A DISCRETE MODEL OF GUIDED MODES AND ANOMALOUS SCATTERING IN PERIODIC STRUCTURES

A Dissertation

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Abstract

We study a discrete prototype of anomalous scattering associated with the interaction of guided modes of a periodic scatterer and plane waves incident upon the scatterer. The transmission anomalies arise because of the non-robustness of a guided mode, a mode that exists only at a specific frequency and wave number pair. The simplicity of the discrete prototype allows one to make certain explicit calculations and proofs, and to examine details of important resonant phenomena of the open wave guides. The main results are (1) a formula for transmission anomalies near a non-robust guided mode with rigorous error estimates that extends the formula of Shipman and Venakides [28] to non-zero Bloch wave number and (2) rigorous analysis of a bifurcation that connects the anomaly for non-zero wave number to that of zero wave number.
Chapter 1
Introduction

This thesis is motivated by resonant behavior observed in problems of scattering of electromagnetic waves by open periodic wave-guides. More specifically, the interaction of incident plane waves with modes of the wave-guide causes anomalies in the reflection of waves from the guide and enhancement of the field produced in the guide. The subject of this thesis is a discrete prototype of this physical problem. The aim is to construct the simplest model that exhibits the same resonant phenomena but that is amenable to direct and explicit calculations. It turns out that many of the results hold in much more general situations than just the discrete model, but that additional conclusions can be drawn for the discrete prototype based on the explicit nature of the problem. Lattice models have a long and distinguished history. Let us see a brief survey before describing the model studied in this work.

The classical publication on “Wave propagation in periodic structures” by Leon Brillouin [8] gives a detailed review of waves in periodic structures. This book deals not with a special branch of physics but with a general method and its applications to different problems which are accessible to the same mathematical treatment. In 1686, Newton attempted to derive a formula for the velocity of sound, by the assumption that sound was propagated in air in the same manner as an elastic wave would be propagated along a discrete lattice of point masses. At that time a continuous structure represented an insoluble problem and nothing was known about partial differential equations. Soon after Newton, John Bernoulli and his son Daniel studied in detail the dynamics of masses connected along a line. They
showed that the system of N masses has exactly N independent modes of vibration [13]. Then, in 1753, Daniel Bernoulli stated that the general motion of a vibrating system is describable as a superposition of its normal modes. That principle of superposition has since been extended to the statement of Fourier’s theorem.

In the 19th century a number of scientists investigated wave propagation in lattices. In 1830, Cauchy used Newton’s model to explain the dispersion of optical waves. In 1841, Baden-Powell computed the velocity of a wave propagation and his problem is equivalent to considering a wave propagation along a one-dimensional lattice of point masses. In 1881, Kelvin discussed the same lattice as Baden-Powell, but took into account that frequency is a function of wave length, something that was missed by Baden-Powell. Kelvin then proceeded to form a theory of dispersion for a 2-partical lattice, and a mechanical model of it was built by Vincent. At the end of the nineteenth century and in the early twentieth century a number of scientists (Vaschy, Pupin, Campbell) [8] used periodic networks to develop electric filters. In the 1950s the interest in periodic structures came mainly from the fields of slow wave structures and antennas. The study of slow wave structures was mainly stimulated by the development of microwave tubes where a periodic structure is used to slow the wave, which would then couple to the relatively slow electron beam [9].

More recently, Balk, et. al., [4, 5] introduce a model of a chain of masses joined by springs with a non-monotone strainstress relation. Numerical experiments are conducted to find the dynamics of that chain under slow external excitation. They describe important applications of these structures for building constructions that are able to withstand sufficiently strong repeated perturbations, e.g., nuclear power plants in seismic areas. The construction is able to absorb the energy of large per-
turbations (like those produced by seismic waves). When the external perturbation is gone, the construction returns to its original state.

One of the simplest examples of inhomogeneous lattices which is represented by a bi-atomic periodic chain of particles connected by springs, can be found in publications on microstructures with defects [20, 17].

A discrete model that describes a linear chain of particles coupled to a single-site defect with instantaneous Kerr nonlinearity was studied by Miroshnichenko et al. [23]. They show that this model can be regarded as a nonlinear generalization of the familiar Fano-Anderson model, and it can generate an amplitude-dependent bistable resonant transmission or reflection.

Movchan et al. analyse Bloch-Floquet waves propagating in doubly-periodic composite structures containing high-contrast interfaces and finite size defects in [24]. The authors give an analysis for discrete lattice structures with defects.

The thesis presents a study of a discrete mathematical prototype of physical phenomena associated with the interaction of acoustic or electromagnetic plane waves with a periodic slab. The discrete plane wave propagates in an ambient space. The ambient space is modeled by a discrete uniform infinite two-dimensional lattice. The periodic slab is presented by a periodic one-dimensional lattice. The lattices can be thought of as a 2D grid of identical beads connected by springs and a string of beads also connected by springs (see Fig. 1.1). The interaction is produced by a coupling of these two systems. The coupling is made by connecting the beads of the one-dimensional lattice with beads of the two-dimensional lattice by springs in such way as to preserve the periodicity of the 1D lattice. It is known that any periodic structure possesses wave guiding properties and under certain conditions transmission anomalies can be observed. The internal dynamics of the coupled system in the model is described by a Schrodinger type equation [10].
Chapter 2 considers the spectral properties of each system separately. For the one-dimensional lattice we find the dispersion relation and conditions when the system admits pseudoperiodical oscillations. By deriving the dispersion relation, the relation between frequency and the 2D wave vector, for the two-dimensional lattice we can see what kind of waves the system allows to propagate before coupling. It is important that the system possess a continuous spectrum. For the one-dimensional lattice there is an analogous dispersion relation. Then the systems are coupled. Mathematically, this process is described by introduction of a coupling operator, which is an infinite matrix. The coupling modifies the dispersion relation for the one-dimensional lattice – in fact, it is replaced by a complex dispersion relation for generalized guided modes. Their interaction with plane waves of the two-dimensional lattice and creation of scattering anomalies is the subject of this work.

Chapter 3 formulates the problem of scattering of plane waves in the two-dimensional lattice by the one-dimensional lattice, and gives a proof that this problem has always a solution. The question of existence of guided modes is considered.

Chapter 4 explores the primary question of resonant scattering for the coupled system. Specifically, we examine transmission anomalies. By transmission anoma-
lies we mean sharp peaks and dips on the graph representing the transmission coefficient, the total energy transmitted across the one-dimensional lattice, when incoming waves propagate in the two-dimensional lattice and meet the 1D lattice as an obstacle. The asymptotic analysis is given near the guided mode. We find that perturbation of one of the physical parameters of the problem leads to a bifurcation.

The primary new results in this dissertation are:

- determination of the part of the two-dimensional lattice that is “recon-structible” from the observer in the one-dimensional lattice (Section 2.4);

- proofs of existence and nonexistence of guided modes in the discrete prototype (Section 3.8);

- extension of approximate formulas for transmission anomalies to non-robust traveling guided modes with rigorous error estimates (Section 4.1);

- analysis of a bifurcation connecting the transmission anomaly for standing waves to those for traveling waves (Section 4.2).
Chapter 2
The Mathematical Prototype

In this chapter we investigate the spectral properties of each lattice separately and determine what part of the two-dimensional lattice can be detected by an observer in the one-dimensional lattice.

2.1 Description of the One-Dimensional Scatterer and Its Spectral Theory

The one-dimensional periodic lattice (system) can be thought of as an infinite sequence of beads connected by springs. In one period there are \( N \) beads with \( N \) different masses connected by springs of \( N \) different spring constants. The internal dynamics (the nearest-neighbor interactions) are described by a Schrödinger-type equation

\[
\mathbb{M}\dot{x} = -iAx, 
\]

where \( x \in H_1 \), the Hilbert space \( \ell^2(\mathbb{Z}) \), \( \mathbb{M} \) is the bounded positive mass operator given by

\[
(\mathbb{M}x)_j := M_j x_j, \quad M_j > 0, 
\]

the internal forcing operator \( A \) is the discrete nonuniform Laplacian

\[
(Ax)_j := -k_j x_{j+1} + (k_j + k_{j-1})x_j - k_{j-1}x_{j-1}, 
\]

and both \( \mathbb{M} \) and \( A \) are taken to be \( N \)-periodic:

\[
M_{j+N} = M_j \text{ and } k_{j+N} = k_j \text{ for all } j \in \mathbb{Z}. 
\]
Let us rewrite $M\dot{x} = -iAx$ as

$$M^{1/2}M^{1/2}\dot{x} = -iAM^{-\frac{1}{2}}M^{1/2}x$$  \hspace{1cm} (2.5)$$

and multiplying by $M^{-\frac{1}{2}}$ on the left we obtain:

$$M^{1/2}\dot{x} = -iM^{-\frac{1}{2}}AM^{-\frac{1}{2}}M^{1/2}x.$$

By introducing a new variable $z = M^{1/2}x$ and denoting the operator $M^{-\frac{1}{2}}AM^{-\frac{1}{2}}$ by $\Omega_1$, we reduce the equation to a simpler form:

$$\dot{z} = -i\Omega_1 z.$$  \hspace{1cm} (2.6)$$

Let us note that $\Omega_1$ is self-adjoint because $A$ and $M$ are and it is represented by a tridiagonal matrix with periodic entries:

$$(\Omega_1 z)_j = -\frac{k_j}{\sqrt{M_jM_{j+1}}}z_{j+1} + \frac{(k_j + k_{j-1})}{M_j}z_j - \frac{k_{j-1}}{\sqrt{M_jM_{j-1}}}z_{j-1}. \hspace{1cm} (2.7)$$

Since we have a physical system with translational symmetry we can define an operator $S$ associated with shifting by one period as follows:

$$(Sz)_j = z_{j+N}. \hspace{1cm} (2.8)$$

The operator $S$ is unitary, that is, $S^* = S^{-1}$ [2]:

$$(x, S^* y) = (S x, y) = \sum_{j=-\infty}^{\infty} (S x)_j \bar{y}_j = \sum_{j=-\infty}^{\infty} x_{j+N} \bar{y}_j = \sum_{n=-\infty}^{\infty} x_n \bar{y}_{n-N} = (x, S^{-1} y). \hspace{1cm} (2.9)$$

Moreover, we have that $\Omega_1 S - S \Omega_1 = 0$ and by the Floquet theory, we can obtain the generalized eigenfunctions of $\Omega_1$ by examining these of $S$ [8, 18]. Let us find the eigenfunctions of the shifting operator $S$,

$$(Sz)_j = \lambda z_j = z_{j+N}.$$
Since the operator $S$ is unitary, its eigenvalues have the form $e^{2\pi i \kappa}$, $\kappa \in [-1/2, 1/2)$. Substituting this into the previous equation yields:

$$(Sz)_j = e^{2\pi i \kappa} z_j = z_{j+N},$$  \hspace{1cm} (2.10)

The shifting operator has a continuous spectrum and all its eigenvalues are on the unit circle and the corresponding eigenvectors are pseudoperiodic. Notice that, since the problem (2.6) is invariant with respect to the translational symmetry, the space of solutions of (2.6) is $N$-dimensional and the restriction of $\Omega_1$ on a such subspace can be found. Let us denote by $P_\kappa$ the eigensubspace for a fixed $\kappa$. The space $P_\kappa$ has $N$ linearly independent orthogonal eigenvectors, which forms a basis for the subspace. The basis vectors have the following form ($l = 1, \ldots, N$):

$$p^{(l)} = (\ldots, e^{2\pi i \kappa}_{(-N+1)\text{th}}, 0, \ldots, 0, (l)_{\text{th}}, 0, \ldots, 0, e^{2\pi i \kappa}_{(N+1)\text{th}}, 0, \ldots, 0, e^{2\pi i 2\kappa}_{(2N+1)\text{th}}, \ldots).$$  \hspace{1cm} (2.11)

Now we can compute the restriction of the operator $\Omega_1$ to the $N$-dimensional subspace of the pseudoperiodic sequences $\Omega_1|_{P_\kappa}$ or simply $\Omega^{(\kappa)}_1$. For this we analyze how $\Omega_1$ acts on the basis vectors:

$$\Omega_1 p^{(l)} = -\frac{k_{l-1}}{\sqrt{M_{l-1}M_l}} p^{(l-1)} + \frac{(k_l + k_{l-1})}{M_l} p^{(l)} - \frac{k_l}{\sqrt{M_{l}M_{l+1}}} p^{(l+1)}.$$  \hspace{1cm} (2.12)

Notice in our calculations $p^{(0)} = e^{2\pi i \kappa} p^{(N)}$ and $p^{(N+1)} = e^{-2\pi i \kappa} p^{(1)}$. Let $q$ be an arbitrary element of $P_\kappa$, then there are $N$ constants say, $c_l$, $c_l \in \mathbb{C}$, such that $q = \sum_{l=1}^{N} c_l p^{(l)}$. By knowing how the linear operator $\Omega_1$ acts on the basis eigenvectors we can obtain the operator $\Omega^{(\kappa)}_1$:

$$\Omega^{(\kappa)}_1 = \begin{pmatrix}
\frac{(k_1 + k_N)}{M_1} & 0 & \cdots & 0 & -\frac{k_N}{\sqrt{M_{N}M_1}} e^{2\pi i \kappa} \\
-\frac{k_1}{\sqrt{M_{2}M_1}} & \frac{(k_2 + k_1)}{M_2} & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
-\frac{k_N}{\sqrt{M_{N}M_{N-1}}} e^{-2\pi i \kappa} & 0 & \cdots & -\frac{k_{N-1}}{\sqrt{M_{N}M_{N-1}}} & \frac{(k_N + k_{N-1})}{M_N}
\end{pmatrix}.$$  \hspace{1cm} (2.13)
The operator $\Omega_1^{(\kappa)}$ is a $N \times N$, $N > 3$, tridiagonal selfadjoint matrix with nonzero top right and bottom left corner entries. The matrix has $N$ eigenvalues in $\mathbb{C}$ and $N$ associated eigenvectors.

Let us consider a simple particular case for two beads of different masses $m$ and $M$ in one period, with $k_1 = k_2 = k$. In this case, the operator $\Omega_1^{(\kappa)}$ is

$$
\Omega_1^{(\kappa)} = \begin{pmatrix}
\frac{2k}{m} & -\frac{k}{\sqrt{mM}}(1 + e^{2\pi i \kappa}) & \frac{2k}{M} \\
-\frac{k}{\sqrt{mM}}(e^{-2\pi i \kappa} + 1) & \frac{2k}{m} & \\
& \frac{2k}{M} & \frac{2k}{m}
\end{pmatrix},
$$

relation between $\lambda$ and $\kappa$ in the equation

$$
\det (\Omega_1^{(\kappa)} - \lambda I) = 0
$$

is the dispersion relation,

$$
\lambda^2 + \left(\frac{2k}{m} + \frac{2k}{M}\right) \lambda + \frac{4k^2}{mM} \sin^2 \left(\frac{2\pi \kappa}{2}\right) = 0,
$$

and the eigenvalues are

$$
\lambda_{1,2}^{(\kappa)} = -\frac{k}{m} - \frac{k}{M} \pm k \sqrt{\frac{1}{m^2} + \frac{1}{M^2} + \frac{2}{mM} \cos 2\pi \kappa}.
$$

**Example 2.1.** $(N = 2)$ Let us demonstrate a different way of getting the dispersion relation. We have a one-dimensional periodic chain of beads with two beads of different masses, $m$ and $M$, in one period. The equations describing the dynamics have the following form:

$$
\begin{align*}
mx_s &= -ik(-x_{s+1} + 2x_s - x_{s-1}), & s &= 2n + 1, & n &\in \mathbb{Z} \\
Mx_s &= -ik(-x_{s+1} + 2x_s - x_{s-1}), & s &= 2n, & n &\in \mathbb{Z}
\end{align*}
$$

Since the masses of beads are different, their amplitudes are different. Therefore let us look for the solutions to the equations in the form of plane waves $[7]$:

$$
\begin{align*}
x_s &= a e^{\pi i s \kappa} e^{-i\omega t}, & s &= 2n + 1, \\
x_s &= b e^{\pi i s \kappa} e^{-i\omega t}, & s &= 2n,
\end{align*}
$$
where $\kappa$ is a wave number or a Bloch wave number and $\omega$ is a frequency of oscillations. Substituting the expressions for the solutions into equations gives a dispersion relation, or a dispersion law:

$$\omega^2 + \left(\frac{2k}{M} + \frac{2k}{m}\right) \omega + \frac{4k^2}{mM} \sin^2(\pi \kappa) = 0,$$

(2.19)

which has two solutions

$$\omega_1 = -\frac{k}{m} - \frac{k}{M} - k \sqrt{\frac{1}{m^2} + \frac{1}{M^2} + \frac{2}{mM} \cos 2\pi \kappa},$$

$$\omega_2 = -\frac{k}{m} - \frac{k}{M} + k \sqrt{\frac{1}{m^2} + \frac{1}{M^2} + \frac{2}{mM} \cos 2\pi \kappa}.$$  

(2.20)

We see the results agree in the two calculations.

## 2.2 Description of the Ambient Two-Dimensional Lattice and Its Spectral Theory

In our model, the ambient space is a two-dimensional lattice composed of beads all having the same mass equal to 1 and placed at the integer points $\mathbb{Z}^2$ in $\mathbb{R}^2$. The beads in the lattice are connected by springs of equal spring constant 1. The internal dynamics (the nearest-neighbor interactions) is given by a Schrodinger type equation [10]

$$\dot{y} = -i \Omega_2 y,$$

(2.21)

where $y = \{y_{mn}\} \in \ell^2(\mathbb{Z}^2) =: H_2$ with $m, n \in \mathbb{Z}$ and $-\Omega_2$ is the discrete uniform Laplacian:

$$(\Omega_2 y)_{mn} = -(y_{(m-1)n} - 2y_{mn} + y_{(m+1)n} + y_{m(n-1)} - 2y_{mn} + y_{m(n+1)}).$$

(2.22)

Let us look for a solution in the steady state form $y_{mn} = e^{-i\omega t} u_{mn}$, where $\omega$ is a frequency. By substituting it into (2.21) we get an eigenvalue problem for the operator $\Omega_2$

$$(\Omega_2 - \omega) u_{mn} = 0.$$

(2.23)
The Fourier transform is used to identify $H_2$ with $L^2([-1/2, 1/2] \times [-1/2, 1/2])$.

Let $U$ map $H_2$ into $L^2([-1/2, 1/2] \times [-1/2, 1/2])$ by

$$U : \{u_{mn}\} \rightarrow \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} u_{mn} e^{2\pi i (m\theta + n\phi)}.$$  \hspace{1cm} (2.24)

The operator $U$ is unitary. Let us introduce the following operators on $H_2$:

$$(S^l u)_{mn} = u_{(m+1)n},$$  \hspace{1cm} (2.25)

shifting to the left,

$$(S^l)^* = S^r, \text{ or } (S^r u)_{mn} = u_{(m-1)n},$$  \hspace{1cm} (2.26)

shifting to the right,

$$(S^{up} y)_{mn} = y_{m(n-1)},$$  \hspace{1cm} (2.27)

shifting up,

$$(S^{up})^* = S^d \text{ with } (S^d u)_{mn} = u_{m(n+1)},$$  \hspace{1cm} (2.28)

shifting down, and a multiplication operator

$$m_{-4} \text{ with } (m_{-4} u)_{mn} = -4u_{mn}.$$  \hspace{1cm} (2.29)

These operators allow us to rewrite $\Omega_2$ in the form

$$\Omega_2 = -(S^l + S^r + S^{up} + S^d + m_{-4}).$$  \hspace{1cm} (2.30)

Note that for any function $f(\theta, \phi)$ from $L^2([-1/2, 1/2] \times [-1/2, 1/2])$ we have:

$$
\begin{aligned}
US^l U^{-1} f(\theta, \phi) &= e^{2\pi i \theta} f(\theta, \phi), \\
US^r U^{-1} f(\theta, \phi) &= e^{-2\pi i \theta} f(\theta, \phi), \\
US^{up} U^{-1} f(\theta, \phi) &= e^{2\pi i \phi} f(\theta, \phi), \\
US^d U^{-1} f(\theta, \phi) &= e^{-2\pi i \phi} f(\theta, \phi) \\
Um_{-4} U^{-1} f(\theta, \phi) &= -4f(\theta, \phi).
\end{aligned}
$$  \hspace{1cm} (2.31)
Therefore we obtain

\[(U\Omega_2 U^{-1}) f(\theta, \phi) = -U(S^l + S^r + S^{\text{up}} + S^{\text{d}} + m_0) U^{-1} f(\theta, \phi) = (4 - 2 \cos(2\pi \theta) - 2 \cos(2\pi \phi)) f(\theta, \phi).\] (2.32)

This means that the operator \( \Omega_2 \) becomes an operator of multiplication in \( L^2([-1/2, 1/2] \times [-1/2, 1/2]) \). Moreover the spectrum of \( \Omega_2 \) on the infinite 2D lattice is equal to the range of \( 4 - 2 \cos(2\pi \theta) - 2 \cos(2\pi \phi) \), that is, \([0, 8]\).

### 2.3 Coupled System

Let us couple the systems \((H_1, \Omega_1)\) and \((H_2, \Omega_2)\) in a simple way by introducing \(N\) constants \(\gamma_i, \gamma_{n+N} = \gamma_n\) that couple \(z_n\) to \(u_{0n}\). For this purpose, we introduce an operator \(\Gamma, \Gamma : H_2 \rightarrow H_1\), which describes the coupling. In \(H_1\) we have an orthonormal basis consisting of \(e_k = (\ldots, 0, 1, 0, \ldots), k \in \mathbb{Z}\) and in \(H_2\) it is \(E_{mn} = \delta_{mn}\), where \(\delta_{mn}\) is the Kronecker delta and \(m, n \in \mathbb{Z}\). To describe \(\Gamma\) it is enough to show how \(\Gamma\) acts on the basis elements. We require that

\[\Gamma(E_{0n}) = \gamma_n e_n, \quad \Gamma(E_{mn}) = 0, \text{ if } m \neq 0.\]

The adjoint of \(\Gamma\) is

\[\Gamma^\dagger(e_k) = \tilde{\gamma}_k E_{0k}.\]

Thus we have a system \((\mathcal{H}, \Omega)\), in which

\[\mathcal{H} = H_1 \oplus H_2,\] (2.33)

and \(\Omega\) has the following form with respect to this decomposition:

\[\Omega = \begin{bmatrix} \Omega_1 & \Gamma \\ \Gamma^\dagger & \Omega_2 \end{bmatrix}.\] (2.34)
The eigenvalue problem

\[ \Omega \begin{pmatrix} z \\ u \end{pmatrix} - \omega \begin{pmatrix} z \\ u \end{pmatrix} = 0 \]  

is equivalent to the equations

\[ \omega z_n = (\Omega_1 z)_n + (\Gamma u)_n, \]  

\[ \omega u_{mn} = (\Gamma^\dagger z)_{mn} + (\Omega_2 u)_{mn}. \]

## 2.4 Reconstructibility from Open Systems

A typical linear open system is often defined as a component of a larger conservative one [11, 12]. Assuming that such an open system is all one is able to observe, it is a question of how big a part of the original conservative system is coupled to the open system. Because of the coupling both the one-dimensional and two-dimensional lattices become open systems viewed by an observer in either system. In this section we are interested in how much information one can ascertain about the two-dimensional lattice from observations made only from within the one-dimensional lattice.

**Definition 2.2.** (orbit) Let \( \Omega \) be a self-adjoint operator in a Hilbert space \( H \) and \( S \) be a subset of vectors in \( H \). Then we define the closed orbit (or simply orbit) \( \mathcal{O}_\Omega(S) \) of \( S \) under action of \( \Omega \) by

\[ \mathcal{O}_\Omega(S) = \text{closure of span} \ \{ f(\Omega)w : f \in C_c(\mathbb{R}), w \in S \}. \]  

If \( H' \) is a subspace of \( H \) such that \( \mathcal{O}_\Omega(H') = H' \), then \( H' \) is said to be invariant with respect to \( \Omega \) or simply \( \Omega \)-invariant [12].
In [11, 12], it is proved that the minimal self-adjoint extension of the system $(\mathcal{H}, \Omega)$ projected to $H_1$ is equal to the subsystem $(\mathcal{H}, \Omega|_{\mathcal{H}})$, where $\mathcal{H} = H_1 \oplus \mathcal{O}_{\Omega_2}(\Gamma^\dagger(H_1))$. This is part of $(\mathcal{H}, \Omega)$ that is reconstructible from the projection to $H_1$ alone.

Let us find $\mathcal{O}_{\Omega_2}(\Gamma^\dagger(H_1))$.

**Theorem 2.3.** The orbit $\mathcal{O}_{\Omega_2}(\Gamma^\dagger(H_1)) = \{\{u_{mn}\} \in H_2 : u_{mn} = u_{-mn} \forall m \in \mathbb{Z}\}$.

**Proof:** In our case, $\Gamma^\dagger(H_1) = \{\{u_{mn}\} \in H_2 : u_{mn} = 0 \text{ for } m \neq 0\}$ and we use the discrete Fourier transform. $U\Omega_2U^{-1} = 4 - 2\cos(2\pi\theta) - 2\cos(2\pi\phi)$, where $\theta \in [-1/2, 1/2]$ and $\phi \in [-1/2, 1/2]$, with

$$S = U(\Gamma^\dagger(H_1)) = \{f(\phi), f(\phi) \in L^2([-1/2, 1/2])\}.$$  

The orbit is defined as the closure in $L^2([-1/2, 1/2] \times [-1/2, 1/2])$:

$$\mathcal{O}_{U(\Omega_2)}(S) = \{f(U\Omega_2U^{-1})w, f \in C_c(\mathbb{R}), w \in S\}, \quad (2.39)$$

with $f(U\Omega_2U^{-1}) = f(4 - 2\cos(2\pi\theta) - 2\cos(2\pi\phi))$.

To prove our claim let us show that if $F \in C([0, 1/2] \times [-1/2, 1/2])$ and $\varepsilon > 0$, then there exist functions $\{f_1, \ldots, f_n\} \subseteq C([0, 8])$ and $\{g_1, \ldots, g_n\} \subseteq C([-1/2, 1/2])$ such that

$$|F(\theta, \phi) - \sum_{i=1}^{n} f_i(U\Omega_2U^{-1})g_i(\phi)| < \varepsilon \quad (2.40)$$
Consider the set

$$\mathfrak{B} = \{ h \in C([0, 1/2] \times [-1/2, 1/2]) : \exists \{ f_1, \ldots, f_n \} \subseteq C([0, 8]),$$

$$\{ g_1, \ldots, g_n \} \subseteq C([-1/2, 1/2]) \}$$

(2.41)

with \( h(\theta, \phi) = \sum_{i=1}^{n} f_i(U\Omega_2U^{-1})g_i(\phi) \) \( \forall (\theta, \phi) \in [0, 1/2] \times [-1/2, 1/2] \)

Then \( \mathfrak{B} \) is an algebra of functions of \([0, 1/2] \times [-1/2, 1/2] \) and \( 1 \in \mathfrak{B} \). On the other hand, if \((\theta_1, \phi_1) \neq (\theta_2, \phi_2)\), then either \( \theta_1 \neq \theta_2 \) or \( \phi_1 \neq \phi_2 \). If \( \theta_1 \neq \theta_2 \), then pick \( f \in C([0, 8]) \) with \( f(4 - 2\cos(2\pi\theta_1) - 2\cos(2\pi\phi)) \neq f(4 - 2\cos(2\pi\theta_2) - 2\cos(2\pi\phi)) \), and let \( F(\theta, \phi) = f(4 - 2\cos(2\pi\theta) - 2\cos(2\pi\phi)) \) for all \((\theta, \phi) \in [0, 1/2] \times [-1/2, 1/2] \). If \( \phi_1 \neq \phi_2 \), then take some \( g \in C([-1/2, 1/2]) \) with \( g(\phi_1) \neq g(\phi_2) \), and put \( F(\theta, \phi) = g(\phi) \). In any case, \( F \in \mathfrak{B} \) and \( F(\theta_1, \phi_1) \neq F(\theta_2, \phi_2) \) holds, so that \( \mathfrak{B} \) separates the points of \([0, 1/2] \times [-1/2, 1/2] \). Now by the Stone-Weierstrass theorem \([3, 26]\), \( \overline{\mathfrak{B}} = C([0, 1/2] \times [-1/2, 1/2]) \). Then we use the theorem \([3]\) that the collection of all continuous functions with compact support is norm dense in \( L^2(\mu) \) equipped with a regular Borel measure \( \mu \), which implies that \( \overline{\mathfrak{B}} \) is norm dense in \( L^2([0, 1/2] \times [-1/2, 1/2]) \). Then, the algebra \( \mathfrak{A} \)

$$\mathfrak{A} = \{ h \in C([-1/2, 1/2] \times [-1/2, 1/2]) : \exists \{ f_1, \ldots, f_n \} \subseteq C([0, 8]),$$

$$\{ g_1, \ldots, g_n \} \subseteq C([-1/2, 1/2]) \}$$

(2.42)

with \( h(\theta, \phi) = \sum_{i=1}^{n} f_i(U\Omega_2U^{-1})g_i(\phi) \forall (\theta, \phi) \in [-1/2, 1/2] \times [-1/2, 1/2] \)

fails to be dense in \( L^2([-1/2, 1/2] \times [-1/2, 1/2]) \), because for every \( G \) in the closure of \( \mathfrak{A} \) we have \( G(-\theta, \phi) = G(\theta, \phi) \). Thus the closure of \( \mathfrak{B} \) is the set of all even in \( \theta \) functions of \( L^2([-1/2, 1/2] \times [-1/2, 1/2]) \). Then using the inverse discrete Fourier transform we get the result stated in the theorem.

The theorem proves that the coupled component of \( H_2 \) to \( H_1 \) is the space of even motions, in other words odd motions of the two-dimensional lattice can not excite the one-dimensional lattice.
Chapter 3
Scattering Problem

3.1 Spatial Fourier Harmonics

Let us look for the solution to (2.6) in the steady-state form [7]

\[ \dot{z}_n = z_n e^{-i\omega t} = \tilde{z}_n e^{\frac{2\pi \imath}{N} n} e^{-i\omega t}, \]  

(3.1)

which satisfies the condition of pseudoperiodicity (2.10) with \( \tilde{z}_{n+N} = \tilde{z}_n \), the periodic part. The general solution for \( z_n \) is

\[ z_n = \sum_{l=0}^{N-1} c_l e^{\frac{2\pi \imath (\kappa + l)}{N} n}, \]  

(3.2)

where \( c_l \) are arbitrary constants. For the two-dimensional lattice we require that \( u_{m(n+N)} = u_{mne^{2\pi \imath \kappa}} \), that is, it is pseudoperiodic in vertical direction. This implies that \( u_{mn} = \sum_{l=0}^{N-1} a_{l}^m e^{\frac{2\pi \imath (\kappa + l)}{N} n} \), where \( a_{l}^m \) are some functions which do not depend on \( \kappa \). Let the operator \( S \) be a shifting operator in the vertical direction defined on the 2D lattice, \( Sy_{m(n+N)} = y_{mn} \). For a fixed frequency \( \omega \), \( \omega \in [0, 8] \) let us seek a solution to \( \partial y_{mn}/\partial t = -i\Omega_2 y_{mn} \) in the form \( y_{mn} = u_{mn} e^{-i\omega t} \). Substituting it into the master equation leads to

\[ (\Omega_2 - \omega) u_{mn} = 0, \]  

(3.3)

which is an eigenvalue problem for \( \Omega_2 \) on the two-dimensional lattice. It is natural (because we have a system with constant coefficients) to seek its eigenfunctions in the form:

\[ u_{mn} = e^{2\pi \imath (m\theta + n\phi)}. \]  

(3.4)
Substituting (3.4) into (3.3) gives that \( \omega, \theta, \) and \( \phi \) satisfy the dispersion relation
\[
\omega = 4 - 2 \cos(2\pi \theta) - 2 \cos(2\pi \phi),
\]
that is \( \omega \) is an eigenvalue for \( \Omega_2 \). From the point of view of the coupled system with Bloch wave number \( \kappa \) in the \( n \)-direction, pseudo-periodic eigenfunctions such that
\[
S u_{mn} = u_{m(n+N)} = e^{2\pi i \kappa} u_{mn}.
\]
For this, we require \( e^{2\pi i \kappa} = e^{2\pi i \phi N} \) or \( \kappa + l = N\phi, \)
\( l = 0, \ldots (N-1) \). For a fixed \( \kappa \) we have \( N \) different values of \( \phi \),
\[
\phi_l = \frac{\kappa + l}{N},
\]
and for each \( \phi \) there are two different values of \( \theta \) (different only by sign), which can be found from (3.5). This implies
\[
u_{mn} = \sum_{l=0}^{N-1} (a_l^+ e^{2\pi i \theta_l m} + a_l^- e^{-2\pi i \theta_l m}) e^{2\pi i \phi_l n}.
\]
The first term in (3.7) corresponds to waves travelling to the right and the second one describes waves traveling to the left, when the time factor \( e^{-i\omega t} \) is taken into account. Because of the periodicity of the structure, each pseudo-periodic function \( u_{mn} \) is characterized by a minimal Bloch wave vector \( \kappa \) lying in the first Brillouin zone \( \kappa \in [-1/2, 1/2] \).

**Definition 3.1. (outgoing and incoming)** A complex-valued function \( \{u_{mn}\} \) is said to be outgoing if there are sequences \( \{a_l\}_{l=0}^{N-1} \) and \( \{b_l\}_{l=0}^{N-1} \) such that
\[
\begin{align*}
u_{mn} &= \sum_{l=0}^{N-1} a_l e^{-2\pi i \theta_l m} e^{2\pi i \phi_l n}, & m < 0, \quad (3.8) \\
u_{mn} &= \sum_{l=0}^{N-1} b_l e^{2\pi i \theta_l m} e^{2\pi i \phi_l n}, & m > 0. \quad (3.9)
\end{align*}
\]
The function \( \{u_{mn}\} \) is said to be incoming if it admits the expansions
\[
\begin{align*}
u_{mn} &= \sum_{l=0}^{N-1} a_l e^{2\pi i \theta_l m} e^{2\pi i \phi_l n}, & m < 0, \quad (3.10) \\
u_{mn} &= \sum_{l=0}^{N-1} b_l e^{-2\pi i \theta_l m} e^{2\pi i \phi_l n}, & m > 0. \quad (3.11)
\end{align*}
\]
Let $\mathcal{P}$ be a set

$$\mathcal{P} = \{ l : \text{Im}(\theta_l) = 0 \}. \tag{3.12}$$

Let us obtain a diagram of $|\mathcal{P}|$, the number of propagating harmonics for real values of $\omega$ and $\kappa$. The procedure is as following for each $l$, $l = 0, \ldots, N - 1$ to graph the functions $\cos(2\pi\theta_l) = \pm 1$ (or $2 - \frac{\omega}{2} - \cos\left(\frac{2\pi(\kappa + l)}{N}\right) = \pm 1$), in other words graph the curves $\theta_l = 0$ and $\theta_l = \frac{1}{2}$ for $\kappa \in [-1/2, 1/2]$ and $\omega \in [0, 8]$. In Figure 3.1 it is shown the diagram for $N = 2$ and $N = 3$ and in Figure 3.2 for $N = 9$ and $N = 10$.

![Diagram](image)

FIGURE 3.1. The diagram of $|\mathcal{P}|$ for $N = 2$ (left) and $N = 3$ (right). The digits 0, 1, 2, and 3 represent the number of propagating harmonics.

In the problem of scattering of source fields given by traveling waves incident upon the one-dimensional lattice, we must exclude exponential or linear growth of $\{u_{mn}\}$ in the two-dimensional lattice as $|m| \to \infty$. The form of the total field
FIGURE 3.2. The diagram of $|\mathcal{P}|$ for $N = 9$ (left) and $N = 10$ (right).

is therefore:

$$u_{mn} = \sum_{l \in \mathcal{P}} a_l \text{inc} e^{2\pi i \theta_l m} e^{2\pi i \phi_l n} + \sum_{l=0}^{N-1} a_l e^{-2\pi i \theta_l m} e^{2\pi i \phi_l n}, \quad m < 0, \quad (3.13)$$

$$u_{mn} = \sum_{l \in \mathcal{P}} b_l \text{inc} e^{-2\pi i \theta_l m} e^{2\pi i \phi_l n} + \sum_{l=0}^{N-1} b_l e^{2\pi i \theta_l m} e^{2\pi i \phi_l n}, \quad m > 0. \quad (3.14)$$

The first sums in these expressions represent the right-traveling source wave incident upon the one-dimensional lattice from the left side and the left-traveling source wave incident upon the one-dimensional lattice from the right side. By definition 3.1 a function $\{u_{mn}\}$ is outgoing if it is of the form (3.13), (3.14) with $a_l \text{inc} = 0$ and $b_l \text{inc} = 0$ for all $l \in \mathcal{P}$.

In our scattering problem, the pseudo-periodic source field is taken to be a superposition of traveling waves incident upon the one-dimensional lattice from left and right. These waves can be thought of as emanating from $m = -\infty$ and $m = \infty$:

$$u_{mn} \text{inc} = \sum_{l \in \mathcal{P}} (a_l \text{inc} e^{2\pi i \theta_l m} + b_l \text{inc} e^{-2\pi i \theta_l m}) e^{2\pi i \phi_l n}. \quad (3.15)$$

The problem of scattering of the incident wave $\{u_{mn} \text{inc}\}$ by the one-dimensional lattice is expressed as a system characterizing the total field $\{u_{mn}\}$, which is the
sum of the incident field \( \{ u_{mn}^{\text{inc}} \} \) and the scattered, or diffracted, field \( \{ u_{mn}^{\text{sc}} \} \), the latter of which is outgoing.

Since we look now for \( \kappa \)-pseudo-periodic fields in \( n \) direction, the scattering problem can be considered in a strip \( \mathcal{R} \) consisting of one period in the variable \( n \), that is between the lines \( n = 0 \) and \( n = N \):

\[
\mathcal{R} = \{(m,n) \in \mathbb{Z}^2 : -\infty \leq m \leq \infty, 0 \leq n \leq N\}. \quad (3.16)
\]

**Problem 3.2.** (Scattering problem, \( P^{sc} \)) Given an incident field (3.15), find a pair of functions \((z,u)\) that satisfies the following conditions:

\[
\omega z_n = (\Omega_1 z)_n + (\Gamma u)_n, \quad (3.17)
\]

\[
\omega u_{mn} = (\Gamma^t z)_{mn} + (\Omega_2 u)_{mn}, \quad (3.18)
\]

\((z,u)\) are \( \kappa \)-pseudoperiodic in \( n \), \( (3.19)\)

\( u = u^{\text{inc}} + u^{\text{sc}} \), with \( u^{\text{sc}} \) outgoing. \( (3.20)\)

Because of condition (3.19) every solution of \( P^{sc} \) can be extended by pseudoperiodicity to a solution of the scattering problem in the whole plane.

### 3.2 Law of Conservation of Energy

In this section we want to show that the coupled system admits a law of conservation of energy [31]. First, we start with the scattering problem for the ambient space alone, then deduce a law for the coupled system.

**Theorem 3.3.** Suppose there is no scatterer coupled to the ambient space. Assume that the solutions to the left and to the right of \( m = 0 \) have representations

\[
m < 0, \quad y_{mn} = u_{mn} e^{-i\omega t} = \sum_{l=0}^{N-1} (a_i^- e^{-2\pi i \theta_l m} + a_i^+ e^{2\pi i \theta_l m}) e^{2\pi i \phi_l n} e^{-i\omega t}, \quad (3.21)
\]
\[ m > 0, \quad y_{mn} = u_{mn} e^{-i\omega t} = \sum_{l=0}^{N-1} (b_l^- e^{-2\pi i \theta_l m} + b_l^+ e^{2\pi i \theta_l m}) e^{2\pi i \phi_l n} e^{-i\omega t}. \]  

(3.22)

where the coefficients \( b_l^+ \), \( a_l^- \) for \( l \in \mathbb{P} \) correspond to outgoing to infinity waves, whereas \( b_l^- \), \( a_l^+ \) for \( l \in \mathbb{P} \) do to incoming from infinity waves. If \( \omega \) is real and \( \theta_l \) such that \( l \in \mathbb{P} \), then for a finite region \([m_1, m_2] \times [0, N]\), where \( m_1 < 0 \) and \( m_2 > 0 \), the incoming energy flux is equal to the outgoing energy flux,

\[
\text{Im} \left( \sum_{n=1}^{N} (\bar{u}u_x)_{n m} \right) = \text{Im} \left( \sum_{n=1}^{N} (\bar{u}u_x)_{n m} \right).
\]

(3.23)

This is expressed in terms of the coefficients as

\[
\sum_{l \in \mathbb{P}} \left( (|b_l|^2 + |a_l^-|^2) - (|a_l^+|^2 + |b_l^-|^2) \right) \sin (2\pi \theta_l) = 0.
\]

(3.24)

**Proof:** We multiply (3.3) by \( \bar{u}_{mn} \) and sum up over the region. Then applying identity (5.11) (see Appendix) with \( n_1 = 0 \) and \( n_2 = N \), and taking into account that \( \Omega_2 = -\Delta \), and the condition of pseudo-periodicity \( u_{mn+1} = e^{2\pi i \omega} u_{mn} \), we have

\[
0 = -\sum_{n=1}^{N} \sum_{m=m_1+1}^{m_2} (\bar{u} \Delta u + \omega \bar{u}u)_{mn}
\]

\[
= -\sum_{n=1}^{N} ((\bar{u}u_x)_{m_2 n} - (\bar{u}u_x)_{m_1 n}) + \sum_{n=1}^{N} \sum_{m=m_1+1}^{m_2} (|\nabla u|^2 + \omega |u|^2)_{mn}.
\]

(3.25)

Since \( \omega \) is real then we have (3.23). The right hand side of (3.23) in terms of the Fourier coefficients is

\[
\text{Im} \sum_{n=1}^{N} (\bar{u}u_x)_{n m} = \text{Im} \left\{ N \sum_{l=0}^{N-1} \left( |a_l^+|^2 (e^{2\pi i \theta_l} - 1) + |a_l^-|^2 (e^{-2\pi i \theta_l} - 1) + 2 \text{Re} \{ a_l^+ a_l^- e^{-4\pi i \theta_l m_2} (e^{-2\pi i \theta_l} - 1) \} \right) \right\}
\]

\[
= N \sum_{l \in \mathbb{P}} (|a_l^+|^2 - |a_l^-|^2) \sin (2\pi \theta_l),
\]

(3.26)

whereas the left hand side is

\[
\text{Im} \sum_{n=1}^{N} (\bar{u}u_x)_{n m} = N \sum_{l \in \mathbb{P}} (|b_l^+|^2 - |b_l^-|^2) \sin (2\pi \theta_l).
\]

(3.27)
Hence
\[ \sum_{l \in \mathcal{P}} \left( (|b^+_l|^2 + |a^-_l|^2) - (|a^+_l|^2 + |b^-_l|^2) \right) \sin (2\pi \theta_l) = 0, \quad (3.28) \]
which means that if \( \theta_l \in (0,1/2) \) the energy of incoming waves is equal to the energy of outgoing waves.

**Theorem 3.4.** Assume for the coupled system the solutions to the left and to the right of \( m = 0 \) have representations
\[
m < 0, \quad y_{mn} = u_{mn} e^{-i\omega t} = \sum_{l=0}^{N-1} (a^-_l e^{-2\pi i \theta_l m} + a^+_l e^{2\pi i \theta_l m}) e^{2\pi i \phi_l n} e^{-i\omega t}, \quad (3.29)
\]
\[
m > 0, \quad y_{mn} = u_{mn} e^{-i\omega t} = \sum_{l=0}^{N-1} (b^-_l e^{-2\pi i \theta_l m} + b^+_l e^{2\pi i \theta_l m}) e^{2\pi i \phi_l n} e^{-i\omega t}, \quad (3.30)
\]
where the coefficients \( b^-_l, a^-_l \) for \( l \in \mathcal{P} \) correspond to outgoing to infinity waves, whereas \( b^+_l, a^+_l \) for \( l \in \mathcal{P} \) do to incoming from infinity waves. For the one-dimensional lattice the solution has the representation
\[
x_n = z_n e^{-i\omega t} = \sum_{l=0}^{N} c_l e^{2\pi i \phi_l n} e^{-i\omega t}. \quad (3.31)
\]
If \( \omega \) is real and \( \theta_l \in (0,1/2), \ l \in \mathcal{P} \), then for a finite region \([m_1,m_2] \times [0,N]\), where \( m_1 < 0 \) and \( m_2 > 0 \), the incoming energy flux is equal to outgoing energy flux.

**Proof:** We need the following:
\[
\sum_{n=1}^{N} (\bar{z} \Omega z)_n = -\frac{\bar{z}_N}{\sqrt{M_N}} \left( \frac{z_{N+1}}{\sqrt{M_{N+1}}} - \frac{z_N}{\sqrt{M_N}} \right) + \frac{\bar{z}_0}{\sqrt{M_0}} \left( \frac{z_1}{\sqrt{M_1}} - \frac{z_0}{\sqrt{M_0}} \right) + \sum_{n=1}^{N} \left( \frac{\bar{z}_n}{\sqrt{M_n}} - \frac{\bar{z}_{n-1}}{\sqrt{M_{n-1}}} \right) \left( \frac{z_n}{\sqrt{M_n}} - \frac{z_{n-1}}{\sqrt{M_{n-1}}} \right). \quad (3.32)
\]
Multiplying (2.36) by \( \bar{z}_n \) and summing up for one period, using the condition of pseudo-periodicity for \( z_n \) we obtain
\[
0 = \sum_{n=1}^{N} (\omega |z_n|^2 - |\frac{z_n}{\sqrt{M_n}} - \frac{z_{n-1}}{\sqrt{M_{n-1}}}|^2) - \sum_{n=1}^{N} \bar{z}_n \gamma_n u_{0n}. \quad (3.33)
\]
Similarly, multiplying (2.37) by $\bar{u}_{mn}$ and using (5.11) we get

$$0 = \sum_{n=1}^{N} \sum_{m=m_1}^{m_2} (\omega |u_{mn}|^2 - |\nabla u_{mn}|^2) + \sum_{n=1}^{N} (\bar{u}u_x)_{m_{2n}} - \sum_{n=1}^{N} (\bar{u}u_x)_{m_{1n}} - \sum_{n=1}^{N} \bar{u}_0 n_\gamma n z_n, \quad (3.34)$$

the boundary values at $n = 0$ and $n = N$ are canceled out because of the pseudo-periodicity of $u_{mn}$.

Adding (3.33) with (3.34) and taking imaginary part of it leads to the condition (3.23).

### 3.3 Formulation in Terms of Fourier Coefficients

Let us consider the problem of finding the outgoing waves in terms of incoming ones. For this purpose, the solutions in the ambient space are given by (3.13) and (3.14), and for the one-dimensional lattice by (3.2). The known values are $a_l^+$, $b_l^-$, $l = 0, \ldots N - 1$, where the coefficients correspond to incoming waves from minus and plus infinity, respectively, whereas the unknown values are $a_l^-$ and $b_l^+$, $l = 0, \ldots N - 1$, which correspond to outgoing waves to minus and plus infinity, respectively (see Fig. 3.3), and unknown coefficients for the 1D lattice, $c_l$. To set the system of equations, we require that the solution for the ambient space be continuous at $m = 0$ and the solutions satisfy to (3.17) and (3.18). Following these three conditions we obtain the system:

$$\begin{cases}
\sum_{l=0}^{N-1} (a_l^- - b_l^+) e^{\frac{2\pi i l}{N} n} = \sum_{l=0}^{N-1} (b_l^- - a_l^+) e^{\frac{2\pi i l}{N} n}, \\
\sum_{l=0}^{N-1} (a_l e^{2\pi i \theta_l} - b_l^+ e^{-2\pi i \theta_l} - \gamma_n c_l) e^{\frac{2\pi i l}{N} n} = \sum_{l=0}^{N-1} (b_l^- e^{2\pi i \theta_l} - a_l^+ e^{-2\pi i \theta_l}) e^{\frac{2\pi i l}{N} n}, \\
\sum_{l=0}^{N-1} (c_l (\omega - \frac{2 \pi i l}{M_n} + \frac{2 \pi i l}{\sqrt{M_n M_{n+1}}} + \frac{2 \pi i l}{\sqrt{M_n M_{n-1}}}) - \gamma_n b_l^+) e^{\frac{2\pi i l}{N} n} = \gamma_n \sum_{l=0}^{N-1} b_l^+ e^{\frac{2\pi i l}{N} n}.
\end{cases} \quad (3.35)$$

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The system (3.35) can be written in the matrix form:

$$\mathbb{B} \vec{X} = \vec{F},$$

where the matrix $\mathbb{B}$ is obtained from the coefficients of the left hand side of (3.35) and $\vec{F}$ is the right hand side.

FIGURE 3.3. Incident and transmitted/reflected waves in terms of the Fourier coefficients.

### 3.4 Reduction to a Bounded Domain

In order to write a variational form of the scattering problem, we first reduce it to a bounded domain in $\mathbb{Z}^2$.

The method consists in writing an equivalent problem, set in a bounded domain with artificial boundaries $m = \mp \mathcal{M}$. The outgoing condition is enforced through the Dirichlet-to-Neumann operator for outgoing fields, $\mathcal{T}$ [6, 16, 19, 22]. It acts on traces on $m = \mp \mathcal{M}$ of functions in the pseudo-periodic space $\mathcal{H}_\kappa(\mathcal{R})$,

$$\mathcal{H}_\kappa(\mathcal{R}) = \{(z, u) \in \mathcal{H}(\mathcal{R}) : z_N = e^{2\pi i \kappa_{0}, u_{mN} = e^{2\pi i \kappa_{0}}u_{m0}\}},$$

(3.37)
and is defined through the Fourier transform as follows. For any function \( u_{mn}, \) with \( n \in \mathbb{Z} \) and \( m \) restricted to the values \(-M - 1\) and \( M\), let \((\hat{u}_m)_l^r\) be the \( l\)th Fourier coefficient of \( u_{mn}e^{-2\pi i \phi n} \), then the map \( \mathcal{T} \) is defined by

\[
(\hat{\mathcal{T}u}_m)_l^r = (1 - e^{2\pi i \theta_l})(\hat{u}_m)_l^r, \quad \text{for } m = -M - 1 \text{ and } m = M. \quad (3.38)
\]

\( \mathcal{T} \) characterizes the normal forward difference of an outgoing function on \( m = \mp M \) as a function of its values on \( m = \mp M \).

\[
(\partial_{\nu} u + \mathcal{T} u)_{\pm M n} = 0, \quad \text{for } u \text{ outgoing}, \quad (3.39)
\]

where

\[
(\partial_{\nu} u)_{-M n} = -u_x \big|_{m = -M - 1} = -u_{-M n} + u_{(-M - 1)n}, \quad (3.40)
\]

\[
(\partial_{\nu} u)_{M n} = u_x \big|_{m = M} = u_{(M + 1)n} - u_{M n}. \quad (3.41)
\]

Then using the decomposition \( u = u^{sc} + u^{inc} \) of the solution to the scattering problem \( P^{sc} \) we obtain

\[
-(\mathcal{T}u^{sc})_{-M n} = \sum_{l=0}^{N-1} a_l^- (e^{2\pi i \theta_l} - 1)e^{2\pi i \theta_l M} e^{2\pi i \frac{n+l}{N}}, \quad (3.42)
\]

\[
-(\mathcal{T}u^{sc})_{M n} = \sum_{l=0}^{N-1} b_l^+ (e^{2\pi i \theta_l} - 1)e^{2\pi i \theta_l M} e^{2\pi i \frac{n+l}{N}}, \quad (3.43)
\]

\[
\partial_{\nu} u + \mathcal{T} u = \partial_{\nu} u^{inc} + \mathcal{T} u^{inc}
\]

\[
= \begin{cases} 
2 \sum_{l \in \mathbb{Z}} (1 - \cos(2\pi \theta_l)) a_l^+ e^{2\pi i \theta_l (-M)} e^{2\pi i \phi n}, & m = -M \\
2 \sum_{l \in \mathbb{Z}} (1 - \cos(2\pi \theta_l)) b_l^- e^{-2\pi i \theta_l M} e^{2\pi i \phi n}, & m = M 
\end{cases}. \quad (3.44)
\]

Thus we are led to the following problem set in the bounded domain \( \mathcal{R}^M \) of \( \mathbb{Z}^2 \):

\[
\mathcal{R}^M = [-M - 1, M] \times [0, N]. \quad (3.45)
\]
Problem 3.5. (Scattering problem reduced to a bounded domain, $P^sc_M$) Find $(z, u)$ in $\mathcal{H}(\mathbb{R}^M)$ such that

$$\omega z_n = (\Omega_1 z)_n + (\Gamma u)_n,$$

(3.46)

$$\omega u_{mn} = (\Gamma^+ z)_{mn} + (\Omega_2 u)_{mn},$$

(3.47)

and $(z, u)$ are $\kappa$-pseudoperiodic in $n$.

(3.48)

$$\partial_\nu u = \partial_\nu u^{inc} - T(u - u^{inc}) \text{ on } m = \mp M.$$  

(3.49)

Problems $P^{sc}$ and $P^{sc}_M$ are equivalent in the sense of the following theorem [6].

Theorem 3.6. If $(z, u)$ is a solution of $P^{sc}$ such that $(\tilde{z}, \tilde{u}) = (z, u)|_{\mathbb{R}^M} \in \mathcal{H}(\mathbb{R}^M)$, then $(\tilde{z}, \tilde{u})$ is a solution of $P^{sc}_M$. Conversely, if $(\tilde{z}, \tilde{u})$ is a solution of $P^{sc}_M$, it can be extended uniquely to a solution $(z, u)$ of $P^{sc}$.

Proof: The first part of the theorem is a direct result since the condition (3.49) is equivalent to (3.20). Conversely, if $(\tilde{z}, \tilde{u})$ is a solution of $P^{sc}_M$, then $\tilde{u}$ can be written as $\tilde{u} = \tilde{u}^{inc} + \tilde{u}^{sc}$. Set $z = \tilde{z}$ and

$$u_{mn} = \begin{cases} 
\tilde{u}_{mn}, & \text{if } |m| \leq M; \\
\sum_{\ell=0}^{N-1} (\tilde{u}^{inc}_\ell e^{2\pi i t_\ell m} + \tilde{u}^{sc}_\ell e^{-2\pi i t_\ell m}) e^{2\pi i \phi_\ell m}, & \text{if } m < -M; \\
\sum_{\ell=0}^{N-1} (\tilde{u}^{inc}_\ell e^{-2\pi i t_\ell m} + \tilde{u}^{sc}_\ell e^{2\pi i t_\ell m}) e^{2\pi i \phi_\ell m}, & \text{if } m > M.
\end{cases}$$

(3.50)

It is clear that the function $u$ is continuous through the boundaries $m = \mp M$ and $(z, u)$ satisfies the problem $P^{sc}$. $lacksquare$

### 3.5 Variational Form of the Scattering Problem

We begin by obtaining a variational form of the scattering problem in the ambient space without coupling to the one-dimensional lattice. We multiply $(\Omega_2 - \omega)u = 0$ by a test function $\tilde{v}, \tilde{v} \in \mathcal{H}_\kappa(\mathbb{R}^M)$, that it is pseudo-periodic. Using the summation
by parts formula (see Appendix) gives
\[
\sum_{n=1}^{N} \sum_{m=-M}^{M} (\omega u \bar{v} - \nabla_- \bar{v} \nabla_- u)_{mn} - \sum_{n=1}^{N} (\bar{v}_{(-M-1)n}(Tu)_{-Mn} - (\bar{v}Tu)_{Mn}) \\
= -\sum_{n=1}^{N} (\bar{v}_{(-M-1)n}(\partial_{\nu}u\text{inc} + Tu\text{inc}))_{-Mn} - \sum_{n=1}^{N} (\bar{v}(\partial_{\nu}u\text{inc} + Tu\text{inc}))_{Mn}.
\] (3.51)

Then we need a formula of summation by parts for the operator $\Omega_1$. For deriving that the operator can be written in the following form:
\[
(\Omega_1 z)_n = -(M^{-1/2} \nabla_- K \nabla_+ M^{-1/2} z)_n \\
= -\frac{1}{\sqrt{M_n}} \nabla_- \left( k_n \left( \frac{z_{n+1}}{\sqrt{M_{n+1}}} - \frac{z_n}{\sqrt{M_n}} \right) \right) \\
= -\frac{1}{\sqrt{M_n}} \left( k_{n+1} \frac{z_{n+1}}{\sqrt{M_{n+1}}} - (k_n - k_{n+1}) \frac{z_n}{\sqrt{M_n}} - k_{n-1} \frac{z_{n-1}}{\sqrt{M_{n-1}}} \right),
\] (3.52)

with $(Kz)_n = k_n z_n$ and $(M^{-1/2} z)_n = \frac{z_n}{\sqrt{M_n}}$. The discrete version of the first Green’s formula is
\[
\sum_{n=1}^{N} (\Omega_1 z)_n \bar{w}_n = -\sum_{n=1}^{N} (M^{-1/2} \nabla_- K \nabla_+ M^{-1/2} z)_n \bar{w}_n \\
= -\sum_{n=1}^{N} (\nabla_- K \nabla_+ M^{-1/2} z)_n (M^{-1/2} \bar{w})_n \\
= \sum_{n=0}^{N-1} (K \nabla_+ M^{-1/2} z)_n (\nabla_- M^{-1/2} \bar{w})_n \\
- (K \nabla_+ M^{-1/2} z)_N (M^{-1/2} \bar{w})_N + (K \nabla_+ M^{-1/2} z)_0 (M^{-1/2} \bar{w})_0.
\] (3.53)

Therefore the problem $P_{sc}^{\omega}$ has the following variational form:

**Problem 3.7.** (Scattering Problem, variational form, $P_{sc}^{\omega}$.) Find a function $(z, u) \in \mathcal{H}_c(R^M)$ such that
\[
\sum_{n=0}^{N-1} (K \nabla_+ M^{-1/2} z)_n (\nabla_+ M^{-1/2} \bar{w})_n + \sum_{n=1}^{N} ((\Gamma u)_n \bar{w}_n - (\omega z)_n \bar{w}_n) = 0,
\]
\[
\sum_{n=1}^{N} \sum_{m=-M}^{M} (\omega u \bar{v} - \nabla_- \bar{v} \nabla_- u - (\Gamma^\dagger z) \bar{v})_{mn} - \sum_{n=1}^{N} (\bar{v}_{(-M-1)n}(Tu)_{-Mn} - (\bar{v}Tu)_{Mn}) \\
= -\sum_{n=1}^{N} (\bar{v}_{(-M-1)n}(\partial_{\nu}u\text{inc} + Tu\text{inc}))_{-Mn} - \sum_{n=1}^{N} (\bar{v}(\partial_{\nu}u\text{inc} + Tu\text{inc}))_{Mn}.
\] (3.54)

for any $(w, v) \in \mathcal{H}_c(R^M)$.

**Theorem 3.8.** The problem (3.54) always has a solution [6].
Proof: For the sake of simplicity let us rewrite (3.54) in the following form

\[(AY, V) = (F, V), \quad (3.55)\]

where \(Y = (z, u), F = (0, f)\) and \(V = (w, v)\). Then to prove the theorem we use the Fredholm alternative [26], which means that the scattering problem (3.54) has a solution \((z, u)\) if and only if \((F, V) = 0\) for all \(V \in \text{Null}(A^*)\) or in other words

\[(F, V) = 0 \text{ for all } V \text{ such that } (AY, V) = 0 \text{ for all } Y. \quad (3.56)\]

Any function \(V\) satisfying the adjoint eigenvalue problem \((AY, V) = 0\) for all \(Y\) satisfies \((AV, V) = 0\) as well. By Theorem 3.4 it follows that \(v\) in \(V\) contains only evanescent harmonics in the Fourier series, that is

\[v_{mn} = \begin{cases} \sum_{\ell \in \mathbb{P}} v_{\ell}^- e^{-2\pi i \theta_{\ell} m} e^{2\pi i \phi_{\ell} n} & \text{for } m \leq 0, \\ \sum_{\ell \in \mathbb{P}} v_{\ell}^+ e^{2\pi i \theta_{\ell} m} e^{2\pi i \phi_{\ell} n} & \text{for } m > 0. \end{cases} \quad (3.57)\]

Thus we have:

\[(F, V) = (f, v) = -2 \sum_{n=1}^{N} \left( (\sum_{\ell \in \mathbb{P}} v_{\ell}^- e^{2\pi i \theta_{\ell} (-\mathcal{M}-1)} e^{-2\pi i \phi_{\ell} n}) \times (\sum_{\ell' \in \mathbb{P}} (1 - \cos(2\pi \theta_{\ell'})) a_{\ell'}^+ e^{2\pi i \theta_{\ell'} (-\mathcal{M})} e^{2\pi i \phi_{\ell'} n} ) \right) -2 \sum_{n=1}^{N} \left( (\sum_{\ell \in \mathbb{P}} \bar{v}_{\ell}^+ e^{-2\pi i \theta_{\ell} \mathcal{M}} e^{-2\pi i \phi_{\ell} n}) \times (\sum_{\ell' \in \mathbb{P}} (1 - \cos(2\pi \theta_{\ell'})) b_{\ell'}^- e^{-2\pi i \theta_{\ell'} \mathcal{M}} e^{2\pi i \phi_{\ell'} n} ) \right) \quad (3.58)\]

Therefore there exists a solution \((z, u)\) to the problem (3.54).

The problems \(P_{\mathcal{M}_1}^{sc}\) and \(P_{\text{var}}^{sc}\) are equivalent:
Theorem 3.9. *(Equivalence of $P_{sc}^M$ and $P_{var}$*) If $(z, u) \in \mathcal{H}_\kappa (\mathcal{R}^M)$ satisfies the scattering problem $P_{sc}^M$, then $(z, u)$ satisfies $P_{var}$. Conversely, if $(z, u)$ satisfies $P_{var}$ for any $(w, v) \in \mathcal{H}_\kappa (\mathcal{R}^M)$, then $(z, u)$ satisfies $P_{sc}^M$ also.

*Proof:* The first part of the theorem comes directly from the derivation of the variational form. For the second part, first, let us show that a solution $(z, u)$ of $P_{sc}^M$ satisfies equations (3.46) – (3.47). Here we use advantage of the discrete prototype, a test function can be taken concentrated at one point. For a continuous case as we know a test function can not be a $\delta$-function, for the case see [15].

For the one-dimensional lattice we are taking the following test function:

$$(w_n, v_{mn}) = \begin{cases} (1, 0) & \text{for single point } (0, n), \ n \in [0, N) \ , \\
(0, 0) & \text{otherwise} \ . \end{cases} \quad (3.59)$$

Substituting the test function into (3.54) yields

$$(K \nabla_+ M^{-1/2} z)_n (\nabla_+ M^{-1/2} w)_n + (K \nabla_+ M^{-1/2} z)_{n-1} (\nabla_+ M^{-1/2} w)_{n-1}$$

$$+ (\Gamma u)_n \bar{w}_n - (\omega z)_n \bar{w}_n = k_n \left( \frac{z_{n+1}}{\sqrt{M_{n+1}}} - \frac{z_n}{\sqrt{M_n}} \right) \frac{-1}{\sqrt{M_n}}$$

$$+ k_{n-1} \left( \frac{z_n}{\sqrt{M_n}} - \frac{z_{n-1}}{\sqrt{M_{n-1}}} \right) \frac{1}{\sqrt{M_n}} + (\Gamma u)_n - (\omega z)_n \quad (3.60)$$

$$= (\Omega_1 z)_n + (\Gamma u)_n - \omega z_n = 0.$$ 

For the two-dimensional lattice first we take a test function concentrated inside of the rectangle $\mathcal{R}^M$ excluding points coupled to the one-dimensional lattice and boundaries $m = -M - 1$ and $m = M$:

$$(w_n, v_{mn}) = \begin{cases} (0, 1) & \text{for some single } (m, n) \text{ such that } m \in (-M - 1, 0) \cup (0, M) \ , \\
(0, 0) & \text{otherwise} \ , \end{cases}$$

we obtain from (3.54) the first equation is zero and the second one is:

$$\omega u_{mn} - ((1, 1) \cdot (u_x, u_y)_{mn} + (-1, 0) \cdot (u_x, u_y)_{(m+1)n} + (0, -1) \cdot (u_x, u_y)_{m(n+1)}) = 0,$$
which leads that \((\Omega_2 u - \omega u)_{mn} = 0\).

Then for the coupled points take the following test function:

\[
(w_n, v_{mn}) = \begin{cases} 
(0, 1) & \text{for a single pair } (0, n), \ n \in [0, N], \\
(0, 0) & \text{otherwise}.
\end{cases}
\]  

(3.61)

which gives the result

\[
\omega u_0 n - ((1, 1) \cdot (u_x, u_y)_{0n} + (-1, 0) \cdot (u_x, u_y)_{1n} + (0, -1) \cdot (u_x, u_y)_{0(n+1)}) \\
-(\Gamma^t z)_{0n} = \omega u_0 n - (u_x + u_y)_{0n} - (u_x)_{1n} - (u_y)_{0(n+1)} - (\Gamma^t z)_{0n} \\
= \omega u_0 n - (\Omega_2 u)_{0n} - (\Gamma^t z)_{0n} = 0.
\]  

(3.62)

On the boundary \(m = -M\) take

\[
(w_n, v_{mn}) = \begin{cases} 
(0, 1) & \text{for } m = -M - 1 \text{ and a single } n, \ n \in [0, N], \\
(0, 0) & \text{otherwise}.
\end{cases}
\]

then we have only one nonzero term in the double sum, namely with \(\nabla_- v|_{m=-M} = (v_-M_{n} - v_{(-M-1)n}, v_-M_{n} - v_{-M(n-1)}) = (-1, 0)\). It leads to the following result

\[
-(1, 0) \cdot (u_x, u_y)_{-Mn} - (T u)_{-Mn} = -(\partial_v u^{inc} + T u^{inc})_{-Mn}.
\]  

(3.63)

Taking into account that \(\partial_v u|_{m=-M} = -u_x|_{m=-M}\), we obtain

\[
-\partial_v u_{-Mn} - (T u)_{-Mn} = -(\partial_v u^{inc} + T u^{inc})_{-Mn},
\]  

(3.64)

which is equivalent to (3.49) for \(m = -M\).

On the boundary \(m = M\) take

\[
(w_n, v_{mn}) = \begin{cases} 
(0, 1) & \text{for } m = M \text{ and a single } n, \ n \in [0, N], \\
(0, 0) & \text{otherwise}.
\end{cases}
\]
then we have the following nonzero term in the double sum, namely

\[
\omega u_M - (\nabla v \cdot \nabla u)_M - (\nabla v \cdot \nabla u)_{M(n+1)}
\]

\[
= \omega u_M - (1, 1) \cdot (u_x, u_y)_M - (0, 1) \cdot (u_x, u_y)_{M(n+1)}
\]

\[
= \omega u_M - (u_x)_M - (u_y)_M + (u_y)_{M(n+1)}
\]

\[
= -u_{(M+1)n} + u_M = -(u_x)_M = -\partial_v u|_{m=M}.
\]

It leads to the following equality at \( m = M \)

\[
-\partial_v u_M - (Tu)_{Mn} = -(\partial_v u_{inc} + Tu_{inc})_{Mn}.
\]

(3.65)

(3.66)

### 3.6 Scattering Problem for Period Two

In the equation (3.35), the matrix \( B \) has the following form

\[
B_2 = \begin{pmatrix}
1 & -1 & 0 & 1 & -1 & 0 \\
1 & -1 & 0 & -1 & 1 & 0 \\
 \varepsilon^{2\pi i \theta_0} & - \varepsilon^{-2\pi i \theta_0} & -\bar{\gamma}_0 & \varepsilon^{2\pi i \theta_1} & - \varepsilon^{-2\pi i \theta_1} & -\bar{\gamma}_0 \\
 \varepsilon^{2\pi i \theta_0} & - \varepsilon^{-2\pi i \theta_0} & -\bar{\gamma}_1 & - \varepsilon^{2\pi i \theta_1} & \varepsilon^{-2\pi i \theta_1} & \bar{\gamma}_1 \\
0 & - \gamma_0 & \omega - \frac{2}{m_0} \frac{\cos(m \varphi)}{\sqrt{m_0 m_1}} & 0 & - \gamma_0 & \omega - \frac{2}{m_0} \frac{\cos(m \varphi)}{\sqrt{m_0 m_1}} \\
0 & - \gamma_1 & \omega - \frac{2}{m_1} \frac{\cos(m \varphi)}{\sqrt{m_0 m_1}} & 0 & \gamma_1 & -(\omega - \frac{2}{m_1} \frac{\cos(m \varphi)}{\sqrt{m_0 m_1}})
\end{pmatrix},
\]

(3.67)

with right hand side

\[
\bar{F} = \begin{pmatrix}
-a_0^+ + b_0^- - a_1^+ + b_1^- \\
-a_0^+ + b_0^- + a_1^+ - b_1^- \\
-a_0 e^{-2\pi i \theta_0} + b_0^- e^{2\pi i \theta_0} - a_1^+ e^{-2\pi i \theta_1} + b_1^- e^{2\pi i \theta_1} \\
-a_0^+ e^{-2\pi i \theta_0} + b_0^- e^{2\pi i \theta_0} + a_1^+ e^{-2\pi i \theta_1} - b_1^- e^{2\pi i \theta_1} \\
\gamma_0 (b_0^- + b_1^-) \\
\gamma_1 (b_0^- - b_1^-)
\end{pmatrix},
\]

(3.68)
and the unknown vector-column written in a row is:

\[
\vec{X} = \left( a_0^-, b_0^+, c_0, a_1^-, b_1^+, c_1 \right). \tag{3.69}
\]

By using algebraic operations the system can be reduced to a form with matrix

\[
\begin{pmatrix}
1 & -1 & 0 & 0 & 0 & 0 \\
2e^{2\pi i\theta_0} & -2e^{-2\pi i\theta_0} & -2\gamma_0 - 2\gamma_1 & 0 & 0 & \gamma_1 - \gamma_0 \\
0 & -2\gamma - \gamma_1 & 2\omega_0 \frac{2}{M_0} \frac{2}{M_1} \frac{\cos(\pi \kappa)}{\sqrt{M_0 M_1}} & 0 & \gamma_1 - \gamma_0 & \gamma_1 - \gamma_0 \\
0 & 0 & 2\gamma - \gamma_1 & 2e^{2\pi i\theta_1} & -2e^{-2\pi i\theta_1} & -2\gamma_0 - 2\gamma_1 \\
0 & \gamma_1 - \gamma_0 & \frac{2}{M_1} - \frac{2}{M_0} & 0 & -2\gamma_0 - 2\gamma_1 & 2\omega_0 \frac{2}{M_0} \frac{2}{M_1} \frac{\cos(\pi \kappa)}{\sqrt{M_0 M_1}} \\
\end{pmatrix} \tag{3.70}
\]

and right hand side:

\[
\begin{pmatrix}
b_0^- - a_0^+ \\
2b_0^- e^{2\pi i\theta_0} - 2a_0^+ e^{-2\pi i\theta_0} \\
(\gamma_0 + \gamma_1) b_0^- + (\gamma_0 - \gamma_1) b_1^- \\
b_1^- - a_1^+ \\
2b_1^- e^{2\pi i\theta_1} - 2a_1^+ e^{-2\pi i\theta_1} \\
(\gamma_0 - \gamma_1) b_0^- + (\gamma_0 + \gamma_1) b_1^- \\
\end{pmatrix}, \tag{3.71}
\]

and with the same unknown vector \( \vec{X} \).

**Example 3.10.** Special case \( M_0 = M_1 = 1 \) and \( \gamma_0 = \gamma_1 = 1 \). In this case, the total structure becomes uniform, but we would like to imagine that it has a period of \( N = 2 \) and still there are two Fourier harmonics for representing solutions. The
matrix (3.70) has a block-diagonal form:

\[
\begin{pmatrix}
1 & -1 & 0 & 0 & 0 & 0 \\
2e^{2\pi i\theta_0} & -2e^{-2\pi i\theta_0} & -2 & 0 & 0 & 0 \\
0 & -2 & 2\omega-4+4\cos(\pi\kappa) & 0 & 0 & 0 \\
0 & 0 & 0 & 2e^{2\pi i\theta_1} & -2e^{-2\pi i\theta_1} & -2 \\
0 & 0 & 0 & 0 & -2 & 2\omega-4-4\cos(\pi\kappa)
\end{pmatrix}.
\] (3.72)

Note that the harmonics can be found independent from each other. To find dispersion relation for the case we set the determinant of (3.72) equal to zero.

Let us find the transmission coefficient for the region \(|\mathcal{P}| = 1\), where \(2 - 2\cos(\pi\kappa) < \omega < 2 + 2\cos(\pi\kappa)\) and \(\kappa \in (0, 1/2)\). By the **transmission coefficient**, we mean a measure of how much of an incident wave passes through the coupled 1D lattice. It is calculated by taking square root of the ratio of the energy of the transmitted wave to that of the incident wave. We consider a particular case and let the incident wave coming from the left to the right be given by

\[
1 \cdot e^{2\pi i\theta_0} e^{2\pi i\phi_0} = 1 \cdot e^{2\pi i\theta_0} e^{\pi i\kappa},
\]

which contains only one propagating harmonic. The energy of the incident wave according to (3.24) is \(|1|^2 \sin(2\pi \theta_0)\), where \(\theta_0\) is real in \(|\mathcal{P}| = 1\) and \(\theta_0 \in (0, \frac{1}{2})\). The energy of the transmitted wave is \(|b_0^+|^2 \sin(2\pi i \theta_0)\), where \(b_0^+\) can be found from the system (3.70) with the right hand side

\[
\vec{F} = (-1, -2e^{2\pi i \theta_0}, 0, 0, 0, 0).
\] (3.73)

The transmission coefficient is

\[
T = \sqrt{\frac{|b_0^+|^2 \sin(2\pi \theta_0)}{|1|^2 \sin(2\pi \theta_0)}} = |b_0^+|.
\] (3.74)
Fig. 3.4 shows three cases of the transmission coefficients for $N = 2$ when masses are different.

### 3.7 Scattering Problem for Period Three

Here, let us give a couple of examples for case $N = 3$.

**Example 3.11.** Transmission coefficient for case $N = 3$ with $\gamma_0 = \gamma_1 = \gamma_2 = 1$. Let us again find the transmission coefficient over the region $|\Psi| = 1$, where $0 < \omega < 3$. In the region there is only one propagating 0-harmonic. The incident wave is given by

$$1 \cdot e^{2\pi i \theta_0} e^{2\pi i \phi_0} = 1 \cdot e^{2\pi i \theta_0} e^{2\pi i \frac{\alpha}{3}}.$$

Fig. 3.5–3.6 show graphs of the transmission coefficient for $N = 3$ obtained using MAPLE.

The anomalies that appear in these graphs are the main interest of this work. We will obtain a formula for them in terms of $\kappa$ and $\omega$ with rigorous error bounds.
3.8 Existence of Guided Modes

For real $\kappa$ let us investigate how continuous perturbation of real $\omega$ into the complex plane change propagating harmonics. If $\omega = \omega_R + i\omega_I$, where $0 < \omega_I < \epsilon$ is sufficiently small, then the values of $\theta_l$ are changed as well and become, say, $\theta_l = \theta_l^R + i\theta_l^I$. From (3.5) we have the following

$$\cos(2\pi(\theta_l^R + i\theta_l^I)) = 2 - \frac{\omega_R}{2} - \frac{i\omega_I}{2} - \cos(2\pi\phi_l).$$

It is clear that

$$\text{Im}(\cos(2\pi(\theta_l^R + i\theta_l^I))) = -\frac{\omega_I}{2},$$
and after simplifying
\[
\sin(2\pi\theta_l^R)(e^{2\pi\theta_l^I} - e^{-2\pi\theta_l^I}) = \omega_I.
\]

Since \( \theta_l \in (0, 1/2) \) for \( l \in \mathcal{P} \), then it follows that the values \( \theta_l^R \) will stay in the same interval and \( \theta_l^I > 0 \) when \( \omega_I > 0 \). It implies that if \( \omega_I > 0 \), then the solution \( u_{mn}e^{-i\omega t} \) grows in time but decays in space. Conversely, if \( \omega_I < 0 \) then \( \theta_l^I < 0 \) and the solution \( u_{mn}e^{-i\omega t} \) decays in time but grows in space.

**Theorem 3.12.** Suppose that \( \{u_{mn}\} \) is a nontrivial, pseudoperiodic in \( n \) solution to the homogeneous (sourceless) problem \( P^{sc} \). Then \( \text{Im}(\omega) \leq 0 \). In addition, \( |u_{mn}| \to 0 \) as \( |m| \to \infty \) if and only if \( \text{Im}(\omega) = 0 \) [27].

**Proof:** Since the field is sourceless then there are no incoming waves from \( \pm \infty \), which implies \( a_l^+ = b_l^- = 0 \), \( l = 0, \ldots, N - 1 \) in the representations for \( u_{mn} \).

Suppose that a nontrivial solution to the problem \( P^{sc} \) decays to zero in the ambient space as \( |m| \to \infty \). It means that in the representation for \( u_{mn} \) in (3.13) and (3.14) the coefficients for propagating harmonics are equal to zero too. It follows the representations contain only evanescent harmonics. Moreover adding (3.33) and (3.34) and taking imaginary part of it we have:

\[
\text{Im}(\omega)(\sum_{n=1}^N |z_n|^2 + \sum_{n=1}^N \sum_{m_1}^{m_2} |u_{mn}|^2) = \text{Im}(\sum_{n=1}^N (\bar{u}u_x)_{m_1n} - \sum_{n=1}^N (\bar{u}u_x)_{m_2n}). \tag{3.75}
\]

When \( m_1 \to -\infty \) and \( m_2 \to +\infty \), then the right hand side of (3.75) tends to zero. Since in the left hand side of (3.75) the term \( \sum_{n=1}^N |z_n|^2 + \sum_{n=1}^N \sum_{m_1}^{m_2} |u_{mn}|^2 \) \( \neq 0 \), it implies that \( \text{Im}(\omega) = 0 \).

Conversely, if \( \text{Im}(\omega) = 0 \), then (3.75) is still valid and the right hand side of it is zero. By theorem 3.4 it follows that \( a_l^+ = b_l^- = 0 \), for \( l \in \mathcal{P} \) and in the representations for \( u_{mn} \) in (3.29) and (3.30) there are only evanescent harmonics, which leads that the solution decays as \( |m| \to \infty \).
If \( \text{Im}(\omega) > 0 \) then \( \text{Im}(\theta_l) > 0 \), which implies that the solution decays as \( |m| \to \infty \), therefore \( \text{Im}(\omega) = 0 \). Then it follows that \( \text{Im}(\omega) \leq 0 \) always. It means that if we continue analytically \( \omega \) into the complex plane the dispersion relation allows to do it only into the lower half plane of the complex plane.

**Definition 3.13.** If a source-free field exists for a real pair \((\kappa, \omega)\), the one-dimensional lattice sustains a traveling or standing wave along the lattice that decays exponentially as \( |m| \to \infty \) so that the one-dimensional lattice acts as a wave-guide. Moreover, if the guided mode ceases to exist at any nearby frequency under a perturbation of the wave number we call it non-robust.

**Theorem 3.14.** For \( N = 2 \) with \( \gamma_0 = \gamma_1 = \gamma \) or \( \gamma_0 = -\gamma_1 = -\gamma \) and any \( M_0 \) and \( M_1 \) there is no non-robust guided mode for any \( \kappa \in [0, 1] \) and \( \omega \in [0, 8] \).

**Proof:** A wave guided mode occurs under solving a scattering problem. Suppose there is a real pair \( \omega \) and \( \kappa \), which corresponds to such a guided mode. By theorem 3.12 the nontrivial solution for the corresponding homogeneous problem (3.35) for the \( \omega \) and \( \kappa \) decays \( |u_{mn}| \to 0 \) as \( |m| \to \infty \). It implies that the solution contains only evanescent harmonic. The situation may arise only in four regions of the \( (\kappa, \omega) \) plane where \( |\mathcal{P}| = 1 \). For simplicity we consider only one region with \( \kappa \in [0, 1/2), 2 - 2 \cos(\pi \kappa) < \omega < 2 + 2 \cos(\pi \kappa) \) (see Fig. 3.1), because other three ones can be treated similarly. The solution has the following form in the region:

\[
\begin{align*}
    u_{mn} &= a_1^- e^{-2\pi i \theta_1 m} e^{2\pi i \phi_1 n}, \\    u_{mn} &= b_1^+ e^{2\pi i \theta_1 m} e^{2\pi i \phi_1 n}, \\    z_n &= c_0 e^{2\pi i \phi_0 n} + c_1 e^{2\pi i \phi_1 n},
\end{align*}
\] (3.76)

with \( a_0^- = b_0^+ = 0 \) which correspond to the propagating harmonics. For finding nontrivial simultaneously \( c_0, a_1^-, b_1^+ \), and \( c_1 \) we substitute the above representations into (3.67) with zero right hand side (3.68).
Case $\gamma_0 = \gamma_1 = \gamma$. The system has the form $B_2 \vec{X} = \vec{F}$, with

$$B_2 = \begin{pmatrix}
1 & -1 & 0 & 0 & 0 & 0 \\
2e^{2\pi i \theta_0} & -2e^{-2\pi i \theta_0} & -2\bar{\gamma} & 0 & 0 & 0 \\
0 & -2\gamma & 2\omega - \frac{2}{\pi} \frac{2}{\sqrt{M_0 M_1}} & 0 & 0 & \frac{2}{M_1 - \frac{2}{\pi}} \\
0 & 0 & 0 & 1 & -1 & 0 \\
0 & 0 & \frac{2}{\gamma} & -2\gamma & 2\omega - \frac{2}{\pi} \frac{2}{\sqrt{M_0 M_1}} & 0 \\
0 & 0 & 0 & 0 & -2\gamma & 2\omega - \frac{2}{\pi} \frac{2}{\sqrt{M_0 M_1}} \end{pmatrix},$$

$$\vec{X} = (0, 0, c_0, a_1^-, b_1^+, c_1), \quad \vec{F} = (0, 0, 0, 0, 0, 0).$$

From the second and third equations of the system it follows $c_0 = c_1 = 0$. The fourth equation gives that $a_1^- = b_1^+$. The fifth equation of the system implies $4i \sin(2\pi i \theta_1) a_1^- = 0$, which is true if $\sin(2\pi \theta_1) = 0$ or $\theta_1 = 0$, but these cases contradict the assumption that the nontrivial evanescent solution is constructed in $|\Psi| = 1$ and $\theta_1$ corresponds to a pure imaginary number. It follows that for case $\gamma_0 = \gamma_1 = \gamma$ there is no guided mode for any $M_0$ and $M_1$.

Case $\gamma_0 = -\gamma_1 = -\gamma$. The system has the form $B_2 \vec{X} = \vec{F}$ with

$$B_2 = \begin{pmatrix}
1 & -1 & 0 & 0 & 0 & 0 \\
2e^{2\pi i \theta_0} & -2e^{-2\pi i \theta_0} & -2\bar{\gamma} & 0 & 0 & 0 \\
0 & 0 & 2\omega - \frac{2}{\pi} \frac{2}{\sqrt{M_0 M_1}} & 0 & -2\gamma & \frac{2}{M_1 - \frac{2}{\pi}} \\
0 & 0 & 0 & 1 & -1 & 0 \\
0 & 0 & -2\gamma & 2e^{2\pi i \theta_1} & -2e^{-2\pi i \theta_1} & 0 \\
0 & 0 & 0 & 0 & -2\gamma & 2\omega - \frac{2}{\pi} \frac{2}{\sqrt{M_0 M_1}} \end{pmatrix},$$

$$\vec{X} = (0, 0, c_0, a_1^-, b_1^+, c_1), \quad \vec{F} = (0, 0, 0, 0, 0, 0).$$

From the second and sixth equations it follows that $c_0 = c_1 = 0$. Similarly as above, the fourth equation gives that $a_1^- = b_1^+$. The fifth equation of the system
implies \( 4i \sin(2\pi \theta_1)a^+_1 = 0 \), which is true if \( \sin(2\pi \theta_1) = 0 \) or \( \theta_1 = 0 \), but these cases contradict the assumption that the nontrivial evanescent solution is constructed in \(|\mathcal{P}| = 1 \) and \( \theta_1 \) corresponds to a pure imaginary number. It follows that for case \( \gamma_0 = \gamma_1 = -\gamma \) there is no guided mode for any \( M_0 \) and \( M_1 \).

Next we formulate a criterion of existence of a non-robust guided mode for period of two, which implies that a minimal model for observing anomalous transmission is a period of two. Let us look at a general case when \( \gamma_0 \neq \gamma_1 \) in the same region \(|\mathcal{P}| = 1 \). Suppose there is a guided mode for some \( \kappa, \kappa \in [0, 1/2) \). It implies there is a real \( \omega \) such that \( \omega \in (2 - 2\cos(\pi \kappa), 2 + 2\cos(\pi \kappa)) \). In the case we have as above \( a^+_0 = b^+_0 = 0 \) and \( a^-_1 = b^+_1 \). The system for finding unknown coefficients for the nontrivial solution \( b^+_1 \), \( c_0 \), \( c_1 \) and the corresponding \( \omega \) is

\[
\begin{pmatrix}
-\gamma_0 & 2i \sin(2\pi \theta_1) & -\gamma_0 \\
-\gamma_1 & -2i \sin(2\pi \theta_1) & \gamma_1 \\
\omega - \frac{2}{M_0} + \frac{2 \cos(\pi \kappa)}{\sqrt{M_0 M_1}} & -\gamma_0 & \omega - \frac{2}{M_0} - \frac{2 \cos(\pi \kappa)}{\sqrt{M_0 M_1}} \\
\omega - \frac{2}{M_1} + \frac{2 \cos(\pi \kappa)}{\sqrt{M_0 M_1}} & \gamma_1 & -\omega - \frac{2}{M_1} - \frac{2 \cos(\pi \kappa)}{\sqrt{M_0 M_1}}
\end{pmatrix}
\begin{pmatrix}
c_0 \\
b^+_1 \\
c_1
\end{pmatrix} = \begin{pmatrix}
0 \\
0 \\
0
\end{pmatrix}.
\]

Adding the first and second equations we get \( c_0 = \frac{(\gamma_1 - \gamma_0)c_1}{(\gamma_0 + \gamma_1)} \). By using this result and the first equation one obtains \( b^+_1 = \frac{\gamma_0 \gamma_1 c_0}{(\gamma_0 + \gamma_1)} \). Adding the third and the fourth equations whereas subtracting the fourth equation from the third one and assuming that a nontrivial solution is looked for we get the following relations:

\[
\frac{(\gamma_1 - \gamma_0)}{(\gamma_0 + \gamma_1)} \left( \frac{2}{M_1} - \frac{2}{M_0} \right) - \frac{\gamma_0 \gamma_1 (\gamma_0 + \gamma_1)}{(\gamma_0 + \gamma_1) \sin(2\pi \theta_1)} + 2\omega - \frac{2}{M_0} - \frac{2}{M_1} - \frac{4 \cos(\pi \kappa)}{\sqrt{M_0 M_1}} = 0, \tag{R1}
\]

\[
\frac{(\gamma_1 - \gamma_0)}{(\gamma_0 + \gamma_1)} \left( 2\omega - \frac{2}{M_0} - \frac{2}{M_1} + \frac{4 \cos(\pi \kappa)}{\sqrt{M_0 M_1}} \right) + \frac{\gamma_0 \gamma_1 (\gamma_1 - \gamma_0)}{(\gamma_0 + \gamma_1) \sin(2\pi \theta_1)} + \frac{2}{M_1} - \frac{2}{M_0} = 0, \tag{R2}
\]

where \( \sin(2\pi \theta_1) = \sqrt{1 - (2 - \frac{\omega}{2} + \cos(\pi \kappa))^2} = i \sqrt{(2 - \frac{\omega}{2} + \cos(\pi \kappa))^2 - 1} \).
Theorem 3.15. To have a non-robust guided mode in the region of \(|\mathcal{P}| = 1\) at some \(\kappa_0, \kappa_0 \in [0, 1/2]\) there should exist a real \(\omega_0\) which satisfies (3.77) and be in the interval \((2 - 2 \cos(\pi \kappa_0), 2 + 2 \cos(\pi \kappa_0))\).

Example 3.16. \(M_0 = 2, M_1 = 1, \gamma_0 = 1\) and \(\gamma_1 = 7\). The above relations get the following forms:

\[
\frac{6}{8} + \frac{7}{\sqrt{(2 - \frac{\pi}{2} + \cos(\pi \kappa))^2 - 1}} + 2 \omega - 3 - 2 \sqrt{2} \cos(\pi \kappa) = 0, \quad (R1)
\]

\[
\frac{6}{8}(2 \omega - 3 + 2 \sqrt{2} \cos(\pi \kappa)) - \frac{42}{8 \sqrt{(2 - \frac{\pi}{2} + \cos(\pi \kappa))^2 - 1}} + 1 = 0. \quad (R2)
\]

If there are \(\kappa, \kappa \in [0, \frac{1}{2})\), and real \(\omega, \omega \in (2 - 2 \cos(\pi \kappa), 2 - 2 \cos(\pi \kappa))\), such that the corresponding relations are true simultaneously, then it implies that there is a guided mode in the region of \(|\mathcal{P}| = 1\). Indeed, in the case we have all real parameters and the solution exists if the corresponding curves cross each other in \((\kappa, \omega)\)-plane (see Fig. 3.7).

![Figure 3.7](image.png)

**FIGURE 3.7.** Left: The intersection of two relations guarantees existence of a guided mode. Right: Real part of the dispersion relation in the region of one propagating harmonic.

In the case indeed there exists a wave guided mode at \(\kappa_0 \approx 0.0616\) and \(\omega_0 \approx 0.9792\), \(\omega_0 \in (2 - 2 \cos(\pi \kappa_0), 2 + 2 \cos(\pi \kappa_0))\).
FIGURE 3.8. The transmission coefficient for $M_0 = 2$, $M_1 = 1$, $\gamma_0 = 1$, $\gamma_1 = 7$ (left) with refining resolution for $\kappa$ (right).

**Example 3.17.** *Non-robust guided mode at $\kappa_0 = 0$.*** On Fig. 3.9 it is shown that when $M_0 = 2$, $M_1 = 1$, $\gamma_0 = 1.029633513$, and $\gamma_1 = 7$ the relations have a tangent point at $\kappa_0 = 0$ and $\omega_0 \approx 0.9778859328$.

**Theorem 3.18.** *There is a non-robust guided mode at $\kappa_0 = 0$ for $N = 3$ with $\gamma_0 = \gamma_1 = \gamma_2 = 1$, $M_1 = M_2 = M$, $0 < M < 3\sqrt{21}$, and $M_0$ is arbitrary, such that $M_0 > 0$ and $M_0 \neq M$.***
FIGURE 3.10. The transmission coefficient for \( M_0 = 2, M_1 = 1, \gamma_0 = 1.029633513, \gamma_1 = 7 \) (left) with refining resolution for \( \kappa \) (right).

**Proof:** We demonstrate the existence of a guided mode at \( \kappa_0 = 0 \) by constructing a nontrivial solution to the homogeneous problem with finding of the corresponding real \( \omega_0 \) in the region of \( |\Psi| = 1 \) where the other two harmonics are evanescent. We look for a particular solution for the one-dimensional lattice with

\[
  c_0 = 0, \quad c_1 = -c_2, \quad (3.78)
\]

while for the ambient space with

\[
  a_0 = b_0^+ = 0, \quad a_1^- = -a_2^-, \quad b_1^+ = -b_2^+, \quad (3.79)
\]

that is we force the coefficients under the propagating harmonics to be equal to zero. Taking into account all these restrictions on the coefficients the system (3.35) gives

\[
\begin{align*}
  a_1^- &= b_1^+, \\
  \sin (2\pi \theta_1) &= \sin (2\pi \theta_2), \quad \cos (2\pi \theta_1) = \cos (2\pi \theta_2), \\
  c_1 &= 2ia_1^- \sin (2\pi \theta_1), \\
  2i \sin (2\pi \theta_1) (\omega - \frac{\beta}{M}) - 1 &= 0,
\end{align*}
\]

where \( \sin (2\pi \theta_1) = i\sqrt{(\frac{\omega - \beta}{M})^2 - 1} \) and the last equation is the reduced dispersion relation. It follows that the frequency \( \omega \) does not depend on the mass \( M_0 \) at all.
Note by choosing in a such way coefficients, the solutions \( \{z_n\} \) and \( \{u_{mn}\} \) remain periodic in \( n \). Indeed,

\[
\begin{align*}
\{z_n\} &= c_1(e^{\frac{2\pi i n}{3}} - e^{-\frac{4\pi i n}{3}}), \\
\{u_{mn}\} &= a_1^- e^{-2\pi i \theta_1 m} (e^{\frac{2\pi i n}{3}} - e^{-\frac{4\pi i n}{3}}), \quad m < 0, \\
\{u_{mn}\} &= a_1^+ e^{2\pi i \theta_1 m} (e^{\frac{2\pi i n}{3}} - e^{-\frac{4\pi i n}{3}}), \quad m \geq 0.
\end{align*}
\] (3.81)

In the construction we use the property of symmetry of the system about a horizontal line coming between the beads of equal masses. ■

For example,

\[
\begin{align*}
\omega &= 1.191465768 \text{ for } M = 2, \\
\omega &= 0.7345704369 \text{ for } M = 3, \\
\omega &= 0.3610874174 \text{ for } M = 5.
\end{align*}
\] (3.82)

The results are obtained numerically using MAPLE.

**Theorem 3.19.** \((N=3)\) If \( \gamma_0 = \gamma_1 = \gamma_2 = \gamma \) and at \( \kappa = 0 \) there is a guided mode in the region of \( |\mathfrak{B}| = 1 \), then the coefficient \( c_0 = 0 \).

**Proof:** In the region of \( |\mathfrak{B}| = 1 \) with \( \kappa \in [0, 1/2) \) there is one propagating harmonic, which corresponds to \( \theta_0 \). Since at \( \kappa = 0 \) there is a guided mode, then in order to have a decaying solution as \( |m| \to \infty \) the coefficients \( a_0^- \) and \( b_0^+ \) should be zero. Moreover in this case \( \theta_1 = \theta_2 \). It follows the coefficients \( a_1^-, b_1^+, a_2^-, b_2^+, c_0, c_1 \) and \( c_2 \) satisfy the following equations:

\[
\begin{align*}
\{a_1^- = b_1^+, \quad a_2^- = b_2^+, \\
\} \gamma c_0 + 2i \sin(2\pi \theta_1) b_1^+ - \gamma c_1 + 2i \sin(2\pi \theta_1) b_2^+ - \gamma c_2 &= 0, \\
\} \gamma c_0 + 2i \sin(2\pi \theta_1) e^{\frac{2\pi i}{3}} b_1^+ - \gamma e^{\frac{2\pi i}{3}} c_1 + 2i \sin(2\pi \theta_1) e^{\frac{4\pi i}{3}} b_2^+ - \gamma e^{\frac{4\pi i}{3}} c_2 &= 0, \\
\} \gamma c_0 + 2i \sin(2\pi \theta_1) e^{\frac{4\pi i}{3}} b_1^+ - \gamma e^{\frac{4\pi i}{3}} c_1 + 2i \sin(2\pi \theta_1) e^{\frac{2\pi i}{3}} b_2^+ - \gamma e^{\frac{2\pi i}{3}} c_2 &= 0.
\end{align*}
\] (3.83)
Subtracting the fifth equation from the fourth one leads to

\[ c_1 = \frac{2i \sin(2\pi \theta_1)}{\bar{\gamma}} (b_1^+ - b_2^+) + c_2. \]

From the third equation using the above equation one can get that

\[ c_0 = \frac{4i \sin(2\pi \theta_1)}{\bar{\gamma}} b_2^+ - 2c_2. \]

The fourth equation implies

\[ c_2 = \frac{2i \sin(2\pi \theta_1) b_2^+}{\bar{\gamma}}. \]

Substituting value of \( c_2 \) into the equation for \( c_0 \) gives that \( c_0 = 0 \).

**Remark 3.20.** If additionally to the conditions of the theorem 3.19 \( M_1 = M_2 = M \), then the corresponding eigenfield admits an antisymmetric solution, that is \( c_1 = -c_2, a_1^- = -a_2^- \) and \( b_1^+ = -b_2^+ \).
Chapter 4
Resonant Scattering

4.1 Asymptotic Analysis of Transmission Near a Guided Mode Frequency

The solutions of the sourceless problem $B\vec{X} = 0$ occur at values of $\kappa$ and $\omega$ where the operator $B$ has a zero eigenvalue $\ell = \ell(\kappa, \omega) = 0$. The relation $\ell(\kappa, \omega) = 0$ or $\omega = W(\kappa)$ when solved for $\omega$ is the dispersion relation. We analyze states that correspond to a simple zero eigenvalue $\ell$ (that is, having multiplicity 1) occurring at a real pair $(\kappa_0, \omega_0)$, which is in a region with a nonzero number of propagating harmonics, say with one propagating 0-harmonic. The imaginary part of $\omega$ for real values $\kappa$ cannot be positive by theorem 3.12. Consequently the simplest form for a local solution of $\ell(\kappa, \omega) = 0$, in which $\omega$ is as a power series in $\kappa$ is

$$\ell(\kappa, \omega) = 0 \iff \omega = \omega_0 + \ell_1(\kappa - \kappa_0) + \ell_2(\kappa - \kappa_0)^2 + \mathcal{O}(|\kappa - \kappa_0|^3),$$

where $\ell_1$ is real, and $\text{Im}\ell_2 \geq 0$. We will validify this form shortly. Following [28], for values of $(\kappa, \omega)$ for which $\ell(\kappa, \omega) \neq 0$ we introduce a plane-wave source field $\varphi$ and normalize its amplitude by the eigenvalue $\ell$,

$$\ell\varphi = \ell e^{2\pi i \theta_0 m} e^{2\pi i \phi_0 n}.$$

The scattering problem is uniquely solvable and the full field corresponding to its solution satisfies the asymptotic relation

$$\psi \sim \ell e^{2\pi i \theta_0 m} e^{2\pi i \phi_0 n} + a e^{-2\pi i \theta_0 m} e^{2\pi i \phi_0 n} \quad m \to -\infty,$$

$$\psi \sim b e^{2\pi i \theta_0 m} e^{2\pi i \phi_0 n} \quad m \to \infty.$$
In this expression \( a(\kappa, \omega) \) is the reflected complex amplitude and \( b(\kappa, \omega) \) is the transmitted amplitude. Both coefficients \( a \) and \( b \) can be extended in the complex variables \( \kappa \) and \( \omega \) into the relation \( \ell(\kappa, \omega) = 0 \) and are analytic in a complex neighborhood of the point \((\kappa_0, \omega_0)\). In our discrete problem, this is evident from the matrix formulation of the problem.

The solution to the scattering problem possesses only one harmonic at \((\kappa_0, \omega_0)\), and therefore the total field resulting from scattering of the source field \( \ell \varphi \) is characterized by a single reflection amplitude \( a \) and a single transmission amplitude \( b \), as mentioned above. According to (3.24) for real \((\kappa, \omega)\) \( |\ell|^2 = |a|^2 + |b|^2 \) it follows that \( a(\kappa_0, \omega_0) = b(\kappa_0, \omega_0) = 0 \). In the following analysis we let \( \bar{\omega} = \omega - \omega_0 \), \( \bar{\kappa} = \kappa - \kappa_0 \). The Weierstraß preparation theorem for analytic functions of two variables [14] dictates the following forms for \( \ell, a, \) and \( b \):

\[
\ell = e^{i\rho_1} [\bar{\omega} + \ell_1 \bar{\kappa} + \ell_2 \bar{\kappa}^2 + O(|\bar{\kappa}|^3)][\ell_0 + O(|\bar{\kappa}| + |\bar{\omega}|)],
\]

\[
a = e^{i\rho_2} [\bar{\omega} + r_1 \bar{\kappa} + r_2 \bar{\kappa}^2 + O(|\bar{\kappa}|^3)][r_0 + O(|\bar{\kappa}| + |\bar{\omega}|)],
\]

\[
b = e^{i\rho_3} [\bar{\omega} + t_1 \bar{\kappa} + t_2 \bar{\kappa}^2 + O(|\bar{\kappa}|^3)][t_0 + O(|\bar{\kappa}| + |\bar{\omega}|)],
\]

where \( \ell_0, r_0, \) and \( t_0 \) are positive real numbers. We thus arrive at the following relations near \((\kappa_0, \omega_0)\):

\[
\ell = 0 \iff \omega = \omega_0 - \ell_1 \bar{\kappa} - \ell_2 \bar{\kappa}^2 + \ldots, \tag{4.1}
\]

\[
a = 0 \iff \omega = \omega_0 - r_1 \bar{\kappa} - r_2 \bar{\kappa}^2 + \ldots, \tag{4.2}
\]

\[
b = 0 \iff \omega = \omega_0 - t_1 \bar{\kappa} - t_2 \bar{\kappa}^2 + \ldots. \tag{4.3}
\]

Without loss of generality we can take \( \ell_0 = 1 \). Inserting the following forms

\[
|\ell|^2 = \ell \bar{\ell}
\]

\[
= [\bar{\omega} + \ell_1 \bar{\kappa} + \ell_2 \bar{\kappa}^2 + O(|\bar{\kappa}|^3)][\bar{\omega} + \ell_1 \bar{\kappa} + \ell_2 \bar{\kappa}^2 + O(|\bar{\kappa}|^3)][1 + O(|\bar{\kappa}| + |\bar{\omega}|)]
\]

\[
= (\bar{\omega}^2 + 2\ell_1 \bar{\kappa} \bar{\omega} + \ell_1^2 \bar{\kappa}^2 + 2Re(\ell_2) \bar{\omega} \bar{\kappa}^2 + 2\ell_1 Re(\ell_2) \bar{\kappa}^3
\]

\[+(|\ell_2|^2 + 2\ell_1 Re(\ell_3)) \bar{\kappa}^4 + \ldots) \times [1 + O(|\bar{\kappa}| + |\bar{\omega}|)], \tag{4.4}
\]

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\[ |\alpha|^2 = a\bar{a} \]
\[ = (\bar{\omega} + r_1\bar{\kappa} + r_2\bar{\kappa}^2 + \mathcal{O}(\bar{\kappa}^3))|\bar{\omega} + r_1\bar{\kappa} + r_2\bar{\kappa}^2 + \mathcal{O}(\kappa^3))| \]  
\[ = (\bar{\omega}^2 + 2\text{Re}(r_1)\bar{\kappa}\bar{\omega} + |r_1|^2\bar{\kappa}^2 + 2\text{Re}(r_2)\bar{\kappa}\bar{\kappa}^2 + 2\text{Re}(r_2\bar{r}_1)\kappa^3) \]
\[ + (|r_2|^2 + 2\text{Re}(r_1\bar{r}_3))\bar{\kappa}^4 + \cdots) \times [r_0^2 + \mathcal{O}(|\kappa| + |\bar{\omega}|)], \]  
\[ |b|^2 = b\bar{b} \]
\[ = (\bar{\omega} + t_1\bar{\kappa} + t_2\bar{\kappa}^2 + \mathcal{O}(\bar{\kappa}^3))|\bar{\omega} + t_1\bar{\kappa} + t_2\bar{\kappa}^2 + \mathcal{O}(\kappa^3))| \]  
\[ = (\bar{\omega}^2 + 2\text{Re}(t_1)\bar{\kappa}\bar{\omega} + |t_1|^2\bar{\kappa}^2 + 2\text{Re}(t_2)\bar{\kappa}\bar{\kappa}^2) \]
\[ + 2\text{Re}(t_2\bar{t}_1)\bar{\kappa}^3 + (|t_2|^2 + 2\text{Re}(t_1\bar{t}_3))\bar{\kappa}^4 + \cdots) \times [t_0^2 + \mathcal{O}(|\kappa| + |\bar{\omega}|)], \]

into the relation \(|\ell|^2 = |a|^2 + |b|^2\) for real \((\kappa, \bar{\omega})\) and matching like terms we get the relations:

\[
\begin{align*}
1 &= r_0^2 + t_0^2 & (\bar{\omega}^2 \text{ term}), \\
\ell_1^2 &= r_0^2|r_1|^2 + t_0^2|t_1|^2 & (\bar{\kappa}^2 \text{ term}), \\
\ell_1 &= r_0^2\text{Re}(r_1) + t_0^2\text{Re}(t_1) & (\bar{\omega}\kappa \text{ term}), \\
\text{Re}(\ell_2) &= r_0^2\text{Re}(r_2) + t_0^2\text{Re}(t_2) & (\bar{\omega}\kappa^2 \text{ term}), \\
\ell_1\text{Re}(\ell_2) &= r_0^2\text{Re}(r_2\bar{r}_1) + t_0^2\text{Re}(t_2\bar{t}_1) & (\bar{\kappa}^3 \text{ term}), \\
|\ell_2|^2 + 2\ell_1\text{Re}(\ell_3) &= r_0^2[|r_2|^2 + 2\text{Re}(r_1\bar{r}_3)] + t_0^2[|t_2|^2 + 2\text{Re}(t_1\bar{t}_3)] \quad (\bar{\kappa}^4 \text{ term}).
\end{align*}
\]

Due to the analyticity in \(\kappa\) and \(\omega\), these expressions are valid also for \((\kappa, \omega)\) in a complex neighborhood of \((\kappa_0, \omega_0)\). Because of equations \(r_0^2 + t_0^2 = 1\) and \(\ell_1 = r_0^2\text{Re}(r_1) + t_0^2\text{Re}(t_1), \ell_1 \) lies between \(\text{Re}(r_1)\) and \(\text{Re}(t_1)\).

**Theorem 4.1.** The values of \(r_1\) and \(t_1\) are real and \(\ell_1 = t_1 = r_1\).

**Proof:** Suppose \(r_1 = r_{1R} + ir_{1I}\) and \(t_1 = t_{1R} + it_{1I}\), then it follows that

\[
\ell_1 = r_0^2r_{1R} + t_0^2t_{1R} \quad \text{and} \quad \ell_1^2 = r_0^2r_{1R}^2 + t_0^2t_{1R}^2 + r_0^2r_{1I}^2 + t_0^2t_{1I}^2.
\]

Since a real quadratic function is convex [30], the first equality implies

\[
\ell_1^2 \leq r_0^2r_{1R}^2 + t_0^2t_{1R}^2.
\]
This is possible if and only if \( r_{1I} = t_{1I} = 0 \) and \( r_{1R} = t_{1R} \), which gives that \( \ell_1 = r_1 = t_1 \).

We show now how to obtain a formula that approximates the transmission anomalies. According to the above theorem we use the expansions for \( a \) and \( b \) including terms of the second order in \( \kappa \), that is

\[
\ell = e^{i\rho_1(\bar{\omega} + \ell_1\kappa + \ell_2\kappa^2 + \ldots)(1 + c_1\bar{\omega} + c_2\kappa + \ldots)},
\]

\[
a = r_0 e^{i\rho_2(\bar{\omega} + \ell_1\kappa + t_2\kappa^2 + \ldots)(1 + p_1\bar{\omega} + p_2\kappa + \ldots)}, \tag{4.8}
\]

\[
b = t_0 e^{i\rho_3(\bar{\omega} + \ell_1\kappa + t_2\kappa^2 + \ldots)(1 + q_1\bar{\omega} + q_2\kappa + \ldots)}.
\]

In the first factors, the higher-order terms are \( \mathcal{O}(|\kappa|^3) \), in the second, they are \( \mathcal{O}(\kappa^2 + \bar{\omega}^2) \). The transmission coefficient \( T \) depends on the absolute value of the ratio \( b/a \) [28],

\[
T = \frac{|b|}{|\ell|} = \frac{|b|}{\sqrt{|a|^2 + |b|^2}} = \frac{|b/a|}{\sqrt{1 + |b/a|^2}}, \tag{4.9}
\]

and \( b/a \) has form

\[
\frac{b}{a} = e^{i\rho} \frac{t_0}{r_0} \frac{(\bar{\omega} + t_1\kappa + t_2\kappa^2 + \mathcal{O}(|\kappa|^3))(1 + \eta_1\bar{\omega} + \eta_2\kappa + \mathcal{O}(|\kappa| + |\bar{\omega}|))}{(\bar{\omega} + r_1\kappa + r_2\kappa^2 + \mathcal{O}(|\kappa|^3))}, \tag{4.10}
\]

in which \( \rho = \rho_3 - \rho_2 \), \( \eta_1 = q_1 - p_1 \), \( \eta_2 = q_2 - p_2 \). Moreover \( \eta_1 \) and \( \text{Re}(\eta_1) \) have values

\[
\eta_1 = e^{-i\rho} \frac{r_0}{t_0} \frac{\partial((b/a)(0, \bar{\omega}))}{\partial \bar{\omega}} \bigg|_{\bar{\omega}=0}, \quad \text{Re}(\eta_1) = \frac{r_0}{t_0} \frac{\partial((b/a)(0, \bar{\omega}))}{\partial \bar{\omega}} \bigg|_{\bar{\omega}=0}. \tag{4.11}
\]

To put \( \text{Re}(\eta_1) \) in terms of \( T \), we use

\[
\frac{r_0}{t_0} \frac{\partial((b/a)(0, \bar{\omega}))}{\partial \bar{\omega}} \bigg|_{\bar{\omega}=0} = \frac{\partial T(0, \bar{\omega})}{\partial \bar{\omega}} \bigg|_{\bar{\omega}=0}
\]

\[
\eta := \text{Re}(\eta_1) = \frac{1}{t_0 r_0^2} \frac{\partial T(0, \bar{\omega})}{\partial \bar{\omega}} \bigg|_{\bar{\omega}=0}. \tag{4.12}
\]

We use approximation

\[
\frac{|b|}{|a|} \approx \frac{t_0 |\bar{\omega} + t_1\kappa + t_2\kappa^2|}{r_0 |\bar{\omega} + r_1\kappa + r_2\kappa^2|} \bigg|_{1 + \eta\bar{\omega}} \tag{4.13}
\]
to get the following approximation for the transmission coefficient

\[
T \approx \frac{t_0|\tilde{\omega} + t_1\kappa + t_2\kappa^2||1 + \eta\tilde{\omega}|}{\sqrt{t_0^2|\tilde{\omega} + r_1\kappa + r_2\kappa^2|^2 + t_0^2|\tilde{\omega} + l_1\kappa + l_2\kappa^2|^2 (1 + \eta\tilde{\omega})^2}},
\]

which very good agrees with the original one (see Fig. 4.1). One can see on those graphs, that a sharp resonance emanates from the guided-mode frequency \(\omega_0\) as the wave number \(\kappa\) is perturbed from \(\kappa_0\). The anomaly widens as \(\kappa\) becomes larger.

We show now that \(T\) is approximated to order \(O(|\kappa| + |\tilde{\omega}|)\).

**Theorem 4.2.** Given that \(\ell, a,\) and \(b\) have a common root at \((\kappa_0, \omega_0) \in \mathbb{R}^2\); that their partial derivatives with respect to \(\omega\) do not vanish at \((\kappa_0, \omega_0)\); and that
Im $\ell_2 \neq 0$ in the form (4.8), the following approximation holds:

$$T(\kappa, \omega) = \left| \frac{b}{\ell} \right| = t_0 \left| \frac{\omega + \ell_1 \kappa + \ell_2 \kappa^2}{\omega + \ell_1 \kappa + \ell_2 \kappa^2} \right| |1 + \zeta_1 \omega| + O(|\kappa| + |\omega|)$$

(4.15)

as $(\kappa, \omega) \to (0, 0)$ in $\mathbb{R}^2$, where $\zeta_1 = q_1 - c_1$.

Proof: Let $k$ be the first index such that $\ell_k \neq 0$, where $k \geq 3$, then we can write

$$T = \left| \frac{b}{\ell} \right| = t_0 \left| \frac{(\omega + \ell_1 \kappa + \ell_2 \kappa^2 + \ell_3 \kappa^3 + \cdots)}{(\omega + \ell_1 \kappa + \ell_2 \kappa^2 + \ell_3 \kappa^3 + \cdots)} \right| (1 + \zeta_1 \kappa + \zeta_2 \kappa + \cdots)$$

(4.16)

Let us consider the ratio

$$\frac{1}{\omega + \ell_1 \kappa + \ell_2 \kappa^2 + \ell_k \kappa^k + O(\|\kappa\|^{k+1})} = \frac{1 \cdot 1}{\omega + \ell_1 \kappa + \ell_2 \kappa^2 + \ell_k \kappa^k + O(\|\kappa\|^{k+1})}$$

(4.17)

Denote $\epsilon = \frac{\ell_k \kappa^k + O(\|\kappa\|^{k+1})}{\omega + \ell_1 \kappa + \ell_2 \kappa^2} = O(\|\kappa\|)$, then using the fact that $|\epsilon| < 1$ we obtain

$$\frac{1}{\omega + \ell_1 \kappa + \ell_2 \kappa^2} \cdot \frac{1}{1 + \epsilon} = \frac{1}{\omega + \ell_1 \kappa + \ell_2 \kappa^2} \cdot (1 - \epsilon + \epsilon^2 - \cdots)$$

(4.18)

We continue with

$$\frac{(\omega + \ell_1 \kappa + \ell_2 \kappa^2 + \ell_3 \kappa^3 + O(\kappa^4))}{(\omega + \ell_1 \kappa + \ell_2 \kappa^2)} (1 - \epsilon + \cdots)$$

$$= \frac{(\omega + \ell_1 \kappa + \ell_2 \kappa^2)}{(\omega + \ell_1 \kappa + \ell_2 \kappa^2)} (1 - \epsilon + \cdots) + \frac{(\sum_{j=3}^{k-1} \ell_j \kappa^j)}{(\omega + \ell_1 \kappa + \ell_2 \kappa^2)} (1 - \epsilon + \cdots)$$

$$+ \frac{(\ell_k \kappa^k + O(\|\kappa\|^{k+1}))}{(\omega + \ell_1 \kappa + \ell_2 \kappa^2)} (1 - \epsilon + \cdots)$$

(4.19)

$$= \frac{(\omega + \ell_1 \kappa + \ell_2 \kappa^2)}{(\omega + \ell_1 \kappa + \ell_2 \kappa^2)} (1 - \epsilon + \cdots) + \frac{(\sum_{j=3}^{k-1} \ell_j \kappa^j)}{(\omega + \ell_1 \kappa + \ell_2 \kappa^2)} (1 - \epsilon + \cdots)$$

$$+ \frac{(\ell_k \kappa^k + O(\|\kappa\|^{k+1}))}{(\ell_k \kappa^k + O(\|\kappa\|^{k+1}))} \epsilon (1 - \epsilon + \cdots)$$
Considering the whole expression under the sign of absolute value in (4.16), which is
\[
\frac{(\bar{\omega} + \ell_1 \bar{\kappa} + t_2 \bar{\kappa}^2)}{(\bar{\omega} + \ell_1 \bar{\kappa} + \ell_2 \bar{\kappa}^2)}(1 - \epsilon + \epsilon^2 - \cdots)(1 + \zeta_1 \bar{\omega} + \cdots)
\]
\[
+ \frac{(\sum_{j=1}^{k-1} l_j \bar{\kappa}^j)}{(\bar{\omega} + \ell_1 \bar{\kappa} + \ell_2 \bar{\kappa}^2)}(1 - \epsilon + \epsilon^2 - \cdots)(1 + \zeta_1 \bar{\omega} + \cdots)
\]
\[
+ \frac{(t_k \bar{\kappa}^3 + \mathcal{O}(|\bar{\kappa}|^{k+1}))}{(\ell_k \bar{\kappa}^k + \mathcal{O}(|\bar{\kappa}|^{k+1}))}(1 - \epsilon + \epsilon^2 - \cdots)(1 + \zeta_1 \bar{\omega} + \cdots)
\]
leads to the following result
\[
T = t_0 \left| \frac{(\bar{\omega} + \ell_1 \bar{\kappa} + t_2 \bar{\kappa}^2)}{(\bar{\omega} + \ell_1 \bar{\kappa} + \ell_2 \bar{\kappa}^2)}(1 + \zeta_1 \bar{\omega}) \right| \mathcal{O}(|\bar{\kappa}| + |\bar{\omega}|). \tag{4.21}
\]

This is formula generalizes that of [28], where it was assumed that \(\ell_1 = 0\).

### 4.2 Analysis Near a Bifurcation Point

The analysis in this section connects the behavior for the case \(\ell_1 = 0\) to that for \(\ell_1 \neq 0\) in the case of period two. For systems of period two there are three cases of how many true guided modes may exist in the region of one propagating harmonic. When the three parameters \(M_0\), \(M_1\), and \(\gamma_1\) are fixed and \(\gamma_0\) is allowed to vary, we may have no true guided mode, either one at \(\kappa_0 = 0\) or two symmetrical with respect to \(\kappa = 0\). This is because every period-two structure has a horizontal line of symmetry. The splitting of the guided mode from one to two when \(\gamma_0\) varies is called bifurcation. We will do perturbation analysis near such a bifurcation point. Before proceeding we need the following lemma.

**Lemma 4.3.** Suppose for fixed real values of \(M_0\), \(M_1\), \(\gamma_0\) and \(\gamma_1\) there is a unique real pair \((\kappa_0, \omega_0)\) in an open set \(U\) of the real \((\kappa, \omega)\)-region of one propagating
harmonic that admits a true guided mode, that is \( \ell(\kappa_0, \omega_0) = 0 \). Assume that the conditions \( \frac{\partial \ell}{\partial \kappa} (\kappa_0, \omega_0) \neq 0 \), \( \frac{\partial \ell}{\partial \omega} (\kappa_0, \omega_0) \neq 0 \), \( \frac{\partial \ell}{\partial \omega} (\kappa_0, \omega_0) \neq 0 \) hold.

1. There are intervals \( I \) about \( \kappa_0 \), \( V \) about \( \omega_0 \) and smooth real-valued functions \( \omega_a, \omega_b : I \to V \) such that \( a(\kappa, \omega_a(\kappa)) = 0 \), \( b(\kappa, \omega_b(\kappa)) = 0 \), that is \( \omega_a(\kappa) \), \( \omega_b(\kappa) \) for \( \kappa \in I \setminus \{ \kappa_0 \} \) describe real frequencies for which transmission \( T \) reaches precisely 100\% (peak) and 0\% (dip), respectively.

2. Either \( \omega_a(\kappa) > \omega_b(\kappa) \), \( \kappa \in I \setminus \{ \kappa_0 \} \), which means the peak in the transmission comes to the right of the dip, or \( \omega_a(\kappa) < \omega_b(\kappa) \), \( \kappa \in I \setminus \{ \kappa_0 \} \), which implies the peak in the transmission comes to the left of the dip.

Proof: According to (3.35) the zero-sets for \( a(\kappa, \omega) \) and \( b(\kappa, \omega) \) are defined by

\[
\begin{vmatrix}
0 & -(\gamma_0 + \gamma_1) & 0 & \gamma_1 - \gamma_0 \\
-(\gamma_0 + \gamma_1) & \tau + \frac{4\cos(\pi \kappa)}{\sqrt{M_0 M_1}} & \gamma_1 - \gamma_0 & \frac{2}{M_1} - \frac{2}{M_0} \\
0 & \gamma_1 - \gamma_0 & 4i \sin(2\pi \theta_1) & -(\gamma_0 + \gamma_1) \\
\gamma_1 - \gamma_0 & \frac{2}{M_1} - \frac{2}{M_0} & -(\gamma_0 + \gamma_1) & \tau - \frac{4\cos(\pi \kappa)}{\sqrt{M_0 M_1}}
\end{vmatrix} = 0,
\]

(4.22)

\[
\begin{vmatrix}
\tau + \frac{4\cos(\pi \kappa)}{\sqrt{M_0 M_1}} & \gamma_1 - \gamma_0 & \frac{2}{M_1} - \frac{2}{M_0} \\
\gamma_1 - \gamma_0 & 4i \sin(2\pi \theta_1) & -(\gamma_0 + \gamma_1) \\
\frac{2}{M_1} - \frac{2}{M_0} & -(\gamma_0 + \gamma_1) & \tau - \frac{4\cos(\pi \kappa)}{\sqrt{M_0 M_1}}
\end{vmatrix} = 0,
\]

(4.23)

respectively, which are real-valued with \( \sin(2\pi \theta_1) = i \sqrt{(2 - \frac{2}{M_0} + \cos(\pi \kappa))^2 - 1} \), \( \tau = 2\omega - \frac{2}{M_0} - \frac{2}{M_1} \). If there is a real pair \( (\kappa_0, \omega_0) \) in the region of one propagating harmonic such that \( \ell(\kappa_0, \omega_0) = 0 \), then by the law of conservation of energy \( a(\kappa_0, \omega_0) = 0 \) and \( b(\kappa_0, \omega_0) = 0 \) too. Since the conditions \( \frac{\partial a}{\partial \omega}(\kappa_0, \omega_0) \neq 0 \) and \( \frac{\partial b}{\partial \omega}(\kappa_0, \omega_0) \neq 0 \) are assumed then by the implicit function theorem there are intervals \( I \) about \( \kappa_0 \), \( V \) about \( \omega_0 \) and smooth real-valued functions \( \omega_a, \omega_b : I \to V \) such that \( a(\kappa, \omega_a(\kappa)) = 0 \), \( b(\kappa, \omega_b(\kappa)) = 0 \) and therefore for real \( \kappa \) in the vicinity of \( \kappa_0 \)
The transmission coefficient reaches 100% at \( \omega_a \) and 0% at \( \omega_b \). For the reason that \( \omega_a(\kappa), \omega_b(\kappa) \) are real-valued that is why all coefficients in the expansions (4.2), (4.3) are real:

\[
\omega_a(\kappa) = \omega_0 - \ell_1(\kappa - \kappa_0) - r_2(\kappa - \kappa_0)^2 - \ldots \tag{4.24}
\]

\[
\omega_b(\kappa) = \omega_0 - \ell_1(\kappa - \kappa_0) - t_2(\kappa - \kappa_0)^2 - \ldots \tag{4.25}
\]

The frequencies \( \omega_a \) and \( \omega_b \) in the expansions (4.24), (4.25) have the same linear terms gives the order in which the peak and dip in \( T \) occur on the real \( \omega \)-axis, and the order is the same for \( \kappa < \kappa_0 \) as it is for \( \kappa > \kappa_0 \) and the curves at \( (\kappa_0, \omega_0) \) touches each other, not cross. Since \( \omega_a(\kappa) \neq \omega_b(\kappa), \kappa \in I \setminus \{ \kappa_0 \} \) otherwise the dispersion relation would have been real what would contradict to the uniqueness of the real pair \( (\kappa_0, \omega_0) \), therefore it leads either \( \omega_a > \omega_b \) or \( \omega_a < \omega_b \) for all \( \kappa \in I \setminus \{ \kappa_0 \} \) (see Fig. 4.2).

The analysis of the transmission anomaly relies on the following conditions:

\[
|\ell(\kappa, \omega, \gamma)|^2 = |a(\kappa, \omega, \gamma_0)|^2 + |b(\kappa, \omega, \gamma_0)|^2 \quad \text{for} \quad \kappa, \omega, \gamma_0 \in \mathbb{R} \tag{4.26}
\]

if \( \ell(\kappa, \omega, \kappa_0) = 0 \) for \( \kappa \in \mathbb{R} \), then \( \text{Im}(\omega) \leq 0 \).

\[
\ell(\kappa_0^*, \omega_0^*, \gamma_0^*) = 0, \quad a(\kappa_0^*, \omega_0^*, \gamma_0^*) = 0, \quad b(\kappa_0^*, \omega_0^*, \gamma_0^*) = 0 \tag{4.27}
\]

where \( (\kappa_0^*, \omega_0^*, \gamma_0^*) \in \mathbb{R}^3 \) is the bifurcation point.
The following conditions hold generically:

\[
\frac{\partial \ell}{\partial \omega}(\kappa_0^*, \omega_0^*, \gamma_0^*) \neq 0, \quad \frac{\partial a}{\partial \omega}(\kappa_0^*, \omega_0^*, \gamma_0^*) \neq 0, \quad \frac{\partial b}{\partial \omega}(\kappa_0^*, \omega_0^*, \gamma_0^*) \neq 0.
\] (4.28)

The curves \(a(\kappa, \omega, \gamma_0) = 0\) and \(b(\kappa, \omega, \gamma_0) = 0\) for real values of \(\kappa\) near the bifurcation point describe frequencies \(\omega_a, \omega_b\) of the reflected and transmitted coefficients, respectively, which correspond peaks and dips of the transmission.

**Theorem 4.4.** Suppose for the fixed real values of \(M_0, M_1,\) and \(\gamma_1\) in the regime of one propagating harmonic, there exists a unique triple \((\kappa_0^*, \omega_0^*, \gamma_0^*) \in \mathbb{R}^3\), such that \(\ell(\kappa_0^*, \omega_0^*, \gamma_0^*) = 0\). Let \(\ell(\kappa, \omega, \gamma_0) = \mathcal{L}_1(\kappa, \omega, \gamma_0) + i\mathcal{L}_2(\kappa, \omega, \gamma_0)\), where \(\mathcal{L}_1 = \text{Re}(\ell), \mathcal{L}_2 = \text{Im}(\ell)\) and \(\mathcal{L}_1, \mathcal{L}_2\) are real-valued functions of the real vector argument \((\kappa, \omega, \gamma_0)\). Assume (4.28) hold and

\[
\det \left( \begin{array}{cc}
\frac{\partial \mathcal{L}_1}{\partial \omega}(\kappa_0^*, \omega_0^*, \gamma_0^*) & \frac{\partial \mathcal{L}_1}{\partial \gamma_0}(\kappa_0^*, \omega_0^*, \gamma_0^*) \\
\frac{\partial \mathcal{L}_2}{\partial \omega}(\kappa_0^*, \omega_0^*, \gamma_0^*) & \frac{\partial \mathcal{L}_2}{\partial \gamma_0}(\kappa_0^*, \omega_0^*, \gamma_0^*)
\end{array} \right) \neq 0.
\] (4.29)

Then there are intervals \(I\) about \(\kappa_0^*\), \(J\) about \(\gamma_0^*\), and \(V\) about \(\omega_0^*\) and smooth real-valued functions \(\omega_a, \omega_b : I \times J \to V, g : I \to J, W : I \to V\) such that \(a(\kappa, \omega_a(\kappa, \gamma_0), \gamma_0) = 0, b(\kappa, \omega_b(\kappa, \gamma_0), \gamma_0) = 0\), \(\ell(\kappa, W(\kappa), g(\kappa)) = 0\) with \(W(\kappa_0^*) = \omega_0^*\), \(g(\kappa_0^*) = \gamma_0^*\), \(g(\kappa) \leq \gamma_0^*\) or \(g(\kappa) \geq \gamma_0^*\) for all \(\kappa \in I\). Without loss of generality let \(g(\kappa) \leq \gamma_0^*\) for \(\kappa \in I\) and \(\omega_a(\kappa, \gamma_0) \leq \omega_b(\kappa, \gamma_0)\) in \(I \times J\). The system undergoes a bifurcation at \(\gamma_0 = \gamma_0^*\):

1. For \(\gamma_0 = \gamma_0^*\) there is a unique \(\kappa = \kappa_0^*\) such that \(g(\kappa_0^*) = \gamma_0^*, W(\kappa_0^*) = \omega_0^*, \omega_a(\kappa_0^*, \gamma_0^*) = \omega_b(\kappa_0^*, \gamma_0^*) = \omega_0^*\) and \(\omega_a(\kappa, \gamma_0) < \omega_b(\kappa, \gamma_0)\) for \(\kappa \in I \setminus \{\kappa_0^*\}\).

2. For \(\gamma_0 < \gamma_0^*\) there are exactly two symmetrical \(\kappa\) in \(I\), say \(\kappa = \mp \kappa_0\) such that \(\gamma_0 = g(\mp \kappa_0), \omega_a(\mp \kappa_0, \gamma_0) = \omega_b(\mp \kappa_0, \gamma_0) = W(\mp \kappa_0) = \omega_0, \ell(\mp \kappa_0, \omega_0, \gamma_0) = 0\) and \(\omega_a(\kappa, \gamma_0) < \omega_b(\kappa, \gamma_0)\) for \(\kappa \in I \setminus \{-\kappa_0, \kappa_0\}\).
3. For $\gamma_0 > \gamma_0^*$ there is no $\kappa$ in $I$ such that $\gamma_0 = g(\kappa)$ and $\omega_a(\kappa, \gamma_0) < \omega_b(\kappa, \gamma_0)$ for all $\kappa \in I$.

Proof: According to the law of conservation of energy $a(\kappa_0^*, \omega_0^*, \gamma_0^*) = b(\kappa_0^*, \omega_0^*, \gamma_0^*) = 0$. Since the conditions (4.28), (4.29) are satisfied then lemma 4.3 together with the implicit function theorem guarantee existence of intervals $I$ about $\kappa_0^*$, $J$ about $\gamma_0^*$, $V$ about $\omega_0^*$ and smooth real-valued functions $\omega_a(\kappa, \gamma_0), \omega_b(\kappa, \gamma_0) : I \times J \to V$, $W : I \to V$, $g : I \to J$. The property that the dispersion relation $\ell(\kappa, \omega, \gamma_0) = 0$ is symmetric with respect to $\kappa$ gives that the functions $W$ and $g$ are symmetric too, that is $W(-\kappa) = W(\kappa)$, $g(-\kappa) = g(\kappa)$ for $\kappa \in I$. Then the Taylor expansion for $g(\kappa)$ can be written as following:

$$g(\kappa) = \gamma_0^* + G_2\kappa^2 + G_4\kappa^4 + \ldots,$$

(4.30)

where coefficients $G_{2j}, j \in \mathbb{Z}$, are real. It implies that either $g(\kappa) \leq \gamma_0^*$ or $g(\kappa) \geq \gamma_0^*$ for all $\kappa \in I$, without loss of generality we pick the case $g(\kappa) \leq \gamma_0^*$ for all $\kappa \in I$. It means a horizontal line, say $\gamma_0 = Y$ intersects the graph of $g(\kappa)$ either at only one point $\kappa = \kappa_0^*$ (the first part of the theorem), or at exactly two points $\kappa = \mp \kappa_0^*$ (the second part of the theorem), or none (the last one). \]

Let us note that the dispersion relation $\ell = \det(\mathbb{H}_2) = 0$ is not analytic in $\gamma_0$, but analytic in $\kappa_0$, the wave number where the true guided mode exists for a given $\gamma_0$. Therefore we use $\kappa_0$ instead of $\gamma_0$ in the analysis and do the perturbation about the point $(\kappa, \omega, \kappa_0) = (0, \omega_0^*, 0)$, where $\omega_0^* = W(\kappa_0^*)$ with respect to three parameters $(\kappa, \omega, \kappa_0)$. As above we let $\widetilde{\omega} = \omega - \omega_0$, and $\tilde{\kappa} = \kappa - \kappa_0$, but now $\kappa_0$ is another complex variable. The Weierstraß preparation theorem for analytic functions of three variables [14] provides the following expansions for $\ell, a,$ and $b$ near $(\tilde{\kappa}, \widetilde{\omega}, \kappa_0) = (0, 0, 0)$:

55
\[ \ell = e^{i\psi_1} [\bar{\omega} + \ell_{1,0} \kappa_0 + \ell_{0,1} \kappa + \ldots + \ell_{i,j} \kappa_0^i \kappa_j^i + \ldots] \times [\lambda_0 + \lambda_1 \bar{\omega} + \lambda_2 \kappa_0 + \lambda_3 \kappa + \ldots] \]  \hspace{1cm} (4.31)

\[ a = e^{i\psi_2} [\bar{\omega} + r_{1,0} \kappa_0 + r_{0,1} \kappa + r_{1,1} \kappa_0 \kappa + \ldots + r_{i,j} \kappa_0^i \kappa_j^i + \ldots] \times [\rho_0 + \rho_1 \bar{\omega} + \rho_2 \kappa_0 + \rho_3 \kappa + \ldots] \]  \hspace{1cm} (4.32)

\[ b = e^{i\psi_3} [\bar{\omega} + t_{1,0} \kappa_0 + t_{0,1} \kappa + t_{1,1} \kappa_0 \kappa + \ldots + t_{i,j} \kappa_0^i \kappa_j^i + \ldots] \times [\tau_0 + \tau_1 \bar{\omega} + \tau_2 \kappa_0 + \tau_3 \kappa + \ldots] \]  \hspace{1cm} (4.33)

These functions are symmetric in the following sense \( \ell(-\kappa, \omega, -\kappa_0) = \ell(\kappa, \omega, \kappa_0) \), \( a(-\kappa, \omega, -\kappa_0) = a(\kappa, \omega, \kappa_0) \), and \( b(-\kappa, \omega, -\kappa_0) = b(\kappa, \omega, \kappa_0) \). This property implies that all coefficients multiplying \( \kappa_0^{2j+1} \kappa^{2k} \) and \( \kappa_0^{2j} \kappa^{2k+1} \), where \( j, k = 0, 1, 2, \ldots \), are zero for all three functions in both brackets. Additionally, for a fixed \( \kappa_0 \) these formulas have to agree with the corresponding formulas in the analysis near guided modes which implies that the coefficients for \( \kappa_0^{2j} \) in both brackets for each function are zero also. Again without loss of generality we can take \( \lambda_0 = 1 \). Taking all these properties into account we obtain

\[ \ell = e^{i\psi_1} [\bar{\omega} + \ell_{1,1} \kappa \kappa_0 + \ell_{0,2} \kappa^2 + \ldots] [1 + L_1 \bar{\omega} + L_2 \kappa \kappa_0 + L_3 \kappa^2 + \ldots] \]  \hspace{1cm} (4.34)

\[ a = e^{i\psi_2} \rho_0 [\bar{\omega} + r_{1,1} \kappa \kappa_0 + r_{0,2} \kappa^2 + \ldots] [1 + P_1 \bar{\omega} + P_2 \kappa \kappa_0 + P_3 \kappa^2 + \ldots] \]  \hspace{1cm} (4.35)

\[ b = e^{i\psi_3} \tau_0 [\bar{\omega} + t_{1,1} \kappa \kappa_0 + t_{0,2} \kappa^2 + \ldots] [1 + Q_1 \bar{\omega} + Q_2 \kappa \kappa_0 + Q_3 \kappa^2 + \ldots] \]  \hspace{1cm} (4.36)

Inserting these expressions into the law of conservation of energy for real \( (\kappa, \bar{\omega}, \kappa_0) \) and matching like terms yields the following relations:

\[(\bar{\omega}^2 \text{ term}) \hspace{1cm} 1 = \rho_0^2 + \tau_0^2 \]

\[(\bar{\omega} \kappa_0 \bar{\kappa} \text{ term}) \hspace{1cm} \text{Re}(\ell_{1,1}) = \rho_0^2 \text{Re}(r_{1,1}) + \tau_0^2 \text{Re}(t_{1,1}) \]

\[(\kappa_0^2 \bar{\kappa}^2 \text{ term}) \hspace{1cm} |\ell_{1,1}|^2 = \rho_0^2 |r_{1,1}|^2 + \tau_0^2 |t_{1,1}|^2 \]

\[(\bar{\omega} \bar{\kappa}^2 \text{ term}) \hspace{1cm} \text{Re}(\ell_{0,2}) = \rho_0^2 \text{Re}(r_{0,2}) + \tau_0^2 \text{Re}(t_{0,2}) \]

\[(\bar{\kappa}^4 \text{ term}) \hspace{1cm} |\ell_{0,2}|^2 = \rho_0^2 |r_{0,2}|^2 + \tau_0^2 |t_{0,2}|^2 \]

\[(\bar{\omega} \kappa_0^2 \bar{\kappa}^2 \text{ term}) \hspace{1cm} |\ell_{1,1}|^2 \text{Re}(L_1) + \text{Re}(\ell_{2,2}) + 2 \text{Re}(\ell_{1,1}) \text{Re}(L_2)
= \rho_0^2 (|r_{1,1}|^2 \text{Re}(P_1) + \text{Re}(r_{2,2}) + 2 \text{Re}(r_{1,1}) \text{Re}(P_2)) + \tau_0^2 (|t_{1,1}|^2 \text{Re}(Q_1) + \text{Re}(t_{2,2}) + 2 \text{Re}(t_{1,1}) \text{Re}(Q_2)) \]

\[56\]
The zero-sets of each function are defined by

\[ \ell = 0 \Leftrightarrow \omega = \omega_0 - \ell_{1,1} \kappa_0 (\kappa - \kappa_0) - \ell_{0,2} (\kappa - \kappa_0)^2 - \ell_{3,1} \kappa_0^3 (\kappa - \kappa_0) - \ldots, \tag{4.38} \]

\[ a = 0 \Leftrightarrow \omega = \omega_0 - r_{1,1} \kappa_0 (\kappa - \kappa_0) - r_{0,2} (\kappa - \kappa_0)^2 - r_{3,1} \kappa_0^3 (\kappa - \kappa_0) - \ldots, \tag{4.39} \]

\[ b = 0 \Leftrightarrow \omega = \omega_0 - t_{1,1} \kappa_0 (\kappa - \kappa_0) - t_{0,2} (\kappa - \kappa_0)^2 - t_{3,1} \kappa_0^3 (\kappa - \kappa_0) - \ldots. \tag{4.40} \]

In terms of new coefficients one arrives at the following relations:

\[ \ell_{2i+1} = \sum_{k=0}^{\infty} \ell_{2k+1,2i+1} \kappa_0^{2k+1}, \quad \ell_{2j+2} = \sum_{k=0}^{\infty} \ell_{2k,2j+2} \kappa_0^{2k}, \quad (j = 0, 1, 2, \ldots), \]

\[ r_{2i+1} = \sum_{k=0}^{\infty} r_{2k+1,2i+1} \kappa_0^{2k+1}, \quad r_{2j+2} = \sum_{k=0}^{\infty} r_{2k,2j+2} \kappa_0^{2k}, \quad (i = 0, 1, 2, \ldots), \tag{4.41} \]

\[ t_{2i+1} = \sum_{k=0}^{\infty} t_{2k+1,2i+1} \kappa_0^{2k+1}, \quad t_{2j+2} = \sum_{k=0}^{\infty} t_{2k,2j+2} \kappa_0^{2k}, \quad (j = 0, 1, 2, \ldots). \]

Here we get a new information about the coefficients in the expansions for zero sets in (4.1)–(4.3) in terms of the new coefficients, namely with true guided mode at the bifurcation point \( \kappa_0 = 0 \) the coefficients in the expansions (4.1)–(4.3) for \( \kappa^{2n+1}, n = 0, 1, \ldots \) are zeros.

Fig. 4.3 demonstrates how the spikes as functions of \( \omega \) emanate away from the bifurcation point and spread, whereas Fig. 4.4 shows that spikes have two origins and to show what happens with the spikes between the split of the guided modes after bifurcation.

### 4.3 Resonant Enhancement

In this section we present a leading-order asymptotic theory of resonant field enhancement of plane wave source field scattered by one-dimensional periodic lattices, a phenomenon accompanies anomalous transmission [28]. We want to demonstrate as the authors did for \( \ell_1 = 0 \) that the emerging high fields have a dominant contribution from the eigenfield of the operator \( B \) corresponding to the simple eigenvalue
FIGURE 4.3. The transmission coefficient for $M_0 = 2, M_1 = 1, \gamma_0 = \gamma^*_0 = 1.029633513, \gamma_1 = 7$ near the true guided mode $\kappa_0^* = 0, (\omega_0^* = 0.9778859328)$. Upper: The pictures by using the original formula for transmission coefficient. Lower: Using the approximation formula (4.14).

$\ell = \ell(\kappa, \omega)$. Since $\ell$ is of multiplicity 1, there is a basis such that the matrix $\mathbb{B}$ has the following form [1]

$$
\mathbb{J} = \begin{pmatrix}
\ell & 0 \\
0 & \mathbb{B}
\end{pmatrix}
$$

(4.42)

where the matrix $\mathbb{B}$ has dimension $(3N - 1) \times (3N - 1)$, note here that the matrix has bounded inverse because of the simplicity of $\ell$. Without loss of generality in our analysis we can consider instead of system $\mathbb{B}\mathbb{X} = \ell F$ the system $\mathbb{J}\mathbb{X} = \ell F$. The source field is uniquely decomposed as $\mathbb{F} = \alpha e_1 + (0, F_2)$, where the complex scalar $\alpha$ and the vector $F_2, F_2 \in \mathbb{C}^{3N-1}$ are analytic, and the vector $e_1 = (1, 0, \ldots, 0) \in \mathbb{C}^{3N}$. One can easily verify that $\mathbb{X} = \alpha e_1 + (0, \ell^{-1}\mathbb{B}F_2)$ is a solution. Indeed,

$$
\mathbb{J}\mathbb{X} = \begin{pmatrix}
\ell & 0 \\
0 & \mathbb{B}
\end{pmatrix}
\begin{pmatrix}
\alpha \\
\ell^{-1}\mathbb{B}F_2
\end{pmatrix}
= \begin{pmatrix}
\ell \alpha \\
\ell F_2
\end{pmatrix}
= \ell F
$$

(4.43)
The source of any measurable amplitude enhancement can be traced to the first component of the field $\vec{X}$. The magnitude of change can be estimated by the ratio $|\alpha/\ell|$, the second component is of order $O(\ell)$ as is the incident field. Let $\alpha$ in the vicinity of $(\kappa_0, \omega_0)$ have the following expansion

$$\alpha = \beta_0 + \beta_1 \kappa + \beta_2 \omega + \cdots$$  \hspace{1cm} (4.44)

**Theorem 4.5.** *In the expansion (4.44) the constant $\beta_0 = 0$.*

**Proof:** By theorem 3.8 at the pair $(\kappa_0, \omega_0)$ there is a solution to the scattering problem with the right hand side $\vec{F} = (\alpha(\kappa_0, \omega_0), F_2)$, that is to

$$\mathcal{J} \vec{X} = \begin{pmatrix} 0 & 0 \\ 0 & \hat{B} \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = \begin{pmatrix} \alpha \\ F_2 \end{pmatrix}$$  \hspace{1cm} (4.45)

where $X_1$ corresponds to the resonant part of the solution and $X_2 \in \mathbb{C}^{3N-1}$. It follows that $\alpha(\kappa_0, \omega_0) = 0$.\[\square\]
FIGURE 4.5. The solid dots represent numerically calculated absolute values of the field in the one-dimensional lattice produced by an incident plane wave of amplitude 1 at various values of $\kappa$ for two cases. Left: $\kappa^*_0 = 0$. Right: $\kappa_0 = 0.061$.

Using the forms for $\alpha$ and (4.8) for $\ell$, we obtain

$$\frac{\alpha}{\ell} = \frac{\beta_1 \widetilde{\kappa} + \beta_2 \tilde{\omega} + \cdots}{(\tilde{\omega} + \ell_1 \widetilde{\kappa} + \ell_2 \widetilde{\kappa}^2 + \cdots)} \left( \frac{1}{e^{i\eta_1}} + \cdots \right)$$

(4.46)

Let $\widetilde{\kappa}$ be a small positive number and allow $\omega$ to range over real values near $\omega_0$ (so that $\tilde{\omega}$ varies over real values near zero), which corresponds to scattering by harmonic plane-wave sources. The magnitude of the denominator in $\alpha/\ell$ is smallest when $\tilde{\omega} + \ell_1 \widetilde{\kappa} + \text{Re}(\ell_2) \widetilde{\kappa}^2 = \mathcal{O}(\widetilde{\kappa}^2)$; the corresponding value of $\omega$ ($\omega = \omega_0 - \ell_1 \widetilde{\kappa} - \text{Re}(\ell_2) \widetilde{\kappa}^2 - \mathcal{O}(\widetilde{\kappa}^2)$). To see the response to an incident plane wave at this optimal frequency, we put

$$\tilde{\omega} = -\ell_1 \widetilde{\kappa} - \text{Re}(\ell_2) \widetilde{\kappa}^2, \text{ or } \omega = \omega_0 - \ell_1 \widetilde{\kappa} - \text{Re}(\ell_2) \widetilde{\kappa}^2,$$

(4.47)

and obtain for the amplitude enhancement $\mathcal{A}$

$$\mathcal{A} = \left| \frac{\alpha}{\ell} \right| = \frac{1}{|\widetilde{\kappa}|} \left| \beta_1 - \ell_1 \beta_2 - \beta_2 \text{Re}(\ell_2) \widetilde{\kappa} + \cdots \right| \text{Im}(\ell_2) + \cdots$$

(4.48)

so that $\mathcal{A}$ has the asymptotic expansion

$$\mathcal{A} \sim \frac{d_1}{|\widetilde{\kappa}|} + d_2 + \cdots (\tilde{\omega} = -\ell_1 \widetilde{\kappa} - \text{Re}(\ell_2) \widetilde{\kappa}^2, \quad \kappa \to \kappa_0)$$

(4.49)

Let us confirm this law by numerical calculations for the field amplitude in the one-dimensional lattice. Since the growth of amplitude of the solution occurs when
the incident wave reaches the one-dimensional lattice at the frequency closest to the
dispersion relation therefore we solve the scattering problem (3.35) for pairs \((\kappa, \omega)\)
such that \(\omega = \omega_0 - \ell_1(\kappa - \kappa_0) - \text{Re}(\ell_2)(\kappa - \kappa_0)^2\) for a given \(\kappa\) in the vicinity of \(\kappa_0\).
Then we calculate the \(\ell^2\)-space norm of the solution in the one-dimensional lattice,
which is \(\sqrt{|c_0|^2 + |c_1|^2 + \cdots + |c_{N-1}|^2}\). Figure 4.11 shows numerical simulations for
the cases of \(N = 2\).
Chapter 5
Conclusions

Before coupling, the spectral properties for each lattice are studied separately. By coupling the lattices the one-dimensional lattice is viewed as a periodic wave-guide that is open to the ambient two-dimensional lattice “space”. We showed that an observer in the wave-guide can only detect the even motions in the two-dimensional lattice. The scattering problem has been reformulated in a variational form and the existence of solutions has been proved. We explore existence of non-robust guided modes, which are known to be connected with anomalous scattering behavior. A non-robust guided mode is associated with the existence of an isolated real pair of wave number and frequency on the complex dispersion relation. This guided mode is supported by the one-dimensional lattice and decays far away from it. We establish for systems of period two a criterion of existence of nonrobust guided modes, which shows that a simplest model to observe the anomalous scattering has period two, and unlike the continuous case, we prove that the transmission reaches precisely 0% (dips) and 100% (peaks) in the vicinity of the non-robust guided modes. This is possible because in the discrete case, we can get explicit formulas. For a system of a period three, we show by examples an algorithm for finding non-robust guided modes. We give an asymptotic analysis of transmission near the non-robust guided mode in the regime of one propagating harmonic for an arbitrary period and derived the order to which the transmission is approximated. We extend the formula for transmission anomalies to genuinely traveling waves (Bloch wave-number nonzero) and give rigorous error estimates. For the systems of a period two, when three physical parameters are fixed and the fourth is allowed
to vary, we find that the system undergoes a bifurcation, in which a guided mode appears and then splits into two during variation of the coupling constants. Finally, we prove the $1/|\kappa|$ law for the resonance enhancement as for a continuous case.
References


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Appendix: The Fundamental Difference Operators

Let us start with formulas for discrete differentiation for functions of a single variable. There are two types of difference derivatives left and right, that is why there are two formulas for difference differentiation for product [25]:

\[
(fg)_x = f_x g + f^{(+1)} g_x = f_x g^{(+1)} + fg, 
\tag{5.1}
\]

\[
(fg)_{x} = f_x g + f^{(-1)} g_{x} = f_x g^{(-1)} + fg_{x}. 
\tag{5.2}
\]

Here we use notations

\[
f^{(\pm)} = f(x \pm h), \quad f_x = \frac{f^{(+1)} - f}{h}, \quad f_{x} = \frac{f - f^{(-1)}}{h}. \tag{5.3}
\]

Let us verify, for instance, formula (5.1). By definition for derivative we have

\[
\frac{f_{j+1}g_{j+1} - f_{j}g_{j}}{h} = \frac{f_{j+1}g_{j+1} - f_{j}g_{j+1}}{h} + \frac{f_{j}g_{j+1} - f_{j}g_{j}}{h}. \tag{5.4}
\]

Now we are ready to write the discrete Divergence Theorem for the 1D lattice for an interval from \(m_1\) to \(m_2\):

\[
\sum_{m=m_1+1}^{m_2} (f_x)_m = f_{m_2} - f_{m_1}. \tag{5.5}
\]

It helps to get an analogue of the discrete version for the first Green’s identity for the one-dimensional lattice lattice:

\[
\sum_{m=m_1+1}^{m_2} (gf_{xx})_{m} = (gf_x)_{m_2} - (gf_x)_{m_1} - \sum_{m=m_1+1}^{m_2} (g_{xx}f_x)_{m}. \tag{5.6}
\]

The same we want to obtain for the 2D lattice. If we did it in a continuous case we would have integration over a rectangular region. In the discrete case we sum up over a discrete rectangular shape region [21]. We need to introduce some
extra notations. Since there are differentiations in horizontal and vertical directions therefore it is introduced two types of gradients

$$\nabla_− = (\partial_x, \partial_y), \quad \nabla_+ = (\partial_x, \partial_y).$$ (5.7)

Let $F$ with $F_{mn} = (F^1_{mn}, F^2_{mn})$, $m, n \in \mathbb{Z}$ be a 2D vector and $w$ be a scalar function of two variables both defined on the 2D lattice. Then the following is true by direct calculations

$$\nabla_− \cdot (wF) = w \nabla_− \cdot F + \nabla_− w \cdot F^{(-1),(-1)}. \quad (5.8)$$

The discrete 2D Divergence Theorem for a rectangular shape region $[m_1, m_2] \times [n_1, n_2]$ has the following form

$$\sum_{n=n_1+1}^{n_2} \sum_{m=m_1+1}^{m_2} (\nabla F)_{mn} = \sum_{n=n_1+1}^{n_2} (F^1_{m_2n} - F^1_{m_1n}) + \sum_{m=m_1+1}^{m_2} (F^2_{mn_2} - F^2_{mn_1}). \quad (5.9)$$

Applying the theorem to the identity:

$$\sum_{n=n_1+1}^{n_2} \sum_{m=m_1+1}^{m_2} (v\Delta u)_{mn} = \sum_{n=n_1+1}^{n_2} \sum_{m=m_1+1}^{m_2} (\nabla_− \cdot (v \nabla_+ u))_{mn}$$

$$- \sum_{n=n_1+1}^{n_2} \sum_{m=m_1+1}^{m_2} (\nabla_− v \cdot \nabla_− u)_{mn}. \quad (5.10)$$

with $F = \nabla_+ u$ and noticing that $(\nabla_+ u)^{(-1),(-1)} = (\partial_x u^{(-1)}, \partial_y u^{(-1)}) = \nabla_− u$ it leads to

$$\sum_{n=n_1+1}^{n_2} \sum_{m=m_1+1}^{m_2} (v\Delta u)_{mn} = \sum_{n=n_1+1}^{n_2} ((vu_x)_{m_2n} - (vu_x)_{m_1n})$$

$$+ \sum_{m=m_1+1}^{m_2} ((vu_y)_{mn_2} - (vu_y)_{mn_1})$$

$$- \sum_{n=n_1+1}^{n_2} \sum_{m=m_1+1}^{m_2} (\nabla_− v \cdot \nabla_− u)_{mn}. \quad (5.11)$$
Vita

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