in the eigenvalue group has series representation given by

$$(10.9) \quad \beta_i(z) = \nu_{j+1}^{-1} + \sum_{n=1}^{\infty} z^n \beta_i^n(z)$$

for z inside the interval $-\bar{r}_j < z < \bar{r}_j$. For $k > \bar{r}_j^{-1}$, let $\nu_{j+1}(k)$ be the minimum of $1/\beta_i(\frac{1}{k})$, with $\beta_i(z)$ in the eigenvalue group, and we have $\nu_{j+1}(k) \rightarrow \nu_{j+1}$ for $k \rightarrow \infty$. Since $\nu_{j+1}(k)$ is increasing with k we conclude

$$(10.10) \quad \nu_{j+1}(k) \leq \nu_{j+1}.$$

We take a min-max ordering for $\sigma(-\Delta_D)$ and suppose that the j th Dirichlet eigenvalue corresponds to an eigenfunction of nonzero mean. The eigenvalue is denoted by δ_j^* . The min-max principle together with the monotonicity of eigenvalues with respect to increasing k delivers the inequality between the Bloch eigenvalues and $\sigma(-\Delta_D)$:

$$(10.11) \quad \lambda_j(k, \alpha) \leq \delta_j^* \quad \text{for } \alpha \in Y^* \text{ and } k > 0.$$

Application of (1.24) and (10.11) gives

$$(10.12) \quad \lambda_m(k, \alpha) \leq \delta_j^* \quad \text{for } m \leq j \quad \text{and} \quad \nu_{j+1}(k) \leq \lambda_m(k, \alpha) \text{ for } j + 1 \leq m,$$

for every $\alpha \in Y^*$, and it is clear that a band gap opens in the Bloch spectrum when $\delta_j^* < \nu_{j+1}(k)$ or equivalently when

$$(10.13) \quad |\nu_{j+1}(k) - \nu_{j+1}| < |\delta_j^* - \nu_{j+1}|.$$

We apply (7.15) and Remark 7.5 to get

$$(10.14) \quad |\nu_{j+1}(k) - \nu_{j+1}| < \frac{\nu_{j+1}^2 d_j}{k\bar{r}_j - 1},$$

and the theorem follows for all k that satisfy

$$(10.15) \quad \frac{\nu_{j+1}^2 d_j}{k\bar{r}_j - 1} < |\delta_j^* - \nu_{j+1}|. \quad \square$$

We now establish Theorem 10.3.

Proof. From the min-max formulation we have that $\lambda_j(k, 0)$ and $\lambda_j(k, \alpha)$ are increasing with k , and from [15] (or [25]) we have

$$(10.16) \quad \lim_{k \rightarrow \infty} \lambda_j(k, 0) = \nu_j \text{ hence } \lambda_j(k, 0) \leq \nu_j \quad \text{for } k > 1$$

and

$$(10.17) \quad \lim_{k \rightarrow \infty} \lambda_j(k, \alpha) = \delta_j^* \text{ hence } \lambda_j(k, \alpha) \leq \delta_j^* \quad \text{for } k > 1$$

With this in mind observe that if $|\delta_j^* - \lambda_j(k, \alpha)| < |\delta_j^* - \nu_j|$ then

$$(10.18) \quad \sigma(L_k) \supset [\nu_j, \lambda_j(k, \alpha)].$$

To proceed we estimate the difference $|\lambda_j(k, \alpha) - \delta_j^*|$. Set $\hat{d} = d_j$ with

$$d_j = \frac{1}{2} \text{dist}(\{(\delta_j^*)^{-1}\}, \sigma(-\Delta_D) \setminus \{(\delta_j^*)^{-1}\})$$

and r_j^* given by (7.3) with $\hat{d} = d_j$. Apply Theorem 7.1 noting that δ_j^* is simple so that $\beta_j^\alpha(z)$ has series representation given by

$$(10.19) \quad \beta_j^\alpha(z) = (\delta_j^*)^{-1} + \sum_{n=1}^{\infty} z^n \beta_j^n(z)$$

for z inside the interval $-r_j^* < z < r_j^*$. For $k > r_j^{*-1}$ we have $\lambda_j(k, \alpha) = \frac{1}{\beta_j^\alpha(k^{-1})}$ and we apply (7.13) to get

$$(10.20) \quad |\delta_j^* - \lambda_j(k, \alpha)| < \frac{(\delta_j^*)^2 d_j}{k r_j^* - 1}.$$

The persistence of band structure described by (10.18) follows for a fixed $\alpha \in Y^*$ for all k that satisfy

$$(10.21) \quad \frac{(\delta_j^*)^2 d_j}{k r_j^* - 1} < |\delta_j^* - \nu_j|.$$

We maximize r_j^* over $\alpha \in [-\pi, \pi]^d$ to find that it is attained for $|\alpha|^2 = d\pi^2$ and the maximum is $r_j^* = r_j$. For this choice we recover the persistence of band structure described by (10.7) and (10.8). \square

11. Derivation of the convergence radius, separation of spectra, and error estimates. Here we prove Theorems 7.3 and 7.4 and part 4 of Theorems 7.1 and 7.2. The Theorems 7.1 and 7.2 parts 1 through 3 and explicit convergence radii for power series representation for the eigenvalue group are proved in [25]. To begin, we recall both the Neumann series (4.6) and (4.12) converge provided that

$$(11.1) \quad \|(A(z) - A(0))R(\zeta, 0)\|_{\mathcal{L}[L_0^2(Y); L_0^2(Y)]} < 1.$$

With this in mind we follow [25] and compute an explicit upper bound $B(z)$ and identify a neighborhood of the origin on the complex plane for which

$$(11.2) \quad \|(A(z) - A(0))R(\zeta, 0)\|_{\mathcal{L}[L_0^2(Y); L_0^2(Y)]} < B(z) < 1$$

holds for $\zeta \in \Gamma$. The inequality $B(z) < 1$ will be used first to derive a lower bound on the radius of convergence of the series expansion of the spectral projection $P(z)$ on the eigenvalue group. It will then be used to provide a lower bound on the neighborhood of $z = 0$ for $z \in \mathbb{C}$ where properties 1 through 3 of Theorem 7.3 hold. The inequality $B(z) < 1$ restricted to real z is then used to prove Theorem 7.4 part 3 and part 4 of Theorem 7.3.

We have the basic estimate given by

$$(11.3) \quad \begin{aligned} & \|(A(z) - A(0))R(\zeta, 0)\|_{\mathcal{L}[L_0^2(Y); L_0^2(Y)]} \\ & \leq \|A(z) - A(0)\|_{\mathcal{L}[L_0^2(Y); L_0^2(Y)]} \|R(\zeta, 0)\|_{\mathcal{L}[L_0^2(Y); L_0^2(Y)]}. \end{aligned}$$

Here $\zeta \in \Gamma$ as defined in Theorem 7.1 and elementary arguments deliver the estimate

$$(11.4) \quad \|R(\zeta, 0)\|_{\mathcal{L}[L_0^2(Y); L_0^2(Y)]} \leq \hat{d}^{-1},$$

where \hat{d} is given by (7.1).

Next we estimate $\|(A(z) - A(0))\|_{\mathcal{L}[L_0^2(Y); L_0^2(Y)]}$. Denote the energy seminorm of u by

$$(11.5) \quad \|u\| = \|\nabla u\|_{L^2(Y)}.$$

To proceed we introduce the standard Poincare and Green's function estimates:

LEMMA 11.1. For $u \in \mathcal{H}$

$$(11.6) \quad \|u\|_{L^2(Y)}^2 \leq \lambda_N^{-1} \|u\|^2,$$

and for $v \in L_0^2(Y)$

$$(11.7) \quad \|-\Delta_N^{-1}\| \leq \lambda_N^{-1/2} \|v\|_{L^2(Y)},$$

where λ_N is the first nonzero Neumann eigenvalue for the period Y , $\lambda_N = \pi^2$ for $Y = (0, 1]^d$.

For any $v \in L_0^2(Y)$, we apply (11.6) to find

$$(11.8) \quad \begin{aligned} & \|(A(z) - A(0))v\|_{L^2(Y)} \\ & \leq |\lambda_N|^{-1/2} \|(A(z) - A(0))v\| \\ & = |\lambda_N|^{-1/2} \|((T_k)^{-1} - (T_0)^{-1})(-\Delta_N)^{-1}v\| \\ & \leq |\lambda_N|^{-1/2} \|((T_k)^{-1} - P_2)\|_{\mathcal{L}[\mathcal{H}_N; \mathcal{H}_N]} \|-\Delta_N^{-1}v\|. \end{aligned}$$

Applying (11.7) and (11.8) delivers the upper bound:

$$(11.9) \quad \|(A(z) - A(0))\|_{\mathcal{L}[L_0^2(Y); L_0^2(Y)]} \leq \lambda_N^{-1} \|((T_k)^{-1} - P_2)\|_{\mathcal{L}[\mathcal{H}_N; \mathcal{H}_N]}.$$

The next step is to obtain an upper bound on $\|((T_k)^{-1} - P_2)\|_{\mathcal{L}[\mathcal{H}_N; \mathcal{H}_N]}$. For all $v \in \mathcal{H}_N$, we have

$$(11.10) \quad \frac{\|((T_k)^{-1} - P_2)v\|}{\|v\|} \leq |z| \left\{ w_0 + \sum_{i=1}^{\infty} w_i |(1/2 + \mu_i) + z(1/2 - \mu_i)|^{-2} \right\}^{1/2},$$

where $w_0 = \|P_1 v\|^2 / \|v\|^2$, $w_i = \|P_i v\|^2 / \|v\|^2$, and $w_0 + \sum_{i=1}^{\infty} w_i = 1$. So maximizing the right-hand side is equivalent to calculating

$$(11.11) \quad \begin{aligned} & \max_{w_0 + \sum w_i = 1} \left\{ w_0 + \sum_{i=1}^{\infty} w_i |(1/2 + \mu_i) + z(1/2 - \mu_i)|^{-2} \right\}^{1/2} \\ & = \sup \{1, |(1/2 + \mu_i) + z(1/2 - \mu_i)|^{-2}\}^{1/2}. \end{aligned}$$

Thus we maximize the function

$$(11.12) \quad f(x) = \left| \frac{1}{2} + x + z \left(\frac{1}{2} - x \right) \right|^{-2}$$

over $x \in [\mu^*, 1/2]$ for z in a neighborhood about the origin. Let $\operatorname{Re}(z) = u$, $\operatorname{Im}(z) = v$ and we write

$$(11.13) \quad \begin{aligned} f(x) &= \left| \frac{1}{2} + x + (u + iv) \left(\frac{1}{2} - x \right) \right|^{-2} \\ &= \left(\left(\frac{1}{2} + x + u \left(\frac{1}{2} - x \right) \right)^2 + v^2 \left(\frac{1}{2} - x \right)^2 \right)^{-1} \\ &\leq \left(\frac{1}{2} + x + u \left(\frac{1}{2} - x \right) \right)^{-2} = g(\operatorname{Re}(z), x) \end{aligned}$$

to get the bound

$$(11.14) \quad \|((T_k)^{-1} - P_2)\|_{\mathcal{L}[\mathcal{H}_N; \mathcal{H}_N]} \leq |z| \sup \left\{ 1, \sup_{x \in [\mu^*, 1/2]} g(u, x) \right\}^{1/2}.$$

We now examine the poles of $g(u, x)$ and the sign of its partial derivative $\partial_x g(u, x)$ when $|u| < 1$. If $\operatorname{Re}(z) = u$ is fixed, then $g(u, x) = ((\frac{1}{2} + x) + u(\frac{1}{2} - x))^{-2}$ has a pole when $(\frac{1}{2} + x) + u(\frac{1}{2} - x) = 0$. For u fixed this occurs when

$$(11.15) \quad \hat{x} = \hat{x}(u) = \frac{1}{2} \left(\frac{1+u}{u-1} \right).$$

On the other hand, if x is fixed, g has a pole at

$$(11.16) \quad u = \frac{\frac{1}{2} + x}{x - \frac{1}{2}}.$$

The sign of $\partial_x g$ is determined by the formula

$$(11.17) \quad \partial_x g(u, x) = N/D,$$

where $N = -2(1 - u)^2 x - (1 - u^2)$ and $D := ((\frac{1}{2} + x) + u(\frac{1}{2} - x))^4 \geq 0$. Calculation shows that $\partial_x g < 0$ for $x > \hat{x}$, i.e., g is decreasing on (\hat{x}, ∞) . Similarly, $\partial_x g > 0$ for $x < \hat{x}$ and g is increasing on $(-\infty, \hat{x})$.

Now we identify all $u = \text{Re}(z)$ for which $\hat{x} = \hat{x}(u)$ satisfies

$$(11.18) \quad \hat{x} < \mu^* < 0.$$

Indeed for such u , the function $g(u, x)$ will be decreasing on $[\mu^*, 1/2]$, so that $g(u, \mu^*) \geq g(u, x)$ for all $x \in [\mu^*, 1/2]$, yielding an upper bound for (11.14).

LEMMA 11.2. *The set U of $u \in \mathbb{R}$ for which $-\frac{1}{2} < \hat{x}(u) < \mu^* < 0$ is given by*

$$U := [z^*, 1],$$

where

$$-1 \leq z^* := \frac{\mu^* + \frac{1}{2}}{\mu^* - \frac{1}{2}} < 0.$$

Proof. Note first that $\mu^* = \inf_{i \in \mathbb{N}} \{\mu_i\} \leq 0$ follows from the fact that zero is an accumulation point for the sequence $\{\mu_i\}_{i \in \mathbb{N}}$, so it follows that $-1 \leq z^*$. Noting $\hat{x} = \hat{x}(u) = \frac{1}{2} \frac{u+1}{u-1}$, we invert and write

$$(11.19) \quad u = \frac{\frac{1}{2} + \hat{x}}{\hat{x} - \frac{1}{2}}.$$

We now show that

$$(11.20) \quad z^* \leq u \leq 1$$

for $\hat{x} \leq \mu^*$. Set $h(\hat{x}) = \frac{\frac{1}{2} + \hat{x}}{\hat{x} - \frac{1}{2}}$. Then

$$(11.21) \quad h'(\hat{x}) = \frac{-1}{(\hat{x} - \frac{1}{2})^2},$$

and so h is decreasing on $(-\infty, \frac{1}{2})$. Since $\mu^* < \frac{1}{2}$, h attains a minimum over $(-\infty, \mu^*]$ at $x = \mu^*$. Thus $\hat{x}(u) \leq \mu^*$ implies

$$(11.22) \quad z^* = \frac{\mu^* + \frac{1}{2}}{\mu^* - \frac{1}{2}} \leq u \leq 1$$

as desired. □

Combining Lemma 11.2 with inequality (11.14), noting that $-|z| \leq \text{Re}(z) \leq |z|$, and on rearranging terms we obtain the following corollary.

COROLLARY 11.3. *For $|z| < |z^*|$*

$$(11.23) \quad \|(A(z) - A(0))\|_{\mathcal{L}[L_0^2(Y); L_0^2(Y)]} \leq \lambda_N^{-2} |z| (-|z| - z^*)^{-1} (\frac{1}{2} - \mu^*)^{-1}.$$

From Corollary 11.3, (11.3), and (11.4) we easily see that

$$(11.24) \quad \|(A(z) - A(0))R(\zeta, 0)\|_{\mathcal{L}[L_0^2(Y); L_0^2(Y)]} \leq B(z) = \lambda_N^{-2} |z| (-|z| - z^*)^{-1} (\frac{1}{2} - \mu^*)^{-1} \hat{d}^{-1}.$$

A straightforward calculation shows that $B(z) < 1$ for

$$(11.25) \quad |z| < r^* := \frac{\lambda_N^2 \hat{d} |z^*|}{\frac{1}{\frac{1}{2} - \mu^*} + \lambda_N^2 \hat{d}},$$

with $\lambda_N = \pi^2$ for the cubic (or square) unit period cell. Since $r^* < |z^*|$ we have established that the Neumann series (4.6) converges. It is also immediate that (4.7) converges for $|z| < r^*$.

Now we establish properties 1 through 3 of Theorem 7.3. First note that inspection of (4.6) shows that if (11.1) holds and if $\zeta \in \mathbb{C}$ belongs to the resolvent of $A(0)$ then it also belongs to the resolvent of $A(z)$. Since (11.1) holds for $\zeta \in \Gamma$ and $|z| < r^*$, property 1 of Theorem 7.3 follows. Formula (4.7) shows that $P(z)$ is analytic in a neighborhood of $z = 0$ determined by the condition that (11.1) holds for $\zeta \in \Gamma$. The set $|z| < r^*$ lies inside this neighborhood and property 2 of Theorem 7.3 is proved. The isomorphism expressed in property 3 of Theorem 7.3 follows directly from Lemma 4.10 ([22], Chapter I, section 4) which is also valid in a Banach space. Properties 1 through 3 of Theorems 7.1 and 7.2 have been derived earlier by the authors and are parts 1 through 3 of Theorems 7.1 and 7.2 of [25]. Property 4 of Theorems 7.1, 7.2, and 7.3 follows from the error estimates given in Theorem 7.4.

We now establish Theorem 7.4. We illustrate the proof of part 3 of this theorem noting that the proof of parts 1 and 2 follow identical arguments. Theorem 7.4 part 3 follows once we establish Cauchy-like inequalities for the coefficients $\beta_i^n(z)$ appearing in (4.14) given by

$$(11.26) \quad |\beta_i^n(z)| \leq \hat{d}(r^*)^{-n}$$

for $|z| < r^*$. From this it is evident that we can recover the estimates

$$(11.27) \quad \left| \beta(z) - \sum_{n=0}^p z^n \beta_i^n \right| \leq \sum_{n=p+1}^{\infty} |z|^n |\beta_i^n| \leq \frac{\hat{d} |z|^{p+1}}{(r^*)^p (r^* - |z|)}$$

for $|z| < r^*$, and part 3 of Theorem 7.4 is established.

Now we establish (11.26). Applying (11) to (4.15) and noting that $|\zeta - \beta_0| = \hat{d}$ on Γ , one obtains the estimate

$$(11.28) \quad |\beta_i^n(z)| \leq \hat{d} \|\mathcal{N}(\zeta, z)\|_{\mathcal{L}[L_0^2(Y); L_0^2(Y)]}^n \leq \hat{d} (\lambda_N^{-2} (|z^*| - |z|)^{-1} (\frac{1}{2} - \mu^*)^{-1} \hat{d}^{-1})^n$$

for $|z| < r^*$. Note that the right-hand side of (11.28) is increasing with $|z| \leq r^* < |z^*|$. The right-hand side is maximized for $|z| = r^*$ and we recover (11.26) on setting $|z| = r^*$ in (11.28) and applying the formula for r^* given by (11.25).

Now we show that the operator $B(k)$ introduced in section 3 is bounded and compact.

THEOREM 11.4. *The operator $B(k) : L_0^2(Y) \rightarrow \mathcal{H}_N$ is bounded for $k \notin Z$.*

Observe for $v \in L_0^2(Y)$ that

$$(11.29) \quad \begin{aligned} \|B(k)v\| &= |T_k^{-1}(-\Delta_N)^{-1}v| \\ &\leq \|(T_k^{-1}\|_{\mathcal{L}[\mathcal{H}_N; \mathcal{H}_N]} - \Delta_N^{-1})v\| \\ &\leq \lambda_N^{-1/2} \|T_k^{-1}\|_{\mathcal{L}[\mathcal{H}_N; \mathcal{H}_N]} \|v\|_{L^2(Y)}, \end{aligned}$$

where the last inequality follows from (11.7). The upper estimate on $\|T_k^{-1}\|_{\mathcal{L}[\mathcal{H}_N; \mathcal{H}_N]}$ is obtained from

$$(11.30) \quad \frac{\|T_k^{-1}v\|}{\|v\|} \leq \left\{ |z|\hat{w} + \tilde{w} + \left| \sum_{i=1}^{\infty} w_i |(1/2 + \mu_i) + z(1/2 - \mu_i)|^{-2} \right| \right\}^{1/2},$$

where $\hat{w} = \|P_1v\|^2/\|v\|^2$, $\tilde{w} = \|P_2v\|^2/\|v\|^2$, $w_i = \|P_iv\|^2/\|v\|^2$. Since $\hat{w} + \bar{w} + \sum_{i=1}^{\infty} w_i = 1$, one recovers the upper bound

$$(11.31) \quad \frac{\|T_k^{-1}v\|}{\|v\|} \leq M,$$

where

$$(11.32) \quad M = \max \left\{ 1, |z|, \sup_i \{ |(1/2 + \mu_i) + z(1/2 - \mu_i)|^{-1} \} \right\},$$

and the proof of Theorem 11.4 is complete.

Remark 11.5. The Poincaré inequality (11.6) together with Theorem 11.4 show that $B(k)$ is a bounded linear operator mapping $L_0^2(Y)$ into itself. The compact embedding of \mathcal{H} into $L_0^2(\alpha, Y)$ shows the operator is compact on $L_0^2(Y)$.

We have the following theorem.

THEOREM 11.6. *$A(z)$ is bounded and compact on $L_0^2(Y)$ for $z \in \mathbb{C}$ and $z \notin S$ and $A^*(z) = A(\bar{z})$. For z real and $z \notin S$ $A(z)$ is self-adjoint.*

The compactness and boundedness of $A(z)$ follows immediately from Theorem 11.4. To see that $A^*(z) = A(\bar{z})$ we write $(A(z)u, v)$ for u and v in $L_0^2(Y)$ and apply the formula

$$(11.33) \quad A(z) = \left(zP_1 + P_2 + z \sum_{-\frac{1}{2} < \mu_i < \frac{1}{2}} [(1/2 + \mu_i) + z(1/2 - \mu_i)]^{-1} P_{\mu_i} \right) (-\Delta_N)^{-1}.$$

We have

$$(11.34) \quad \begin{aligned} (A(z)u, v) &= z(P_1(-\Delta_N)^{-1}u, v) + (P_2(-\Delta_N)^{-1}u, v) + \\ &+ z \sum_{-\frac{1}{2} < \mu_i < \frac{1}{2}} [(1/2 + \mu_i) + z(1/2 - \mu_i)]^{-1} (P_{\mu_i}(-\Delta_N)^{-1}u, v). \end{aligned}$$

For $v \in \mathcal{H}_N$ the projections $P_{\mu_i}v$ are of the form

$$(11.35) \quad P_{\mu_i}v(x) = \sum_{\ell=1}^{m_i} \langle \Psi_{\ell}^i, v \rangle \Psi_{\ell}^i(x) \quad \text{for } x \in Y,$$

where $\{\Psi_{\ell}^i\}_{\ell=1}^{m_i}$ is an orthonormal basis for the subspace $P_{\mu_i}(\mathcal{H}_N)$. The projections P_1 and P_2 are defined similarly. Without loss of generality we show that $P_{\mu_i}(-\Delta_N)^{-1}$ is a self-adjoint operator on $L_0^2(Y)$. For p and q in $L_0^2(Y)$ we apply (2.18) to write

$$(11.36) \quad \begin{aligned} (P_{\mu_i}(-\Delta_N)^{-1}p, q) &= \sum_{\ell=1}^{m_i} \langle \Psi_{\ell}^i, (-\Delta_N)^{-1}p \rangle \langle \Psi_{\ell}^i, q \rangle \\ &= \sum_{\ell=1}^{m_i} \langle \Psi_{\ell}^i, p \rangle \langle \Psi_{\ell}^i, q \rangle. \end{aligned}$$

Applying this observation and straightforward calculation in (11.34) shows that $A^*(z) = A(\bar{z})$ for $z \in \mathbb{C}$ and that $A(z)$ is self-adjoint for real z .

Remark 11.7. Identical arguments apply to $A^\alpha(z)$. Here $(A^\alpha)^(z) = A^\alpha(\bar{z})$ and $A^\alpha(z)$ is self-adjoint for $z \in \mathbb{R}$.*

12. Reciprocal relation and its applications. We introduce a reciprocal relation for both Bloch and Neumann spectra and use it to understand band structure for crystals with coefficient $a = \frac{1}{k} < 1$ inside Ω and $a = 1$ outside. We denote the eigenvalue associated with a choice of coefficient $a(x) = a^{in}$ for points $x \in D$ and $a = a^{out}$ for points $x \in Y \setminus D$ by $\omega^2 = \omega^2(a^{in}, a^{out})$. The spectral problem is given by the solution u of

$$(12.1) \quad a^{in} \int_D \nabla u(x) \cdot \nabla \bar{v}(x) dx + a^{out} \int_{Y \setminus D} \nabla u(x) \cdot \nabla \bar{v}(x) dx = \omega^2 \int_Y u(x) \bar{v}(x) dx$$

for all test functions v . The Bloch spectrum is associated with u and v in $H_{\#}^1(\alpha, Y)$ and the Neumann spectrum is associated with u and v in \mathcal{H}_N . Now let t be scalar, and the spectrum satisfies the homogeneity property

$$(12.2) \quad \omega^2(ta^{in}, a^{out}) = t\omega^2(a^{in}, t^{-1}a^{out}),$$

so for $a = \frac{1}{k}$ in D and 1 in $Y \setminus D$ we have the reciprocal relation

$$(12.3) \quad \omega^2\left(\frac{1}{k}, 1\right) = \frac{1}{k}\omega^2(1, k).$$

The reciprocal relation (12.3) provides the relation between the band structure for the operator L_k described by (1.1) and

$$(12.4) \quad \tilde{L}_k = -\nabla \cdot ((1 - \chi_\Omega) + k^{-1}\chi_\Omega)\nabla$$

and is given by

$$(12.5) \quad \sigma(\tilde{L}_k) = \frac{1}{k}\sigma(L_k).$$

As an application we return to the photonic crystal given by the periodic dispersion of N disks, each separated by a minimum distance as described section 1. We suppose that the dielectric constant inside each disk is now greater than 1 and is given by k , while the surrounding material has dielectric constant 1. For this case the operator is taken to be (12.4) and we apply (12.5) together with Theorems 1.1 and 1.2 to recover the following theorem on existence of band gaps and persistence of spectral bands for H-polarized modes.

THEOREM 12.1 (Opening a band gap). *Given δ_{0j}^* define the set σ_N^+ to be elements $\nu \in \sigma_N$ for which $\nu > \delta_{0j}^*$. The element in σ_N^+ closest to δ_{0j}^* is denoted by ν_{j+1} . Set d_j according to*

$$(12.6) \quad d_j = \frac{1}{2} \min \{ |\nu_{j+1}^{-1} - \nu^{-1}|; \nu \in \sigma_N \}.$$

We define \bar{r}_j to be

$$(12.7) \quad \bar{r}_j = \frac{\pi^2 d_j (b^2 - a^2)}{(b^2 + a^2) + \pi^2 d_j (b^2 + 3a^2)}.$$

Then one has the band gap

$$(12.8) \quad \sigma(\tilde{L}_k) \cap \frac{1}{k} \left(\delta_{0j}^*, \nu_{j+1} \left(1 - \frac{\nu_{j+1} d_j}{k \bar{r}_j - 1} \right) \right) = \emptyset$$

if

$$(12.9) \quad k > \bar{k}_j = \bar{r}_j^{-1} \left(1 + \frac{d_j \nu_{j+1}}{1 - \frac{\delta_{0j}^*}{\nu_{j+1}}} \right).$$

Next we provide an explicit condition on k sufficient for the persistence of a spectral band together with explicit formulas describing its location and bandwidth.

THEOREM 12.2 (Persistence of passbands). *Given δ_{0j}^* define the set σ_N^- to be elements $\nu \in \sigma_N$ for which $\nu < \delta_{0j}^*$. The element in σ_N^- closest to δ_{0j}^* is denoted by ν_j . Set d_j according to*

$$(12.10) \quad d_j = \frac{1}{2} \min \{ |(\delta_{j0}^*)^{-1} - \delta^{-1}|; \delta \in \sigma(-\Delta_D) \}.$$

Define \underline{r}_j to be

$$(12.11) \quad \underline{r}_j = \frac{2\pi^2 d_j (b^2 - a^2)}{(b^2 + a^2) + 2\pi^2 d_j (b^2 + 3a^2)}.$$

Then one has a passband in the vicinity of δ_{0j}^* and

$$(12.12) \quad \sigma(\tilde{L}_k) \supset \frac{1}{k} \left[\nu_j, \delta_{0j}^* \left(1 - \frac{\delta_{0j}^* d_j}{k \underline{r}_j - 1} \right) \right]$$

if

$$(12.13) \quad k > \underline{k}_j = \underline{r}_j^{-1} \left(1 + \frac{d_j \delta_{0j}^*}{1 - \frac{\nu_j}{\delta_{0j}^*}} \right).$$

We conclude and point out that the results developed here provide rigorous criteria based on geometry and material properties for opening band gaps in both two- and three-dimensional periodic materials; see Theorems 1.1, 1.2, 10.2, 10.3, 12.1, and 12.2.

REFERENCES

- [1] H. AMMARI, H. KANG, S. SOUSSI, AND H. ZRIBI, *Layer potential techniques in spectral analysis. Part 2: Sensitivity analysis of spectral properties of high contrast band-gap materials*, Multiscale Model. Simul., 5 (2006), pp. 646–663.
- [2] M. BENDSOE AND O. SIGMUND, *Topology Optimization Theory, Methods, and Applications*, Springer, Berlin, 2004.
- [3] D. BERGMAN, *The dielectric constant of a composite material - a problem in classical physics*, Phys. Rep., 43 (1978), pp. 377–407.
- [4] D. BERGMAN, *The dielectric constant of a simple cubic array of identical spheres*, J. Phys. C, 12 (1979), pp. 4947–4960.
- [5] O. BRUNO, *The effective conductivity of strongly heterogeneous composites*, Proc. Roy. Soc. London. A, 433 (1991), pp. 353–381.
- [6] M. COSTABEL, *Boundary integral operators on Lipschitz domains: Elementary results*, SIAM J. Math. Anal., 19 (1988), pp. 613–625.
- [7] S. COX AND D. DOBSON, *Band structure optimization of two-dimensional photonic crystals in h-polarization*, J. Comput. Phys., 158 (2000), pp. 214–224.
- [8] A. ELBERT, *Some recent results on the zeros of Bessel functions and orthogonal polynomials*, Journal of Computational and Applied Mathematics, 133 (2001), pp. 65–83.

- [9] A. FIGOTIN AND P. KUCHMENT, *Band-gap structure of the spectrum of periodic Maxwell operators*, J. Stat. Phys., 74 (1994), pp. 447–455.
- [10] A. FIGOTIN AND P. KUCHMENT, *Band-gap structure of spectra of periodic dielectric and acoustic media. 1. Scalar model*, SIAM J. Appl. Math., 56 (1996), pp. 68–88.
- [11] A. FIGOTIN AND P. KUCHMENT, *Spectral properties of classical waves in high-contrast periodic media*, SIAM J. Appl. Math., 58 (1998), pp. 683–702.
- [12] L. FRIEDLANDER, *On the density of states of periodic media in the large coupling limit*, Comm. Partial Differential Equations, 27 (2002), pp. 355–380.
- [13] K. GOLDEN AND G. PAPANICOLAOU, *Bounds for effective parameters of heterogeneous media by analytic continuation*, Comm. Math. Phys., 90 (1983), pp. 473–491.
- [14] D. GREBENKOV AND B. NGUYEN, *Geometrical structure of Laplacian eigenfunctions*, SIAM Rev., 55 (1983), pp. 601–667.
- [15] R. HEMPEL AND K. LIENAU, *Spectral properties of periodic media in the large coupling limit*, Comm. Partial Differential Equations, 25 (2000), pp. 1445–1470.
- [16] S. JOHN, *Strong localization of photons in certain disordered dielectric superlattices*, Phys. Rev. Lett., 58 (1987), pp. 2486–2489.
- [17] I. JOO, *On the control of a circular membrane*, Acta Math. Hungar., 61 (1993), pp. 302–325.
- [18] H. KANG, *Layer potential approaches to interface problems*, in Inverse Problems and Imaging: Panoramas et Synthèses 44, Société Mathématique de France, Paris, 2013.
- [19] C. KAO, S. OSHER, AND E. YABLONOVITCH, *maximizing band gaps in two-dimensional photonic crystals by using level set methods*, Appl. Phys. B, 81 (2005), pp. 235–244.
- [20] T. KATO, *On the convergence of the perturbation method, 1*, Progr. Theor. Phys., 4 (1949), pp. 514–523.
- [21] T. KATO, *On the convergence of the perturbation method, 2*, Progr. Theor. Phys., 5 (1950), pp. 95–101.
- [22] T. KATO, *Perturbation Theory for Linear Operators*, Springer, Berlin, 1995.
- [23] D. KHAVINSON, M. PUTINAR, AND H. SHAPIRO, *Poincaré’s variational problem in potential theory*, Arch. Ration. Mech. Anal., 185 (2007), pp. 143–184.
- [24] P. KUCHMENT, *Floquet Theory for Partial Differential Equations*, Birkhauser, Basel, 1993.
- [25] R. LIPTON AND R. VIATOR, *Bloch waves in crystals and periodic high contrast media*, ESAIM Math. Model. Numer. Anal., 51 (2017), pp. 889–918.
- [26] R. MCPHEDRAN AND G. MILTON, *Bounds and exact theories for transport properties of inhomogeneous media*, Appl. Phys. A, 26 (1981), pp. 207–220.
- [27] H. MEN, K. LEE, R. FREUND, J. PERAIRE, AND S. JOHNSON, *Robust topology optimization of three-dimensional photonic-crystal band-gap structures*, Opt. Express 22634, 22 (2014), <https://doi.org/10.1364/OE.22.022632>.
- [28] G. MILTON, *The Theory of Composites*, Cambridge University Press, Cambridge, 2002.
- [29] F. ODEH AND J. KELLER, *Partial differential equations with periodic coefficients and Bloch waves in crystals*, J. Math. Phys., 5 (1964), pp. 1499–1504.
- [30] M. REED AND B. SIMON, *Methods of Modern Mathematical Physics*, Vol. IV: Analysis, Academic Press, New York, 1978.
- [31] J. SELDEN, *Periodic operators in high-contrast media and the integrated density of states function*, Comm. Partial Differential Equations, 30 (2005), pp. 1021–1037.
- [32] B. SZ.-NAGY, *Perturbations des transformations autoadjoints dans l’espace de hilbert*, Comment. Math. Helv., 19 (1946), pp. 347–366.
- [33] F. WANG, J. S. JENSEN, AND O. SIGMUND, *Robust topology optimization of photonic crystal waveguides with tailored dispersion properties*, J. Opt. Soc. Am. B, 28 (2011), pp. 767–784.
- [34] C. WILCOX, *Theory of Bloch waves*, J. Anal. Math., 33 (1978), pp. 146–167.
- [35] E. YABLONOVITCH, *Inhibited spontaneous emission in solid-state physics and electronics*, Phys. Rev. Lett., 63 (1987), pp. 2059–2062.