Waves in complex media:
Scattering of waves by periodic structures

Math 4999-5 (VIR course)
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1 Physical overview

Consider three-dimensional space filled with a medium, which may be homogeneous or inhomogeneous. In acoustic or elasticity theory, the medium can be distorted from its resting state by displacement of the molecules. We say that the medium supports a *displacement field*, and this displacement at each point of the medium induces stresses, which cause the molecules to move in response. Displacement fields can propagate as *waves*. Alternatively, we could consider electromagnetic fields in space filled with materials that respond to electric and magnetic fields in different ways.

We will be examining the idealized problem, where space consists of an ambient homogeneous medium in which an obstacle is placed. A material wave or electromagnetic wave that is traveling in the ambient medium will be diffracted, or scattered, by the obstacle because its material properties contrast with those of the ambient space. One may think of a radar signal bouncing off of an airplane or car or X-rays scattered by the bones of a patient. We will deal with scattering of waves by *periodic structures*, and in particular, *diffraction gratings* and *periodic slabs* (Fig. 1). This is a rather specialized problem from the general point of view of waves in complex media, but it is also a subject of much research that exhibits a large variety of interesting phenomena and unsolved problems.

Periodic slab structures act as *open waveguides*, in which the fields guided by the slab interact with fields arising from sources exterior to the slab. Applications include filters, antennas, lasers, and other devices, where light needs to be guided in specialized ways.

Some of the physics concepts associated with scattering by periodic structures are

1. diffractive orders (see Fig. 1),
2. guided modes,
3. resonant transmission and reflection,
4. frequency pass-bands and stop-bands,
5. resonant amplitude enhancement,
6. leaky modes (guided waves that lose energy to radiation),

7. lossy modes (guided waves that lose energy to heat).

Here are some good words to google:

photonic crystal

distributed feedback laser

open waveguide

Bloch waves

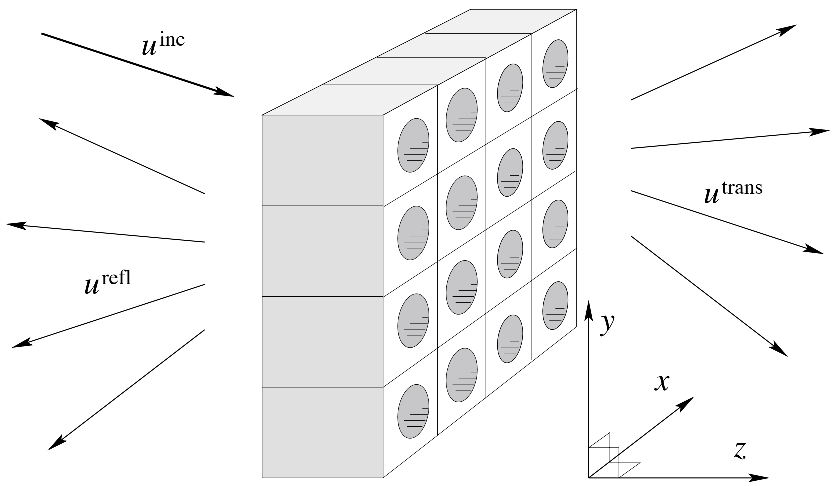
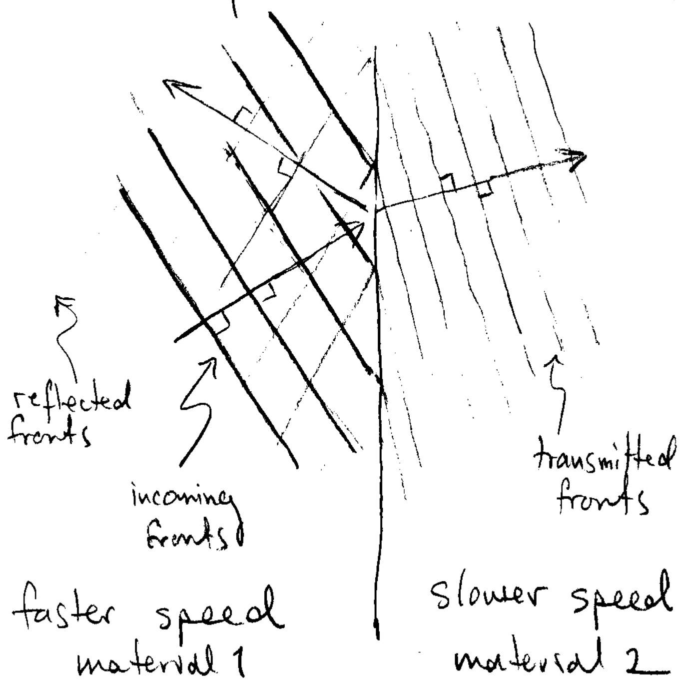


Figure 1. An example of a periodic slab scatterer. The slab is infinite and periodic in the x and y directions (only sixteen periods are shown) but of finite thickness in the z direction. Boundary conditions on the value or derivative of the field could be imposed, or the slab could be in natural contact with the ambient space to its left and right. This figure shows a slab consisting of two homogeneous materials. The reflected and transmitted fields depict the *diffractive orders* associated with the angle of incidence of the source field. The reason for the the diffraction in a finite number of directions is explained in section 2.5.2.

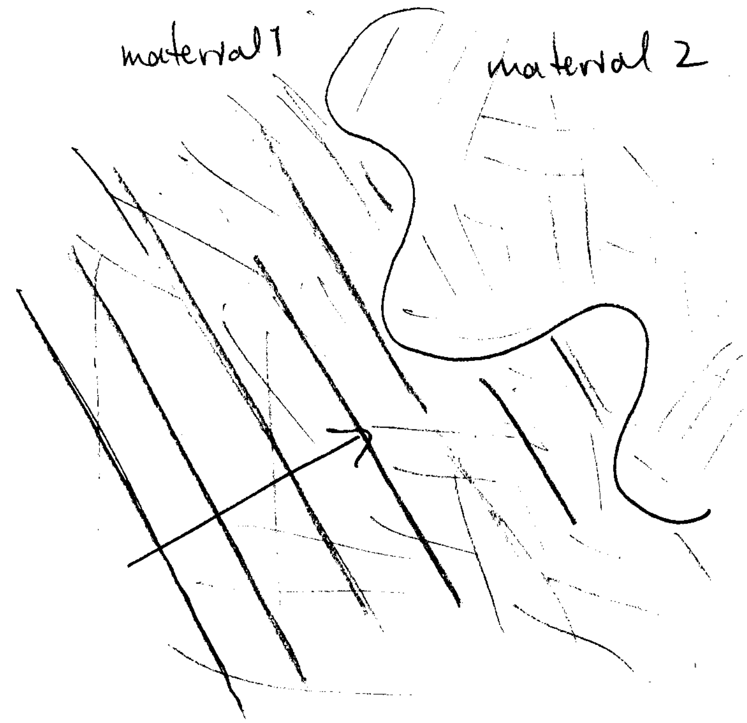
Concepts on wave propagation and scattering

- Transmission of monochromatic (fixed-frequency) plane waves across an interface or reflection from a boundary

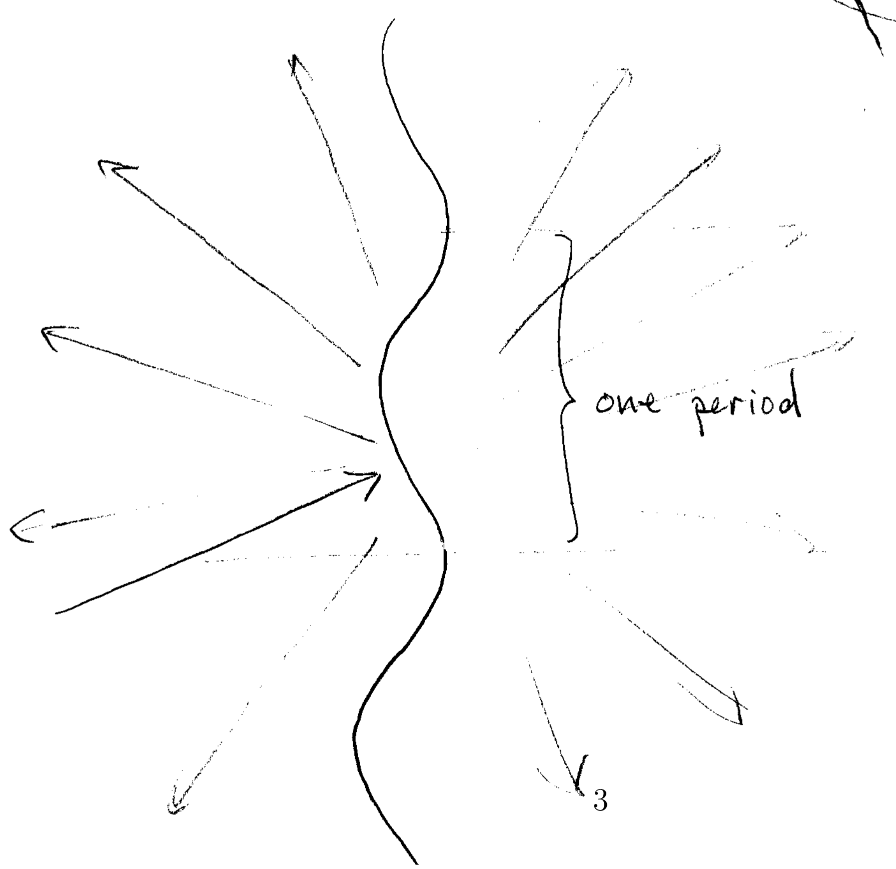
Reflection and transmission is determined by continuity of the wave structure and energy flux.



Planar interface: a plane wave is reflected in one direction and transmitted in one direction



Arbitrary interface: a plane wave is scattered in all directions.



A periodic interface: a plane wave is scattered in a finite number of directions – the propagating diffractive orders

2 Mathematical foundations

2.1 Notation

$\mathbb{R}^3$ = three-dimensional real Cartesian space, with coordinates (x, y, z),

Let $u : \mathbb{R}^3 \to \mathbb{R}$ be a scalar field,

Let $\mathbf{F} : \mathbb{R}^3 \to \mathbb{R}^3$ be a vector field with coordinates
$$\mathbf{F}(x, y, z) = \langle F_1(x, y, z), F_2(x, y, z), F_3(x, y, z)\rangle,$$

$u_t = \dfrac{\partial u}{\partial t}$, $u_{xx} = \dfrac{\partial^2 u}{\partial x^2}$, etc.,

$\nabla = \left\langle \dfrac{\partial}{\partial x}, \dfrac{\partial}{\partial y}, \dfrac{\partial}{\partial z} \right\rangle$ is the gradient operator,

$\nabla u = \left\langle \dfrac{\partial u}{\partial x}, \dfrac{\partial u}{\partial y}, \dfrac{\partial u}{\partial z} \right\rangle$, the gradient of u,

$\nabla\cdot \mathbf{F} = \dfrac{\partial F_1}{\partial x} + \dfrac{\partial F_2}{\partial y} + \dfrac{\partial F_3}{\partial z}$, the divergence of $\mathbf{F}$,

$\triangle = \nabla\cdot\nabla$ is the "Laplace operator", or "Laplacian",

$\triangle u = \nabla\cdot\nabla u$ is the Laplacian of the scalar field u, the divergence of the gradient of u.

2.2 Fundamental equations for fields

2.2.1 The wave equation

Denote a scalar acoustic field in $\mathbb{R}^3$ by $u(x, y, z; t)$. We assume that u satisfies the **wave equation**,

$$\rho\, u_{tt} = \nabla\cdot \tau \nabla u\,, \quad \text{(wave equation)} \tag{2.1}$$

in which $\rho(x, y, z)$ and $\tau(x, y, z)$ are physical properties of the medium. If ρ and τ are constant scalars, then, by appropriate choice of units, both can be taken to be 1, and the equation becomes the standard wave equation

$$u_{tt} = \triangle u\,. \quad \text{(wave equation)} \tag{2.2}$$

2.2.2 Harmonic fields and the Helmholtz equation

We will be considering "harmonic" solutions of the wave equation, solutions that oscillate at a particular **frequency** ω. This means that the field u has the form.

$$u(x, y, z; t) = u(x, y, z) \cos(\omega t)\,. \tag{2.3}$$

[Note that this is a mild abuse of notation, as we use the same symbol u to denote a function of four variables as well as a function of three variables.] It is convenient to take the time-dependent oscillatory factor to be of the form $e^{-i\omega t}$ and to take u to be complex-valued[1],

$$u(x,y,z;t) = u(x,y,z)e^{-i\omega t}\,. \tag{2.4}$$

Then the physical field is taken to be the real part of $u(x,y,z;t)$, and this is expressed conveniently in terms of the modulus and phase of $u(x,y,z)$,

$$u(x,y,z) = |u(x,y,z)|e^{i\theta(x,y,z)}, \tag{2.5}$$

$$\operatorname{Re} u(x,y,z;t) = |u(x,y,z)|\cos(\theta(x,y,z)-\omega t). \tag{2.6}$$

When we insert the form (2.4) into the wave equation (2.1), we obtain the **Helmholtz equation** for the spatial factor of the field,

$$\nabla\cdot\tau\nabla u + \omega^2\rho\, u = 0\,. \quad \text{(Helmholtz equation)} \tag{2.7}$$

2.3 The Helmholtz equation in homogeneous media

Separable solutions. Let us first consider the simple case in which the material coefficients are constant in $\mathbb{R}^3$, say $\epsilon = \epsilon_0 > 0$ and $\tau = \tau_0 > 0$. By setting $k^2 = \omega^2\epsilon_0/\tau_0 > 0$, we obtain the simpler Helmholtz equation

$$\triangle u + k^2 u = \partial_{xx}u + \partial_{yy}u + \partial_{zz}u + k^2 u = 0. \tag{2.8}$$

We will find special solutions of this equation by **separation of variables**, that is, we seek separable solutions,

$$u(x,y,z) = u_1(x)u_2(y)u_3(z). \tag{2.9}$$

Inserting this form into (2.8) and dividing by u, we obtain

$$\frac{u_1''(x)}{u(x)} + \frac{u_2''(y)}{u(y)} + \frac{u_3''(z)}{u(z)} + k^2 = 0, \tag{2.10}$$

and, from this, we see that each term is constant. This yields the system of equations

$$\frac{u_1''(x)}{u(x)} = \kappa_1^2\,, \quad \frac{u_2''(y)}{u(y)} = \kappa_2^2\,, \quad \frac{u_3''(z)}{u(z)} = \kappa_3^2\,, \tag{2.11}$$

$$\kappa_1^2 + \kappa_2^2 + \kappa_3^2 = k^2\,. \tag{2.12}$$

The general solution to the first equation is

$$u_1(x) = c_1 e^{i\kappa_1 x} + c_2 e^{-i\kappa_1 x}, \quad \text{if } \kappa_1 \neq 0\,, \tag{2.13}$$

$$u_1(x) = c_1 + c_2 x\,, \quad \text{if } \kappa_1 = 0\,. \tag{2.14}$$

and the equations for u_2 and u_3 have analogous solutions. Therefore u is a linear combination of separable functions of the form

$$u_{\text{sep}}(x,y,z) = e^{\pm i\kappa_1 x}e^{\pm i\kappa_2 y}e^{\pm i\kappa_3 z} = e^{\pm i\kappa_1 x \pm i\kappa_2 y \pm i\kappa_3 z}\,. \tag{2.15}$$

[1] Recall that $e^{s+i\theta} = e^s(\cos(\theta) + i\sin(\theta))$.

Traveling waves. Suppose that $\kappa_j^2 > 0$ for $j = 1, 2, 3$. In this case, we can take κ_i to be real and positive, and we have a solution of the Helmholtz equation,

$$u(x, y, z) = e^{i(\kappa_1 x + \kappa_2 y + \kappa_3 z)}. \tag{2.16}$$

The corresponding time-dependent solution of the wave equation is

$$u(x, y, z; t) = u(x, y, z)e^{-i\omega t} = e^{i(\kappa_1 x + \kappa_2 y + \kappa_3 z - \omega t)}, \tag{2.17}$$

and the physical field that it represents is

$$\mathrm{Re}\, u(x, y, z; t) = \cos(\kappa_1 x + \kappa_2 y + \kappa_3 z - \omega t). \tag{2.18}$$

This solution is a **traveling wave**; it is traveling in the direction of the **wavevector** $\boldsymbol{\kappa} = \langle \kappa_1, \kappa_2, \kappa_3 \rangle$ with velocity $v = \omega/|\boldsymbol{\kappa}|$. It is typically more convenient to work with the complex-exponential form of the solution, (2.16) or (2.17). The traveling wave can be expressed more concisely by using $\boldsymbol{\kappa}$ and the spatial vector $\boldsymbol{x} = \langle x, y, z \rangle$,

$$u(x, y, z; t) = e^{i(\boldsymbol{\kappa}\cdot\boldsymbol{x} - \omega t)}. \tag{2.19}$$

Multiplying by a complex constant $c = re^{i\theta}$ modifies the amplitude and shifts the phase,

$$c\, e^{i(\boldsymbol{\kappa}\cdot\boldsymbol{x} - \omega t)} = re^{i(\boldsymbol{\kappa}\cdot\boldsymbol{x} - \omega t + \theta)}. \tag{2.20}$$

Standing waves. A standing wave can be obtained as the sum of waves traveling in opposite directions and with the the same amplitude, for example,

$$\mathrm{Re}\, \left(e^{i(\boldsymbol{\kappa}\cdot\boldsymbol{x} - \omega t)} + e^{i(-\boldsymbol{\kappa}\cdot\boldsymbol{x} - \omega t)}\right) = 2\cos(\boldsymbol{\kappa}\cdot\boldsymbol{x})\cos(\omega t), \tag{2.21}$$

$$\mathrm{Re}\, \left(e^{i(\boldsymbol{\kappa}\cdot\boldsymbol{x} - \omega t)} - e^{i(-\boldsymbol{\kappa}\cdot\boldsymbol{x} - \omega t)}\right) = -2\sin(\boldsymbol{\kappa}\cdot\boldsymbol{x})\cos(\omega t). \tag{2.22}$$

Similarly, a traveling wave can be obtained as the sum of standing waves, for example,

$$\cos(\boldsymbol{\kappa}\cdot\boldsymbol{x})\cos(\omega t) - \sin(\boldsymbol{\kappa}\cdot\boldsymbol{x})\cos(\omega t) = \mathrm{Re}\, e^{i(\boldsymbol{\kappa}\cdot\boldsymbol{x} - \omega t)}. \tag{2.23}$$

Evanescent waves. Suppose that $\kappa_1^2 < 0$, whereas $\kappa_2^2 > 0$ and $\kappa_3^2 > 0$. In this case, κ is purely imaginary, and we can take $i\kappa_1 = -\nu_1 < 0$ (so $-i\kappa_1 = \nu_1 > 0$). The solution is

$$u(x, y, x; t) = e^{-\nu_1 x} e^{i(\kappa_2 y + \kappa_3 z - \omega t)}. \tag{2.24}$$

It is traveling parallel to the (y, z)-plane in the direction of the two-dimensional wave vector $\langle \kappa_2, \kappa_3 \rangle$ and exponentially decaying (or **evanescent**) in the direction of x (and exponentially growing in the opposite direction).

2.4 The Helmholtz equation in heterogeneous media.

Boundary conditions. Consider an obstacle occupying a region R in $\mathbb{R}^3$, with boundary ∂R, that is impenetrable by the waves represented by the function u. The properties of the surface of the obstacle determine the way that u behaves as it interacts with it. An acoustically soft obstacle is one whose surface can deform (minutely) to accommodate strains in the carrier medium. The result is that u vanishes on ∂R,

$$u = 0 \text{ on } \partial R. \quad \text{(soft obstacle)} \tag{2.25}$$

An acoustically hard obstacle is one whose surface is rigid. This corresponds to the condition $\tau\partial_n u = 0$ on ∂R,

$$\tau\partial_n u = 0 \text{ on } \partial R. \quad \text{(hard obstacle)} \tag{2.26}$$

A typical obstacle is neither perfectly soft nor hard, and instead admits a boundary condition of the "Robin" type

$$au + b\,\tau\partial_n u = 0 \text{ on } \partial R. \quad \text{(general obstacle)} \tag{2.27}$$

Interface conditions. The Helmholtz equation (2.7) makes sense if $\tau(\boldsymbol{x})$ is a differentiable function. In typical applications, however, there are abrupt changes in the material coefficients at the interfaces between two different (perhaps homogeneous) materials, such as between air and brick, or water and metal.

Suppose that we have two different media separated by an interface that is given by a surface S in $\mathbb{R}^3$. The material on one side is characterized by coefficients ϵ_1 and τ_1, and the material on the other side by ϵ_2 and τ_2. At the interface, the Helmholtz equation does not have meaning in the classical sense of derivatives. To determine how a solution on one side of the interface should connect with a solution on the other side, we return to the more fundamental formulation of the Helmholtz equation, the conservation law. This says that, for any bounded region R in $\mathbb{R}^3$, with boundary ∂R (a two-dimensional surface) and outward-directed normal vector n on ∂R, we have

$$\int_{\partial R} \tau\nabla u \cdot n\, dS \,+\, \omega^2 \int_R \epsilon u\, dV \;=\; 0\,. \tag{2.28}$$

This law allows us to speak of the divergence of $\tau\nabla u$ in the interior of R, even though it is not differentiable. All that is required is that $\tau\nabla u \cdot n$ be well defined on ∂R. Suppose that S divides R into two subdomains, R_1 (with $\epsilon = \epsilon_1$ and $\tau = \tau_1$) and R_2 (with $\epsilon = \epsilon_1$ and $\tau = \tau_1$), and set $\Gamma = S \cap R$, the part of the surface S that intersects the region R. Suppose that the normal vector n to Γ is directed into R_2. Now, we apply (2.28) to R, R_1, and R_2, and, for $i = 1, 2$, let $\tau_i\nabla u_i$ denote the limit of $\tau\nabla u$ to ∂R_i from inside R_i.

$$\int_{\partial R} \tau\nabla u \cdot n \,+\, \omega^2 \int_R \epsilon u = 0\,, \tag{2.29}$$

$$\int_{\partial R_1} \tau_1\nabla u_1 \cdot n \,+\, \omega^2 \int_{R_1} \epsilon_1 u = 0\,, \tag{2.30}$$

$$\int_{\partial R_2} \tau_2\nabla u_2 \cdot n \,+\, \omega^2 \int_{R_2} \epsilon_2 u = 0\,. \tag{2.31}$$

$$\tag{2.32}$$

If we subtract the second two equations from the first, the second term vanishes and only the integrals over Γ remain from the first term,

$$\int_\Gamma \tau_1\nabla u_1 \cdot n \,-\, \int_\Gamma \tau_2\nabla u_2 \cdot n \;=\; 0. \tag{2.33}$$

Since R is arbitrary, (2.33) holds for all sections Γ of S, we infer the continuity of $\tau\nabla u \cdot n$ across the interface,

$$\tau_1 \nabla u_1 \cdot n = \tau_2 \nabla u_2 \cdot n \quad \text{on } S. \tag{2.34}$$

If τ and ϵ are scalars (i.e., not tensors), then $\tau\nabla u \cdot n = \tau\partial_n u$, the (directional) derivative of u in the direction of n. This, together with the assumption of continuity of u gives two conditions on the interface,

$$\left.\begin{array}{l} u_1 = u_2 \\ \tau_1 \partial_n u_1 = \tau_2 \partial_n u_2 \end{array}\right\} \quad \text{on } S. \tag{2.35}$$

We can simply say that **"u and $\tau\partial_n u$ are continuous across the interface S."**

2.5 Periodic structures

The quantum mechanics of particles and radiation in periodic molecular structures has been studied and understood for a long time. But only a couple of decades ago did periodic structures in classical electromagnetics begin to receive widespread attention. These are structures in which the geometry of a cell is repeated periodically in three (or one or two) directions, such as a grating, a lincoln-log-type "logpile", an array of cylinders, or, in the simplest case, a repeating sequence of planar layers. They are called **photonic crystals**.

2.5.1 Photonic and acoustic crystals

The primary attraction of photonic crystals is that they are able to prohibit propagation of waves in certain frequency bands, called "stop-bands", whereas in the "pass-bands", they allow propagation. The idea is that the organized scattering of light waves by the periodic structure can cause coherent destructive interference of waves at stop-band frequencies. If a channel is carved through the crystal, frequencies that are disallowed in the bulk of the crystal may resonate in the channel and propagate along it, effectively allowing one to control the flow of light (photons), theoretically at any wavelength. *These band-gap and resonant phenomena are present at wavelengths of light that are comparable to the period of the structure.* The rigorous mathematical foundations of photonic crystals were laid down by several people, including P. Kuchment, A. Figotin, and A. Klein.

Acoustic and phononic crystals host sound and elastic waves with similar band-gap and wave-guideing behavior.

A periodic structure is represented mathematically by the wave equation or Helmholtz equation with periodic coefficients, that is, the functions ϵ and τ are periodic in $\boldsymbol{x}$. In certain foundational theoretical work, we often study structures whose period lattice is square, often normalized to 2π or 1,

$$\epsilon(x + 2\pi, y, z) = \epsilon(x, y + 2\pi, z) = \epsilon(x, y, z + 2\pi) = \epsilon(x, y, z)\,, \tag{2.36}$$
$$\tau(x + 2\pi, y, z) = \tau(x, y + 2\pi, z) = \tau(x, y, z + 2\pi) = \tau(x, y, z)\,. \tag{2.37}$$

for all $(x, y, z) \in \mathbb{R}^3$. This condition of periodicity can be written in the more compact form

$$\epsilon(\boldsymbol{x} + 2\pi\boldsymbol{n}) = \epsilon(\boldsymbol{x}) \quad \text{and} \quad \tau(\boldsymbol{x} + 2\pi\boldsymbol{n}) = \tau(\boldsymbol{x}) \quad \text{for all } \boldsymbol{n} \in \mathbb{Z}^3, \tag{2.38}$$

for all $(x, y, z) \in \mathbb{R}^3$ ($\mathbb{Z}$ is the set of integers.)

In a periodic structure, simple traveling waves of the complex-exponential form (2.19) are no longer admitted, as the coefficients are not constant. Instead, one seeks solutions of the form of a periodic function modulated by traveling wave,

$$u(x, y, z; t) = u_{\text{per}}(x, y, z)e^{i(\boldsymbol{\kappa}\cdot\boldsymbol{x}-\omega t)}. \tag{2.39}$$

The frequencies for which such a solution exists (for real wave vector $\boldsymbol{\kappa}$) compose the pass-bands, and frequencies for which no such solution exists make up the stop-bands.

2.5.2 Periodic slab scatterers

A periodic slab structure as in Figure 1 is periodic in two directions (x and y) but not in the third direction (z). In fact, outside a finite interval in z, the material coefficients $\rho = \epsilon$ and $\tau = \mu^{-1}$ are constant, say for $z < z_-$ and $z > z_+$, $\epsilon(x, y, z) = \epsilon_0$ and $\mu(x, y, z) = \mu_0$. This means that the physical structure is of finite thickness in the z-direction and ϵ_0 and μ_0 characterize the ambient space in which the structure is embedded.

Let us consider, for simplicity, a two-dimensional reduction of the three-dimensional problem of scattering of an incident plane wave by a periodic slab. This means that we suppose that ϵ and μ are constant in the y-direction, leaving only two variables of variation, a periodic one (x) and one in which the structure is bounded (z). So we can write $\epsilon(x, z)$ and $\mu(x, z)$, which are periodic in x but not in z. So we have

$$\epsilon(x + 2\pi, z) = \epsilon(x, z) \quad \text{and} \quad \mu(x + 2\pi, z) = \mu(x, z), \tag{2.40}$$

$$\epsilon(x, z) = \epsilon_0 \text{ and } \mu(x, z) = \mu_0 \quad \text{for } z < z_- \, , \; z > z_+. \tag{2.41}$$

As source fields, we will consider plane waves, traveling to the right and incident upon the slab from the left, that depend only on x and z so that we can disregard y in the mathematical formulation and pose the problem in the xz-plane. The incident plane wave is

$$u^{\text{inc}}(x, z) = e^{i(\kappa x + \eta_0 z)}, \tag{2.42}$$

in which κ and η_0 are chosen such that

$$\kappa^2 + \eta_0^2 = \epsilon_0\mu_0\omega^2 = k^2 \tag{2.43}$$

and $\eta_0 > 0$ (recall equation (2.13)—here, $\kappa_1 = \kappa$, $\kappa_2 = 0$, and $\kappa_3 = \eta_0$). Since we want both κ and η_0 to be real, neither is not allowed to exceed k in magnitude. Remember that, since the time-dependent factor is taken to be $e^{-i\omega t}$, the function u^{inc} represents a field traveling to the right at an angle of

$$\theta_{\text{inc}} = \arcsin(\kappa/k) \tag{2.44}$$

to the line perpendicular, or "normal", to the slab.

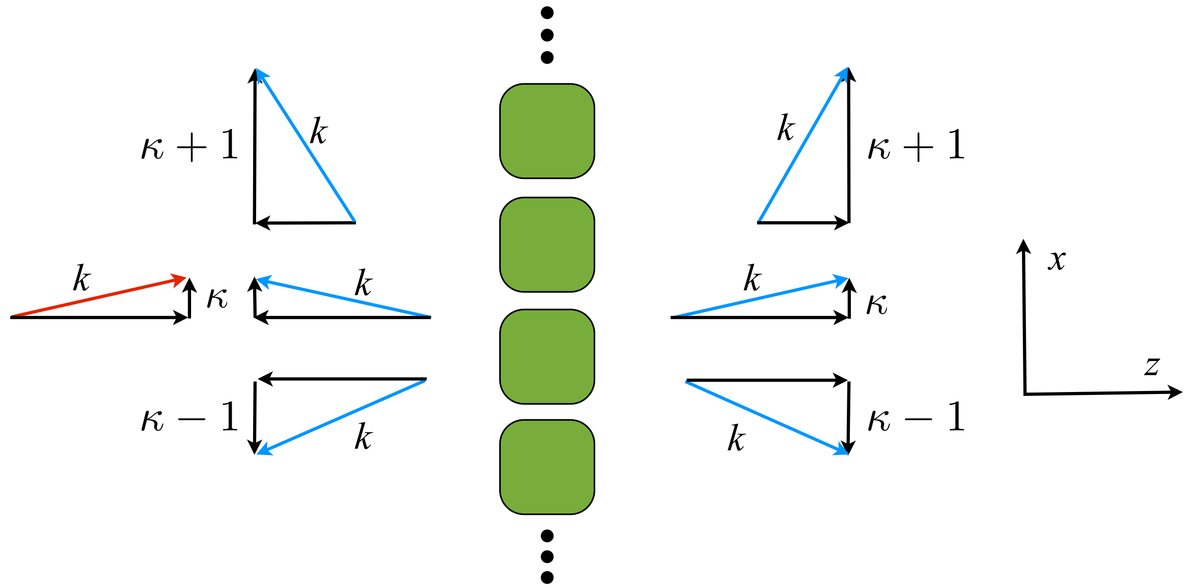


Figure 2. The green structure represents a two-dimensional periodic slab structure (a planar cross section of the physical three-dimensional structure). It continues periodically in the x-direction and is of finite width in the z-direction. The blue arrows represent the wavevectors of the outward propagating, or radiating, diffractive orders. The red arrow represents the wavevector of the incident field that we take in this exposition. In this diagram, $\kappa = 0.36$ and $k = 1.58$. Thus the only integers m for which $|\kappa + m| \leq k$ are $m = -1, 0, 1$.

Notice that, if you are observing this incoming wave from a given point (x, z) and you move parallel to the slab a distance of $2\pi n$ ($n \in \mathbb{Z}$), or n periods, then the structure looks exactly the same and the wave looks the same except for a phase factor of

$$e^{i2\pi n\kappa}. \tag{2.45}$$

We therefore expect the field $u(x, z)$ that results when $u^{\mathrm{inc}}(x, z)$ is scattered by the slab to look the same from either observation point, except for this phase. This means that, except for the phase factor, u should be periodic in the x-direction—it is a periodic part times the x-dependent factor of the incident field $e^{i\kappa x}$

$$u(x, z) = \breve{u}(x, z)\, e^{i\kappa x}, \tag{2.46}$$

in which $\breve{u}$ is 2π-periodic in x. In this context, the factor $e^{i2\pi\kappa}$, which represents the phase advance over one period, is called the *Bloch* or *Floquet* factor. A field of the form (2.46) is called *pseudoperiodic*, or, more specifically, κ-pseudoperiodic.

The total field has two parts: the *incident source field* u^{inc} and the *scattered, or diffracted, field* u^{sc}, which itself is κ-pseudoperiodic, $u^{\mathrm{sc}}(x, z) = \breve{u}^{\mathrm{sc}}(x, z)e^{i\kappa x}$. Each is equal to a periodic part multiplied by $e^{i\kappa x}$. Here is the decomposition of u into incident and scattered parts, written in terms of the pseudoperiodic field and in terms of the periodic factors:

$$u(x, z) = u^{\mathrm{inc}}(x, z) + u^{\mathrm{sc}}(x, z), \tag{2.47}$$

$$\breve{u}(x, z) = e^{i\eta_0 z} + \breve{u}^{\mathrm{sc}}(x, z). \tag{2.48}$$

In order to formulate the scattering problem correctly and unambiguously, we need to understand the conditions that the scattered field satisfies. Essentially, we need a condition that characterizes the property that u^{sc} radiates energy away from the slab to the left and right—it should be composed of plane waves traveling outward, as opposed to the incident field, which is traveling toward the slab (from the left). To do this, we need to understand how periodic functions of x are composed out of an infinite number of *spatial harmonics*. An essentially arbitrary 2π-periodic function f of x can be written uniquely as an infinite series

$$f(x) = \sum_{m\in\mathbb{Z}} c_m e^{imx}, \tag{2.49}$$

which is called the *Fourier series* of f. The c_m are called the *Fourier coefficients* of f, and they are unique. The essential feature of the Fourier harmonics is that *they are mutually orthogonal with respect to the inner product of integration over a period*:

$$\int_0^{2\pi} e^{imx} e^{-inx}\, dx \;=\; 2\pi\delta_{mn}, \tag{2.50}$$

where $\delta_{mn} = 0$ if $m \neq n$ and $\delta_{mn} = 1$ if $m = n$. This is known as the Kronecker delta symbol.

Now, lets expand the field $\breve{u}^{\mathrm{sc}}(x,z)$, which is periodic in x, in its Fourier series *as a function of x, for each fixed value of z*. The coefficients will depend on z because $\breve{u}^{\mathrm{sc}}$ does.

$$\breve{u}^{\mathrm{sc}}(x,z) = \textstyle\sum_{m\in\mathbb{Z}} c_m(z) e^{imx}, \tag{2.51}$$

$$u^{\mathrm{sc}}(x,z) = \textstyle\sum_{m\in\mathbb{Z}} c_m(z) e^{i(m+\kappa)x}. \tag{2.52}$$

Now, u^{sc} satisfies the two-dimensional Helmholtz equation, and *to the left and right of the slab, in the homogeneous ambient medium,* this is

$$u_{xx} + u_{zz} + k^2 u = 0. \tag{2.53}$$

Inserting the expansions (2.51) into this Helmholtz equation and differentiating term by term (ignoring the rigorous justification for today), we obtain

$$0 = u^{\mathrm{sc}}_{xx} + u^{\mathrm{sc}}_{zz} + k^2 u^{\mathrm{sc}} = \sum_{m\in\mathbb{Z}} [c''_m(z) + (k^2 - (m+\kappa)^2) c_m(z)] e^{i(m+\kappa)x}. \tag{2.54}$$

Since Fourier expansions are unique and the coefficients for the constant function 0 are all zero, we find that

$$c''_m(z) + (k^2 - (m+\kappa)^2) c_m(z) = 0 \quad \text{for all } m \in \mathbb{Z} \tag{2.55}$$

and conclude that $c_m(z)$ must have the simple form

$$c_m(z) = c_m^+ e^{i\eta_m z} + c_m^- e^{-i\eta_m z}, \quad \text{if } \eta_m \neq 0 \tag{2.56}$$

$$c_m(z) = c_m^+ + c_m^- z, \quad \text{if } \eta_m = 0. \tag{2.57}$$

where $c_m^\pm$ are constants

$$\eta_m^2 = k^2 - (m+\kappa)^2. \tag{2.58}$$

Upon multiplying by the spatial harmonic in the variable x, $e^{i(m+\kappa)x}$, we obtain

$$c_m(z)e^{i(m+\kappa)x} = \begin{cases} c_m^+ e^{i((m+\kappa)x+\eta_m z)} + c_m^- e^{i((m+\kappa)x-\eta_m z)} & \text{if } \eta_m \neq 0, \\ c_m^+ e^{i(m+\kappa)x} + c_m^- z e^{i(m+\kappa)x} & \text{if } \eta_m = 0. \end{cases} \tag{2.59}$$

The functions $e^{i((m+\kappa)x\pm\eta_m z)}$ represent what is known as the *diffractive orders* (or diffraction orders) or *propagating space harmonics* of the periodic structure. We see from the definition (2.58) of η_m^2 that $\eta_m^2 > 0$ for a finite number of integers m and $\eta_m^2 < 0$ for infinitely many. If κ is chosen such that $|\kappa + m| = k$ for some integer m, then $\eta_m = 0$ for such m. We make the following definitions:

$$\begin{array}{llll} m \in \mathcal{Z}_p & \Longleftrightarrow \;\; \eta_m^2 > 0, & \eta_m > 0 & \text{(propagating harmonics)}, \\ m \in \mathcal{Z}_\ell & \Longleftrightarrow \;\; \eta_m^2 = 0, & \eta_m = 0 & \text{(linear harmonics)}, \\ m \in \mathcal{Z}_e & \Longleftrightarrow \;\; \eta_m^2 < 0, & -i\eta_m > 0 & \text{(evanescent harmonics)}. \end{array} \tag{2.60}$$

Let us examine the reasons for using these appellations.

If $m \in \mathcal{Z}_p$, η_m is real and positive, and therefore the terms of (2.59) are traveling waves, or *propagating diffractive orders*. Keeping in mind the time-harmonic factor that we are suppressing in the notation, observe that the $+$-term is traveling to the right and the $-$-term is traveling to the left at a certain angle to the normal. This is illustrated in Figure 2. In order to be consistent with the physical requirement of radiation away from the slab, the finite number of propagating harmonics in the space-harmonic (Fourier) expansion (2.51)) of u^{sc} must contain only right-traveling terms ($+$-sign) for $z > z_+$ and only left-traveling terms ($-$-sign) for $z < z_-$.

In the anomalous case that $m \in \mathcal{Z}_\ell$, η_m is zero and (2.59) are linear in the z-variable and propagating parallel to the slab with wave number $\pm k$. The physical requirement that the amplitude of the the field not become unbounded as $|z| \to \infty$ precludes the term with the factor z in the second line of (2.59). One would perhaps do better call these harmonics the "grazing" harmonics, as they represent plane-wave fields that run exactly parallel to, or graze, the slab.

Finally, if $m \in \mathcal{Z}_e$, η_m is positive imaginary, and the functions $e^{i((m+\kappa)x+\eta_m z)}$ are exponential in z and propagating parallel to the slab with wave number $m + \kappa$. To wit, the z-dependent factor $e^{\pm i\eta_m z}$ is exponentially decaying as z moves to the right (and growing as z moves to the left) if the $+$-sign is taken, whereas the opposite occurs if the $-$-sign is taken. In order to exclude unbounded growth as $|z| \to \infty$, only the $+$-term in (2.59) must be taken in the the space-harmonic expansion (2.51) of u^{sc} for $z > z_+$ and only the minus sign for $z < z_-$. This ensures that each $m \in \mathcal{Z}_e$ contributes only an *evanescent* field to u^{sc}, that is, a field that decays exponentially as an observer moves away from the slab, to the left or right. These harmonics travel at a speed greater than the wave speed in the ambient medium (exterior to the slab), and are called "fast modes" or the like.

We now can state the *radiation condition*, or *outgoing condition*, that must be imposed on the scattered field for physical correctness: propagating space harmonics must be traveling outward, linear harmonics must be of constant amplitude, and exponential harmonics must evanesce as $|z| \to \infty$.

Condition 1. *(outgoing, or radiating) The scattered field u^{sc} must be* outgoing *(or* radiating*), that is, there are sequences $\{a^{\mathrm{s}}_m\}_{-\infty}^{\infty}$ and $\{b^{\mathrm{s}}_m\}_{-\infty}^{\infty}$ such that*

$$u^{\mathrm{sc}}(x,z) = \sum_{m\in\mathbb{Z}} a^{\mathrm{s}}_m e^{-i\eta_m z} e^{i(m+\kappa)x} \quad \text{for } z \le z_-, \tag{2.61}$$

$$u^{\mathrm{sc}}(x,z) = \sum_{m\in\mathbb{Z}} b^{\mathrm{s}}_m e^{i\eta_m z} e^{i(m+\kappa)x} \quad \text{for } z \ge z_+. \tag{2.62}$$

Voilà! The astute reader will have noticed that, as $|z| \to \infty$, all the evanescent harmonics decay toward zero, and what remains at the far field (actually, you don't have to go to far out) is a *finite number of waves traveling at different angles!* These angles, which are illustrated in Figure 2, are

$$\theta_m = \arcsin((m+\kappa)/k) \quad \text{for } m \in \mathcal{Z}_p \cup \mathcal{Z}_\ell. \tag{2.63}$$

The total field, being $u = u^{\mathrm{inc}} + u^{\mathrm{sc}}$, has on the left one incoming harmonic (from u^{inc}) and a finite number of outgoing harmonics, whereas on the right, it has a finite number of outgoing harmonics (from u^{inc} and u^{sc}). Thus u has the form

$$u(x,z) = \begin{cases} e^{i(\kappa x + \eta_0 z)} + \displaystyle\sum_{m\in\mathbb{Z}} a_m e^{-i\eta_m z} e^{i(m+\kappa)x} & \text{for } z \le z_-, \\ \displaystyle\sum_{m\in\mathbb{Z}} b_m e^{i\eta_m z} e^{i(m+\kappa)x} & \text{for } z \ge z_+, \end{cases} \tag{2.64}$$

in which $a_m = a^{\mathrm{s}}_m$ and $b_m = b^{\mathrm{s}}_m + \delta_{m0}$. The sum with the a_m is called the *reflected field*, and the a_m are the *reflection coefficients*; the sum with the b_m is called the *transmitted field*, and the b_m are the *transmission coefficients*.

If the coefficients ϵ and μ are real-valued, we can derive a law that expresses the conservation of energy in the sense that the (outward) energy flux of the reflected and transmitted fields equals the (inward) flux of the incident field: what comes in must also go out; there is no loss of energy to movement of the molecular structure of the material itself. The argument goes like this (you can fill in the details). Given that u satisfies the Helmholtz equation

$$\nabla\cdot \frac{1}{\mu}\nabla u + \omega^2 \epsilon u \;=\; 0, \tag{2.65}$$

we multiply this equation by the conjugate $\bar{u}$ of the field and integrate over a rectangle R, containing one period of the slab structure, with right and left boundaries $\Gamma_\pm$ placed at $z_\pm$, (Fig. 3) and outward-directed normal vector n. We use a two-dimensional version of the product rule, or "integration by parts" as well a the pseudoperiodicity of u to obtain

$$0 = \int_R \left[(\nabla\cdot \frac{1}{\mu}\nabla u)\bar{u} + \omega^2 \epsilon u \bar{u} \right] dA = \int_R \left[-\frac{1}{\mu}|\nabla u|^2 + \omega^2 \epsilon u \bar{u} \right] dA + \int_{\Gamma_\pm} \frac{1}{\mu}(\partial_n u)\bar{u}\, ds. \tag{2.66}$$

Assuming that μ and ϵ are real-valued, the imaginary part of this equation is contained only in the integral over $\Gamma_\pm$, and, using the expansions (2.64) together with the orthogonality of the spatial harmonics, we obtain

$$0 = \mathrm{Im} \int_{\Gamma_\pm} \frac{1}{\mu}(\partial_n u)\bar{u}\, ds = -\eta_0 + \sum_{m\in\mathcal{Z}_p} \eta_m (|a_m|^2 + |b_m|^2). \tag{2.67}$$

Thus we conclude

$$\sum_{m\in\mathcal{Z}_p} \eta_m(|a_m|^2 + |b_m|^2) = \eta_0, \tag{2.68}$$

which is the statement that the sum of the energy fluxes contained in each of the finite number of outgoing diffractive orders on both sides of the slab is equal to the energy flux of the incoming wave. Notice that, the greater the angle of the m^{th} propagating harmonic to the normal is, the smaller η_m is, and the less energy flux there is through $\Gamma_\pm$.

The *transmission coefficient* T is typically defined to by the square root of the ratio of transmitted energy flux to the incident energy flux,

$$T^2 = \frac{1}{\eta_0\mu_0}\int_{\Gamma_+}(\partial_n u)\bar{u}\,ds = \frac{1}{\eta_0}\sum_{m\in\mathbb{Z}}\eta_m|b_m|^2. \tag{2.69}$$

The *reflection coefficient* is defined similarly,

$$R^2 = 1 - T^2 = \frac{1}{\eta_0}\sum_{m\in\mathbb{Z}}\eta_m|a_m|^2. \tag{2.70}$$

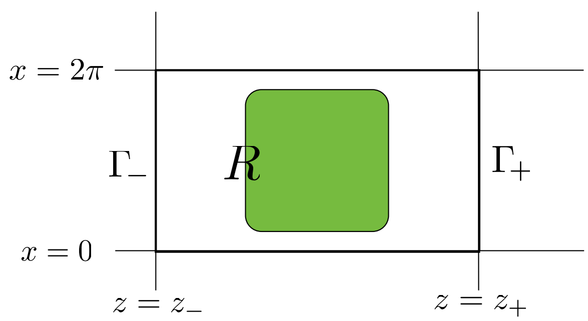


Figure 3. The rectangle R, bounded on the left and right by the segments $\Gamma_\pm$ and above and below by lines one period apart.