Resonant scattering by open periodic waveguides[1]

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Abstract. This article concerns the interaction between guided electromagnetic or acoustic modes of a penetrable periodic planar waveguide and plane waves originating from sources exterior to the waveguide. The interaction causes resonant enhancement of fields in the waveguide and anomalous transmission of energy across it. A guided mode is an eigenfunction of a member of the family of operators in the Floquet-Bloch decomposition of the periodic differential operator underlying the waveguide structure. The theory of existence or nonexistence of modes in ideal lossless waveguides is founded on variational principles. The mechanism for resonant scattering behavior is the dissolution of an embedded eigenvalue into the continuous spectrum, which corresponds to the destruction of a guided mode of a waveguide, upon perturbation of the wavevector or the material properties or geometry of the structure. Analytic perturbation of functions that unify the guided modes and the extended scattering states gives rise to asymptotic formulas for transmission anomalies.

Key words: guided mode, scattering, resonance, photonic crystal slab, boundary-integral equations.

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5. Resonance

The transmission resonances that result from the interaction of plane waves and guided modes are akin to those in quantum mechanics that are associated with the names of Feshbach, Breit-Wigner, or Fano. The unifying idea is that, when one perturbs a system that admits a bound state whose frequency is embedded in the continuous spectrum, the eigenvalue dissolves as a result of the coupling of the bound state to the extended states corresponding to the frequencies of the continuum. We give proofs of asymptotic formulas for transmission anomalies and analysis of resonant amplitude enhancement.

1 Overview

A planar structure acts both as a guide of electromagnetic or acoustic waves as well as a scatterer of waves that originate from sources exterior to it. An open waveguide is one that is in contact with the ambient space; the effect of this contact is twofold: (1) Fields produced by sources in the guide lose energy through radiation into the ambient space; and (2) fields originating in the ambient space interact with the guided modes of the slab. This Chapter is concerned with the latter, and, in particular, with resonant phenomena that result from this interaction.

Consider, for example, a periodically perforated film, an infinite wall of dielectric pillars, or the slab structure in Fig. 1. If a field strikes the structure, the coherent scattering by the periodic geometry can result in enhanced transmission or reflection of energy in narrow frequency intervals, causing the structure to act as a frequency-specific filter. In many cases, the explanation for this anomalous transmission is understood to be the resonant interaction between the incident field and the guided modes of the structure. There is a large body of literature dedicated to this phenomenon; we shall discuss some of it later on.

The fundamental mechanism of resonance can be understood as follows. A waveguide (closed or open) possesses a "dispersion relation" relating the frequency of a guided wave to its wavevector, which in the case of a slab waveguide is two-dimensional. The ambient space has its own dispersion relation, and, there, the wavevector is three-dimensional. This means that a two-dimensional wavevector parallel to the waveguide admits a discrete set of frequencies corresponding to guided modes but a continuum of frequencies corresponding to plane waves in the ambient space because of the additional spatial degree of freedom there. Resonance occurs when the frequency of a plane wave and the component of its wavevector parallel to the slab lie close to the dispersion relation for the waveguide itself. This is an expression of the idea of interaction between plane waves and guided modes.

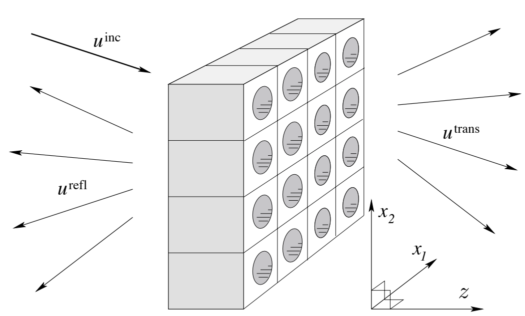

Figure 1: A slab waveguide that is doubly periodic in $x = (x_1, x_2)$ and finite in z (sixteen periods are shown). It is in contact with a homogeneous ambient space.

The periodicity of the slab acts as a mechanism for this type of resonance. It causes incident plane waves to be diffracted into a finite number outward-propagating plane waves (Rayleigh-Bloch scattering), which are accompanied by slow surface waves that fall off exponentially with the distance from the slab (Rayleigh-Bloch surface waves). Periodicity causes the frequencies for (real) wavevectors of guided modes to be complex because of "coupling" to the Rayleigh-Bloch scattered waves. In physical terms, the mode is not truly guided but is "leaky". When the imaginary part of the frequency is very small, plane waves in the ambient medium that oscillate at the real part of the frequency scatter resonantly in the slab. We will analyze in detail the situation in which the slab structure admits a true guided mode (with real frequency) that is *isolated* in the sense that nearby frequencies of guided modes are leaky (with complex frequency). The frequency of such a guided mode can be conceived as an eigenvalue that is embedded in the continuous spectrum corresponding to a specific wavevector, and the dissolution of the eigenvalue upon perturbation of the wavevector or structural parameters corresponds to the destruction of the guided mode. This gives rise to anomalous transmission of plane-wave energy across the slab and resonant enhancement of the field in the structure. Some of these anomalies are seen in Figs. 6,7,8,9 in Sec. 5.

Most of the analysis in the following sections is presented for the case of scalar waves in a penetrable and lossless doubly periodic slab waveguide in three-dimensional space. The ideas and results are not specific to any particular geometry, such as layers or gratings. Moreover, they extend to the Maxwell system and slabs fabricated from perfect conductors or acoustically hard or soft components, as well as lattice models. The focus is on lossless materials, although much of the analysis is extensible to lossy materials.

Let us set the notation for scalar waves. The periodic slab structure is defined through two material coefficients, $\varepsilon(x,z)$ and $\mu(x,z)$, where

$$x \in \mathbb{R}^2, \quad z \in \mathbb{R},$$

that are doubly 2π-periodic in x between the parallel planes $z = z_-$ and $z = z_+$ and constant in the homogeneous ambient space outside the region between these planes. Both coefficients are positive measurable functions bounded from below and above:

$$\begin{aligned}
&\varepsilon(x+2\pi n, z) = \varepsilon(x,z),\ n \in \mathbb{Z}^2,\\
&\mu(x+2\pi n, z) = \mu(x,z),\ n \in \mathbb{Z}^2,\\
&0 < \varepsilon_- \leq \varepsilon(x,z) \leq \varepsilon_+, \quad 0 < \mu_- \leq \mu(x,z) \leq \mu_+,\\
&\varepsilon(x,z) = \varepsilon_0,\ \mu(x,z) = \mu_0 \ \text{ if } z \leq z_- \text{ or } z \geq z_+.
\end{aligned}$$

The scalar wave equation in this open slab structure is

$$\varepsilon \frac{\partial^2 u}{\partial t^2} - \nabla\cdot\mu^{-1}\nabla u = 0. \tag{1}$$

The assumption of harmonic time dependence

$$u(x,z;t) = u(x,z)e^{-i\omega t}$$

results in the Helmholtz equation for the spatial factor $u(x,z)$,

$$\nabla\cdot\mu^{-1}\nabla u + \omega^2 \varepsilon u = 0. \tag{2}$$

2 Scattering by a periodic slab

The purpose of this section is to expound the role that structural periodicity plays in the coupling of plane waves and guided modes of an open slab waveguide, as this mechanism will be central to the analysis of resonance later on. We then sketch how the problem of plane-wave scattering fits into the general context of time dynamics.

2.1 Effects of periodicity

We begin in a nontechnical way by examining the simplest time-harmonic solutions of the wave equation in the presence of the slab. We shall progress from the simple case of scattering of plane waves by a slab with no genuine periodicity to scattering by a general lossless periodic slab in order to understand the concepts of Rayleigh-Bloch diffraction, robust and nonrobust (embedded) guided modes, cutoff frequencies, and the interaction between extended (scattering) states and guided modes.

Fig. 2A shows a two-dimensional cross-section of a homogeneous slab, invariant in the x-variables. A plane wave w^{inc} with wavevector $\langle \kappa, \eta \rangle$, $\kappa = \langle \kappa_1, \kappa_2 \rangle$, satisfying the wave equation (1) is traveling to the right at an angle of $\arctan(|\kappa|/\eta)$ with the line perpendicular to the slab,

$$
\begin{gathered}
w^{\text{inc}}(x,z;t) = \cos(\kappa \cdot x + \eta z - \omega t), \\
|\kappa|^2 + \eta^2 = \varepsilon_0 \mu_0 \omega^2, \\
\omega > 0, \quad \eta > 0,
\end{gathered}
$$

and strikes the slab from the left. Part of the energy is reflected back to the left and part is transmitted through to the right.

The incident field w^{inc} is the real part of $u^{\text{inc}}(x,z)e^{-i\omega t} = e^{i(\kappa \cdot x + \eta z)}e^{-i\omega t}$, and the spatial part u^{inc} satisfies the Helmholtz equation (2). Dropping the time factor, we can write the total field as $u(x,z) = e^{i\kappa \cdot x}\phi(z)$, where

$$
\phi(z) = \begin{cases} e^{i\eta z} + a e^{-i\eta z}, & z < z_-, \\ c e^{i\nu z} + d e^{-i\nu z}, & z_- < z < z_+, \\ b e^{i\eta z}, & z_+ < z. \end{cases} \tag{3}
$$

The common x-factor is necessary for continuity, and, in the slab,

$$
|\kappa|^2 + \nu^2 = \varepsilon_1 \mu_1 \omega^2. \tag{4}
$$

The complex reflection and transmission coefficients a and b, as well as c and d, are determined by the interface conditions at $z = z_-$ and $z = z_+$,

$$
\begin{aligned}
&u(x, z_\pm - 0) = u(x, z_\pm + 0), \\
&\mu_0^{-1} \tfrac{\partial}{\partial z} u(x, z_- - 0) = \mu_1^{-1} \tfrac{\partial}{\partial z} u(x, z_- + 0), \\
&\mu_1^{-1} \tfrac{\partial}{\partial z} u(x, z_+ - 0) = \mu_0^{-1} \tfrac{\partial}{\partial z} u(x, z_+ + 0).
\end{aligned}
$$

An analogous problem describes the scattering of a plane wave $u^{\text{inc}}(x,z) = e^{i(\kappa \cdot x - \eta z)}e^{-i\omega t}$ incident upon the slab from the right.

For each of these solutions,

$$
|\kappa| < \omega\sqrt{\varepsilon_0 \mu_0}. \tag{5}
$$

This conical region in (κ, ω)-space is the *light cone* for the exterior medium (blue region in Fig. 2A), and for each pair in this region, there is a two-parameter family of *scattering states* spanned by the solution with z-dependent factor (3) and its counterpart with incident field from the right.

Assuming that $\varepsilon_0\mu_0 < \varepsilon_1\mu_1$, Fig. 2A depicts three regions in (κ, ω)-space,

$$
\begin{aligned}
&0 < \omega^2 \varepsilon_0 \mu_0 - |\kappa|^2 < \omega^2 \varepsilon_1 \mu_1 - |\kappa|^2, \\
&\omega^2 \varepsilon_0 \mu_0 - |\kappa|^2 < 0 < \omega^2 \varepsilon_1 \mu_1 - |\kappa|^2, \\
&\omega^2 \varepsilon_0 \mu_0 - |\kappa|^2 < \omega^2 \varepsilon_1 \mu_1 - |\kappa|^2 < 0.
\end{aligned}
$$

The first region parameterizes the scattering states. It is the (κ, ω)-region in which $\phi(z)$ is oscillatory inside and outside the slab. In the third region, there are no scattering states because the pair (κ, ω) violates (5). In fact, $\phi(z)$ is exponential inside and outside the slab, and there are therefore no solutions that are uniformly bounded in magnitude over $z \in \mathbb{R}$, which we require for our Helmholtz fields (exponentially growing solutions do not play a direct role in the spectral decomposition).

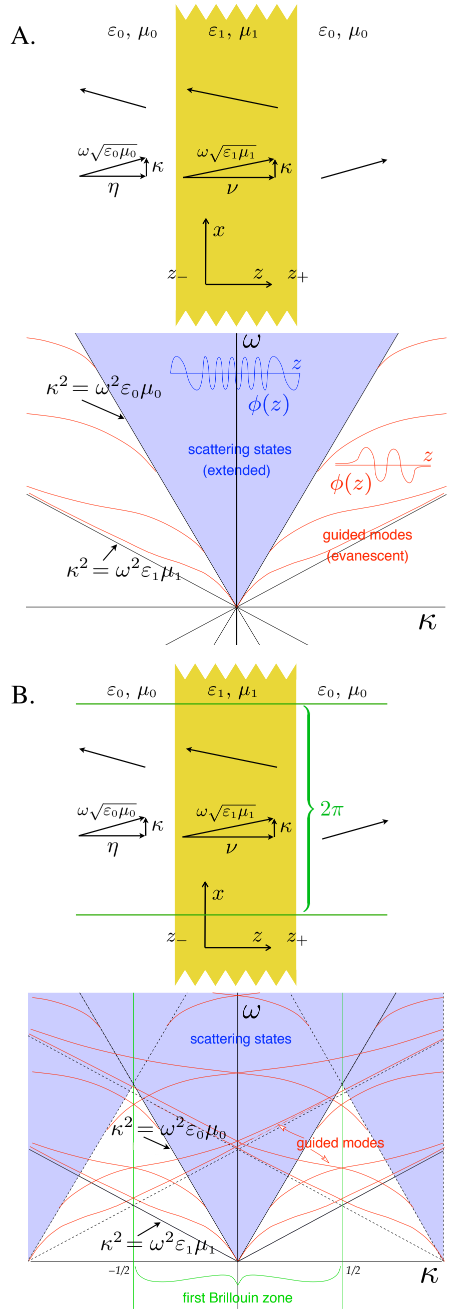

Figure 2: **A.** A homogeneous 2D slab scatters a plane wave incident on the left. The arrows indicate the directions of the plane-wave components of the total field. The (κ, ω) for all scattering states lies in the blue light cone for the exterior medium. Dispersion relations (red) for guided modes lie between the interior and exterior light cones. The behavior of the z-factor in the separable fields $\phi(z)e^{i\kappa x}$ is indicated by the inset graphs. **B.** By imposing an artificial period of 2π in a uniform slab, the extended and guided Bloch (pseudo-periodic) states can be represented by their reduced wavenumber in the first Brillouin zone by shifting the wavenumber by an integer.

In the second region, there are no scattering states either. But, although $\phi(z)$ is exponential outside the slab, it is still oscillatory inside. The requirement that a solution to the Helmholtz equation be bounded in magnitude leads to solutions of the form

$$\phi(z) = \begin{cases} e^{\gamma z}, & z < z_-, \\ ce^{i\nu z} + de^{-i\nu z}, & z_- < z < z_+, \\ be^{-\gamma z}, & z_+ < z, \end{cases} \tag{6}$$

where $\gamma > 0$. The solution $e^{i(\kappa\cdot x - \omega t)}\phi(z)$ is a *guided mode* of the slab, exponentially decaying as $|z| \to \infty$ and propagating along the slab in the direction of κ with phase velocity

$$v_{\text{ph}} = \omega/|\kappa|. \tag{7}$$

This velocity is less than that of waves in the ambient medium.

The condition that ϕ decay on both sides of the slab is satisfied only on certain relations between κ and ω that are branches of the *dispersion relation* for guided modes. There is one branch for each nonnegative integer n, and one computes that they are expressed in the form

$$L\Theta(\kappa,\omega) - 2\Phi(\kappa,\omega) = n\pi\,,\;\; n \in \mathbb{N}, \tag{8}$$

in which

$$\begin{aligned} &L = z_+ - z_-, \\ &\Theta = (\omega^2\varepsilon_1\mu_1 - |\kappa|^2)^{1/2}, \\ &\alpha = \frac{\mu_1}{\mu_0}\frac{(|\kappa|^2 - \omega^2\varepsilon_0\mu_0)^{1/2}}{(\omega^2\varepsilon_1\mu_1 - |\kappa|^2)^{1/2}}, \\ &\Phi = \arctan\alpha. \end{aligned}$$

These relations define a sequence of functions $W_n(\kappa)$ with domains $\mathscr{D}(W_n) = \mathbb{R}\setminus[-\kappa_n,\kappa_n]$ and images (ω_n,∞), such that (8) is expressed as the union of the graphs

$$\omega = W_n(\kappa),\; \kappa \in \mathscr{D}(W_n),\; n \in \mathbb{N}.$$

These graphs are the *branches* of the dispersion relation for guided modes and are shown in red in Fig. 2A. One can show that each function W_n is increasing, emanates tangentially from the light cone for the exterior medium at $(\pm\kappa_n,\omega_n)$, and is asymptotically tangent to the light cone for the interior medium as $|\kappa| \to \infty$. The points (κ_n,ω_n) are

$$(\kappa_n,\omega_n) = \frac{n\pi}{L\sqrt{\varepsilon_1\mu_1 - \varepsilon_0\mu_0}}(\sqrt{\varepsilon_0\mu_0},1).$$

Fig. 2A shows that, for each value of κ, there is a continuous spectrum of frequencies $\omega \in (|\kappa|/\sqrt{\varepsilon_0\mu_0},\infty)$ that admit scattering states and a finite number of guided mode frequencies given by $W_n(\kappa)$ for all n such that $\kappa_n < |\kappa|$. The frequency $|\kappa|/\sqrt{\varepsilon_0\mu_0}$ on the light cone is the *cutoff frequency* for the slab structure and wavevector κ.

We must keep in mind that the solutions we have constructed are purely monochromatic fields with infinite energy (but finite energy density), and, as such, are idealized fields that are not truly physically viable in isolation. The incident fields in the scattering states are thought of as originating from sources infinitely far away from the slab, and the guided modes are thought of as being excited by sources in or near the slab but infinitely far from an observer in the slab. Integral superpositions of monochromatic fields form finite-energy solutions of the wave equation; this spectral theory is discussed below.

In Fig. 3C we see a two-dimensional depiction of a slab with a genuine periodicity of 2π. Solutions of the Helmholtz equation no longer have the separable form $u(x,z) = u_1(x)u_2(z)$. But since the slab is periodic and the incident field in the scattering problem exhibits only a phase difference of $2\pi\kappa\cdot n$ between the points (x,z) and $(x+2\pi n,z)$, we may take the point of view that, when the incident field is scattered by the slab, an observer at $(x+2\pi n,z)$

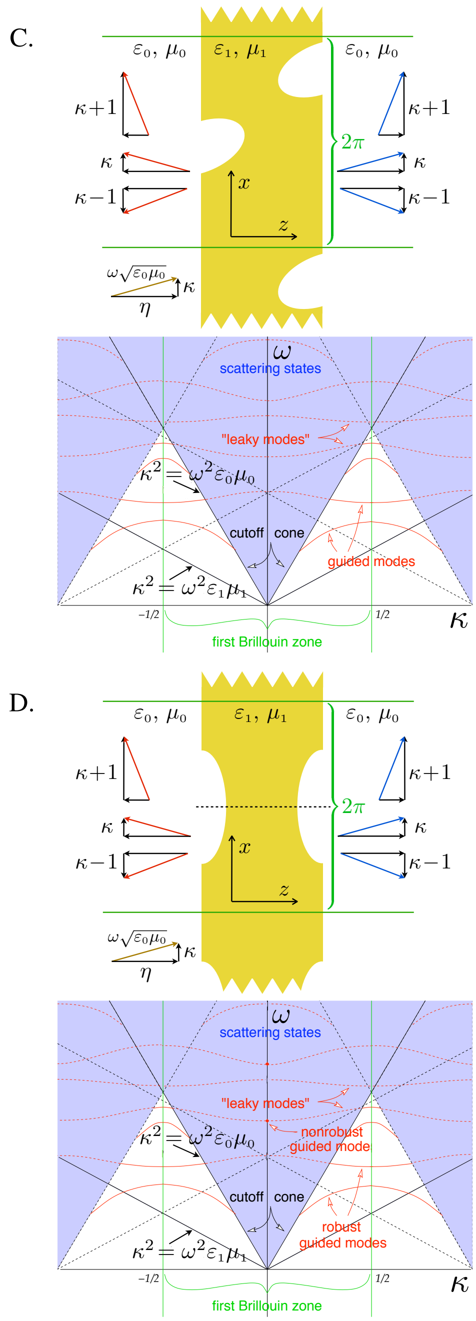

Figure 3: **C.** The periodicity of the slab causes an incident plane wave (brown) to be scattered into a finite number of directions. The reflected diffractive orders are indicated in red and the transmitted in blue. Real dispersion relations split apart (cf. Fig. 2B) at the crossing points (this diagram is qualitative and some of the branches are not drawn). The dotted curves indicate the real part of the frequency that has become complex due to the periodicity. **D.** Because of the symmetry of the structure about the dotted line, the frequency on the dispersion relation may be real for $\kappa = 0$. Such isolated real points on a complex dispersion relation correspond to nonrobust guided slab modes.

will experience a field that differs from that experienced by an observer at (x,z) only by a phase of $2\pi\kappa\cdot n$. This means that we are interested in *pseudo-periodic*, or *quasi-periodic*, solutions of the Helmholtz equation

$$u(x,z;\kappa) = e^{i\kappa\cdot x}\tilde{u}(x,z;\kappa), \tag{9}$$

in which $\tilde{u}(x,z;\kappa)$ is periodic in x. Such a solution u is a *Bloch wave* with *Bloch wavevector* κ, *Bloch factor* $e^{i\kappa\cdot x}$, and *Floquet multiplier* $e^{2\pi i\kappa\cdot n}$. The corresponding physical solution (with the (κ,ω)-dependence suppressed) is

$$\mathrm{Re}\,(\tilde{u}(x,z)e^{i(\kappa\cdot x-\omega t)}) = |\tilde{u}(x,z)|\cos(\theta(x,z)+\kappa\cdot x-\omega t) \tag{10}$$

($\theta(x,z) = \arg\tilde{u}(x,z)$), which is a wave that is distorted in a periodic fashion in the x-variables by the slab structure.

Now, the periodic factor in a Bloch wave can be written as a Fourier series in the variable x parallel to the slab, with coefficients that depend on the transverse variable z,

$$\tilde{u}(x,z) = \sum_{m\in\mathbb{Z}^2}\phi_m(z)e^{im\cdot x}. \tag{11}$$

Because u satisfies a homogeneous Helmholtz equation exterior to the slab, there, ϕ_m must have the form

$$\phi_m(z) = c_m^1\phi_m^1(z)+c_m^2\phi_m^2(z), \tag{12}$$

in which $\phi^{1,2}$ are independent solutions of the ordinary differential equation $\phi_m''+\eta_m^2\phi_m = 0$, where the numbers η_m are defined through

$$\eta_m^2+|m+\kappa|^2 = \omega^2\varepsilon_0\mu_0. \tag{13}$$

The functions $\phi_m^{\pm}$ are either oscillatory, linear, or exponential, depending on the numbers η_m. The Fourier components of u are known as the *spatial harmonics* or the *diffractive (or diffraction) orders* associated with the periodic structure. There are many references that expound these ideas, including C. Wilcox [90] and M. Nevière [63]. We distinguish between the following classes of spatial harmonics, for fixed parameters (κ,ω):

$$\begin{array}{ll} m\in\mathscr{Z}_p \Leftrightarrow \eta_m^2>0,\ \eta_m>0 & \text{(propagating)},\\ m\in\mathscr{Z}_\ell \Leftrightarrow \eta_m^2=0,\ \eta_m=0 & \text{(linear)},\\ m\in\mathscr{Z}_e \Leftrightarrow \eta_m^2<0,\ -i\eta_m>0 & \text{(evanescent)}. \end{array} \tag{14}$$

The first class $\mathscr{Z}_p$ of oscillatory harmonics is finite, the class $\mathscr{Z}_\ell$ of linear harmonics is generically empty but always finite, and the class $\mathscr{Z}_e$ of exponential harmonics is infinite. The latter harmonics are called evanescent because of the requirement that the component that is exponentially growing as $|z|\to\infty$ vanish.

The general bounded pseudo-periodic solution of the Helmholtz equation can be interpreted as the field resulting from scattering of plane waves by the slab:

$$u(x,z) = \sum_{m\in\mathscr{Z}_p}a_m^{\text{inc}}e^{i\eta_m z}e^{i(m+\kappa)\cdot x}+\sum_{m\in\mathbb{Z}^2}a_m e^{-i\eta_m z}e^{i(m+\kappa)\cdot x} \quad (z<z_-), \tag{15}$$

$$u(x,z) = \sum_{m\in\mathscr{Z}_p}b_m^{\text{inc}}e^{-i\eta_m z}e^{i(m+\kappa)\cdot x}+\sum_{m\in\mathbb{Z}^2}b_m e^{i\eta_m z}e^{i(m+\kappa)\cdot x} \quad (z>z_+). \tag{16}$$

The sums over $\mathscr{Z}_p$ represent traveling source waves incident upon the slab from the left and right, generalizing the incident field to a sum of plane waves, each of whose Bloch wavevector differs from κ by an integer pair $m\in\mathscr{Z}_p$. The sums over $\mathbb{Z}^2$ represent the reflected and transmitted fields. The scattered, or diffracted, field is the difference $u(x,z)-u^{\text{inc}}(x,z)$, which is radiating. We say that a function u is *radiating* (or *outgoing*) if it is of the form (15,16) with $a_m^{\text{inc}}=0$ and $b_m^{\text{inc}}=0$ for all $m\in\mathscr{Z}_p$.

Condition 1 (Radiation) *A complex-valued function u defined on $\mathbb{R}^3$ is said to satisfy the* radiation condition *for the slab for the real pair (κ,ω), with $\omega>0$, if there exist a real number z_0 and complex coefficients $\{c_m^{\pm}\}_{m\in\mathbb{Z}^2}$ in $\ell^2(\mathbb{Z}^2)$ such that*

$$u(x,z) = \sum_{m\in\mathbb{Z}^2}c_m^{\pm}e^{\pm i\eta_m z}e^{i(m+\kappa)\cdot x} \quad \textit{for } \pm z>z_0.$$

Because the Bloch form $u(x,z) = e^{i\kappa\cdot x}\tilde{u}(x,z)$, is equivalent to the form $u(x,z) = e^{i(\kappa+m)\cdot x}\tilde{u}(x,z)$ by the change of periodic part $\tilde{u}(x,z) \mapsto \tilde{u}(x,z)e^{-im\cdot x}$, one can always assume that κ lies in the first *Brillouin zone*,

$$B = [-1/2, 1/2)^2, \tag{17}$$

shown in Fig. 3C for the two-dimensional case. It is then guaranteed that $|\kappa + m| \geq |\kappa|$ for all $m \in \mathbb{Z}^2$. This value of κ is called the *reduced wavevector* for u.

The harmonic pseudo-periodic scattering problem is stated below. Proof that it has a solution that is typically unique is achieved through a weak formulation of the problem, which we present later.

Problem 2 (Plane-wave scattering) *Given $\omega > 0$ and $\kappa \in B$, find a function u on $\mathbb{R}^3$ that is doubly 2π-pseudo-periodic in x with Bloch wavevector κ and that satisfies the Helmholtz equation* (2) *and such that*

$$u(x,z) = u^{inc}(x,z) + u^{sc}(x,z),$$

in which

$$u^{inc}(x,z) = \sum_{m\in\mathscr{Z}_p} (a_m^{inc} e^{i\eta_m z} + b_m^{inc} e^{-i\eta_m z}) e^{i(m+\kappa)\cdot x}$$

and u^{sc} satisfies the radiation Condition 1.

A **guided mode** is a nontrivial solution to Problem 2 such that $a_m^{inc} = b_m^{inc} = 0$ for all $m \in \mathscr{Z}_p$. As long as $\mathscr{Z}_\ell = \emptyset$, such solutions necessarily fall off exponentially with $|z|$ because of the conservation of energy law for Helmholtz fields with the expansions (15,16),

$$\sum_{m\in\mathscr{Z}_p} \eta_m(|a_m^{inc}|^2 + |b_m^{inc}|^2) = \sum_{m\in\mathscr{Z}_p} \eta_m(|a_m|^2 + |b_m|^2).$$

This can be proved by integration by parts applied to the Helmholtz equation (2) multiplied by $\bar{u}$.

Because of the periodicity of the slab, all the spatial harmonics for a given wavevector $\kappa \in B$ are coupled. They cannot exist in isolation; rather, in each Helmholtz field, all harmonics are generally present. A distinctive structure emerges from this observation: when a plane-wave source is scattered by a periodic slab, the energy of the scattered, or diffracted, field that propagates away from the slab is split into a finite number of distinct plane waves traveling at prescribed angles. These are known as *Rayleigh-Bloch waves*, and their angles α_m, depicted in Fig. 3C are

$$\alpha_m = \arcsin\frac{|\kappa + m|}{\omega\sqrt{\varepsilon_0\mu_0}}, \quad m \in \mathscr{Z}_p. \tag{18}$$

The angles α_m depend only on κ, ω, the exterior material coefficients ε_0 and μ_0, and the periodicity of the slab (which we always normalize to 2π and therefore does not appear in the expression for α_m), and not on any other attributes of the structure. The evanescent diffractive orders do not carry energy away from the slab, but only along it. They are known as slow *Rayleigh-Bloch surface waves* because they have a phase velocity that is less than the wave speed of the ambient space. In the special case that $\eta_m = 0$ for some $m \in \mathbb{Z}^2$, the corresponding linear harmonic is exactly grazing the slab; it carries no energy away from it yet is extended in the z-variable.

If a pair (κ, ω) admits no propagating harmonics, then no incident field in (15,16) is available and there is no notion of scattering of plane waves originating from sources exterior to the slab. A nontrivial bounded pseudo-periodic solution of the Helmholtz equation is, in this case, always a guided mode, assuming $\mathscr{Z}_\ell = \emptyset$.

Because of the coupling of spatial harmonics due to the periodicity, we have seen that a pseudo-periodic solution of the Helmholtz equation is typically composed of all harmonics with wavevectors $\kappa + m$. It can be ascribed a unique Bloch wavevector κ in B, but, among the possible wavevectors $\kappa + m$, there is in general no preferred one. This is in contrast to the case of the x-invariant slab we considered first, in which the periodicity is absent. It is instructive to impose a periodicity artificially and view this case from the point of view of the Bloch theory to understand just how the transition from flat to periodic takes place. This is illustrated in Fig. 2B, where all pairs (κ, ω) admitting scattering or guided states are shifted in κ by an integer into B. Thus all Bloch states are represented by a pair (κ, ω) in $B \times \mathbb{R}$.

By assigning a wavevector $\kappa \in B$ to each state of the flat (nonperiodic) slab, we view it as having a Fourier expansion in spatial harmonics for which all but one coefficient vanishes: indeed, by writing $\kappa = \bar{\kappa} + \bar{m}$, with $\bar{\kappa} \in B$ and $\bar{m} \in \mathbb{Z}^2$, and $\phi_{\bar{m}}(z) = \phi(z)$, a solution of the form $e^{i\kappa\cdot x}\phi(z)$ can be written as

$$\phi_{\bar{m}}(z)e^{(\bar{m}+\bar{\kappa})\cdot x},\ \bar{\kappa} \in B. \tag{19}$$

If the flat slab is perturbed periodically, we expect its Bloch states to be perturbed from their special form and typically attain all spatial harmonics. For those guided modes corresponding to (κ, ω) in the white region below the light cone, or below the cutoff frequency for $\kappa \in B$, all spatial harmonics are evanescent, and the guided mode should persist. We call these guide modes *robust*. Guided mode frequencies above the cutoff frequency (the blue region of Fig. 2B) are embedded in the continuous spectrum of scattering states. If we expect a typical state of the periodically perturbed slab to have a full expansion in spatial harmonics, then a guided mode can typically no longer exist because of the presence of propagating harmonics. The destruction of a guided mode under this perturbation of the structure corresponds to the dissolution of an embedded eigenvalue into the continuous spectrum. Sharp transmission anomalies that emerge are treated in a physical model by Fan and Joannopoulos [22], which takes into account a direct (nonresonant) transmission process as well as an indirect (resonant) one mediated by the excitation of the guided mode.

The dissolution of the dispersion relations in the (κ, ω)-region of scattering states, as well as the typical splitting of crossings of dispersion relations is depicted in Fig. 3C. In fact, the dispersion relation does not actually disappear, but the frequency becomes complex. The dotted curves correspond to the real part of a generalized dispersion relation, which we discuss in Sec. 4 and 5. Fields corresponding to points on the complex dispersion curve are *generalized guided modes*. Generalized modes whose frequency ω has a small but nonzero imaginary part form the theoretical basis of *leaky modes* or *quasi-guided modes*. Discussions of the topic of leaky modes as well as methods for computation of their dispersion relations can be found in [67, 85, 68, 32] and references therein.

Wave phenomena connected with periodicity of waveguide structures and applications are treated for a large class of structures in the nice review paper [17] of Elachi.

Even for periodic slabs, embedded guided mode frequencies can exist. The two-dimensional structure in Fig. 3D, for example, is symmetric about a horizontal line, and we can therefore seek states for $\kappa = 0$ that are symmetric or antisymmetric about this line. In the (κ, ω)-region of one propagating harmonic, $m = 0$, this harmonic $e^{i\eta_0 z}$ is constant in x and therefore absent in antisymmetric states, making them exponentially decaying as $|z| \to \infty$. Because a perturbation of κ from 0 breaks the symmetry of the propagating harmonic, the guided mode is destroyed and ω takes on a nonzero imaginary part. We refer to such a guided mode as *nonrobust*. The destruction of a guided mode, this time due to a perturbation of κ, corresponds again to the dissolution of an embedded eigenvalue. The eigenvalue is characterized by an isolated pair (κ, ω) on the complex dispersion relation at which ω and κ are *real* and is illustrated in Fig. 3D. Isolated true guided modes are discussed in [67] and [85]. We deal with their mathematical existence in Sec. 3.2.

It is the interaction between nonrobust guided slab modes and incoming plane waves that causes anomalous scattering behavior, including transmission anomalies, and this is the subject of Sec. 5. The analysis involves an analytic connection of generalized guided modes to scattering states and perturbation analysis in the vicinity of a nonrobust true guided mode pair (κ_0, ω_0), where κ_0 and ω_0 are both real.

2.2 Broader context

Let us step back to the time-dependent wave equation (1) and consider its free solutions in $\mathbb{R}^3$ in the presence of the slab. To place the wave equation into the proper functional-analytic setting, we should write it as a first-order system by defining $v = \frac{\partial u}{\partial t}$:

$$\frac{\partial}{\partial t}\begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} 0 & I \\ \varepsilon^{-1}\nabla\cdot\mu^{-1}\nabla & 0 \end{bmatrix}\begin{bmatrix} u \\ v \end{bmatrix}, \tag{20}$$

which may be supplemented by initial data $u(x,z;0)$ and $v(x,z;0)$. The appropriate functional spaces are the Hilbert spaces

$$\mathscr{H} = L^2(\mathbb{R}^3, \mathbb{C}, \varepsilon dV),$$
$$\mathscr{K} = L^2(\mathbb{R}^3, \mathbb{C}^3, \mu^{-1} dV),$$

with inner products

$$(u,w)_{\mathscr{H}} = \int_{\mathbb{R}^3} \varepsilon\, u\bar{w}\, dV,$$
$$(F,G)_{\mathscr{K}} = \int_{\mathbb{R}^3} \mu^{-1}\, F\cdot\bar{G}\, dV.$$

The symbol ∇ denotes the usual gradient operator in $\mathscr{H}$ (defined independently of the measure εdV). It is a closed operator, which takes values in $\mathscr{K}$ and whose domain is $\mathscr{D}(\nabla) = H^1(\mathbb{R}^3) \subset \mathscr{H}$, the Sobolev space of L^2 functions with weak L^2 derivatives. Similarly, the symbol $\nabla\cdot$ denotes the usual divergence operator in $\mathscr{K}$, with values in $\mathscr{H}$. With respect to the inner products in $\mathscr{H}$ and $\mathscr{K}$, one can verify that the adjoint of ∇ is $\nabla^\dagger = -(\varepsilon^{-1}\nabla\cdot)\mu^{-1}$.

The operator matrix in (20), which we denote by A, has a natural domain,

$$A = \begin{bmatrix} 0 & I \\ -\nabla^\dagger\nabla & 0 \end{bmatrix}, \quad \mathscr{D}(A) = \mathscr{D}(\nabla^\dagger\nabla) \oplus \mathscr{D}(\nabla),$$

and, thus defined, is an anti-self-adjoint operator in the Hilbert space

$$\mathscr{D}(\nabla) \oplus \mathscr{H}$$

with inner product

$$\left(\begin{bmatrix} \nabla^\dagger\nabla & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ v_1 \end{bmatrix}, \begin{bmatrix} u_2 \\ v_2 \end{bmatrix} \right)_{\mathscr{H}\oplus\mathscr{H}} = (\nabla u_1, \nabla u_2)_{\mathscr{K}} + (v_1, v_2)_{\mathscr{H}}.$$

Let E_λ be the standard spectral resolution of the identity in $\mathscr{H}$ for the operator $\nabla^\dagger\nabla$ (see [1], Ch. VI, for example). This means that, for each $\lambda \in \mathbb{R}$, E_λ is an orthogonal projection in $\mathscr{H}$; for each $u \in \mathscr{H}$, $(E_\lambda u, u)$ is a nondecreasing function of λ; and

$$\begin{aligned} u &= \int_0^\infty dE_\lambda u \qquad \forall u \in \mathscr{H}, \\ \nabla^\dagger\nabla u &= \int_0^\infty \lambda\, dE_\lambda u \quad \forall u \in \mathscr{D}(\nabla^\dagger\nabla). \end{aligned} \tag{21}$$

These integrals of $\mathscr{H}$-valued functions exist in the Lebesgue-Stieljes sense, and the lower limits are zero because the positivity of $\nabla^\dagger\nabla$ implies that $E_\lambda = 0$ if $\lambda < 0$.

Since A is anti-self-adjoint, it admits a spectral resolution of the identity in $\mathscr{D}(\nabla) \oplus \mathscr{H}$ with purely imaginary spectrum. For the wave equation, it is convenient to split the resolution into two projection-valued functions F_ω^+ and F_ω^- such that

$$\begin{aligned} \begin{bmatrix} u \\ v \end{bmatrix} &= \int_0^\infty dF_\omega^+ \begin{bmatrix} u \\ v \end{bmatrix} + \int_0^\infty dF_\omega^- \begin{bmatrix} u \\ v \end{bmatrix}, \\ A \begin{bmatrix} u \\ v \end{bmatrix} &= \int_0^\infty i\omega dF_\omega^+ \begin{bmatrix} u \\ v \end{bmatrix} + \int_0^\infty -i\omega dF_\omega^- \begin{bmatrix} u \\ v \end{bmatrix}. \end{aligned} \tag{22}$$

In order to obtain $F_\omega^\pm$ in terms of E_λ, we write A in terms of E_λ,

$$A \begin{bmatrix} u \\ v \end{bmatrix} = \int_0^\infty \begin{bmatrix} 0 & 1 \\ -\lambda & 0 \end{bmatrix} \begin{bmatrix} dE_\lambda u \\ dE_\lambda v \end{bmatrix}, \tag{23}$$

and use the spectral resolution of the matrix in this expression,

$$\begin{aligned} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} &= P_\omega^+ + P_\omega^-, \\ \begin{bmatrix} 0 & 1 \\ -\omega^2 & 0 \end{bmatrix} &= i\omega P_\omega^+ - i\omega P_\omega^-, \end{aligned} \tag{24}$$

in which the projection matrices $P^\pm$ are orthogonal (self-adjoint) with respect to the natural inner product

$$\left(\begin{bmatrix} \lambda & 0 \\ 0 & 1 \end{bmatrix} \cdot,\ \cdot \right)$$

($\lambda \neq 0$) in $\mathbb{C}^2$. These projections are given by

$$P_\omega^+ = \frac{1}{2}\begin{bmatrix} 1 & (i\omega)^{-1} \\ i\omega & 1 \end{bmatrix},\ P_\omega^- = \frac{1}{2}\begin{bmatrix} 1 & -(i\omega)^{-1} \\ -i\omega & 1 \end{bmatrix}.$$

By inserting (24) into (23), with $\lambda = \omega^2$ and $\omega \geq 0$, we deduce that the resolutions $F_\omega^\pm$ in (22) are given by

$$F_\omega^\pm \begin{bmatrix} u \\ v \end{bmatrix} = \int_0^{\omega^2} P_{\omega'}^\pm \begin{bmatrix} dE_{\omega'^2} u \\ dE_{\omega'^2} v \end{bmatrix}, \tag{25}$$

or, equivalently,

$$dF_\omega^\pm \begin{bmatrix} u \\ v \end{bmatrix} = P_\omega^\pm \begin{bmatrix} dE_{\omega^2} u \\ dE_{\omega^2} v \end{bmatrix}. \tag{26}$$

Because A is anti-self-adjoint, there exists a unique strongly continuous unitary group of operators in $\mathscr{D}(\nabla) \oplus \mathscr{H}$, denoted by e^{tA}, whose generator is A (see Stone's Theorem §VIII.4 of [74]). This means that

$$\tfrac{\partial}{\partial t} e^{tA} w = A e^{tA} w$$

for $w \in \mathscr{D}(A)$. The solution of the initial-value problem

$$\tfrac{\partial}{\partial t} \begin{bmatrix} u \\ v \end{bmatrix} = A \begin{bmatrix} u \\ v \end{bmatrix}, \quad \begin{bmatrix} u(0) \\ v(0) \end{bmatrix} = \begin{bmatrix} u_0 \\ v_0 \end{bmatrix},$$

in terms of the resolution (22) of A is

$$\begin{bmatrix} u(t) \\ v(t) \end{bmatrix} = e^{tA} \begin{bmatrix} u_0 \\ v_0 \end{bmatrix} = \int_0^\infty e^{i\omega t} dF_\omega^+ \begin{bmatrix} u_0 \\ v_0 \end{bmatrix} + \int_0^\infty e^{-i\omega t} dF_\omega^- \begin{bmatrix} u_0 \\ v_0 \end{bmatrix}$$

(the dependence on (x,z) is suppressed in $u(t)$).

Let us understand this solution more concretely in terms of generalized eigenfunctions. Since $F_\omega^\pm$ are expressed in terms of E_λ, we may focus our attention on $\nabla^\dagger \nabla = -\varepsilon^{-1} \nabla \cdot \mu^{-1} \nabla$. Suppose a pair $(u,v)^t \in \mathscr{D}(A)$ is expressed through integral superpositions

$$u(x,z) = \int_0^\infty w_1(x,z;\lambda)\, d\lambda,$$
$$v(x,z) = \int_0^\infty w_2(x,z;\lambda)\, d\lambda,$$

in which w_i satisfy the Helmholtz equation

$$-\varepsilon^{-1} \nabla \cdot \mu^{-1} \nabla w_i(x,z;\lambda) = \lambda w_i(x,z;\lambda)$$

in $\mathbb{R}^3$ but do not necessarily have finite L^2 norm. Then

$$\nabla^\dagger \nabla u(x,z) = \int_0^\infty \lambda w_1(x,z;\lambda)\, d\lambda.$$

The decomposition of $(w_1,w_2)^t$ according to $P_\omega^\pm$ for $\lambda = \omega^2$ ($\omega \geq 0$) is

$$\begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} u_+ \\ i\omega u_+ \end{bmatrix} + \begin{bmatrix} u_- \\ -i\omega u_- \end{bmatrix},$$

in which

$$u_\pm(x,z;\omega) = \tfrac{1}{2}\big(w_1(x,z;\omega^2) \pm (i\omega)^{-1} w_2(x,z;\omega^2)\big).$$

In the time dynamics, this represents a decomposition into harmonic fields oscillating with the time factors $e^{i\omega t}$ and $e^{-i\omega t}$:

$$\begin{bmatrix} u(x,z,t) \\ v(x,z,t) \end{bmatrix} = \int_0^\infty \left(e^{i\omega t} \begin{bmatrix} u_+(x,z;\omega) \\ i\omega\, u_+(x,z;\omega) \end{bmatrix} + e^{-i\omega t} \begin{bmatrix} u_-(x,z;\omega) \\ -i\omega\, u_-(x,z;\omega) \end{bmatrix} \right) d(\omega^2).$$

The functions $w_i(x,z;\lambda)$ in the generalized eigenfunction expansions include scattering states and guided modes for the slab, in other words, Helmholtz fields with the behavior (15,16). A rigorous development of a generalized Fourier transform in terms of generalized eigenfunctions that concretely realizes the spectral resolution E_λ through a unitary transformation is not given here. For specific related problems, the reader is referred to Theorem 4.1 of Goldstein [27] for infinite cylindrical scatterers, Theorem 8.5 of Wilcox [90] for diffraction gratings, and Theorem 3 of Groves [29] for an obstacle in a closed waveguide.

The treatment of scattering and resonance in this Chapter will remain in the frequency domain, that is, we study scattering of time-harmonic fields. The theory of scattering of general finite-energy disturbances for a diffraction grating is treated rigorously in [90]; other references on scattering theory include Lax and Phillips [48], Barut [7], Reed and Simon [75], and Newton [64].

The consideration of scattering of time-harmonic fields by a slab may begin with a field produced by a single harmonic monopole source off the guide, in other words, a fundamental solution of the Helmholtz equation, in the presence of the scatterer. One must determine from physical principles an appropriate radiation condition that makes the solution unique. Typically, this condition is obtained by means of the *principle of limiting absorption*, by which one begins with the unique finite-energy solution in a lossy ambient space and passes to the limit of vanishing loss (see [16, 88]). For scalar waves and a bounded obstacle in space, the condition is known as the "Sommerfeld radiation condition",

$$\lim_{r\to\infty} r\left(\tfrac{\partial u}{\partial r} - iku\right) = 0.$$

In the two-dimensional case, the factor of r is replaced by $\sqrt{r}$. For the Maxwell system, the same condition applies to all components of the electromagnetic field, and the additional conditions of Silver-Müller on the orthogonality of E, H, and the radial vector at the far field, are also satisfied [61, 62].

For unbounded scatterers, the Sommerfeld condition does not apply in general. This is because energy can be radiated not only into free space but also along the scatterer in the form of guided modes, which are excited by the evanescent waves emanating from the source. The contribution of the guided modes in addition to the scattering states appears in the radiating fundamental solution, which can then be used to derive the correct radiation condition for general sources. For the case of an impedance plane, the fundamental solution and radiation condition are treated rigorously by Nosich; see equations 20 and 24 in [66]. Equation 2 in the same reference gives the radiation condition for a closed waveguide, which is analogous to Condition 1. There is large body of literature on scattering by open waveguides and resonators, including discussions of radiation conditions; see, for example, [65, 78, 87].

Because our slab structure is invariant under the action of the group $2\pi\mathbb{Z}^2$ of transformations of $\mathbb{R}^3$ in the x-variables, the operator

$$S = \nabla^\dagger\nabla = -\varepsilon^{-1}\nabla\cdot\mu^{-1}\nabla \tag{27}$$

can be decomposed into components that act on pseudo-periodic functions. This is accomplished through the *Floquet transform*, by which a function on $\mathbb{R}^3$ is expressed as an integral superposition of pseudo-periodic functions. It is defined by

$$(\mathscr{F}u)(x,z;\kappa) = \sum_{n\in\mathbb{Z}^2} u(x+2\pi n, z)e^{-2\pi i\kappa\cdot n}.$$

For each κ, $\mathscr{F}u$ is doubly pseudo-periodic in x with fundamental domain $W\times\mathbb{R}$, $W=[0,2\pi)^2$, and Bloch wavevector κ. It is also periodic in κ with fundamental domain equal to the first Brillouin zone B. The function $u(x,z)$ is reconstructed from its Floquet transform through

$$u(x,z) = \int_B (\mathscr{F}u)(x,z;\kappa)\,d\kappa.$$

The Floquet transform is unitary in L^2,

$$\int_{\mathbb{R}^3} |u(x,z)|^2 dV = \int_{W\times\mathbb{R}}\int_B |(\mathscr{F}u)(x,z;\kappa)|^2 dA\,dV,$$

and it commutes with S in the sense that

$$(\mathscr{F}Su)(x,z;\kappa) = S_\kappa((\mathscr{F}u)(x,z;\kappa)),$$

where S_κ is essentially the restriction of S to pseudo-periodic functions and will be defined precisely in the next section. The solutions to the scattering Problem 2 are generalized eigenfunctions of S_κ.

The family $\{S_\kappa\}_{\kappa\in B}$ provides an integral decomposition of S,

$$S = \int_B^{\oplus} S_\kappa \, d\kappa. \tag{28}$$

Direct integrals of operators such as this one are treated in §XIII.16 of [73], and more on application of the Floquet transform to waves in periodic structures can be found in [43] and references therein.

3 Plane-wave scattering and guided modes

Because of the decomposition (28), solutions of the Helmholtz equation are integral superpositions of pseudo-periodic solutions, which we will investigate in the remainder of this Chapter. Specifically, we consider the problems of plane-wave scattering and guided modes, which are the inhomogeneous and homogeneous ($u^{\text{inc}} = 0$) versions of the same Problem 2. The existence of a guided mode at (κ, ω) is equivalent to the nonuniqueness of solutions (for $\mathscr{Z}_\ell = \emptyset$).

3.1 Spectrum for a periodic slab

We may restrict analysis to one period in $\mathbb{R}^3$ of the functions ε and μ, which is the strip

$$\mathscr{S} = \{(x,z) \in \mathbb{R}^3 : x \in (0, 2\pi)^2\}. \tag{29}$$

If ε or μ has a jump discontinuity along a surface Σ with normal vector n, the Helmholtz equation (2) must be supplemented by matching conditions

$$u \text{ and } \mu^{-1}\frac{\partial u}{\partial n} \text{ are continuous on } \Sigma. \tag{30}$$

By passing to a weak form of the equation, ε and μ are only required to be measurable, u is only required to have weak L^2 derivatives, and the matching conditions and pseudo-periodicity are automatically imposed. For this, we introduce the functional spaces[2]

$$H^1_{\kappa,\text{loc}}(\mathscr{S}) = \{u \in H^1_{\text{loc}}(\mathscr{S}) : u(x_1, 2\pi, z) = e^{2\pi i\kappa_2} u(x_1, 0, z), u(2\pi, x_2, z) = e^{2\pi i\kappa_1} u(0, x_2, z)\}, \tag{31}$$

in which the boundary values of u are understood in the sense of the usual trace of H^1 functions, and

$$H^1_\kappa(\mathscr{S}) = H^1_{\kappa,\text{loc}}(\mathscr{S}) \cap H^1(\mathscr{S}). \tag{32}$$

The pseudo-periodic scattering problem in weak form is as follows, where $C^\infty_{0,\kappa}(\mathscr{S})$ is the space of infinitely differentiable functions with compact support in the closure of $\mathscr{S}$ and that satisfy the same pseudo-periodic condition as the functions in $H^1_{\kappa,\text{loc}}(\mathscr{S})$.

Problem 3 (Scattering, weak form 1) *Find a function $u \in H^1_{\kappa,\text{loc}}(\mathscr{S})$ such that*

$$\int_{\mathscr{S}} (\mu^{-1}\nabla u \cdot \nabla \bar{v} - \omega^2 \varepsilon u \bar{v}) dV = 0 \;\; \forall v \in C^\infty_{0,\kappa}(\mathscr{S})$$

and

$$u(x,z) = u^{inc}(x,z) + u^{sc}(x,z),$$

where u^{inc} is a sum of plane waves as in Problem 2 and u^{sc} satisfies the radiation Condition 1.

[2] $H^1_{\text{loc}}(\mathscr{S})$ denotes the subspace of locally L^2 functions on $\mathscr{S}$ with locally L^2 weak gradients, and $H^1(\mathscr{S})$ denotes the Hilbert space of functions $u \in H^1_{\text{loc}}(\mathscr{S})$ for which the norm $\|u\|_{H^1} = (\int_{\mathscr{S}} (|u|^2 + |\nabla u|^2))^{\frac{1}{2}}$ is finite.

It can be shown that this is equivalent to the strong form of the scattering Problem 2 if all functions involved are smooth.

A useful functional-analytic framework for Problem 3 is the Hilbert space $L^2(\mathscr{S},\varepsilon dV)$ of square-Lebesgue-integrable complex-valued functions in the strip with inner product

$$b(u,v) = \int_{\mathscr{S}} \varepsilon\, u\bar{v}\, dV \tag{33}$$

and the unbounded symmetric nonnegative quadratic form in $L^2(\mathscr{S},\varepsilon dV)$, with form domain $H^1_\kappa(\mathscr{S})$, defined by

$$a(u,v) := \int_{\mathscr{S}} \mu^{-1}\nabla u\cdot\nabla\bar{v}\, dV,\;\; u,v\in H^1_\kappa(\mathscr{S}). \tag{34}$$

This form is closed, and the associated positive operator S_κ is given by[3]

$$S_\kappa u = -\varepsilon^{-1}\nabla\cdot\mu^{-1}\nabla u, \quad u\in\mathscr{D}(S_\kappa)\subset H^1_\kappa(\mathscr{S}). \tag{35}$$

Of course, there is a close relationship between the spectrum $\sigma(S_\kappa)$ of S_κ and the harmonic Bloch states of the slab. An eigenfunction of S_κ is a nontrivial function in $H^1_\kappa(\mathscr{S})$ that satisfies the Helmholtz equation; it can be extended to a pseudo-periodic solution in $\mathbb{R}^3$. By the general form (15,16), the coefficients of all propagating and linear harmonics must vanish, and the field is therefore a guided mode. The continuous spectrum corresponds to scattering states.

The spectrum of S_κ is characterized in part by the min-max principle (see [73], Ch. XIII, or [89], for example). The sequence $\{\lambda_j(\kappa)\}_{j=1}^\infty$ defined by

$$\lambda_j(\kappa) = \sup_{V^{j-1}<L^2(\mathscr{S})} \inf_{\substack{u\in(V^{j-1})^\perp\setminus\{0\}\\ u\in H^1_\kappa(\mathscr{S})}} \frac{a(u,u)}{b(u,u)}, \tag{36}$$

in which the supremum is taken over all $(j-1)$-dimensional subspaces, is nondecreasing, and converges to the infimum λ_- of the essential spectrum of S_κ. If $\lambda_n\neq\lambda_-$, then λ_n is the n^{th} eigenvalue of S_κ, counting from the bottom and including multiplicity. In fact, as we expect, we will see that $\lambda_- = |\kappa|^2/(\varepsilon_0\mu_0)$, $\lambda_1 > |\kappa|^2/(\varepsilon_+\mu_+)$, and there are only finitely many eigenvalues below the essential spectrum.

Much of the analysis in sections 3.1 and 3.2 is adapted from the work of Bonnet-Bendhia and Starling [8]. We include proofs for completeness and consistency within the present framework.

Theorem 4 (spectrum) *The essential spectrum of S_κ, for $\kappa\in B$, consists of all $\lambda=\omega^2$, where ω is above the light cone for the medium exterior to the slab; there are only finitely many eigenvalues below the essential spectrum. Precisely,*

1. $\sigma(S_\kappa)\subset[\frac{|\kappa|^2}{\varepsilon_+\mu_+},\infty)$;
2. $\sigma_{ess}(S_\kappa) = [\frac{|\kappa|^2}{\varepsilon_0\mu_0},\infty)$;
3. *there are only finitely many eigenvalues λ_j strictly less than $\frac{|\kappa|^2}{\varepsilon_0\mu_0}$.*

Proof. 1. Each $u\in H^1_\kappa(\mathscr{S})$ admits the Fourier series

$$u(x,z) = \sum_{m\in\mathbb{Z}^2} u_m(z)e^{i(m+\kappa)\cdot x}, \tag{37}$$

from which we obtain

$$\int_{\mathscr{S}} |u|^2 = 4\pi^2\int_{\mathbb{R}}\sum_{m\in\mathbb{Z}^2}|u_m(z)|^2\,dz,$$

$$\int_{\mathscr{S}} |\nabla_x u|^2 = 4\pi^2\int_{\mathbb{R}}\sum_{m\in\mathbb{Z}^2}|m+\kappa|^2|u_m(z)|^2\,dz.$$

[3]The operator $-\varepsilon^{-1}\nabla\cdot\mu^{-1} : \mathscr{D}(\varepsilon^{-1}\nabla\cdot\mu^{-1})\subset L^2(\mathscr{S},\mathbb{C}^3,\mu^{-1}dV)\to L^2(\mathscr{S},\mathbb{C},\varepsilon dV)$ is the adjoint of $\nabla_0 : H^1_0(\mathscr{S})\subset L^2(\mathscr{S},\mathbb{C},\varepsilon dV)\to L^2(\mathscr{S},\mathbb{C}^3,\mu^{-1}dV)$, where $H^1_0(\mathscr{S})$ is the subspace of $H^1(\mathscr{S})$ with vanishing trace on $\partial\mathscr{S}$. ∇_0 is the restriction to $H^1_0(\mathscr{S})$ of the usual weak gradient operator ∇, and $\nabla\cdot$ is the usual weak divergence operator.

Since $|m+\kappa| \geq |\kappa|$ for $m \in \mathbb{Z}^2$ and $\kappa \in B$, we obtain

$$\int_{\mathscr{S}} \mu^{-1}|\nabla u|^2 \geq \mu_+^{-1} \int_{\mathscr{S}} |\nabla_x u|^2 \geq \frac{|\kappa|^2}{\varepsilon_+\mu_+} \int_{\mathscr{S}} \varepsilon |u|^2.$$

In view of (36), part (1) follows.

2. Let $\psi(z)$ be a smooth function on $\mathbb{R}$ with compact support that vanishes in $[z_-, z_+]$. If $\lambda \geq |\kappa|^2/(\varepsilon_0\mu_0)$, then $\eta^2 = \lambda\varepsilon_0\mu_0 - |\kappa|^2 \geq 0$, and one can verify that the functions

$$u^n(x,z) := n^{-\frac{1}{2}} \psi(z/n) e^{i(\eta z + \kappa\cdot x)}, \quad n \in \mathbb{N}_+,$$

are in $\mathscr{D}(S_\kappa)$ and are bounded from below in $L^2(\mathscr{S}, \varepsilon dV)$ uniformly in n and that

$$\varepsilon^{-1}\nabla\cdot\mu^{-1}\nabla u^n + \lambda u^n \to 0 \quad \text{as } n \to \infty$$

in $L^2(\mathscr{S}, \varepsilon dV)$. Conversely, for $\lambda \in \sigma_{ess}(S_\kappa)$, Weyl's criterion (Theorem 7.2 of [34]) provides a sequence u^n from $\mathscr{D}(S_\kappa)$ such that, in $L^2(\mathscr{S}, \varepsilon dV)$, u^n has norm 1 and tends weakly to 0 and $(S_\kappa - \lambda)u^n \to 0$ strongly. These conditions imply

$$\int_{\mathscr{S}} \mu^{-1}|\nabla u^n|^2 = \int_{\mathscr{S}} \varepsilon \bar{u}^n S_\kappa u^n \to \lambda,$$
$$\int_{\mathscr{S}\setminus\Omega} \varepsilon|u^n|^2 - \int_{\mathscr{S}} \varepsilon|u^n|^2 \to 0,$$

as $n \to \infty$, where Ω is defined below (41, Fig. 4), and, as in part (1), we have

$$\int_{\mathscr{S}} \mu^{-1}|\nabla u^n|^2 \geq \mu_0^{-1} \int_{\mathscr{S}\setminus\Omega} |\nabla_x u^n|^2 \geq \frac{|\kappa|^2}{\varepsilon_0\mu_0} \int_{\mathscr{S}\setminus\Omega} \varepsilon|u^n|^2.$$

We conclude that $\lambda \geq |\kappa|^2/(\varepsilon_0\mu_0)$.

3. We show below that $\lambda_j = \hat{\lambda}_j$ for $\lambda_j < |\kappa|^2/(\varepsilon_0\mu_0)$, where the $\hat{\lambda}_j$ arise from an equivalent formulation of the scattering problem in Ω and tend to infinity as $n \to \infty$. ■

The scattering Problem 3 can also be formulated in terms of the x-periodic part $\tilde{u}$ of the field $u(x,z) = \tilde{u}(x,z)e^{i\kappa\cdot x}$. The Helmholtz equation implies

$$(\nabla + i\kappa)\cdot\mu^{-1}(\nabla + i\kappa)\,\tilde{u} + \omega^2\varepsilon\,\tilde{u} = 0, \tag{38}$$

and its weak form is

$$\int_{\mathscr{S}} (\mu^{-1}(\nabla + i\kappa)\tilde{u}\cdot(\nabla - i\kappa)\bar{v} - \omega^2\varepsilon\,\tilde{u}\bar{v})dV = 0 \tag{39}$$

$\forall\, v \in C^\infty_{0,\mathrm{per}}(\mathscr{S})$ $(= C^\infty_{0,\kappa}(\mathscr{S})$ with $\kappa = 0)$, or, in expanded form,

$$\int_{\mathscr{S}} \mu^{-1}\big(\nabla\tilde{u}\cdot\nabla\bar{v} + i\kappa\cdot(\tilde{u}\nabla_x\bar{v} - \bar{v}\nabla_x\tilde{u}) + +(|\kappa|^2 - \omega^2\varepsilon\mu)\tilde{u}\bar{v}\big)dV = 0. \tag{40}$$

The relevant quadratic form in $H^1_{\mathrm{per}}(\mathscr{S})$ is

$$a_\kappa(u,v) = \int_{\mathscr{S}} \mu^{-1}\big(\nabla u\cdot\nabla\bar{v} + i\kappa\cdot(u\nabla_x\bar{v} - \bar{v}\nabla_x u) + |\kappa|^2 u\bar{v}\big)dV.$$

An equally important formulation of the scattering problem for a fixed pair (κ, ω) is obtained by truncating the strip $\mathscr{S}$ to a domain Ω finite length, outside of which $\varepsilon = \varepsilon_0$ and $\mu = \mu_0$ (Fig. 4),

$$\begin{gathered}\Omega = \{(x,z) \in \mathscr{S} : z_- < z < z_+\}, \\ \Gamma_\pm = \mathscr{S} \cap \{(x, z_\pm) : x \in \mathbb{R}^2\}, \\ \Gamma = \Gamma_- \cup \Gamma_+.\end{gathered} \tag{41}$$

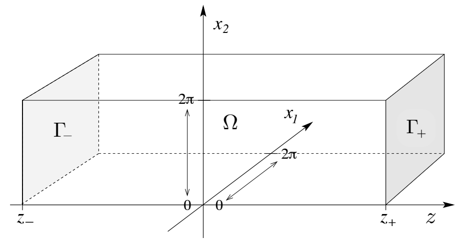

Figure 4: The domain Ω, comprising one truncated period of the functions ε and μ.

The normal vector n on Γ is taken to be directed out of Ω.

The radiation condition is enforced through a Dirichlet-to-Neumann operator $T = T^{\kappa,\omega}$ that characterizes radiating fields in the sense that, for pseudo-periodic Helmholtz fields u,

$$\partial_n u + Tu = 0 \text{ on } \Gamma \iff u \text{ is radiating.} \tag{42}$$

Technically, $T : H^{\frac{1}{2}}(\Gamma) \to H^{-\frac{1}{2}}(\Gamma)$ acts on traces on Γ of functions in $H^1_\kappa(\Omega)$ and is defined through the Fourier transform as follows. For any $f \in H^{\frac{1}{2}}(\Gamma)$, let $\hat{f}_m$ be the Fourier coefficients of $e^{-i\kappa\cdot x}f$; this is a pair of numbers $\hat{f}_m = (\hat{f}^-_m, \hat{f}^+_m)$, one giving the m^{th} pseudoperiodic Fourier component of f on Γ_- and the other on Γ_+,

$$f(x, z_\pm) = \sum_{m\in\mathbb{Z}^2} \hat{f}^\pm_m e^{i(m+\kappa)\cdot x}. \tag{43}$$

Then T is defined by

$$T : H^{\frac{1}{2}}(\Gamma) \to H^{-\frac{1}{2}}(\Gamma), \quad (\widehat{Tf})_m = -i\eta_m \hat{f}_m. \tag{44}$$

The operator T has a nonnegative real part T_r and a nonpositive imaginary part T_i:

$$T = T_r + iT_i, \tag{45}$$

$$(\widehat{T_r f})_m = \begin{cases} -i\eta_m \hat{f}_m & \text{if } m \in \mathscr{Z}_e, \\ 0 & \text{otherwise.} \end{cases} \tag{46}$$

$$(\widehat{T_i f})_m = \begin{cases} -\eta_m \hat{f}_m & \text{if } m \in \mathscr{Z}_p, \\ 0 & \text{otherwise.} \end{cases} \tag{47}$$

For each pair (κ, ω), define the sesquilinear forms in $H^1_\kappa(\Omega)$ (we suppress the dependence on κ),

$$\begin{aligned} \hat{a}^\omega(u,v) &= \int_\Omega \mu^{-1}\nabla u\cdot\nabla\bar{v} + \mu_0^{-1}\int_\Gamma (T^\omega u)\bar{v}, \\ \hat{a}^\omega_r(u,v) &= \int_\Omega \mu^{-1}\nabla u\cdot\nabla\bar{v} + \mu_0^{-1}\int_\Gamma (T^\omega_r u)\bar{v}, \\ \hat{a}^\omega_i(u,v) &= \mu_0^{-1}\int_\Gamma (T^\omega_i u)\bar{v}, \\ \hat{b}(u,v) &= \int_\Omega \varepsilon u\bar{v}. \end{aligned}$$

We have $\hat{a}^\omega = \hat{a}^\omega_r + i\hat{a}^\omega_i$. Define also the bounded conjugate-linear functional f^ω_Γ on $H^1_\kappa(\Omega)$,

$$f^\omega_\Gamma(v) = \mu_0^{-1}\int_\Gamma (\partial_n + T^\omega)u^{\text{inc}}\,\bar{v} \quad \forall v \in H^1_\kappa(\Omega).$$

The frequency dependence of T is exhibited because we will consider the problem for fixed κ, with ω^2 playing the role of an eigenvalue. Problem 3 is equivalent to the following one:

Problem 5 (Scattering, weak form 2) *Find a function $u \in H^1_\kappa(\Omega)$ such that*

$$\hat{a}^\omega(u,v) - \omega^2 \hat{b}(u,v) = f^\omega_\Gamma(v) \;\; \forall v \in H^1_\kappa(\Omega). \tag{48}$$

The equivalence of Problems 2, 3, and 5 is in the sense of the following Proposition, whose proof we leave to the reader. The space $H^1_{\kappa,\mathrm{loc}}(\mathbb{R}^3)$ consists of those functions in $H^1_{\mathrm{loc}}(\mathbb{R}^3)$ that are pseudo-periodic with Bloch wavevector κ.

Proposition 6 (Equivalence of problems) *If $u \in H^1_{\kappa,\mathrm{loc}}(\mathbb{R}^3)$ solves Problem 2, then $u|_{\mathscr{S}}$ solves Problem 3 and $u|_\Omega$ solves Problem 5. If $u \in H^1_\kappa(\Omega)$ solves Problem 5, then there exists a unique extension $\tilde{u} \in H^1_{\kappa,\mathrm{loc}}(\mathbb{R}^3)$ of u that solves Problem 2.*

The scattering problem in the form of Problem 5 can be generalized to include harmonic pseudo-periodic source fields originating from sources interior to and exterior to Ω; these sources are realized by generalizing the right-hand side of (48) to an arbitrary element of the conjugate dual of $H^1_\kappa(\Omega)$.

Now, a guided mode of the slab for the pair (κ,ω) (with $\mathscr{Z}_\ell = \emptyset$) is the extension to $\mathbb{R}^3$ of a nontrivial solution to Problem 5 in the absence of a source field, that is, a function $u \in H^1_\kappa(\Omega)$ that satisfies the nonlinear eigenvalue problem

$$\hat{a}^\omega(u,v) - \omega^2 \hat{b}(u,v) = 0 \quad \forall v \in H^1_\kappa(\Omega). \tag{49}$$

The form $\hat{a}^\omega$ is not real if ω lies above the cutoff frequency, or if $\omega^2 > |\kappa|^2/(\varepsilon_0\mu_0)$ because of the presence of propagating spatial harmonics for the pair (κ,ω). Because $\hat{a}^\omega_i$ is definite in sign, the condition (49) is equivalent to a pair of conditions; this is straightforward to prove.

Proposition 7 (Real eigenvalues) *If $\omega^2 \in \mathbb{R}$, then a function $u \in H^1_\kappa(\Omega)$ satisfies the homogeneous problem* (49) *if and only if it satisfies the equation*

$$\hat{a}^\omega_r(u,v) - i\hat{a}^\omega_i(u,v) - \omega^2 \hat{b}(u,v) = 0 \;\; \forall v \in H^1_\kappa(\Omega) \tag{50}$$

and if and only if it satisfies the pair

$$\begin{aligned} &\hat{a}^\omega_r(u,v) - \omega^2 \hat{b}(u,v) = 0 \;\; \forall v \in H^1_\kappa(\Omega), \\ &(\widehat{u|_\Gamma})_m = 0 \;\; \forall m \in \mathscr{Z}_p. \end{aligned} \tag{51}$$

The solutions u of the first condition in (51) are of the form (15,16), in which the normal derivatives of all the propagating harmonics vanish on Γ. The second condition requires that the propagating harmonics vanish altogether, leaving only those that are linear or evanescent. In the case that all η_m are nonzero, the field u is exponentially confined to the slab waveguide and is a true guided mode.

By means of the min-max principle applied to the real form $\hat{a}^\omega_r$, one obtains a sequence of frequencies $\{\omega_j\}$ that subsumes the frequencies of the guided modes. This is proved in the next theorem. We denote the set of square frequencies of the guided modes by $\hat{\lambda}_j$:

$$\{(\hat{\lambda}_j)^{\frac{1}{2}}\}_{j=1}^N \;:\; \text{guided-mode frequencies},$$

in which N may be ∞. Because of Proposition 6, the values $\hat{\lambda}_j$ that lie below $|\kappa|^2/(\varepsilon_0\mu_0)$ coincide with the eigenvalues λ_j:

$$\hat{\lambda}_j = \lambda_j \;\;\text{for}\;\; \lambda_j < |\kappa|^2/(\varepsilon_0\mu_0).$$

Theorem 8 (Guided-mode frequencies) *Given $\kappa \in B$, the frequencies ω for which the equation $\hat{a}^\omega_r(u,\cdot) - \omega^2\hat{b}(u,\cdot) = 0$ admits a nontrivial solution $u \in H^1_\kappa(\Omega)$ are the elements of a nondecreasing sequence $\{\omega_j\}_{j=1}^\infty$ of positive numbers that tends to ∞ and their additive inverses. The nonnegative frequencies for which the slab admits a guided mode with Bloch wavevector κ is a subset of this family that includes all ω_j less than $|\kappa|/\sqrt{\varepsilon_0\mu_0}$.*

Proof. For a fixed value of $\omega > 0$, the set of numbers α for which $\hat{a}_r^\omega(u,\cdot) - \alpha\hat{b}(u,\cdot) = 0$ admits a nontrivial solution is a nondecreasing nonnegative sequence $\alpha_j(\omega)$. This is seen as follows. Since $\hat{a}_r^\omega$ and $\hat{b}$ are bounded forms in $H^1_\kappa(\Omega)$, there exist linear operators A_r^ω and B from $H^1_\kappa(\Omega)$ to itself defined through

$$(A_r^\omega u, v) = \hat{a}_r^\omega(u,v) + \hat{b}(u,v),$$
$$(Bu,v) = \hat{b}(u,v).$$

The operator A_r^ω is bijective with bounded inverse because $\hat{a}_r^\omega + \hat{b}$ is coercive:

$$\hat{a}_r^\omega(u,u) + \hat{b}(u,u) \geq \mu_+^{-1}\int_\Omega |\nabla u|^2 + \varepsilon_-\int_\Omega |u|^2 \geq \min\{\mu_+^{-1}, \varepsilon_-\}\|u\|^2_{H^1_\kappa(\Omega)}.$$

The operator B is compact because of the compact embedding of $H^1_\kappa(\Omega)$ into $L^2(\Omega)$. Therefore the set of α that admit a nontrivial solution to $(A_r^\omega - (\alpha+1)B)u = 0$ is a sequence converging to infinity. That the α_j must be positive is seen through their construction by the min-max principle,

$$\alpha_j(\omega) = \sup_{V^{j-1} < L^2(\Omega)} \inf_{\substack{u \in (V^{j-1})^\perp \setminus \{0\} \\ u \in H^1_\kappa(\Omega)}} \frac{\hat{a}_r^\omega(u,u)}{\hat{b}(u,u)}. \tag{52}$$

One shows that each α_j is a nonincreasing continuous function of ω (details can be found in the proof of Theorem 3.3 of [8]). Therefore, for each $j = 1,2,\dots$, there is exactly one number $\omega_j \geq 0$ such that $\alpha_j(\omega_j) = \omega_j^2$, and the sequence $\{\omega_j\}_{j=1}^\infty$ tends to infinity. These are the values of ω for which $\hat{a}_r^\omega(u,\cdot) - \omega^2\hat{b}(u,\cdot) = 0$ admits a nontrivial solution.

By the characterization (49) of guided modes and Proposition 7, the set of guided mode frequencies $\{(\hat{\lambda}_j)^{\frac{1}{2}}\}_{j=1}^N$ is a subset of $\{\omega_j\}_{j=1}^\infty$. If $\omega_j < |\kappa|/\sqrt{\varepsilon_0\mu_0}$, then $\hat{a}^{\omega_j} = \hat{a}_r^{\omega_j}$, and, as (κ,ω_j) admits only evanescent harmonics, ω_j is a guided-mode frequency. ■

The existence of guided modes is treated in the next subsection. What we can say at this point is that, because the eigenvalues $\hat{\lambda}_j$ tend to infinity, their multiplicities must be finite. If a real pair (κ,ω) admits a guided mode, then any solution to the scattering problem is not unique because the addition of a guided mode results in another solution. For plane-wave sources there always exists a solution ([8]). This will turn out to be important in calculating the leading-order resonant amplitude enhancement in Sec. 5.5.

Theorem 9 (Existence of scattered fields) *Problem 5 has a solution, and the space of solutions is finite-dimensional.*

Proof. Rewrite (48) in the following way:

$$\hat{a}^\omega(u,v) + \hat{b}(u,v) - (\omega^2+1)\hat{b}(u,v) = f_\Gamma^\omega(v). \tag{53}$$

As in the proof of Theorem 8, we may define the linear operators A^ω and C^ω from $H^1_\kappa(\Omega)$ into itself, as well as an element $\tilde{f} \in H^1_\kappa(\Omega)$ through

$$(A^\omega u, v) = \hat{a}^\omega(u,v) + \hat{b}(u,v),$$
$$(C^\omega u, v) = -(\omega^2+1)\hat{b}(u,v),$$
$$(\tilde{f}, v) = f(v).$$

Now (53) takes the form

$$(A^\omega + C^\omega)u = \tilde{f}. \tag{54}$$

The operator C^ω is compact, and A^ω is bijective with a bounded inverse because $\hat{a}^\omega + \hat{b}$ is coercive: As we have shown,

$$\mathrm{Re}\,(\hat{a}^\omega(u,u) + \hat{b}(u,u)) \geq \min\{\mu_+^{-1}, \varepsilon_-\}\|u\|^2_{H^1_\kappa(\Omega)}.$$

By the Fredholm alternative, (54) has a solution if and only if $(\tilde{f}, v) = 0$ for all $v \in \mathrm{Null}(A^\omega + C^\omega)^\dagger$, that is, for all v that satisfy

$$(w, (A^\omega + C^\omega)^\dagger v) = 0 \;\; \forall w \in H^1_\kappa(\Omega). \tag{55}$$

By using the relation

$$(w,(A^{\omega}+C^{\omega})^{\dagger}v)=\hat{a}_r^{\omega}(w,v)+i\hat{a}_i^{\omega}(w,v)-\omega^2\hat{b}(w,v),$$

(55) becomes

$$\hat{a}_r^{\omega}(v,w)-i\hat{a}_i^{\omega}(v,w)-\omega^2\hat{b}(v,w)=0$$

for all $w\in H^1_\kappa(\Omega)$. By Proposition 7, the propagating harmonics of such a function v vanish on Γ, and therefore, by the definitions of $\tilde{f}$ and f^{ω}_{Γ}, $(\tilde{f},v)$ vanishes.

The space of solutions is finite-dimensional because A^{ω} is invertible and C^{ω} is compact. ■

3.2 Guided modes

We turn to proving (mathematical) existence of isolated and embedded guided-mode frequencies, as well as the the nonexistence of guided modes in certain structures for which $\varepsilon(x,z)\le\varepsilon_0$ and $\mu(x,z)\le\mu_0$. An example of the latter is an infinite homogeneous ceramic matrix in which a "slab" is created by a doubly periodic array of air holes.

At the end of this section, we will indicate a variety of related results in the literature, especially on guided modes on periodic surfaces and trapped modes in closed waveguides containing an obstacle.

3.2.1 Existence and nonexistence

The following Theorem is adapted from Theorems 4.3 and 4.4 of [8]. It guarantees the existence of guided modes below the cutoff frequency for any $\kappa\in B$. If $\mu=\mu_0$, the converse of part (1) is also true. Let $\mathscr{N}(\kappa)$ be the number of eigenvalues λ_j less than $|\kappa|^2/(\varepsilon_0\mu_0)$.

Theorem 10 (Existence of guided modes)

1. If $\varepsilon\mu>\varepsilon_0\mu_0$ on a set of positive measure and

$$\int_{\mathscr{S}}\left(\frac{\varepsilon}{\varepsilon_0}-\frac{\mu_0}{\mu}\right)dV\ge 0, \tag{56}$$

then, for all $\kappa\in B\setminus\{0\}$, $\mathscr{N}(\kappa)\ge 1$, that is, there exists a guided mode at a frequency below $|\kappa|/\sqrt{\varepsilon_0\mu_0}$.

2. Let K be an open set in S, and let $\{\beta_j\}_{j=1}^{\infty}$ be the spectrum of the Dirichlet Laplacian in K ($-\nabla^2$ with $u=0$ on ∂K). If $\kappa\in B\setminus\{0\}$ and $\varepsilon>\varepsilon_*$, $\mu>\mu_*$ on K, with $\varepsilon_*\mu_*>\beta_j\frac{\varepsilon_0\mu_0}{|\kappa|^2}$, then $\mathscr{N}(\kappa)\ge j$, that is, there are at least j independent guided modes with Bloch wavevector κ and frequency below $|\kappa|/\sqrt{\varepsilon_0\mu_0}$.

Proof. We adapt the arguments of [8].

1. Set $H_0=\max\{|z_-|,|z_+|\}$, and define, for $H>H_0$,

$$u^H(x,z)=\begin{cases}1 & \text{if } |z|<H,\\ \frac{2H-|z|}{H} & \text{if } H<|z|<2H,\\ 0 & \text{if } |z|>2H,\end{cases}$$

on $\mathscr{S}$. By the assumption that $\varepsilon\mu>\varepsilon_0\mu_0$ on a set of positive measure, there exists a real-valued test function $w\in C^{\infty}_{0,\mathrm{per}}(\mathscr{S})$ with support in $|z|<H_0$ such that

$$\int_{\mathscr{S}}\left(\frac{\mu_0}{\mu}-\frac{\varepsilon}{\varepsilon_0}\right)w\,dV\;<\;0. \tag{57}$$

From the definition of a_κ, if u is real-valued,

$$a_\kappa(u,u)=\int\mu^{-1}[|\nabla u|^2+|\kappa|^2|u|^2].$$

Let α be an arbitrary real number, and define

$$w^H_\alpha=u^H+\alpha w, \tag{58}$$

which is real-valued on $\mathscr{S}$. Thus

$$\frac{a_\kappa(w_\alpha^H,w_\alpha^H)}{\int \varepsilon(w_\alpha^H)^2} - \frac{|\kappa|^2}{\varepsilon_0\mu_0} = \frac{1}{\int \varepsilon(w_\alpha^H)^2}\left[\frac{8\pi^2}{\mu_0 H} + \alpha^2\int \mu^{-1}|\nabla w|^2 + + \frac{|\kappa|^2}{\mu_0}\int\left(\frac{\mu_0}{\mu} - \frac{\varepsilon}{\varepsilon_0}\right)(1+2\alpha w+\alpha^2 w^2)\right].$$

In the case of strict inequality in (56), this expression is negative for $\alpha = 0$ and sufficiently large H. In the case of equality, the expression is negative for sufficiently small nonzero α and sufficiently large H.

2. If $u \in H^1_\kappa(\mathscr{S})$ has support in the closure of K, then

$$\frac{\int \mu^{-1}|\nabla u|^2}{\int \varepsilon |u|^2} \le \frac{1}{\varepsilon_* \mu_*}\frac{\int_K |\nabla u|^2}{\int_K |u|^2}.$$

Since each function $u \in H^1_0(K)$ is extensible to a function in $H^1_\kappa(\Omega)$, this inequality, together with the min-max principle for $\{\lambda_j\}$ and $\{\beta_j\}$ imply

$$\lambda_j(\kappa) \le \frac{1}{\varepsilon_*\mu_*}\beta_j.$$

As long as $\varepsilon_*\mu_* > \beta_j \frac{\varepsilon_0\mu_0}{|\kappa|^2}$, we obtain $\lambda_j(\kappa) \le \frac{|\kappa|^2}{\varepsilon_0\mu_0}$. ∎

Theorem 11 states that there are continuous dispersion relations for robust guided modes. The condition $\varepsilon\mu \ge \varepsilon_0\mu_0$ can be eliminated if $\mu = \mu_0$.

Theorem 11 (Dispersion relations)

1. The eigenvalues $\lambda_j(\kappa)$ are continuous functions of $\kappa \in B$.

2. If $\varepsilon\mu \ge \varepsilon_0\mu_0$, then, for each unit vector $\hat{\kappa} \in \mathbb{R}^2$, the functions $\lambda_j(s\hat{\kappa}) - \frac{s^2}{\varepsilon_0\mu_0}$ are nonincreasing in s for $s\hat{\kappa} \in B$, and therefore $\mathscr{N}(s\hat{\kappa})$ is nondecreasing.

Proof. The proof follows [8]. For part (1), assume that $\int_{\mathscr{S}} |u|^2 = 1$, and, for arbitrary κ^1 and κ^2 in B, consider the difference

$$a_{\kappa^1}(u,u) - a_{\kappa^2}(u,u) = 2(\kappa^1-\kappa^2)\cdot\int_{\mathscr{S}} \mu^{-1}\mathrm{Im}\,\bar{u}\nabla_x u\, dV + +(|\kappa^1|^2 - |\kappa^2|^2)\int_{\mathscr{S}} \mu^{-1}|u|^2\, dV,$$

which yields

$$|a_{\kappa^1}(u,u) - a_{\kappa^2}(u,u)| \le |\kappa^1-\kappa^2|\frac{2}{\mu_-}\left[\left(\textstyle\int_{\mathscr{S}} |\nabla_x u|^2\right)^{\frac12} + \max(|\kappa^1|,|\kappa^2|)\right]. \tag{59}$$

In order to replace the L^2-norm of $\nabla_x u$ with an expression involving a_{κ^2}, we use Young's inequality

$$|2\mathrm{Im}\,(\kappa\cdot\nabla u)\bar{u}| \le \tfrac12|\nabla_x u|^2 + 2|\kappa|^2|u|^2$$

to obtain the coercivity estimate

$$a_\kappa(u,u) + |\kappa|^2\int_{\mathscr{S}} \mu^{-1}|u|^2 \ge \int_{\mathscr{S}} \mu^{-1}(|\partial_z u|^2 + \tfrac12|\nabla_x u|^2).$$

Using this in the estimate (59) yields

$$a_{\kappa^1}(u,u) \le a_{\kappa^2}(u,u) + |\kappa^1-\kappa^2|\frac{2}{\mu_-}\left[\left(2\mu_+(a_{\kappa^2}(u,u) + \tfrac{|\kappa^2|^2}{\mu_-})\right)^{\frac12} + \max(|\kappa^1|,|\kappa^2|)\right].$$

This implies the inequality

$$\lambda_j(\kappa^1) \le \lambda_j(\kappa^2) + |\kappa^1-\kappa^2|\frac{2}{\mu_-}\left[\left(2\mu_+(\lambda_j(\kappa^2) + \tfrac{|\kappa^2|^2}{\mu_-})\right)^{\frac12} + \max(|\kappa^1|,|\kappa^2|)\right].$$

Using this and its analog with κ^1 and κ^2 interchanged, we obtain

$$\limsup_{\kappa^2\to\kappa^1}\lambda_j(\kappa^2) \le \lambda_j(\kappa^1) \le \liminf_{\kappa^2\to\kappa^1}\lambda_j(\kappa^2),$$

which implies continuity of λ_j at κ^1.

To prove part (2), assume again that $\int_{\mathscr{S}} |u|^2 = 1$ and observe that, since $\lambda_j \leq \frac{|\kappa|^2}{\varepsilon_0\mu_0}$ for $\kappa \in B$,

$$\lambda_j(\kappa) - \frac{|\kappa|^2}{\varepsilon_0\mu_0} = \sup\inf\min\left(\frac{a_\kappa(u,u) - |\kappa|^2\varepsilon_0^{-1}\mu_0^{-1}\int\varepsilon|u|^2dV}{\int\varepsilon|u|^2dV}, 0\right). \tag{60}$$

One computes that

$$a_\kappa(u,u) - \frac{|\kappa|^2}{\varepsilon_0\mu_0}\int_{\mathscr{S}}\varepsilon|u|^2dV = a|\kappa|^2 + b\cdot\kappa + c,$$

where

$$a = \int_{\mathscr{S}} \mu^{-1}(1 - \tfrac{\varepsilon\mu}{\varepsilon_0\mu_0})|u|^2\,dV \leq 0,$$
$$c = \int_{\mathscr{S}} \mu^{-1}|\nabla u|^2 \geq 0,$$

and this implies that

$$\min\left(a_\kappa(u,u) - |\kappa|^2\varepsilon_0^{-1}\mu_0^{-1}\int\varepsilon|u|^2dV, 0\right),$$

with $\kappa = s\hat{\kappa}$ is nonincreasing as a function of s as long as $s\hat{\kappa} \in B$. This, in turn, implies that

$$\lambda_j(s\hat{\kappa}) - \frac{s^2}{\varepsilon_0\mu_0} \tag{61}$$

is nonincreasing. ■

As we have discussed, real dispersion relations for guided modes in a (κ,ω) region of $\mathbb{R}^3$ that admits at least one propagating spatial harmonic typically do not exist. Instead, the imaginary part of the frequency corresponding to κ vanishes only for isolated real values of κ, giving rise to isolated real pairs in (κ,ω)-space that admit guided modes. At these isolated pairs, the frequency, wavevector, and structure are in such a relation that all propagating harmonics of the solutions u of the first equation in (51) vanish, that is, the second condition in (51) is satisfied. This situation occurs, for example, if the the structure has symmetry about a plane transverse to the waveguide and $\kappa_1 = 0$ or $\kappa_2 = 0$; this is treated in [82].

Theorem 12 (Embedded eigenvalues)
If $\kappa = (0,\kappa_2)$ (resp. $\kappa = (\kappa_1, 0)$) is in the interior of B, then there exist functions $\varepsilon(x,z)$ and $\mu(x,z)$ that are symmetric about the x_2z-plane (resp. the x_1z-plane) that admit a guided-mode frequency above the cutoff frequency $|\kappa|/\sqrt{\varepsilon_0\mu_0}$.

Proof. We give a sketch of the proof. If $\varepsilon(x)$ and $\mu(x)$ are symmetric about the x_2z-plane and $\kappa = (0,\kappa_2)$, then the symmetric part $H_\kappa^{1\,\mathrm{sym}}(\Omega)$ and antisymmetric part $H_\kappa^{1\,\mathrm{ant}}(\Omega)$ of $H_\kappa^1(\Omega)$ with respect to the x_2z-plane are orthogonal with respect to $\hat{a}^\omega$ and $\hat{b}^\omega$. Thus a function that is antisymmetric about the x_2z-plane and satisfies $\hat{a}^\omega(u,v) - \omega^2\hat{b}(u,v) = 0$ for all $v \in H_\kappa^{1\,\mathrm{ant}}(\Omega)$ also satisfies the equation for all $v \in H_\kappa^1(\Omega)$. The frequencies of antisymmetric modes are therefore a subset of a sequence $\{\omega_j^{ant}\}_{j=1}^\infty$ defined in analogy to the ω_j in Theorem 8 by restricting the evaluation of the forms in the Rayleigh quotient (52) to functions in $H_\kappa^{1\,\mathrm{ant}}(\Omega)$. By making ε_+ and/or μ_+ large enough, at least one of the ω_j^{ant} can be adjusted so that

$$0 < \varepsilon_0\mu_0(\omega_j^{ant})^2 - \kappa_2^2 < 1$$

and $\mathscr{Z}_\ell = \emptyset$. In this regime, there is at least one propagating spatial harmonic and all of them have $m = (0,m_2)$. Since all harmonics with $\kappa_1 = m_1 = 0$ are symmetric about the x_2z-plane and the corresponding field that satisfies $\hat{a}_r^\omega(u,v) - (\omega_j^{ant})^2\hat{b}(u,v) = 0$ for all $v \in H_\kappa^1(\Omega)$ is antisymmetric, the coefficients of these harmonics for u must vanish and u is therefore a guided mode. ■

The existence of these antisymmetric guided modes with zero Bloch wavenumber in the variable of structural symmetry can also be proved using a harmonic Lippmann-Schwinger equation [81]. Embedded eigenvalues at nonzero wavenumber are constructed in the two-dimensional case for periodic slabs with metal inclusions [8], and analogous results are obtained for a two-dimensional lattice model [70].

Theorem 13 (Nonexistence of guided modes) *Let ω and κ be real, and let one of the following conditions be satisfied:*

1. In Ω, $\varepsilon_- < \varepsilon(x,z) \le \varepsilon_0$ and $\mu_- < \mu(x,z) \le \mu_0$, and

$$L(\omega^2\varepsilon_0\mu_0 - |\kappa|^2)^{1/2} < \pi \ \text{if } \mathscr{Z}_p \neq \emptyset; \tag{62}$$

2. There is a real number z_0 such that $\varepsilon(x,z_0+z)$, $\varepsilon(x,z_0-z)$, $\mu(x,z_0+z)$, and $\mu(x,z_0-z)$ are nondecreasing functions of z for all $x \in \mathbb{R}^2$.

Then there exists no function $u \in H^1_\kappa(\Omega)$ for which (49) *holds. This means that the periodic slab structure admits no guided modes at the pair (κ,ω).*

Condition (62) imposes no restriction on the width of the slab if there are no propagating spatial harmonics for the parameters ω, κ, ε_0, and μ_0. Otherwise, the restriction is interpreted as demanding that the width be less than half the wavelength in the direction perpendicular to the slab of the spatial harmonic whose propagation direction is closest to the normal ($m = 0$), and, in fact, less than half that of all propagating spatial harmonics. Thus the restriction becomes more severe as the frequency increases. Whether this or some weaker restriction is necessary for the prohibition of guided modes is an open question.

Proof. Following Shipman and Volkov [82], we take a different approach to making the form $a(u,v)$ real. Instead of eliminating its imaginary part, we restrict the form to a subspace $X \subset H^1_\kappa(\Omega)$ on which the imaginary part vanishes,

$$u \in X \iff \int_{\Gamma_\pm} u(x,z)e^{-i(m+\kappa)x}dA = 0 \ \ \forall m \notin \mathscr{Z}_e.$$

In other words, the nonevanescent spatial harmonics must vanish on Γ_- and Γ_+, a condition we know must be satisfied for guided modes. The form a is closed on its domain X, and $a(u,u) \ge 0$ for $u \in X$.

Suppose that $u \in X$ satisfies

$$\hat{a}^\omega(u,v) - \omega^2\hat{b}(u,v) = 0 \tag{63}$$

for all $v \in X$. In order that u be extensible to a solution of the Helmholtz equation in the strip $\mathscr{S}$, it must satisfy (63) for all $v \in H^1_\kappa(\Omega)$, or (49). (This amounts to a finite number of additional constraints, given by taking, say, $v = ze^{i(m+\kappa)x}$ and $v = (L-z)e^{i(m+\kappa)x}$ for each $m \notin \mathscr{Z}_e$, and is equivalent to setting the nonevanescent spatial harmonics of $\partial_n u$ equal to zero on $\Gamma_\pm$ when the normal derivative exists.)

Let us fix ω and κ and turn to the problem of finding the numbers γ for which there exists a nontrivial function $u \in X$ such that

$$\hat{a}^\omega(u,v) - \gamma\hat{b}(u,v) = 0 \ \ \forall v \in X. \tag{64}$$

These nonnegative numbers $\gamma = \gamma_j^{\kappa,\omega}(\varepsilon,\mu)$ are given by the min-max expression (52), but with the infimum taken over $u \in X$. For the special choice of material coefficients $\varepsilon \equiv \varepsilon_0$ and $\mu \equiv \mu_0$, when the slab ceases to exist, they can be calculated explicitly.

Finding solutions to (64) with these constant coefficients amounts to solving

$$\Delta u + \gamma\varepsilon_0\mu_0 u = 0 \tag{65}$$

in Ω with pseudo-periodic conditions on the planes parallel to the z-axis and appropriate boundary conditions on the sides $\Gamma_\pm$. As $\gamma\varepsilon_0\mu_0$ is constant, it suffices to seek separable solutions

$$u(x,z) = e^{i(m+\kappa)x}u_1(z), \tag{66}$$

where u_1 is a combination of $e^{\pm i\nu z}$ with

$$|m+\kappa|^2 + \nu^2 = \gamma\varepsilon_0\mu_0. \tag{67}$$

For $m \in \mathscr{Z}_p \cup \mathscr{Z}_\ell$, $u \in X$ requires that $u_1(0) = u_1(L) = 0$, so that

$$u(x,z) = e^{i(m+\kappa)x}\sin(\nu z), \ \nu L = \pi j, \tag{68}$$

where $j \in \mathbb{N}_+$. Thus, we have a set of eigenvalues γ_{mj} of (64) given by

$$\gamma_{mj} = \frac{1}{\varepsilon_0\mu_0}\left(|m+\kappa|^2 + \left(\frac{\pi j}{L}\right)^2\right),\; m \notin \mathscr{Z}_e,\; j \in \mathbb{N}_+.$$

For $m \in \mathscr{Z}_e$, because of the term of $\hat{a}^\omega$ containing the Dirichlet-to-Neumann map T^ω, we have $u_1'(0) = \alpha_m u_1(0)$ and $u_1'(L) = -\alpha_m u_1(L)$, with $\alpha_m = -i\eta_m > 0$, and these conditions require that u_1 be oscillatory, or $\nu^2 > 0$ in (67). But $\eta_m^2 < 0$ in the equation $|m+\kappa|^2 + \eta_m^2 = \omega^2\varepsilon_0\mu_0$, and we infer that $\gamma > \omega^2$.

From this we see that the lowest eigenvalue $\gamma_1^{\omega,\kappa}(\varepsilon_0,\mu_0)$ is greater than ω^2 if and only if either $\mathscr{Z}_p \cup \mathscr{Z}_\ell = \emptyset$ or $\mathscr{Z}_p \cup \mathscr{Z}_\ell \neq \emptyset$ and $\gamma_{01} > \omega^2$. This is equivalent to the condition

$$L(\omega^2\varepsilon_0\mu_0 - |\kappa|^2)^{1/2} < \pi \;\text{ if } \mathscr{Z}_p \cup \mathscr{Z}_\ell \neq \emptyset. \tag{69}$$

Now since $0 < \varepsilon(x,z) \leq \varepsilon_0$ and $0 < \mu(x,z) \leq \mu_0$ in Ω, the quotient $\hat{a}^\omega(u,u)/\hat{b}(u,u)$ with coefficients (ε,μ) is greater than or equal to the quotient with coefficients (ε_0,μ_0) so that

$$\gamma_1^{\kappa,\omega}(\varepsilon,\mu) \geq \gamma_1^{\kappa,\omega}(\varepsilon_0,\mu_0) > \omega^2.$$

Thus (63) is never satisfied for all $v \in X$, and therefore neither is (49) satisfied for any $u \in H^1_\kappa(\Omega)$. Finally, we observe that, if $\mathscr{Z}_p = \emptyset$ and $\mathscr{Z}_\ell \neq \emptyset$, then $\omega^2\varepsilon_0\mu_0 - |\kappa|^2 = 0$, so (69) can be replaced by (62).

To prove the Theorem subject to condition (2), we follow Theorem 3.5 of [8]. It is convenient to take $z_- < z_0 < z_+$ with $z_0 = 0$. For pseudo-periodic u, we begin with the identity

$$\int_\Omega z\frac{\partial u}{\partial z}\nabla\cdot\mu^{-1}\nabla\bar{u} + \int_\Omega \mu^{-1}\nabla\bar{u}\cdot\left(\frac{\partial u}{\partial z}e_z + z\frac{\partial}{\partial z}\nabla u\right) = \mu_0^{-1}\int_\Gamma z\frac{\partial u}{\partial z}\frac{\partial\bar{u}}{\partial n},$$

($e_z = \langle 0,0,1\rangle$) use the Helmholtz equation in the first term on the left, and add the complex conjugate of the equation to obtain

$$-\omega^2\int_\Omega \varepsilon z\frac{\partial}{\partial z}|u|^2 + \int_\Omega \mu^{-1}\left(2\left|\frac{\partial u}{\partial z}\right|^2 + z\frac{\partial}{\partial z}|\nabla u|^2\right) = 2\mu_0^{-1}\int_\Gamma |z|\left|\frac{\partial u}{\partial z}\right|^2.$$

Then use integration by parts in z on the two terms with the symbol $z\frac{\partial}{\partial z}$ and replace $\int \mu^{-1}|\nabla u|^2$ using

$$\int_\Omega(-\mu^{-1}|\nabla u|^2 + \omega^2\varepsilon|u|^2) = \mu_0^{-1}\int_\Gamma \bar{u}\,T_r u$$

to obtain

$$\int_\Omega\left[2\mu^{-1}\left|\frac{\partial u}{\partial z}\right|^2 + \omega^2 z|u|^2\frac{\partial\varepsilon}{\partial z} - z|\nabla u|^2\frac{\partial\mu^{-1}}{\partial z}\right] + +\mu_0^{-1}\int_\Gamma \bar{u}\,T_r u$$
$$= \mu_0^{-1}\int_\Gamma |z|\left[\omega^2\mu_0\varepsilon_0|u|^2 + \left|\frac{\partial u}{\partial z}\right|^2 - |\nabla_x u|^2\right]. \tag{70}$$

By condition (2) of the Theorem (with $z_0 = 0$), $z\frac{\partial\varepsilon}{\partial z}$ and $-z\frac{\partial\mu^{-1}}{\partial z}$ are nonnegative, so the left-hand side is nonnegative. If we assume that u is a guided mode and write and u in its expansion in spatial harmonics, we see that the integral on the right-hand side is a sum over $m \in \mathscr{Z}_e$ of terms that are multiples of

$$\omega^2\mu_0\varepsilon_0 + |\eta_m|^2 - |m+\kappa|^2. \tag{71}$$

But for $m \in \mathscr{Z}_e$, $\eta_m^2 < 0$, and by the definition of η_m, (71) vanishes. Therefore the right-hand side of (70) vanishes and we conclude that u vanishes identically in Ω. ∎

3.2.2 Modes in related problems

It is worth mentioning a few problems in wave propagation that are closely related to guided modes in open slab scatterers.

The problem of waves guided by periodically corrugated planar surfaces (diffraction gratings) is in many ways no different from ours. There is no transmission of energy across the surface, but the concepts of Rayleigh-Bloch scattering and the mathematical techniques for their analysis are essentially the same. Existence of scalar surface waves is treated by Linton and McIver [51] using variational techniques, by Grikurov, *et. al.,* [28] using the "augmented scattering matrix", as well as others [10, 36, 58, 69, 90]. Guided modes for the Maxwell equations in metal strip gratings over a substrate, in which the strips or the space between the strips is very thin, are established by Ammari, *et. al.* [2, 3].

One can consider a complementary structure to our slab system in which the ambient space is replaced by a photonic crystal and the slab is replaced by a homogeneous material. In fact, one of the primary attractions of photonic crystals is that they can be used to guide electromagnetic fields along paths carved out of the crystal at frequencies whose propagation is prohibited in the bulk. Guided modes of planar defects in two-dimensional photonic crystals are discussed by Ammari and Santosa [4], and the existence of modes in linear defects in three-dimensional photonic crystals is proved by Kuchment and Ong [44].

There is a large body of literature concerning the closely related problem in which closed waveguides with an obstacle placed inside admit trapped modes whose energy is concentrated at the obstacle. Much of this literature is presented in the context of water or sound waves by Evans, Linton, McIver, Ursell, and others. Trapped modes for water waves in a channel with a free surface were shown to exist by Ursell [86]. There, the governing equation is the Laplace equation, which admits no propagating spatial harmonics in the channel. The method of matched spatial harmonics and the residue calculus (see [60]) can be used to construct trapped acoustic (Helmholtz) modes [18, 20]. A variety of methods are demonstrated in [52]. Infinite sequences of trapped mode frequencies are treated in [50], and results on the dependence of the number of trapped modes on the structure are given in [15, 38].

Of particular interest are trapped modes whose frequencies are embedded in the continuous spectrum for a waveguide with an obstacle. Several techniques have been used to construct them, such as multipole expansions [9], variational formulations [19], generalized eigenfunction expansions [29], boundary integrals [57], construction of obstacles from trial trapped-mode solutions [58], and mode-matching and residue calculus [21]. In the latter, one can observe how the presence of a propagating spatial harmonic imposes an additional condition that is not present for trapped modes at frequencies below the cutoff. This condition corresponds to the second condition in the characterization (51).

4 Complex (κ,ω) and boundary-integral equations

Rigorous analysis of resonance near nonrobust guided modes requires a formulation of the scattering problem for complex (κ,ω) and the complex dispersion relation for generalized guided modes. This is achieved by "reducing" the problem to an auxiliary one that is posed on a bounded domain. The method we expound in this section is that of boundary integrals.

Another approach, which we shall not expound, is to allow (κ,ω) to be complex in the weak formulation 5 and thereby extend the resolvent of the operator S_κ. The poles in the closed lower half ω-plane (Im $\omega \leq 0$) of this extension for real κ are the branches of the dispersion relation discussed in Sec. 2, on which a real value of ω corresponds to a true guided mode (exponentially decaying in space). This approach is taken by Lenoir, *et. al.*, for acoustic scattering by a rigid bounded obstacle. The poles are in the open lower half plane, Im $\omega < 0$, which expresses the fact that a bounded scatterer can support no bound (exponentially localized) acoustic modes.

Regardless of the method of reduction, the resulting auxiliary problem is an equation

$$A(\kappa,\omega)\psi(\kappa,\omega) = \phi(\kappa,\omega),$$

in which A is an operator that is jointly analytic in (κ,ω) and acts in a suitable function space that is independent of (κ,ω). The function ϕ is determined by the source field and the solution ψ contains data about the total field (source plus scattered) that is sufficient for reconstructing the total physical field in space. A generalized guided mode is represented by a solution to the homogeneous equation

$$A(\kappa,\omega)\psi(\kappa,\omega)=0,$$

and the locus of (κ,ω) pairs in $\mathbb{C}^3$ (or $\mathbb{C}^2$ in the two-dimensional case) for which a nontrivial solution exists is the complex multi-branched dispersion relation.

If the open waveguide is constructed from homogeneous components with smooth interfaces, the auxiliary problem is naturally formulated in terms of boundary integrals. The functions ϕ and ψ are traces of the source and total fields on the interfaces, and the operator A is composed of layer potentials. For simplicity, we shall suppose that our structure is composed of a homogeneous and isotropic medium occupying a region $\tilde{D}$ that is bounded in the z variable and periodic in the x variables and that has a smooth boundary and outwardly directed normal vector $n(\mathbf{r})$ for $\mathbf{r}\in\partial\tilde{D}$. Let $D=\tilde{D}\cap\mathscr{S}$ be one period of the structure, set $D^c=\mathscr{S}\setminus\bar{D}$, and denote by ∂D the part of the boundary of $\tilde{D}$ that lies in $\mathscr{S}$. Denote the dielectric and magnetic constants in D by ε_1 and μ_1 and those in the ambient medium by ε_0 and μ_0.

We will first describe the extension of the problems of scattering and guided modes to complex (κ,ω) and introduce the outgoing pseudo-periodic Green function for the Helmholtz equation. The Green function underlies the boundary-integral equations from which the auxiliary problem we described above is constructed. The associated Calderón boundary-integral projectors allow for an elegant and organized approach.

4.1 Extension to complex frequency and wavevector

The extension to the complex domain is not only important for the mathematical analysis of resonant behavior at real (κ,ω); the fields themselves for complex (κ,ω) have physical significance. As we have already understood, true guided slab modes are nonzero pseudo-periodic solutions to the Helmholtz equation with real (κ,ω) that fall of exponentially away from the slab. If we keep κ real but now allow the frequency ω of a generalized guided mode to have a nonzero imaginary part, it turns out (Theorem 15) that this imaginary part must be negative. This means that the mode decays in time but grows exponentially with distance away from the slab; this is made clear through the analytic continuation of the spatial harmonics as we discuss presently. The physical interpretation of these modes as leaky modes must be treated with care, and we refer the reader to the literature, for example [67, 85, 32]. If, on the other hand, ω remains real while the κ of a generalized mode attains an imaginary part, the mode is a harmonic field that is attenuated due to radiation losses as it travels along the slab; see [68] and the chapter by Tausch of this book.

In the definition (14) of the numbers η_m,

$$\eta_m=\left[\varepsilon_0\mu_0\omega^2-(m_1+\kappa_1)^2-(m_2+\kappa_2)^2\right]^{\frac{1}{2}},$$

the choice of square root was made to give the correct radiation Condition 1. For each $m\in\mathbb{Z}^2$, the branch cut for the square root can be taken to be the negative imaginary axis. When ω decreases through a real value at which η_m vanishes, we say that the m^{th} Rayleigh diffractive order is cut off, as this spatial harmonic passes from propagating to evanescent. For ω just above the cutoff frequency, this harmonic is at a grazing angle with the slab and gives rise to an anomaly in the transmission coefficient known as the Wood anomaly (see [85, 53], for example). In the regime of leaky modes in which $\kappa\in\mathbb{R}^2$ and ω has a small imaginary part, η_m must jump from one branch of the square root function to another as the real part of ω passes a cutoff value. We will not treat this important case but focus on anomalies that are the result of nonrobust guided modes at real (κ,ω) at which all η_m are nonzero; this type of resonance is also discussed in [85]. We will show how these anomalies generalize the Fano resonance derived originally in the context of quantum mechanics.

If $(\kappa,\omega)\in\mathbb{R}^3$ and $\mathscr{Z}_\ell$ is empty, that is, for all $m\in\mathbb{Z}^2$,

$$\varepsilon_0\mu_0\omega^2-|m+\kappa|^2\neq 0,$$

then the numbers η_m can be extended analytically in a complex neighborhood of (κ,ω) in $\mathbb{C}^3$. If ω attains a small negative imaginary part, the outgoing propagating harmonics become exponentially growing as $|z|\to\infty$ (recall that we take $\operatorname{Re}\omega>0$) and the incoming harmonics become decaying; the reverse occurs if ω attains a small positive imaginary part. The evanescent harmonics remain evanescent under small perturbations of ω and κ. The radiation Condition 1 extends in this neighborhood to a *generalized outgoing condition*.

Condition 14 (Outgoing) *A complex-valued function u defined on* $\mathbb{R}^3$ *is said to satisfy the* generalized outgoing condition *for the slab for the complex pair* (κ,ω)*, with Re* $\omega>0$*, if there exist a real number* z_0 *and complex coefficients* $\{c_m^\pm\}_{m\in\mathbb{Z}^2}$ *in* $\ell^2(\mathbb{Z}^2)$ *such that*

$$u(x,z)=\sum_{m\in\mathbb{Z}^2} c_m^\pm e^{\pm i\eta_m z}e^{i(m+\kappa)\cdot x}\quad \textit{for } \pm z>z_0.$$

An analogous condition holds for the two-dimensional Helmholtz equation.

The outgoing condition is extended to electromagnetic fields by requiring that each component of the electric and magnetic fields satisfy Condition 14. Additional constraints are imposed by the Maxwell system: the E and H fields of each propagating harmonic are perpendicular to each other and to the propagation direction ([35] §7.1).

The outgoing pseudo-periodic Green function $G(\mathbf{r})$ ($\mathbf{r}=(x,z)$) for the Helmholtz equation in a homogeneous medium with coefficients (ε_0,μ_0) is a function that satisfies the equation in $\mathbb{R}^3$ except on a two-dimensional periodic array of source points $(2\pi n,0)$, whose strengths differ by a phase determined by the Bloch wavevector κ:

$$(\nabla^2+\omega^2\varepsilon_0\mu_0)G(\mathbf{r})=-\sum_{n\in\mathbb{Z}^2}\delta(x-2\pi n,z)e^{i\kappa\cdot x}.$$

Its representation in spatial Fourier harmonics is

$$G(\mathbf{r})=-\frac{1}{8\pi^2}\sum_{m\in\mathbb{Z}^2}\frac{1}{i\eta_m}e^{i\eta_m|z|}e^{i(m+\kappa)\cdot x}. \tag{72}$$

For $z\neq 0$, the convergence is exponential in m and one can see that G satisfies the Helmholtz equation; G also satisfies the outgoing Condition 14. A proof of the two-dimensional analog is given in [79]. The two-dimensional Green function looks the same except that the sum is taken over $\mathbb{Z}$ and $8\pi^2$ is replaced by 4π.

The scattering Problem 2 can be generalized by means of the outgoing condition, as can the definition of a guided mode. A *generalized guide mode* is a function that satisfies the Helmholtz equation as well as the outgoing condition. This means that it exists in the absence of generalized source fields ($u^{\text{inc}}=0$). If $\operatorname{Im}\kappa=\operatorname{Im}\omega=0$, the propagating harmonics necessarily vanish and the field falls off exponentially with distance from the slab. (Note that the outgoing condition encompasses exponentially decaying fields.)

The following theorem from plays a crucial role in the analysis of resonant transmission anomalies in Sec. 5. It asserts that generalized guided modes can exist only for $\operatorname{Im}\omega\leq 0$. (We always take $\operatorname{Re}\omega>0$.) We prove it here in the case of the Helmholtz equation; it extends generally to other harmonic wave equations, continuous and discrete.

Theorem 15 (Generalized modes) *Suppose that* (κ,ω) *is such that* $\mathscr{Z}_\ell=\emptyset$ *and that u is pseudo-periodic with real wavevector* κ *and satisfies the Helmholtz equation and the generalized outgoing Condition 14. Then Im* $\omega\leq 0$*. In addition,* $u\to 0$ *as* $|z|\to\infty$ *if and only if* ω *is real.*

Proof. For this proof, let $z_0=-z_-=z_+>0$. The Helmholtz equation and integration by parts gives

$$0=\int_\Omega\left(\nabla\cdot\mu^{-1}\nabla u+\omega^2\varepsilon u\right)\bar{u}=\int_\Omega\left(-\mu^{-1}|\nabla u|^2+\omega^2\varepsilon|u|^2\right)+\int_\Gamma\mu_0^{-1}(\partial_n u)\bar{u}.$$

Using the outgoing condition, one computes that, for sufficiently large $z_0>0$,

$$\int_\Gamma\mu_0^{-1}(\partial_n u)\bar{u}=\frac{4\pi^2}{\mu_0}\sum_{m\in\mathbb{Z}^2}i\eta_m(|c_m^-|^2+|c_m^+|^2)e^{-2\operatorname{Im}\eta_m|z_0|}.$$

These equations yield

$$-\operatorname{Im}(\omega^2)\int_\Omega\varepsilon|u|^2=\frac{4\pi^2}{\mu_0}\sum_{m\in\mathbb{Z}^2}\operatorname{Re}\eta_m(|c_m^-|^2+|c_m^+|^2)e^{-2\operatorname{Im}\eta_m|z_0|}. \tag{73}$$

Let κ be real and ω be in a neighborhood of a point on the real axis for which all numbers η_m are analytic functions of ω. If $\operatorname{Im}\omega>0$ (with our convention that $\operatorname{Re}\omega>0$), then $\operatorname{Im}\eta_m>0$ for all $m\in\mathbb{Z}^2$ and we obtain a contradition by letting z_0 tend to ∞. If $\operatorname{Im}\omega=0$, then, for all $m\in\mathscr{Z}_p$, $\eta_m>0$ and thus $c_m^\pm=0$. Therefore, u is exponentially decaying as $|z|\to\infty$. Conversely, if $u\to 0$ as $|z|\to\infty$, then, because $\operatorname{Im}\omega\leq 0$, all harmonics with $m\in\mathscr{Z}_p$ are exponentially growing in $|z|$ and therefore $c_m^\pm=0$ for all $m\in\mathscr{Z}_p$. The rest of the terms decay exponentially; hence letting $z_0\to\infty$ in (73) shows that $\operatorname{Im}\omega^2$ and therefore also $\operatorname{Im}\omega$ vanishes. ■

4.2 The Helmholtz equation

We seek a solution of the Helmholtz equation in $\mathbb{R}^3$ such that

$$\begin{aligned} \nabla^2 u + \omega^2 \alpha_1 u = f \quad & \text{in } D, \\ \nabla^2 u + \omega^2 \alpha_0 u = f \quad & \text{in } D^c, \end{aligned} \tag{74}$$

in which $\alpha_k = \varepsilon_k \mu_k$, $k = 1,2$, subject to the interface conditions

$$\left.\begin{aligned} u(\mathbf{r} - 0n(\mathbf{r})) = u(\mathbf{r} + 0n(\mathbf{r})), \\ \mu_1^{-1} \partial_n u(\mathbf{r} - 0n(\mathbf{r})) = \mu_0^{-1} \partial_n u(\mathbf{r} + 0n(\mathbf{r})) \end{aligned}\right\} \mathbf{r} \in \partial D \tag{75}$$

(the notation ± 0 indicates limits as $h \to 0^{\pm}$) and the pseudo-periodicity condition for wavevector κ. We may restrict analysis to the strip $\mathscr{S}$.

We will show how a solution u to the generalized scattering problem can be elegantly decomposed into source and scattered fields in the interior of D and in the exterior of D separately,

$$\begin{aligned} u|_D = u^{\text{int}} = u^{\text{int}}_{\text{so}} + u^{\text{int}}_{\text{sc}}, \\ u|_{D^c} = u^{\text{ext}} = u^{\text{ext}}_{\text{so}} + u^{\text{ext}}_{\text{sc}}. \end{aligned}$$

The scattered field should satisfy the homogeneous equation, and the source field is produced by the sources represented by f:

$$\begin{aligned} (\nabla^2 + \omega^2 \alpha_1) u^{\text{int}}_{\text{so}} = f|_D, \\ (\nabla^2 + \omega^2 \alpha_1) u^{\text{int}}_{\text{sc}} = 0, \\ (\nabla^2 + \omega^2 \alpha_0) u^{\text{ext}}_{\text{so}} = f|_{D^c}, \\ (\nabla^2 + \omega^2 \alpha_0) u^{\text{ext}}_{\text{sc}} = 0, \end{aligned}$$

so that the equations (74) are satisfied.

We will see that unique determination of u is generically guaranteed by the following additional conditions, which complete the formulation of the physical problem.

1. $u^{\text{int}}_{\text{so}}$ is taken to be the restriction to D of the outgoing pseudo-periodic field $U^{\text{int}}_{\text{so}}$ in $\mathscr{S}$ satisfying

$$(\nabla^2 + \omega^2 \alpha_1) U^{\text{int}}_{\text{so}} = f \chi_D \quad \text{in } \mathscr{S},$$

where χ_D is the characteristic function of D. This field is given by

$$U^{\text{int}}_{\text{so}}(\mathbf{r}) = -\int_D G(\mathbf{r} - \mathbf{r}') f(\mathbf{r}')\, dV.$$

2. $u^{\text{ext}}_{\text{so}}$ is taken to be the restriction to D^c of a pseudo-periodic field $U^{\text{ext}}_{\text{so}}$ in $\mathscr{S}$ satisfying

$$(\nabla^2 + \omega^2 \alpha_0) U^{\text{ext}}_{\text{so}} = f \chi_{D^c} \quad \text{in } \mathscr{S}.$$

Such a field $U^{\text{ext}}_{\text{so}}$ is not unique, as it could be modified by a field emanating from sources at infinity, such as a plane wave U^{∞}_{so} satisfying $(\nabla^2 + \omega^2 \alpha_0) U^{\infty}_{\text{so}} = 0$ in $\mathscr{S}$.

3. $u^{\text{ext}}_{\text{sc}}$ satisfies the generalized outgoing condition.

4. The interface conditions (75) must hold on ∂D.

The scattering problem can be reduced to integral equations on the boundary of D that involve the interface data of the total field u as unknown variables and the interface data of the source fields $u^{\text{int}}_{\text{so}}$ and $u^{\text{ext}}_{\text{so}}$ as the term of inhomogeneity. The interface data of a field u consists of the limits of u and $\mu^{-1} \partial_n u$ to ∂D, which are taken from the interior or exterior of D. We refer to this data collectively as the interior or exterior trace of u.

$$\psi_{\text{int}}(\mathbf{r}) = \begin{bmatrix} u^{\text{int}}(\mathbf{r}) \\ \mu_1^{-1} \partial_n u^{\text{int}}(\mathbf{r}) \end{bmatrix}, \; \psi_{\text{ext}} = \begin{bmatrix} u^{\text{ext}}(\mathbf{r}) \\ \mu_0^{-1} \partial_n u^{\text{ext}}(\mathbf{r}) \end{bmatrix},$$

for $\mathbf{r} \in \partial D$. The traces are naturally considered in the space $H^{\frac{1}{2}}(\partial D) \oplus H^{-\frac{1}{2}}(\partial D)$.

We shall omit the details of the proper function spaces for the fields and their traces as well as technical aspects of the proofs and focus on the mathematical structure and how a boundary-integral formulation of the scattering problem arises from it. A through rigorous treatment of the theory, including the ensuing theory of layer potentials for the Helmholtz equation with applications to acoustic scattering is available in Costabel and Stephan [12] or Nédélec [62] §3.1, as well as Colton and Kress [11], Kress [40], and many other works. The first two works make explicit reference to the Calderón boundary-integral projectors, which we use below in the formulation of the auxiliary problem for scattering by a slab. Our presentation essentially follows that presented for the two-dimensional case by Shipman and Venakides [79].

The development of a boundary-integral formulation begins with the boundary-integral representations of Helmholtz fields in D and in D^c. Let us first take ε and μ to be constant over all of $\mathbb{R}^3$, as if the structure were not present, but retain the knowledge of the domain D. We will see how an arbitrary pair of functions (ξ, η) on ∂D can be decomposed uniquely into the sum of the boundary data of an interior Helmholtz field and the boundary data of an exterior outgoing Helmholtz field, both with the same coefficients ε and μ.

If u satisfies $(\nabla^2 + \omega^2\alpha)u = 0$ with $\alpha = \varepsilon\mu$ in D, then u can be reconstructed from its boundary data on ∂D,

$$\begin{bmatrix} u(\mathbf{r}) \\ \mu^{-1}\partial_n u(\mathbf{r}) \end{bmatrix}, \quad \mathbf{r} \in \partial D, \tag{76}$$

through

$$u(\mathbf{r}) = \int_{\partial D} \left[-\frac{\partial G(\mathbf{r}-\mathbf{r}')}{\partial n_{\mathbf{r}'}} u(\mathbf{r}') + \; + \mu G(\mathbf{r}-\mathbf{r}')\mu^{-1}\frac{\partial u}{\partial n}(\mathbf{r}') \right] ds_{\mathbf{r}'}, \;\; \mathbf{r} \in D. \tag{77}$$

If u satisfies $(\nabla^2 + \omega^2\alpha)u = 0$ in D^c and the generalized outgoing condition, then

$$u(\mathbf{r}) = \int_{\partial D} \left[\frac{\partial G(\mathbf{r}-\mathbf{r}')}{\partial n_{\mathbf{r}'}} u(\mathbf{r}') + \; - \mu G(\mathbf{r}-\mathbf{r}')\mu^{-1}\frac{\partial u}{\partial n}(\mathbf{r}') \right] ds_{\mathbf{r}'}, \;\; \mathbf{r} \in D^c. \tag{78}$$

Both equations are proved by using the divergence theorem (or Green's identities) in the truncated period Ω of the slab structure. The contributions from the sides of $\mathscr{S}$ that are parallel to the z-axis vanish because of the pseudo-periodicity of u and G, and the contributions from the perpendicular sides $\Gamma_\pm$ vanish because of the outgoing condition satisfied by both u and G.

These representations show one way in which u is generated by a combination of single- and double-layer potentials. It is natural to extend these formulas to allow an arbitrary pair (ξ, η) of functions on ∂D in place of the trace of u and to define

$$u^{\text{int}}(\mathbf{r}) = \int_{\partial D} \left[-\frac{\partial G(\mathbf{r}-\mathbf{r}')}{\partial n_{\mathbf{r}'}} \xi(\mathbf{r}') + \; + \mu G(\mathbf{r}-\mathbf{r}')\eta(\mathbf{r}') \right] ds_{\mathbf{r}'}, \;\; \mathbf{r} \in D, \tag{79}$$

$$u^{\text{ext}}(\mathbf{r}) = \int_{\partial D} \left[\frac{\partial G(\mathbf{r}-\mathbf{r}')}{\partial n_{\mathbf{r}'}} \xi(\mathbf{r}') + \; - \mu G(\mathbf{r}-\mathbf{r}')\eta(\mathbf{r}') \right] ds_{\mathbf{r}'}, \;\; \mathbf{r} \in D^c. \tag{80}$$

The function u^{int} satisfies $(\nabla^2 + \omega^2\alpha)u = 0$ in D, and the function u^{ext} satisfies the same equation in D^c plus the outgoing condition because the Green function G does. Both fields have traces in $H^{\frac{1}{2}}(\partial D) \oplus H^{-\frac{1}{2}}(\partial D)$.

Taking the limits of u and $\partial_n u$ as $\mathbf{r} \to \partial D$ leads to the following representations. The analysis of the singularity in the integral is subtle and is based on the Sokhotski-Plemelj formulas.

$$\begin{aligned}
u^{\text{int}}(\mathbf{r}) &= \tfrac{1}{2}\xi(\mathbf{r}) + \int_{\partial D} \left[-\frac{\partial G(\mathbf{r}-\mathbf{r}')}{\partial n_{\mathbf{r}'}} \xi(\mathbf{r}') + \mu G(\mathbf{r}-\mathbf{r}')\eta(\mathbf{r}') \right] ds_{\mathbf{r}'}, \\
\mu^{-1}\partial_n u^{\text{int}}(\mathbf{r}) &= \tfrac{1}{2}\eta(\mathbf{r}) + \int_{\partial D} \left[-\mu^{-1}\frac{\partial^2 G(\mathbf{r}-\mathbf{r}')}{\partial n_{\mathbf{r}}\partial n_{\mathbf{r}'}} \xi(\mathbf{r}') + \frac{\partial G(\mathbf{r}-\mathbf{r}')}{\partial n_{\mathbf{r}}} \eta(\mathbf{r}') \right] ds_{\mathbf{r}'}, \\
u^{\text{ext}}(\mathbf{r}) &= \tfrac{1}{2}\xi(\mathbf{r}) + \int_{\partial D} \left[\frac{\partial G(\mathbf{r}-\mathbf{r}')}{\partial n_{\mathbf{r}'}} \xi(\mathbf{r}') - \mu G(\mathbf{r}-\mathbf{r}')\eta(\mathbf{r}') \right] ds_{\mathbf{r}'},
\end{aligned} \tag{81}$$

$$\mu^{-1}\partial_n u^{\text{ext}}(\mathbf{r}) = \tfrac{1}{2}\eta(\mathbf{r}) + \int_{\partial D}\left[\mu^{-1}\frac{\partial^2 G(\mathbf{r}-\mathbf{r}')}{\partial n_{\mathbf{r}}\partial n_{\mathbf{r}'}}\xi(\mathbf{r}') - \frac{\partial G(\mathbf{r}-\mathbf{r}')}{\partial n_{\mathbf{r}}}\eta(\mathbf{r}')\right]ds_{\mathbf{r}'}. \tag{82}$$

These formulas are composed of four operators giving the values and normal derivatives on ∂D of the single- and double-layer potentials,

$$(S\eta)(\mathbf{r}) = \int_{\partial D} G(\mathbf{r}-\mathbf{r}')\eta(\mathbf{r}')ds_{\mathbf{r}'},$$
$$(K\xi)(\mathbf{r}) = \int_{\partial D} \frac{\partial G(\mathbf{r}-\mathbf{r}')}{\partial n_{\mathbf{r}'}}\xi(\mathbf{r}')ds_{\mathbf{r}'},$$
$$(K'\eta)(\mathbf{r}) = \int_{\partial D} \frac{\partial G(\mathbf{r}-\mathbf{r}')}{\partial n_{\mathbf{r}}}\xi(\mathbf{r}')ds_{\mathbf{r}'},$$
$$(T\xi)(\mathbf{r}) = \int_{\partial D} \frac{\partial^2 G(\mathbf{r}-\mathbf{r}')}{\partial n_{\mathbf{r}}\partial n_{\mathbf{r}'}}\xi(\mathbf{r}')ds_{\mathbf{r}'}.$$

The singular integrals, especially T, must be treated carefully (see [12]). These operators are such that the following matrix operator A is bounded in $H^{\frac{1}{2}}(\partial D) \oplus H^{-\frac{1}{2}}(\partial D)$,

$$A = \begin{bmatrix} K & -\mu S \\ \mu^{-1}T & -K' \end{bmatrix}.$$

Let I be the identity operator, and define the operators

$$P_{\text{int}} = \tfrac{1}{2}I - A, \quad P_{\text{ext}} = \tfrac{1}{2}I + A.$$

The equations (81) and (82) are expressed in terms of P_{int} and P_{ext} as

$$\begin{bmatrix} u^{\text{int}} \\ \mu^{-1}\partial_n u^{\text{int}} \end{bmatrix} = P_{\text{int}}\begin{bmatrix} \xi \\ \eta \end{bmatrix}, \quad \begin{bmatrix} u^{\text{ext}} \\ \mu^{-1}\partial_n u^{\text{ext}} \end{bmatrix} = P_{\text{ext}}\begin{bmatrix} \xi \\ \eta \end{bmatrix}.$$

Now, because of the integral representations (77) and (78), we also have

$$\begin{bmatrix} u^{\text{int}} \\ \mu^{-1}\partial_n u^{\text{int}} \end{bmatrix} = P_{\text{int}}\begin{bmatrix} u^{\text{int}} \\ \mu^{-1}\partial_n u^{\text{int}} \end{bmatrix},$$
$$\begin{bmatrix} u^{\text{ext}} \\ \mu^{-1}\partial_n u^{\text{ext}} \end{bmatrix} = P_{\text{ext}}\begin{bmatrix} u^{\text{ext}} \\ \mu^{-1}\partial_n u^{\text{ext}} \end{bmatrix}.$$

This shows that P_{int} and P_{ext} are projection operators, and, by their definition, they are complementary. These are the *Calderón projectors* for the Helmholtz equation in the doubly pseudo-periodic setting. They depend on the parameters ω, κ, and α. In summary, we have

1. $P_{\text{int}} + P_{\text{ext}} = I$,
2. $P_{\text{int}}^2 = P_{\text{int}}$ and $P_{\text{ext}}^2 = P_{\text{ext}}$,
3. The range of P_{int} is the subspace consisting of traces of free κ-pseudo-periodic Helmholtz fields in D.
4. The range of P_{ext} is the subspace consisting of traces of free κ-pseudo-periodic Helmholtz fields in D^c that satisfy the outgoing condition.

Let us return to the interior and exterior constants $\alpha_1 = \varepsilon_1\mu_1$ and $\alpha_0 = \varepsilon_0\mu_0$ and the scattering problem and put

$$\bar{\varepsilon} = \tfrac{1}{2}(\varepsilon_0 + \varepsilon_1), \quad \bar{\mu} = \tfrac{1}{2}(\mu_0 + \mu_1).$$

Consider the traces of all the fields involved:

$$\psi = \begin{bmatrix} u \\ \mu^{-1}\partial_n u \end{bmatrix},$$
$$\phi_{\text{so}}^{\text{int}} = \begin{bmatrix} u_{\text{so}}^{\text{int}} \\ \mu_1^{-1}\partial_n u_{\text{so}}^{\text{int}} \end{bmatrix}, \ \phi_{\text{sc}}^{\text{int}} = \begin{bmatrix} u_{\text{sc}}^{\text{int}} \\ \mu_1^{-1}\partial_n u_{\text{sc}}^{\text{int}} \end{bmatrix}, \tag{83}$$
$$\phi_{\text{so}}^{\text{ext}} = \begin{bmatrix} u_{\text{so}}^{\text{ext}} \\ \mu_0^{-1}\partial_n u_{\text{so}}^{\text{ext}} \end{bmatrix}, \ \phi_{\text{sc}}^{\text{ext}} = \begin{bmatrix} u_{\text{sc}}^{\text{ext}} \\ \mu_0^{-1}\partial_n u_{\text{sc}}^{\text{ext}} \end{bmatrix}.$$

Because of the requirement of continuity of the boundary data,

$$\begin{aligned}\psi &= \phi^{\text{int}}_{\text{so}} + \phi^{\text{int}}_{\text{sc}},\\ \psi &= \phi^{\text{ext}}_{\text{so}} + \phi^{\text{ext}}_{\text{sc}}.\end{aligned} \tag{84}$$

Recall that the interior scattered field $u^{\text{int}}_{\text{sc}}$ is a free pseudo-periodic Helmholtz field in D with constant α_1 and that the interior source field $u^{\text{int}}_{\text{so}}$, by our definition, extends to a free outgoing Helmholtz field $U^{\text{int}}_{\text{so}}$ in D^c with the same constant α_1. This means that $\phi^{\text{int}}_{\text{sc}}$ is in the nullspace of P^1_{ext} and $\phi^{\text{int}}_{\text{so}}$ is in the range (the superscript refers to the value α_1). Similarly, the exterior scattered field $u^{\text{ext}}_{\text{sc}}$ is a free pseudo-periodic outgoing Helmholtz field in D^c with constant α_0 and the exterior source field $u^{\text{ext}}_{\text{so}}$ extends to a free Helmholtz field in D also with α_0; thus $\phi^{\text{ext}}_{\text{sc}}$ is in the nullspace of P^0_{int} and $\phi^{\text{ext}}_{\text{so}}$ is in the range. This all means that we can project the trace of the field we seek onto traces of the known interior and exterior source fields that produce it:

$$\begin{aligned}P^1_{\text{ext}}\psi &= \phi^{\text{int}}_{\text{so}},\\ P^0_{\text{int}}\psi &= \phi^{\text{ext}}_{\text{so}}.\end{aligned} \tag{85}$$

For the problem of scattering of a plane wave $u^{\text{inc}}(x,z) = e^{i(\bar{m}+\kappa)x}e^{i\eta_{\bar{m}}z}$, the source traces are

$$\phi^{\text{ext}}_{\text{so}} = \begin{bmatrix} 1 \\ i\mu_0^{-1}(\bar{m}+\kappa, \eta_{\bar{m}})\cdot n \end{bmatrix} u^{\text{inc}}(x,z), \quad \phi^{\text{int}}_{\text{so}} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

The Calderón projectors in the equations (85) have a second-order derivative of G in the integral kernel with leading singularities differing by a multiplicative constant. To cause these to cancel in a linear combination, we can multiply them by the matrices

$$\Lambda_k = \begin{bmatrix} 1 & 0 \\ 0 & \mu_k/\bar{\mu} \end{bmatrix}, \tag{86}$$

for $k = 0,1$, to obtain

$$[\Lambda_1 P^1_{\text{ext}} + \Lambda_0 P^0_{\text{int}}]\psi = \Lambda_1\phi^{\text{int}}_{\text{so}} + \Lambda_0\phi^{\text{ext}}_{\text{so}}. \tag{87}$$

With the notation

$$\eta(\mathbf{r}) = \mu_1^{-1}\frac{\partial u^{\text{int}}}{\partial n}(\mathbf{r}) = \mu_0^{-1}\frac{\partial u^{\text{ext}}}{\partial n}(\mathbf{r}), \quad r \in \partial D,$$

the resulting system of boundary-integral equations for $[u(\mathbf{r}), \eta(\mathbf{r})]^t$ is

$$u(\mathbf{r}) + \int_{\partial D}\left[\frac{\partial(G_1 - G_0)(\mathbf{r}-\mathbf{r}')}{\partial n_{\mathbf{r}'}}u(\mathbf{r}') + -(\mu_1 G_1 - \mu_0 G_0)(\mathbf{r}-\mathbf{r}')\,\eta(\mathbf{r}')\right]ds_{\mathbf{r}'} = u^{\text{int}}_{\text{so}}(\mathbf{r}) + u^{\text{ext}}_{\text{so}}(\mathbf{r}), \tag{88}$$

$$\eta(\mathbf{r}) + \bar{\mu}^{-1}\int_{\partial D}\left[\frac{\partial^2(G_1 - G_0)(\mathbf{r}-\mathbf{r}')}{\partial n_{\mathbf{r}}\partial n_{\mathbf{r}'}}u(\mathbf{r}') + -(\mu_1 G_1 - \mu_0 G_0)(\mathbf{r}-\mathbf{r}')\,\eta(\mathbf{r}')\right]ds_{\mathbf{r}'} = \bar{\mu}^{-1}\frac{\partial}{\partial n}(u^{\text{int}}_{\text{so}}(\mathbf{r}) + u^{\text{ext}}_{\text{so}}(\mathbf{r})). \tag{89}$$

The system in which we are interested is the pair (85), for the trace of the scattered field is recovered from the decomposition (84) and this or the total field is then used to determine the scattered field in D and D^c by means of boundary-integral representation formulas (77,78). Any solution of the pair (85) is also a solution to the combination (87). What we must now determine is if a solution to the combination is also a solution of the pair. To ascertain this, we observe that (87) is equivalent to

$$\left.\begin{aligned}\Lambda_1 P^1_{\text{ext}}\psi &= \Lambda_1\phi^{\text{int}}_{\text{so}} + f\\ \Lambda_0 P^0_{\text{int}}\psi &= \Lambda_0\phi^{\text{ext}}_{\text{so}} - f\end{aligned}\right\}\text{ for some } f, \tag{90}$$

or, alternatively,

$$\left.\begin{aligned}P^1_{\text{ext}}\psi &= \phi^{\text{int}}_{\text{so}} + \Lambda_1^{-1}f\\ P^0_{\text{int}}\psi &= \phi^{\text{ext}}_{\text{so}} - \Lambda_0^{-1}f\end{aligned}\right\}\text{ for some } f. \tag{91}$$

Such a function pair $f=[f_1,f_2]^t$ is characterized by the property that $\Lambda_1^{-1}f$ is in the range of the projection P^1_{ext} (because $\phi^{\text{int}}_{\text{so}}$ is) and $\Lambda_0^{-1}f$ is in the range of P^0_{int} (because $\phi^{\text{ext}}_{\text{so}}$ is), or, equivalently,

$$P^1_{\text{int}}\Lambda_1^{-1}f=0,\quad P^0_{\text{ext}}\Lambda_0^{-1}f=0. \tag{92}$$

Now, one can calculate that the Calderón projectors for the *reciprocal* coefficients

$$\begin{aligned}\varepsilon^0&=\frac{2\varepsilon_1\mu_1}{\mu_0+\mu_1},\quad \mu^0=\frac{\mu_0+\mu_1}{2},\\ \varepsilon^1&=\frac{2\varepsilon_0\mu_0}{\mu_0+\mu_1},\quad \mu^1=\frac{\mu_0+\mu_1}{2},\end{aligned} \tag{93}$$

are related to those of the original coefficients by conjugation by $\Lambda_{0,1}$. In particular, if we distinguish the projectors for the reciprocal coefficients by a bar,

$$\bar{P}^0_{\text{int}}=\Lambda_1P^1_{\text{int}}\Lambda_1^{-1} \tag{94}$$

is the interior Calderón projector for the coefficients (ε^0,μ^0) and

$$\bar{P}^1_{\text{ext}}=\Lambda_0P^0_{\text{ext}}\Lambda_0^{-1} \tag{95}$$

is the exterior projector for the coefficients (ε^1,μ^1).

Then, because of (92), we obtain the pair

$$\begin{aligned}\bar{P}^0_{\text{int}}f&=0,\\ \bar{P}^1_{\text{ext}}f&=0.\end{aligned}\qquad\text{(reciprocal system)} \tag{96}$$

A function f that satisfies this pair is simultaneously the trace of an exterior pseudo-periodic outgoing Helmholtz field with constants (ε^0,μ^0) and the trace of an interior Helmholtz field with constants (ε^1,μ^1). If $f\neq 0$, this field corresponds to a generalized guided mode of a *reciprocal structure* characterized by these new constants. Since

$$\begin{aligned}\alpha_0&=\varepsilon_0\mu_0=\varepsilon^1\mu^1,\\ \alpha_1&=\varepsilon_1\mu_1=\varepsilon^0\mu^0,\end{aligned}$$

the mode satisfies the Helmholtz equation with the interior and exterior valus of α switched relative to those of the original structure, but the multiplicative jump in the normal derivative is replaced by continuity because $\mu^0=\mu^1$.

If no guided mode exists in the reciprocal structure, that is, if the pair (96) admits only the trivial solution, then the combination (87) is equivalent to the pair (85). In other words, uniqueness of the solution of the reciprocal scattering problem, in which the ambient medium is characterized by (ε^0,μ^0) and periodic structure are characterized by (ε^1,μ^1), implies equivalence of the original scattering Problem 2 and the boundary integral equations (88,89).

The essential results can be summarized in the following theorem.

Theorem 16 *If the (reciprocal) periodic structure with coefficients*

$$\begin{aligned}\varepsilon=\varepsilon^1,\ \mu=\mu^1\quad &\text{in } D,\\ \varepsilon=\varepsilon^0,\ \mu=\mu^0\quad &\text{in } D^c,\end{aligned}$$

defined in terms of given constants (ε_1,μ_1) *and* (ε_0,μ_0) *by* (93) *does not admit a free pseudo-periodic outgoing Helmholtz field in the absence of a source (a generalized guided mode), then the boundary-integral system (88,89) is equivalent to the scattering Problem 2 in the (original) structure with*

$$\begin{aligned}\varepsilon=\varepsilon_1,\ \mu=\mu_1\quad &\text{in } D,\\ \varepsilon=\varepsilon_0,\ \mu=\mu_0\quad &\text{in } D^c.\end{aligned}$$

More specifically, with ϕ^{int}_{so} *and* ϕ^{ext}_{so} *defined as in* (83)*, the scattered field* u^{sc} *of the scattering problem with source fields* u^{int}_{so} *and* u^{ext}_{so} *is obtained by using the solution to (88,89),*

$$\begin{bmatrix}u(\mathbf{r})\\ \eta(\mathbf{r})\end{bmatrix}=\begin{bmatrix}u(\mathbf{r})\\ \mu^{-1}\partial_n u(\mathbf{r})\end{bmatrix},\quad \mathbf{r}\in\partial D,$$

in the representation formulas (77) *and* (78)*.*

The reciprocal relations have the property that, if R is defined by

$$R(\varepsilon_0,\mu_0;\varepsilon_1,\mu_1) = (\varepsilon^0,\mu^0;\varepsilon^1,\mu^1),$$

subject to the relations (93), then

$$R^2(\varepsilon_0,\mu_0;\varepsilon_1,\mu_1) = (\varepsilon_0\tfrac{\mu_0}{\bar{\mu}},\bar{\mu};\varepsilon_1\tfrac{\mu_1}{\bar{\mu}},\bar{\mu})$$

and

$$R^3 = R^1;$$

and the image of R is those sets of coefficients for which $\mu_0 = \mu_1$.

4.3 Two-dimensional reduction

In its two-dimensional form, the Helmholtz equation describes a variety of harmonic waves, including acoustic waves in structures that are invariant in one direction, water waves in certain regimes, and polarized electromagnetic waves. If the periodicity of the slab degenerates to invariance in, say, the x_2-direction and we assume that the electromagnetic waves are also invariant in the x_2-direction, then the Maxwell system decouples into two polarizations.

In the E-polarized case, the E field is directed out of the x_1z-plane and H lies in the plane. If we denote by u this out-of-plane component, then $H = (i\omega\mu)^{-1}\langle -u_z, 0, u_{x_1}\rangle$. The Maxwell system implies the Helmholtz equation for u:

$$\nabla\cdot\mu^{-1}\nabla u + \omega^2\varepsilon u = 0, \tag{97}$$

which, considered in the distributional sense, implies continuity of u and $\mu^{-1}\partial_n u$ at ∂D. The foregoing analysis of the boundary-integral equations is valid in two dimensions if the Green functions are replaced with their two-dimensional analogues.

In the H-polarized case, the H field is directed out of the x_1z-plane and E lies in the plane. If u is this out-of-plane component, then $E = -(i\omega\varepsilon)^{-1}\langle -u_z, 0, u_{x_1}\rangle$. The equation in distributional form is

$$\nabla\cdot\varepsilon^{-1}\nabla u + \omega^2\mu u = 0, \tag{98}$$

which implies continuity of u and $\varepsilon^{-1}\partial_n u$ at ∂D. In this case, the results on the boundary-integral formulation must be modified by interchanging the roles of ε and μ.

Let us examine the case of nonmagnetic materials, or $\mu\equiv 1$. In the E-polarized case, we wish to solve the scattering problem with

$$\begin{aligned} \varepsilon = \varepsilon_1,\ \mu = 1 \quad &\text{in } D,\\ \varepsilon = \varepsilon_0,\ \mu = 1 \quad &\text{in } D^c. \end{aligned}$$

The system of boundary-integral equations, with $\eta = \partial_n u$ continuous on ∂D, is

$$u(\mathbf{r}) + \int_{\partial D}\left[\frac{\partial(G_1-G_0)(\mathbf{r}-\mathbf{r}')}{\partial n_{\mathbf{r}'}}u(\mathbf{r}') - (G_1-G_0)(\mathbf{r}-\mathbf{r}')\,\eta(\mathbf{r}')\right]ds_{\mathbf{r}'} = u^{\text{int}}_{\text{so}}(\mathbf{r}) + u^{\text{ext}}_{\text{so}}(\mathbf{r}), \tag{99}$$

$$\eta(\mathbf{r}) + \int_{\partial D}\left[\frac{\partial^2(G_1-G_0)(\mathbf{r}-\mathbf{r}')}{\partial n_{\mathbf{r}}\partial n_{\mathbf{r}'}}u(\mathbf{r}') - (G_1-G_0)(\mathbf{r}-\mathbf{r}')\,\eta(\mathbf{r}')\right]ds_{\mathbf{r}'} = \frac{\partial}{\partial n}(u^{\text{int}}_{\text{so}}(\mathbf{r}) + u^{\text{ext}}_{\text{so}}(\mathbf{r})). \tag{100}$$

The reciprocal problem of Theorem 16 for E-polarization has

$$\begin{aligned} \varepsilon = \varepsilon_0,\ \mu = 1 \quad &\text{in } D,\\ \varepsilon = \varepsilon_1,\ \mu = 1 \quad &\text{in } D^c. \end{aligned}$$

In the H-polarized case, we wish to solve the scattering problem with the following replacement in the forgoing analysis:

$$\begin{aligned} \varepsilon\mapsto 1,\ \mu\mapsto\varepsilon_1 \quad &\text{in } D,\\ \varepsilon\mapsto 1,\ \mu\mapsto\varepsilon_0 \quad &\text{in } D^c. \end{aligned}$$

The system of boundary-integral equations in the H-polarization case, with $\eta = \varepsilon^{-1}\partial_n u$ continuous on ∂D, is

$$u(\mathbf{r}) + \int_{\partial D}\left[\frac{\partial(G_1 - G_0)(\mathbf{r}-\mathbf{r}')}{\partial n_{\mathbf{r}'}}\,u(\mathbf{r}') \;-\; (\varepsilon_1 G_1 - \varepsilon_0 G_0)(\mathbf{r}-\mathbf{r}')\,\eta(\mathbf{r}')\right]ds_{\mathbf{r}'} = u^{\text{int}}_{\text{so}}(\mathbf{r}) + u^{\text{ext}}_{\text{so}}(\mathbf{r}), \tag{101}$$

$$\eta(\mathbf{r}) + \bar{\varepsilon}^{-1}\int_{\partial D}\left[\frac{\partial^2(G_1 - G_0)(\mathbf{r}-\mathbf{r}')}{\partial n_{\mathbf{r}}\partial n_{\mathbf{r}'}}\,u(\mathbf{r}') \;-\; (\varepsilon_1 G_1 - \varepsilon_0 G_0)(\mathbf{r}-\mathbf{r}')\,\eta(\mathbf{r}')\right]ds_{\mathbf{r}'} = \bar{\varepsilon}^{-1}\frac{\partial}{\partial n}(u^{\text{int}}_{\text{so}}(\mathbf{r}) + u^{\text{ext}}_{\text{so}}(\mathbf{r})). \tag{102}$$

The reciprocal problem has

$$\begin{aligned} \varepsilon = \varepsilon_0\bar{\varepsilon}^{-1},\ \mu = \bar{\varepsilon} \quad &\text{in } D,\\ \varepsilon = \varepsilon_1\bar{\varepsilon}^{-1},\ \mu = \bar{\varepsilon} \quad &\text{in } D^c. \end{aligned}$$

But Helmholtz fields in a structure with these coefficients coincide with fields in a structure with ε replaced with $c\varepsilon$ and μ replaced with $c^{-1}\mu$, with c a constant. By taking $c = \bar{\varepsilon}$, the reciprocal problem is seen to be identical to that for the E-polarized case.

In summary, we have obtained Theorem 4.4 of [79].

Theorem 17 *If the (reciprocal) two-dimensional structure with dielectric constants*

$$\varepsilon = \varepsilon_1 \text{ in } D^c,\ \ \varepsilon = \varepsilon_0 \text{ in } D,$$

and magnetic constant $\mu = 1$ *admits no nontrivial E-polarized field in the absence of a source, (generalized guided mode) then the systems (99,100) and (101,102) are equivalent to the E-polarized and H-polarized scattering problems, respectively, with* $\mu = 1$.

We have seen already that the condition in this theorem is satisfied when ω and κ are real, $\varepsilon_1 > \varepsilon_0$, $\mu = 1$, and an additional condition from Theorem 13 holds.

4.4 The harmonic Maxwell system

For the harmonic Maxwell system, rigorous treatment of the technical aspects of the boundary-integral operators can be found, for example, in Müller [61] and [62], and the Calderón projectors are treated for bounded objects in $\mathbb{R}^3$ in [62] §5.5.

The development of the boundary-integral equations and the reciprocal problem for the Maxwell system parallels that of the Helmholtz equation. We present the framework, leaving the technical details to the references cited above.

We seek a pseudo-periodic solution of the harmonic Maxwell system in $\mathbb{R}^3$,

$$\begin{aligned} \nabla\times H + i\omega\varepsilon E = J_1,\\ \nabla\times E - i\omega\mu H = J_2, \end{aligned}$$

subject to continuity of the tangential traces of E and H on ∂D. The sources J_1 and J_2 are electric and magnetic currents. If we put

$$v = \begin{bmatrix} H \\ E \end{bmatrix}, \quad f = \begin{bmatrix} J_1 \\ J_2 \end{bmatrix},$$

$$L = \begin{bmatrix} \nabla\times & i\omega\varepsilon \\ -i\omega\mu & \nabla\times \end{bmatrix}, \quad L_k = \begin{bmatrix} \nabla\times & i\omega\varepsilon_k \\ -i\omega\mu_k & \nabla\times \end{bmatrix},$$

for $k = 1, 2$, the Maxwell system is written compactly as

$$Lv = f. \tag{103}$$

A solution v can be decomposed into source and scattered fields in the interior of D and in the exterior of D,

$$\begin{aligned} v|_D = v^{\text{int}} = v^{\text{int}}_{\text{so}} + v^{\text{int}}_{\text{sc}},\\ v|_{D^c} = v^{\text{ext}} = v^{\text{ext}}_{\text{so}} + v^{\text{ext}}_{\text{sc}}. \end{aligned} \tag{104}$$

The scattered field should satisfy the homogeneous Maxwell system,

$$\left\{\begin{array}{l} L_1 v^{\text{int}}_{\text{so}} = f|_D \\ L_1 v^{\text{int}}_{\text{sc}} = 0 \end{array}\right. \implies L_1 v^{\text{int}} = f|_D.$$

$$\left\{\begin{array}{l} L_0 v^{\text{ext}}_{\text{so}} = f|_{D^c} \\ L_0 v^{\text{ext}}_{\text{sc}} = 0 \end{array}\right. \implies L_0 v^{\text{ext}} = f|_{D^c}.$$

The conditions that generically determine a unique solution v are the following:

1. $v^{\text{int}}_{\text{so}}$ is taken to be the restriction to D of the outgoing pseudo-periodic field $V^{\text{int}}_{\text{so}}$ satisfying

$$L_1 V^{\text{int}}_{\text{so}} = f\chi_D \quad \text{in } \mathscr{S}.$$

2. $v^{\text{ext}}_{\text{so}}$ is taken to be the restriction to D^c of a field $V^{\text{ext}}_{\text{so}}$ satisfying

$$L_0 V^{\text{ext}}_{\text{so}} = f\chi_{D^c} \quad \text{in } \mathscr{S}.$$

Such a field is not unique, as it could be modified by fields emanating from sources at infinity, such as plane waves V^{∞}_{so} satisfying $L_0 V^{\infty}_{\text{so}} = 0$ in $\mathscr{S}$.

3. $v^{\text{ext}}_{\text{sc}}$ satisfies the generalized outgoing condition.
4. The tangential traces of the fields v^{int} and v^{ext} must match on ∂D.

The integral representation formulas for a Maxwell field $[H,E]^t$ involve the tangential traces of H and E, or the electric current j and magnetic current m,

$$\begin{array}{l} j(\mathbf{r}) = -n(\mathbf{r}) \times H(\mathbf{r}) \\ m(\mathbf{r}) = n(\mathbf{r}) \times E(\mathbf{r}) \end{array} \quad (\mathbf{r} \in \partial D). \tag{105}$$

If $[H,E]^t$ is an outgoing pseudo-periodic Maxwell field in D^c with constant coefficients ε and μ,

$$\begin{aligned} E(\mathbf{r}) &= -i\omega\mu \int_{\partial D} G(\mathbf{r}-\mathbf{r}')j(\mathbf{r}')dS(\mathbf{r}') + \frac{1}{i\omega\varepsilon}\nabla\int_{\partial D} G(\mathbf{r}-\mathbf{r}')\text{div}_{\partial D} j(\mathbf{r}')dS(\mathbf{r}') + \nabla\times\int_{\partial D} G(\mathbf{r}-\mathbf{r}')m(\mathbf{r}')dS(\mathbf{r}'), \\ H(\mathbf{r}) &= -i\omega\varepsilon \int_{\partial D} G(\mathbf{r}-\mathbf{r}')m(\mathbf{r}')dS(\mathbf{r}') + \frac{1}{i\omega\mu}\nabla\int_{\partial D} G(\mathbf{r}-\mathbf{r}')\text{div}_{\partial D} m(\mathbf{r}')dS(\mathbf{r}') - \nabla\times\int_{\partial D} G(\mathbf{r}-\mathbf{r}')j(\mathbf{r}')dS(\mathbf{r}'), \end{aligned} \tag{106}$$

and the integral representation for interior fields has an additional factor of -1 in each term of the right-hand sides (see [5, 62]).

The boundary-integral formulation of the scattering problem involves the tangential traces $[j(\mathbf{r}),m(\mathbf{r})]^t$ of the total field $v = [H,E]^t$ as unknown variables and the tangential traces of the source fields $v^{\text{int}}_{\text{so}}$ and $v^{\text{ext}}_{\text{so}}$ in the term of inhomogeneity,

$$\begin{array}{l} q_1(\mathbf{r}) = \frac{\mu_1}{\bar{\mu}}(-n\times H^{\text{int}}_{\text{so}}) + \frac{\mu_0}{\bar{\mu}}(-n\times H^{\text{ext}}_{\text{so}}), \\ q_2(\mathbf{r}) = \frac{\varepsilon_1}{\bar{\varepsilon}}(n\times E^{\text{int}}_{\text{so}}) + \frac{\varepsilon_0}{\bar{\varepsilon}}(n\times E^{\text{ext}}_{\text{so}}). \end{array} \quad (\mathbf{r}\in\partial D)$$

The analogue of the system (88,89) is the pair

$$\begin{aligned} j(\mathbf{r}) - \frac{1}{\bar{\mu}}\int_{\partial D} n(\mathbf{r})\times[j(\mathbf{r}')\times\nabla(\mu_1 G_1 - \mu_0 G_0)]dS(\mathbf{r}') - \frac{1}{i\omega\bar{\mu}}\int_{\partial D}[n(\mathbf{r})\times m(\mathbf{r}')][\omega^2\varepsilon_1\mu_1 G_1 - \omega^2\varepsilon_0\mu_0 G_0]|dS(\mathbf{r}') + \\ - \frac{1}{i\omega\bar{\mu}}\int_{\partial D} n(\mathbf{r})\times[(m(\mathbf{r}')\cdot\nabla)\nabla(G_1 - G_0)]dS(\mathbf{r}') = q_1(\mathbf{r}), \end{aligned} \tag{107}$$

$$\begin{aligned} m(\mathbf{r}) - \frac{1}{\bar{\varepsilon}}\int_{\partial D} n(\mathbf{r})\times[m(\mathbf{r}')\times\nabla(\varepsilon_1 G_1 - \varepsilon_0 G_0)]dS(\mathbf{r}') + \frac{1}{i\omega\bar{\varepsilon}}\int_{\partial D}[n(\mathbf{r})\times j(\mathbf{r}')][\omega^2\varepsilon_1\mu_1 G_1 - \omega^2\varepsilon_0\mu_0 G_0]dS(\mathbf{r}') + \\ + \frac{1}{i\omega\bar{\varepsilon}}\int_{\partial D} n(\mathbf{r})\times[(j(\mathbf{r}')\cdot\nabla)\nabla(G_1 - G_0)]dS(\mathbf{r}') = q_2(\mathbf{r}), \end{aligned} \tag{108}$$

in which the functions G_0 and G_1 are evaluated at $\mathbf{r}-\mathbf{r}'$.

To derive these equations, we begin as before by letting ε and μ be constant over all of $\mathbb{R}^3$. We will see how arbitrary pairs of tangential fields (j,m) on ∂D can be decomposed uniquely into the sum of the tangential trace of an interior Maxwell field and the tangential trace of an exterior outgoing Maxwell field, both with Bloch wavevector κ. We shall omit the details of the proper functional spaces for the fields and their traces as well as technical aspects of the proofs; the reader can find this material in [62], Ch. 5, as well as [5, 61]. Instead, we present the analogue of the structure developed above for the Helmholz equation.

Define the boundary-integral operator

$$\mathscr{A}\begin{bmatrix} j \\ m \end{bmatrix} = \begin{bmatrix} A \\ A' \end{bmatrix}\begin{bmatrix} j \\ m \end{bmatrix}, \tag{109}$$

in which

$$A\begin{bmatrix} j \\ m \end{bmatrix}(\mathbf{r}) = \int_{\partial D} n(\mathbf{r})\times[j(\mathbf{r}')\times\nabla_{\mathbf{r}'}G(\mathbf{r}-\mathbf{r}')]dS(\mathbf{r}') - \frac{1}{i\omega\mu}\int_{\partial D}[n(\mathbf{r})\times m(\mathbf{r}')]\omega^2\varepsilon\mu G(\mathbf{r}-\mathbf{r}')dS(\mathbf{r}') + \\ - \frac{1}{i\omega\mu}\int_{\partial D} n(\mathbf{r})\times[(m(\mathbf{r}')\cdot\nabla_{\mathbf{r}'})\nabla_{\mathbf{r}'}G(\mathbf{r}-\mathbf{r}')]dS(\mathbf{r}'),$$

$$A'\begin{bmatrix} j \\ m \end{bmatrix}(\mathbf{r}) = \int_{\partial D} n(\mathbf{r})\times[m(\mathbf{r}')\times\nabla_{\mathbf{r}'}G(\mathbf{r}-\mathbf{r}')]dS(\mathbf{r}') + \frac{1}{i\omega\varepsilon}\int_{\partial D}[n(\mathbf{r})\times j(\mathbf{r}')]\omega^2\varepsilon\mu G(\mathbf{r}-\mathbf{r}')dS(\mathbf{r}') + \\ + \frac{1}{i\omega\varepsilon}\int_{\partial D} n(\mathbf{r})\times[(j(\mathbf{r}')\cdot\nabla_{\mathbf{r}'})\nabla_{\mathbf{r}'}G(\mathbf{r}-\mathbf{r}')]dS(\mathbf{r}').$$

Let $\mathscr{I}$ be the identity operator $\mathscr{I}[j,m]^t = [j,m]^t$. The Calderón projectors for the Maxwell system are

$$\mathscr{P}_{\text{int}} = \tfrac{1}{2}\mathscr{I} - \mathscr{A}; \quad \mathscr{P}_{\text{ext}} = \tfrac{1}{2}\mathscr{I} + \mathscr{A}. \tag{110}$$

The following statements can be proved; the first is trivial, and the others are nontrivial and involve the representation formulas (106) and the Sokhotski-Plemelj formulas.

1. $\mathscr{P}_{\text{int}} + \mathscr{P}_{\text{ext}} = \mathscr{I}$,
2. $\mathscr{P}_{\text{int}}^2 = \mathscr{P}_{\text{int}}$ and $\mathscr{P}_{\text{ext}}^2 = \mathscr{P}_{\text{ext}}$,
3. The range of $\mathscr{P}_{\text{int}}$ is the space of tangential traces $\begin{bmatrix} -n\times H \\ n\times E \end{bmatrix}$ of pseudo-periodic interior free Maxwell fields $\begin{bmatrix} H \\ E \end{bmatrix}$.
4. The range of $\mathscr{P}_{\text{ext}}$ is the space of tangential traces $\begin{bmatrix} -n\times H \\ n\times E \end{bmatrix}$ of pseudo-periodic exterior free Maxwell fields $\begin{bmatrix} H \\ E \end{bmatrix}$ that satisfy the outgoing condition.

Returning to the scattering problem with interior and exterior material constants (ε_1,μ_1) and (ε_0,μ_0), consider the traces of all the fields involved:

$$\begin{gathered} \psi = \begin{bmatrix} -n\times H \\ n\times E \end{bmatrix}, \\ \phi_{\text{so}}^{\text{int}} = \begin{bmatrix} -n\times H_{\text{so}}^{\text{int}} \\ n\times E_{\text{so}}^{\text{int}} \end{bmatrix}, \ \phi_{\text{sc}}^{\text{int}} = \begin{bmatrix} -n\times H_{\text{sc}}^{\text{int}} \\ n\times E_{\text{sc}}^{\text{int}} \end{bmatrix}, \\ \phi_{\text{so}}^{\text{ext}} = \begin{bmatrix} -n\times H_{\text{so}}^{\text{ext}} \\ n\times E_{\text{so}}^{\text{ext}} \end{bmatrix}, \ \phi_{\text{sc}}^{\text{ext}} = \begin{bmatrix} -n\times H_{\text{sc}}^{\text{ext}} \\ n\times E_{\text{sc}}^{\text{ext}} \end{bmatrix}. \end{gathered} \tag{111}$$

Because of the requirement of continuity of the tangential electric and magnetic fields, we have

$$\begin{aligned} \psi &= \phi_{\text{so}}^{\text{int}} + \phi_{\text{sc}}^{\text{int}}, \\ \psi &= \phi_{\text{so}}^{\text{ext}} + \phi_{\text{sc}}^{\text{ext}}. \end{aligned} \tag{112}$$

In analogy with the Helmholtz case, the interior scattered field $v_{\rm sc}^{\rm int}=[H_{\rm sc}^{\rm int},E_{\rm sc}^{\rm int}]^t$ satisfies the homogeneous Maxwell system in D and the interior source field extends to a field in D^c that satisfies the homogeneous Maxwell system with (ε_1,μ_1) and the outgoing condition. This means that $\phi_{\rm sc}^{\rm int}$ is in the nullspace of $\mathscr{P}_{\rm ext}^1$ and $\phi_{\rm so}^{\rm int}$ is in the range. Similarly, the exterior scattered field $v_{\rm sc}^{\rm ext}=[H_{\rm sc}^{\rm ext},E_{\rm sc}^{\rm ext}]^t$ satisfies the homogeneous Maxwell system in D^c and the interior source field extends to a field in D that satisfies the homogeneous Maxwell system with (ε_0,μ_0); thus $\phi_{\rm sc}^{\rm ext}$ is in the nullspace of $\mathscr{P}_{\rm int}^0$ and $\phi_{\rm so}^{\rm ext}$ is in the range. By projecting to the source fields, we obtain

$$\begin{aligned}\mathscr{P}_{\rm ext}^1\psi&=\phi_{\rm so}^{\rm int},\\ \mathscr{P}_{\rm int}^0\psi&=\phi_{\rm so}^{\rm ext}.\end{aligned}\tag{113}$$

For the problem of scattering of plane waves, the source traces are

$$\phi_{\rm so}^{\rm ext}=\begin{bmatrix}j_{\rm inc}\\ m_{\rm inc}\end{bmatrix},\quad \phi_{\rm so}^{\rm int}=\begin{bmatrix}0\\0\end{bmatrix}$$

where $\phi_{\rm so}^{\rm ext}$ is the tangential trace of a plane electromagnetic wave.

To cause the leading-order singularity in the Calderón projectors to cancel in a linear combination, we multiply them by the matrices

$$\Lambda_k=\begin{bmatrix}\mu_k/\bar\mu & 0\\ 0 & \varepsilon_k/\bar\varepsilon\end{bmatrix},$$

for $k=0,1$,

$$\left[\Lambda_1\mathscr{P}_{\rm ext}^1+\Lambda_0\mathscr{P}_{\rm int}^0\right]\psi=\Lambda_1\phi_{\rm so}^{\rm int}+\Lambda_0\phi_{\rm so}^{\rm ext}.\tag{114}$$

This equation is the boundary-integral system (107,108) for $j(\mathbf{r})$ and $m(\mathbf{r})$.

We are interested in solving the pair (113); the solution of the scattering problem is obtained from ψ through the decomposition (112) and the boundary-integral representation formulas (106). Any solution of the pair (113) is also a solution to the combination (114), and we must determine if a solution to the combination of the equations is a solution of the pair. As before, we find that (114) is equivalent to

$$\left.\begin{aligned}\mathscr{P}_{\rm ext}^1\psi&=\phi_{\rm so}^{\rm int}+\Lambda_1^{-1}f\\ \mathscr{P}_{\rm int}^0\psi&=\phi_{\rm so}^{\rm ext}-\Lambda_0^{-1}f\end{aligned}\right\}\text{ for some } f.\tag{115}$$

The reciprocal coefficients for the Maxwell system are

$$\begin{aligned}\varepsilon^0&=\mu_1\frac{\varepsilon_0+\varepsilon_1}{\mu_0+\mu_1},\quad \mu^0=\varepsilon_1\frac{\mu_0+\mu_1}{\varepsilon_0+\varepsilon_1}\quad\text{in } D,\\ \varepsilon^1&=\mu_0\frac{\varepsilon_0+\varepsilon_1}{\mu_0+\mu_1},\quad \mu^1=\varepsilon_0\frac{\mu_0+\mu_1}{\varepsilon_0+\varepsilon_1}\quad\text{in } D^c.\end{aligned}\tag{116}$$

and one can check that

$$\bar{\mathscr{P}}_{\rm int}^0=\Lambda_1\mathscr{P}_{\rm int}^1\Lambda_1^{-1}$$

is the interior Calderón projector for the constants (ε^0,μ^0) and that

$$\bar{\mathscr{P}}_{\rm ext}^1=\Lambda_0\mathscr{P}_{\rm ext}^0\Lambda_0^{-1}\tag{117}$$

is the exterior projector for the coefficients (ε^1,μ^1).

The pair (115) implies that $\mathscr{P}_{\rm int}^1\Lambda_1^{-1}f=0$ and $\mathscr{P}_{\rm ext}^0\Lambda_0^{-1}f=0$, or

$$\begin{aligned}\bar{\mathscr{P}}_{\rm int}^0 f&=0,\\ \bar{\mathscr{P}}_{\rm ext}^1 f&=0.\end{aligned}\qquad\text{(reciprocal system)}\tag{118}$$

A function f that satisfies this pair is simultaneously the trace of an exterior outgoing Maxwell field with constants (ε^0,μ^0) and the trace of an interior Maxwell field with constants (ε^1,μ^1). The extension of this field to $\mathbb{R}^3$ is a generalized guided mode of the reciprocal structure characterized by these new constants. Notice that

$$\varepsilon_0\mu_0=\varepsilon^1\mu^1,\quad \varepsilon_1\mu_1=\varepsilon^0\mu^0.\tag{119}$$

As in the case of the Helmholtz equation, uniqueness of the solution of the reciprocal scattering problem implies equivalence of the original scattering problem and the boundary integral equations (107,108). This result is summarized in the following theorem.

Theorem 18 *If the (reciprocal) structure with coefficients*

$$\begin{aligned} \varepsilon = \varepsilon^1,\ \mu = \mu^1 \quad & \text{in } D, \\ \varepsilon = \varepsilon^0,\ \mu = \mu^0 \quad & \text{in } D^c, \end{aligned}$$

defined in terms of given constants (ε_1, μ_1) *and* (ε_0, μ_0) *by* (116) *does not admit a free Maxwell field in the absence of a source (a generalized guided mode), then the boundary-integral system (107,108) is equivalent to the scattering problem for the harmonic Maxwell system in the (original) structure with*

$$\begin{aligned} \varepsilon = \varepsilon_1,\ \mu = \mu_1 \quad & \text{in } D, \\ \varepsilon = \varepsilon_0,\ \mu = \mu_0 \quad & \text{in } D^c. \end{aligned}$$

More specifically, with ϕ_{so}^{int} *and* ϕ_{so}^{ext} *defined as in* (111)*, the scattered field* $v_{sc} = [H_{sc}, E_{sc}]$ *with source fields* $v_{so}^{int} = [H_{so}^{int}, E_{so}^{int}]$ *and* $v_{so}^{ext} = [H_{so}^{ext}, E_{so}^{ext}]$ *is obtained by using the solution to (107,108),*

$$\begin{bmatrix} j(\mathbf{r}) \\ m(\mathbf{r}) \end{bmatrix} = \begin{bmatrix} -n(\mathbf{r}) \times H(\mathbf{r}) \\ n(\mathbf{r}) \times E(\mathbf{r}) \end{bmatrix}, \quad \mathbf{r} \in \partial D \tag{120}$$

in the representation formula (106) *for* $\mathbf{r} \in D$ *and its analog for* $\mathbf{r} \in D^c$.

For the Maxwell system, the reciprocal relations (116) satisfy

$$R^2 = I.$$

This means that every structure is the reciprocal of its own reciprocal.

Theorems 16 and 18 lead to a condition for the existence of guided modes in periodic slab structures. The following theorem can be strengthened somewhat by the condition $R^2(\varepsilon_0, \mu_0, \varepsilon_1, \mu_1) = (\varepsilon_0, \mu_0, \varepsilon_1, \mu_1)$, which holds for the Helmholtz equation with $\mu_0 = \mu_1$ and for the Maxwell system. It is given in [79] for polarized electromagnetic fields in two-dimensional nonmagnetic structures.

Theorem 19 (Existence of guided modes)

1. If the boundary-integral system (88,89) with zero source field, or equivalently,

$$(\Lambda_1 P^1_{ext} + \Lambda_0 P^0_{int})\psi = 0 \tag{121}$$

has a nontrivial solution, then the periodic structure with interior constants (ε_1, μ_1) *and exterior constants* (ε_0, μ_0) *or the reciprocal structure with constants given by the relations* (93) *admits a generalized guided mode of the Helmholtz equation (at the frequency and wavevector appearing in the projectors).*

2. If the boundary-integral system (107,108) with $q_1 = q_2 = 0$*, or equivalently,*

$$(\Lambda_1 \mathscr{P}^1_{ext} + \Lambda_0 \mathscr{P}^0_{int})\psi = 0 \tag{122}$$

has a nontrivial solution, then the periodic structure with interior constants (ε_1, μ_1) *and exterior constants* (ε_0, μ_0) *or the reciprocal structure with constants given by the relations* (116) *admits a generalized guided mode of the Maxwell equation.*

5 Resonance

Let us recapitulate what we have learned about resonant interaction of guided modes with plane waves and make clear the nature of the resonance that we wish to investigate.

We have seen that, if a slab admits a true guided mode at a real pair (κ_0, ω_0) in a (κ, ω)-regime for which at least one spatial harmonic is propagating, the frequency ω_0 of the guided mode is embedded in the spectrum of the pseudo-periodic Helmholtz or Maxwell operator in $\mathscr{S}$ for the Bloch wavevector κ. Restricted to the strip, the guided mode is a finite-energy eigenfunction. An embedded eigenvalue is typically nonrobust with respect to perturbation of (real) κ from κ_0 or perturbation of the geometry or material coefficients of the waveguide. The dissolution of the embedded eigenvalue coincides with the frequency's attaining an imaginary part as (κ, ω) remains on the complex dispersion relation for generalized guided modes. As we have discussed, the corresponding generalized modes with small imaginary part are leaky: they interact with the propagating spatial harmonics and therefore cannot persist as true guided modes. This resonant interaction lies behind the phenomenon of transmission anomalies and the enhancement of field intensity within the waveguide when the guide is illuminated by a plane wave. We will focus on perturbations of κ.

Physically speaking, true guided modes are idealized entities. They exist in a mathematical sense, as exact solutions to the Helmholtz or Maxwell equations in the absence of any external sources, oscillating with undiminished intensity for all time in an infinite waveguide. Every physical structure, in contrast, is subject to thermal and radiation losses due to material and fabrication limitations, and thus all guided modes in the laboratory or in nature must be initiated and sustained by a source of energy.

It is often useful to take the point of view that resonance in physical systems is the result of the proximity of the system to a idealized one that admits mathematically a guided mode or bound (finite-energy) state. The energy of the idealized bound state is embedded within a continuous spectrum corresponding to extended states. As the system is perturbed from the idealized one, the bound and extended states become coupled. The eigenvalue dissolves into the continuous spectrum and the bound state is destroyed, that is, the perturbed system possesses no finite-energy state. Instead, extended states near the bound-state frequency are sharply modified by the perturbation, and the perturbed system exhibits behavior that we call resonant.

In the context of quantum mechanics, this type of resonance is often called Feshbach resonance. Let us briefly discuss this setting. The autoionizing (Auger) states of the Helium atom provide the simplest example, which is treated in detail by Reed and Simon in §XXII.6 [73]. The idealized system in this case is described by the Hamiltonian of two *uncoupled* electrons in the presence of the (fixed) potential created by the positively charged Helium nucleus. The energy associated with a bound state in which both electrons are excited (above the ground state) is an eigenvalue of the idealized Hamiltonian that is embedded in the continuous spectrum corresponding to the extended states. When this idealized Hamiltonian is perturbed through a Coulomb coupling between the electrons, the eigenvalue disappears, and, instead of possessing a bound state, the physical system exhibits sharply modified states that are extended in the variable of one of the electrons; in other words, one of the electrons breaks free from the atom, causing it to ionize.

This Coulomb interaction between the electrons gives rise to anomalies in the graph of absorption *vs.* energy of the atom that are close to the energies of the idealized bound state of two excited electrons. An approximate formula for the anomalies is derived in [73] by continuation of the resolvent of the perturbed operator into the lower half complex energy plane. The graph of the function is the familiar Lorentzian, or Breit-Wigner, resonance shape

$$f(E) = \text{const.} \frac{1}{(E - E_{\mathrm{r}})^2 + (\Gamma/2)^2}, \tag{123}$$

in which E_{r} is a resonant frequency. The width Γ of the resonance at half the maximum height is given by the Fermi golden rule; a similar principle, as we shall show, arises for the double-spiked anomaly observed in the transmission of classical waves across periodic slabs.

The term "Fano resonance" is commonly applied to this double-spiked anomaly, which is observed in many resonant systems, including the Auger states of the noble gases (as Helium). The name originates from the work of Ugo Fano [23], in which he derived a formula for the anomaly with a parameter q that controls the relative size of the peak and dip as a function of energy,

$$f_q(\mathrm{e}) = \text{const.} \frac{|q + \mathrm{e}|^2}{1 + \mathrm{e}^2}, \tag{124}$$

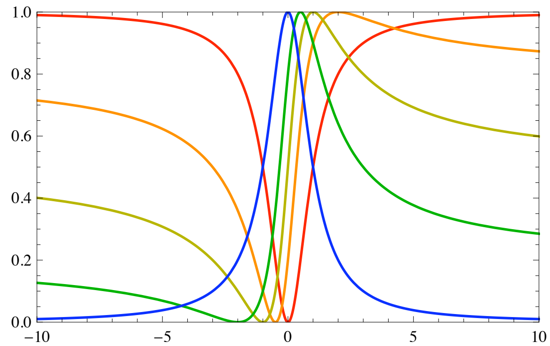

Figure 5: The Fano resonance (124), with $q = 0, \frac{1}{2}, 1, 2, \infty$, normalized to a maximum height of 1.

in which e represents the energy normalized to a characteristic width Γ of the anomaly,

$$\mathrm{e} = \frac{E - E_{\mathrm{res}}}{\Gamma/2}. \tag{125}$$

As q ranges over real numbers from infinity to zero, the graph morphs from a Lorentzian $1/(1+\mathrm{e}^2)$ to an inverted Lorentzian $\mathrm{e}^2/(1+\mathrm{e}^2)$, as illustrated in Fig. 5.

Our discussions treat resonance as a phenomenon observed in the frequency domain. The coupling of a bound state to extended states also has interesting and important implications for the time dynamics of the system. Soffer and Weinstein [83] approach the time-dependent resonant theory in quantum systems by treating the perturbed Schrödinger equation as a dynamical system under very general hypotheses. They demonstrate the Fermi golden rule for decay of transient fields and derive intermediate- and long-time behavior of the coupled system. We will restrict our analysis to the frequency domain.

5.1 Fano resonance

Fano's model is the simplest one that describes the linear coupling of a bound state to extended states under a perturbation of a system. One begins with a self-adjoint operator H_0 that admits an eigenvalue corresponding to a bound (finite-energy) state embedded within a continuous spectrum corresponding to extended states. As the operator is modified by a self-adjoint perturbation W that couples the bound and extended states of H_0, the eigenvalue dissolves into the continuous spectrum. The operator $H = H_0 + W$ possesses no finite-energy state, and extended states with energy near that of the bound state of H_0 are sharply modified.

A careful discussion of the derivation and application of the Fano formula is provided by Rau [72], whose close collaboration with Fano provides important insight into the subtleties of the physical context.

In $\mathbb{C} \times L^2(\mathbb{R})$, define the "unperturbed" self-adjoint operator H_0 by its explicit spectral representation,

$$H_0 : \begin{bmatrix} a \\ b(E) \end{bmatrix} \mapsto \begin{bmatrix} E_0\, a \\ E\, b(E) \end{bmatrix},$$

in which E_0 is real. The domain of H_0 is

$$\mathscr{D}(H_0) = \{[a, b(E)]^t : b(E), Eb(E) \in L^2(\mathbb{R})\},$$

and its spectrum is $\sigma(H_0) = \mathbb{R}$. The vector $[1,0]^t$ is a proper eigenfunction with embedded eigenvalue E_0, and the rest of the spectrum is absolutely continuous. For $\hat{E} \in \sigma(H_0)$, $[0, \delta(E - \hat{E})]^t$ are generalized eigenfunctions.

Define the perturbation

$$W : \begin{bmatrix} a \\ b(E) \end{bmatrix} \mapsto \begin{bmatrix} V_0 a + \int V^*(E')b(E')dE' \\ V(E)a + \int V_1(E,E')b(E')dE' \end{bmatrix},$$

in which V_0 and V_1 are real valued. If we assume that V and V_1 satisfy

$$V(E)(E+i)^{-1} \in L^2(\mathbb{R}),$$
$$V_1(E,E')(E'+i)^{-1} \in L^2(\mathbb{R}^2),$$

then W is symmetric on $\mathscr{D}(H_0)$ and, since $W(H_0+i)^{-1}$ is of Hilbert-Schmidt class, W is compact relative to H_0. Therefore H_0+W is self-adjoint with domain $\mathscr{D}(H_0+W) = \mathscr{D}(H_0)$ and the essential spectrum is unchanged,

$$\sigma_{\text{ess}}(H_0+W) = \sigma_{\text{ess}}(H_0) = \mathbb{R}.$$

This is an instance of a Theorem of Weyl; see Corollary 2 in §XIII.4 of [73].

Consider the generalized eigenvalue problem

$$H \begin{bmatrix} a \\ b(E) \end{bmatrix} = \hat{E} \begin{bmatrix} a \\ b(E) \end{bmatrix},$$

which is equivalent to the following equations:

$$\begin{aligned} &(\hat{E}-E)b(E) - \int V_1(E,E')b(E')dE' = V(E)a, \\ &\int V^*(E')b(E')dE' = (\hat{E}-E_0-V_0)a. \end{aligned} \tag{126}$$

We allow b to be a distribution (which depends on $\hat{E}$), with at most a δ-singularity at $E = \hat{E}$,

$$b(E) = \tilde{b}(E) + c\,\delta(E-\hat{E}),$$

in which c is a constant to be determined and $\tilde{b}$ is a function. Both c and $\tilde{b}$ depend on $\hat{E}$. The system (126) becomes

$$\begin{aligned} &(\hat{E}-E)\tilde{b}(E) - \int V_1(E,E')\tilde{b}(E')dE' \\ &\qquad\qquad = cV_1(E,\hat{E}) + aV(E), \\ &\int V^*(E')\tilde{b}(E')dE' = a(\hat{E}-E_0-V_0) - cV^*(\hat{E}). \end{aligned} \tag{127}$$

Fano's calculation. Fano's result in Sec. 2 of [23] is obtained if we set $V_1 = 0$ (he also has $V_0 = 0$). System (127) reduces to

$$\begin{aligned} &(\hat{E}-E)\tilde{b}(E) = aV(E), \\ &\int V^*(E')\tilde{b}(E')\,dE' + cV^*(\hat{E}) = a(\hat{E}-E_0-V_0). \end{aligned}$$

For the solution, we obtain

$$\begin{bmatrix} a \\ b(E) \end{bmatrix} = \begin{bmatrix} a \\ a\dfrac{V(E)}{\hat{E}-E} + c\delta(E-\hat{E}) \end{bmatrix}, \tag{128}$$

(the function $V(E)/(\hat{E}-E)$ is understood in the sense of distributions as a principal value) subject to the relation between a and c,

$$cV^*(\hat{E}) = a(\hat{E} - \mathring{E}(\hat{E})), \tag{129}$$

in which the shifted resonant frequency $\mathring{E}(\hat{E})$ is

$$\begin{aligned} &\mathring{E}(\hat{E}) = E_0 + V_0 + F(\hat{E}), \\ &F(\hat{E}) = \text{P.V.}\!\int \frac{|V(E')|^2}{\hat{E}-E'}dE'. \end{aligned} \tag{130}$$

For nonresonant $\hat{E}$, it is enlightening to set $c = C(\hat{E} - \mathring{E}(\hat{E}))$ with C a fixed arbitrary constant independent of $\hat{E}$ and write

$$\begin{bmatrix} a \\ b(E) \end{bmatrix} = C \begin{bmatrix} V^*(\hat{E}) \\ V^*(\hat{E}) \dfrac{V(E)}{\hat{E} - E} + (\hat{E} - \mathring{E}(\hat{E}))\delta(E - \hat{E}) \end{bmatrix} \quad \text{if } \hat{E} \neq \mathring{E}(\hat{E}). \tag{131}$$

Then, as $\hat{E} - \mathring{E}(\hat{E})$ vanishes and $V^*(\hat{E}) \neq 0$ when $\hat{E} - \mathring{E}(\hat{E}) = 0$, the δ part of the generalized eigenfunction vanishes, and we obtain

$$\begin{bmatrix} a \\ b(E) \end{bmatrix} = a \begin{bmatrix} 1 \\ \dfrac{V(E)}{\hat{E} - E} \end{bmatrix}, \ \hat{E} = \mathring{E}(\hat{E}) \text{ and } V(\hat{E}) \neq 0.$$

When both $\hat{E} - \mathring{E}(\hat{E}) = 0$ and $V^*(\hat{E}) = 0$, the generalized eigenspace for $\hat{E}$ is two-dimensional:

$$\begin{bmatrix} a \\ b(E) \end{bmatrix} = \begin{bmatrix} a \\ a\dfrac{V(E)}{\hat{E} - E} + c\delta(E - \hat{E}) \end{bmatrix} \quad \text{if } \hat{E} = \mathring{E}(\hat{E}) \text{ and } V(\hat{E}) = 0.$$

Let us now assume, as Fano does, that $V(E) \neq 0$ for all E and fix a generalized eigenvector, that is, choose C in (131). By defining the real-valued functions of real $\hat{E}$

$$z(\hat{E}) = \frac{\hat{E} - \mathring{E}(\hat{E})}{|V(\hat{E})|^2} \tag{132}$$

and

$$\Delta(\hat{E}) = \operatorname{arccot}(-z(\hat{E})/\pi), \tag{133}$$

an appropriately scaled eigenvector is written conveniently as

$$\begin{aligned} a_{\hat{E}} &= \frac{\sin\Delta(\hat{E})}{\pi V(\hat{E})}, \\ b_{\hat{E}}(E) &= \frac{\sin\Delta(\hat{E})}{\pi V(\hat{E})} \frac{V(E)}{\hat{E} - E} - \cos\Delta(\hat{E})\delta(E - \hat{E}). \end{aligned} \tag{134}$$

With this definition, $[a_{\hat{E}}, b_{\hat{E}}(E)]^t$ coincides with the generalized eigenvectors $\pm[0, \delta(E - \hat{E})]^t$ of H_0 as $\hat{E} \to \pm\infty$.

Fano considers the concrete situation in which the vector $[1,0]^t$ corresponds to a bound state $\varphi(x)$ of H_0 in $\mathbb{R}^3$, exponentially decaying as $|x| = r \to \infty$ ($x \in \mathbb{R}^3$), and the generalized eigenfunctions correspond to extended states $\psi_E(x)$ of H_0 that have oscillatory far-field behavior:

$$\psi_E(x) \to \sin(k(E)r + \alpha(E)), \quad (r \to \infty).$$

Through a generalized Fourier transform, an arbitrary state represented by $[a, b(E)]^t$ can be expressed as a superposition of the bound state and the extended states:

$$\begin{bmatrix} a \\ b(E) \end{bmatrix} \rightsquigarrow a\,\varphi(x) + \int b(E)\psi_E(x)\,dE. \tag{135}$$

To determine the far-field behavior of the spatial state $\Psi_{\hat{E}}(x)$ corresponding to the generalized eigenfunction (134) of the perturbed operator $H = H_0 + W$, we must compute

$$\Psi_{\hat{E}}(x) \to \int b_{\hat{E}}(E) \sin\big(k(E)r + \alpha(E)\big)\,dE, \ (r \to \infty).$$

In the limit as $r \to \infty$, the δ part of the integral contributes $-\cos\Delta(\hat{E})\sin(k(\hat{E})r+\alpha(\hat{E}))$ and the principal-value part contributes $-\sin\Delta(\hat{E})\cos(k(\hat{E})r+\alpha(\hat{E}))$. In the case that $k(\hat{E}) = m\hat{E}$ (space is homogeneous far from the origin), the latter is shown as follows.

Let us assume $V \in L^2(\mathbb{R})$, and define

$$U(\hat{E}) = \text{P.V.}\!\int \frac{V(E)}{\hat{E}-E}\sin(mEr+\alpha(E))dE,$$
$$f_\pm(E) = V(E)e^{\pm i\alpha(E)};$$

then

$$U(\hat{E}) = \frac{1}{2i}\int \frac{1}{\hat{E}-E}\left(f_+(E)e^{imEr} - f_-(E)e^{-imEr}\right)dE.$$

Now go over to the Fourier variable and use the representation of the Hilbert transform there (*e.g.* [13] §2.3),

$$g(\hat{E}) = -\frac{1}{\pi i}\int \frac{1}{\hat{E}-E}f(E)dE,$$
$$\iff \mathscr{F}g(\xi) = \text{sgn}(\xi)\mathscr{F}f(\xi),$$

to obtain

$$\mathscr{F}U(\xi) = -\tfrac{\pi}{2}\text{sgn}(\xi)\left[\mathscr{F}f_+(\xi - \tfrac{mr}{2\pi}) - \mathscr{F}f_-(\xi + \tfrac{mr}{2\pi})\right],$$

which tends to

$$-\tfrac{\pi}{2}\left[\mathscr{F}f_+(\xi - \tfrac{mr}{2\pi}) + \mathscr{F}f_-(\xi + \tfrac{mr}{2\pi})\right]$$

in $L^2(\mathbb{R})$ as $r \to \infty$. Thus,

$$\left\| -\tfrac{\pi}{2}\left[f_+(\hat{E})e^{im\hat{E}r} + f_-(\hat{E})e^{-im\hat{E}r}\right] - U(\hat{E})\right\| \to 0$$

in $L^2(\mathbb{R})$ as $r \to \infty$, and the term in brackets is $2V(\hat{E})\cos(m\hat{E}r+\alpha(\hat{E}))$, as desired.

The result is that

$$\Psi_{\hat{E}}(x) \to -\left[\sin\Delta(\hat{E})\cos(k(\hat{E})r+\alpha(\hat{E})) + \cos\Delta(\hat{E})\sin(k(\hat{E})r+\alpha(\hat{E}))\right] = -\sin[k(\hat{E})r+\alpha(\hat{E})+\Delta(\hat{E})] \quad (r \to \infty).$$

As $\hat{E}$ traverses the real line, $z(\hat{E})$ passes from $-\infty$, through zero near the shifted resonance frequency $\mathring{E}(\hat{E})$ (assuming this frequency is unique), to ∞. This means that $\Delta(\hat{E})$ runs from 0 to π as $\hat{E}$ traverses $\mathbb{R}$, and therefore, the spatial asymptotic behavior of $\Psi_{\hat{E}}$ is as $-\psi_{\hat{E}}$ for $\hat{E}$ large and negative and as $\psi_{\hat{E}}$ for $\hat{E}$ large and positive. Thus the extended states are modified sharply near the resonant frequency but remain unaltered far from resonance.

Fano was interested more particularly in the way observable properties are modified by the resonance. Let T be a linear functional represented by a smooth function in the spectral variable E so that T can be applied to generalized eigenfunctions[4]. Evaluation at $x \in \mathbb{R}^3$ described above is an example. We are interested in comparing the effect of the perturbation W on the values that $|T|^2$ takes on generalized eigenfunctions, that is, we wish to compare $|T(\Psi_{\hat{E}})|^2$ to $|T(\psi_{\hat{E}})|^2$. By inserting the solution $[a_{\hat{E}}, b_{\hat{E}}(E)]^t$(134) into the general Fourier integral (135) and defining

$$\Phi_{\hat{E}} = \varphi + \text{P.V.}\!\int \frac{V(E)}{\hat{E}-E}\psi_E\, dE,$$

we find that $T(\Psi_{\hat{E}})$ is related to $T(\psi_{\hat{E}})$ through

$$T(\Psi_{\hat{E}}) = \sin\Delta(\hat{E})\frac{T(\Phi_{\hat{E}})}{\pi V(\hat{E})} - \cos\Delta(\hat{E})T(\psi_{\hat{E}}).$$

In terms of Fano's reduced energy variable

$$\text{e} = -\cot\Delta(\hat{E}) = \frac{\hat{E}-\mathring{E}(\hat{E})}{\pi|V(\hat{E})|^2} = \frac{\hat{E}-\mathring{E}(\hat{E})}{\Gamma_{\hat{E}}/2},$$

[4]Fano [23] considers the conjugate-linear functional $(\Psi_E|T|i)$, which is the "matrix element of a suitable transition operator T between an initial state i and the state Ψ_E", and whose square modulus is "the probability of excitation of the stationary state Ψ_E."

the spectral width of the resonance

$$\Gamma_{\hat{E}} = 2\pi |V(\hat{E})|^2,$$

and the shape parameter

$$q = \frac{T(\Phi_{\hat{E}})}{\pi V(\hat{E}) T(\psi_{\hat{E}})},$$

the ratio we seek is

$$\frac{|T(\Psi_{\hat{E}})|^2}{|T(\psi_{\hat{E}})|^2} = \frac{|q+\mathrm{e}|^2}{1+\mathrm{e}^2}. \tag{136}$$

The idea now is to use e instead of $\hat{E}$ a vicinity of the resonant frequency $\hat{E}^*$ for which $\hat{E}^* = \mathring{E}(\hat{E}^*)$ and hold q fixed. Such an approximation is justified if $V(\hat{E}) \ll 1$ near $\hat{E}^*$, allowing q and Γ to be approximated by their values at $\hat{E}^*$ for values of $\hat{E}$ with $|\hat{E} - \hat{E}^*|$ on the order of a few times $\Gamma_{\hat{E}^*}$. This is the situation in which the coupling of continuum to bound states is weak near $\hat{E}^*$ and the width Γ of the resonance is therefore narrow.

If one linearly interpolates of the graph of the Fano anomaly through the resonance, the result is flat, whereas experimental data show a nonzero "background" slope. Fano treats this discrepancy for the Helium atom by fitting a modified formula with a nonzero slope to the data. He also extends his treatment to systems with multiple continua or multiple bound states. It has become common in the literature on resonance in classical and quantum systems to fit a Fano formula to experimental data.

5.2 Transmission resonance

Examples of anomalous transmission of energy through slab structures and related resonant systems abound in the literature. Since the late 1990s, there has appeared a vast amount of literature on enhanced transmission of electromagnetic waves through periodic structures, in particular, optical transmission of through metallic sheets with sub-wavelength arrays of holes or dimples. In the case of metal structures, it is generally understood that the transmission is enhanced or inhibited because of coupling of incident plane waves with the surface plasmons of the structure. In fact, there has been quite a lively discussion and controversy surrounding the mechanism. We cannot adequately represent the scope of the recent literature here, but we will presently indicate some of the basic issues and provide some references.

The theory that we present in this Chapter is a part of the story. While one does not expect the ensuing analysis to extend to all cases of anomalous transmission, it is reasonable to expect that it can be adapted to those situations in which one can identify an idealized (lossless) structure that is somehow close to the resonant one. One important phenomenon that does not fall into the setting of the dissolution of an embedded eigenvalue is the Wood anomaly that occurs at cutoff frequencies of the spatial harmonics; this phenomenon also plays a role in enhanced transmission, and is treated mathematically in [53]. The peaks observed in the transmission of plane-wave energy across metal slabs with thin slits or in Fabry-Perot resonance (the mirror effect of organized reflection from the walls of a slab) [41, 77] are also not generally connected with guided modes.

We will analyze in detail the particular case of perturbation of the Bloch wavenumber in scalar (acoustic or polarized electromagnetic) waves in lossless two-dimensional slabs, which encompasses those composed of lossless penetrable materials as well as perfect conductors and acoustically hard or soft surfaces. A numerical example is shown in Fig. 6. If the source field is taken to be incident upon the slab from the left,

$$u^{\text{inc}}(x,z) = \sum_{m \in \mathscr{Z}_p} a_m^{\text{inc}} e^{i\eta_m z} e^{i(m+\kappa)\cdot x},$$

with all $b_m^{\text{inc}} = 0$ in (16), the transmitted time-averaged energy flux of one period of the scattered field through a plane parallel to the slab is given by

$$\mathscr{E}^{\text{trans}} = \operatorname{Im} \int_{\Gamma_+} \mu_0^{-1} \bar{u} \partial_n u = \mu_0^{-1} \sum_{m \in \mathscr{Z}_p} \eta_m |b_m|^2.$$

The corresponding energy flux $\mathscr{E}^{\text{inc}}$ for the incident field is obtained by using a_m^{inc} in place of b_m in the rightmost expression, and we define

$$T^2 = \frac{\mathscr{E}^{\text{trans}}}{\mathscr{E}^{\text{inc}}}.$$

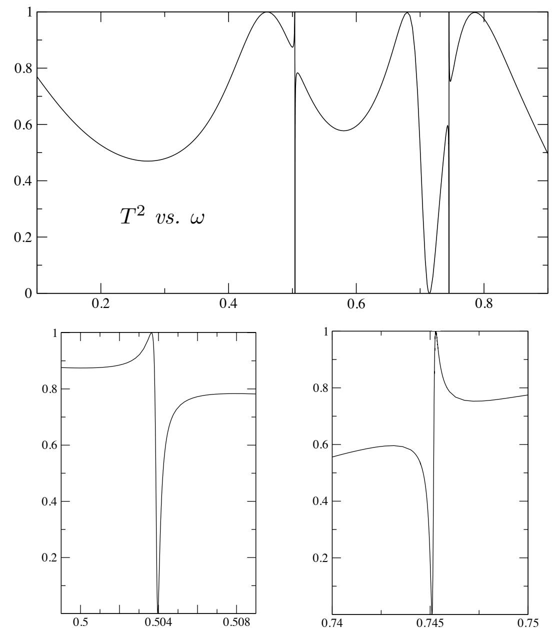

Figure 6: Numerical computation of the transmitted energy T^2 as a function of reduced frequency ω, with $\kappa = 0.02$. The scatterer is a single infinite 2π-periodic row of infinitely tall rods with radius $\pi/2$, $\varepsilon_1 = 10$, and $\mu_1 = 1$. In the exterior medium, $\varepsilon_0 = \mu_0 = 1$. There are guided modes at the (κ, ω) pairs $(0, \sim 0.5039)$ and $(0, \sim 0.7452)$. In this frequency range, there is exactly one propagating spatial harmonic.

The extension of the analysis of transmission resonance to doubly periodic structures and the full Maxwell system as well as to perturbations of the geometry and material properties, including small losses, of the structure will certainly lead to new interesting features and formulas. Several categories of transmission anomalies at normal incidence that arise from the introduction of a channel after every six rows of an otherwise perfect square-lattice photonic crystal slab are reported in [31], and it appears that the sharpest of them, which coincide with very high field amplitude enhancement in the slab, are a result of the dissolution of a guided mode.

In [14], Ebbesen, *et. al.*, reported the extraordinary transmission of light through metal sheets with a periodic array of holes whose spacing is smaller than the wavelength of the incident light. Since then, there has been much literature by many authors expounding the role of plasmons and the Wood anomaly in the theory of enhanced transmission, [6, 25, 26, 30, 39, 42, 45, 46, 47, 54, 56, 59], and the role of evanescent fields [49]. Many investigations involve coupled-mode analysis, in which the slab/ambient-space system is modeled by the prominent features of the waves it supports: the incoming waves, the surface plasmon polaritons, and the modes of the holes in a metal sheet, [54, 67]. Electric circuit models have also been successfully used to compute transmission anomalies [59]. A review of literature on this subject is given in [24].

Our analysis of transmission anomalies is based on an analytic connection of the scattering states of a slab to the generalized guided modes and analytic perturbation about an isolated real point (κ_0, ω_0) on the complex dispersion relation for generalized guided modes. This is accomplished through the auxiliary problem

$$A(\kappa, \omega)\psi(\kappa, \omega) = \phi(\kappa, \omega)$$

described at the beginning of Sec. 4. The operators $A(\kappa, \omega)$ act in a common Banach space $\mathscr{H}$. In the case of acoustic or electromagnetic scattering by a homogeneous periodic slab with a smooth boundary, the operator A is the boundary-integral operator derived in Sec. 4.2 and 4.4,

$$A = \Lambda_1 P^1_{\text{ext}} + \Lambda_0 P^0_{\text{int}}.$$

It can be shown that this operator is of the form $I + C$, where C is compact. For the two-dimensional scalar case, this is shown in [79]; the operator is posed in $\mathscr{H} = H^s(\partial D) \oplus H^{s-1}(\partial D)$, where s is most naturally taken to be $1/2$.

The following exposition follows that of [80] and [71] for two-dimensional problems in which the scatterer is periodic in one direction so that κ is scalar, and where the guided mode is simple. We shan't treat the case of guided modes of multiplicity greater than one, which are associated with multiple anomalies that emanate from the modes' characteristic (κ,ω) pair.

Consider a nonrobust guided slab mode corresponding to the simple eigenvalue 0 of $A(\kappa_0,\omega_0)$. This means that there is a neighborhood $U\subset\mathbb{C}^2$ of (κ_0,ω_0) and a simple closed curve C encircling the origin in the complex λ plane such that, for all $(\kappa,\omega)\in U,\ A(\kappa,\omega)$ has a unique, simple eigenvalue $\tilde{\ell}(\kappa,\omega)$ contained in the region bounded by C and that $(\kappa,\omega)=(\kappa_0,\omega_0)$ is the unique point in $U\cap\mathbb{R}^2$ satisfying $\tilde{\ell}(\kappa,\omega)=0$. The relation

$$\tilde{\ell}(\kappa,\omega)=0 \quad \text{(dispersion relation)}$$

is a dispersion relation in U for generalized guided modes, and (κ_0,ω_0) represents an isolated point on the relation corresponding to a true guided mode, which falls off exponentially with distance from the slab.

By projecting onto the eigenspace corresponding to $\tilde{\ell}(\kappa,\omega)$, one is able to split the source and scattered fields into "resonant" and "nonresonant" components. Specifically, the spectral projection

$$P_1(\kappa,\omega)=\frac{1}{2\pi i}\oint_C(\lambda I-A(\kappa,\omega))^{-1}d\lambda,$$

in which C is a sufficiently small circle about 0 in the complex λ-plane, is jointly analytic in (κ,ω) at (κ_0,ω_0) (*i.e.,* in a neighborhood U of (κ_0,ω_0)). P_1 is a rank-one projection-valued function of (κ,ω) that commutes with A and whose image is the eigenspace of $A(\kappa,\omega)$ with eigenvalue $\tilde{\ell}(\kappa,\omega)$. An analytic eigenvector $\hat{\psi}(\kappa,\omega)$ is obtained by fixing an eigenvector $\hat{\psi}_0$ of $A(\kappa_0,\omega_0)$ and setting

$$\hat{\psi}(\kappa,\omega)=P_1(\kappa,\omega)\hat{\psi}_0.$$

To see that $\tilde{\ell}(\kappa,\omega)$ is analytic, observe that

$$P_1(\kappa_0,\omega_0)\hat{\psi}(\kappa,\omega)=\beta(\kappa,\omega)\hat{\psi}_0,$$

where $\beta(\kappa_0,\omega_0)=1$ and $\beta(\kappa,\omega)$ is analytic because $\hat{\psi}(\kappa,\omega)$ is, and that

$$P_1(\kappa_0,\omega_0)A(\kappa,\omega)\hat{\psi}(\kappa,\omega)=\tilde{\ell}(\kappa,\omega)\beta(\kappa,\omega)\hat{\psi}_0$$

is also analytic. Theory of spectral projections and analytic perturbation of eigenvalues can be found in many classic references, including Ch. 7 §3 of Kato [37], §XII.2 of [73], §5.6 of Hille and Phillips [33], Ch. XI of Riesz and Sz.-Nagy [76], as well as Steinberg [84].

The projection P_1 together with its complement $P_2=I-P_1$ form a partial spectral resolution of the identity on $\mathscr{H}$:

$$I=P_1+P_2,$$
$$A=\tilde{\ell}P_1+AP_2.$$

Now write A as

$$A=(\tilde{\ell}-1)P_1+\tilde{A},$$

where $\tilde{A}=P_1+AP_2$, and observe that $\tilde{A}$ is analytic with analytic inverse in a neighborhood of (κ_0,ω_0) and commutes with P_1 and P_2. One obtains the relation

$$AP_2\tilde{A}^{-1}P_2=P_2. \tag{137}$$

An analytic connection between scattering states and generalized guided modes is made as follows. Choose an analytic vector $\phi(\kappa,\omega)$ that represents a source field (such as the incident plane wave we take below) and split it into its resonant and nonresonant parts

$$\phi=P_1\phi+P_2\phi=\alpha\hat{\psi}+\phi_2.$$

The multiple α is analytic at (κ_0,ω_0). Indeed, since $\hat{\psi}$ and $\alpha\hat{\psi}$ are analytic, so are $P_1(\kappa_0,\omega_0)\hat{\psi}=\beta\hat{\psi}(\kappa_0,\omega_0)$ and $P_1(\kappa_0,\omega_0)\alpha\hat{\psi}=\alpha\beta\hat{\psi}(\kappa_0,\omega_0)$ and therefore also the functions α and $\alpha\beta$. Since $\beta(\kappa_0,\omega_0)=1$, α is analytic at (κ_0,ω_0).

For (κ,ω) near the dispersion relation $\tilde{\ell}(\kappa,\omega)=0$, the "resonant part" $\alpha\hat{\psi}$ of the source field will induce a proportionally high field, and we therefore normalized the source by a constant multiple (to be specified soon) $\ell = c\tilde{\ell}$ of the eigenvalue. The equation $A\psi = \ell\phi$ has a solution $\psi(\kappa,\omega)$ that is analytic at (κ_0,ω_0), namely

$$\psi = c\alpha\hat{\psi} + \ell\tilde{A}^{-1}\phi_2,$$

where we have used (137) and $\phi_2 = P_2\phi_2$. This is seen clearly in the matrix form,

$$A\psi = \begin{bmatrix} \tilde{\ell} & 0 \\ 0 & AP_2 \end{bmatrix} \begin{bmatrix} c\alpha\hat{\psi} \\ \ell\tilde{A}^{-1}\phi_2 \end{bmatrix} = \begin{bmatrix} \ell\alpha\hat{\psi} \\ \ell\phi_2 \end{bmatrix} = \ell\phi.$$

It is the analytic field $\psi(\kappa,\omega)$ that connects scattering states with guided modes. If $\tilde{\ell}(\kappa,\omega)=0$, $\psi(\kappa,\omega)$ represents a generalized guided mode, and otherwise, it represents a scattering state.

Let us return to the concrete situation in which the source field ϕ represents the incident plane waves $e^{i(\kappa\cdot x+\eta_0 z)}$. In the case of the Helmholtz equation or the Maxwell system, the integral representation formulas (77,78) or (106), together with the form (72) of the Green function, show that the coefficients of the propagating spatial harmonics of the reflected and transmitted fields are analytic functions of (κ,ω) at (κ_0,ω_0). We shall consider the regime in which there is exactly one propagating harmonic and therefore a single complex reflected coefficient $a(\kappa,\omega)$ and a single transmitted coefficient $b(\kappa,\omega)$. Because of the conservation of energy relation $|\ell|^2 = |a|^2+|b|^2$ for real pairs (κ,ω), we deduce the important condition that *ℓ, a, and b have a common root at* (κ_0,ω_0). We continue to assume that $\mathrm{Re}\,\omega_0>0$, so that $\mathrm{Im}\,\omega \le 0$ whenever $\ell(\kappa,\omega)=0$ for real κ near κ_0 (Theorem 15), as well as the generic condition that $\partial\ell/\partial\omega$, $\partial a/\partial\omega$, and $\partial b/\partial\omega$ do not vanish at (κ_0,ω_0). The analysis of transmission anomalies is based on the following conditions alone:

$$\begin{aligned}
&\ell(\kappa_0,\omega_0) = a(\kappa_0,\omega_0) = b(\kappa_0,\omega_0) = 0 \qquad \text{with } (\kappa_0,\omega_0)\in\mathbb{R}^2, \\
&|\ell(\kappa,\omega)|^2 = |a(\kappa,\omega)|^2 + |b(\kappa,\omega)|^2 \qquad \forall(\kappa,\omega)\in\mathbb{R}^2, && (138)\\
&\ell(\kappa,\omega)=0 \text{ with } \kappa\in\mathbb{R} \implies \mathrm{Im}\,\omega\le 0, && (139)\\
&\tfrac{\partial\ell}{\partial\omega}\neq 0,\ \tfrac{\partial a}{\partial\omega}\neq 0,\ \tfrac{\partial b}{\partial\omega}\neq 0, \text{ at } (\kappa_0,\omega_0). && (140)
\end{aligned}$$

The analytic perturbation theory of these three analytic functions about the true guided mode pair (κ_0,ω_0) is facilitated by the Weierstraß Preparation Theorem ([55] §16), which, because of conditions (138) and (140) provides the following forms in the variables $\tilde{\omega}=\omega-\omega_0$ and $\tilde{\kappa}=\kappa-\kappa_0$:

$$\begin{aligned}
\ell &= \left[\tilde{\omega} + \ell_1\tilde{\kappa} + \ell_2\tilde{\kappa}^2 + O(|\tilde{\kappa}|^3)\right]\left[1+O(|\tilde{\kappa}|+|\tilde{\omega}|)\right],\\
a &= \left[\tilde{\omega} + r_1\tilde{\kappa} + r_2\tilde{\kappa}^2 + O(|\tilde{\kappa}|^3)\right]\left[r_0 e^{i\theta_1} + O(|\tilde{\kappa}|+|\tilde{\omega}|)\right], \qquad (141)\\
b &= \left[\tilde{\omega} + t_1\tilde{\kappa} + t_2\tilde{\kappa}^2 + O(|\tilde{\kappa}|^3)\right]\left[t_0 e^{i\theta_2} + O(|\tilde{\kappa}|+|\tilde{\omega}|)\right].
\end{aligned}$$

All series are convergent for $(\tilde{\kappa},\tilde{\omega})$ in a neighborhood of $(0,0)$. The constant c has been chosen so that the leading coefficient in the second factor for ℓ is unity, and both r_0 and t_0 are positive. These forms guarantee an explicit analytic dispersion relation $\ell(\kappa,\omega)=0$ near (κ_0,ω_0),

$$\omega = W(\kappa) := \omega_0 - \ell_1(\kappa-\kappa_0) - \ell_2(\kappa-\kappa_0)^2 + \dots$$

and similar explicit expressions for the zero sets of a and b.

Theorem 20 *The following relations hold among the coefficients in the forms* (141)*:*

1. $r_0>0,\ t_0>0,\ r_0^2+t_0^2=1,$
2. $\ell_1 = r_1 = t_1 \in\mathbb{R},$
3. $\mathit{Im}\,\ell_2\ge 0,$
4. $\ell_2\in\mathbb{R} \iff r_2=t_2\in\mathbb{R} \iff \ell_2=r_2=t_2\in\mathbb{R}.$

If r_2 and t_2 are real and ℓ_2 is imaginary, then

5. $r_2 t_2 = -|\ell_2|^2$.

If $\ell_1 = 0$*, then*

6. $\mathit{Re}\,\ell_2 = r_0^2 \mathit{Re}\, r_2 + t_0^2 \mathit{Re}\, t_2$,

7. $|\ell_2|^2 = r_0^2 |r_2|^2 + t_0^2 |t_2|^2$.

Proof. The positivity of r_0 and t_0 is a consequence of the Weierstraß Preparation Theorem, and the third relation in (1.) follows from (138). Because of condition (139), ℓ_1 must be real and $\mathrm{Im}\,\ell_2$ positive.

To prove (2.), let $(\tilde{\kappa},\tilde{\omega})$ tend to $(0,0)$ along the set $\{(\tilde{\kappa},\tilde{\omega}) : \tilde{\omega}+\ell_1\tilde{\kappa}=0\} \subset \mathbb{R}^2$. The forms (141) imply

$$\begin{aligned}
&|\ell|^2 = O(\tilde{\kappa}^4),\\
&|a|^2 = r_0^2(|\mathrm{Re}\, r_1-\ell_1|^2+|\mathrm{Im}\, r_1|^2)\tilde{\kappa}^2 + O(|\tilde{\kappa}|^3),\\
&|b|^2 = t_0^2(|\mathrm{Re}\, t_1-\ell_1|^2+|\mathrm{Im}\, t_1|^2)\tilde{\kappa}^2 + O(|\tilde{\kappa}|^3),\\
&\qquad\qquad (\tilde{\kappa},\tilde{\omega})\to(0,0),\ \tilde{\omega}+\ell_1\tilde{\kappa}=0.
\end{aligned}$$

The balance of these powers in equation (138) implies $\ell_1 = r_1 = t_1$.

Now assume that r_2 and t_2 are real and let $(\tilde{\kappa},\tilde{\omega})$ tend to $(0,0)$ along the set $\{(\tilde{\kappa},\tilde{\omega}) : \tilde{\omega}+\ell_1\tilde{\kappa}+t_2\tilde{\kappa}^2=0\} \subset \mathbb{R}^2$ to obtain

$$\begin{aligned}
&|\ell|^2 = (|\mathrm{Re}\,\ell_2-t_2|^2+|\mathrm{Im}\,\ell_2|^2)\tilde{\kappa}^4 + O(|\tilde{\kappa}|^5),\\
&|a|^2 = r_0^2(r_2-t_2)^2\kappa^4 + O(|\tilde{\kappa}|^5),\\
&|b|^2 = O(\tilde{\kappa}^6),\\
&\qquad\qquad (\tilde{\kappa},\tilde{\omega})\to(0,0),\ \tilde{\omega}+\ell_1\tilde{\kappa}+t_2\tilde{\kappa}^2=0,
\end{aligned}$$

and then along the set $\{(\tilde{\kappa},\tilde{\omega}) : \tilde{\omega}+\ell_1\tilde{\kappa}+r_2\tilde{\kappa}^2=0\} \subset \mathbb{R}^2$ to obtain

$$\begin{aligned}
&|\ell|^2 = (|\mathrm{Re}\,\ell_2-r_2|^2+|\mathrm{Im}\,\ell_2|^2)\tilde{\kappa}^4 + O(|\tilde{\kappa}|^5),\\
&|a|^2 = O(\tilde{\kappa}^6),\\
&|b|^2 = t_0^2(t_2-r_2)^2\kappa^4 + O(|\tilde{\kappa}|^5),\\
&\qquad\qquad (\tilde{\kappa},\tilde{\omega})\to(0,0),\ \tilde{\omega}+\ell_1\tilde{\kappa}+r_2\tilde{\kappa}^2=0,
\end{aligned}$$

Using (138) again, each of these asymptotic regimes yields a relation among the coefficients, and the sum of them gives

$$(r_2-t_2)^2 = (\mathrm{Re}\,\ell_2-r_2)^2+(\mathrm{Re}\,\ell_2-t_2)^2+2|\mathrm{Im}\,\ell_2|^2 \qquad (\mathrm{Im}\, r_2=\mathrm{Im}\, t_2=0). \tag{142}$$

If ℓ_2 is imaginary, this relation simplifies to (5.). If $r_2=t_2$, then it implies $\ell_2=r_2=t_2$, which proves part of (4.).

To complete the proof of (4.), assume that $\ell_2\in\mathbb{R}$ and let $(\tilde{\kappa},\tilde{\omega})$ tend to $(0,0)$ along the set $\{(\tilde{\kappa},\tilde{\omega}) : \tilde{\omega}+\ell_1\tilde{\kappa}+\ell_2\tilde{\kappa}^2=0\} \subset \mathbb{R}^2$ to obtain

$$\begin{aligned}
&|\ell|^2 = O(\tilde{\kappa}^6),\\
&|a|^2 = r_0^2(|\mathrm{Re}\, r_2-\ell_2|^2+|\mathrm{Im}\, r_2|^2)\tilde{\kappa}^4 + O(|\tilde{\kappa}|^5),\\
&|b|^2 = t_0^2(|\mathrm{Re}\, t_2-\ell_2|^2+|\mathrm{Im}\, t_2|^2)\tilde{\kappa}^4 + O(|\tilde{\kappa}|^5),\\
&\qquad\qquad (\tilde{\kappa},\tilde{\omega})\to(0,0),\ \tilde{\omega}+\ell_1\tilde{\kappa}+\ell_2\tilde{\kappa}^2=0.
\end{aligned}$$

It follows from balancing powers in (138) that $\ell_2=r_2=t_2$.

To prove the last two relations, we compute $|\ell|^2$, $|a|^2$, and $|b|^2$ using the forms (141):

$$\ell\bar{\ell} = \left[\tilde{\omega}^2+\ell_1^2\tilde{\kappa}^2+2\ell_1\tilde{\omega}\tilde{\kappa}+2\mathrm{Re}\,\ell_2\tilde{\omega}\tilde{\kappa}^2+2\ell_1\mathrm{Re}\,\ell_2\tilde{\kappa}^3+(2\ell_1\mathrm{Re}\,\ell_3+|\ell_2|^2)\tilde{\kappa}^4+\dots\right][1+O(|\tilde{\kappa}|+|\tilde{\omega}|)],$$

$$a\bar{a} = \left[\tilde{\omega}^2+|r_1|^2\tilde{\kappa}^2+2r_1\tilde{\omega}\tilde{\kappa}+2\mathrm{Re}\, r_2\tilde{\omega}\tilde{\kappa}^2+2r_1\mathrm{Re}\, r_2\tilde{\kappa}^3+(2r_1\mathrm{Re}\, r_3+|r_2|^2)\tilde{\kappa}^4+\dots\right][r_0^2+O(|\tilde{\kappa}|+|\tilde{\omega}|)],$$

and there is a similar expression for $|b|^2$. Provided $\ell_1=0$, the $\tilde{\kappa}^4$ and $\tilde{\omega}\tilde{\kappa}^2$ terms simplify to

$$\begin{aligned}
&\tilde{\kappa}^4 \text{ term:} &&|\ell_2|^2 = r_0^2|r_2|^2+t_0^2|t_2|^2,\\
&\tilde{\omega}\tilde{\kappa}^2 \text{ term:} &&\mathrm{Re}\,\ell_2 = r_0^2\mathrm{Re}\, r_2+t_0^2\mathrm{Re}\, t_2.
\end{aligned}$$

■

The condition $\ell_1 = r_1 = t_1$ leads to useful expressions for the zero sets of ℓ, a, and b near (κ_0, ω_0):

$$\begin{aligned} \ell(\kappa,\omega) = 0 &\iff \omega = \omega_0 - \ell_1(\kappa-\kappa_0) - \ell_2(\kappa-\kappa_0)^2 - \dots, \\ a(\kappa,\omega) = 0 &\iff \omega = \omega_0 - \ell_1(\kappa-\kappa_0) - r_2(\kappa-\kappa_0)^2 - \dots, \\ b(\kappa,\omega) = 0 &\iff \omega = \omega_0 - \ell_1(\kappa-\kappa_0) - t_2(\kappa-\kappa_0)^2 - \dots. \end{aligned} \tag{143}$$

The statement that the guided mode at (κ_0, ω_0) is nonrobust with respect to perturbations of κ is implied by the generic inequality $\operatorname{Im}\ell_2 > 0$. While we are interested in calculating transmission anomalies near nonrobust guided modes, the ensuing analysis does not exclude the case that ℓ_2 is real.

Figs. 7 and 8 show resonant anomalies in the transmission coefficient

$$T(\kappa,\omega) = \left| \frac{b(\kappa,\omega)}{\ell(\kappa,\omega)} \right|, \tag{144}$$

which is the square root of the time-averaged energy flux transmitted across one period the slab relative to that of the incident wave.

Using the expansions (141), approximate formulas for ℓ, a, and b give an analytic formula for T^2 to any desired degree of accuracy. In order to capture the essential features of the anomaly, one must include the second-order terms in (143). Assuming $\operatorname{Im}\ell_2 > 0$, the resulting approximation has an error of first order in κ, as stated in Theorem 21 below.

Four of the graphs in Figs. 7 and 8 exhibit peaks and dips that reach 100% and 0%. This occurs when all of the coefficients r_n and t_n are real and the zero set of each of $a(\kappa,\omega)$ and $b(\kappa,\omega)$ in $\mathbb{C}^2$ intersects $\mathbb{R}^2$ in a curve (rather than just a point) described by the real function given in (143). The zero set of a in $\mathbb{R}^2$ describes the frequency ω as a function of κ at which 100% transmission is achieved, whereas the zero set of b describes the frequencies of 0% transmission.

The graphs exhibit noteworthy features that are established rigorously by the expansions. Assuming the coefficients of a and b are real, we observe the following:

1. For $\kappa = \kappa_0$, the structure supports a guided mode at frequency ω_0, yet there is no anomaly present in the graph of T *vs.* ω.

2. As κ is perturbed from κ_0, a guided mode is no longer supported, and a peak and a dip in the graph of T *vs.* ω emanate from the frequency ω_0 of the destroyed mode. To order $O((\kappa-\kappa_0)^2)$, both the peak and dip occur at $\omega \approx \omega_0 - \ell_1(\kappa-\kappa_0)$. Thus, if $\ell_1 \neq 0$, the spike passes through ω_0 at a speed of $-\ell_1$ as κ passes through κ_0 and for each $\kappa \neq \kappa_0$, both the peak and the dip are on the same side of ω_0.

3. To order $O((\kappa-\kappa_0)^3)$, the frequencies of the peak and the dip differ from one another by $(t_2 - r_2)(\kappa-\kappa_0)^2$. As long as $r_2 \neq t_2$, this implies that they appear in the same order, regardless of whether they are to the left or to the right of or straddling ω_0.

We will show presently that T^2 can approximated to order $O(|\tilde\kappa| + \tilde\omega^2)$ by an expression involving seven real parameters. For real (κ, ω),

$$\begin{aligned} |\ell(\kappa,\omega)| &= \left[\left| \tilde\omega + \ell_1\tilde\kappa + \ell_2\tilde\kappa^2 \right| + O(|\tilde\kappa|^3) \right] [1 + c_1\tilde\omega + c_2\tilde\kappa + O(\tilde\kappa^2 + \tilde\omega^2)], \\ |a(\kappa,\omega)| &= \left[r_0 \left| \tilde\omega + \ell_1\tilde\kappa + r_2\tilde\kappa^2 \right| + O(|\tilde\kappa|^3) \right] [1 + a_1\tilde\omega + a_2\tilde\kappa + O(\tilde\kappa^2 + \tilde\omega^2)], \\ |b(\kappa,\omega)| &= \left[t_0 \left| \tilde\omega + \ell_1\tilde\kappa + t_2\tilde\kappa^2 \right| + O(|\tilde\kappa|^3) \right] [1 + b_1\tilde\omega + b_2\tilde\kappa + O(\tilde\kappa^2 + \tilde\omega^2)], \end{aligned}$$

in which the coefficients of the second factors are real. The $\tilde\kappa^2$-terms in the first factors have been retained because, as we shall see, they are necessary for ensuring an error of $O(|\tilde\kappa|)$ in the ratio, which is possible if we assume that $\operatorname{Im}\ell_2 \neq 0$.

Now, we have

$$\left| \frac{a}{b} \right| = \frac{r_0|\tilde\omega + \ell_1\tilde\kappa + r_2\tilde\kappa^2| + O(|\tilde\kappa|^3)}{t_0|\tilde\omega + \ell_1\tilde\kappa + t_2\tilde\kappa^2| + O(|\tilde\kappa|^3)} (1 + \zeta\tilde\omega + O(|\tilde\kappa| + \tilde\omega^2)), \tag{145}$$

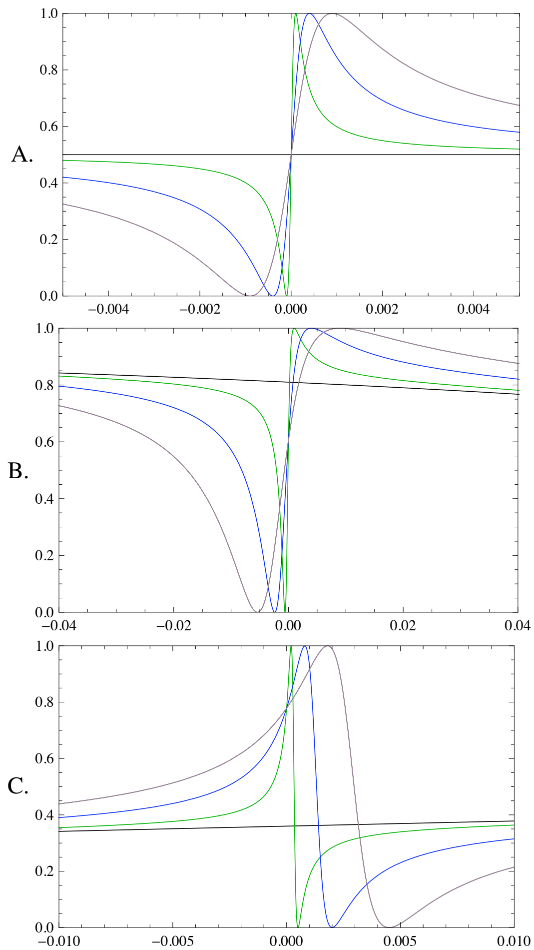

Figure 7: Transmission anomaly (T^2 *vs.* $\tilde{\omega}$) using the approximate formulas in Theorem 21 with $\ell_1 = 0$ and various values of the parameters $(t_0, \ell_1, t_2, r_2, \zeta)$.
A. $(2^{-\frac{1}{2}}, 0, 1, -1, 0)$; $\tilde{\kappa} = 0.0$, 0.01, 0.02, 0.03.
B. $(0.9, 0, 1.5, -2.5, 3)$; $\tilde{\kappa} = 0.0$, 0.02, 0.04, 0.06.
C. $(0.6, 0, -5, -2, -4)$; $\tilde{\kappa} = 0.0$, 0.01, 0.02, 0.03.

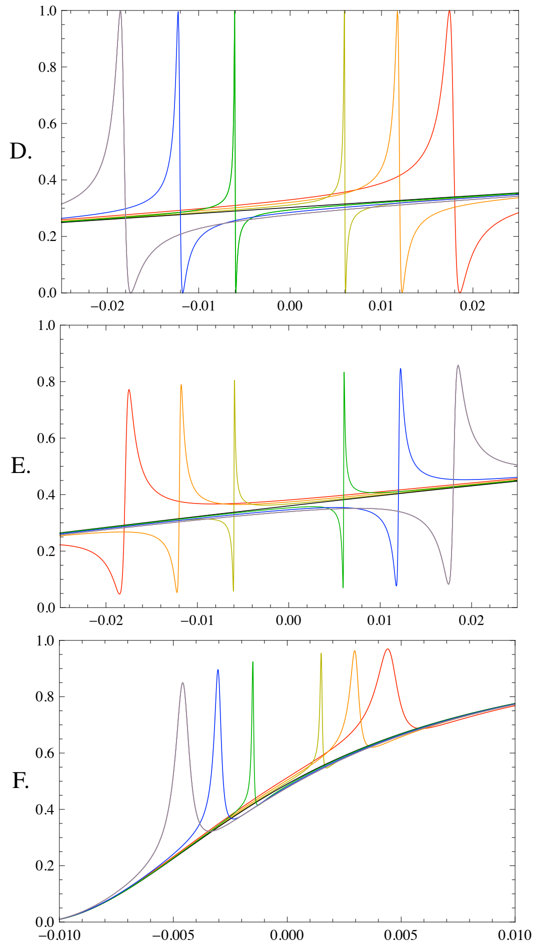

Figure 8: Transmission anomaly (T^2 *vs.* $\tilde{\omega}$) using the approximate formulas in Theorem 21 with $\ell_1 \neq 0$ and various values of the parameters $(t_0, \ell_1, t_2, r_2, \zeta)$; $\tilde{\kappa} = -0.009$, -0.006, -0.003, 0.0, 0.003, 0.006, 0.009.
D. $(0.55, 2, -7, 7, -5)$
E. $(0.6, -2, 5+4i, -5+4i, -8)$
F. $(0.7, 0.5, -1-8i, 1-2i, -90)$

where $\zeta = a_1 - b_1 \in \mathbb{R}$, and by means of this ratio, T^2 expressed as

$$T^2 = \frac{|b|^2}{|b|^2 + |a|^2} = \frac{1}{1 + |a/b|^2}. \tag{146}$$

More terms in both factors of the expansions of $|b|$ and $|a|$ would be needed in order to obtain an approximation of order $(\tilde{\kappa}^2 + \tilde{\omega}^2)$.

The validity of Theorem 20 relies on the assumption that $\operatorname{Im} \ell_2 \neq 0$, which, by part 4 of Theorem 20, is equivalent to $r_2 \neq t_2$ in the case that these are both real. The case that $t_2 = r_2 = \ell_2 \in \mathbb{R}$ is a singular situation in which there is nearly a real dispersion relation for guided modes in the presence of a propagating harmonic; the formula degenerates and exhibits no anomaly. In this case, higher orders in the expansions of a, b, and ℓ should be taken, up to the first coefficient of ℓ with a nonzero imaginary part, in order to capture the anomaly. A true real dispersion relation exists in the highly degenerate case that all coefficients ℓ_n vanish, in which case the guided mode at (κ_0, ω_0) is in fact robust with respect to perturbations of κ and no anomaly is present. This situation occurs, for example, if the structure is not genuinely periodic, as illustrated in Fig. 2B.

As we have discussed, the coefficient ℓ_1 controls the position of the transmission anomaly as a function of $\tilde{\kappa}$. If $\ell_1 \neq 0$, it is the derivative of a sort of dispersion relation for leaky modes, giving the real part of the frequency as a function of real κ.

The parameters in the formulas of the theorem have the following significance.

1. If $\ell_1 \neq 0$, then $\lim_{(\kappa,\omega)\to(\kappa_0,\omega_0)} T(\kappa, \omega) = t_0$. Thus, $T(\kappa, \omega)$ is continuous at (κ_0, ω_0).
2. If $\ell_1 = 0$, then $\lim_{\omega\to\omega_0} T(\kappa_0, \omega) = t_0$ and

$$\lim_{\kappa\to\kappa_0} T(\kappa, \omega_0) = \frac{t_0 |t_2|}{(t_0^2 |t_2|^2 + r_0^2 |r_2|^2)^{\frac{1}{2}}}. \tag{147}$$

The different limits can be seen in Fig. 7.

3. $\frac{\partial}{\partial \omega} T(\kappa_0, \omega)|_{\omega_0} = -2\zeta \frac{r_0^2 t_0^2}{(r_0^2 + t_0^2)^2}$.

It is also possible to derive an approximate formula for the phase of the transmitted field, which undergoes sharp variation near the resonant pair (κ_0, ω_0).

Theorem 21 *Given that ℓ, a, and b have a common root at $(\kappa_0, \omega_0) \in \mathbb{R}^2$; that their partial derivatives with respect to ω do not vanish at (κ_0, ω_0); and that $\operatorname{Im} \ell_2 \neq 0$ in the form* (141)*, the following approximations hold.*

$$\begin{aligned} T^2(\kappa, \omega) &= \frac{1}{1 + D_0^2} + O(|\tilde{\kappa}| + \tilde{\omega}^2) \\ &= \frac{E_0^2}{E_0^2 + 1} + O(|\tilde{\kappa}| + \tilde{\omega}^2) \\ &= \frac{t_0^2 |\tilde{\omega} + \ell_1 \tilde{\kappa} + t_2 \tilde{\kappa}^2|^2}{|\tilde{\omega} + \ell_1 \tilde{\kappa} + \ell_2 \tilde{\kappa}^2|^2} (1 + c_1 \tilde{\omega})^2 + O(|\tilde{\kappa}| + \tilde{\omega}^2), \end{aligned}$$

as $(\tilde{\kappa}, \tilde{\omega}) \to (0, 0)$ in $\mathbb{R}^2$, where D_0 and E_0 are defined by

$$D_0 = \frac{r_0 |\tilde{\omega} + \ell_1 \tilde{\kappa} + r_2 \tilde{\kappa}^2|}{t_0 |\tilde{\omega} + \ell_1 \tilde{\kappa} + t_2 \tilde{\kappa}^2|} (1 + \zeta \tilde{\omega}),$$

$$E_0 = \frac{t_0 |\tilde{\omega} + \ell_1 \tilde{\kappa} + t_2 \tilde{\kappa}^2|}{r_0 |\tilde{\omega} + \ell_1 \tilde{\kappa} + r_2 \tilde{\kappa}^2|} (1 - \zeta \tilde{\omega}).$$

Proof. The treatment of the asymptotics as $(\tilde{\kappa},\tilde{\omega})\to(0,0)$ is subtle. What allows obtention of the $O(|\kappa|)$ part of the estimate is the assumption that $\mathrm{Im}\,\ell_2\neq 0$. To prove the first approximation (the second and third are handled similarly), let us define A and B to be the numerator and denominator of the first factor in (145) and C to be the second factor. Their approximations that appear in D_0 are

$$\begin{aligned}&A_0=r_0|\tilde{\omega}+\ell_1\tilde{\kappa}+r_2\tilde{\kappa}^2|,\;\; A=A_0+O(|\tilde{\kappa}|^3),\\ &B_0=t_0|\tilde{\omega}+\ell_1\tilde{\kappa}+t_2\tilde{\kappa}^2|,\;\; B=B_0+O(|\tilde{\kappa}|^3),\\ &C_0=1+\zeta\tilde{\omega},\quad C=C_0+O(|\tilde{\kappa}|+\tilde{\omega}^2).\end{aligned}$$

With these definitions, we have

$$\begin{aligned}T^2&=\frac{B^2}{B^2+A^2C^2},\\ \frac{1}{1+D_0^2}&=\frac{B_0^2}{B_0^2+A_0^2C_0^2}.\end{aligned}\tag{148}$$

The crucial inequality is the lower bound

$$A_0^2+B_0^2\geq\tfrac{1}{4}(A_0+B_0)^2\geq\tfrac{1}{4}\min(t_0^2,r_0^2)(|\tilde{\omega}+\ell_1\tilde{\kappa}+r_2\tilde{\kappa}^2|+|\tilde{\omega}+\ell_1\tilde{\kappa}+t_2\tilde{\kappa}^2|)^2\geq m_0^2\tilde{\kappa}^4,\tag{149}$$

in which

$$m_0=\tfrac{1}{4}\min(t_0,r_0)\left[|\mathrm{Re}\,(r_2-t_2)|+|\mathrm{Im}\,r_2|+|\mathrm{Im}\,t_2|\right].$$

By the assumption that $\mathrm{Im}\,\ell_2\neq 0$ and part (4) of Theorem 20, m_0 is strictly positive.

In what follows, the symbol $O(|\tilde{\kappa}|^n)$ is used in place of any function that is "big-oh" of $|\tilde{\kappa}|^n$ as $(\tilde{\kappa},\tilde{\omega})\to(0,0)$, that is any function that is bounded in magnitude by a constant multiple by $|\tilde{\kappa}|^n$ for sufficiently small $(\tilde{\kappa},\tilde{\omega})$.

Since C_0^2 and C^2 as well as their reciprocals are $O(1)$, it follows that

$$\begin{aligned}&A_0^2=(B_0^2+A_0^2C_0^2)O(1),\\ &B_0+A_0C^2=(A_0+B_0)O(1)=(A_0^2+B_0^2)^{\frac{1}{2}}O(1),\\ &A_0^2+B_0^2=(B_0^2+A_0^2C^2)O(1).\end{aligned}\tag{150}$$

We compare the denominators in (148):

$$B^2+A^2C^2=B_0^2+A_0^2C_0^2+A_0^2O(|\tilde{\kappa}|+\tilde{\omega}^2)+(B_0+A_0C^2)f_1(\tilde{\kappa})+f_2(\tilde{\kappa}),\tag{151}$$

in which $f_1(\tilde{\kappa})=O(|\tilde{\kappa}|^3)$ and $f_2(\tilde{\kappa})=O(\tilde{\kappa}^6)$. The lower bound (149) gives

$$f_1(\tilde{\kappa})=O(|\tilde{\kappa}|^3)=m_0|(t_2-r_2)\tilde{\kappa}^2|O(|\tilde{\kappa}|)=(A_0^2+B_0^2)^{\frac{1}{2}}O(|\tilde{\kappa}|).\tag{152}$$

This, together with the second and third equations in (150), gives

$$(B_0+A_0C^2)f_1(\tilde{\kappa})=(A_0^2+B_0^2)O(|\tilde{\kappa}|)=(B_0^2+A_0^2C_0^2)O(|\tilde{\kappa}|).\tag{153}$$

The term $f_2(\tilde{\kappa})$ is estimated similarly:

$$f_2(\tilde{\kappa})=O(\tilde{\kappa}^6)=m_0^2|(t_2-r_2)\tilde{\kappa}^2|^2O(\tilde{\kappa}^2)=(A_0^2+B_0^2)O(\tilde{\kappa}^2)=(B_0^2+A_0^2C_0^2)O(\tilde{\kappa}^2).\tag{154}$$

This, together with (153) and the first equation in (150), give

$$B^2+A^2C^2=(B_0^2+A_0^2C_0^2)(1+O(|\tilde{\kappa}|+\tilde{\omega}^2)).\tag{155}$$

Next, we compare B^2 and B_0^2:

$$B^2=B_0^2+A_0g_2(\tilde{\kappa})+g_2(\tilde{\kappa}),\tag{156}$$

where $g_1(\tilde\kappa) = O(|\tilde\kappa|^3)$ and $g_2(\tilde\kappa) = O(\tilde\kappa^6)$. In a similar fashion, we obtain

$$A_0 g_1(\tilde\kappa) = A_0(A_0^2+B_0^2)^{\frac{1}{2}} O(|\tilde\kappa|) = (A_0^2+B_0^2)O(|\tilde\kappa|) = (B_0^2+A_0^2C_0^2)O(|\tilde\kappa|), \tag{157}$$

$$g_2(\tilde\kappa) = (B_0^2+A_0^2C_0^2)O(|\tilde\kappa|^2). \tag{158}$$

This gives

$$B^2 = B_0^2 + (B_0^2+A_0^2C_0^2)O(|\tilde\kappa|) \tag{159}$$

Finally, using (155) and (159), we obtain the result of the theorem:

$$\begin{aligned}(B^2+A^2C^2)^{-1}B^2 &= (B_0^2+A_0^2C_0^2)^{-1}(1+O(|\tilde\kappa|+\tilde\omega^2))\left[B_0^2+(B_0^2+A_0^2C_0^2)O(|\tilde\kappa|)\right] \\ &= \left[(B_0^2+A_0^2C_0^2)^{-1}B_0^2+O(|\tilde\kappa|)\right](1+O(|\tilde\kappa|+\tilde\omega^2)) = (B_0^2+A_0^2C_0^2)^{-1}B_0^2+O(|\tilde\kappa|+\tilde\omega^2).\end{aligned}$$

■

5.3 Relation to Fano resonance

The approximations of T^2 given in Theorem 21 generalize the Fano resonance (124) when viewed as functions of $\tilde\omega$. The seven real parameters reduce to two if the following conditions are satisfied (Fig. 7A):

1. $\ell_1 = 0$ (the anomaly remains at about ω_0);
2. r_2 and t_2 are real (the extremal values of the anomaly are 0 and 1);
3. $\mathrm{Re}\,\ell_2 = 0$ (the dispersion relation is purely imaginary up to order $\tilde\kappa^2$);
4. $\zeta = 0$ (the background transmission is flat).

Under these conditions, the connection between T^2 and the Fano resonance is made through

$$\begin{aligned}\Gamma &= 2\tilde\kappa^2 \mathrm{Im}\,\ell_2, \\ q &= \frac{t_2}{\mathrm{Im}\,\ell_2}, \\ \mathrm{e} &= \frac{\tilde\omega}{\tilde\kappa^2\,\mathrm{Im}\,\ell_2}.\end{aligned} \tag{160}$$

The relation between the width of the resonance and the imaginary part of ℓ_2 should be compared with the formulation of Fermi's golden rule by Reed and Simon at the end of §12.6 of [73].

With only the first three conditions, there arises a description of the parameter Γ in terms of r_2 and t_2. The relations (5) and (6) in Theorem 20 imply

$$\begin{aligned}t_2 &= \pm \mathrm{Im}\,\ell_2 \frac{r_0}{t_0}, \\ r_2 &= \mp \mathrm{Im}\,\ell_2 \frac{t_0}{r_0}.\end{aligned}$$

In particular, t_2 and r_2 are of opposite sign. This leads to

$$\Gamma = 2\tilde\kappa^2 \mathrm{Im}\,\ell_2 = 2\tilde\kappa^2 \frac{t_0}{r_0}|t_2| = 2\tilde\kappa^2 \frac{r_0}{t_0}|r_2|.$$

5.4 Structural perturbations and bifurcation of anomalies

As Figs. 7 and 8 illustrate, if $\ell_1 \neq 0$, the entire anomaly (peak and dip) is always to one side of ω_0 because it travels with speed $-\ell_1$ as a function of κ near κ_0 and widens proportionally to $\tilde\kappa^2$. But when $\ell_1 = 0$, the peak and dip may straddle the resonant frequency ω_0. For symmetric structures with $\kappa_0 = 0$, the dispersion relation (ω *vs.* κ) is necessarily even in κ, and we obtain $\ell_1 = 0$. In this case, the nonrobust mode at κ_0 is a standing wave exponentially confined to the slab. These two types of behavior can be connected through a variation of the structure where the guided mode pair (κ_0, ω_0) is a function of a structural parameter γ. There are two scenarios.

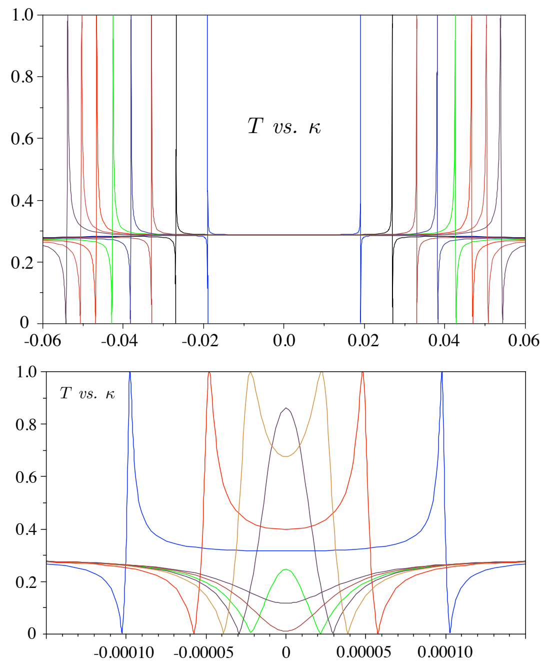

Figure 9: The bifurcation discussed in point (2) of Sec. 5.4. **Top:** At the critical value $\gamma = \gamma_0$ for which there is a single guided mode at $(\kappa_0(\gamma_0), \omega_0(\gamma_0)) = (0, \sim 0.977886)$, T is graphed as a function of κ for values of ω that run from $\omega_0 - 0.001$ to $\omega_0 - 0.008$ in increments of -0.001 as the colors run from blue to violet. **Bottom:** For a value of γ after bifurcation, the transmission is graphed as a function of κ for several fixed values of ω greater than the guided mode frequency $\omega_0(\gamma)$. The values of κ lie between the guided mode wavenumbers $\pm\kappa_0(\gamma)$.

1. One can choose a parameter γ that controls the asymmetry of the slab, with $\gamma = 0$ corresponding to a symmetric one. An example of this is a two-dimensional slab whose period consists of an elliptical rod that, for $\gamma = 0$, has the z-axis (perpendicular to the slab) as one of its principle axes, and where γ is an angle of rotation of the rod. The wavenumber κ_0 of the guided mode is an odd function of γ, as is ℓ_1, which passes from negative to positive as γ passes through zero.

2. One can define γ so that, for $\gamma < 0$ there are no guided mode pairs (κ_0, ω_0) in an open set $U \subset \mathbb{R}^2$ but that, for $\gamma = 0$, there is a single pair that bifurcates into two for $\gamma > 0$. The simplest model for which such a bifurcation can be constructed is a discrete one, in which the open waveguide is modeled by a one-dimensional lattice that is coupled to a uniform two-dimensional lattice, where the masses and spring constants of the waveguide as well as the coupling have period two. Any such structure is symmetric, so if the real pair (κ_0, ω_0) admits a guided mode, so does the pair $(-\kappa_0, \omega_0)$. In [70], Ptitsyna uses one of the two coupling constants as the structural parameter γ and analyzes this type of bifurcation in detail. The bifurcation is most clearly seen if the anomaly is graphed as function of κ for different fixed values of ω; it is shown in Fig. 9.

5.5 Amplitude enhancement

When resonant scattering occurs due to a perturbation that results in the destruction of a guided mode, the transmission anomalies that we have analyzed are accompanied by the phenomenon of enhancement of the field amplitude in the waveguide.

We have seen that the transmission coefficient exhibits no anomaly as a function of real ω at the wavenumber of the nonrobust guided mode $\kappa = \kappa_0$, whereas a very sharp anomaly appears near the frequency of the guided mode for arbitrarily small deviations $\tilde{\kappa} = \kappa - \kappa_0$. In numerical simulations of scattering of scalar plane waves by two-dimensional periodic dielectric waveguides, we observe a corresponding phenomenon in the field in the waveguide: There is no significant field amplitude enhancement near the guided mode frequency for fixed wavenumber $\kappa = \kappa_0$, whereas very high enhancement is observed for small nonzero $\tilde{\kappa}$, for ω in the vicinity of the transmission anomaly.

Determination of the field amplitude enhancement as a function of κ involves a subtlety of the source field ϕ that did not play a role in the derivation of the transmission anomaly, namely, that the resonant part in the decomposition of the trace of a plane-wave source field vanishes at the guided-mode pair (κ_0, ω_0). This is seen as follows. Recall the decomposition of the trace $\phi(\kappa, \omega)$ of an analytic source field

$$\phi(\kappa,\omega) = \alpha(\kappa,\omega)\hat{\psi}(\kappa,\omega) + \phi_2(\kappa,\omega). \tag{161}$$

We have shown that the multiple α is analytic at (κ_0, ω_0). If ϕ is the trace of a plane-wave source field for the Helmholtz equation,

$$u^{\text{inc}}(x,z) = e^{i(\tilde{m}+\kappa)x} e^{i\eta_{\tilde{m}} z}, \tag{162}$$

with $\eta_{\tilde{m}} > 0$ at (κ_0, ω_0), then $\phi(\kappa, \omega)$ is analytic at (κ_0, ω_0). We will prove that $\alpha(\kappa_0, \omega_0) = 0$. Because of Theorem 9, there is a solution to the scattering problem at (κ_0, ω_0) (although a solution is not unique). Let ψ be the trace of a solution, and let its partial spectral decomposition be

$$\psi = \gamma\hat{\psi} + \psi_2, \tag{163}$$

in which γ is a complex constant. Using the decompositions $A = \tilde{\ell}P_1 + AP_2$, (161), and (163) in the equation

$$A(\kappa_0,\omega_0)\psi = \phi(\kappa_0,\omega_0),$$

we obtain

$$\gamma\tilde{\ell}(\kappa_0,\omega_0)\hat{\psi} + A(\kappa_0,\omega_0)\psi_2 = \alpha(\kappa_0,\omega_0)\hat{\psi} + \phi_2(\kappa_0,\omega_0).$$

Since $\tilde{\ell}(\kappa_0, \omega_0) = 0$, we obtain $\alpha(\kappa_0, \omega_0) = 0$ and therefore an expansion

$$\alpha(\kappa,\omega) = \alpha_1\tilde{\kappa} + \alpha_2\tilde{\omega} + \dots. \tag{164}$$

The enhancement of the field amplitude should be manifest in the ratio

$$\left|\frac{\psi}{\ell\phi}\right| = \frac{|c\alpha\hat{\psi} + \ell\tilde{A}^{-1}\phi_2|}{|\ell\alpha\hat{\psi} + \ell\phi_2|}.$$

Since the nonresonant component of ψ as well as the source are of order ℓ, any meaningful enhancement may be measured by the ratio

$$\mathscr{A} = \frac{|c\alpha|}{|\ell|} = \frac{|\alpha|}{|\tilde{\ell}|} = \frac{|\alpha_1\tilde{\kappa} + \alpha_2\tilde{\omega}| + O(\tilde{\kappa}^2 + \tilde{\omega}^2)}{|\tilde{\omega} + \ell_1\tilde{\kappa} + \ell_2\tilde{\kappa}^2| + O(|\tilde{\kappa}|^3)}(|c| + O(|\tilde{\kappa}| + |\tilde{\omega}|), \quad (165)$$

as $(\kappa, \omega \to 0)$.

The numerical observations we mentioned above, namely the absence of field enhancement at the wavenumber of the guided mode and enhancement inversely proportional to $\tilde{\kappa}$ in the vicinity of the anomaly for small $\tilde{\kappa} \neq 0$, are borne out through analysis of $\mathscr{A}$.

By setting $\tilde{\kappa} = 0$ in (165), we obtain

$$\mathscr{A} = |c\alpha_2| + O(|\omega|), \quad \tilde{\kappa} = 0, \tilde{\omega} \to 0,$$

which demonstrates the absence of field enhancement at $\tilde{\kappa} = 0$. Assuming that $\mathrm{Im}\,\ell_2 \neq 0$, for nonzero $\tilde{\kappa}$, the denominator in (165) reaches its minimal value to order $O(|\tilde{\kappa}|^3)$ when $\tilde{\omega} = -\ell_1\tilde{\kappa} - \mathrm{Re}\,\ell_2\tilde{\kappa}^2$. Part 6 of Theorem 20 shows that, if $\ell_1 = 0$, this frequency is between the peak and the dip of the transmission coefficient. Under this relation between $\tilde{\omega}$ and $\tilde{\kappa}$, (165) yields

$$\mathscr{A} = \frac{1}{|\tilde{\kappa}|}\frac{|\alpha_1 - \alpha_2\ell_1|}{|\mathrm{Im}\,\ell_2|}(|c| + O(|\tilde{\kappa}|), \tilde{\omega} + \ell_1\tilde{\kappa} + \mathrm{Re}\,\ell_2\tilde{\kappa}^2 = 0\ , \tilde{\kappa} \to 0.$$

The leading order behavior of $1/|\tilde{\kappa}|$ is confirmed by numerical data in the two-dimensional Helmholtz case [80] and for a two-dimensional lattice model [70].

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