Exceptional Points in Real Potential Scattering

by

Sezin Su Elden

A Dissertation Submitted to the
Graduate School of Sciences and Engineering
in Partial Fulfillment of the Requirements for
the Degree of

Master of Science

in

Physics

KOÇ ÜNİVERSİTESİ

September, 2023

Exceptional Points in Real Potential Scattering

Koç University

Graduate School of Sciences and Engineering

This is to certify that I have examined this copy of a master's thesis by

Sezin Su Elden

and have found that it is complete and satisfactory in all respects,

and that any and all revisions required by the final

examining committee have been made.

Committee Members:

Prof. Ali Mostafazadeh (Advisor)

Assoc. Prof. O. Teoman Turgut

Assist. Prof. Menderes Işkın

Date:

ABSTRACT

Exceptional Points in Real Potential Scattering
Sezin Su Elden
Master of Science in Physics
September, 2023

Exceptional points are non-Hermitian degeneracies that appear in parameter-dependent eigenvalue problems, where two or more eigenvalues and their corresponding eigenvectors coalesce. These types of degeneracies can only be observed in non-Hermitian operators, which leads to the idea that exceptional points are exclusive to open quantum systems. We utilized the dynamical formulation of stationary scattering to study the scattering of waves by two- and three-dimensional finite-length waveguides filled with inactive and lossless material. With this formulation, the transfer matrix for these higher-dimensional setups is associated with the pseudo-Hermitian Hamiltonian of a two-level effective quantum system. This Hamiltonian is related to the transfer matrix by a function that exhibits exceptional points. Although these scattering setups are modeled by real potentials, we demonstrate that exceptional points can have a physical effect in these systems. Moreover, we use the composition property of the transfer matrix to solve the scattering problem for a system consisting of multiple finite waveguides and show that exceptional points also have physical realizations at these points.

ACKNOWLEDGMENTS

I would like to express my sincere gratitude and appreciation to all those who have contributed to the successful completion of my M.Sc thesis. This research would not have been possible without their support, guidance, and encouragement.

First and foremost, I extend my heartfelt thanks to my thesis advisor, Prof Ali Mostafazadeh, for his invaluable mentorship, patience, and expertise. His unwavering support and insightful feedback were instrumental in shaping this thesis and enhancing its quality.

I am grateful to Koc University for providing me with the resources and facilities needed to conduct this research.

I am deeply appreciative of my family for their unwavering support, encouragement, and understanding during this challenging journey. Their love and belief in me provided the motivation to persevere and achieve my goals.

I would also like to thank the members of my thesis committee, Dr. Menderes Iskın and Dr. Teoman Turgut, for their kind support.

Last but not least, I want to express my gratitude to my friends and colleagues who provided emotional support and valuable insights throughout this endeavor. Your encouragement was a source of motivation during both the high and low points of this research journey.

To everyone mentioned here and to all those who have contributed in their own way, I am truly thankful. Your support has been invaluable, and I could not have completed this M.Sc thesis without you.

Sezin Su Elden

September 2023

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

ABBREVIATIONS

EP - exceptional point,

DP - diabolic point,

DFSS - dynamical formulation of stationary scattering

Chapter 1

INTRODUCTION

Singularities are a significant part of physics that appear in many research areas. One of the types of singularities that will be the focal point of this thesis are exceptional points, which appear in eigenvalue problems that depend on parameters. At an exceptional point, two or more eigenvalues and their corresponding eigenvectors coalesce. It is a well known fact that this cannot happen for a Hermitian operator. This is the reason why the main focus on exceptional points involves open quantum systems where the Hamiltonian is a non-Hermitian operator.

EPs first appeared in physics literature while studying the perturbation of linear non-Hermitian operators [1]. Later works illustrated the physical significance of EPs [2, 3]. Experimental studies showed the topological structure of EPs [4, 5].

Recently the interest in EPs turned to non-Hermitian Hamiltonians that are symmetric under the combined parity and time reversal operators ($\mathcal{PT}$-symmetric operators). The fact that the spectrum of these Hamiltonians can be real made them interesting to study [6, 7]. $\mathcal{PT}$-symmetric Hamiltonians can go under symmetry breaking where the eigenvalues become complex. This happens as a result of parametric variation of the Hamiltonian. The point when this happens on the parameter space turns out to be the exceptional point of the system [8, 9, 10]. The theoretical effects of this phenomena [11, 12, 13, 14, 15]. Optics and photonics include active or lossy material, which require non-Hermitian Hamiltonians. The effects of EPs can be observed in optics and photonics [16, 17, 18, 19, 20, 21, 22].

Recently, [23] showed that affects of EPs appear in quantum problems concerning real potentials in particular, in the scattering of a wave by a two-dimensional finite waveguide. In this thesis, we will investigate scattering of a wave by a three dimensional finite waveguide, illustrate the consequences of the existence of an exceptional point in this scattering setup, and discuss the similarities and differences between scattering from two- and three-dimensional waveguide. We show the emergence of EPs in the treatment of scattering by a potential of the form,

$$v(x,y,z) = \begin{cases} V(x,y) & \text{for } z \in [a_-, a_+] \\ 0 & \text{for } z \notin [a_-, a_+] \end{cases}, \tag{1.1}$$

where $V(x,y)$ is a real-valued function and $a_\pm$ are real parameters that satisfies $a_- < a_+$. We study the scattering of by this potential by utilizing a newly developed multidimensional generalization of the transfer-matrix [24, 25]. This is a generalization of the dynamical formulation of stationary scattering (DFSS) in one dimension, where the transfer matrix is associated with the S-matrix of an effective two-level non-unitary quantum system [26, 27]. The fact that the resulting effective quantum system is described by a non-Hermitian Hamiltonian allows exceptional points to be possible in the treatment of scattering by the potential (1.1). In order to find the transfer matrix for this potential we have to find an explicit expression for the Hamiltonian $\hat{\mathbf{H}}(z)$ of the fore mentioned effective quantum system.

The organization of this thesis is as follows. In Chapter 2 we give a brief introduction to non-Hermitian operators and exceptional points, as well as, some mathematical tools that we used in the following chapters. In Chapters 3 we discuss dynamical formulation of stationary scattering (DFSS), and in chapter 4 we introduce the transfer matrix and generalize DFSS for higher dimensional scattering. We derive results of Ref. [23] and generalize them to three-dimensions in chapter 5. Here we also discuss the differences between scattering from two- and three-dimensional finite waveguides. In chapter 6 we make use of the composition property of the transfer matrix to investigate the scattering problem for a configuration of different waveguides.

Chapter 2

NON-HERMITIAN OPERATORS AND EXCEPTIONAL POINTS

In standard quantum mechanics the Hamiltonian is required to be a Hermitian operator. This Hermiticity condition for the Hamiltonian offers significant advantages. Most notably, it ensures that energy eigenvalues are real, and it establishes the existence of a complete set of orthonormal basis vectors comprising the Hamiltonian's eigenvectors. This property greatly simplifies computational tasks. Additionally, the Hermitian nature guarantees the unitary behavior of the time-evolution operator, thus upholding the conservation of probability for isolated systems. However, there are open systems that exchanges energy with their surrounding environment . In such cases, the probabilities are not conserved, making Hermitian Hamiltonians inadequate for the describtion these systems.

Non-Hermitian operators exhibit distinct characteristics. The realness of eigenvalues is not guaranteed, in general eigenvalues are complex numbers. The inherent orthogonality of eigenvectors and existence of an eigenbasis are no longer certain. Another notable contrast concerns degeneracies: non-Hermitian operators manifest distinct behaviours from their Hermitian counterparts.

Particularly intriguing are the "exceptional points" that emerge within non-Hermitian operators in their parameter space. These points signify instances where eigenvalues and the corresponding eigenvectors coalesce. This phenomenon diverges significantly from the diabolic points in Hermitian systems, where eigenvalues coincide while their corresponding eigenvectors remain linearly independent.

The primary objective of this chapter is to delve into exceptional points while providing useful tools to work with non-Hermitian operators. The chapter sets out to establish key definitions and outcomes in linear algebra, offering a foundation to comprehend the spectra of parameter-dependent linear operators. These tools will be instrumental in handling non-Hermitian Hamiltonians in subsequent chapters.

2.1 Vector Spaces

Consider an inner product space V. The sum of vector spaces $\bigoplus_{i=1}^{N} U_i$ is called a direct sum, if every $u \in \bigoplus_{i=1}^{N} U_i$ can be written uniquely as a sum $u_1 + u_2 + \cdots u_n$ where $u_j \in U_j$ for all $j \in \{1, 2, \cdots, n\}$.

A list of vectors $v_1, v_2, \cdots v_n$ is said to be linearly independent if $a_1 v_1 + a_2 v_2 + \cdots a_n v_n = 0$ implies $a_1 = a_2 = \cdots a_n = 0$. The largest number of linearly independent vectors that can exist in V is called the *dimension* of V and denoted by $\mathrm{dim}V$. If there is no such finite number V is said to be an infinite-dimensional vector space and we set $\mathrm{dim}V = \infty$.

A set of linearly independent vectors $\{v_1, v_2, \cdots v_N\}$ is said to be a basis, if every element $v \in V$ can be written uniquely as

$$v = \sum_{n=1}^{N} c_n v_n, \tag{2.1}$$

for complex coefficients c_n. However, for the infinite-dimensional case this summation must be convergent. In the rest of this text we assume this condition holds for every basis. Here the norm for the convergence is derived by the inner product.

A basis $v_1, v_2, \cdots, v_N$ of an inner product space V is said to be *orthonormal* if

$$\langle v_i | v_j \rangle = \delta_{ij} \text{ for all } i, j \in \{1, 2, \cdots, N\}, \tag{2.2}$$

where δ_{ij} is the Kronecker delta symbol defined as

$$\delta_{ij} = \begin{cases} 1 & \text{if} i = j, \\ 0 & \text{if} i \neq j, \end{cases} \tag{2.3}$$

However, we note that the orthonormality of vectors depend on the choice of inner product. For details see [28].

If the basis is orthonormal for this inner product space, terms that appear in (2.1) are given by

$$c_n = \langle v_n | v \rangle. \tag{2.4}$$

Moreover we have,

$$\langle u|v\rangle = \sum_{n=1}^{N}\langle u|v_n\rangle\langle v_n|v\rangle = \langle u|\big(\sum_{n=1}^{N}|v_n\rangle\langle v_n|\big)|v\rangle \tag{2.5}$$

for all $u, v \in V$. This implies the completeness relation,

$$I = \sum_{n=1}^{N}|v_n\rangle\langle v_n|, \tag{2.6}$$

where I is the identity operator on V. Any given basis can be transformed to an orthonormal basis with the Gram-Schimidt process [29].

For $V = \mathbb{C}^N$, the standard basis $e_1, e_2, \cdots, e_N$ consists of vectors e_i whose ith entry in equal to 1 all other entries are zeros.

Now, we introduce a generalization of orthogonal basis. A system of vectors $v_1, \cdots, v_m, u_1, \cdots u_m$ is called a biorthonormal system if

$$\langle v_i|u_j\rangle = \delta_{ij} \tag{2.7}$$

for all $i, j \in \{1, \cdots, m\}$. A biorthonormal system that satisfies

$$\sum_{i=1}^{N}|v_i\rangle\langle u_i| = I \tag{2.8}$$

is said to be complete.

Given a basis $\{v_i\}$ of a finite-dimensional inner product space V, it is possible to construct another basis $\{u_i\}$ such that $\{v_i, u_i\}$ is a complete biorthogonal system. To see this let $\{e_n\}$ be an orthonormal basis of V. Then we have,

$$v_n = \sum_m \langle e_m|v_n\rangle e_m. \tag{2.9}$$

Since $\{v_i\}$ is a basis of V we have

$$e_n = \sum_m A_{nm}v_m, \tag{2.10}$$

for some complex coefficients A_{nm}. By substituting equation (2.9) into equation (2.10), we obtain

$$e_n = \sum_{k,m} A_{nm}\langle e_k|v_m\rangle e_k. \tag{2.11}$$

Since $\{e_i\}$ is a orthonormal basis we must have

$$\sum_{k,m} A_{nm}\langle e_k|v_m\rangle = \delta_{km},$$

which implies $A_{nm} \neq 0$. Consequently,let $A^{-1}_{nm} = \langle e_m|v_k\rangle$ and define

$$u_n := \sum_m (A^{-1}_{nm})^* e_m \tag{2.12}$$

for all $i \in \{1, \cdots, N\}$. It is straight forward to show that $\{u_i\}$ a basis of V and $\{v_1, \cdots, v_N, u_1, \cdots, u_N\}$ is a biorthonormal system. The basis $\{u_i\}$ is called the biorthonormal extension of $\{v_i\}$. In order to see the completeness of this biorthonormal system note that,

$$\begin{aligned}\sum_k |v_k\rangle\langle u_k| = I\sum_k |v_k\rangle\langle u_k|I &= \sum_j |e_j\rangle\langle e_j|\sum_k |v_k\rangle\langle u_k|\sum_l |e_l\rangle\langle e_l| \\ &= \sum_{k,l,j}\langle e_j|v_k\rangle\langle u_k|e_l\rangle|e_j\rangle\langle e_l| = \sum_{k,l,j}(A_{jk},^{-1})^* A^*_{kl}|e_j\rangle\langle e_l| \\ &= \sum_j |e_j\rangle\langle e_j| = I.\end{aligned}$$

Here, we made use of (2.9) and (2.11).

For the infinite-dimensional case, constructing and biorthonormal extension for a given basis is not possible in general. For such basis to exist, the right-hand side of (2.12) must be convergent. This happens if and only if $\sum_m (A^{-1}_{nm})^* < \infty$ [28].

A theorem by Bari states that, if $\{v_n\}$ is a Riesz basis, then $\{u_n\}$ is also a Riesz basis and $\{(v_n, u_n)\}$ is the unique biorthonormal extension of $\{v_n\}$. [30].

2.2 Linear operators

An operator $T : \mathcal{D}(T) \subseteq V \to V$ is said to be linear if $T(au + bv) = aTu + bTv$ for all $u, v \in V$ and $a, b \in \mathbb{C}$. Here $\mathcal{D}(T)$ is called the domain of T. We assume the all operators considered in this thesis to be bounded operators [28].

The null space of a linear operator T, denoted by null$T$, is the subspace of V consisting of the vector that T maps to 0, i.e, $\text{null}(T) = \{v \in V|Tv = 0\}$. Nullity of the operator T on a finite inner product space is defined as $\text{null}(T) = \dim(\text{null}(T))$.

The range of an operator T is the subspace of V that can be expressed as Tu for some $u \in V$, i.e, range $= TV := \{Tv|v \in V\}$. The dimension of the range of T on a finite dimensional inner product space is called the rank of T and denoted by rank(T).

If null$T = 0$ and $\mathcal{D}(T) = V$, the linear operator T is invertible, that is, there exist a unique linear operator, say T^{-1}, such that $TT^{-1} = T^{-1}T = I$. If T^{-1} does not exist T is called a singular operator. Let $v_1, v_2, \cdots v_N$ be a basis and $v_1', v_2', \cdots, v_N'$ be orthonormal basis of V. Then the matrix representation $\mathcal{M}(T)$ of T, is a $N \times N$ matrix whose entries defined as

$$\mathcal{M}(T)_{ij} = \langle v_i'|Tv_j\rangle \text{ for each } i, j \in \{1, \cdots, N\}. \tag{2.13}$$

A subspace U of V is said to be an invariant subspace of T, if $Tu \in U$ for all $u \in U$. In this case T induces a linear operator $T_U : U \to U$, which is defined by $T_U u = Tu$ for $u \in U$ and it is called the restriction of T on U. If there exists subspaces $U_1, \cdots, U_n$ such that $V = \bigoplus_{i=1}^n U_i$ and each U_i is invariant under the operator T, we can write $T = \bigoplus_{i=1}^n T_i$, where $T_i := T_{U_i}$.

A linear operator P is a projection if $P^2 = P$ and $\mathcal{D}(P) = V$. This means P leaves its range unchanged. Notice that if P is a projection $I - P$ is also a projection. Let M be the image of the projection operator P and let N be the image of $I - P$. P is said to be the projection on M along N. For any element v of V can be decomposed uniquely as have $v = v' + v''$ where $v' = Pv$ and $v'' = (1 - P)v$. This shows that, $V = M \oplus N$. Assume that the subspaces $U_1, U_2, \cdots U_s$ satisfy $V = \oplus_{k=1}^s U_k$. Then each $u \in V$ can be decomposed uniquely as $u = \sum_{k=1}^s u_k$ where $u_k \in U$. The operator defined as $P_j u = u_j$ is the projection on U_j along $N_j := \oplus_{k=1, k\neq j}^s U_k$. Notice that we have,

$$P_k P_j = \delta_{kj} P_j, \qquad \sum_{j=1}^s P_j = I. \tag{2.14}$$

Another important property of projection operators is the fact that when U is an invariant subspace of T, then T and the projection defined on U commute.

Now let V be a finite-dimensional vector space. A linear operator N is called a nilpotent if $N^n = 0$ for some $n \in \mathbb{N}^+$, note that this implies $N^{\dim(V)} = 0$. Another important property of a nilpotent operator N, is that there exists vectors $v_1, \cdots, v_n$ such that $\{N^{m_1}v_1, \cdots, Nv_1, v_1, \cdots N^{m_n}v_n, \cdots v_n\}$ is a basis of V and $N^{m_i+1}v_i = 0$ for every $i \in \{1, 2, \cdots, n\}$, for the verification of existence of such an basis see [29]. Notice that, for $i \in \{1, \cdots, n\}$, in this choice of basis,the list of vectors $\{N^{m_i}v_i, \cdots, Nv_i, v_i\}$, the operator N takes the jth element of list to $(j-1)$st element for $j \in \{2, \cdots, m_i - 1\}$ and N takes N^{m_i} to 0. This demonstrates that, with respect to this choice of basis, the matrix representation of N has the form,

$$\begin{bmatrix} 0 & 1 & & & \\ & 0 & 1 & & \\ & & \ddots & \ddots & \\ & & 0 & 0 & 1 \\ & & 0 & 0 & 0 \end{bmatrix}, \tag{2.15}$$

where unspecified elements are zero.

2.3 The Eigenvalue Problem

A complex number λ is called an eigenvalue of an linear operator $T : V \to V$ if there exists a nonzero vector $v \in V$ such that

$$Tv = \lambda v. \tag{2.16}$$

Any vector that satisfies (2.16) is called an eigenvector of T corresponding to the eigenvalue λ. In the rest of the text we assume that all the linear operators defined on infinite-dimensional inner product spaces have discrete spectrum. It is important to note that eigenvectors corresponding to distinct eigenvalues are linearly dependent. The eigenspace of T corresponding to the eigenvalue λ is denoted by $E(\lambda, T)$ and defined as

$$E(\lambda, T) := \big\{u \in V | Tu = \lambda I\big\} = \text{null}(T - \lambda I). \tag{2.17}$$

It is easy to see that eigenspaces of T are invariant under T. The dimension of $E(\lambda, T)$ is called the geometric multiplicity of the eigenvalue λ, i.e., $m^g_\lambda = dim(E(\lambda, T))$.

Solving the eigenvalue problem involves determining the eigenvalues and their corresponding eigenvectors. Notice that if λ is an eigenvalue of T, $T - \lambda I$ is a singular operator. If V is a finite-dimensional vector space, this is equivalent to $det(T - \lambda I) = 0$. For this case, the characteristic polynomial of the operator T is defined as

$$p_T(\lambda) := det(T - \lambda I) \tag{2.18}$$

This is a polynomial of degree $N = dimV$, with zeros corresponding to the eigenvalues of T. This shows that T can have at most N eigenvalues.

2.3.1 Generalized eigenvectors

We wish to express the vector space V as a direct sum of invariant subspace of a given linear operator T. While the eigenspaces are invariant under T, in general, the direct sum of these eigenspaces is smaller than a proper subspace V.

A vector $v \in V$ is called a generalized eigenvector of T corresponding to an eigenvalue λ if there exists $m \in \mathbb{Z}^+$ such that

$$(T - \lambda I)^m v = 0. \tag{2.19}$$

The subspace consisting of all generalized eigenvalues of T corresponding to the eigenvalue λ is called the generalized eigenspace of T. We denote it by $G(\lambda, T)$, i.e,

$$G(\lambda, T) := \big\{v \in V | (T - \lambda I)^m v = 0 \text{ for some } m \in \mathbb{N}\big\}. \tag{2.20}$$

The dimension of the generalized eigenspace corresponding to λ is called the algebraic multiplicity of the eigenvalue λ, let $m^a_\lambda := dim(G(\lambda, T))$. Notice that, $E(\lambda, T) \subseteq G(\lambda, T)$, which implies

$$m^g_\lambda \leq m^a_\lambda. \tag{2.21}$$

It is easy to show that generalized eigenspaces are invariant under the operator they are defined for. Additionally, generalized eigenvectors corresponding to different eigenvalues are linearly independent.

The most significant result about the generalized eigenspaces is that the a finite-dimensional vector space V can be decomposed into a direct sum of all generalized eigenspaces of T [29], that is,

$$V = \bigoplus_{i=N}^{S} G(\lambda_i, T). \tag{2.22}$$

2.3.2 Diagonalizability

An operator is said to be diagonalizable if there is a basis in the operator is represented by a diagonal matrix. Diagonalizability of an operator is equivalent to the existence of a basis of V consisting of the eigenvectors of that operator. This, in turn, implies that if the operator is diagonalizable, the generalized eigenspace and eigenspace corresponding to all eigenvalues coinside. Consequently, $m_\lambda^a = m_\lambda^g$ holds for all eigenvalues, and if the vector space V is finite-dimensional it can be expressed as a direct sum of eigenspaces of the operator.

2.3.3 The Hermitian Adjoint

The Hermitian adjoint of a operator T is denoted by $T^\dagger$ and satisfies

$$\langle v_1 | T v_2 \rangle = \langle T^\dagger v_1 | v_2 \rangle, \tag{2.23}$$

for every $v_1, v_2 \in V$. An operator is called Hermitian if it is equal to its Hermitian adjoint, $T = T^\dagger$, i.e.,

$$\langle v_1 | T v_2 \rangle = \langle v_1 | v_2 \rangle \tag{2.24}$$

for every $v_1, v_2 \in V$. It is a very well known fact that the eigenvalues of Hermitian operators is defined on a finite vector space are real, and they possess a complete set of orthonormal eigenvectors, which implies that Hermitian operators are diagonalizable. The matrix representation of a Hermitian operator with respect to its eigenbasis is a diagonal matrix whose diagonal entries are the eigenvalues of the operator.

Let λ_n be an eigenvalue of a Hermitian operator A with algebraic multiplicity m_n^a, and $\{v_{n,1}, \cdots v_{n,m_n^a}\}$ be the corresponding eigenvectors which are orthonormal.

Then the completeness relation holds,

$$I = \sum_{n}^{S} \sum_{a}^{m_n^a} |v_{n,a}\rangle\langle v_{n,a}|, \tag{2.25}$$

here S is the number of distinct eigenvalues of A. This leads to

$$A = \sum_{n} \sum_{a}^{m_n^a} \lambda_n |v_{n,a}\rangle\langle v_{n,a}|, \tag{2.26}$$

which is known as the spectral representation of A.

A more general class of operators than Hermitian ones are the normal operators, which commute with their Hermitian adjoint, that is, an operator $\mathcal{N}$ is said to be a normal operator if

$$[\mathcal{N}, \mathcal{N}^\dagger] = 0. \tag{2.27}$$

It is obvious that a Hermitian operator is also a normal operator. Similar to Hermitian operators, normal operators admit a orthonormal basis consisting of its eigenvectors, which shows that normal operators are diagonalizable.

Let A be a non-Hermitian linear operator which is diagonalizable and has a discrete spectrum. Let λ_n be a eigenvalue of A of multiplicity m_n^a and let $v_{n,a}$ for $a \in \{1, \cdots, d_n\}$ be the corresponding eigenvectors. Then there exists a complete biorthonormal system of eigenvectors $\{|v_{n,a}\rangle, |u_{n,a}\rangle\}$ which satisfies the following relations.

$$H|v_{n,a}\rangle = \lambda_n |v_{n,a}\rangle, \qquad H^\dagger |u_{n,a}\rangle = \lambda_n^* |u_{n,a}\rangle, \tag{2.28}$$

$$\langle u_{m,b}|v_{n,a}\rangle = \delta_{mn}\delta_{ab}, \tag{2.29}$$

$$\sum_{n}^{N} \sum_{a=1}^{d_n} |u_{n,a}\rangle\langle v_{n,a}| = I, \tag{2.30}$$

2.3.4 Pseudo-Hermitian Operators

A linear operator A is said to be pseudo-Hermitian if there exists a Hermitian automorphism η such that

$$A^\dagger = \eta A \eta^{-1}. \tag{2.31}$$

In this case, we call it a η-pseudo Hermitian operator. Notice that if an operator is pseudo-Hermitian the operator η is not unique [28].

let λ be an eigenvalue of η-pseudo Hermitian operator A. Then $A - \lambda I$ is not invertible which implies $\eta(A - \lambda I)\eta^{-1} = A^{\dagger} - \lambda I$ is not invertible. This shows that λ is also an eigenvalue of $A^{\dagger}$ which in turn shows that λ^{*} is an eigenvalue of A. In other words if a pseudo-Hermitian operator has a discrete spectrum, this spectrum consists of real or complex conjugate pairs of eigenvalues.

2.3.5 The Jordan Normal Form

Any linear operator T defined on a finite-dimensional complex vector space can be written in the following form.

$$T = \mathcal{S} + N, \tag{2.32}$$

Here S is a diagonalizable operator defined as

$$\mathcal{S} = \sum_{i=1}^{S} \lambda_i P_i \tag{2.33}$$

where P_i is a projection onto the generalized eigenspace corresponding to eigenvalue λ_i. This projection is called the eigenprojection corresponding to λ_i. The operator N is a nilpotent operator that can be defined as

$$N = \sum_{i=1}^{S} N_i \tag{2.34}$$

where N_i is called the eigennilpotent corresponding to the eigenvalue λ_i and defined as

$$N_i := T_{G(\lambda_i,T)} - \lambda_i P_i. \tag{2.35}$$

It is straight forward to show that $N_i^{m^a_{\lambda_i}} = 0$, thus they are nilpotent operators. This also implies that N is a nilpotent operator.

Notice that since P_i commutes with $T_{G(\lambda_i,T)}$ for every $i \in \{1, \cdots, S\}$, N and S commutes.

The equality given by (2.26) is called the Jordan-Chevallay decomposition.

Previously, we showed that it is possible to find a basis for a nilpotent operator so that the matrix representation with respect to this bases has the form (2.18). Then we can choose a basis, say $\mathcal{B}_n := \{v_{n,1}, \cdots, v_{n,m_n^a}\}$, in $G(\lambda_n, T)$ such that, the eigennilpotent N_n defined as (2.34) has this form. Note that, in this basis the term $\lambda_n P_n$ has a diagonal matrix representation with λ_n on the diagonal. Combining these bases for all $G(\lambda_n, T)$, which is equal to $\mathcal{B} = \bigcup_{n=1}^{S} \mathcal{B}_n = \{v_{1,1}, \cdots, v_{1,m_1^a}, \cdots, v_{S,1}, \cdots v_{S,m_S^a}\}$, is called a Jordan basis. The matrix representation of T in this basis has the form,

$$J = \begin{pmatrix} J_{1,1} & 0 & \cdots & & & & 0 \\ \vdots & \ddots & & & & & \vdots \\ & & J_{1,m_1} & & & & \\ & & & \ddots & & & \\ & & & & J_{S,1} & & \\ & & & & & \ddots & 0 \\ 0 & \cdots & & & & 0 & J_{S,m_S} \end{pmatrix} \tag{2.36}$$

where S is the number of distinct eigenvalues of T and $J_{j,n}$ for $j \in \{1, \cdots, S\}$ and $m \in \{1, \cdots, m_j\}$,

$$J_{j,m} = \begin{pmatrix} \lambda_j & 1 & \cdots & 0 \\ 0 & \lambda_j & \ddots & 0 \\ \vdots & & \ddots & 1 \\ 0 & & 0 & \lambda_j \end{pmatrix} \tag{2.37}$$

where the unspecified elements of both matrices are zero. A matrix of the form (2.33) is called a Jordan block and n_j for each j is the number of Jordan blocks for λ_j.

Note that, for every $j \in \{1, \cdots, S\}$, the matrix representation of T restricted to $G(\lambda_j, T)$ is equal to the direct sum of Jordan blocks for λ_j

$$\mathcal{M}(T_{G(\lambda_j,T)}) = \bigoplus_{k=1}^{j_n} J_{j,k}. \tag{2.38}$$

Let $n_{j,k}$ be the size of the kth Jordan form of eigenvalue λ_j.

The number of Jordan blocks for a given eigenvalue is equal to its geometric multiplicity, which in turn is equal to linearly independent eigenvectors corresponding to that eigenvalue. Moreover, the number of times a eigenvalue appears in the total Jordan normal or equivalently the summation of sizes of all Jordan blacks for that eigenvalue is the algebraic multiplicity of that eigenvalue. Considering, these facts about the algebraic and geometric multiplicity of an eigenvalue λ_j, it is easy to show that the number 1's that appear in the super-diagonal of (2.38) is equal to the difference of $m_j^a - m_j^g$, which is equal to number of linearly independent generalized eigenvector not including the eigenvectors corresponding to λ_j.

2.3.6 Function of an operator

Let $f(z) : \mathbb{C} \to \mathbb{C}$ be an analytical function. Then [1] shows that,

$$f(T) = \sum_{j=1}^{S} f(\lambda_j) P_j + D'_j \tag{2.39}$$

where

$$D'_j = \sum_{l=1}^{m_j^a - 1} \frac{f^{(l)}(\lambda_j)}{l!} D_j^l, \tag{2.40}$$

and $f^{(l)}$ is the lth derivative of f with respect to η. In the Jordan basis of T, $f(T)$ has the form The Jordan block becomes

$$f(J_{j,n}) \begin{bmatrix} f(\lambda_j) & f'(\lambda_j) & \frac{f''(\lambda_j)}{2} & \ddots & \frac{f^{(m_i^a-1)}(\lambda_j)}{(n_i-1)!} \\ 0 & f(\lambda_j) & f'(\lambda_j) & \ddots & \frac{f^{(n_i-2)}(\lambda_J)}{(m_i^a-2)!} \\ \vdots & & \ddots & \ddots & \\ 0 & 0 & & & f(\lambda_J) \end{bmatrix}. \tag{2.41}$$

Moreover, the matrix representation of $f(T)$ with respect to the Jordan basis that gives (2.36) is in the form

$$f(J) = \bigoplus_{l=1}^{S} f(J_{j,n}) \tag{2.42}$$

2.4 Parameter-Dependent Operators

We want to examine the eigenvalue problem for an analytic operator valued function that dependent on a complex parameter ξ. A linear operator T is said to be analytic in a region G, if $T(\xi)$ for all $\xi \in G$ and if in a neighbourhood of each point $\xi_0 \in G$, the operator valued function $T(\xi)$ can be expended in a series

$$T(\xi) = T(\xi_0) + \sum_{j=1}^{\infty} (\xi - \xi_0)^j C_j \tag{2.43}$$

where C_j is a linear operator for every $j \in \{1, \cdots\}$ [30]. Here, the convergence of the series id defined with the uniform form, which is defined as

$$|T| = \sup_{|v|=1} |Av|.$$

2.4.1 The Eigenvalue Problem

We can find the eigenvalues of $T(\xi)$ in the previous section, λ is an eigenvalue if there exist a non-zero vector v that satisfies $T(\xi)v = \lambda v$, notice that λ is a function of ξ. Now, we examine the behavior of λ as we change the parameters. For the finite-dimensional case, consider the function

$$(p(\lambda))(\xi) := det(T(\xi) - \lambda I). \tag{2.44}$$

This is a polynomial of degree $N = dimV$ whose coefficients are functions of ξ. The zeros of (2.40) are the eigenvalues of $T(\xi)$. There are some important properties of this function which are listed below.

1. Coefficients are analytical functions of ξ.
2. There is at most N distinct zeros of $(p(\lambda))(\xi)$.
3. Zeros of $(p(\lambda))(\xi)$ are almost everywhere analytical functions except at some isolated points.
4. The number of zeros of $(p(\lambda))(\xi)$ is constant almost everywhere.
5. The number of zeros can only decrease at these isolates points and remain constant at other points.

Property 1 can be seen by considering the determinant of a matrix representation of the operator T. As shown in [29], the coefficients are sums and products of entries of the matrix representation of T which are analytical functions. The second property is trivial. The third property is a well-known result [31] which implies the fourth. The fifth property can be seen by considering the opposite, if the number of zeros increase this violates the continuity of the zeros which contradicts the third property [32]. These facts show that, the eigenvalues of $T(\eta)$ are analytical functions of ξ, the number of eigenvalues is constant smaller or equal to the dimension of the vector space except some isolated points, where this number decreases. In the book [1], these points where the number of eigenvalues decreases are labeled as exceptional points. It is important to note that this is a more extensive definition that the exceptional points considered in physics literature.

2.4.2 The Jordan Normal Form

$T(\xi)$ is a linear operator, then it has a Jordan normal form. However, like the eigenvalues, the Jordan normal form changes with the parameter ξ. In this subsection, we study the relationship of Jordan normal form of $T(\xi)$ and the parameter ξ. In particular, we examine the structural changes of the Jordan normal form.

Changes in the Jordan normal form can appear in the diagonal part with the eigenvalues, since the eigenvalues are continuous function of the parameter ξ the diagonal elements vary continuously, and as we explained in the previous chapter the number of eigenvalues is constant almost everywhere. This implies that the algebraic multiplicities of the eigenvalues are constant except at some isolated points. A structural change in the diagonal happens, if the number of eigenvalues decreases, that is some of the eigenvalues coalesce and the number of times that particular eigenvalue appears on the diagonal increases.

The other type of change in the Jordan form is the change in the super-diagonal which consists of zeros and ones. The number of ones can increase or decrease. Obviously there is two ways this can happen; if the eigenvalue is permanently degenerate the number of corresponding eigenvectors can increase or decrease or when some of the eigenvalues coalesce some of the corresponding eigenvectors can also coalesce, resulting in more ones in the super-diagonal of the corresponding part of the Jordan normal form.

We will examine these possibilities separately, which are

1. Only eigenvalues coalesce,
2. Only eigenvectors coalesce,
3. Both eigenvalues and some of the corresponding eigenvectors coalesce.

For first possibility, where just the eigenvalues coalesce, consider the operator T_1, which has the following matrix representation with respect to the standard basis.

$$\mathbb{T}_1(\xi) = \begin{bmatrix} \lambda & 0 \\ 0 & \xi \end{bmatrix}, \tag{2.45}$$

The eigenvalues are λ and ξ. When $\xi \neq \lambda$, there is two eigenvalues, the multiplicity of each is equal to one. There is two 1×1 Jordan blocks. The Jordan normal form is equal to $\mathbb{T}_1(\xi)$. At $\xi = \lambda$, the eigenvalues are equal the multiplicity becomes two. Notice in both cases the operator is diagonizable and it has two distinct eigenvectors $v_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $v_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$.

For the second case consider a permanently degenerate operator T_2, with matrix representation

$$\mathbb{T}_1(\xi) = \begin{bmatrix} \lambda & \xi \\ 0 & \lambda \end{bmatrix}. \tag{2.46}$$

The only eigenvalue is λ. The number of eigenvalues is 1 with algebraic multiplicity 2 for all ξ. For $\xi \neq 0$. The Jordan normal form of this operator is

$$\begin{bmatrix} \lambda & 1 \\ 0 & \lambda \end{bmatrix}. \tag{2.47}$$

In this case there is one eigenvector of this matrix, namely $v_1 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$. The eigenspace which is given by $E(\lambda, T_1) = \mathrm{span}(v_1)$ is one-dimensional. Therefor its geometric multiplicity $m^g(\lambda) = 1$. At the point $\xi = 0$, the operator becomes diagonalizable and its Jordan normal form takes the form

$$\begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix}. \tag{2.48}$$

A discontinuous change happens at this point. The number of ones at the superdiagonal changes. In this case there is another eigenvector $v_2 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ in addition to v_1. The eigenspace is $E(\lambda, T_1) = \text{span}(v_1, v_2)$ which is equal to the algebraic eigenspace. The geometric multiplicity becomes 2.

For the third case, consider the operator with the following matrix representation.

$$\mathbb{T}_3(\xi) = \begin{bmatrix} 0 & 1 \\ \xi & 0 \end{bmatrix}. \tag{2.49}$$

The eigenvalues are $\lambda_\pm = \pm\sqrt{\xi}$ and the corresponding eigenvectors are $v_\pm = (1, \pm\sqrt{\xi})^T$. The eigenvalues coalesce at $\xi = 0$. When $\xi \neq 0$ there is two linearly independent eigenvectors, so the matrix is diagonalizable. In this case the Jordan normal form is

$$\begin{bmatrix} \sqrt{\xi} & 0 \\ 0 & -\sqrt{\xi} \end{bmatrix} \tag{2.50}$$

At $\xi = 0$ the two eigenvalues coalesce and vanish, the multiplicity becomes two. At this point the eigenvectors also coalesce and become $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$. The matrix becomes non-diagonalizble and the Jordan normal form becomes

$$\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}. \tag{2.51}$$

2.5 Exceptional Points

The term exceptional point was first introduces by Kato [1] as points that are branch points of some of the eigenvalues or regular points for all eigenvalues but at this regular points some of the eigenvalues coincide. Notice that this description is different from the definition given at the beginning of this chapter. This description includes two type of points examined in the previous section, the first and the third kind. In the physics literature the third type of points, where both eigenvalues and eigenvector coalesce are considered exceptional points. This definition is also equivalent to branch point singularities of some of the eigenvalues [32]. In the previous section, we defined this points for linear operators defined on finite vector spaces. However, in an infinite-dimensional inner-product space, if an operator-valued function has a discrete basis, we can define the exceptional points as we defined for the finite-dimensional cases. This is the definition used for exceptional points in the remainder of the text. The first type of points where just the eigenvalues coalesce are called diabolic points.

It is clear that normal operators cannot have exceptional points. In particular, Hermitian operators cannot exhibit exceptional points. In the physical applications of non-Hermitian operators, the operators that are considered are diagonalizable except at their exceptional points where they become non-diagonalizable.

As an example that appears in many physical systems we consider the following 2×2 non-Hermitian matrix Hamiltonian

$$H = \begin{bmatrix} w_1 - i\gamma_1 & \kappa \\ \kappa & w_2 - i\gamma_2 \end{bmatrix}. \tag{2.52}$$

The eigenvalues of H are given by

$$\lambda_\pm = w_+ - i\gamma_+ \pm \Delta, \tag{2.53}$$

where

$$w_\pm := \frac{w_1 \pm w_2}{2}, \qquad \gamma_\pm := \frac{\gamma_1 \pm \gamma_2}{2}, \qquad \Delta := \sqrt{(w_- + i\gamma_-)^2 + \kappa^2} = 0 \tag{2.54}$$

The eigenvalues can coalesce when Δ vanishes. This can happen when $w_- = 0$ and $\kappa = \pm\gamma_-$,or $\gamma_- = 0$ and $\kappa = \pm i w_-$. We continue with the second case and define $\gamma_1 = -\gamma_2 =: \gamma$ and $\delta_1 = -\delta_2 =: \delta$. The Hamiltonian becomes,

$$H = \begin{bmatrix} w - i\gamma & \kappa \\ \kappa & w + i\gamma_2 \end{bmatrix} \tag{2.55}$$

and the eigenvalues and the corresponding eigenvectors become

$$\lambda_\pm = w \pm \sqrt{\kappa^2 - \delta^2}, \qquad v_\pm = \begin{bmatrix} \frac{i\gamma \mp \sqrt{\kappa^2-\gamma^2}}{\kappa} \\ 1 \end{bmatrix}. \tag{2.56}$$

There are two exceptional points $\kappa_\pm^{EP} = \pm\gamma$, where the eigenvalues are equal to $\lambda(\pm\gamma) = w$ and the eigenvectors are equal to $v(\pm\gamma) = [\pm i, 1]^T$.

Figure 1 shows how the real and imaginary parts of the eigenvalues given by the first equation of (2.53) for $w =, \delta = 1$ and $\kappa \in (0, 2)$. When $\kappa = \delta = 1$, both the real and imaginary parts of the eigenvalues are equal.

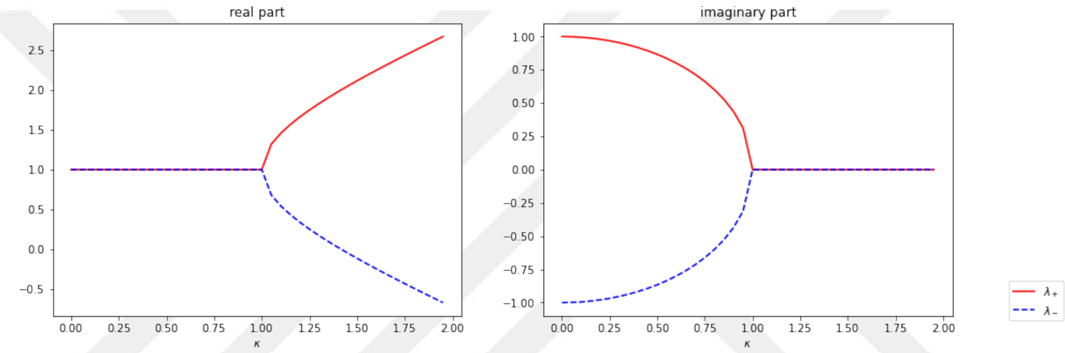

Figure 2.1: real and imaginary part of eigenvalues

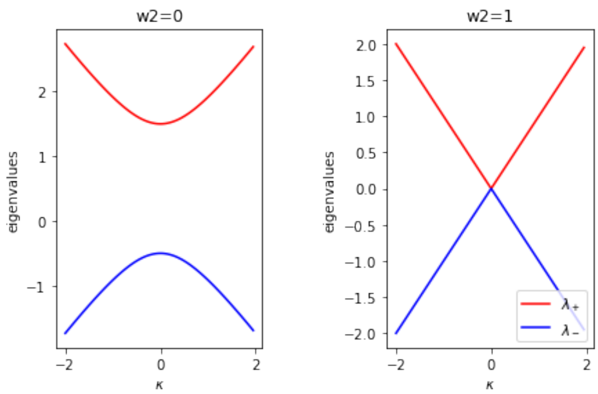

Figure 2.2: eigenvalues of Hermitian Hamiltonian for different w_2

The Hamiltonian (2.49) is Hermitian only when $\delta_1 = \delta_2 = 0$,

$$\begin{bmatrix} w_1 & \kappa \\ \kappa & w_2 \end{bmatrix} \tag{2.57}$$

with eigenvalues

$$\lambda_{\pm} = w_{+} \pm \sqrt{\kappa^2 + w_{-}^2}. \tag{2.58}$$

A diabolic point occurs when $\kappa = 0$ and $w_1 = w_2 =: w$ where the eigenvalues become $\lambda_+ = \lambda_- = w$. At this point the eigenvectors become $(1,0)^T$ and $(0,1)^T$ and (56) is no longer valid. There is still two orthogonal eigenvectors as we expected. Figure 2 shows the eigenvalues (2.55) for $w_1 = 1$ in two cases for $w_2 = 0$ and $w_2 = 1$. A diabolic point occurs just in the second case where $w_1 = w_2$ and $\kappa = 0$.

2.6 Function of a linear operator at an exceptional point

Let $T(\xi)$ be a bounded linear operator on an inner product space of infinite or finite degree. Moreover, assume that this operator has a discrete spectrum and all the bases that is discussed in this chapter are Riesz bases. Assume this operator is diagonalizable every where except a point ξ_{EPn}, at which it has a exceptional point of order n and the first n distinct eigenvalues and the corresponding eigenvectors coalesce.

Let $\mathcal{B}$ be a basis consisting of eigenvectors of T

$$\mathcal{B} := \{v_{1,1}, \cdots, v_{1,m_1^a}, \cdots, v_{S,1}, \cdots, v_{s,m_s^a}\}, \tag{2.59}$$

where s is the number of distinct eigenvalues of T, m_j^a is the algebraic multiplicity of the jth eigenvalue of T, and for all $j \in \{1, \cdots, s\}$ and $a \in \{1, \cdots, m_j^a\}$ $v_{j,a}$ are the eigenvectors corresponding to jth eigenvalue. This basis exists for every ξ except at ξ_{EPn}. In subsection (2.3.3), we showed that when $\xi \neq \xi_{EPn}$ the operator T can be written as

$$T = \sum_{j=1}^{S} \sum_{a=1}^{m_j^a} \lambda_j |u_{j,a}\rangle\langle v_{j,a}|, \tag{2.60}$$

where $\mathcal{B}^{\perp} := \{v_{n,a}\}$ is the biorthonormal extension of $\mathcal{B}$.

At the exceptional point the first n eigenvalues and the corresponding eigenvectors coalesce. Define $\lambda := \lambda_1(\xi_{EPn}) = \cdots = \lambda_1(\xi_{EPn})$ and v_0 be the eigenvector corresponding this eigenvector. At this point the set of eigenvector is not a complete basis, however, we can extend it to a complete basis with the addition of generalized eigenvectors corresponding to λ, there must be $n-1$ generalized eigenvectors, that can be defined as the vectors that satisfy $(T-\lambda I)^{k+1}v_k = 0$ for each $k \in \{1, \cdots, n-2\}$. Note that this also implies

$$(T-\lambda I)v_k = v_{k-1}, \tag{2.61}$$

for all $k \in \{1, \cdots, n-2\}$. Then the set of generalized eigenvectors

$$\mathcal{B}_{EP} := \{v_0, v_1, \cdots, v_{n-1}\} \cup \bigcup_{j=1}^{N} \{v_{j,2}, \cdots, v_{j,m_j^a}\} \cup \bigcup_{j=N+1}^{S} \{v_{j,1}, \cdots, v_{j,m_j^a}\}, \tag{2.62}$$

is a complete basis, and has the following biorthonormal extension

$$\mathcal{B}_{EP}^{\perp} := \{u_0, u_1, \cdots, u_{n-1}\} \cup \bigcup_{j=1}^{N} \{u_{j,2}, \cdots, u_{j,m_j^a}\} \cup \bigcup_{j=N+1}^{S} \{u_{j,1}, \cdots, u_{j,m_j^a}\}. \tag{2.63}$$

Since $\{\mathcal{B}_{EP}, \mathcal{B}_{EP}^{\perp}\}$ is a complete biorthonormal system and the vector u_j for $j \in \{1, \cdots, N-1\}$ are the generalized eigenvectors of the operator $T^\dagger$ corresponding to the eigenvalue λ^*,i.e, they satisfy $(T^\dagger - \lambda^* I)^{j+1} u_j = 0$. With these, identity operator can be written as

$$I = \sum_{j=0}^{N-1} |v_j\rangle\langle u_j| + \sum_{j=1}^{N} \sum_{a=2}^{m_j^a} |v_{j,a}\rangle\langle u_{j,a}| + \sum_{j=2}^{S} \sum_{a=1}^{m_j^a} |v_{j,a}\rangle\langle u_{j,a}|. \tag{2.64}$$

Making use of this and (2.79) we get

$$T = \sum_{j=0}^{N-1} \lambda|v_j\rangle\langle u_j| + \sum_{j=1}^{N} |v_j\rangle\langle u_{j-1}| + \sum_{j=1}^{N} \sum_{a=2}^{m_j^a} \lambda_j |v_{j,a}\rangle\langle u_{j,a}| + \sum_{j=2}^{S} \sum_{a=1}^{m_j^a} \lambda_j |v_{j,a}\rangle\langle u_{j,a}|. \tag{2.65}$$

Here the second summation is a result of (2.79). For a finite dimensional vector space the expression (2.82) gives the Jordan Normal form of the operator at ξ_{EPn}, which has the form

$$T(\xi_{EP_n}) = T_1(\xi_{EP_n}) \oplus T_2(\xi_{EP_n}) \oplus T_3(\xi_{EP_n}) \tag{2.66}$$

where the term $T_1(\xi_{EPn})$ is the matrix representation of the first and the second summation of (2.82) and has the form

$$T_1(\xi_{EP_n}) = \begin{pmatrix} \lambda & 1 & 0 & \cdots & 0 \\ 0 & \lambda & 1 & & \\ & & \lambda & \ddots & \\ & & & \ddots & 1 \\ 0 & & & 0 & \lambda \end{pmatrix}_{(n\times n)} . \tag{2.67}$$

The terms $T_2(\xi_{EPn})$ and $T_3(\xi_{EPn})$ correspond to the third and the forth summations in (2.83) respectivly and they have the following matrix representations.

$$T_2(\xi_{EP_n}) = \begin{pmatrix} \lambda & 0 & 0 & \cdots & 0 \\ 0 & \lambda & 0 & \vdots & \\ & & \lambda & \ddots & \\ & & & \ddots & 0 \\ 0 & & & 0 & \lambda \end{pmatrix}_{(n' \times n')} \tag{2.68}$$

,

$$T(\xi_{EP_n}) = \begin{pmatrix} \lambda_{N+1}(\xi) & 0 & 0 & & & & 0 \\ 0 & \ddots & 0 & & & & \\ & & \lambda_{N+1}(\xi) & & & & \\ & & & \ddots & & & \\ & & & & \lambda_S(\xi) & & 0 \\ & & & & & \ddots & \\ 0 & & & & & 0 & \lambda_S(\xi) \end{pmatrix}_{(n'' \times n'')} .$$

Here $n' := \sum_{j=1}^{N}(m_j^a - 1)$ and $n'' := \sum_{j=N+1}^{S} m_j^a$. Note that by m_j^a, we mean the algebraic multiplicity of the jth eigenvalue at the points except the exceptional point.

The function of a linear operator T is defined as

$$f(T) := \sum_{n=0}^{\infty} a_n T^n. \tag{2.69}$$

It is easy to see that when T satisfies the conditions given in the beginning of this chapter, (2.78) and (2.86) implies

$$f(T) = \sum_{j=0}^{\infty} \sum_{a=1}^{m_j^a} f(\lambda) |u_{j,a}\rangle\langle v_{j,a}|, \tag{2.70}$$

however this relation does not hold if the operator is not diagonalizable. Then in order to find an expression for $f(T)$ at an exceptional point, we need to find how T^n acts on a generalized eigenvector of T, which can be found with the following result.

$$f(T)v_k = \sum_{i=0}^{k} \frac{f^{(k-i)}(\lambda)}{(k-i)!} v_{k-i}, \tag{2.71}$$

here $f^{(k-i)}(\lambda)$ is the $(k-i)$th derivative of $f(z)$ evaluated at λ. Then (2.83), (2.87) and (2.89) implies that

$$\begin{aligned} f(T) = & \sum_{j=0}^{N-1} \sum_{l=0}^{j} \frac{f^{(j-l)}(\lambda)}{(j-l)!} |v_l\rangle\langle u_j| + \sum_{j=1}^{N} \sum_{a=2}^{m_j^a} f(\lambda)|v_{j,a}\rangle\langle u_{j,a}| \\ & + \sum_{j=2}^{S} \sum_{a=1}^{m_i^a} f(\lambda_j)|v_{j,a}\rangle\langle u_{j,a}|, \end{aligned} \tag{2.72}$$

rearranging the terms we get

$$\begin{aligned} f(T) = & \left(\sum_{j=0}^{N-1} f(\lambda)|v_j\rangle\langle u_j| + \sum_{j=1}^{N} \sum_{a=2}^{m_j^a} f(\lambda)|v_{j,a}\rangle\langle u_{j,a}| + \sum_{j=2}^{S} \sum_{a=1}^{m_i^a} f(\lambda_j)|v_{j,a}\rangle\langle u_{j,a}| \right) \\ & + \sum_{j=1}^{N-1} \sum_{l=0}^{j-1} \frac{f^{(j-l)}(\lambda)}{(j-l)!} |v_l\rangle\langle u_j| \end{aligned} \tag{2.73}$$

The summation inside the parenthesis has the same structure of $f(T)$ for a regular point, at the exceptional the summation outside the parenthesis appears as extra terms. Note that the equation is valid for a diabolic point, which shows another different features of exceptional points that cannot occur in diabolic points. For a second degree EP, the extra term becomes

$$\frac{f'(\lambda)}{2}|v_0\rangle\langle u_1|, \tag{2.74}$$

and for a third degree EP, the extra term is

$$\frac{f'(\lambda)}{2}|v_0\rangle(\langle u_1| + \langle u_2|) + \frac{f''(\lambda)}{3!}|v_1\rangle\langle u_2|. \tag{2.75}$$

Notice that, if the operator is defined on a vector space, (2.92) implies the results given in subsection (2.3.6).

Chapter 3

STATIONARY SCATTERING IN ONE DIMENSION

In this chapter we introduce the basics of stationary scattering in one-dimensional systems, the transfer matrix and a dynamical formulation of one-dimensional scattering recently developed by [26, 27].

Consider the one-dimensional time-independent Schrödinger equation,

$$-\psi''(x) + v(x)\psi(x) = k^2\psi(x), \tag{3.1}$$

where $v(x) : \mathbb{R} \to \mathbb{C}$ and $k \in \mathbb{R}^+$ is the wavenumber. If this potential vanishes as $x \to \pm\infty$, it is called a scattering potential. A short range potential is a special kind of scattering potential that satisfies

$$|v(x)| \leq \frac{C}{|x|^\alpha} \text{ for } |x| \geq M, \tag{3.2}$$

for some positive real numbers $C, M, \alpha > 1$ and all $x \in \mathbb{R}$.

Every solution of (3.1) with a short range potential tends to the solution of this equation for a free particle far away from the origin, that is, if $\psi(x)$ is such a solution, it must satisfy the following asymptotic boundary condition.

$$\psi(x) \to \begin{cases} A_- e^{ikx} + B_- e^{-ikx} & \text{for } x \to -\infty, \\ A_+ e^{ikx} + B_+ e^{-ikx} & \text{for } x \to \infty, \end{cases} \tag{3.3}$$

for some $A_\pm, B_\pm \in \mathbb{C}$. It is important to note that, this does not hold for solutions to (3.1) for any scattering potential, the short-range criteria for the potential is necessary [33]. Here the terms $e^{\pm ikx}$ are called right/left moving wave respectively.

A potential $v(x)$ is said to be finite range if it vanishes outside some interval $[a_-, a_+]$ where $a_+ > a_-$, i.e,

$$v(x) = \begin{cases} V(x) \text{ for } x \in [a_-, a_+], \\ 0 \text{ for } x \notin [a_-, a_+], \end{cases} \tag{3.4}$$

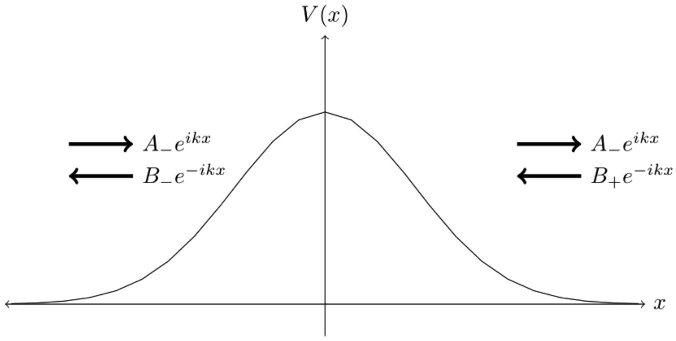

Figure 3.1: Scattering from a short-range potential

for some function $V(x) : [a_-, a_+] \to \mathbb{C}$. The support of a finite-range potential is the largest interval outside which the potential vanishes. It is easy to see that a finite range potential is a short range potential and its solutions satisfy

$$\psi(x) = \begin{cases} A_-e^{ikx} + B_-e^{-ikx} & \text{for } x \leq a_-, \\ A_+e^{ikx} + B_+e^{-ikx} & \text{for } x \geq a_+. \end{cases} \tag{3.5}$$

3.1 *Scattering from the left and the right*

A scattering experiment consists of three ingredients:

1. The source of the incident wave,

2. The scattering potential,

3. The detectors.

The source and the detectors can be placed at $x = \pm\infty$ and $x = \pm\infty$ respectively.

Assume the source of the incident wave is placed at $x = -\infty$, then it moves towards the right. We name it left-incident wave $\psi^l(x)$. When the incident wave interacts with the potential it will be partially reflected and partially transmitted. The reflected wave must propagate towards the source and it is a left-moving wave that propagates towards $x = -\infty$. Then the reflected wave is a wave that is proportional to e^{-ikx} at $x = -\infty$. The transmitted wave must be a right-moving wave and moves towards $x = \infty$, thus the transmitted wave is proportional to e^{ikx} as $x = \infty$. In order to distinguish a left-incident wave, we use the superscript $'l'$ for the coefficients $A^l_\pm, B^l_\pm$ that appear at (3.3). Notice that, for a left-incident wave there must not be a term that is left-moving at $x = \infty$, that is, $B^l_+ = 0$. Then (3.3) for a left-incident wave becomes

$$\psi^l(x) \to \begin{cases} A^l_- e^{ikx} + B^l_- e^{-ikx} & \text{for } x \to -\infty, \\ A^l_+ e^{ikx} & \text{for } x \to \infty. \end{cases} \tag{3.6}$$

We can take the coefficient A^l_- o utside of this expression and find

$$\psi^l(x) \to A^l_- \begin{cases} e^{ikx} + B^l_-/A^l_- e^{-ikx} & \text{for } x \to -\infty, \\ A^l_+/A^l_- e^{ikx} & \text{for } x \to \infty. \end{cases}$$

According to the description above we define,

$$R^l := \frac{B^l_-}{A^l_-}, \qquad T^l := \frac{A^l_+}{A^l_-}. \tag{3.7}$$

Here $R^l, T^l \in \mathbb{C}$ are called left reflection and transmission amplitudes respectively.

Now, assume the source of the incident wave is placed at $x = \infty$. It is a right-moving wave and we name it right-incident wave $\psi^r(x)$. When the wave interacts with the potential, the reflected wave will be a left-moving wave that travels towards $x = \infty$ and the transmitted wave will a right-moving wave $x = -\infty$. So, $\psi^r(x)$ must have the following form,

$$\psi^r(x) \to \begin{cases} A^r e^{-ikx} & \text{for } x \to -\infty, \\ B^r_+ e^{-ikx} + B^-_r e^{ikx} & \text{for } x \to \infty, \end{cases} \tag{3.8}$$

Similarly to a left-incident wave, we define

$$R^r = \frac{A^r_+}{B^r_+}, \qquad T^r = \frac{B^r_-}{B^r_+}, \tag{3.9}$$

where $R^r, T^r \in \mathbb{C}$ which are called right reflection and transmission amplitudes respectively.

Now consider $\phi(x) = (\psi^{l*}(x) - R^{l*}\psi^{l}(x))/T^{l*}$. For a real potential $v(x)$, $\psi^{l*}(x)$ is also a solution of (3.1), then $\phi(x)$ is a solution of (3.1) as it is a linear combination of solutions. Notice that,

$$\phi(x) \to \begin{cases} (1-|R^l|^2)/T^{l*}e^{-ikx} & \text{for } x \to -\infty, \\ T^{l*}/T^{l*}e^{-ikx} - R^{l*}T^l/T^{l*}e^{ikx} & \text{for } x \to \infty. \end{cases} \tag{3.10}$$

Comparing (3.10) and (3.12) we can see that

$$\frac{1-|R^l|^2}{T^{l*}} = T^r, \qquad \frac{T^{l*}}{T^{l*}} = 1, \qquad \frac{R^{l*}T^l}{T^{l*}} = R^l. \tag{3.11}$$

Therefore we have $T^l = T^r$, this is called transmission reciprocity. In the remainder of this text we drop the superscripts for the transmission coefficient and define

$$T := T^l = T^r. \tag{3.12}$$

The transmission reciprocity is also valid for complex potentials, for the proof see [33].

Another implication of equations (3.13) is the fact that if the potential is real R^l and R^r differ only by a phase factor. It is important to note that, this result does not hold for complex potentials.

Solving the scattering problems for a short range potential $v(x)$ means finding $R^{l/r}$ and T for wavenumber k.

3.2 Transfer matrix and the S-matrix

Now, we summarize the results of chapter 2.2, [33], which defines the transfer matrix.

Consider a finite range potential in the form (3.4) and let $\psi(x)$ be a solution of (3.1) for this potential. Then $\psi(x)$ and $\psi'(x) := \partial_x\psi(x)$ must be continuous everywhere. Let,

$$\psi(x) = \begin{cases} \psi_- \text{ for } x < a_-, \\ \psi_0 \text{ for } a_- \leq x \leq a_+, \\ \psi_+ \text{ for } x > a_+, \end{cases}$$

which must satisfy

$$\partial_x^2\psi_- = k^2\psi_- \text{ for } x < a_-, \tag{3.13}$$

$$\big(\partial_x^2 - V(x)\big)\psi_0 = k^2\psi_0 \text{ for } a_- \leq x \leq a_+, \tag{3.14}$$

$$\partial_x^2\psi_+ = k^2\psi_+ \text{ for } x < a_+, \tag{3.15}$$

The solutions of (3.13) and (3.15) are in the form

$$\psi_\pm(x) = A_\pm e^{ikx} + B_\pm e^{-ikx}, \text{ for } \pm x > \pm a_\pm. \tag{3.16}$$

and the solution of (3.14) is in the form

$$\psi_0(x) = c_1\psi_1(x) + c_2\psi_2(x), \tag{3.17}$$

where ψ_1 and ψ_2 are twice differentiable solutions of (3.1) that vanish outside $[a_-, a_+]$ and $c_{1,2}$ are complex coefficients. Then, we must have

$$\lim_{z\to a_+^-}\psi_+(x) = \lim_{z\to a_+^+}\psi_0(x), \qquad \lim_{z\to a_-^+}\psi_-(x) = \lim_{z\to a_-^-}\psi_0(x), \tag{3.18}$$

$$\lim_{z\to a_+^-}\psi'_+(x) = \lim_{z\to a_+^+}\psi_0(x) \qquad \lim_{z\to a_-^+}\psi'_-(x) = \lim_{z\to a_-^-}\psi_0(x), \tag{3.19}$$

Here the superscripts + and − mean that the limit approaches to the limiting point from left and right respectively. Taking (3.16) and (3.17) we can write this conditions in the following form.

$$A_\pm e^{ika_\pm} + B_\pm e^{-ika_\pm} = \psi_1(a_\pm) + \psi_2(a_\pm),$$

$$ikA_\pm e^{ika_\pm} - ikB_\pm e^{-ika_\pm} = \psi'_1(a_\pm) + \psi'_2(a_\pm),$$

which can be written as

$$\begin{bmatrix} e^{ika_\pm} & e^{-ika_\pm} \\ ike^{ika_\pm} & -ike^{-ika_\pm} \end{bmatrix}\begin{bmatrix} A_\pm \\ B_\pm \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ ik & -ik \end{bmatrix} e^{ika_\pm\boldsymbol{\sigma}_3}\begin{bmatrix} A_\pm \\ B_\pm \end{bmatrix} = \begin{bmatrix} \psi_1(a_\pm) & \psi_2(a_\pm) \\ \psi'_1(a_\pm) & \psi'_2(a_\pm) \end{bmatrix}\begin{bmatrix} c_1 \\ c_2 \end{bmatrix}.$$

Here $\boldsymbol{\sigma}_3$ is the third Pauli matrix

$$e^{ika_\pm\boldsymbol{\sigma}_3} := \sum_{n=1}^{\infty}\frac{(ika_\pm\boldsymbol{\sigma}_3)^n}{n!} = \begin{bmatrix} e^{ika_\pm} & 0 \\ 0 & e^{-ika_\pm} \end{bmatrix} \tag{3.20}$$

Define

$$\mathbf{K} := \begin{bmatrix} 1 & 1 \\ ik & -ik \end{bmatrix}, \qquad \mathbf{F}(x) := \begin{bmatrix} \psi_1(x) & \psi_2(x) \\ \psi_1'(x) & \psi_2'(x) \end{bmatrix}. \tag{3.21}$$

Note that we have

$$\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \mathbf{F}^{-1}(a_\pm)\mathbf{K}e^{ika_\pm\boldsymbol{\sigma}_3} \begin{bmatrix} A_\pm \\ B_\pm \end{bmatrix},$$

Here, we note that, $\mathbf{F}(x)$ is invertible for every x, since $det(\mathbf{F}(x)) = W[\psi_1(x), \psi_2(x)]$ is the Wronskian of ψ_1 and ψ_2 which is always nonzero. Then we have

$$\mathbf{F}^{-1}(a_+)\mathbf{K}e^{ika_+\boldsymbol{\sigma}_3} \begin{bmatrix} A_+ \\ B_+ \end{bmatrix} = \mathbf{F}^{-1}(a_-)\mathbf{K}e^{ika_-\boldsymbol{\sigma}_3} \begin{bmatrix} A_- \\ B_- \end{bmatrix}$$

which implies

$$\begin{bmatrix} A_+ \\ B_+ \end{bmatrix} = \mathbf{M} \begin{bmatrix} A_- \\ B_- \end{bmatrix} \tag{3.22}$$

where

$$\mathbf{M} := e^{-ia_+k\boldsymbol{\sigma}_3}\mathbf{K}^{-1}\mathbf{F}(a_+)\mathbf{F}^{-1}(a_-)\mathbf{K}e^{ika_-\boldsymbol{\sigma}_3} \tag{3.23}$$

The matrix $\mathbf{M}$ that satisfies (3.22) is called the transfer matrix. Equation (3.23) agrees with the formula of the transfer matrix given by [33].

Equations (3.6), (3.8) and (3.22) imply

$$\begin{bmatrix} A_+^l \\ 0 \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} A_-^l \\ B_-^l \end{bmatrix}, \qquad \begin{bmatrix} A_+^r \\ B_+^r \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} 0 \\ B_-^r \end{bmatrix}. \tag{3.24}$$

Solving these for the entries M_{ij} of the transfer matrix $\mathbf{M}$ we find

$$\mathbf{M} = \begin{bmatrix} T - \dfrac{R^l R^r}{T} & \dfrac{R^r}{T} \\ -\dfrac{R^l}{T} & \dfrac{1}{T} \end{bmatrix}. \tag{3.25}$$

Notice that the transmission reciprocity and (3.18) implies

$$\det\mathbf{M} = 1. \tag{3.26}$$

We can use (3.7), (3.9) and (3.25) to find the reflection and the transmission amplitudes in terms of the entries of $\mathbf{M}$,

$$R^l = -\frac{M_{21}}{M_{22}}, \qquad R^r = \frac{M_{12}}{M_{22}}, \qquad T = \frac{1}{M_{22}}. \tag{3.27}$$

This shows that finding the transfer matrix is enough to solve the scattering problem.

Another important property of the transfer matrix is its composition property which motivated its definition [34]. Suppose v_1 and v_2 are short range potentials vanishing outside intervals $I_1 = [a_1, a_2]$ and $I_2 = [a_2, a_3]$ such that I_1 and I_2 do not intersect, and I_1 lies the to the right of I_2. Let $v = v_1 + v_2$ and, $\mathbf{M}, \mathbf{M}_1$, and $\mathbf{M}_2$ be transfer matrices for v, v_1 and v_2 respectively. We can find these transfer matrices using (3.23).

$$\begin{aligned}
\mathbf{M} &= e^{-ia_3k\boldsymbol{\sigma}_3}\mathbf{K}^{-1}\mathbf{F}(a_3)\mathbf{F}^{-1}(a_1)\mathbf{K}e^{ika_1\boldsymbol{\sigma}_3},\\
\mathbf{M}_1 &= e^{-ia_2k\boldsymbol{\sigma}_3}\mathbf{K}^{-1}\mathbf{F}(a_2)\mathbf{F}^{-1}(a_1)\mathbf{K}e^{ika_1\boldsymbol{\sigma}_3},\\
\mathbf{M}_2 &= e^{-ia_3k\boldsymbol{\sigma}_3}\mathbf{K}^{-1}\mathbf{F}(a_3)\mathbf{F}^{-1}(a_2)\mathbf{K}e^{ika_2\boldsymbol{\sigma}_3},
\end{aligned}$$

which implies

$$\mathbf{M} = \mathbf{M}_2\mathbf{M}_1. \tag{3.28}$$

Let us repeat the same procedure for the short-range potentials defined as,

$$v_j = \begin{cases} v(x) & \text{for } x \in [a_{j-1}, a_j) \\ 0 & \text{for } x \notin [a_{j-1}, a_j) \end{cases} \tag{3.29}$$

with transfer matrices $\mathbf{M}_j$ for $j \in \{1, 2, \cdots, n\}$ and $a_n > a_{n_1} > \cdots > a_1$. Then the transfer matrix $\mathbf{M}$ for the potential $v = v_1 + v_2 + \cdots + v_n$ can be written as

$$\mathbf{M} = \mathbf{M}_n\mathbf{M}_{n-1}\cdots\mathbf{M}_1. \tag{3.30}$$

The decomposition property can be generalized to potentials with overlapping supports [35].

Scattering Matrix

The scattering matrix or the **S**-matrix for potential v is defined by the relation

$$\begin{bmatrix} A_+ \\ B_- \end{bmatrix} = \mathbf{S} \begin{bmatrix} A_- \\ B_+ \end{bmatrix}. \tag{3.31}$$

Combining equations (3.6), (3.8) and (3.31) we arrive at

$$\begin{bmatrix} A_+^l \\ B_-^l \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} A_-^l \\ 0 \end{bmatrix}, \qquad \begin{bmatrix} A_+^r \\ B_-^r \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} 0 \\ B_+^r \end{bmatrix} \tag{3.32}$$

and solving for the components for **S** and using (3.7), (3.11) and (3,14) we get

$$S_{11} = S_{22} = T, \qquad S_{12} = R^r, \qquad S_{21} = R^l. \tag{3.33}$$

The transfer matrix takes the coefficients of the left side of the potential to the right side, while the S-matrix takes the coefficients of incoming waves to coefficients of outgoing waves.

Comparing (3.27) and (3.33), solving the scattering problem with **S** seems more efficient compared to **M**. However, **S** does not have the composition property that **M** has, which makes it a useful tool for a variety of physical problems including modeling and numerical investigation of optics [36, 37, 38]; condensed matter physics [39, 40, 41] and acoustics [42, 43, 44]. Designing optical potential with interesting properties useful in condensed matter and atomic physics described with transfer matrix approach [45, 46].

3.3 Dynamical formulation of one-dimensional stationary scattering

Similar to the transfer matrix, the evolution operator $U(t, t_0)$ of any Hamiltonian also has the composition property. This relation leads to searching a connection between the evolution operator of a quantum system and the transfer matrix **M** of a short-range potential [26, 27]. Since **M** is a 2×2 matrix the quantum system we are looking for must be a two-level system.

Additionally, for every linear ordinary differential equation of order n, there is an equivalent system of n linear first order equations. The time independent

Schrödinger equation (3.1) is a second order linear differential equation, then we can find a system of two first order linear differential equations that is equivalent to it. This system of equations can be related to the time-dependent Schrödinger equation for a two level quantum system

$$i\partial_x \boldsymbol{\Psi}(x) = \boldsymbol{\mathcal{H}}(x)\boldsymbol{\Psi}(x), \tag{3.34}$$

where x takes the role of time. Here the state vector $\boldsymbol{\Psi}(x)$ is an element of the Hilbert space $\mathscr{H} := \mathbb{C}^2 \otimes \mathcal{H}$ and $\boldsymbol{\mathcal{H}}(x) : \mathscr{H} \to \mathscr{H}$ is a linear operator. Notice that this system of equations is not unique. Since (3.34) is equivalent to (3.1), the components of $\boldsymbol{\Psi}(x)$ must be linear combinations of a solution ψ of (3.1) and its first derivative ψ'. Define

$$\boldsymbol{\Psi}(x) = \begin{bmatrix} f_{11}(x)\psi(x) + f_{12}(x)\psi'(x) \\ f_{21}(x)\psi(x) + f_{22}(x)\psi'(x) \end{bmatrix} \tag{3.35}$$

for some functions f_{ij} for $i, j \in \{1, 2\}$. We have infinitely many choices for these functions. However, there is a choice for these functions that is significant to the motivation mentioned in the beginning of this chapter. We want to set $\mathbf{M} = \boldsymbol{\mathcal{U}}(x_+, x_-)$ for some $x_\pm$, then we must have

$$\boldsymbol{\Psi}(x_+) = \boldsymbol{\mathcal{U}}(x_+, x_-)\boldsymbol{\Psi}(x_-). \tag{3.36}$$

Looking at (3.15) we let $z_\pm = \pm\infty$ and arrive at,

$$\mathbf{M} = \boldsymbol{\mathcal{U}}(\infty, -\infty) = \lim_{x_\pm \to \pm\infty} \boldsymbol{\mathcal{U}}(x_+, x_-) \tag{3.37}$$

then the wavevector must satisfy the following.

$$\lim_{x\to\pm\infty} \boldsymbol{\Psi}(x) = \begin{bmatrix} A_\pm \\ B_\pm \end{bmatrix}. \tag{3.38}$$

If we enforce (3.38) on (3.35) and use the boundary condition (3.3), we arrive at

$$\lim_{x\to\pm\infty} \boldsymbol{\Psi}(x) = \begin{bmatrix} f_{11}(x)(A_\pm e^{ikx} + B_\pm e^{-ikx}) + ikf_{12}(x)(A_\pm e^{ikx} - B_\pm e^{-ikx}) \\ f_{21}(x)(A_\pm e^{ikx} + B_\pm e^{-ikx}) + ikf_{22}(x)(A_\pm e^{ikx} - B_\pm e^{-ikx}) \end{bmatrix} = \begin{bmatrix} A_\pm \\ B_\pm \end{bmatrix}$$

Rearranging this we get,

$$\lim_{x\to\pm\infty} \{A_\pm(f_{11} + ikf_{12})e^{ikx} + B_\pm(f_{11} - ikf_{12})e^{-ikx}\} = A_\pm,$$

and

$$\lim_{x\to\pm\infty}\{A_\pm(f_{21}+ikf_{22})e^{ikx}+B_\pm(f_{21}-ikf_{22})e^{-ikx}\}=B_\pm.$$

The coefficients of $A_\pm$ and $B_\pm$ in these equations must be equal.

$$f_{11}+ikf_{12}=e^{-ikx}, \qquad f_{11}-ikf_{12}=0,$$
$$f_{21}(x)+ikf_{22}=0, \qquad f_{21}-ikf_{22}=e^{ikx}.$$

There are unique functions that can satisfy these equations,

$$f_{11}=\frac{1}{2}e^{-ikx}, \qquad f_{12}=-\frac{i}{2k}e^{-ikx},$$
$$f_{21}=\frac{1}{2}e^{ikx} \qquad f_{22}=-\frac{i}{2k}e^{ikx}.$$

Then we can write equation (3.35) as,

$$\mathbf{\Psi}(x)=\frac{1}{2}e^{-ikx\boldsymbol{\sigma}_3}\begin{bmatrix}\psi(x)-ik^{-1}\psi'(x)\\ \psi(x)+ik^{-1}\psi'(x)\end{bmatrix} \tag{3.39}$$

where

$$\boldsymbol{\sigma}_3=\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} \tag{3.40}$$

is the third Pauli matrix, and

$$\begin{aligned} e^{-ikx\boldsymbol{\sigma}_3}:&=\sum_{n=1}^{\infty}(-ikx)^n\boldsymbol{\sigma}_3^n=\sum_{n=1}^{\infty}(-1)^n(kx)^{2n}\mathbf{I}+i\sum_{n=1}^{\infty}(-1)^n(kx)^{2n+1}\boldsymbol{\sigma}_3\\ &=\begin{bmatrix}e^{-ikx} & 0\\ 0 & e^{ikx}\end{bmatrix}\end{aligned} \tag{3.41}$$

We find the left-hand side of equation (3.34) becomes by differentiating (3.39) with respect to x and find

$$i\partial_x\mathbf{\Psi}(x)=-i\frac{v(x)\psi(x)}{2k}e^{-ikx\boldsymbol{\sigma}_3}\begin{bmatrix}1\\ -1\end{bmatrix} \tag{3.42}$$

where we used (3.1). We can find $\boldsymbol{\mathcal{H}}(x)$ by inserting (3.39) and (3.42) into (3.34).

$$\boldsymbol{\mathcal{H}}(x)=\frac{v(x)}{2k}e^{-ikx\boldsymbol{\sigma}_3}\boldsymbol{\mathcal{K}}e^{-ikx\boldsymbol{\sigma}_3} \tag{3.43}$$

where

$$\boldsymbol{\mathcal{K}} = \begin{bmatrix} 1 & 1 \\ -1 & -1 \end{bmatrix}. \tag{3.44}$$

If we identify $\boldsymbol{\mathcal{U}}(x, x_0)$ with the evolution operator for the system in the interaction picture, (3.29) implies $\mathbf{M}$ is the S-matrix of the of the quantum system described with the Hamiltonian $\boldsymbol{\mathcal{H}}(x)$ [47].

We let $\boldsymbol{\mathcal{H}}(x)$ be the interaction picture Hamiltonian, then (3.43) gives us the free Hamiltonian,

$$\mathbf{H}_0 = -k\boldsymbol{\sigma}_3. \tag{3.45}$$

and the interaction Hamiltonian

$$\mathbf{H}_1 = \frac{v(x)}{2k}\boldsymbol{\mathcal{K}} \tag{3.46}$$

Then the Schrödinger picture state vector and Hamiltonian are

$$\boldsymbol{\Phi}(x) = \frac{1}{2}\begin{bmatrix} \psi(x) - ik^{-1}\psi'(x) \\ \psi(x) + ik^{-1}\psi'(x) \end{bmatrix}, \tag{3.47}$$

$$\mathbf{H}(x) = \frac{v(x)}{2k}\boldsymbol{\mathcal{K}} - k\boldsymbol{\sigma}_3 = \frac{1}{2k}\begin{bmatrix} v(x) - 2k^2 & v(x) \\ -v(x) & -v(x) + 2k^2 \end{bmatrix}. \tag{3.48}$$

Notice that if $v(x)$ is a real-valued function both $\boldsymbol{\mathcal{H}}(x)$ and $\mathbf{H}(x)$ are $\boldsymbol{\sigma}_3$-pseudo Hermitian. The advantage of $\mathbf{H}(x)$ over $\boldsymbol{\mathcal{H}}(x)$ is the fact that the former is diagonalizable and has a biorthonormal system.

Next we use the result of Appendix A to show that

$$\mathbf{M} = \boldsymbol{\mathcal{U}}(+\infty, -\infty) = \lim_{x_\pm \to \pm\infty} e^{-ikx_+\boldsymbol{\sigma}_3}\mathbf{U}(x_+, x_-)e^{-ikx_-\boldsymbol{\sigma}_3}, \tag{3.49}$$

where we let $x = 0$. In particular, for a finite range potential with support $[a_-, a_+]$ we have

$$\begin{aligned} \mathbf{M} &= \boldsymbol{\mathcal{U}}(+\infty, -\infty) = \boldsymbol{\mathcal{U}}(\infty, a_+)\boldsymbol{\mathcal{U}}(a_+, a_-)\boldsymbol{\mathcal{U}}(a_-, -\infty) \\ &= \boldsymbol{\mathcal{U}}(a_+, a_-) = e^{-ika_+\boldsymbol{\sigma}_3}\mathbf{U}(a_+, a_-)e^{-ika_-\boldsymbol{\sigma}_3}. \end{aligned} \tag{3.50}$$

where we used (3.48) to show if $x \notin [a_-, a_+]$

$$\boldsymbol{\mathcal{H}}(x) = 0, \qquad \boldsymbol{\mathcal{U}}(x, x_0) = \mathbf{I}. \tag{3.51}$$

Chapter 4

DYNAMICAL FORMULATION OF STATIONARY SCATTERING IN HIGHER DIMENSIONS

We discussed the significant role of the transfer matrix and its composition property in the previous chapter, however their applications are limited to one-dimensional scattering problems. The usual higher dimensional generalization of the transfer matrix involves discretization of the momentum or configuration space that is normal to the scattering axis. These transfer matrices are large numerical matrices and require numerical treatments. Refs. [24],[25], give a different higher-dimensional generalization of transfer matrix that do not require discretization. In fact, instead of complex numbers like its one-dimensional counterpart, this definition of the transfer matrix gives a linear operator acting on an infinite-dimensional function space. In addition, these references generalize the dynamical formulation of stationary scattering to higher dimensions by relating the transfer matrix to the time-evolution of an effective quantum system. Moreover, this transfer matrix shares the composition property of the one-dimensional transfer matrix. The first half of this chapter explains some of the results found in these papers for d-dimensional cases.

Generally, the standard approach to two- and three-dimensional scattering assumes that the scattering potential vanishes at spatial infinities. However with the DFSS in higher dimensions, it is possible to solve the scattering problem for potentials that are nonzero in an infinitely extended region of space. The authors of [23] use DFSS to study the scattering properties of this kind of potential in two-dimensions. In particular, they derive an explicit form of the transfer matrix for two-dimensional potentials that are short range along the scattering axis but get infinitely strong as its gets away from the origin along normal directions to this axis. In the remainder of the chapter, we derive the transfer matrix for this kind of potentials in d-dimensions.

In both dimensions, the scattering axis is the z-axis, the source of the incident wave and the detector are placed on the planes $z = \pm\infty$.

4.1 Basic setup for stationary scattering in d-dimensions

First, focus on two dimensional stationary scattering. We define the polar coordinates of our system as

$$r := \sqrt{x^2 + z^2}. \qquad \theta = \arctan x/z,$$

where $\theta \in [-\pi/2, 3\pi/2]$. The two-dimensional time-independent Schödinger equation for a short-range potential $v : \mathbb{R}^2 \to \mathbb{C}$ and a wavenumber $k \in \mathbb{R}^+$ has the form

$$-\partial_x^2\psi(x,z) - \partial_z^2\psi(x,z) + v(x,z)\psi(z) = k^2\psi(x,z), \tag{4.1}$$

A potential is said to be short-range if it satisfies

$$r|v| \to 0 \text{ as } r \to \infty. \tag{4.2}$$

There is a unique solution of this equation that satisfies the following asymptotic boundary equation.

$$\psi(\vec{r}) \to e^{i\boldsymbol{k}_0\vec{r}} + \sqrt{\frac{i}{kr}}f(\theta)\frac{e^{ikr}}{r} \quad \text{for} \quad r \to \infty, \tag{4.3}$$

Here, the term $e^{i\vec{k}_0\vec{r}}$ is the incident plane wave, $\vec{k}_0 = k(\cos\theta_0\hat{e}_z + \sin\theta_0\hat{e}_x) \in \mathbb{R}^2$ is the incident wavevector, and θ_0 is the incidence angle. The second term which involves e^{ikr}/r is the scattered spherical wave and the function $f(\theta)$ is the scattering amplitude. Solving the scattering problem is equivalent to find the scattering amplitude for each wavenumber k and incident angle θ_0.

Now, consider a potential whose support lies $z = a_\pm$ for some real number $a_+ > a_-$, i.e.,

$$v(x,z) = 0 \text{ for } z \notin [a_-, a_+]. \tag{4.4}$$

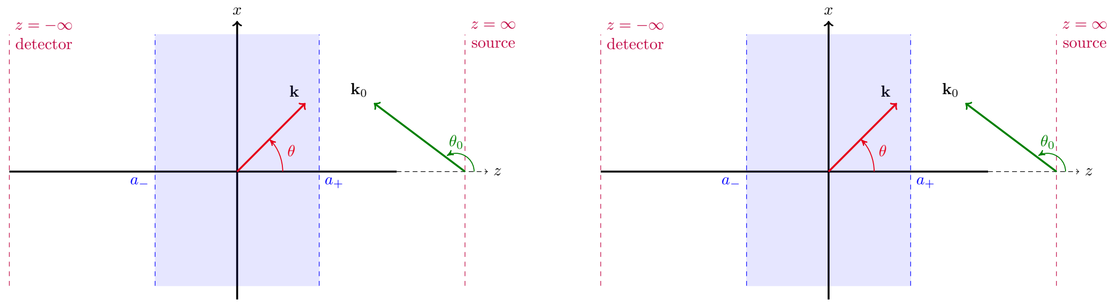

Figure 4.1: Schematic view of scattering of left-and right-incident waves. The figure on the right is a right-incident wave with incidence angle $\theta \in (\pi/2, 3\pi/2)$. The left figure represents a left-incident wave with the incidence angle $\theta \in (-\pi/2, \pi/2)$. In both figures the support of the potential lies between the lines $z = a_-$ and $z = a_+$.

There is ,however, no restriction on the value of the potential in the region bounded by the lines. The solution of (4.1) for this equation satisfies the asymptotic boundary condition (4.3), except in the vicinity of the x-axis, that is when $\theta = \pm\pi/2$.

Consider the case where the source is located at $z = -\infty$, then the $\theta_0 \in (-\pi/2, \pi/2)$, and we call it a left-incident wave. Similarly, if the source of the wave is located at $z = \infty$, $\theta_0 \in (\pi/2, 3\pi/2)$, and we have a right-incident wave. Let $f^l(\theta)$ and $f^r(\theta)$ be the scattering amplitudes for left- and right-incident waves respectively. In the following we use superscripts l/r to label the scattering amplitudes of the left and right incident waves respectively. Then

$$f(\theta) = \begin{cases} f^l(\theta) & \text{for } \theta_0 \in (-\pi/2, \pi/2), \\ f^r(\theta) & \text{for } \theta_0 \in (\pi/2, 3\pi/2). \end{cases} \tag{4.5}$$

Now, consider the three-dimensional case, where we use the spherical coordinates defined as follows

$$r := \sqrt{x^2 + y^2 + z^2}, \qquad \theta := \arccos\left(z/\sqrt{x^2 + y^2}\right), \qquad \varphi := \arctan\left(x/y\right).$$

where $\theta \in [0, \pi]$ and $\varphi \in [0, 2\pi)$. The solution of the stationary time-independent Schrödinger equation in three dimensions

$$-(\partial_x^2 + \partial_x^2 + \partial_x^2)\psi(x, y, z) + v(x, y, z)\psi(x, y, z) = k^2\psi(x, y, z) \tag{4.6}$$

where $v(x, y, z) : \mathbb{R}^3 \to \mathbb{C}$ is a short range potential, satisfies the following boundary condition

$$\psi(\mathbf{r}) \to e^{i\boldsymbol{k}_0\vec{r}} + f(\theta, \varphi)\frac{e^{ikr}}{r} \quad \text{for} \quad r \to \infty. \tag{4.7}$$

Here $e^{i\vec{k}_0\boldsymbol{r}}$ is the incident plane wave and $\vec{k}_0 \in \mathbb{R}^+$ is the incident wave vector, which is defined as $\vec{k}_0 \in \mathbb{R}^3 = k(\sin\theta_0 \cos\varphi_0, \sin\theta_0 \sin\varphi_0, \cos\theta_0)$ where θ_0 and φ_0 are incidence angles. The term $f(\theta, \varphi)e^{ikr}/r$ is the scattered spherical wave and $f(\theta, \varphi)$ is the scattering amplitude.

For a potential that is supported between the planes $z = \pm a_\pm$, need not to vanish along the x- and y-axes. In this case the solutions of (4.6) satisfies (4.7) when $\theta \neq \pi/2$.

If the incident wave is located at the plane $z = -\infty$ we name it a left-incident wave. In this case the incidence angle θ_0 ranges over $[0, \frac{\pi}{2})$. Similarly for a right-incident wave $\theta_0 \in (\frac{\pi}{2}, \pi]$, and we have

$$f(\theta, \varphi) = \begin{cases} f^l(\theta, \varphi) \text{ for } \theta_0 \in (0, \frac{\pi}{2}], \\ f^r(\theta, \varphi) \text{ for } \theta_0 \in (\frac{\pi}{2}, \pi]. \end{cases} \tag{4.8}$$

We aim to express both two and three dimensional cases in the same expressions. Let $d \in \{2, 3\}$ be the dimension of the space. d-dimensional vectors are denoted by bold symbols and $(d - 1)$ dimensional vectors are denoted with symbols with arrows on them. Let $\hat{e}_j$ be the unit vector along the j-axis for $j \in \{x, y, z\}$. Let $\boldsymbol{r} := (\vec{r}, z) \in \mathbb{R}^d$ where, $\boldsymbol{r}$ is a $(d - 1)$ dimensional vector defined as

$$\vec{r} := \begin{cases} x & \text{for } d = 2, \\ (x, y) & \text{for } d = 3. \end{cases}$$

Let $\hat{r} := \vec{r}/r$, where r is the norm of the vector $\vec{r}$. Define the angle θ as the angle $\theta = \arccos z/|\vec{r}|$ in the respective ranges for each d. For $d = 3$, define $\phi :=$ $\arctan{(y/x)} \in [0, 2\pi)$. Let

$$\hat{\boldsymbol{\Omega}} := \begin{cases} \theta & \text{for } d = 2, \\ (\theta, \phi) & \text{for } d = 3. \end{cases} \tag{4.9}$$

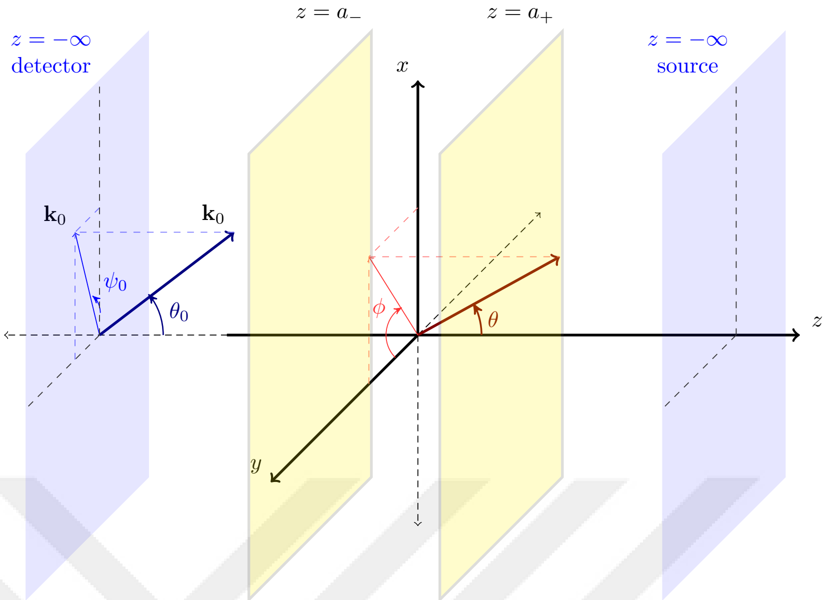

Figure 4.2: Schematic view of scattering of left-incident wave. The incidence angle $\theta \in (0, \pi/2]$. The support of the potential lies between the surfaces $z = a_-$ and $z = a_+$.

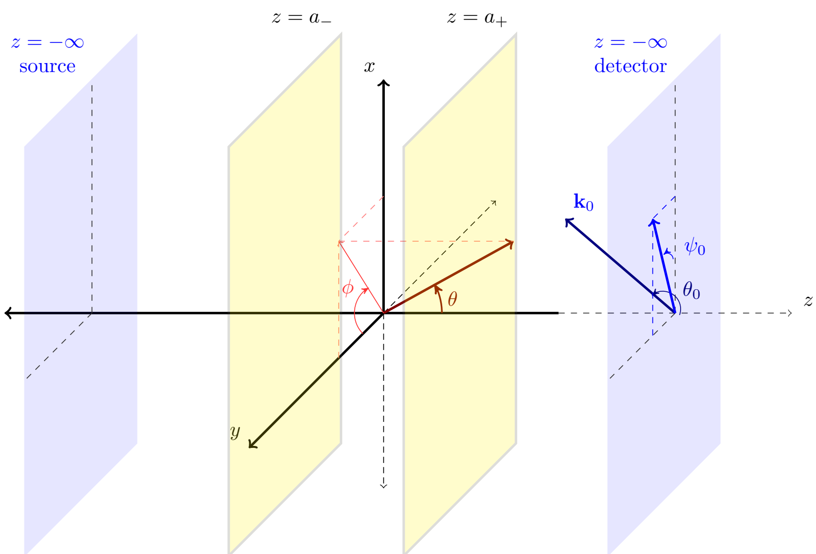

Figure 4.3: Schematic view of scattering of right-incident wave. The incidence angle $\theta \in (\pi/2, \pi]$. The support of the potential lies between the surfaces $z = a_-$ and $z = a_+$.

With this notation the time dependent Schrödinger equations (4.1) and (4.5) can be written as

$$\big(-\nabla_{d-1}^2 - \partial_z^2 + v(\vec{r}, z)\big)\psi(\vec{r}, z) = k^2\psi(\vec{r}, z), \tag{4.10}$$

where ∇_{d-1}^2 is the $(d-1)$ dimensional Laplacian. Consider a potential that is supported between $z = a_\pm$, i.e,

$$v(\vec{r}, z) = 0 \text{ for } z \notin [a_-, a_+]. \tag{4.11}$$

The solutions of (4.10) for this choice of potential have the following asymtotic boundary condition.

$$\psi(\vec{r}) \to \frac{1}{(2\pi)^{3-d}}\left[e^{i\vec{k}_0\cdot\vec{r}} + \left(\frac{i}{k}\right)^{\frac{3-d}{2}} f(\hat{\mathbf{\Omega}})\frac{e^{ikr}}{r^{\frac{d-1}{2}}}\right] \text{ as } r \to \infty. \tag{4.12}$$

The term $\psi_{incident}(\vec{r}) := e^{i\vec{k}_0\cdot\vec{r}}$, is the incident plane wave that travels towards the potential. The incident wave vector $\vec{k}_0 = k\big(\cos\theta_0, \sin\theta_0\hat{r}\big)$, where $\hat{r}$ is the unit vector in the direction of $\vec{r}$. The second term is the scattered wave,

$$\psi_{scattered}(\vec{r}) := \big(ik^{-1}\big)^{3-d} f(\hat{\mathbf{\Omega}})\frac{e^{ikr}}{r^{\frac{d-1}{2}}} \text{ as } r \to \infty.$$

where the complex valued function $f(\hat{\mathbf{\Omega}})$ is the scattering amplitude. Solving the scattering problem for a given potential is to determine f for every incident wave vector $\vec{k}_0$.

The conditions for θ_0 we discussed above for a left- and right-incident waves is equivalent to $\cos\theta > 0$ and $\cos\theta < 0$ respectively. Again we use the terms f^l and f^r to label scattering amplitude for right- and left-incident waves,

$$f(\hat{\mathbf{\Omega}}) = \begin{cases} f^l(\hat{\mathbf{\Omega}}) & \text{for } \cos\theta_0 > 0, \\ f^r(\hat{\mathbf{\Omega}}) & \text{for } \cos\theta_0 < 0. \end{cases} \tag{4.13}$$

Let the Fourier transformation and its inverse be defined by,

$$\mathcal{F}_{\vec{r},\vec{p}}\{f(\vec{r})\} := \tilde{f}(\vec{p}) := \int_{\mathbb{R}^{d-1}} d\vec{r} e^{-i\vec{p}\cdot\vec{r}} f(\vec{r}), \tag{4.14}$$

$$\mathcal{F}_{\vec{r},\vec{p}}^{-1}\{g(\vec{p})\} := \tilde{g}(\vec{r}) := \frac{1}{(2\pi)^{d-1}}\int_{\mathbb{R}^{d-1}} d\vec{r}\, e^{i\vec{p}\cdot\vec{r}} g(\vec{p}), \tag{4.15}$$

where $f, g : \mathbb{R}^{d-1} \to \mathbb{C}$ are functions. Equation (4.10) is a second degree partial differential equation. Taking its Fourier transform with respect to $\vec{r}$ we arrive a the following second order ordinary differential equation

$$-\tilde{\psi}''(\vec{p}, z) + \big(\widehat{\mathscr{V}}\tilde{\psi}\big)(\vec{p}, z) = \varpi^2(\vec{p})\tilde{\psi}(\vec{p}, z), \tag{4.16}$$

where

$$\tilde{\psi}(\vec{p}, z) := \mathcal{F}_{\vec{r},\vec{p}}\{\psi(\vec{r}, z)\}, \tag{4.17}$$

$$\big(\widehat{\mathscr{V}}\tilde{\psi}\big)(\vec{p}, z) := \mathcal{F}_{\vec{r},\vec{p}}\{v(\vec{r}, z), \psi(\vec{r}, z)\} = (2\pi)^{d-1} \int_{\mathbb{R}^{d-1}} d\vec{q}\tilde{v}(\vec{p} - \vec{q}, z)\tilde{\psi}(\vec{p}, z) \tag{4.18}$$

and

$$\varpi(\vec{p}) := \begin{cases} \sqrt{k^2 - p^2} & \text{for } p < k, \\ i\sqrt{p^2 - k^2} & \text{for } p \geq k. \end{cases} \tag{4.19}$$

where $p := |\vec{p}|$.

Since the potential is supported between the planes $z = a_+$ and $z = a_-$, $\big(\widehat{\mathscr{V}}\tilde{\psi}\big)$ vanishes outside the support of the potential and (4.16) becomes

$$\tilde{\psi}''(\vec{p}, z) + \varpi(\vec{p})^2\tilde{\psi}(\vec{p}, z) = 0 \text{ for } z \notin [a-, a_+]. \tag{4.20}$$

It is easy to see that the bounded solution of this equation has the form

$$\tilde{\psi}(\vec{p}, z) = \varpi^{-1} \times \begin{cases} A_\pm(\vec{p})e^{i\varpi(\vec{p})z} + B_\pm(\vec{p})e^{-i\varpi(\vec{p})z}, & \text{for } \pm z \geq a_\pm \text{ and } k > |\vec{p}|, \\ C_\pm(\vec{p})e^{\mp\varpi(\vec{p})z} & \text{for } \pm z \geq a_\pm \text{ and } k \leq |\vec{p}|, \end{cases} \tag{4.21}$$

where $A_\pm, B_\pm, C_\pm \in \mathcal{F}$, where we define $\mathcal{F}$ as the set of complex valued generalized functions of $d-1$ real variables. Without loss of generality we set $A_\pm, B_\pm = 0$ for $p < k$ and $C_\pm = 0$ for $p \geq k$. Here the factor ϖ^{-1} to ensure that the coefficient functions $A_\pm, B_\pm, C_\pm$ are dimensionless. Note that there is no term of the form $e^{\pm\varpi(\boldsymbol{p})z}$ for $\pm z \geq a_\pm$, since, otherwise we would have $||\psi(\vec{p}, z)|| = ||\psi(\vec{r}, z)|| \to \infty$ as $z \to \infty$, which contradicts with the the boundedness of the solutions. We can recover the solution of (4.10) by taking the inverse Fourier transform of (4.21). This gives

$$\psi(\vec{r}, z) = \psi^\pm_{os}(\vec{r}, z) + \psi^\pm_{ev}(\vec{r}, z) \text{ for } \pm z > \pm a_\pm \tag{4.22}$$

where

$$\psi_{os}^{\pm}(\vec{r},z) = \int_{\mathcal{D}_k} \frac{d\vec{p}}{(2\pi)^{d-1}\varpi(\vec{p})}\left[A_{\pm}(\vec{p})e^{i\varpi(\vec{p})z} + B_{\pm}(\vec{p})e^{-i\varpi(\vec{p})z}\right]e^{-i\vec{r}\cdot\vec{p}}, \tag{4.23}$$

$$\psi_{ev}^{\pm}(\vec{r},z) = \int_{\mathbb{R}^{d-1}\setminus\mathcal{D}_k} \frac{d\vec{p}}{(2\pi)^{d-1}\varpi(\boldsymbol{p})}C_{\pm}(\vec{p})e^{\mp\varpi(\vec{p})z}e^{-i\vec{r}\cdot\vec{p}}, \tag{4.24}$$

where $\mathcal{D}_k := \{\vec{p} \in \mathbb{R}^{(d-1)} | |\vec{p}| \leq k\}$. The part of the solution (4.32) that is labeled as ψ_{os} and defined by (4.33) describes the oscillating part of the solution. The other part is the evanescent wave and it satisfies $|\psi_{ev}^{\pm}| \to 0$ as $z \to \pm\infty$ which implies

$$\psi \to \psi_{os}^{\pm} \text{ as } z \to \pm\infty. \tag{4.25}$$

Define

$$(\widehat{\Pi}_k\phi)(p) := \begin{cases} \phi(\vec{p}) & \text{for } |\vec{p}| < k, \\ 0 & \text{for } |\vec{p}| \geq k. \end{cases} \tag{4.26}$$

Notice that we have $\widehat{\Pi}_k^2 = \widehat{\Pi}_k$, which indicates that this is a projection operator and its range is $\mathcal{F}_k := \{\psi \in \mathcal{F} | \psi(\vec{p}) = 0 \text{ for } k < |\vec{p}|\}$. To simplify the expression (4.23) we define

$$\mathscr{A}_+ = A_+ + C_+, \qquad \mathscr{B}_- = B_- + C_-. \tag{4.27}$$

Notice that,

$$\hat{\Pi}_k\mathscr{A}_+ = A_+, \qquad \hat{\Pi}_k\mathscr{B}_- = B_-. \tag{4.28}$$

Then (4.21) can be written as

$$\tilde{\psi}(\vec{p},z) = \varpi^{-1}\begin{cases} A_- e^{i\varpi(\vec{p})z} + \mathscr{B}_- e^{-i\varpi(\vec{p})z}, & \text{for } z < a_-, \\ \mathscr{A}_+ e^{i\varpi(\vec{p})z} + B_+ e^{-i\varpi(\vec{p})z} & \text{for } z > a_+, \end{cases} \tag{4.29}$$

and we can get the solution to the Schrödinger equation outside the range of the potential by calculating the Fourier transform (4.29) and get

$$\psi(\vec{r},z) = \begin{cases} \int_{\mathbb{R}^{d-1}} \frac{d\vec{p}}{(2\pi)^{d-1}\varpi(\vec{p})} \; [A_-(\vec{p})e^{i\varpi(p)z} + \mathscr{B}_-(\vec{p})e^{-i\varpi(\vec{p})z}]e^{i\vec{p}\cdot\vec{r}} & \text{for } z < a_-, \\ \int_{\mathbb{R}^{d-1}} \frac{d\vec{p}}{(2\pi)^{d-1}\varpi(\vec{p})} \; [\mathscr{A}_+(\vec{p})e^{i\varpi(\vec{p})z} + B_+(\vec{p})e^{-i\varpi(\vec{p})z}]e^{i\vec{p}\cdot\vec{r}} & \text{for } z \geq a_+. \end{cases}$$

(4.30)

Now, we combine the two boundary conditions (4.25) and (4.30) using [[35],Appendix A] and [[35],Appendix B]. Following the example of the one-dimensional case we use the superscripts l/r to distinguish between left- and right-incident waves.

For a left-incident wave we have

$$B^l_+ = 0, \qquad A^l_- = (2\pi)^{d-1}\varpi(\vec{p}_0)\delta_{\vec{p}_0}. \tag{4.31}$$

Then the scattering function becomes

$$f^l(\hat{\vec{\Omega}}) = -\frac{i}{(2\pi)^{\frac{d-1}{2}}} \times \begin{cases} A^l_+(\vec{p}) - (2\pi)^{d-1}\varpi(\vec{p}_0)\delta(\vec{p}-\vec{p}_0) & \text{for } \cos\theta > 0, \\ B^l_-(\vec{p}) & \text{for } \cos\theta < 0. \end{cases} \tag{4.32}$$

For a right incident wave we must have

$$A^r_- = 0, \qquad B^r_+ = (2\pi)^{d-1}\varpi(\vec{p}_0)\delta_{\vec{p}_0} \tag{4.33}$$

and we get

$$f^r(\hat{\vec{\Omega}}) = -\frac{i}{(2\pi)^{\frac{d-1}{2}}} \times \begin{cases} A^r_+(\vec{p}) & \text{for } \cos\theta > 0, \\ B^r_-(\vec{p}) - (2\pi)^{d-1}\varpi(\vec{p})\delta(\vec{p}-\vec{p}_0) & \text{for } \cos\theta < 0. \end{cases} \tag{4.34}$$

where

$$\vec{p}_0 = \vec{k}_0 \sin\theta_0, \qquad \vec{p} = k\sin\theta\hat{\vec{r}}. \tag{4.35}$$

Note that, (4.19) and (4.35) implies

$$\varpi(\vec{p}_0) = k|\cos\theta_0|. \tag{4.36}$$

We also define the reflection and transmission coefficients as

$$R^l(\vec{p}) := -\frac{i}{(2\pi)^{\frac{d-1}{2}}}B^l_-(\vec{p}), \qquad T^l(\vec{p}) := -\frac{i}{(2\pi)^{\frac{d-1}{2}}}A^l_+(\boldsymbol{p}), \tag{4.37}$$

$$R^r(\vec{p}) := -\frac{i}{(2\pi)^{\frac{d-1}{2}}}A^r_+(\vec{p}), \qquad T^r(\vec{p}) := -\frac{i}{(2\pi)^{\frac{d-1}{2}}}B^r_-(\vec{p}). \tag{4.38}$$

4.2 Transfer matrix in higher dimensions

In analogy with one dimension, we define the transfer matrix $\widehat{\mathbf{M}}$ by,

$$\begin{bmatrix} A_+ \\ B_+ \end{bmatrix} = \widehat{\mathbf{M}} \begin{bmatrix} A_- \\ B_- \end{bmatrix} \tag{4.39}$$

$$M_{ij} : \mathcal{F}_k \to \mathcal{F}_k,$$
$$\widehat{\mathbf{M}} : \mathbb{C}^{2\times 1} \otimes \mathcal{F}_k \to \mathbb{C}^{2\times 1} \otimes \mathcal{F}_k$$

Here the entries of the transfer matrix are not complex numbers like its one-dimensional counterpart, but are operators acting on $\mathcal{F}_k$. Similarly, we define the scattering matrix $\widehat{\mathbf{S}}$ as the 2×2 matrix with operator entries that satisfy

$$\widehat{\mathbf{S}} \begin{bmatrix} A_- \\ B_+ \end{bmatrix} = \begin{bmatrix} A_+ \\ B_- \end{bmatrix}. \tag{4.40}$$

Applying (4.31) and (4.33) to (4.39) we get

$$\widehat{\mathbf{M}} \begin{bmatrix} (2\pi)^{d-1}\varpi(\vec{p}_0)\delta_{\vec{p}_0} \\ B_-^l \end{bmatrix} = \begin{bmatrix} A_+^l \\ 0 \end{bmatrix}, \qquad \widehat{\mathbf{M}} \begin{bmatrix} 0 \\ B_-^l \end{bmatrix} = \begin{bmatrix} A_+^l \\ (2\pi)^{d-1}\varpi(\vec{p}_0)\delta_{\vec{p}_0} \end{bmatrix},$$

which is equivalent to

$$(2\pi)^{d-1}\widehat{M}_{11}\varpi(\vec{p}_0)\delta_{\vec{p}_0} + \widehat{M}_{12}B_-^l = A_-^l,$$
$$(2\pi)^{d-1}\widehat{M}_{21}\varpi(\vec{p}_0)\delta_{\vec{p}_0} + \widehat{M}_{22}B_-^l = 0,$$
$$\widehat{M}_{12}B_-^r = A_+^r,$$
$$\widehat{M}_{22}B_-^r = (2\pi)^{d-1}\varpi(\vec{p}_0)\delta_{\vec{p}_0}.$$

Solving these we arrive at

$$B_-^l = -(2\pi)^{d-1}\varpi(\vec{p}_0)\widehat{M}_{22}^{-1}\widehat{M}_{11}\delta_{\vec{p}_0}, \tag{4.41}$$
$$A_+^l = (2\pi)^{d-1}\varpi(\vec{p}_0)\big(\widehat{M}_{11} - \widehat{M}_{12}\widehat{M}_{22}^{-1}\widehat{M}_{11}\big)\delta_{\vec{p}_0}, \tag{4.42}$$
$$B_-^r = (2\pi)^{d-1}\varpi(\vec{p}_0)\widehat{M}_{22}^{-1}\delta_{\vec{p}_0}, \tag{4.43}$$
$$A_+^r = (2\pi)^{d-1}\varpi(\vec{p}_0)\widehat{M}_{12}\widehat{M}_{22}^{-1}\delta_{\vec{p}_0}, \tag{4.44}$$

where

$$(\widehat{M}_{ij}\delta_{\vec{p}_0})(\vec{p}) = \langle\vec{p}|\widehat{M}_{ij}|\vec{p}_0\rangle \text{ for } i,j \in 1,2, \qquad \delta_{\vec{p}_0} := \delta_{\vec{p}-\vec{p}_0} \tag{4.45}$$

We can find the scattering amplitude $f^{l/r}(\hat{\Omega})$ by inserting (4.41) and (4.42) to (4.32), and (4,43) and (4,44) to (4,34). This means that, the scattering problem can be solved with the transfer matrix. Similarly for the scattering matrix we get

$$\widehat{\mathbf{S}}\begin{bmatrix}(2\pi)^{d-1}\varpi(\vec{p}_0)\delta_{\vec{p}_0}\\ 0\end{bmatrix} = \begin{bmatrix}A_+^l\\ B_-^l\end{bmatrix}. \qquad \widehat{\mathbf{S}}\begin{bmatrix}0\\ (2\pi)^{d-1}\varpi(\vec{p}_0)\end{bmatrix} = \begin{bmatrix}A_+^r\\ B_-^r\end{bmatrix}.$$

which imply

$$(2\pi)^{d-1}\varpi(\vec{p}_0)\widehat{\mathbf{S}}\delta_{\vec{p}_0} = \begin{bmatrix}A_+^l & A_+^r\\ B_-^l & B_-^r\end{bmatrix}. \tag{4.46}$$

where

$$(\widehat{S}_{ij}\delta_{\vec{p}_0})(\vec{p}) = \langle\vec{p}|\widehat{S}_{ij}|\vec{p}_0\rangle \text{ for } i,j \in 1,2. \tag{4.47}$$

Again, we can insert the entries of $\widehat{\mathbf{S}}$ to (4,40)-(4,43) to (4.32) and (4.34) to solve the scattering problem.

4.3 Dynamical Formulation of Higher Dimensional Stationary Scattering

Following the example of dynamical formulation of one-dimensional stationary scattering , we seek to relate the transfer matrix for a given potential v to the time-evolution operator of an effective quantum system. In order to achieve this, we follow the steps of the previous chapter for equation (4.16). Since this is a second order ordinary differential equation of second order , we can find a system of two first order ordinary differential equations that is equivalent to (4.16). Which can be described by the time-dependent Scrödinger equation of a two-level system,

$$i\partial_z\mathbf{\Psi}(z) = \widehat{\boldsymbol{\mathcal{H}}}\mathbf{\Psi}(z), \tag{4.48}$$

where z plays the role of time and $\mathbf{\Psi}(z) : \mathbb{R}^{d-2} \to \mathbb{C}$. Following the example of the previous chapter we define,

$$(\mathbf{\Psi}(z))(\vec{p}) = \frac{1}{2} e^{-i\varpi(\vec{p})z\boldsymbol{\sigma}_3} \begin{bmatrix} \varpi(\vec{p})\tilde{\psi}(\vec{p},z) - i\tilde{\psi}'(\vec{p},z) \\ \varpi(\vec{p})\tilde{\psi}(\vec{p},z) + i\tilde{\psi}'(\vec{p},z) \end{bmatrix}, \tag{4.49}$$

where $\tilde{\psi}'(\vec{p},z) = \partial_z \tilde{\psi}(\vec{p},z)$. The left-hand side of (4.48) is given by

$$i\partial_z \mathbf{\Psi}(z) = \frac{1}{2} e^{-i\varpi(\vec{p})z\boldsymbol{\sigma}_3} \begin{bmatrix} \widehat{\mathscr{V}}\tilde{\psi} \\ -\widehat{\mathscr{V}}\tilde{\psi} \end{bmatrix},$$

where we used (4.16). Inserting this and (4.49) to equation (4.48) we find

$$\widehat{\boldsymbol{\mathcal{H}}}(z) = \frac{1}{2} e^{-i\varpi(\vec{p})z\boldsymbol{\sigma}_3} \widehat{\mathscr{V}}(\vec{p},z)\widehat{\varpi}^{-1}(\vec{p})\boldsymbol{\mathcal{K}} e^{-i\varpi(\vec{p})z\boldsymbol{\sigma}_3}, \tag{4.50}$$

where $\boldsymbol{\mathcal{K}}$ is given by (3.44) and

$$\widehat{\varpi} := \varpi(\hat{\vec{p}}, z) = \int_{\mathbb{R}^{(d-1)}} d\vec{p}\varpi(\vec{p})|\vec{p}\rangle\langle\vec{p}|. \tag{4.51}$$

Notice that (4.29) and (4.49) imply

$$(\mathbf{\Psi}(z))(\vec{p}) = \begin{bmatrix} A_-(\vec{p}) \\ \mathscr{B}_-(\vec{p}) \end{bmatrix} \text{for } z \le a_-, \quad (\mathbf{\Psi}(z))(\vec{p}) = \begin{bmatrix} \mathscr{A}_+(\vec{p}) \\ B_+(\vec{p}) \end{bmatrix} \quad \text{for } z \ge a_+. \tag{4.52}$$

The time-evolution operator $\boldsymbol{\mathcal{U}}(z, z_0)$ is a 2×2 matrix with operator entries, defined as,

$$\mathbf{\Psi}(z) = \boldsymbol{\mathcal{U}}(z, z_0)\mathbf{\Psi}(z_0) \tag{4.53}$$

Inserting (4.52) to (4.53) we find

$$\begin{bmatrix} \mathscr{A}_+(\vec{p}) \\ B_+(\vec{p}) \end{bmatrix} = \widehat{\boldsymbol{\mathcal{U}}}(a_+, a_-) \begin{bmatrix} A_-(\vec{p}) \\ \mathscr{B}_-(\vec{p}) \end{bmatrix}. \tag{4.54}$$

Equation (4.39) shows that the evolution operator $\widehat{\boldsymbol{\mathcal{U}}}$ is not the same as the transfer matrix. However it turns out to be useful, so we define the auxiliary transfer matrix $\widehat{\boldsymbol{\mathcal{M}}}$ as,

$$\widehat{\boldsymbol{\mathcal{M}}} = \widehat{\boldsymbol{\mathcal{U}}}(+\infty, -\infty) := \lim_{z_\pm \to \pm\infty} \widehat{\boldsymbol{\mathcal{U}}}(z_+, z_-). \tag{4.55}$$

If the support of the potential $v(\boldsymbol{r})$ lies between the surfaces $z = a_\pm$, the Hamiltonian $\widehat{\boldsymbol{\mathcal{H}}}(z)$ vanishes outside the this region. This shows $\widehat{\boldsymbol{\mathcal{U}}}(z_+, z_-) = \widehat{\mathbf{I}}$ for $z_\pm \notin [a_-, a_+]$. Using the composition property of the evolution operator we get,

$$\widehat{\boldsymbol{\mathcal{U}}}(+\infty, -\infty) = \widehat{\boldsymbol{\mathcal{U}}}\ (+\infty, -a_+)\, \widehat{\boldsymbol{\mathcal{U}}}(a_+, a_-)\, \widehat{\boldsymbol{\mathcal{U}}}(a_-, -\infty) = \widehat{\boldsymbol{\mathcal{U}}}(a_+, a_-).$$

This implies

$$\widehat{\boldsymbol{\mathcal{M}}} = \widehat{\boldsymbol{\mathcal{U}}}(a_+, a_-), \tag{4.56}$$

for a finite range potential whose support lies on $[a_-, a_+]$. Define,

$$\widehat{\mathbf{\Pi}}_k := \widehat{\Pi}_k \widehat{\mathbf{I}}, \tag{4.57}$$

where $\widehat{\Pi}_k$ is defined by (4.26). Notice that, (4.28) implies

$$\begin{bmatrix} A_-(\vec{p}) \\ B_-(\vec{p}) \end{bmatrix} = \widehat{\mathbf{\Pi}}_k \begin{bmatrix} A_-(\vec{p}) \\ \mathscr{B}_-(\vec{p}) \end{bmatrix}, \qquad \begin{bmatrix} A_+(\vec{p}) \\ B_+(\vec{p}) \end{bmatrix} = \widehat{\mathbf{\Pi}}_k \begin{bmatrix} \mathscr{A}_+(\vec{p}) \\ B_+(\vec{p}) \end{bmatrix}. \tag{4.58}$$

Then equations (4.39), (4.54), (4.55) and (4.58) imply,

$$\widehat{\mathbf{M}} = \widehat{\mathbf{\Pi}}_k\, \widehat{\boldsymbol{\mathcal{M}}}\, \widehat{\mathbf{\Pi}}_k. \tag{4.59}$$

We call $\widehat{\mathbf{M}}$ the fundamental transfer matrix.

It is possible to recover the fundamental transfer matrix in another way. Assume the Hamiltonian $\widehat{\boldsymbol{\mathcal{H}}}(z)$ defined by the equation (4.41) is the interaction picture Hamiltonian, then the free Hamiltonian as,

$$\widehat{\mathbf{H}}_0 := -\widehat{\varpi}(\vec{p})\widehat{\boldsymbol{\sigma}}_3. \tag{4.60}$$

and the Schrödinger picture Hamiltonian and and the Schrödinger picture state vector are given by

$$\widehat{\mathbf{H}} := \frac{1}{2}\widehat{\mathscr{V}}(z)\boldsymbol{\mathcal{K}}\widehat{\varpi}^{-1}(\vec{p}) - \varpi(\vec{p})\widehat{\boldsymbol{\sigma}}_3, \tag{4.61}$$

$$(\mathbf{\Phi}(z))(\vec{p}) = \frac{1}{2}\begin{bmatrix} \varpi(\vec{p})\tilde{\psi}(\vec{p}, z) - i\tilde{\psi}'(\vec{p}, z) \\ \varpi(\vec{p})\tilde{\psi}(\vec{p}, z) + i\tilde{\psi}'(\vec{p}, z) \end{bmatrix}. \tag{4.62}$$

Then time evolution operator $\widehat{\mathbf{U}}(z_+, z_-)$ satisfies,

$$\widehat{\mathbf{M}} = \widehat{\mathbf{U}}(+\infty, -\infty) := \lim_{z_\pm \to \pm\infty} \widehat{\mathbf{U}}(z_+, z_-). \tag{4.63}$$

where we made use of (4.38), (4.62) and (4.64).

We can use the relationship between $\widehat{\mathbf{U}}(z_+, z_-)$ and $\widehat{\boldsymbol{\mathcal{U}}}(z_+, z_-)$ given in Appendix A to show that,

$$\widehat{\mathbf{U}}(z_+, z_-) = e^{-iz_+ \widehat{\varpi}(\vec{p})\widehat{\boldsymbol{\sigma}}_3} \widehat{\boldsymbol{\mathcal{U}}}(z_+, z_-)\, e^{iz_- \widehat{\varpi}(\vec{p})\widehat{\boldsymbol{\sigma}}_3} \tag{4.64}$$

which together with (4.63) imply

$$\widehat{\mathbf{M}} = \lim_{z_\pm \to \pm\infty} e^{-iz_+ \varpi(\vec{p})\,\widehat{\boldsymbol{\sigma}}_3} \widehat{\boldsymbol{\mathcal{U}}}(+z, -z)\, e^{iz_- \varpi(\vec{p})\widehat{\boldsymbol{\sigma}}_3} \tag{4.65}$$

In particular for a potential that is supported in the region $[a_-, a_+]$ we have,

$$\widehat{\mathbf{M}} = e^{-ia_+ \varpi(\vec{p})\boldsymbol{\sigma}_3} \widehat{\boldsymbol{\mathcal{U}}}(a_+, a_-)\, e^{ia_- \varpi(\vec{p})\boldsymbol{\sigma}_3}. \tag{4.66}$$

Notice that neither of $\widehat{\boldsymbol{\mathcal{H}}}(z)$ and $\widehat{\mathbf{H}}(z)$ is a Hermitian operator. However, these are $\boldsymbol{\sigma}_3$-pseudo Hermitian operators if the potential v is real valued. Moreover, $\widehat{\mathbf{H}}(z)$ is diagonalizable can be diagonalizable unlike $\widehat{\boldsymbol{\mathcal{H}}}(z)$.

Assume the potential (4.11) is z-independent for $z \in [a_-, a_+]$, i.e.,

$$v(\vec{r}, z) = \begin{cases} \mathscr{V}(\vec{r}) & \text{for } z \in [a_-, a_+], \\ 0 & \text{for } z \notin [a_-, a_+]. \end{cases} \tag{4.67}$$

Then $\widehat{\mathbf{H}}$ is z-independent and we have $\widehat{\mathbf{U}}(z_+, z_-) = e^{-i(z_+ - z_-)\widehat{\mathbf{H}}}$. Using (4.56) we find

$$\widehat{\boldsymbol{\mathcal{M}}} = e^{-ia_+ \widehat{\varpi}\boldsymbol{\sigma}_3} e^{-ia\widehat{\mathbf{H}}} e^{ia_- \widehat{\varpi}\boldsymbol{\sigma}_3} \tag{4.68}$$

and, using (4.59) we get,

$$\widehat{\mathbf{M}} = \widehat{\boldsymbol{\Pi}}_k e^{-ia_+ \hat{\varpi}\boldsymbol{\sigma}_3} e^{-ia\widehat{\mathbf{H}}} e^{ia_- \hat{\varpi}\boldsymbol{\sigma}_3} \widehat{\boldsymbol{\Pi}}_k \tag{4.69}$$

$$= e^{-ia_+ \hat{\varpi}\boldsymbol{\sigma}_3} \widehat{\boldsymbol{\Pi}}_k e^{-ia\widehat{\mathbf{H}}} \widehat{\boldsymbol{\Pi}}_k e^{ia_- \hat{\varpi}\boldsymbol{\sigma}_3} \tag{4.70}$$

This shows that for this kind of potentials, finding the transfer matrix reduces to calculating $e^{-ia\widehat{\mathbf{H}}}$.

4.4 The composition property of the transfer matrix in d-dimensions

Now we can show that the auxiliary transfer matrix has the composition property. First we arbitrarily slice a part of the z-axis where the support of the potential lies. Let $n \in \mathbb{N}^+$, and $a_0, a_1, \cdots, a_n$ and $z_\pm$ be real numbers such that

$$z_- \leq a_- = a_0 < a_1 < a_2 < \cdots < a_{n-1} < a_n = a_+ \leq z_+. \tag{4.71}$$

The evolution operator $\widehat{\boldsymbol{\mathcal{U}}}(z_+, z_-)$ has the composition property, then we can write

$$\widehat{\boldsymbol{\mathcal{U}}}(z_+, z_-) = \widehat{\boldsymbol{\mathcal{U}}}(z_+, a_n)\widehat{\boldsymbol{\mathcal{U}}}(a_n, a_{n_1}) \cdots \widehat{\boldsymbol{\mathcal{U}}}(a_1, a_0)\widehat{\boldsymbol{\mathcal{U}}}(a_0, z_-). \tag{4.72}$$

Now, divide the potential v into potentials v_j with smaller supports defined as,

$$v_j(\vec{r}, z) := \begin{cases} v(\vec{r}, z) & \text{for } z \in (a_{j-1}, a_j], \\ 0 & \text{for } \quad z \notin (a_{j-1}, a_j], \end{cases} \tag{4.73}$$

This implies $\widehat{\mathscr{V}}_j(\vec{p}, z) = 0$, then equation (4.50) implies

$$\widehat{\boldsymbol{\mathcal{H}}}_j(z) := \begin{cases} \widehat{\boldsymbol{\mathcal{H}}}(z) & \text{for } z \in [a_{j-1}, a_j], \\ \widehat{\mathbf{0}} & \text{for } z \notin [a_{j-1}, a_j], \end{cases} \tag{4.74}$$

$$\widehat{\boldsymbol{\mathcal{U}}}_j(z_+, z_-) = \begin{cases} \widehat{\mathbf{I}} & \text{for } z_- \leq z \leq a_{j-1}, \\ \widehat{\boldsymbol{\mathcal{U}}}(z_+, z_-) & \text{for } a_{j-1} \leq z_- \leq a_j, \\ \widehat{\mathbf{I}} & \text{for } a_j \leq z_- \leq z_+, \end{cases} \tag{4.75}$$

where $\widehat{\boldsymbol{\mathcal{H}}}_j(z)$ and $\widehat{\boldsymbol{\mathcal{U}}}_j(z_+, z_-)$ are defined by equation (4.50) and (4.55) for potential v_j. Moreover we define the auxiliary transfer matrix for potential v_j as,

$$\begin{aligned} \widehat{\boldsymbol{\mathcal{M}}}_j := \lim_{z_\pm \to \pm\infty} \widehat{\boldsymbol{\mathcal{U}}}_j(z_+, z_-) &= \widehat{\boldsymbol{\mathcal{U}}}_j(\infty, z_-)\boldsymbol{\mathcal{U}}_j(a_j, a_{j-1})\widehat{\boldsymbol{\mathcal{U}}}_j(a_{j-1}, -\infty) \\ &= \boldsymbol{\mathcal{U}}_j(a_j, a_{j-1}). \end{aligned} \tag{4.76}$$

Here we used the composition property of $\widehat{\boldsymbol{\mathcal{U}}}_j$ and equation (4.75). Notice that (4.71) also implies $\widehat{\boldsymbol{\mathcal{U}}}(z_+, a_n) = \widehat{\boldsymbol{\mathcal{U}}}(z_+, a_n) = \hat{\mathbf{I}}$, then we have,

$$\begin{aligned} \widehat{\boldsymbol{\mathcal{U}}}(z_+, z_-) &= \widehat{\boldsymbol{\mathcal{U}}}(z_+, a_n)\widehat{\boldsymbol{\mathcal{U}}}_n(a_n, a_{n-1})\widehat{\boldsymbol{\mathcal{U}}}_{n-1}(a_{n-1}, a_{n-2}) \cdots \widehat{\boldsymbol{\mathcal{U}}}_1(a_1, a_0)\widehat{\boldsymbol{\mathcal{U}}}(a_0, z_-) \\ &= \widehat{\boldsymbol{\mathcal{U}}}_n(a_n, a_{n-1})\widehat{\boldsymbol{\mathcal{U}}}_{n-1}(a_{n-1}, a_{n-2}) \cdots \widehat{\boldsymbol{\mathcal{U}}}_1(a_1, a_0). \end{aligned} \tag{4.77}$$

Then (4.55), (4.76) and (4.77) proves the composition property of the auxiliary transfer matrix,

$$\widehat{\boldsymbol{\mathcal{M}}} = \widehat{\boldsymbol{\mathcal{M}}}_n \widehat{\boldsymbol{\mathcal{M}}}_{n-1} \cdots \widehat{\boldsymbol{\mathcal{M}}}_1 \tag{4.78}$$

Note that $\widehat{I} = \widehat{\boldsymbol{\mathcal{U}}}(z_+, a_n) = e^{iz_+\varpi(\vec{p})}\widehat{\mathbf{U}}(z_+, a_n)e^{-ia_n\varpi(\vec{p})}$ implies $\widehat{\mathbf{U}}(z_+, a_n) = e^{-i(z_+-a_n)\varpi(\vec{p})}$. Similarly we find $\widehat{\mathbf{U}}(a_0, z_-) = e^{i(z_--a_0)\varpi(\vec{p})}$ These, (4.63) and the composition property of the evolution operator $\widehat{\mathbf{U}}(z_+, z_-)$ imply

$$\widehat{\mathbf{M}} = \lim_{z_\pm \to \pm\infty} e^{-iz_+\varpi(\vec{p})}\widehat{\mathbf{U}}_n(a_n, a_{n-1})\widehat{\mathbf{U}}_{n-1}(a_n, a_{n-1}) \cdots \widehat{\mathbf{U}}_1(a_1, a_0)e^{iz_-\varpi(\vec{p})}. \tag{4.79}$$

Note that, we cannot apply the same procedure to the fundamental transfer matrix since the Schrödinger picture evolution operator $\widehat{\mathbf{U}}_j(z_+, z_-)$ for potential v_j does not have the form (4.75). As a consequence, $\widehat{\mathbf{U}}_j(z_+, z_-) \neq \widehat{\mathbf{I}}$ for $z_- \notin [a_{j-1}, a_j]$ and (4.76) and (4.737 does not hold. This shows the importance of including the evanescent waves in the DFSS in higher dimensions.

4.5 An explicit formula for the transfer matrix

The Hamiltonians $\widehat{\mathbf{H}}(z)$ and $\widehat{\boldsymbol{\mathcal{H}}}(z)$ are not Hermitian, so there is no spectral theorem that guarantee the existence of a complete set of eigenfunctions. This makes finding an explicit formula for the transfer matrix difficult. However, [23] shows that if we restrict the scattering systems such that $\widehat{\mathbf{H}}(z)$ has a discrete spectrum, it is possible to construct a biorthogonal system for $\widehat{\mathbf{H}}(z)$. In the rest of this chapter we give the details of this construction.

We focus our attention on potentials of the form (4.67) where $\mathscr{V}(\vec{r})$ is a real confining potential, that is $\mathscr{V}(\vec{r}) \to \infty$ as $r := |\vec{r}| \to \infty$. Define the operator $\hat{h} := \hat{\vec{p}}^2 + \widehat{\mathscr{V}}(\vec{r})$, where $\hat{\vec{p}}$ be the $(d-1)$ dimensional momentum operator acting on the Hilbert space $L^2(\mathbb{R}^{d-1})$ and $\hat{\vec{p}}^2 = \hat{\vec{p}} \cdot \hat{\vec{p}}$. Then this operator has a real discrete spectrum $\{E_n\}$ and a complete set of orthonormal eigenbasis $\{|\phi_n, a\rangle\}$ such that

$$\left(\hat{\boldsymbol{p}}^2 + \widehat{\mathscr{V}}(\boldsymbol{r})\right)|\phi_n, a\rangle = E_n|\phi_n, a\rangle, \tag{4.80}$$

$$\sum_{n=1}^{\infty}\sum_{a=1}^{d_n} |\phi_n, a\rangle\langle\phi_n, a| = \hat{I}, \tag{4.81}$$

$$|\phi_m, b\rangle\langle\phi_n, a| = \delta_{mn}\delta_{ab} \tag{4.82}$$

where $n \in \mathbb{N}^+$, d_n is the multiplicity of the eigenvalue E_n, $\hat{I}$ is the identity operator defined on $L^2(\mathbb{R}^{d-1})$ and $a, b \in \{1, \cdots, d_n\}$. Define,

$$\widehat{W} := \sqrt{\widehat{\varpi}^2 - \widehat{\mathscr{V}}}. \tag{4.83}$$

Equations (4.19), (4.51) and (4.83) imply,

$$(\widehat{\varpi}^2 - \widehat{\mathscr{V}})|\phi_n, a\rangle = w_n^2|\phi_n, a\rangle \tag{4.84}$$

where

$$w_n = \begin{cases} \sqrt{k^2 - E_n} & \text{for } E_n \leq k^2, \\ i\sqrt{E_n - k^2} & \text{for } E_n > k^2, \end{cases} \tag{4.85}$$

then we get,

$$\widehat{W} = \sum_{n=1}^{\infty}\sum_{a=1}^{d_n} w_n|\phi_n, a\rangle\langle\phi_n, a|. \tag{4.86}$$

It is easy to show that the vectors given by [23]

$$|\mathbf{\Psi}_{n,a}^{\pm}\rangle := \frac{1}{2k}\begin{bmatrix} \widehat{\varpi} \mp \widehat{W} \\ \widehat{\varpi} \pm \widehat{W} \end{bmatrix}|\phi_n, a\rangle, \quad |\mathbf{\Phi}_{n,a}^{\pm}\rangle := \frac{1}{2k}\begin{bmatrix} \widehat{\varpi}^{-1\dagger} \mp \widehat{W}^{-1\dagger} \\ \widehat{\varpi}^{-1\dagger} \pm \widehat{W}^{-1\dagger} \end{bmatrix}|\phi_n, a\rangle, \tag{4.87}$$

satisfy

$$\widehat{\mathbf{H}}|\mathbf{\Psi}_{n,a}^{\pm}\rangle = \pm\omega_n|\mathbf{\Psi}_{n,a}^{\pm}\rangle, \qquad \widehat{\mathbf{H}}^{\dagger}|\mathbf{\Phi}_{n,a}^{\pm}\rangle = \pm\omega_n^*|\mathbf{\Phi}_{n,a}^{\pm}\rangle, \tag{4.88}$$

$$\langle\mathbf{\Phi}_{m,b}^{\pm}|\mathbf{\Psi}_{n,a}^{\pm}\rangle = \delta_{mn}\delta_{ab}, \tag{4.89}$$

$$\sum_{n=1}^{\infty}\sum_{a=1}^{d_n}\left(|\mathbf{\Psi}_{n,a}^{+}\rangle\langle\mathbf{\Phi}_{n,a}^{+}| + |\mathbf{\Psi}_{n,a}^{-}\rangle\langle\mathbf{\Phi}_{n,a}^{-}|\right) = \widehat{\mathbf{I}}, \tag{4.90}$$

where $\widehat{\mathbf{I}}$ is the identity operator on $\mathbb{C}^2 \otimes L^2(\mathbb{R}^2)$. The definitions in section 2 show that $\{|\mathbf{\Psi}_{n,a}^{\pm}\rangle, |\mathbf{\Phi}_{n,a}^{\pm}\rangle\}$ forms a complete biorthonormal basis. As we expected the spectrum of $\widehat{\mathbf{H}}$ consists of real and complex conjugate pairs of imaginary eigenvalues. The definition of the eigenvalues (4.85) shows that there is finitely many or no real eigenvalues of $\widehat{\mathbf{H}}$ and there are infinitely many complex conjugate eigenvalues.

When $k=\sqrt{E_n}$, both the eigenvalues $\pm w_n$ vanishes, which shows that these eigenvalues coalesce. Moreover the first relation in (4.87) shows that the corresponding eigenvectors $|\boldsymbol{\Psi}^{\pm}_{n,a}\rangle$ also coalesce at this value of k. Then the wavenumber $k=\sqrt{E_n}$ is an exceptional point. We name $k_*=\sqrt{E_{n_*}}$ as exceptional wavenumber. Since the eigenvectors coalesce, there is no longer a complete set of biorthonormal eigenvectors and $\widehat{\mathbf{H}}$ is no longer diagonalizable, this makes w_{n_*} a defective eigenvalue of $\widehat{\mathbf{H}}$.

In order to get an explicit form of the transfer matrix. First we assume there is no exceptional point, that is $k^2\neq E_n$ for any $n\in\mathbb{N}^+$. Then the system of vector $\Big\{|\boldsymbol{\Psi}_{n,a}\rangle, |\boldsymbol{\Phi}_{n,a}\rangle,\Big\}$ forms a complete biorthonormal system of eigenvectors of $\widehat{\mathbf{H}}$ and $\widehat{\mathbf{H}}^\dagger$ for the Hilbert space $\mathscr{H}$.

$$|\boldsymbol{\Psi}^{\pm}_{n},a\rangle\langle\boldsymbol{\Phi}^{\pm}_{n},a| = \frac{1}{4}\begin{bmatrix} 2\mp(\hat{\varpi}\widehat{W}^{-1}+\widehat{W}\hat{\varpi}^{-1}) & \pm(\hat{\varpi}\widehat{W}^{-1}-\widehat{W}\hat{\varpi}^{-1}) \\ \mp\hat{\varpi}\widehat{W}^{-1}-\widehat{W}\hat{\varpi}^{-1} & 2\pm(\hat{\varpi}\widehat{W}^{-1}+\widehat{W}\hat{\varpi}^{-1})\end{bmatrix}|\phi_n,a\rangle\langle\phi_n,a|, \tag{4.91}$$

where we used (4.87).

Moreover we have the following spectral representation for $\widehat{\mathbf{H}}(z)$.

$$\widehat{\mathbf{H}} = \sum_{n=1}^{\infty}\sum_{a=1}^{d_n}\big(w_n|\boldsymbol{\Psi}^{+}_{n,a}\rangle\langle\boldsymbol{\Phi}^{+}_{n,a}| - w_n|\boldsymbol{\Psi}^{-}_{n,a}\rangle\langle\boldsymbol{\Phi}^{-}_{n,a}|\big) \tag{4.92}$$

$$= \frac{1}{2}\sum_{n=1}^{\infty}\sum_{a=1}^{d_n} w_n\begin{bmatrix} -(\hat{\varpi}\widehat{W}^{-1}+\widehat{W}\hat{\varpi}^{-1}) & (\hat{\varpi}\widehat{W}^{-1}-\widehat{W}\hat{\varpi}^{-1}) \\ -(\hat{\varpi}\widehat{W}^{-1}-\widehat{W}\hat{\varpi}^{-1}) & (\hat{\varpi}\widehat{W}^{-1}+\widehat{W}\hat{\varpi}^{-1})\end{bmatrix}|\phi_n,a\rangle\langle\phi_n,a|, \tag{4.93}$$

and

$$e^{-iz\widehat{\mathbf{H}}} = \sum_{n=1}^{\infty}\sum_{a=1}^{d_n}\big(e^{-izw_n}|\boldsymbol{\Psi}^{+}_{n,a}\rangle\langle\boldsymbol{\Phi}^{+}_{n,a}| + e^{izw_n}|\boldsymbol{\Psi}^{-}_{n,a}\rangle\langle\boldsymbol{\Phi}^{-}_{n,a}|\big) \tag{4.94}$$

$$= \sum_{n=1,n_i}^{\infty}\frac{1}{2}\Big\{\hat{\varpi}\hat{C}(z)\hat{\varpi}^{-1}(\mathbf{I}+\boldsymbol{\sigma}_1)+\hat{C}(z)(\mathbf{I}-\boldsymbol{\sigma}_1)+i(\widehat{W}^2\hat{S}(z)\hat{\varpi}^{-1}\boldsymbol{\mathcal{K}}+\hat{\varpi}\hat{S}(z)\boldsymbol{\mathcal{K}}^T]\Big\} \tag{4.95}$$

where

$$\widehat{C}(z) := \sum_{n=1}^{\infty}\sum_{a}^{d_n}\cos(w_n z)|\phi_n,a\rangle\langle\phi_n,a| = \cos(\widehat{W}), \tag{4.96}$$

and

$$\widehat{S}(z) := \sum_{n=1}^{\infty}\sum_{a}^{d_n} {w_n}^{-1}\sin(w_n z)|\phi_n, a\rangle\langle\phi_n, a| = \widehat{W}^{-1}\sin(\widehat{W}). \tag{4.97}$$

Inserting (4.95) to (4.70) we find the explicit formula of the transfer matrix found by [23]

$$\widehat{\mathbf{M}} = \frac{1}{2}e^{-ia_+\widehat{\varpi}\boldsymbol{\sigma}_3}\big[\widehat{\varpi}\widehat{\mathcal{C}}\widehat{\varpi}^{-1}(\mathbf{I}+\boldsymbol{\sigma}_1)+\widehat{\mathcal{C}}(\mathbf{I}-\boldsymbol{\sigma}_1)+i(\widehat{\mathcal{R}}\widehat{\varpi}^{-1}\boldsymbol{\mathcal{K}}+\widehat{\varpi}\hat{\mathcal{S}}\boldsymbol{\mathcal{K}}^T)\big]e^{-a_-\widehat{\varpi}\boldsymbol{\sigma}_3} \tag{4.98}$$

where

$$\widehat{\mathcal{C}} := \widehat{\Pi}_k\widehat{C}(a)\widehat{\Pi}_k, \qquad \widehat{\mathcal{R}} := \widehat{\Pi}_k\widehat{W}^2\widehat{S}(a)\widehat{\Pi}_k, \qquad \widehat{\mathcal{S}} := \widehat{\Pi}_k\widehat{S}(a)\widehat{\Pi}_k, \tag{4.99}$$

We introduce new operators

$$\widehat{\mathcal{C}}_\pm = \widehat{\varpi}\widehat{\mathcal{C}}\hat{\varpi}^{-1} \pm \widehat{\mathcal{C}}, \qquad \widehat{\mathcal{S}}_\pm = i(\hat{\mathcal{R}}\hat{\varpi}^{-1} \pm \hat{\varpi}\hat{\mathcal{S}}), \tag{4.100}$$

to simplify the expression (4.98) and we arrive at

$$\widehat{\mathbf{M}} = \begin{bmatrix} e^{-ia_+\widehat{\varpi}}(\widehat{\mathcal{C}}_+ + \widehat{\mathcal{S}}_+)e^{ia_-\widehat{\varpi}} & e^{-ia_+\widehat{\varpi}}(\widehat{\mathcal{C}}_- + \widehat{\mathcal{S}}_-)e^{-ia_-\widehat{\varpi}} \\ e^{ia_+\widehat{\varpi}}(\widehat{\mathcal{C}}_- - \widehat{\mathcal{S}}_-)e^{ia_-\widehat{\varpi}} & e^{ia_+\widehat{\varpi}}(\widehat{\mathcal{C}}_+ - \widehat{\mathcal{S}}_+)e^{-ia_-\widehat{\varpi}} \end{bmatrix}. \tag{4.101}$$

Now, consider the case when we have a exceptional wavenumber $k_{n_*} = \sqrt{E_{n_*}}$. Then $w_{n_*} = 0$, $\widehat{W}$ is not invertible and $\widehat{\mathbf{H}}$ is not diagonalizable. In section two we showed that it is possible to get a complete basis by extending the previous basis with the generalized eigenvector corresponding to the defective eigenvalue. The corresponding eigenvectors of $\pm w_{n_*}$ become

$$|(\boldsymbol{\Psi}_{n_*,a})_+\rangle := |\boldsymbol{\Psi}^+_{n_*,a}\rangle = |\boldsymbol{\Psi}^-_{n_*,a}\rangle = \frac{\widehat{\varpi}}{2k}\begin{bmatrix}1\\1\end{bmatrix}|\psi_{n_*,a}\rangle, \quad \text{for each } a \in d_{n_*} \tag{4.102}$$

The generalized eigenvectors are the vectors $|(\boldsymbol{\Psi}_{n_*,a})_-\rangle$ that satisfies

$$\widehat{\mathbf{H}}|(\boldsymbol{\Psi}_{n_*,a})_-\rangle = w_{n_*}|(\boldsymbol{\Psi}_{n_*,a})_+\rangle = 0, \quad \text{for each } a \in d_{n_*}$$

Equations (4.92) shows that

$$|(\boldsymbol{\Psi}_{n_*,a})_-\rangle = \frac{1}{2}\begin{bmatrix}-1\\1\end{bmatrix}|\psi_{n_*,a}\rangle, \quad \text{for each } a \in d_{n_*} \tag{4.103}$$

are the vectors we are looking for.

Similarly w_{n_*} is an defective eigenvalue of $\widehat{\mathbf{H}}^\dagger$ and the corresponding eigenvectors $|\mathbf{\Phi}^\pm_{n_*,a}\rangle$ coalesce and we define

$$|(\mathbf{\Phi}_{n_*,a})^+\rangle = k \begin{bmatrix} 1 \\ 1 \end{bmatrix} \widehat{\varpi}^{-1\dagger}|\phi_{n_*,a}\rangle \quad \text{for each } a \in d_{n_*}. \tag{4.104}$$

We find that the generalized eigenvector corresponding to w_{n_*} is

$$|(\mathbf{\Psi}_{n_*,a})^-\rangle = \begin{bmatrix} -1 \\ 1 \end{bmatrix} |\phi_{n_*,a}\rangle \quad \text{for each } a \in d_{n_*}. \tag{4.105}$$

Now, define the sets

$$\mathcal{B} := \left\{|\mathbf{\Psi}^\pm_{n,a}\rangle \;\middle|\; n \in \mathbb{Z}^+ \setminus \{n_*\}\right\} \cup \left\{|(\mathbf{\Psi}_{n_*,a})^+\rangle, |(\mathbf{\Psi}_{n_*,a})^-\rangle\right\}, \tag{4.106}$$

$$\mathcal{B}_\perp := \left\{|\mathbf{\Phi}^\pm_{n,a}\rangle \;\middle|\; n \in \mathbb{Z}^+ \setminus \{n_*\}\right\} \cup \left\{|(\mathbf{\Phi}_{n_*,a})^+\rangle, |(\mathbf{\Phi}_{n_*,a})^-\rangle\right\}. \tag{4.107}$$

Considering the fact that (4.95) is an analytical function of the operator $\widehat{\mathbf{H}}$ and equation (2.74) shows that the expression (4.101) still holds for exceptional wavenumbers. This agrees with the results of [23]. Note that, for an exceptional wavenumber, the operator $\widehat{W}$ is not invertible, however, the operator $\widehat{S}(z)$ is still can be defined as $\widehat{S}(z) = \sum_n (-1)^n \widehat{W}^{2n}/(2n+1)$.

At the exceptional point $e^{-ia\widehat{\mathbf{H}}}$ has an extra term which can be found by (2.76).

$$\begin{aligned}
&\sum_{a=1}^{d_{n_*}} \left(e^{-iaw_{n_*}} |(\mathbf{\Psi}_{n_*,a})_+\rangle\langle(\mathbf{\Phi}_{n_*,a})_+| + e^{iaw_{n_*}} |(\mathbf{\Psi}_{n_*,a})_-\rangle\langle(\mathbf{\Phi}_{n_*,a})_-| \right) \\
&= \sum_{a=1}^{d_{n_*}} \left(|(\mathbf{\Psi}_{n_*,a})_+\rangle\langle(\mathbf{\Phi}_{n_*,a})_+| + | + |(\mathbf{\Psi}_{n_*,a})_-\rangle\langle(\mathbf{\Phi}_{n_*,a})_-| \right). \\
&= \sum_{a=1}^{d_n} \frac{i}{2} a \hat{\Pi}_k \hat{\varpi} |\phi_{n_*,a}\rangle\langle\phi_{n_*,a}| \,\hat{\Pi}_k \boldsymbol{\mathcal{K}}^T.
\end{aligned}$$

Therefore the contribution of the exceptional point to the fundamental transfer matrix is linear in a.

4.6 Solution of the scattering problem

Solving the scattering problem requires to find the scattering amplitude $f(\hat{\mathbf{\Omega}})$ for all wavenumbers and incident angles. This can be achieved by calculation the scattering matrix $\widehat{\mathbf{S}}$ or finding $\widehat{\mathbf{M}}$ and solving for the coefficients $A_\pm, B_\pm$. Then we can insert the reflection and transmission amplitudes to (4.32) and (4.34).

First, we solve the scattering problem using $\widehat{\mathbf{M}}$. We begin by calculating $B^l_-(\vec{p})$.

$$\begin{aligned} B^l_-(\vec{p}) &= -(2\pi)^{(d-1)}\widehat{\varpi}\widehat{M}_{22}^{-1}\widehat{M}_{21}\delta_{\vec{p}_0} \\ &= -\langle\vec{p}|\widehat{\varpi}e^{-ia_-\widehat{\varpi}}(\widehat{\mathcal{C}}_+ - \widehat{\mathcal{S}}_+)^{-1}e^{ia_+\widehat{\varpi}}e^{-ia_+\widehat{\varpi}}(\widehat{\mathcal{C}}_- - \widehat{\mathcal{S}}_-)e^{ia_-\widehat{\varpi}}|\vec{p}_0\rangle \\ &= -e^{ia_-(-\varpi(\boldsymbol{p})+\varpi(\vec{p}_0))}\widehat{\varpi}(\vec{p})\langle\vec{p}|(\widehat{\mathcal{C}}_+ - \widehat{\mathcal{S}}_+)^{-1}(\widehat{\mathcal{C}}_- - \widehat{\mathcal{S}}_-)|\vec{p}_0\rangle \\ &= -e^{ia_-k(\cos\theta_0-\cos\theta)}\widehat{\varpi}(\vec{p})\langle\vec{p}|(\widehat{\mathcal{C}}_+ - \widehat{\mathcal{S}}_+)^{-1}(\widehat{\mathcal{C}}_- - \widehat{\mathcal{S}}_-)|\vec{p}_0\rangle. \end{aligned}$$

Here we have used (4.41) and (4.101) and the fact that $\cos\theta_0 > 0$ for a left-incident wave. Similarly, we find

$$R^l(\vec{p}) = i(2\pi)^{\frac{d-1}{2}}e^{ia_-k(\cos\theta_0-\cos\theta)}\varpi(\vec{p})\langle\vec{p}|(\widehat{\mathcal{C}}_+ - \widehat{\mathcal{S}}_+)^{-1}(\widehat{\mathcal{C}}_- - \widehat{\mathcal{S}}_-)|\vec{p}_0\rangle, \tag{4.108}$$

$$T^l(\vec{p}) = i(2\pi)^{\frac{d-1}{2}}\varpi(\vec{p})\langle\vec{p}|(\widehat{\mathcal{C}}_+ + \widehat{\mathcal{S}}_+) - (\widehat{\mathcal{C}}_- - \widehat{\mathcal{S}}_-)(\widehat{\mathcal{C}}_+ - \widehat{\mathcal{S}}_+)^{-1}(\widehat{\mathcal{C}}_- + \widehat{\mathcal{S}}_-)|\vec{p}_0\rangle, \tag{4.109}$$

$$R^r(\vec{p}) = i(2\pi)^{\frac{d-1}{2}}e^{ia_+k(\cos\theta_0-\cos\theta)}\varpi(\vec{p})\langle\vec{p}|(\widehat{\mathcal{C}}_+ + \widehat{\mathcal{S}}_+)^{-1}(\widehat{\mathcal{C}}_- - \widehat{\mathcal{S}}_-)|\vec{p}_0\rangle, \tag{4.110}$$

$$T^r(\vec{p}) = i(2\pi)^{\frac{d-1}{2}}e^{ik(a_+\cos\theta_0 - a_-\cos\theta)}\varpi(\vec{p})\langle\vec{p}|(\widehat{\mathcal{C}}_+ - \widehat{\mathcal{S}}_+)^{-1}|\vec{p}_0\rangle. \tag{4.111}$$

Here we used $\varpi(\vec{p}) = k\cos\theta_0$ and $\varpi(\vec{p}_0) = k|\cos\theta_0|$, also the fact that $\cos\theta_0 > 0$ for a left-incident wave and $\cos\theta_0 < 0$ for a right-incident wave. The authors of [23] showed that the scattering matrix $\widehat{\mathbf{S}}$ for this system is given by the following expression.

$$\widehat{\mathbf{S}} = \widehat{\Pi}_k\widehat{\varpi}\widehat{\mathbf{E}}_+\widehat{\Gamma}\widehat{\mathbf{E}}_-\widehat{\varpi}^{-1} \tag{4.112}$$

where

$$\widehat{\mathbf{E}}_\pm = \begin{bmatrix} e^{\mp ia_\pm\widehat{\varpi}} & 0 \\ 0 & e^{\pm ia_\mp\widehat{\varpi}}, \end{bmatrix} \qquad \widehat{\boldsymbol{\Gamma}} = \begin{bmatrix} \widehat{\Gamma}_+ & \widehat{\Gamma}_- \\ \widehat{\Gamma}_- & \widehat{\Gamma}+ \end{bmatrix}. \tag{4.113}$$

where

$$\widehat{\Gamma}_\pm := \frac{1}{2}(\widehat{\Omega}_{1-}^{-1}\widehat{\Omega}_{1+} \pm \widehat{\Omega}_{2-}^{-1}\widehat{\Omega}_{2-}) \tag{4.114}$$

and

$$\widehat{\Omega}_{1\pm} = \widehat{W}\cos(\frac{a}{2}\widehat{W}) \pm \sin(\frac{a}{2}\widehat{W})\widehat{\varpi}, \widehat{\Omega}_{2\pm} = \cos(\frac{a}{2}\widehat{W})\widehat{\varpi} + \pm i\widehat{W}\sin(\frac{a}{2}\widehat{W}). \tag{4.115}$$

Inserting (4.35) and (4.36) to (4.34) we get

$$\begin{bmatrix} T^l & R^r \\ R^l & T^r \end{bmatrix} = -i(2\pi)^{d-1}\varpi(\vec{p_0})\widehat{\mathbf{S}}\delta_{\vec{p}_0}, \tag{4.116}$$

These imply

$$\widehat{\mathbf{S}} = \begin{bmatrix} e^{-ia_+\widehat{\varpi}}\widehat{\Gamma}_+ e^{ia_-\widehat{w}} & e^{-ia_+\widehat{\varpi}}\widehat{\Gamma}_- e^{-ia_+\widehat{\varpi}} \\ e^{ia_-\widehat{\varpi}}\widehat{\Gamma}_- e^{ia_-\widehat{\varpi}} & e^{ia_-\widehat{\varpi}}\widehat{\Gamma}_+ e^{-ia_+\widehat{w}}. \end{bmatrix} \tag{4.117}$$

Using (4.116) we get the left/right reflection and transmission amplitudes.

$$R^l(\theta,\varphi) = i(2\pi)^{\frac{d-1}{2}} k\cos\theta e^{ia_- k(\cos\theta_0-\cos\theta)}\Gamma_-(\vec{p},\vec{p_0}), \tag{4.118}$$

$$T^l(\theta,\varphi) = -i(2\pi)^{\frac{d-1}{2}} k\cos\theta e^{ik(a_-\cos(\theta_0)-a_+\cos(\theta))}\Gamma_+(\vec{p},\vec{p_0}), \tag{4.119}$$

$$R^r(\theta,\varphi) = -i(2\pi)^{\frac{d-1}{2}} k\cos\theta e^{ia_+ k(\cos(\theta_0)-\cos(\theta))}\Gamma_-(\vec{p},\vec{p_0}), \tag{4.120}$$

$$T^r(\theta,\varphi) = i(2\pi)^{\frac{d-1}{2}} k\cos\theta e^{ik(a_+\cos(\theta_0)-a_-\cos(\theta))}\Gamma_+(\vec{p},\vec{p_0}), \tag{4.121}$$

where

$$\Gamma_\pm(\vec{p},\vec{p_0}) = \langle\vec{p}|\widehat{\Gamma}_\pm|\vec{p_0}\rangle. \tag{4.122}$$

This shows that solving the scattering problem reduces to calculation of $\Gamma_\pm(\vec{p},\vec{p_0})$.

Chapter 5

FINITE LENGTH WAVEGUIDES

In this chapter we use the machinery developed in the previous chapter to study scattering of wave from a finite length waveguide with impenetrable walls of infinite thickness filled with a homogeneous inactive and lossless material. Fig. 5.1 and Fig. 5.7 show the schematic views of such waveguide for two- and three-dimensions respectively. The two dimensional case of this problem is studied in [23], where the scattering from the finite length waveguide is due to two different parts; from the impenetrable walls and from the material inside the waveguide. We generalize this approach to three-dimensional finite waveguide and discuss its differences and similarities with its two-dimensional counterpart.

5.1 *Scattering from a* d*-dimensional finite length waveguide*

Consider potentials defined as (4.67) where

$$\mathscr{V}(\vec{r}) := \begin{cases} \mathscr{V}_0 & \text{for } \vec{r} \in box, \\ +\infty & \text{for } \vec{r} \notin box, \end{cases} \tag{5.1}$$

$\mathscr{V}_0 \in \mathbb{R}$,

$$box := \begin{cases} [0, L_x] & \text{for } d = 2, \\ [0, L_x] \times [0, L_y] & \text{for } d = 3, \end{cases} \tag{5.2}$$

and L_x and L_y are positive real parameters. This potential describes a d-dimensional rectangular waveguide of length a, width L_x, and height L_y for $d = 3$. The waveguide is filled with passive and lossless material and it has impenetrable walls with infinite thickness. The scattering properties of the material is determined by the parameter $\mathscr{V}_0$. Figures (5.1) and (5.3) show schematic view of such waveguides in two- and three-dimensions respectively.

With the choice of the potential (5.1), the operator $\hat{h} := \hat{\vec{p}}^2 + \widehat{\mathscr{V}}$ becomes the Hamiltonian of the quantum system describing a particle confined in a $(d-1)$-dimensional infinite rectangular well. The energy eigenvalues and the corresponding eigenvectors can be found in every introductory quantum mechanics textbook. Generally, this problem is considered in the Hilbert space $L^2(box)$, however, in order to take the impenetrable walls into consideration, we examine the problem in the Hilbert space $L^2[\mathbb{R}^{d-1}]$. It is easy to see that

$$L^2[\mathbb{R}^{d-1}] = L^2[box] \oplus L^2[\mathbb{R}^{d-1} \setminus box] \tag{5.3}$$

where $\oplus$ stands for direct sum. This means that for every $\phi \in L^2[\mathbb{R}^{d-1}]$ there exist unique functions $\mathring{\phi} \in L^2(box)$ and $\breve{\phi} \in L^2(R^{(d-1)} \setminus box)$ such that,

$$\phi(\boldsymbol{r}) = \begin{cases} \mathring{\phi}(\vec{r}) & \text{for } \vec{r} \in box, \\ \breve{\phi}(\vec{r}) & \text{for } \vec{r} \notin box. \end{cases} \tag{5.4}$$

Let $\widehat{\Lambda}$ be the projection onto $L^2[box]$ defined as

$$\widehat{\Lambda}\phi(\vec{r}) = \begin{cases} \mathring{\phi}(\vec{r}) & \text{for } \vec{r} \in box, \\ 0 & \text{for } \vec{r} \notin box. \end{cases} \tag{5.5}$$

Since we are working in a Hilbert space, $\widehat{\Lambda}$ is an orthogonal projection. This implies that $(\hat{I} - \widehat{\Lambda})$ is the orthogonal projection onto $L^2[\mathbb{R}^{d-1} \setminus box]$;

$$(\hat{I} - \widehat{\Lambda})\phi(\vec{r}) = \begin{cases} 0 & \text{for } \vec{r} \in box, \\ \breve{\phi}(\vec{r}) & \text{for } \vec{r} \notin box. \end{cases} \tag{5.6}$$

In particular we have

$$L^2[box] = \widehat{\Lambda} L^2[\mathbb{R}^{d-1}], \qquad L^2[\mathbb{R}^{d-1} \setminus box] = (\widehat{I} - \widehat{\Lambda}) L^2[\mathbb{R}^{d-1}]. \tag{5.7}$$

The energy eigenvalue E and corresponding eigenfunction $\phi(\vec{r}) = \langle \vec{r} | \psi \rangle \in L^2[\mathbb{R}^{(d-1)}]$ of $\hat{h}$ must satisfy $\langle \vec{r} | (\hat{\vec{p}}^2 + \widehat{\mathscr{V}}) | \phi \rangle = E\phi(\vec{r})$. Outside the *box*, the potential is infinite. Therefore eigenvalue problem becomes

$$\langle \boldsymbol{r} | (\hat{\boldsymbol{p}}^2 + \widehat{\mathscr{V}}) | \phi \rangle = \begin{cases} -\nabla^2_{d-1}\mathring{\phi}(\vec{r}) + \mathscr{V}\mathring{\phi}(\vec{r}) & \text{for } \vec{r} \in box, \\ 0 & \text{for } \vec{r} \notin box, \end{cases} \tag{5.8}$$

where $\mathring{\phi}$ are twice differentiable functions of $\vec{r}$, that satisfy

$$\mathring{\phi}(0) = \mathring{\phi}(L_x) = 0 \text{ for } d = 2, \tag{5.9}$$

$$\mathring{\phi}(0, y) = \mathring{\phi}(L_x, y) = \mathring{\phi}(x, 0) = \mathring{\phi}(x, L_y) = 0 \text{ for } d = 3. \tag{5.10}$$

Equation (5.8) shows that the eigenvalues of $\widehat{\Lambda}\hat{h}\widehat{\Lambda} = -\nabla^2_{d-1} + \widehat{\mathscr{V}}$ are also eigenvalues of $\hat{h}$ with the same eigenvectors which vanish when $\vec{r} \notin box$. Moreover, zero is an infinitely degenerate eigenvalue of $\hat{h}$ and the corresponding eigenvectors are all functions in $L^2[\mathbb{R}^{(d-1)} \setminus box]$. The total spectrum of $\hat{h}$ becomes the spectrum of $\widehat{\Lambda}\hat{h}\widehat{\Lambda}$ combined with zero. The following are the eigenvalues and and the corresponding eigenfunctions of $\hat{h}$.

$$E_n = \mathcal{E}_n + \mathscr{V}_0, \qquad \phi_{n,a}(\vec{r}) = \begin{cases} \mathring{\phi}_{n,a}(\vec{r}) & \text{for } \vec{r} \in box, \\ 0 & \text{for } \vec{r} \notin box. \end{cases} \tag{5.11}$$

Here $\mathcal{E}_n$ and $\mathring{\phi}_{n,a} \in L^2[box]$ are eigenvalues and the corresponding eigenfunctions of $\widehat{\Lambda}\hat{h}\widehat{\Lambda}$, i.e., they satisfy

$$\nabla^2_{d-1}\mathring{\phi}_{n,a} + \mathcal{E}_n\mathring{\phi}_{n,a} = 0.$$

for all $n \in \mathbb{Z}^+$.

Notice that the regular completeness relation for the eigenfunctions of $\hat{h}$ does not hold. Instead we get

$$\sum_{n=1}^{\infty}\sum_{a=1}^{d_n} |\phi_{n,a}\rangle\langle\phi_{n,a}| = \widehat{\Lambda}. \tag{5.12}$$

The scattering from the potential (5.1) is due to two different interactions, namely the interactions with the walls and the material inside the waveguide. The part of the wave that interacts with the vertical boundaries of impenetrable walls gets reflected. The remaining part of the wave interacts with the material inside the waveguide and gets partially reflected and partially transmitted. The linearity of the Schrödinger equation allows us to consider the scattered wave as the superposition of the contribution of interior of the waveguide and the vertical boundaries of the impenetrable wall. The vertical boundaries of impenetrable walls are represented by thick dark red lines in Figure (5.1) and pink walls dashed with dark red lines in Figure (5.3).

Let $\psi(\vec{r}, z)$ be a solution of the Schrödinger equation (4.10) that satisfies the boundary condition (4.12). Let $|\psi(z)\rangle$ be the function that satisfies $\langle \vec{r}|\psi(z)\rangle = \psi(\vec{r}, z)$. This allows us to consider $\tilde{\psi}(\vec{p}, z) := \langle \vec{p}|\psi(z)\rangle$. In particular, (4.21) implies

$$|\psi(z)\rangle = \frac{\widehat{\varpi}^{-1}}{2\pi^{\frac{d-1}{2}}} \times \begin{cases} e^{iz\widehat{\varpi}}|A_-\rangle + e^{-iz\widehat{\varpi}}|\mathscr{B}_-\rangle & \text{for } z \leq a_-, \\ e^{iz\widehat{\varpi}}|\mathscr{A}_+\rangle + e^{-iz\widehat{\varpi}}|B_+\rangle & \text{for } z \geq a_+, \end{cases} \tag{5.13}$$

where we used the fact that $\langle \vec{r}|\vec{p}\rangle = (2\pi)^{\frac{1-d}{2}} e^{i\vec{p}\cdot\vec{r}}$ and $\langle \vec{p}|\hat{\varpi} = \langle \vec{p}|\varpi(\vec{p})$.

As a solution of the Schr̆odinger equation (4.10) for potential (5.1), $\psi(\vec{r}, z)$ must be a continuous function that vanishes inside the vertical boundaries of the impenetrable walls. This is equivalent to the condition, $\psi(\vec{r}, a_\pm) = 0$ when $\vec{r} \notin box$, which implies

$$(\widehat{I} - \widehat{\Lambda})|\psi(a_\pm)\rangle = 0. \tag{5.14}$$

Inserting (5.14) to (5.13), we get

$$(\widehat{\Lambda} - \widehat{I})|\mathscr{B}_-\rangle = (\widehat{I} - \widehat{\Lambda})e^{2ia_-\widehat{\varpi}}|A_-\rangle, \tag{5.15}$$

$$(\widehat{\Lambda} - \widehat{I})|\mathscr{A}_+\rangle = (\widehat{I} - \widehat{\Lambda})e^{-2ia_+\widehat{\varpi}}|B_+\rangle. \tag{5.16}$$

We want to solve these for $|\mathscr{B}_-\rangle, |\mathscr{A}_+\rangle$ respectively. Since these are non-homogeneous linear equations, the solutions are of the form

$$|\mathscr{B}_-\rangle = |\mathscr{B}_{0-}\rangle + (\widehat{I} - \widehat{\Lambda})e^{2ia_-\widehat{\varpi}}|A_-\rangle, \tag{5.17}$$

$$|\mathscr{A}_+\rangle = |\mathscr{A}_{0+}\rangle + (\widehat{I} - \widehat{\Lambda})e^{-2ia_+\widehat{\varpi}}|B_+\rangle, \tag{5.18}$$

where

$$(\widehat{\Lambda} - \widehat{I})|\mathscr{B}_{0-}\rangle = 0, \qquad (\widehat{\Lambda} - \widehat{I})|\mathscr{A}_{0+}\rangle = 0, \tag{5.19}$$

which show that $|\mathscr{B}_{0-}\rangle$ and $|\mathscr{A}_{0+}\rangle$ are solutions of the homogeneous linear equation $(\widehat{\Lambda} - \widehat{I})|\psi\rangle = 0$. Noting that $(\widehat{I} - \widehat{\Lambda})^2 = (\widehat{I} - \widehat{\Lambda})$, it is easy to check that (5.17) and (5.18) are solutions of (5.15) and (5.16) respectively.

In view of (5.19) $|\mathscr{B}_{0-}\rangle$ and $|\mathscr{A}_{0+}\rangle$ are associated with the Hilbert space $L^2[box]$, and $(\widehat{I}-\widehat{\Lambda})e^{2ia_-\widehat{\varpi}}|A_-\rangle$ and $(\widehat{I}-\widehat{\Lambda})e^{-2ia_+\widehat{\varpi}}|B_+\rangle$ are associated with $L^2[\mathbb{R}^d\setminus box]$.

Consider a left-incident wave where according to (4.31) $|B^l_+\rangle = 0$ and $|A^l_-\rangle = (2\pi)^{d-1}\varpi(\vec{p}_0)|\vec{p}_0\rangle$. This implies $A^l_-(\vec{p}) = \langle\vec{p}|A^l_-\rangle = (2\pi)^{d-1}\varpi(\vec{p}_0)\delta_{\vec{p}_0}$. Next consider (5.15) and (5.16) for a left incident wave, and apply $\widehat{\Pi}_k$ to both sides of these equations to obtain

$$|B^l_-\rangle = \widehat{\Pi}_k|\mathscr{B}^l_{0-}\rangle + (2\pi)^{d-1}\varpi(\vec{p}_0)e^{2ia_-\widehat{\varpi}}\widehat{\Pi}_k(\widehat{I}-\widehat{\Lambda})|\vec{p}_0\rangle, \tag{5.20}$$

$$|A^l_+\rangle = \widehat{\Pi}_k|\mathscr{A}^l_{0+}\rangle. \tag{5.21}$$

Applying $\langle\vec{p}|$ from left to both sides of this equation we get

$$B^l_-(\vec{p}) = \mathscr{B}^l_{0-}(\vec{p}) + B^l_{1-}(\vec{p}), \tag{5.22}$$

$$A^l_+(\vec{p}) = \mathscr{A}^l_{0+}, \tag{5.23}$$

where

$$\begin{aligned} B^l_{1-}(\vec{p}) &:= \langle\vec{p}|(2\pi)^{d-1}\varpi(\vec{p}_0)e^{2ia_-\widehat{\varpi}}(\widehat{I}-\widehat{\Lambda})|\vec{p}_0\rangle \\ &= \varpi(\vec{p}_0)e^{2ia_-\widehat{\varpi}}\Big[(2\pi)^{d-1}\delta_{\vec{p}_0} - \sum_{n=1}^{\infty}\sum_{a=1}^{d_n}\tilde{\phi}_{n,a}(\vec{p}_0)^*\tilde{\phi}_{n,a}(\vec{p})\Big] \end{aligned} \tag{5.24}$$

and $\tilde{\phi}_{n,a}(\vec{p}) = (2\pi)^{d-1}\langle\vec{p}|\phi\rangle$ is the Fourier transform of $\phi_{n,a}(\vec{r})$.

The functions B^l_- and A^l_+ describe the reflection and transmission of the left-incident wave respectively. $\mathscr{B}^l_{0-}(\vec{p})$ and $\mathscr{A}^l_{0+}(\vec{p})$ are associated with the Hilbert space describing the interaction of the wave with the interior of the waveguide. We can identify them with the reflection and transmission coefficients of the part of the left-incident wave that interacts with the interior of the waveguide. The same argument applies to B^l_{1-} and we associate it with the reflection from the vertical boundaries at $z = a_-$ of the impenetrable walls.

Following the same procedure for right-incident waves we have

$$B^+_-(\vec{p}) = \mathscr{B}^r_{0-}(\vec{p}), \tag{5.25}$$

$$A^r_+(\vec{p}) = \mathscr{A}^r_{0+}(\vec{p}) + A^r_{1+}(\vec{p}), \tag{5.26}$$

where

$$A^r_{1+}(\vec{p}) = \varpi(\vec{p_0})e^{-2ia_+\varpi(\vec{p}_0)}((2\pi)^{d-1}\delta(\vec{p}-\vec{p}_0) - \sum_{n=1}^{\infty}\sum_{a=1}^{d_n}\tilde{\phi}^*_{n,a}(\vec{p}_0)\tilde{\phi_{n,a}(\vec{p})}) \tag{5.27}$$

Again, we associate the functions $\mathscr{B}^r_{0-}(\vec{p})$ and $\mathscr{A}^+_{0+}(\vec{p})$ with the interior of the waveguide and $A^r_{1+}(\vec{p})$ with the vertical boundary of the walls located at $z = a_+$.

Notice that, as expected, equations (5.22) and (5.25) show that there is no contribution to transmission amplitude from the impenetrable walls.

The scattering problem can be solved by inserting (5.22), (5.23) to (4.32), and (5.25), (5.26) to (4.34). This reduces to the calculation of $\mathscr{A}^{l/r}_{0+}$ and $\mathscr{B}^{l/r}_{0-}$, which can be done with the results of section 4 either with the transfer matrix or the scattering matrix.

5.1.1 The contribution of the interior of the waveguide to the scattering problem

We aim to use the machinery developed in chapter 4 to determine the contribution of the interior of the waveguide. To achieve this, we need to redefine some operators defined in the section 4 so they are associated with the interior of the waveguide. The operator $\widehat{W}$ can be expressed in the form (4.86) with the eigenvectors (5.11) and considering $\phi_{n,a}(\vec{r}) = \langle \vec{r} | \phi_{n,a} \rangle$, which implies

$$\widehat{W}\widehat{\Lambda} = \widehat{\Lambda}\widehat{W} = \widehat{W}. \tag{5.28}$$

Note that this shows $\widehat{W}\psi(\vec{r}) = 0$ if $\psi(\vec{r}) \in L^2[\mathbb{R}^{d-1} \setminus box]$ which implies that zero is an infinitely degenerate eigenvalue of $\widehat{W}$ with corresponding eigenvectors being the elements of $L^2[\mathbb{R}^{d-1} \setminus box]$. This implies

$$\widehat{W} = \sum_{n=1}^{\infty} \sum_{a=1}^{d_n} w_n |\phi_{n,a}\rangle\langle\phi_{n,a}|, \tag{5.29}$$

where

$$w_n = \begin{cases} \sqrt{k^2 - \mathcal{E}_n - \mathscr{V}_0} & \text{for } \sqrt{\mathcal{E}_n + \mathscr{V}_0} \leq k, \\ i\sqrt{\mathcal{E}_n + \mathscr{V}_0 - k^2} & \text{for } \sqrt{\mathcal{E}_n + \mathscr{V}_0} > k. \end{cases} \tag{5.30}$$

Now, we consider the operator $\widehat{\varpi}$ defined by (4.51). Let $\psi(\vec{r}, z)$ be a solution of the time-independent Schödinger equation (4.21) with potential (5.1). Then $\psi(\vec{r}, z) = 0$ when $\vec{r} \notin box$ and $z \in [a_-, a_+]$. This can be written as $(\widehat{I} - \widehat{\Lambda})|\psi(z)\rangle = 0$, which implies $\psi(\vec{r}, z) \in L^2[box]$. Equation (4.57) shows that this is also true for the solution

$\boldsymbol{\Psi}(z)$ of the time-dependent Schödinger equation (4.48). Let us define

$$\widehat{\varpi} := \widehat{\Lambda}\varpi(\hat{\vec{p}})\widehat{\Lambda}. \tag{5.31}$$

which together with (5.1) imply

$$\widehat{\boldsymbol{\mathcal{H}}}(z) = \frac{\mathscr{V}_0}{2}\widehat{\Lambda}e^{-i\widehat{\varpi}z\boldsymbol{\sigma}_3}\boldsymbol{\mathcal{K}}e^{-i\widehat{\varpi}z\boldsymbol{\sigma}_3}\widehat{\varpi}^{-1}(\vec{p})\widehat{\Lambda}, \text{ for } z \in [a_-, a_+]. \tag{5.32}$$

Using (5.29), (5.31) and (5.32), we can employ the methods developed in chapter 4 to solve the scattering problem for the interior of the waveguide.

First we observe that (5.31) implies

$$[\widehat{\varpi}, \widehat{\Lambda}] = 0. \tag{5.33}$$

Now, we consider $\widehat{\varpi}|\phi_{n,a}\rangle$, since $\widehat{\varpi}$ is a function of $\vec{p}^2$, we need to find how $\vec{p}^2$ act on $|\mathring{\psi}_{n,a}\rangle$. By definition we have

$$\langle\vec{r}|\vec{p}^2|\mathring{\phi}_{n,a}\rangle = -\nabla^2_{d-1}\mathring{\phi}_{n,a}(\boldsymbol{r}) = \mathcal{E}_n\mathring{\phi}_{n,a}(\vec{r}).$$

Combining this, (4.19), (4.51) and (5.11), we obtain

$$\langle\boldsymbol{r}|\widehat{\varpi}|\mathring{\phi}_{n,a}\rangle = \begin{cases} \varpi_n\phi_{n,a}(\vec{r}) & \text{for } \vec{r} \in box, \\ 0 & \text{for } \vec{r} \notin box, \end{cases}$$

where

$$\varpi_n := \begin{cases} \sqrt{k^2 - \mathcal{E}_n} & \text{for } \sqrt{\mathcal{E}_n} \leq k, \\ i\sqrt{\mathcal{E}_n - k^2} & \text{for } \sqrt{\mathcal{E}_n} > k. \end{cases} \tag{5.34}$$

This in turn implies

$$\widehat{\varpi}|\phi_{n,a}\rangle = \varpi_n|\phi_{n,a}\rangle, \tag{5.35}$$

and we find

$$\widehat{\varpi} = \widehat{\varpi}\widehat{\Lambda} = \sum_{n=1}^{\infty}\sum_{a=1}^{d_n}\varpi_n|\phi_{n,a}\rangle\langle\phi_{n,a}|. \tag{5.36}$$

In particular we can show that $\widehat{\varpi}$ and $\widehat{W}$ commute,

$$\begin{aligned}[\widehat{W},\widehat{\varpi}] &= \widehat{W}\widehat{\varpi} - \widehat{\varpi}\widehat{W} = \widehat{W}\widehat{\varpi}\widehat{\Lambda} - \widehat{\varpi}\widehat{W} \\ &= \widehat{W}\sum_{n=1}^{\infty}\sum_{a=1}^{d_n}\varpi_n|\phi_{n,a}\rangle\langle\phi_{n,a}| - \widehat{\varpi}\sum_{n=1}^{\infty}\sum_{a=1}^{d_n}w_n|\phi_{n,a}\rangle\langle\phi_{n,a}| \\ &= \sum_{n=1}^{\infty}\sum_{a=1}^{d_n}w_n\varpi_n|\phi_{n,a}\rangle\langle\phi_{n,a}| - \sum_{n=1}^{\infty}\sum_{a=1}^{d_n}\varpi_n w_n|\phi_{n,a}\rangle\langle\phi_{n,a}| = 0.\end{aligned} \tag{5.37}$$

This property simplifies the calculations of $\widehat{\Gamma}_\pm$ and the elements of the transfer matrix $\widehat{\mathbf{M}}$. In particular, for non-exceptional wavenumbers we get

$$e^{-ia\widehat{H}} = \frac{e^{-ia\widehat{W}}}{2\widehat{W}\widehat{\varpi}}\begin{bmatrix}\left[e^{2ia\widehat{W}}(\widehat{\varpi}+\widehat{W})^2 - (\widehat{\varpi}-\widehat{W})^2\right] & (\widehat{\varpi}^2-\widehat{W}^2)\left(1-e^{2ia\widehat{W}}\right) \\ (\widehat{W}^2-\widehat{\varpi}^2)\left(1-e^{2ia\widehat{W}}\right) & \left[e^{2ia\widehat{W}}(\widehat{\varpi}-\widehat{W})^2 - (\widehat{\varpi}+\widehat{W})^2\right]\end{bmatrix}, \tag{5.38}$$

which can be inserted to first (4.70) and then (4.41)-(4.44) to solve the scattering problem. Moreover, $\widehat{\Gamma}_\pm$ become

$$\widehat{\Gamma}_+ = \left[\frac{4\widehat{\varpi}\widehat{W}e^{ia\widehat{W}}}{(\widehat{\varpi}+\widehat{W})^2 - (\widehat{\varpi}-\widehat{W})^2 e^{2ia\widehat{W}}}\right]\widehat{\Lambda}, \tag{5.39}$$

$$\widehat{\Gamma}_- = \left[\frac{(\widehat{W}^2-\widehat{\varpi}^2)(\widehat{I}-e^{2ia\widehat{W}})}{(\widehat{\varpi}+\widehat{W})^2 - (\widehat{\varpi}-\widehat{W})^2 e^{2ia\widehat{W}}}\right]\widehat{\Lambda}. \tag{5.40}$$

These can be inserted to (4.118)-(4.121) in order to solve the scattering problem. These equations also hold for exceptional wavenumbers if $\mathscr{V}_0 \neq 0$. The same expressions can be found for an empty waveguide with an exceptional wavenumber by taking the limit $\mathscr{V}_0 \to 0$.

It is straight forward to show that

$$\begin{aligned}\widehat{M}_{22}^{-1} &= -\left(\widehat{M}_{11} - \widehat{M}_{12}\widehat{M}_{22}^{-1}\widehat{M}_{21}\right) = -\widehat{\Gamma}_+, \\ \widehat{M}_{22}^{-1}\widehat{M}_{21} &= -\widehat{M}_{12}\widehat{M}_{22}^{-1} = \widehat{\Gamma}_-.\end{aligned}$$

Let n_* be the largest positive integer such that $k \leq \sqrt{\mathcal{E}_{n_*} + \mathscr{V}_0}$. If $n_* \geq 1$, (5.30) implies $w_n = |w_n|$ if $n \leq n_*$ and $w_n = i|w_n|$ if $n > n_*$, which allows us to write $\widehat{\Gamma}_\pm$ as

$$\widehat{\Gamma}_\pm = \sum_{n=1}^{n_*}\sum_{a=1}^{d_n} r_\pm^n|\phi_{n,a}\rangle\langle\phi_{n,a}| + \sum_{n=n_*+1}^{\infty}\sum_{a=1}^{d_n} s_\pm^n|\phi_{n,a}\rangle\langle\phi_{n,a},| \tag{5.41}$$

where

$$r_n^+ := \frac{4|\omega_n|\varpi_n e^{ia|\omega_n|}}{(\varpi_n + |\omega_n|)^2 - (\varpi_n - |\omega_n|)^2 e^{2ia|\omega_n|}}, \tag{5.42}$$

$$s_n^+ := \frac{4i|\omega_n|\varpi_n e^{-a|\omega_n|}}{(\varpi_n + i|\omega_n|)^2 - (\varpi_n - i|\omega_n|)^2 e^{-2a|\omega_n|}}, \tag{5.43}$$

$$r_n^- := \frac{(|\omega_n|^2 - \varpi_n^2)(1 - e^{2ia|\omega_n|})}{(\varpi_n + |\omega_n|)^2 - (\varpi_n - |\omega_n|)^2 e^{2ia|\omega_n|}}, \tag{5.44}$$

$$s_n^- := -\frac{(|\omega_n|^2 + \varpi_n^2)(1 - e^{-2a|\omega_n|})}{(\varpi_n + i|\omega_n|)^2 - (\varpi_n - i|\omega_n|)^2 e^{-2a|\omega_n|}}. \tag{5.45}$$

Then inserting (4.122) to (5.41) we find

$$\begin{aligned} \widehat{\Gamma}_\pm(\vec{p}, \vec{p}_0) &= \langle \vec{p}_0 | \widehat{\Gamma} | \vec{p} \rangle \\ &= (2\pi)^{1-d} \left[\sum_{n=1}^{n_*} \sum_{a=1}^{d_n} r_n^\pm \tilde{\phi}(\vec{p}_0)^* \tilde{\phi}(\vec{p}) + \sum_{n=n_*+1}^{\infty} \sum_{a=1}^{d_n} s_n^\pm \tilde{\phi}(\vec{p}_0)^* \tilde{\phi}(\vec{p}) \right]. \end{aligned} \tag{5.46}$$

5.2 Two-dimensional finite waveguide

Now, we focus on the two dimensional case, and derive the results of [23]. For $d = 2$, we drop the label for degeneracy and the summation over d_n since energy eigenvalues particle trapped in a two-dimensional rectangular box are non-degenerate. Then (5.10) becomes

$$E_n = \mathcal{E}_n + \mathscr{V}_0, \qquad E_{0,n} = \left(\frac{\pi n}{L_x}\right)^2, \tag{5.47}$$

$$\phi_n(x) = \begin{cases} \sqrt{2/L_x} \sin \frac{\pi n x}{L_x} & \text{for } x \in [0, L_x], \\ 0 & \text{for } x \notin [0, L_x]. \end{cases} \tag{5.48}$$

Moreover, (5.28) and (5.33) become

$$w_n = \begin{cases} \sqrt{k^2 - (\pi n/L_x)^2 - \mathscr{V}_0} & \text{for } \sqrt{(\pi n/L_x)^2 + \mathscr{V}_0} \le k, \\ i\sqrt{(\pi n/L_x)^2 + \mathscr{V}_0 - k^2} & \text{for } \sqrt{(\pi n/L_x)^2 + \mathscr{V}_0} > k. \end{cases} \tag{5.49}$$

$$\varpi_n = \begin{cases} \sqrt{k^2 - (\pi n/L_x)^2 - \mathscr{V}_0} & \text{for } (\pi n/L_x) \le k, \\ i\sqrt{(\pi n/L_x)^2 + \mathscr{V}_0 - k^2} & \text{for } (\pi n/L_x) > k. \end{cases} \tag{5.50}$$

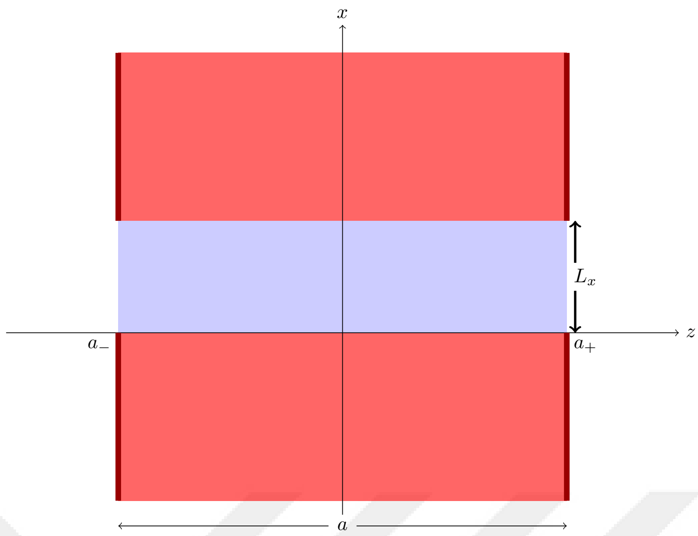

Figure 5.1: Schematic view of two dimensional waveguide of finite length a and height L_x. The potential is infinite inside the impenetrable walls which are illustrated as pink walls. Inside the waveguide there is a homogeneous lossless material(the region colored in blue). The thick dark red lines are the vertical boundaries of the impenetrable walls which contribute to the reflection of the waves.

Also we have,

$$\tilde{\phi_n}(p) = \begin{cases} \frac{\pi n\sqrt{2L_x}[e^{-i(L_x p - \pi n)}]}{((L_x p^2) - (\pi n)^2)} & \text{for } p \neq \pi n/L_x, \\ -i\sqrt{L_x/2} & \text{for } p = \pi n/L_x, \end{cases} \tag{5.51}$$

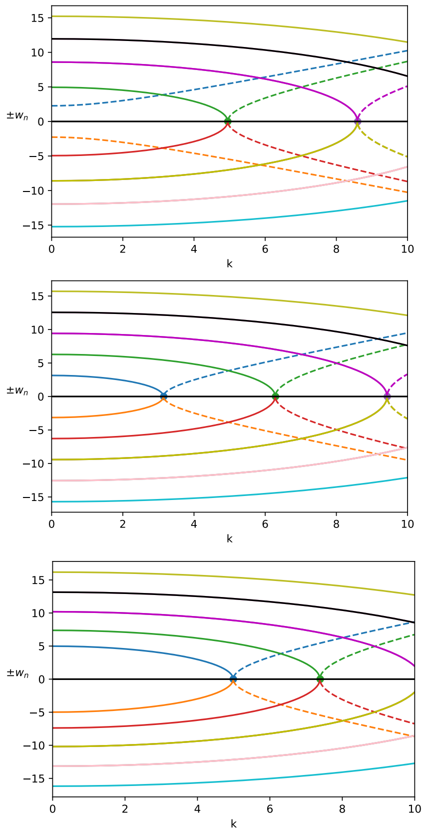

Figure 5.2: The eigenvalues $\pm w_n$ of $\widehat{\mathbf{H}}$ of a two dimensional waveguide for different potentials inside the waveguide. The solid lines are the real parts and the dashed lines are the imaginary parts of $\pm w_n$. The points of crossing with the k-axis are the exceptional points. The blue and orange, green and light red, magenta and yellow, black and pink, light green and light blue curves correspond to w_n and $-w_n$ respectively for $n = 1, 2, 3, 4, 5$. The upper figure has negative potential, the middle has no potential and lower figure has positive potential.

Fig (5.2) shows the plots of the eigenvalues $\pm w_n$ of the effective Hamiltonian $\widehat{\mathbf{H}}$ for $n = 1, 2, 3, 4, 5$ for negative, zero and positive potentials. The points where $\pm w_n$ intersect are the exceptional points of $\widehat{\mathbf{H}}$. As the parameter k increases, the values $\pm w_n$ decrease and eventually reach zero at the exceptional point. Beyond this exceptional point, they transition into imaginary values.

The largest integer n_* that makes $\pm w_n$ real is

$$n_* = \left\lfloor \frac{b}{n} \sqrt{k^2 - \mathscr{V}_0} \right\rfloor, \tag{5.52}$$

where $\lfloor x \rfloor$ is the largest integer that is smaller than x.

Now, we examine some limiting cases. Assume that the length of the waveguide is much larger than its width, that is $a \gg L_x$. Then for $n > n_*$ we find

$$\big(a|w_n|\big)^2 = a^2\left[\left(\frac{\pi n}{L_x}\right)^2 + \mathscr{V}_0 - k^2\right] \geq a^2\left[\left(\frac{\pi}{L_x}\right)^2(2n_* - 1)\right] > \left[\frac{a}{L_x}\right]^2.$$

This implies $a|w_n| \gg 1$ for $n > n_*$. Also we have

$$s_n^+ \to 0 \text{ as } a|w_n| \to \infty, \tag{5.53}$$

$$s_n^- \to t_n \text{ as } a|w_n| \to \infty, \tag{5.54}$$

where $s^\pm$ are defined as (5.43) and (5.45), and

$$t_n := \frac{|w_n| + i\varpi_n}{|w_n| - i\varpi_n} \tag{5.55}$$

Using these results and (5.46) become

$$\widehat{\Gamma}_+(\vec{p}_0, \vec{p}) \approx \frac{1}{2\pi}\sum_{n=1}^{n_*} r_n^+ \tilde{\phi}_n(\vec{p}_0)^* \tilde{\phi}_n(\vec{p}), \tag{5.56}$$

$$\widehat{\Gamma}_-(\vec{p}_0, \vec{p}) \approx \frac{1}{2\pi}\left[\sum_{n=1}^{n_*} r_n^- \tilde{\phi}_n(\vec{p}_0)^* \tilde{\phi}_n(\vec{p}) + \sum_{n=n_*+1}^{\infty} t_n \tilde{\phi}_n(\vec{p}_0)^* \tilde{\phi}_n(\vec{p})\right]. \tag{5.57}$$

This shows that the transmitted wave is determined by the Fourier transform of the first n_* eigenfunctions of the particle trapped in $[0, L_x]$.

In the limit $a \to \infty$ the approximations (5.56) and (5.57) become exact which agrees with the fact that there are finitely many waves that can propagate through a regular infinitely long waveguide.

Next, we focus on the cases where the wavenumber is smaller than any possible exceptional wavenumber, that is $k^2 < \pi^2/L_x^2 + \mathscr{V}_0$. Then $w_n = i|w_n|$ for all $n \in \mathbb{N}^+$ and (5.46) becomes

$$\widehat{\Gamma}_\pm(p, p_0) = \frac{1}{2\pi}\sum_{n=1}^{\infty} s_n^\pm \tilde{\phi}_n(p_0)^* \tilde{\phi}_n(p). \tag{5.58}$$

In addition with the condition $a \gg L_x$ we can use (5.53) and (5.54) to show that (5.58) becomes

$$\widehat{\Gamma}_+(p, p_0) \approx 0, \qquad \widehat{\Gamma}_+(p, p_0) \approx \frac{1}{2\pi}\sum_{n=1}^{\infty} t_n \tilde{\phi}_n(p_0)^* \tilde{\phi}_n(p). \tag{5.59}$$

The first approximation indicates that there is no transmitted wave from the waveguide whose length is much larger than its width i.e, act like a filter for waves with wavenumber $k^2 < \pi^2/L_x^2 + \mathscr{V}_0$.

Now, assume that the waveguide is empty, i.e., $\mathscr{V}_0 = 0$, which implies $w_n = \varpi_n$, which suggests $\widehat{W} = \widehat{\varpi}$, (5.39) and (5.40) reduce to

$$\widehat{\Gamma}_+ = e^{ia\widehat{W}}, \qquad \widehat{\Gamma}_- = 0, \tag{5.60}$$

and $\langle p_0|\widehat{\Gamma}_\pm|p\rangle$ become

$$\widehat{\Gamma}_+(p,p_0) = \frac{1}{2\pi}\sum_{n=1}^{\infty} e^{iaw_n}\tilde{\phi}(p_0)^*\tilde{\phi}(p), \qquad \widehat{\Gamma}_+(p,p_0) = 0. \tag{5.61}$$

The second equality shows that there is no contribution to the reflection from the interior of the waveguide as expected. We can express the first equality as

$$\widehat{\Gamma}_+(p,p_0) = \frac{1}{2\pi}\sum_{n=1}^{n_*} e^{ia|w_n|}\tilde{\phi}_n(p_0)^*\tilde{\phi}_n(p) + \sum_{n=n_*+1}^{\infty} e^{-a|w_n|}\tilde{\phi}_n(p_0)^*\tilde{\phi}_n(p) \tag{5.62}$$

and if we have $a \gg L_x$ we find

$$\widehat{\Gamma}_+(p,p_0) \approx \frac{1}{2\pi}\sum_{n=1}^{n_*} e^{ia\sqrt{k^2-(\pi n/L_x)^2}}\tilde{\phi}_n(p_0)^*\tilde{\phi}_n(p). \tag{5.63}$$

Then the transmission is determined by $\tilde{\phi}_n$ where $<\leq n_*$ Fourier transform of $\phi(x)$. Let k be the smallest possible exceptional wavenumber, i.e., $k = \pi n/L_x$, then (194) reduces to

$$\widehat{\Gamma}_+(p,p_0) \approx \frac{1}{2\pi}\tilde{\phi}_1(p_0)^*\tilde{\phi}_1(p). \tag{5.64}$$

This shows that the transmitted part of the scattered wave is independent of the length of the waveguide a. This is consequence of the emergence an exceptional point in the scattering problem.

Note that, for a nonempty waveguide, if $k = \pi/L_x + \mathscr{V}_0$, (5.56) reduces to

$$\widehat{\Gamma}_+(p,p_0) \approx \frac{1}{2\pi}r_1^+\tilde{\phi}_1(p_0)^*\tilde{\phi}_1(p), \tag{5.65}$$

where r_1^+ can be calculated from (5.42) by taking the limit $|w_1| \to 0$. Using L'Hopital rule, we can show that

$$\lim_{|w_n|\to 0} r_n^+ = 4\lim_{w_n\to 0}\frac{\frac{d}{dw_1}\left[|\omega_n|\varpi_n e^{ia|\omega_n|}\right]}{\frac{d}{dw_1}\left[(\varpi_n+|\omega_n|)^2-(\varpi_n-|\omega_n|)^2e^{2ia|\omega_n|}\right]} = \frac{1}{1-\frac{ia\varpi_{n*}}{2}} \tag{5.66}$$

where we assume $a \gg L_x$ for a non-empty waveguide

$$\varpi_{n_*} = \begin{cases} \sqrt{\mathscr{V}_0} & \text{for } \mathscr{V}_0 \geq 0, \\ i\sqrt{\mathscr{V}_0} & \text{for } \mathscr{V}_0 < 0. \end{cases} \tag{5.67}$$

(5.65) is not independent of the length a of the waveguide. The a dependence is given by (5.66).

Consider an empty two-dimensional waveguide of length a and height L_x, located between the lines $z = 0$ and $z = -a$, and $a \gg L_x$. We send a left-incident wave with wavenumber $k = \sqrt{2}\pi/L_x$ and incidence angle $\theta = 0$. In this case, $p_0 = k \sin\theta_0 = 0$ and $\varpi(p_0) = k$. Since the waveguide is empty, there is no reflection from the interior of the waveguide, we focus on the transmission which can be calculated using (5.63). With this choice of the wavenumber, only the Fourier transform of the first eigenfunction of particle in a box determines the transmission, and (5.63) becomes

$$\widehat{\Gamma}_{1,+}(\theta, 0) = \frac{1}{2\pi} e^{i\pi a/L_x} \tilde{\phi}_1^*(0)\tilde{\phi}_1(p). \tag{5.68}$$

Using (5.51) we find,

$$\tilde{\phi}_1(p = \frac{\sqrt{2}\pi}{L_x}\sin\theta) = \begin{cases} \frac{\sqrt{2L_x}(e^{-i\sqrt{2}\pi\sin\theta}+1)}{\pi\cos 2\theta} & \text{for } \theta \neq \pm\frac{\pi}{4}, \\ -i\sqrt{\frac{L_x}{2}} & \text{for } \theta = \pm\frac{\pi}{4}, \end{cases},$$

$$\tilde{\phi}_1^*(p_0 = 0) = i\sqrt{\frac{L_x}{2}}$$

Inserting these to (5.68) and making use of (4.121) we find the transmission amplitude,

$$T_1^l(\theta) = \cos\theta e^{i\pi c(\theta)} \begin{cases} \frac{(e^{-i\sqrt{2}\pi\sin\theta}+1)}{\pi\cos 2\theta} & \text{for } \theta \neq \frac{\pi}{4}, \\ -i\frac{\sqrt{\pi}}{2} & \text{for } \theta = \frac{\pi}{4}, \end{cases}$$

where $c(\theta) := [(1 - \sqrt{2}\cos\theta)a_+ + (\sqrt{2} - 1)a_-]/L_x$.

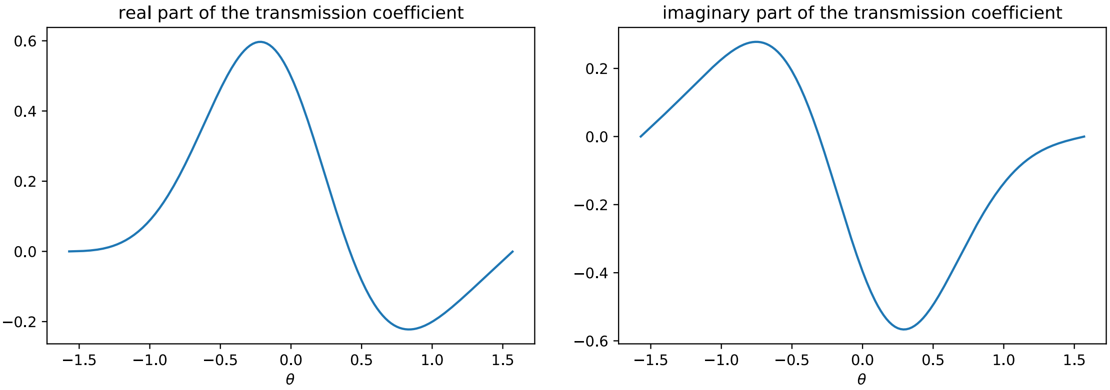

Figure 5.3: Real and imaginary parts of transmission amplitude of an empty 2D finite waveguide, for $a_+ = 0, a_- = -1000L_x$ and $k = \sqrt{2}\pi/L_x$ and incidence angle $\theta_0 = 0$.

Using (4.12) for $d = 2$, the transmitted wave becomes

$$\phi_{trans} = (1-i)e^{\sqrt{2}\pi r/L_x}\sqrt{\frac{L_x}{r}}\cos\theta e^{i\pi c(\theta)} \times \begin{cases} \frac{(e^{-i\sqrt{2}\pi\sin\theta}+1)}{\sqrt{\pi^3}\cos 2\theta} & \text{for } \theta \neq \frac{\pi}{4}, \\ -i\frac{1}{2} & \text{for } \theta = \frac{\pi}{4}, \end{cases}$$

where we used (4.12).

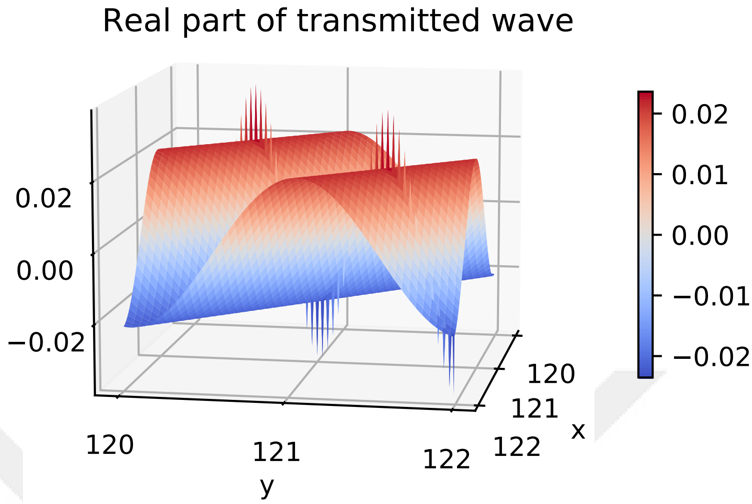

Figure 5.4: Real part of transmitted wave from a finite waveguide, where $a_+ = 0, a_- = -1000L_x$ and $k = \sqrt{2}\pi/L_x$ and incident angle $\theta = 0$, in the range $120 \leq x \leq 122$

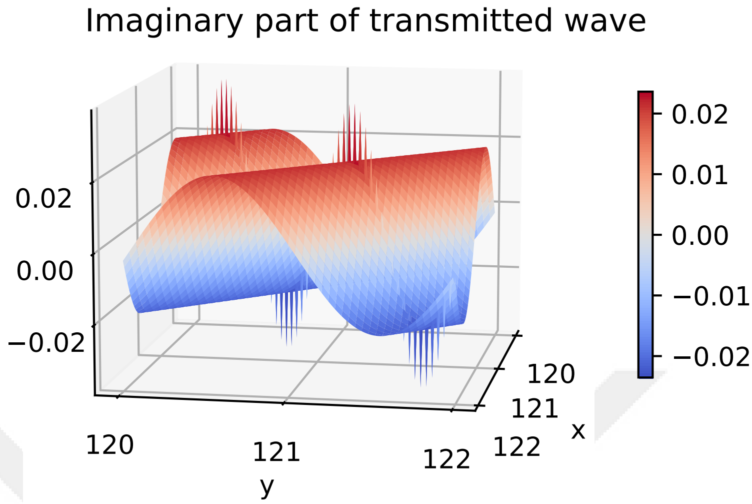

Figure 5.5: Real part of transmitted wave from a finite waveguide, where $a_+ = 0, a_- = -1000L_x$ and $k = \sqrt{2}\pi/L_x$ and incident angle $\theta = 0$, in the range $120 \leq x \leq 122$

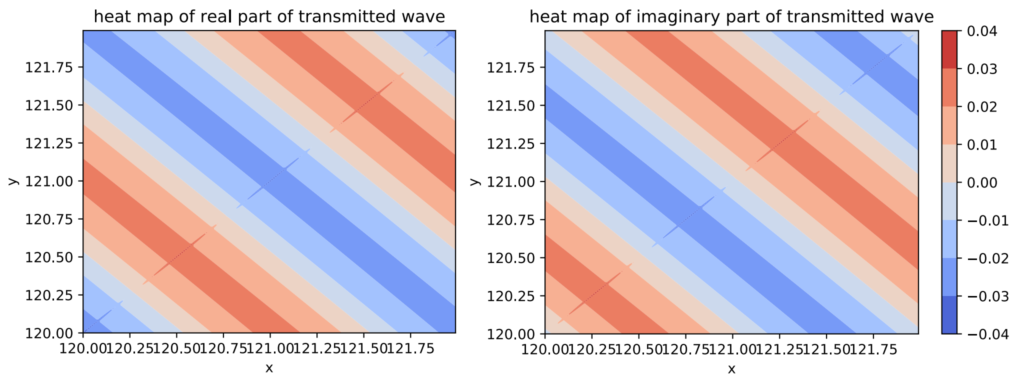

Figure 5.6: Heat map of real and imaginary parts of transmitted wave from a finite waveguide, where $a_+ = 0, a_- = -1000L_x$ and $k = \sqrt{2}\pi/L_x$ and incident angle $\theta = 0$, in the range $120 \leq x \leq 122$

5.3 Three dimensional finite waveguide

Now, we focus on a three-dimensional finite waveguides. In this case the operator $\hat{h}$ describes the problem of a quantum particle trapped in a two-dimensional rectangular well $[0, L_x] \times [0, L_y]$. The energy eigenvalues and corresponding eigenvectors of this problem are given by

$$E_{n_x,n_y} = \mathcal{E}_{n_x,n_y} + \mathscr{V}_0, \qquad \mathcal{E}_{n_x,n_y} = \left(\frac{\pi n_x}{L_x}\right)^2 + \left(\frac{\pi n_y}{L_y}\right)^2, \tag{5.69}$$

$$\phi_{n_x,n_y}(\boldsymbol{r}) = \begin{cases} \sqrt{2/L_x}\sin\frac{\pi n_x x}{L_x}\sqrt{2/L_y}\sin\frac{\pi n_y y}{L_y} & \text{if } (x,y) \in box, \\ 0 & \text{if } (x,y) \notin box, \end{cases} \tag{5.70}$$

where $n_x, n_y \in \mathbb{Z}^+$.

$$\phi_{n_x,n_y}(\boldsymbol{r}) = \begin{cases} \phi_{n_x}(x)\phi_{n_y}(y) & \text{if } (x,y) \in box, \\ 0 & \text{if } (x,y) \notin box, \end{cases}$$

where

$$\phi_{n_x}(x) = \sqrt{2/L_x}\sin\frac{\pi n_x x}{L_x},$$
$$\phi_{n_y}(x) = \sqrt{2/L_y}\sin\frac{\pi n_y y}{L_y},$$

Moreover we have

$$\tilde{\phi}_{n_x,n_y} = \tilde{\phi}_{n_x}\tilde{\phi}_{n_y}$$

where $\tilde{\phi}_{n_x}$ and $\tilde{\phi}_{n_y}$ can be found by (5.51) replacing n and L with n_x and L_x, and n_y and L_y respectively. Unlike its one dimensional counterpart, the energy eigenvalues of particle trapped in a two-dimensional rectangular well can be degenerate depending on the ratio L_x/L_y. We examine all the possible cases of degeneracies below.

1. If $\frac{L_x}{L_y} = p \in \mathbb{Q}^+$, then energy levels E_{n_x,n_y} and $E_{n'_x,n'_y}$ are equal if $n_x = Na, n_y = b$ and $n'_x = a, n'_y = Nb$, where $p = a/b$ and $gcd(a,b) = 1$.

2. If $\left(\frac{L_x}{L_y}\right)^2 = p = a/b \in \mathbb{Q}^+$, the energy levels E_{n_x,n_y} and $E_{n'_x,n'_y}$ are equal if $b(n_x^2 - n_x'^2) = a(n_y'^2 - n_y^2)$. For example if $\frac{L_x}{L_y} = \sqrt{2}$, $E_{2,5} = E_{6,3}$.

3. If $\left(\frac{L_x}{L_y}\right)^2$ is an irrational number, there are no energy levels E_{n_x,n_y} and $E_{n'_x,n'_y}$, that are equal for distinct pairs of (n_x, n_y) and (n'_x, n'_y).

We aim to use the machinery developed in section 5.1, which requires to label energy eigenvalues and the corresponding eigenvectors like the two-dimensional problem, where $\mathcal{E}_n$ denotes the nth smallest energy eigenvalue. Clearly, the labels (n_x, n_y) introduced in (5.69) do not fulfill this condition. To fix this, let E_n be the nth energy eigenvalue of $\hat{h}$ and let $(n_x, n_y) \in \mathbb{N}^+$ such that $\mathcal{E}_n := \mathcal{E}_{n_x,n_y}$ and let $\mathring{\psi}_n := \mathring{\psi}_{n_x,n_y}$. If there is degeneracy there can be multiple pairs of (n_x, n_y) that correspond to n. Let d_n be the degeneracy level of E_n, in this case n is still the label for the nth largest eigenvalue nothing changes for the energy levels. To differentiate between two different eigenvectors, we use the label a as $\mathring{\phi}_{n,a} := \mathring{\phi}_{n_x,n_y}$, where $a \in 1, 2, \cdots, d_n$. Then each pair (n_x, n_y) is uniquely mapped to the pair (n, a)i and we can express (5.69) and (5.70) as

$$E_n = \mathcal{E}_n + \mathscr{V}_0, \qquad\qquad \mathcal{E}_n = \mathcal{E}^0_{n_x,n_y} = \left(\frac{\pi n_x}{L_x}\right)^2, \tag{5.71}$$

$$\phi_{n,a}(x,y) = \begin{cases} \mathring{\phi}_{n,a}(x,y) & \text{for } (x,y) \in box, \\ 0 & \text{for } (x,y) \notin box, \end{cases} \tag{5.72}$$

Here,

$$\mathring{\phi}_{n,a} := \sqrt{2/L_x}\sin\frac{\pi n_x x}{L_x}\sqrt{2/L_y}\sin\frac{\pi n_y y}{L_y}$$

and (n_x, n_y) are the pair of positive natural numbers associated uniquely with (n, a).

Fig. (5.4) shows the eigenvalues $\pm w_n$ of the effective Hamiltonian $\widehat{\mathbf{H}}$ for the three-dimensional waveguide. Then following the example of the previous section we define

$$\widehat{\varpi} = \sum_{n=1}^{\infty}\sum_{a=1}^{d_n} \varpi_n |\phi_{n,a}\rangle\langle\phi_{n,a}|, \tag{5.73}$$

where

$$\varpi_n := \begin{cases} \sqrt{k^2 - \mathcal{E}_n} & \text{for } k \geq \sqrt{\mathcal{E}_n}, \\ i\sqrt{\mathcal{E}_n - k^2} & \text{for } k < \sqrt{\mathcal{E}_n}. \end{cases} \tag{5.74}$$

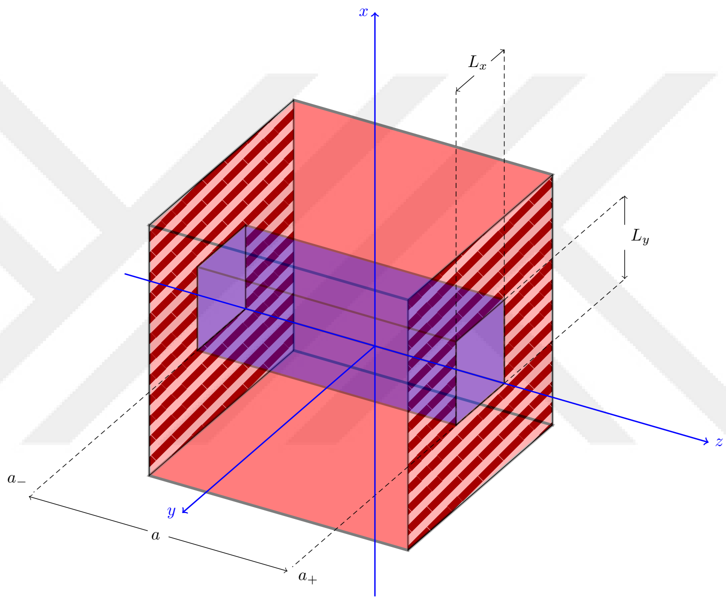

Figure 5.7: Schematic view of three-dimensional waveguide of finite length a, height L_x and width L_y. The potential is infinite inside the impenetrable walls which are illustrated as pink walls. Inside the waveguide there is a homogeneous lossless material(the region colored in blue). The pinks walls with red dashed lines are the vertical boundaries of the impenetrable walls which contribute to the reflection of the waves.

Similarly, the operator $\widehat{W}$ is

$$\widehat{W} = \sum_{n=1}^{\infty} \sum_{a=1}^{d_n} w_n |\phi_{n,a}\rangle\langle\phi_{n,a}|, \tag{5.75}$$

where

$$w_n := \begin{cases} \sqrt{k^2 - \mathcal{E}_n - \mathscr{V}_0} & \text{for } k \geq \sqrt{\mathcal{E}_n + \mathscr{V}_0}, \\ i\sqrt{\mathcal{E}_n + \mathscr{V}_0 - k^2} & \text{for } k < \sqrt{\mathcal{E}_n + \mathscr{V}_0}. \end{cases} \tag{5.76}$$

Here we used (4.85),(4.86) and (5.71).

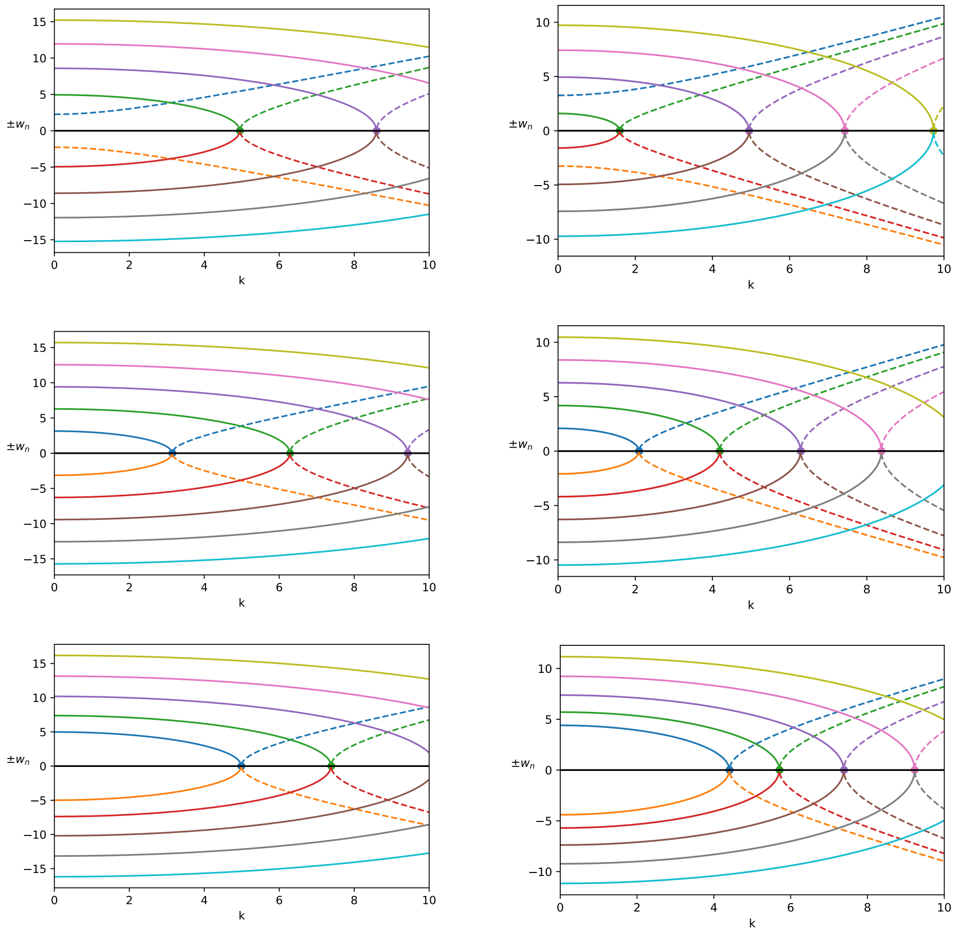

Figure 5.8: Plots of real and imaginary parts of the eigenvalues $\pm w_n$ of $\widehat{\mathbf{H}}$ for three-dimensional waveguides $L_x = L_y$ (on the left) and $L_y = 1.5L_x$ (on the right) for $n = 1, 2, 3$, $\mathscr{V}_0 = 0$. The solid lines are real parts and dashed lines are imaginary part of $\pm w_n$. The points of crossing with the k-axis are the exceptional points. The blue and orange, green and light red, magenta and yellow, black and pink, light green and light blue curves correspond to w_n and $-w_n$ respectively for $n = 1, 2, 3, 4, 5$. The upper figures have negative potential, the middle figures have no potential and lower figures have positive potential.

Another difference of the three dimensional problem is that we have two length scales (L_x, L_y) instead of one (L_x). This changes the comparison between the length of the waveguide a with its width. First assume that the length of the waveguide is much larger than both its width L_x and its height L_y, that is $a \gg L_x$ and $a \gg L_y$. For simplicity assume $L_x = L_y$. Let n_* be the largest integer such that $E_{n_*} \geq k$.

Then for $n > n_*$ we find

$$\begin{aligned}\big(a|w_n|\big)^2 &= a^2\left[\left(\frac{\pi n_x}{L_x}\right)^2 + \left(\frac{\pi n_y}{L_y}\right)^2 + \mathscr{V}_0 - k^2\right]\\ &\geq a^2\left[\left(\frac{\pi}{L_x}\right)^2(n_x^2 - n_{x*}^2) + \left(\frac{\pi}{L_y}\right)^2(n_y^2 - n_{y*}^2)\right]\\ &= a^2\left[\left(\frac{\pi}{L_x}\right)^2(2n_{x*} - 1)\right] > \left[\frac{a}{L_x}\right]^2 \gg 1.\end{aligned}$$

where (n_x, n_y) are one of the pair of labels that is associated to n and (n_{x*}, n_{y*}) are one of the pair of labels that is associated with n_*.

Now we consider the waveguide where its width L_y is comparable to its length a, i.e., $L_y \sim a$ and its height L_x is mush smaller than its length, i.e., $a \gg L_y$. In order to make the calculations easier let $a = L_x$. Then for $n > n_*$ we get

$$\begin{aligned}\big(a|w_n|\big)^2 &= a^2\left[\left(\frac{\pi n_x}{L_x}\right)^2 + \left(\frac{\pi n_y}{L_y}\right)^2 + \mathscr{V}_0 - k^2\right]\\ &\geq a^2\left[\left(\frac{\pi}{L_x}\right)^2(n_x^2 - n_{x*}^2) + \left(\frac{\pi}{L_y}\right)^2(n_y^2 - n_{y*}^2)\right]\\ &\geq a^2\left[\left(\frac{\pi}{L_x}\right)^2 + \left(\frac{\pi}{L_y}\right)^2\right] = a^2\pi^2 + \left[\frac{a}{L_y}\right]^2 > \left[\frac{a}{L_y}\right]^2 \gg 1.\end{aligned}$$

It is easy to see that this holds for $a \gg L_x$ and and $L_y \sim L_x$. In the following we assume $L_y \geq L_x$.

In both cases, $a \gg L_x, L_y$ and $L_x \sim L_y$, and $a \sim L_y$ and $a \gg L_x$, we have $a|w_n| \gg 1$ which implies that the limits (5.53) and (5.54) hold for the three-dimensional problems and we find

$$\widehat{\Gamma}_+(\boldsymbol{p}_0, \boldsymbol{p}) \approx \frac{1}{4\pi^2}\sum_{n=1}^{n_*}\sum_{a=1}^{d_n} r_n^+ \tilde{\phi}_{n,a}(\vec{p}_0)^*\tilde{\phi}_{n,a}(\vec{p}), \tag{5.77}$$

$$\begin{aligned}\widehat{\Gamma}_-(\boldsymbol{p}_0, \boldsymbol{p}) \approx \frac{1}{4\pi^2}&\left[\sum_{n=1}^{n_*}\sum_{a=1}^{d_n} r_n^- \tilde{\phi}_{n,a}(\vec{p}_0)^*\tilde{\phi}_{n,a}(\vec{p})\right.\\ &\left. + \sum_{n=n_*+1}^{\infty}\sum_{a=1}^{d_n} t_n\tilde{\phi}_{n,a}(\vec{p}_0)^*\tilde{\phi}_{n,a}(\vec{p}).\right.\end{aligned} \tag{5.78}$$

where t_n is given by (5.55). Similar to the two-dimensional waveguide, in the limit $a \to \infty$, the approximations become exact, which agrees with the fact that there are finitely many modes that are allowed to travel inside an infinite waveguide. For the case $a \sim L_y$ this is equivalent to a parallel plate waveguide.

Assume the wavenumber is smaller than all possible exceptional wavenumbers, i.e., $k < \pi\sqrt{(1/L_x)^2 + (1/L_y)^2}$. Then $w_n = i|w_n|$ for all $n \in \mathbb{N}^+$ and (5.46) becomes

$$\widehat{\Gamma}_\pm(p, p_0) = \frac{1}{4\pi^2}\sum_{n=1}^{\infty}\sum_{a=1}^{d_n} s_n^\pm \tilde{\phi}_n(p_0)^* \tilde{\phi}_n(p). \tag{5.79}$$

In addition with the condition $a \gg L_x$, (5.77) and (5.78) reduce to

$$\widehat{\Gamma}_+(p, p_0) \approx 0, \qquad \widehat{\Gamma}_-(p, p_0) \approx \frac{1}{4\pi^2}\sum_{n=1}^{\infty}\sum_{a=1}^{d_n} t_n \tilde{\phi}_n(p_0)^* \tilde{\phi}_n(p). \tag{5.80}$$

The first approximation indicates that there is no transmission which means a waveguide filled with inactive material, whose length is much larger than its width acts like a filter for waves with wavenumber $k^2 < \pi^2(1/L_x^2 + 1/L_y^2) + \mathscr{V}_0$.

If the waveguide is empty, that is, $\mathscr{V}_0 = 0$, we have $\widehat{W} = \widehat{\varpi}$ and (5.46) becomes

$$\widehat{\Gamma}_+ = e^{ia\widehat{W}}\widehat{\Lambda}, \qquad \widehat{\Gamma}_- = 0 \tag{5.81}$$

$$\widehat{\Gamma}_+(p, p_0) = \frac{1}{4\pi^2}\sum_{n=1}^{\infty}\sum_{n,a}^{d_n} e^{iaw_n} \tilde{\phi}_{n,a}(p_0)^* \tilde{\phi}_{n,a}(p), \qquad \widehat{\Gamma}_-(p, p_0) = 0. \tag{5.82}$$

The second equality implies that there is no contribution to reflection from the interior of the waveguide as expected. We can express the first equality as

$$\widehat{\Gamma}_+(p, p_0) = \frac{1}{4\pi^2}\sum_{n=1}^{n_*}\sum_{n,a}^{d_n} e^{ia|w_n|} \tilde{\phi}_{n,a}(p_0)^* \tilde{\phi}_{n,a}(p) + \frac{1}{4\pi^2}\sum_{n=n_*+1}^{\infty}\sum_{n,a}^{d_n} e^{-a|w_n|} \tilde{\phi}_{n,a}(p_0)^* \tilde{\phi}_{n,a}(p) \tag{5.83}$$

and if $a \gg L_x$ or $a \sim L_x$ and $a \gg L_y$, then $a|w_n| \gg 1$ for $n > n_*$ and we find

$$\widehat{\Gamma}_+(p, p_0) \approx \frac{1}{4\pi^2}\sum_{n=1}^{n_*}\sum_{a=1}^{d_n} e^{ia\sqrt{k^2 - \mathcal{E}_n}} \tilde{\phi}_n(p_0)^* \tilde{\phi}_n(p). \tag{5.84}$$

Let k be the smallest possible exceptional wavenumber, i.e., $k = \mathcal{E}_1 = \pi\sqrt{1/L_x^2 + 1/L_y^2}$, then (5.84) reduces to

$$\widehat{\Gamma}_+(p, p_0) \approx \frac{1}{4\pi^2}\tilde{\phi}_1(p_0)^* \tilde{\phi}_1(p). \tag{5.85}$$

Here we dropped the label of degeneracy since the first energy level is always non degenerate. This implies that the transmitted part of the scattered wave is independent of the length of the waveguide a. Again this is a direct result of exceptional points in the scattering problem.

Note that, for a nonempty waveguide, if $k = \pi\sqrt{1/L_x^2 + 1/L_y^2}$, (5.77) reduces to

$$\widehat{\Gamma}_+(p, p_0) \approx \frac{1}{4\pi^2} r_1^+ \tilde{\phi}_1(p_0)^* \tilde{\phi}_1(p), \tag{5.86}$$

where r_{n*}^+ for any exceptional wavenumber is given by (5.66).

Let $k = \sqrt{2}\pi/L_x$ and the incident angle $\theta_0 = 0$ and $\psi_0 = 0$. This makes $p_x = \sqrt{2}\pi/L_x \sin\theta\cos\varphi$, $p_y = \sqrt{2}\pi/L_x \sin\theta\sin\varphi$, $\boldsymbol{p}_0 = 0$ and $\varpi(p_0) = k$.

Assume that the waveguides has equal height and width $L_x = L_y$. For this choice of the wavenumber we have an exceptional point, (5.85) applies and

$$\widehat{\Gamma}_+ = \frac{1}{4\pi^2} \tilde{\phi}_{1,1}(0)^* \tilde{\phi}_{1,1}(\vec{p}) \tag{5.87}$$

Here,

$$\tilde{\phi}_{1,1}(\vec{p}) = \tilde{\phi}_1(\vec{p}_x)\tilde{\phi}_1(\vec{p}_y), \qquad \tilde{\phi}_{1,1}(\vec{p}_0 = 0) = \tilde{\phi}_1(0)\tilde{\phi}_1(0)$$

where $\tilde{\phi}_1(\vec{p}_{x,y})$ can be found using (5.51). Here we focus on $\varphi = 0$ and $\varphi = \pi/4$.

For $\varphi = 0$, $p_x = p$ and $p_y = 0$ and $\tilde{\phi}_{1,1}(0)^* \tilde{\phi}_{1,1}(\vec{p})$ becomes

$$\begin{aligned}
\tilde{\phi}_{1,1}(0)^* \tilde{\phi}_{1,1}(\vec{p}) &= i\left(\frac{L_x}{2}\right)^{3/2} \times \begin{cases} \frac{\sqrt{2L_x}(e^{-i\sqrt{2}\pi\sin\theta}+1)}{\pi\cos 2\theta} & \text{for } \theta \neq \frac{\pi}{4} \\ & \text{for } \theta = \frac{\pi}{4}, \end{cases} \\
&= \begin{cases} \frac{L_x^2(e^{-i\sqrt{2}\pi\sin\theta}+1)}{2\pi\cos 2\theta} & \text{for } \theta \neq \frac{\pi}{4} \\ \frac{L_x^2}{4} & \text{for } \theta = \pi/4 \end{cases}
\end{aligned}$$

Inserting this to (5.85) we find

$$\widehat{\Gamma}_+(\theta, 0) = \begin{cases} \frac{L_x^2(e^{-i\sqrt{2}\pi\sin\theta}+1)}{8\pi^3\cos 2\theta} & \text{for } \theta \neq \frac{\pi}{4}, \\ \frac{L_x^2}{16\pi^2} & \text{for } \theta = \pi/4. \end{cases}$$

Then, the transmission coefficient for $\phi = 0$ becomes

$$T^l(\theta, 0) = i\cos\theta e^{ik(a_- - a_+\cos\theta)} \times \begin{cases} \frac{L_x(e^{-i\sqrt{2}\pi\sin\theta}+1)}{2\sqrt{2}\pi^2\cos 2\theta} & \text{for } \theta \neq \frac{\pi}{4}, \\ \frac{L_x}{4\sqrt{2}\pi} & \text{for } \theta = \pi/4. \end{cases}$$

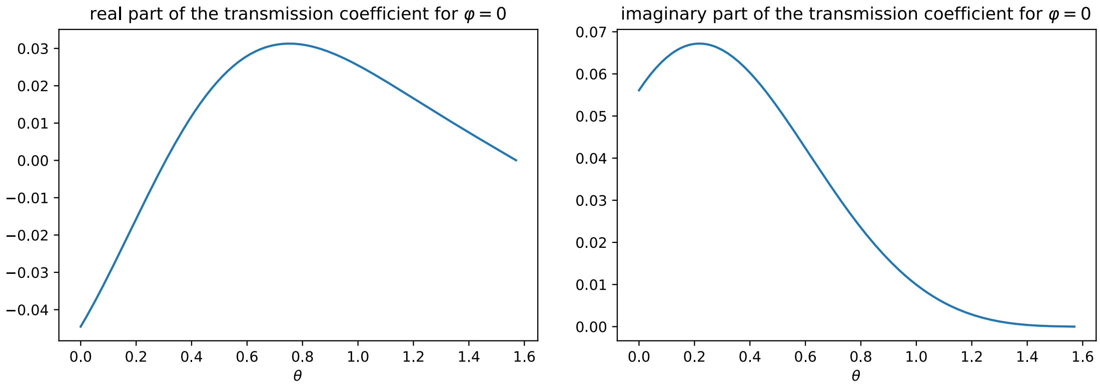

Figure 5.9: Real and imaginary part of transmission coefficient of a three-dimensional waveguide of height and width L_x, located between the planes $z = -1000L_x$ and $z = 0$, where the incident wavenumber is $k = \sqrt{2}\pi/L_x$ and incident angle $\theta_0 = 0, \varphi_0 = 0$, calculated at $\varphi = 0$.

Inserting the transmission coefficient to equation (4.12), we find the scattered wave,

$$\phi^l_{trans} = \frac{e^{ikr} L_x}{r} \cos\theta e^{ik(a_- - a_+ \cos\theta)} \times \begin{cases} \frac{i(e^{-i\sqrt{2}\pi \sin\theta}+1)}{2\sqrt{2}\pi^2 \cos 2\theta} & \text{for } \theta \neq \frac{\pi}{4}, \\ \frac{i}{4\sqrt{2}\pi} & \text{for } \theta = \pi/4. \end{cases} \quad (5.88)$$

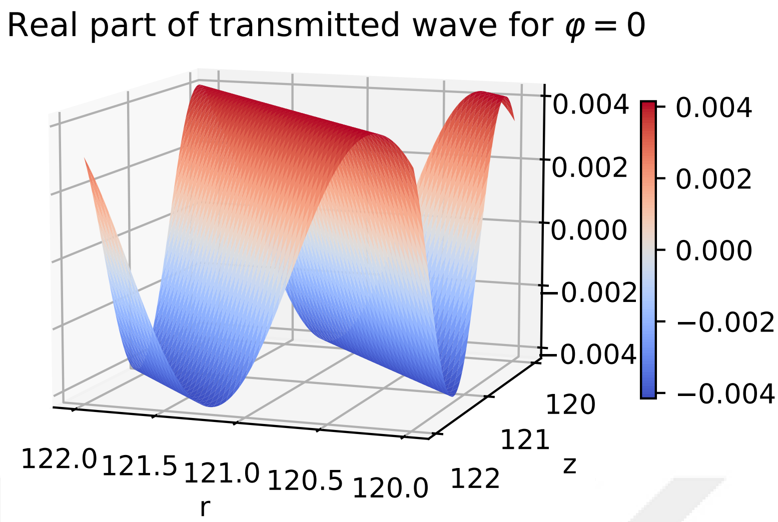

Figure 5.10: Real part of transmitted wave from a three-dimensional finite of height and width $L_x$waveguide, located between the planes $z = 0, z = -1000L_x$, in the range $120 \leq r \leq 122$ and $\varphi = 0$. The incident wavenumber is $k = \sqrt{2}\pi/L_x$ and incident angles are $\theta_0, \varphi_0 = 0$.

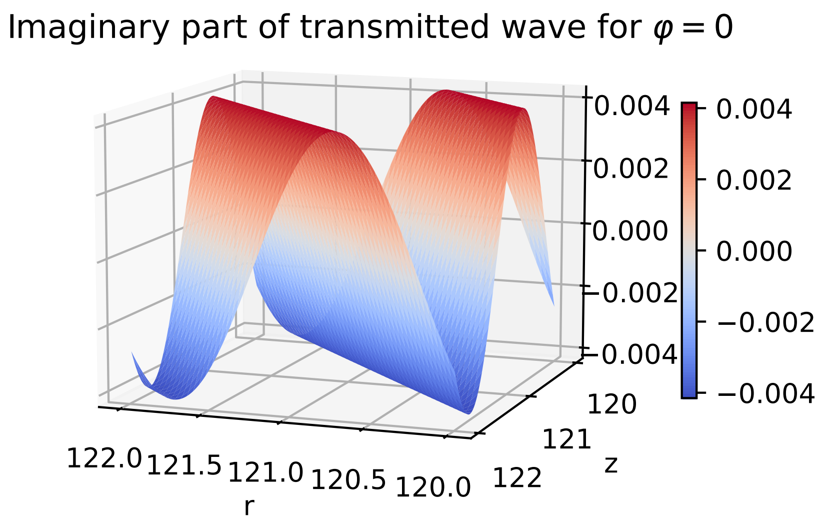

Figure 5.11: Real part of transmitted wave from a three-dimensional finite of height and width $L_x$waveguide, located between the planes $z = 0, z = -1000L_x$, in the range $120 \leq r \leq 122$ and $\varphi = 0$. The incident wavenumber is $k = \sqrt{2}\pi/L_x$ and incident angles are $\theta_0, \varphi_0 = 0$.

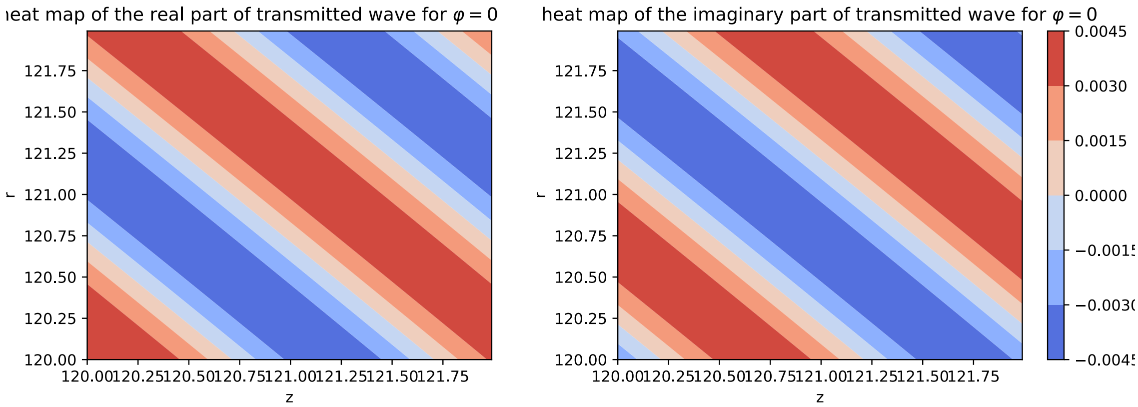

Figure 5.12: Heat map of the real and the imaginary parts of transmitted wave from a three-dimensional finite waveguide where $\varphi = 0$.

For $\varphi = \pi/4$, $p_x = p_y = \pi/L_x \sin\theta$ and the (5.84) becomes

$$\widehat{\Gamma}_+(\theta, 0) = \frac{L_x^2(e^{-i\pi\sin\theta} + 1)^2}{4\pi^4\cos^2\theta}.$$

Inserting this to (4.119) we find the transmission coefficient for $\varphi = \pi/4$,

$$T^l(\theta, 0) = -i\frac{L_x(e^{-i\pi\sin\theta} + 1)^2}{\sqrt{2}\pi^3\cos\theta}.$$

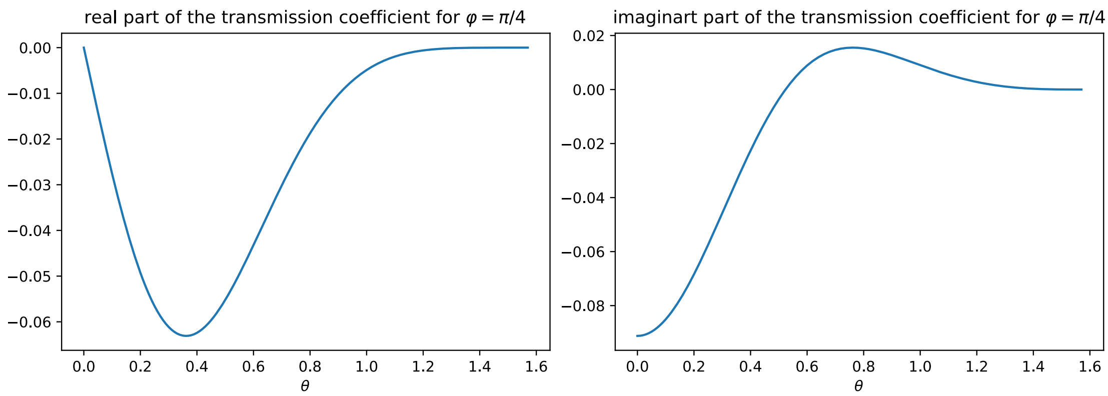

Figure 5.13: CReal and imaginary part of transmission coefficient of a three-dimensional waveguide of height and width L_x, located between the planes $z = -1000L_x$ and $z = 0$, where the incident wavenumber is $k = \sqrt{2}\pi/L_x$ and incident angle $\theta_0 = 0, \varphi_0 = 0$, calculated at $\varphi = \pi/4$.

Using (4.12), we get the transmitted wave,

$$\phi_{trans} = -i\frac{e^{i\sqrt{2}\pi r/L_x} L_x}{r} \frac{(e^{-i\pi\sin\theta}+1)^2}{\sqrt{2}\pi^3\cos\theta}.$$

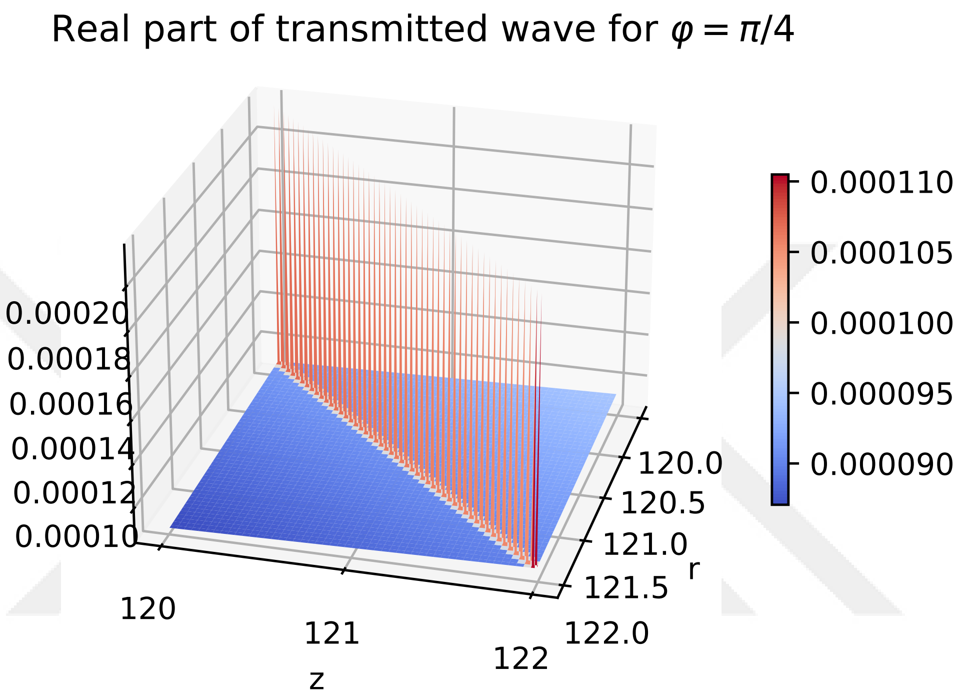

Figure 5.14: Real part of transmitted wave from a three-dimensional finite of height and width $L_x$waveguide, located between the planes $z = 0, z = -1000L_x$, in the range $120 \leq r \leq 122$ and $\varphi = 0$. The incident wavenumber is $k = \sqrt{2}\pi/L_x$ and incident angles are $\theta_0, \varphi_0 = \pi/4$.

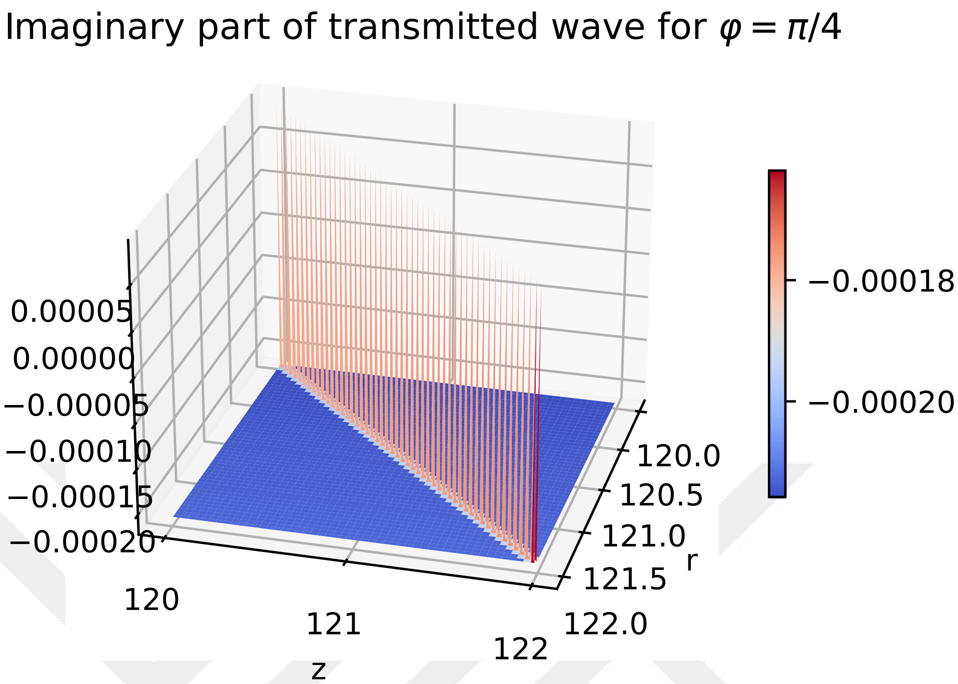

Figure 5.15: Imaginary part of transmitted wave from a three-dimensional finite of height and width $L_x$waveguide, located between the planes $z = 0, z = -1000L_x$, in the range $120 \leq r \leq 122$ and $\varphi = 0$. The incident wavenumber is $k = \sqrt{2}\pi/L_x$ and incident angles are $\theta_0, \varphi_0 = \pi/4$.

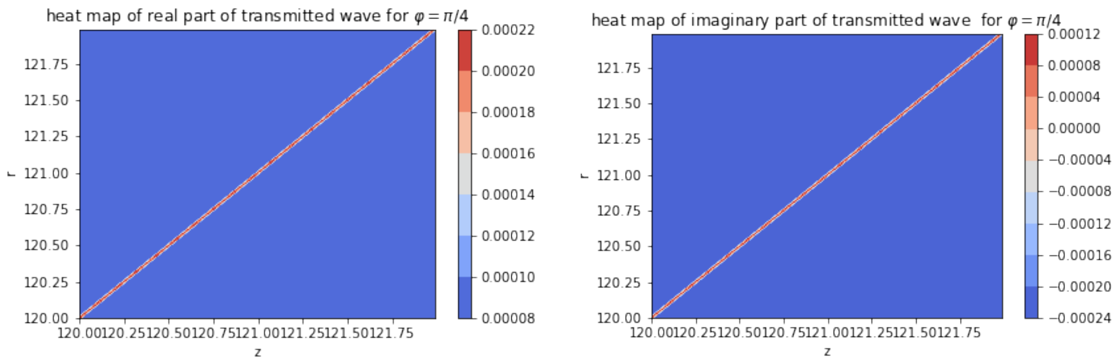

Figure 5.16: Caption

5.4 Comparision of two-dimensional and three-dimensional waveguides

The properties of two- and three-dimensional waveguides are mostly similar. Consider cases when the waveguides whose length a is much larger than its height L_x for both dimensions. Then the transmission amplitude is determined by the Fourier transform of $\phi_{n,a}$ for $n \leq n_*$. If the incident wavenumber is smaller than the smallest possible wavenumber, the waveguides act like a filter for these wavenumbers. For an empty waveguide, if the wavenumber is equal to the smallest possible wavenumber, the transmission is independent of the length of the waveguide.

There is two additional properties of the three-dimensional case over the two-dimensional one; the effective Hamiltonian $\widehat{\mathbf{H}}$ of the three-dimensional case can have degenerate eigenvalues and there is an extra length parameter L_y. Fig (5.8) shows that the exceptional wavenumbers of a three- dimensional waveguide gets closer to each other as L_y increases. This happens because the differences between energy levels of the particle trapped in a two-dimensional rectangular well gets smaller as L_y increases.

As k increases the number of $\tilde{\phi}_{n,a}$ that are included in the summations (5.63) and (5.82) increases. Since the exceptional wavenumbers of a three-dimensional waveguide gets closer as L_y increases, wider three-dimensional waveguides are more sensitive to the changes in k, than other three-dimensional waveguides and two-dimensional waveguides of the same height. Here more sensitive we mean that as k increases a larger number of $\tilde{\phi}_{n,a}$ determine the transmission amplitude. Since the restriction $a \gg L_x$ is enough for (5.82), we are free to choose L_y.

To see this difference we consider six empty waveguides of the same length a and same height L_x. The first waveguide is two-dimensional. The second, third, fourth, fifth and sixth waveguides are three-dimensional of width $L_x, (\pi/3)L_x, 10L_x$, $50L_x$ and $100L_x$. Fig (5.17) shows the exceptional wavenumbers of each waveguide. The number of dots that appears it the left-hand side of a vertical line gives the largest positive integer that makes w_n for each waveguide positive, that is it is n_* we used in this chapter. Consider the transmission amplitudes of these waveguides. The fact that $a \gg L_x$ for all waveguides allows us to use (5.62) for the two-dimensional

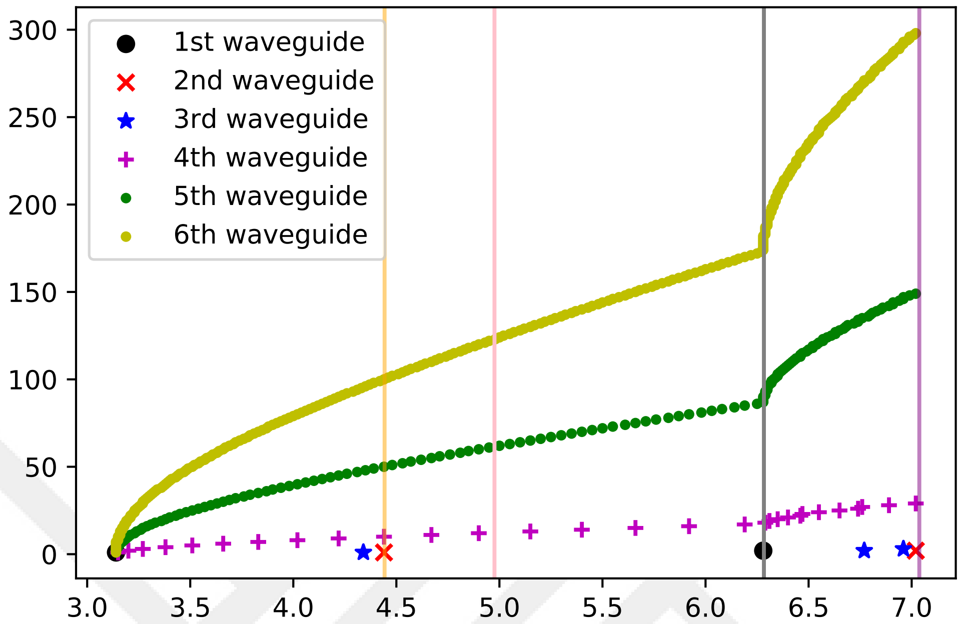

Figure 5.17: Plot of exceptional points of different waveguides all of thich have the same heigth L_x. Each point indicates that k is the nth smallest exceptional wavenumber, that is $k^2 = \mathcal{E}_n$ for different waveguides. The black and the grey vertical lines is equal to $k/Lx = \sqrt{2}\pi$ and $k/Lx = 2\pi$, the pink and the purple vertical lines are 12% larger than k, respectively.

waveguide and (5.80) for the three-dimensional waveguides. Table (5.1) shows n_* and the number of $\tilde{\phi}_{n,a}$ that determine the transmission amplitudes. Both n_* and the number of $\tilde{\phi}_{n,a}$ for waveguides that have larger width compared to their height grow faster as k increases. Note that the number of $\tilde{\phi}_{n,a}$ and n_* for $k = 1.12k_2$ are different for the second, forth, fifth and the sixth waveguides. This is because there are degenerate energy levels. This cannot happen for the first and the third waveguides. Also note that the the third waveguide is wider than the second waveguide, so n_* for the third waveguide is larger than or equal to n_* for the second waveguide for any wavenumber. However, for $k = 1.12k_2$, the number of Fourier transforms of $\phi_{n,a}$ that determines the transmission from the third waveguide is smaller than the number that determined the transmission of the second one. This is a result of degeneracy in our systems.

	1st wg		2nd wg		3rd wg		4th wg		5th wg		6th wg	
	n_*	$\#\tilde{\phi}_{n,a}$	n_*	$\#\tilde{\phi}_{n,a}$	n_*	$\#\tilde{\phi}_{n,a}$	n_*	$\#\tilde{\phi}_{n,a}$	n_*	$\#\tilde{\phi}_{n,a}$	n_*	$\#\tilde{\phi}_{n,a}$
k_1	1	1	1	1	1	1	9	9	49	49	99	99
$1.12k_1$	1	1	1	1	1	1	12	12	61	61	122	122
k_2	1	1	1	1	1	1	17	17	86	86	173	173
$1.12k_2$	2	2	2	3	2	2	29	30	149	150	298	300

Table 5.1: Table of n_* and the number of $\tilde{\phi}_{n,a}$, denoted as $(\#\tilde{\phi}_{n,a})$,that determines the transmission coefficient for six different waveguides. The wavenumbers $k_1 = \sqrt{2}\pi/L_x$ and $k_2 = 2\pi/L_x$.

Chapter 6

CONNECTING DIFFERENT FINITE LENGTH WAVEGUIDES

In this chapter we solve the scattering from a system of N, d-dimensional, finite waveguides of different sizes and filled with different, homogeneous, non-active material. First, we introduce new notation to distinguish between each waveguide. Consider the jth waveguide where $j \in \{1, 2, \cdots, N\}$, which is bounded between the walls $z = a_{j+}$ and $z = a_{j-}$ where $a_{j\pm}$ are real parameters such that $a_{j+} > a_{j-}$, and define $I_j = [a_{j-}, a_{j+}] \subset \mathbb{R}$. Also we require that, either the support of the potentials separate and nonadjacent, i.e., $I_j \cap I_k = \varnothing$ for $k \in \{1, 2, \cdots, N\}$ and $k \neq j$,and $a_{j+} > a_{k+}$ if $k < j$ or the supports potentials of different waveguides are separate but adjacent, i.e., $I_j \cap I_k = \varnothing$ for $k \in \{1, 2, \cdots, N\}$, $k \neq j$ and $j \neq k \pm 1$, and $a_{j\mp} = a_{k\pm}$ if $j = k \pm 1$. Then, analog of potential (4.11) that describes the jth waveguide is given by

$$v_j(\boldsymbol{r}, z) := \begin{cases} \mathscr{V}_j(\boldsymbol{r}) & \text{for } z \in I_j, \\ 0 & \text{for } z \notin I_j. \end{cases} \tag{6.1}$$

where

$$\mathscr{V}_j(\boldsymbol{r}) := \begin{cases} \mathscr{V}_j & \text{for } \boldsymbol{r} \in box_j, \\ +\infty & \text{for } \boldsymbol{r} \notin box_j. \end{cases} \tag{6.2}$$

Here $\mathscr{V}_j$ is a real parameter and

$$box_j := \begin{cases} [0, L_{x,j}] & \text{for } d = 2, \\ [0, L_{x,j}] \times [0, L_{y,j}] & \text{for } d = 3, \end{cases} \tag{6.3}$$

where $L^+_{x/y,j} > L^-_{x/y,j}$ are real parameters. Define $l_j := a_{j+} - a_{j-}$, which are the height the jth waveguide. The size parameters of waveguide j, are its height and width.

The transfer matrix $\widehat{\mathbf{M}}_j$ and the auxiliary transfer matrix $\widehat{\boldsymbol{\mathcal{M}}}_j$ associated with the jth waveguide are

$$\widehat{\boldsymbol{\mathcal{M}}}_j = e^{-ia_{j+}\widehat{\varpi}\boldsymbol{\sigma}_3} e^{-il_j\widehat{\mathbf{H}}_j} e^{ia_{j-}\widehat{\varpi}\boldsymbol{\sigma}_3}, \tag{6.4}$$

$$\widehat{\mathbf{M}}_j = e^{-ia_{j+}\widehat{\varpi}\boldsymbol{\sigma}_3}\widehat{\boldsymbol{\Pi}}_k e^{-il_j\widehat{\mathbf{H}}_j}\widehat{\boldsymbol{\Pi}}_k e^{ia_{j-}\widehat{\varpi}\boldsymbol{\sigma}_3}, \tag{6.5}$$

where

$$\widehat{\mathbf{H}}_j = \frac{1}{2}\widehat{\mathscr{V}}_j\widehat{\varpi}^{-1}\boldsymbol{\mathcal{K}} - \widehat{\varpi}\boldsymbol{\sigma}_3, \tag{6.6}$$

and $\widehat{\mathscr{V}}_j = \mathscr{V}_j(\hat{\boldsymbol{r}})$.

The total potential of the total system is

$$v(\boldsymbol{r}, z) = \sum_{j=1}^{N} v_j, \tag{6.7}$$

which is bounded between the planes $z = a_{1-}$ and $z = a_{N+}$. We can utilize the composition property of the auxiliary transfer matrix to find the fundamental transfer matrix $\widehat{\mathbf{M}}$ of the whole system. Equations (4.59) and (4.80) imply

$$\begin{aligned}\widehat{\mathbf{M}} &= \widehat{\boldsymbol{\Pi}}_k\widehat{\boldsymbol{\mathcal{M}}}_N\widehat{\boldsymbol{\mathcal{M}}}_{N-1}\cdots\widehat{\boldsymbol{\mathcal{M}}}_1\widehat{\boldsymbol{\Pi}}_k \\ &= \widehat{\boldsymbol{\Pi}}_k e^{-ia_{N+}\widehat{\varpi}\boldsymbol{\sigma}_3} e^{-il_N\widehat{\mathbf{H}}_N} e^{ia_{N-}\widehat{\varpi}\boldsymbol{\sigma}_3}\cdots e^{-ia_{1+}\widehat{\varpi}\boldsymbol{\sigma}_3} e^{-il_1\widehat{\mathbf{H}}_1} e^{ia_{1-}\widehat{\varpi}\boldsymbol{\sigma}_3}\widehat{\boldsymbol{\Pi}}_k\end{aligned}. \tag{6.8}$$

Define

$$\widehat{\mathbf{T}} := e^{ia_{N,+}\widehat{\varpi}\boldsymbol{\sigma}_3}\widehat{\boldsymbol{\Pi}}_k\widehat{\mathbf{M}}\widehat{\boldsymbol{\Pi}}_k e^{-ia_{1,-}\widehat{\varpi}\boldsymbol{\sigma}_3}, \tag{6.9}$$

which can be written as

$$\widehat{\mathbf{T}} = \widehat{\boldsymbol{\Pi}}_k e^{-il_N\widehat{\mathbf{H}}_N} e^{ia_{N-}\widehat{\varpi}_N\boldsymbol{\sigma}_3}\left[\prod_{n=1}^{N-2} e^{-ia_{N-n,+}\widehat{\varpi}_{N-n}\boldsymbol{\sigma}_3} e^{-il_{N-n}\widehat{\mathbf{H}}_{N-n}} e^{ia_{N-n,-}\widehat{\varpi}_{N-n}\boldsymbol{\sigma}_3}\right] e^{-ia_{1-}\widehat{\varpi}_1\boldsymbol{\sigma}_3} e^{il_1\widehat{\mathbf{H}}_1}\widehat{\boldsymbol{\Pi}}_k. \tag{6.10}$$

Then $\widehat{\mathbf{M}}$ becomes

$$\widehat{\mathbf{M}} = e^{-ia_{N,+}\boldsymbol{\sigma}_3}\widehat{\mathbf{T}}e^{ia_{1,-}\boldsymbol{\sigma}_3} = \begin{bmatrix} e^{-ia_{N+}\widehat{\varpi}}\widehat{T}_{11}e^{ia_{1-}\widehat{\varpi}} & e^{-ia_{N+}\widehat{\varpi}}\widehat{T}_{12}e^{-ia_{1-}\widehat{\varpi}} \\ e^{ia_{N+}\widehat{\varpi}}\widehat{T}_{21}e^{ia_{1-}\widehat{\varpi}} & e^{ia_{N+}\widehat{\varpi}}\widehat{T}_{22}e^{-ia_{1-}\widehat{\varpi}} \end{bmatrix} \tag{6.11}$$

and equations (4.41)-(4.44) can be written as

$$B_-^l = -(2\pi)^{d-1}\varpi(\vec{p}_0)e^{ia_1-k(\cos\theta+\cos\theta_0)}\langle\vec{p}|\widehat{T}_{22}^{-1}\widehat{T}_{21}|\vec{p}_0\rangle, \tag{6.12}$$

$$A_+^l = (2\pi)^{d-1}\varpi(\vec{p}_0)e^{-ik(a_{N+}\cos\theta-a_{1-}\cos\theta_0)}\langle\vec{p}|\big(\widehat{T}_{11}-\widehat{T}_{12}\widehat{T}_{22}^{-1}\widehat{T}_{21}\big)|\vec{p}_0\rangle, \tag{6.13}$$

$$B_-^r = (2\pi)^{d-1}\varpi(\vec{p}_0)e^{ia_1-k(\cos\theta-\cos\theta_0)}\langle\vec{p}|\widehat{T}_{22}^{-1}|\vec{p}_0\rangle, \tag{6.14}$$

$$A_+^r = (2\pi)^{d-1}\varpi(\vec{p}_0)e^{-ik(a_{N+}\cos\theta+a_{1-}\cos\theta_0)}\langle\vec{p}|\widehat{T}_{12}\widehat{T}_{22}^{-1}|\vec{p}_0\rangle, \tag{6.15}$$

where we used $\varpi(\vec{p}) = k|\cos\theta|$ and $\varpi(\vec{p}_0) = k|\cos\theta_0|$. These equations show that solving the scattering problem reduces to calculating the operator $\widehat{\mathbf{T}}$.

The machinery introduced in section 5.1 is still valid for the jth waveguide. To see this, note that with the choise of potential (6.2), the operator $\hat{h}_j := \hat{\boldsymbol{p}}^2 + \widehat{\mathscr{V}}_j$, describes the problem of a particle trapped in a $(d-1)$-dimensional, infinite rectangular well considered in the Hilbert space $L^2[\mathbb{R}^{d-1}]$, instead of the usual Hilbert space $L^2(box_j)$ this problem descibed in. Following the example of section 5.1, we consider this problem on the Hilbert space $L^2(box_j)$, instead of the usual Hilbert space $L^2[\mathbb{R}^{d-1}]$. Let $\widehat{\Lambda}_j$ be the orthogonal projection operator onto $L^2[box_j]$. Then $(\widehat{I} - \widehat{\Lambda}_j)$ is the orthogonal projection onto $L^2[\mathbb{R}^{d-1}\backslash box_j]$ and we have the direct sum decomposition

$$L^2[\mathbb{R}^{d-1}] = L^2[box_j] \oplus L^2[\mathbb{R}^{d-1} \setminus box_j].$$

This implies that for every $\mathring{\phi} \in L^2[box_j]$, there exist unique $\mathring{\phi} \in L^2[box_j]$ and $\breve{\phi} \in L^2[\mathbb{R}^{d-1}]$ such that $\phi = \mathring{\phi} + \breve{\phi}$. Let $\mathcal{E}_{j,n}$ be the energy eigenvalue and $\mathring{\phi}_{n,a}^{(j)} \in L^2[box_j]$ be the corresponding eigenfunction of $\widehat{\Lambda}_j\hat{h}_j\widehat{\Lambda}_j$, that is,

$$\widehat{\Lambda}_j\hat{h}_j\widehat{\Lambda}_j\mathring{\phi}_{n,a}^{(j)} = \mathcal{E}_{j,n}$$

$E_{j,n}$ and $\mathring{\phi}_{n,a}^{(j)}$ are given by the equations (5.47) and (5.48) for $d = 2$, and by equations (5.71) and (5.72) for $d = 3$. Then the eigenvalues and the corresponding eigenfunctions of $\hat{h}_j$ are

$$E_{j,n} = \mathcal{E}_{j,n} + \mathscr{V}_j, \qquad \phi_{n,a}^j(\boldsymbol{r}) = \begin{cases} \mathring{\phi}_{n,a}^{(j)}(\boldsymbol{r}) & \text{for } \boldsymbol{r} \in box_j, \\ 0 & \text{for } \boldsymbol{r} \notin box_j. \end{cases} \tag{6.16}$$

Moreover, the regular completeness relation becomes

$$\sum_{n=1}^{\infty}\sum_{a=1}^{d_n} |\phi_{n,a}^{(j)}\rangle\langle\phi_{n,a}^{(j)}| := \widehat{\Lambda}_j \tag{6.17}$$

where $\widehat{\Lambda}_j$ is the orthogonal projection operator onto $L^2[box_j]$.

The scattering of the incident wave by the system of N finite length waveguides is due to two different interactions, a part of the incident wave enters to the waveguide, interacts with the material inside it, and gets partially reflected and partially transmitted. The other part of the wave hits the vertical boundaries of impenetrable walls of the first waveguide at $z = a_{1-}$ or the impenetrable walls of the Nth waveguide at $z = a_{N+}$, gets fully reflected back. If there is a vertical boundary of a impenetrable wall inside, the part of the incident wave that enters inside the waveguide will get reflected by this boundary, if there is a potential before this boundary, the reflection gets complicated. In order to avoid this complication, we consider the cases $box_1 = box_N \subseteq box_j$ for $j \in \{2, \cdots, N-1\}$. See fig (6.1). Then a part of the left-incident wave interacts with the vertical boundaries of the impenetrable wall of the first waveguide and a part of the right-incident wave hits impenetrable wall of the Nth waveguide and get fully reflected. In this case, the boundary condition analog to the scattering from a single finite length waveguide becomes, $\psi(\boldsymbol{r}, a_{1-}) = 0$ when $\boldsymbol{r} \notin box_1$ and$\psi(\boldsymbol{r}, a_{N+}) = 0$ when $\boldsymbol{r} \notin box_N$, which allows is equivalent to

$$(\widehat{I} - \widehat{\Lambda})|\psi(a_{1,-})\rangle = 0, \qquad (\widehat{I} - \widehat{\Lambda})|\psi(a_{N,+})\rangle = 0, \tag{6.18}$$

where $\widehat{\Lambda} := \widehat{\Lambda}_1 = \widehat{\Lambda}_N$. Inserting these to (5.13) we find

$$(\widehat{\Lambda} - \widehat{I})|\mathscr{B}_-\rangle = (\widehat{I} - \widehat{\Lambda})e^{2ia_{1-}\widehat{\varpi}}|A_-\rangle, \tag{6.19}$$

$$(\widehat{\Lambda} - \widehat{I})|\mathscr{A}_+\rangle = (\widehat{I} - \widehat{\Lambda})e^{-2ia_{N+}\widehat{\varpi}}|B_+\rangle, \tag{6.20}$$

Solving these for $|\mathscr{B}_-\rangle$ and $|\mathscr{A}_+\rangle$, we find

$$|\mathscr{B}_-\rangle = |\mathscr{B}_{0-}\rangle + (\widehat{I} - \widehat{\Lambda})e^{2ia_{1-}\widehat{\varpi}}|A_-\rangle, \tag{6.21}$$

$$|\mathscr{A}_+\rangle = |\mathscr{A}_{0+}\rangle + (\widehat{I} - \widehat{\Lambda})e^{-2ia_{+}\widehat{\varpi}}|B_+\rangle, \tag{6.22}$$

where $|\mathscr{B}_{0-}\rangle$ and $|\mathscr{A}_{0+}\rangle$ are the solutions of the homogeneous linear equations $(\widehat{\Lambda} - \widehat{I})|\psi\rangle = 0$ and $(\widehat{\Lambda} - \widehat{I})|\psi\rangle = 0$ respectively. Following the procedure of section 5.1, we consider left- and right-incident weaves separately and find that (5.22), (5.23), (5.25) and (5.26) still hold and can be written as

$$B^l_-(\vec{p}) = \mathscr{B}^l_{0-}(\vec{p}) + B^l_{1-}(\vec{p}), \tag{6.23}$$

$$A^l_+(\vec{p}) = \mathscr{A}^+_{0+}, \tag{6.24}$$

$$B^r_-(\vec{p}) = \mathscr{B}^r_{0-}(\vec{p}) \tag{6.25}$$

$$A^l_+(\vec{p}) = \mathscr{A}^+_{0+} + A^r_{1-}(\vec{p}) \tag{6.26}$$

where

$$\begin{aligned} B^l_{1-}(\vec{p}) &:= \langle \boldsymbol{p}|(2\pi)^{d-1}\varpi(\boldsymbol{p}_0)e^{2ia_{1-}\widehat{\varpi}}(\widehat{I}-\widehat{\Lambda})|\boldsymbol{p}_0\rangle \\ &= \varpi(\boldsymbol{p}_0)e^{2ia_{1-}\widehat{\varpi}}\Big[(2\pi)^{d-1}\delta_{\boldsymbol{p}_0} - \sum_{n=1}^{\infty}\sum_{a=1}^{d_n}\tilde{\phi}^{(1)}_{n,a}(\boldsymbol{p}_0)^*\tilde{\phi}^{(1)}_{n,a}(\boldsymbol{p})\Big], \end{aligned} \tag{6.27}$$

$$\begin{aligned} A^l_{1-}(\vec{p}) &:= \langle \boldsymbol{p}|(2\pi)^{d-1}\varpi(\boldsymbol{p}_0)e^{-2ia_{N+}\widehat{\varpi}}(\widehat{I}-\widehat{\Lambda})|\boldsymbol{p}_0\rangle \\ &= \varpi(\boldsymbol{p}_0)e^{-2ia_{N+}\widehat{\varpi}}\Big[(2\pi)^{d-1}\delta_{\boldsymbol{p}_0} - \sum_{n=1}^{\infty}\sum_{a=1}^{d_n}\tilde{\phi}^{(N)}_{n,a}(\boldsymbol{p}_0)^*\tilde{\phi}^{(N)}_{n,a}(\boldsymbol{p})\Big]. \end{aligned} \tag{6.28}$$

The terms $\mathscr{B}^{l/r}_{0-}(\boldsymbol{p})$ and $\mathscr{A}^{l/r}_{0+}(\boldsymbol{p})$ are associated with the scattering due to interior part of the waveguide system. The solution of the scattering problem reduces to calculating these functions.

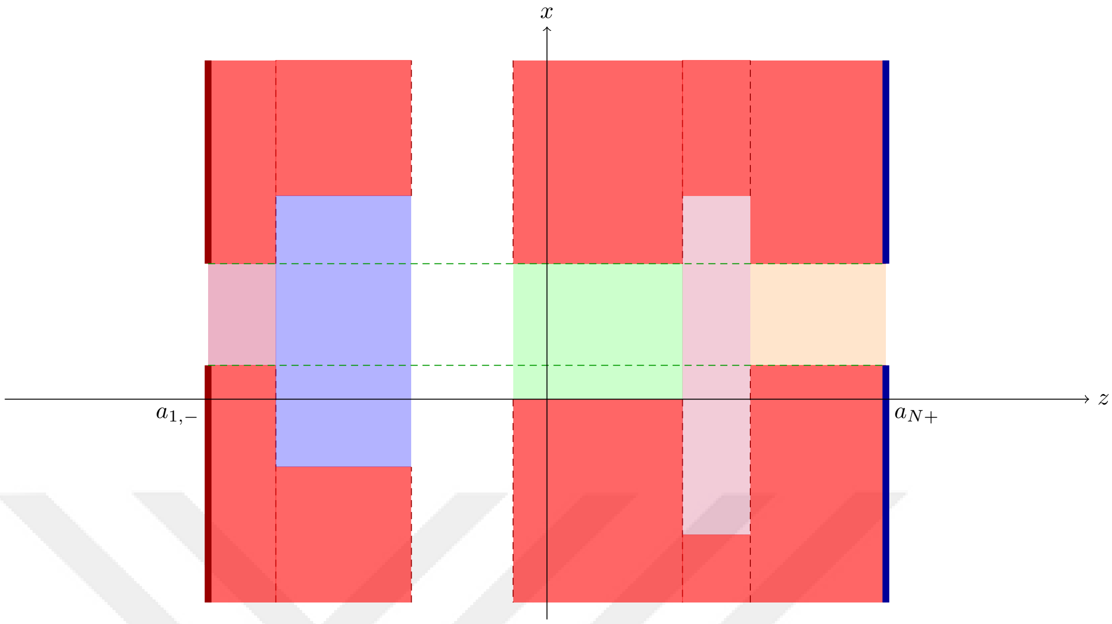

Figure 6.1: Schematic views of a system of waveguides. In both pictures, light red parts describes impenetrable walls, and the vertical boundaries of impenetrable walls that a left- and right incident wave are shown as thick dark red and blue lines respectively. The light purple, blue, green pink and yellow parts represent the different potentials of the waveguides.

6.1 Contribution of the interior to the scattering problem

We can use the composition property of the transfer matrix to determine the contribution of the interior of the waveguide system to the scattering problem. Let $\widehat{\mathbf{M}}$ be the transfer matrix associated with the interior of the waveguide. Considering equation (4.58) and (4.79) we find

$$\widehat{\mathbf{M}} = \widehat{\mathbf{\Pi}}_k \widehat{\boldsymbol{\mathcal{M}}}_N \widehat{\boldsymbol{\mathcal{M}}}_{N-1} \cdots \widehat{\boldsymbol{\mathcal{M}}}_1 \widehat{\mathbf{\Pi}}_k \tag{6.29}$$

where $\widehat{\boldsymbol{\mathcal{M}}}_j$ is the auxiliary transfer matrix associated with the interior of the jth waveguide, which we aim to calculate. In order to achieve this, we follow the example of subsection (5.1.1) and define the operator $\widehat{W}_j$ for the interior of the j waveguide as (4.98) with eigenvector $|\phi^j_{n,a}\rangle$, i.e.,

$$\widehat{W}_j = \sum_{n=1}^{N} w_{j,n} |\phi^j_{n,a}\rangle\langle\phi^j_{n,a}|, \tag{6.30}$$

where

$$w_{j,n} = \begin{cases} \sqrt{k^2 - \mathcal{E}_{j,n} - \mathscr{V}_j} & \text{for } k \leq \sqrt{\mathcal{E}_{j,n} + \mathscr{V}_j}, \\ i\sqrt{\mathcal{E}_{j,n} - \mathscr{V}_j - k^2} & \text{for } k > \sqrt{\mathcal{E}_{j,n} + \mathscr{V}_j}, \end{cases} \tag{6.31}$$

Additionally, we define

$$\widehat{\varpi}_j = \widehat{\Lambda}_j \varpi(\hat{\boldsymbol{p}}) \widehat{\Lambda}_j \tag{6.32}$$

equations (4.30) and (5.11) imply

$$\widehat{\varpi}_j = \sum_{n=1}^{\infty} \sum_{a=1}^{d_n} \varpi_{j,n} |\phi^j_{n,a}\rangle\langle\phi^j_{n,a}|, \tag{6.33}$$

where

$$\varpi_{j,n} = \begin{cases} \sqrt{k^2 - \mathcal{E}_{j,n}} & \text{for } k \leq \sqrt{\mathcal{E}_{j,n}}, \\ i\sqrt{\mathcal{E}_{j,n} - k^2} & \text{for } k > \sqrt{\mathcal{E}_{j,n}}. \end{cases} \tag{6.34}$$

Equations (6.30) and (6.33) imply,

$$[\widehat{W}_j, \widehat{\varpi}_j] = 0, \tag{6.35}$$

which allows us to write

$$e^{-il_j \widehat{\mathbf{H}}_j} = \frac{e^{-il_j \widehat{W}_j}}{2\widehat{W}_j \widehat{\varpi}_j} \begin{bmatrix} \widehat{d}_j^- & -\widehat{o}_j \\ \widehat{o}_j & \widehat{d}_j^+ \end{bmatrix}, \tag{6.36}$$

where

$$\widehat{d}_j^\pm := \mp \widehat{\mathbf{\Pi}}_k ((\widehat{\varpi}_j \pm \widehat{W}_j)^2) - e^{2il_j \widehat{W}_j} (\widehat{\varpi}_j \mp \widehat{W}_j)^2) \widehat{\mathbf{\Pi}}_k \tag{6.37}$$

$$\widehat{o}_j := \widehat{\mathbf{\Pi}}_k (\widehat{W}_i^2 - \widehat{\varpi}_i^2)(1 - e^{2il_i \widehat{W}_i}) \widehat{\mathbf{\Pi}}_k. \tag{6.38}$$

Here, we used the expression (5.38). Also we have

$$\begin{aligned} \widehat{d}_j^\pm = \widehat{\Lambda}_j \widehat{d}_j^\pm &= \sum_{n=1}^{\infty} \sum_{a=1}^{d_n} \widehat{d}_j^\pm |\phi_{n,a}\rangle\langle\phi_{n,a}| \\ &= \sum_{n=1}^{\infty} \sum_{a=1}^{d_n} \mp \big((\varpi_{j,n} \pm w_{j,n})^2 - e^{2il_j w_{j,n}} (w_{j,n} \mp \varpi_{j,n})^2 \big) |\phi_{n,a}\rangle\langle\phi_{n,a}|. \end{aligned} \tag{6.39}$$

Similarly we get

$$\pm\widehat{o}_j = \pm\sum_{n=1}^{\infty}\sum_{a=1}^{d_n}(w_{j,n}^2 - \varpi_{j,n}^2)(1 - e^{2il_j w_{j,n}})|\phi_{n,a}\rangle\langle\phi_{n,a}|. \tag{6.40}$$

Let us define

$$d_{j,n}^{\pm} := \mp\big((\varpi_{j,n} \pm w_{j,n})^2 - e^{2il_j w_{j,n}}(w_{j,n} \mp \varpi_{j,n})^2\big), \tag{6.41}$$

$$o_{j,n} := (w_{j,n}^2 - \varpi_{j,n}^2)(1 - e^{2il_j w_{j,n}}). \tag{6.42}$$

These definitions allows us to write (6.44) and (6.45) as

$$\widehat{d}_j^{\pm} = \sum_{n=1}^{\infty}\sum_{a=1}^{d_n} d_{j,n}^{\pm}|\phi_{n,a}\rangle\langle\phi_{n,a}|, \qquad \widehat{o}_j = \sum_{n=1}^{\infty}\sum_{a=1}^{d_n} o_{j,n}|\phi_{n,a}\rangle\langle\phi_{n,a}|. \tag{6.43}$$

Inserting these in (6.4) we find

$$e^{-il_j\widehat{\mathbf{H}}_j} = \sum_{n=1}^{\infty}\sum_{a=1}^{d_n}\frac{e^{-il_j w_{j,n}}}{2w_{j,n}\varpi_{j,n}}\begin{bmatrix} d_{j,n}^- & -o_{j,n} \\ o_{j,n} & d_{j,n}^+ \end{bmatrix}|\phi_{n,a}\rangle\langle\phi_{n,a}| \tag{6.44}$$

It is easy to see that if $\phi_{n,a}^{(j)} \neq \phi_{n,a}^{(k)}$ for $k \neq j$, the operators $e^{-il_j\widehat{\mathbf{H}}_j}$ and $e^{-il_j\widehat{\mathbf{H}}_j}$ do not commute, which makes the calculation of the transfer matrix for the whole system complicated. To avoid this, we assume that for all the waveguides the functions $\phi_{n,a}^{(j)}$ are equal, this can happen if $L_{x/y,j} = L_{x/y,k}$ for all $j,k \in \{1,\cdots,N\}$. Notice that if this condition holds we have $\mathcal{E}_{j,n} = \mathcal{E}_{k,n}$ and $\widehat{\varpi}_j = \widehat{\varpi}_k$. In the remainder we drop the label j from box_j, $|\phi_{n,a}^{(j)}\rangle$, $\mathcal{E}_{j,n}$, $\widehat{\varpi}_j$ and $\varpi_{n,j}$.

6.2 Adjacent waveguides with same size parameters

In this section, we consider waveguides that are adjacent, i.e., $a_j^- = a_{j-1}^+$ $j \in \{2,\cdots,N\}$, and have same size parameters ,i.e., and $L_{x/y,j}^{\pm} = L_{x/y,k}^{\pm}$ for all $j,k \in \{1,\cdots,N\}$. In this case we have $[\widehat{W}_j,\widehat{W}_k] = 0$, and $\widehat{\varpi} := \widehat{\varpi}_j = \widehat{\varpi}_k$ for all $j,k \in \{1,\cdots,N\}$. In this case, (6.9) reduces to

$$\widehat{\mathbf{T}} = \widehat{\mathbf{\Pi}}_k \prod_{n=0}^{N-1} e^{-il_{N-n}\widehat{\mathbf{H}}}\widehat{\mathbf{\Pi}}_k, \tag{6.45}$$

or taking (6.37) and (6.36) into consideration we get

$$\widehat{\mathbf{T}} = \frac{e^{-i(\sum_{n=1}^{N} l_n\widehat{W}_n)}}{2^n\widehat{\varpi}^n\prod_{n=1}^{N}\widehat{W}_n}\prod_{n=0}^{N-1}\begin{bmatrix} \widehat{d}_{N-n}^- & -\widehat{o}_{N-n} \\ \widehat{o}_{N-n} & \widehat{d}_{N-n}^+ \end{bmatrix}. \tag{6.46}$$

For simplicity, we let $L^-_{x/y,j} = 0$ and $L^+_{x/y,j} = L_{x/y}$ for all $j \in \{1, \cdots, N\}$. Additionally, since all box_j are the same, we drop the label (j) and define $\phi_{n,a} := \phi^{(j)}_{n,a}$ and $\mathcal{E}_n := \mathcal{E}_{j,n}$ for all $j \in \{1, \cdots, N\}$.

6.2.1 Three adjacent waveguides

Consider three adjacent waveguides with the same size parameters, where the first and the third waveguides are empty and the second waveguide is filled, i.e., $\mathscr{V}_1 = \mathscr{V}_3 = 0$ and $\mathscr{V}_2 \neq 0$. Then, we can define $\widehat{\varpi} := \widehat{W}_1 = \widehat{W}_3 = \widehat{\varpi}_1 = \widehat{\varpi}_2 = \widehat{\varpi}_3$. Then $\widehat{\mathbf{T}}$ becomes,

$$\widehat{\mathbf{T}} = \frac{e^{-il_2\widehat{W}_2}}{2\widehat{\varpi}\widehat{W}_2} \begin{bmatrix} e^{il_3\widehat{\varpi}} & 0 \\ 0 & e^{-il_3\widehat{\varpi}} \end{bmatrix} \begin{bmatrix} \widehat{d}_2^- & -\widehat{o}_2 \\ \widehat{o}_2 & \widehat{d}_2^+ \end{bmatrix} \begin{bmatrix} e^{il_1\widehat{\varpi}} & 0 \\ 0 & e^{-il_1\widehat{\varpi}} \end{bmatrix} \tag{6.47}$$

$$= \frac{e^{-il_2\widehat{W}_2}}{2\widehat{\varpi}\widehat{W}_2} \begin{bmatrix} e^{i(l_3+l_1)\widehat{\varpi}}\widehat{d}_2^- & -e^{i(l_3-l_1)\widehat{\varpi}}\widehat{o}_2 \\ e^{-i(l_3-l_1)\widehat{\varpi}}\widehat{o}_2 & e^{-i(l_3+l_1)\widehat{\varpi}}\widehat{d}_2^+ \end{bmatrix}. \tag{6.48}$$

Let n_* and m_* be largest integers such that $w_{2,n}$ and ϖ_n are real. Then we have the following relationship between them.

$$\begin{aligned} &n_* < m_* \text{ if } \mathscr{V}_2 > 0, \\ &m_* < n_* \text{ if } \mathscr{V}_2 < 0. \end{aligned} \tag{6.49}$$

Consider the transmission and reflection coefficients for a right-incident wave, which is determined by T_{22}^{-1} and $T_{12}T_{22}^{-1}$ respectively. Using (6.48) we get

$$T_{22}^{-1} = \frac{2\widehat{\varpi}\widehat{W}_2 e^{il_2\widehat{W}_2}}{e^{-i(l_3+l_1)\widehat{\varpi}}\widehat{d}_2^+} = \frac{2\widehat{\varpi}\widehat{W}_2 e^{i(l_3+l_1)\widehat{\varpi}} e^{il_2\widehat{W}_2}}{\widehat{d}_2^+}, \tag{6.50}$$

and

$$T_{12}T_{22}^{-1} = -\frac{e^{2il_3\widehat{\varpi}}\widehat{o}_2}{\widehat{d}_2^+}. \tag{6.51}$$

.

Consider, the right-reflection coefficient.

$$\langle \vec{p} | T_{12}T_{22}^{-1} | \vec{p}_0 \rangle = -\frac{e^{2il_3\varpi_n} o_{2,n}}{d^+_{2,n}} \tag{6.52}$$

Positive Potential

If $\mathscr{V}_2 > 0$, (6.50) and (6.51= can be expressed as

$$\begin{aligned} T_{22}^{-1} &= \sum_{n=1}^{n_*}\sum_{a=1}^{d_n} r_+|\phi_{n,a}\rangle\langle\phi_{n,a}| \\ &+ \sum_{n=n_*+1}^{m_*}\sum_{a=1}^{d_n} u_+|\phi_{n,a}\rangle\langle\phi_{n,a}| + \sum_{n=m_*+1}^{\infty}\sum_{a=1}^{d_n} s_+|\phi_{n,a}\rangle\langle\phi_{n,a}|, \end{aligned} \tag{6.53}$$

and

$$\begin{aligned} T_{12}T_{22}^{-1} &= \sum_{n=1}^{n_*}\sum_{a=1}^{d_n} r_-|\phi_{n,a}\rangle\langle\phi_{n,a}| \\ &+ \sum_{n=n_*+1}^{m_*}\sum_{a=1}^{d_n} u_-|\phi_{n,a}\rangle\langle\phi_{n,a}| + \sum_{n=m_*+1}^{\infty}\sum_{a=1}^{d_n} s_-|\phi_{n,a}\rangle\langle\phi_{n,a}|, \end{aligned} \tag{6.54}$$

where

$$r_+ = \frac{2|\varpi_n||w_{n,2}|e^{i(l_1+l_3)|\varpi_n|}e^{il_2|w_{n,2}|}}{d_{2,n}^+}, \qquad r_- = -\frac{e^{2il_3|\varpi_n|}o_{2,n}}{d_{2,n}^+}, \tag{6.55}$$

$$u_+ = \frac{2i|\varpi_n||w_{n,2}|e^{i(l_1+l_3)|\varpi_n|}e^{-l_2|w_{n,2}|}}{d_{2,n}^+}, \qquad u_- = -\frac{e^{2il_3|\varpi_n|}o_{2,n}}{d_{2,n}^+}, \tag{6.56}$$

$$s_+ = \frac{-2|\varpi_n||w_{n,2}|e^{-(l_1+l_3)|\varpi_n|}e^{-l_2|w_{n,2}|}}{d_{2,n}^+}, \qquad s_- = -\frac{e^{-2l_3|\varpi_n|}o_{2,n}}{d_{2,n}^+}. \tag{6.57}$$

We can solve the scattering problem for a right-incident wave by ea $\langle\vec{p}|$ from the left and $|\vec{p}_0\rangle$ to (6.53) and (6.54) and inserting the result to (6.14) and (6.15). First, we focus on the reflection. Consider

$$\begin{aligned} \left(T_{12}T_{22}^{-1}\right)(\vec{p}_0,\vec{p}) &= \sum_{n=1}^{n_*}\sum_{a=1}^{d_n} r_n^-\tilde{\phi}^*_{n,a}(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}) \\ &+ \sum_{n=n_*+1}^{m_*}\sum_{a=1}^{d_n} u_n^-\tilde{\phi}^*_{n,a}(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}) + \sum_{n=m_*+1}^{\infty}\sum_{a=1}^{d_n} s_n^-\tilde{\phi}^*_{n,a}(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}) \end{aligned} \tag{6.58}$$

Let $l_1 \gg L_x$, then we have $l_1|\varpi_n| \gg 1$ for all $n \leq m_*$. Then is the length of a waveguide is much larger than its height, the reflection is determined by

$$(T_{21}T_{22}^{-1})(\vec{p}_0,\vec{p}) \approx \sum_{n=1}^{n_*}\sum_{a=1}^{d_n} r_n^-\tilde{\phi}^*_{n,a}(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}) + \sum_{n=n_*+1}^{m_*}\sum_{a=1}^{d_n} u_n^-\tilde{\phi}^*_{n,a}(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}). \tag{6.59}$$

This shows that the reflection is determined by the Fourier transform $\phi_{n,a}$ that corresponds to the the first m_* energy levels. As we showed in the previous section, this is not possible for a single finite waveguide.

Now, let's consider the transmission of a right-incident wave.

$$T_{22}^{-1}(\vec{p},\vec{p}_0) = \sum_{n=1}^{n_*}\sum_{a=1}^{d_n} r_n^+ \tilde{\phi}_{n,a}^*(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}) + \sum_{n=n_*+1}^{m_*}\sum_{a=1}^{d_n} u_n^+ \tilde{\phi}_{n,a}^*(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}) + \sum_{n=m_*+1}^{\infty}\sum_{a=1}^{d_n} s_n^+ \tilde{\phi}_{n,a}^*(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}). \tag{6.60}$$

Now, we consider the cases where the length of the first waveguide l_3 is much larger than the height of the system, but not the length of the second waveguide,that is, $l_3 \gg L_x$ but $l_2 \sim L_x$. Then (6.60) reduces to

$$T_{22}^{-1}(\vec{p},\boldsymbol{p}_0) \approx \sum_{n=1}^{n_*}\sum_{a=1}^{d_n} r_n^+ \tilde{\phi}_{n,a}^*(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}) + \sum_{n=n_*+1}^{m_*}\sum_{a=1}^{d_n} u_n^+ \tilde{\phi}_{n,a}^*(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}), \tag{6.61}$$

which means that the transmission is determined by the Fourier transform of the $\phi_{n,a}$ that corresponds to the first m_*. Now, assume the incident wave is the mth exceptional wavenumber of the empty waveguides, i.e, $k^2 = \mathcal{E}_{m_*}$. Then we get $\varpi_{m_*} = 0$ and (6.56) implies

$$u_{m_*}^+ = 0. \tag{6.62}$$

Then there is no contribution of $\tilde{\phi}_{m_*,a}$, the transmission of the left-incident wave is determined by $\tilde{\phi}_{n,a}$ for $1 \leq n \leq m_* - 1$.

Let $\mathscr{V}_2 = \mathcal{E}_2 - \mathcal{E}_1$ and $k = \mathcal{E}_1 + \mathscr{V}_2 = \mathcal{E}_2$, which is the first exceptional wavenumber of the second waveguide and the second exceptional wavenumbers of the first and the third waveguide. Then, $|w_{2,1}| = 0$ and $|\varpi_2| = 0$. Additionally, when $l_1 = l_3 \gg L_x$,

$$\widehat{\Gamma}_{\pm}(\vec{p},\vec{p}_0) \approx \sum_{n=1}^{n_*}\sum_{a=1}^{d_n} r_n^- \tilde{\phi}_{n,a}^*(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}) + \sum_{n=n^*+1}^{m_*}\sum_{a=1}^{d_n} u_n^- \tilde{\phi}_{n,a}^*(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}). \tag{6.63}$$

With these choices of potential and the wavenumber, $r_1^{\pm}$ and $u_2^{\pm}$ can be calculated by taking the limit $|w_{2,1}| \to 0$ of (6.55) and $|\varpi_2| \to 0$ of (6.56). The later gives

$$u_2^- = \frac{|w_{22}|^2(1 - e^{-2l_2|w_{2,2}|})}{-|w_{22}|^2(e^{-2l_2|w_{2,2}|} - 1))} = 1,$$

$$u_2^+ = 0$$

Using the L'Hopitals rule for $r_1^{\pm}$ we get

$$\lim_{|w_{2,1}|\to 0} r_1^- = \frac{e^{2il_1|\mathscr{V}_2|}}{1+\frac{i}{l_2\sqrt{\mathscr{V}_2}}}$$
$$\lim_{|w_{2,1}|\to 0} r_1^+ = \frac{e^{i(l_1+l_3)}\sqrt{\mathscr{V}_2}}{il_2\sqrt{\mathscr{V}_2}-2}$$

where we made use of the fact $\varpi_1 = \sqrt{(}\mathscr{V}_2)$ for this choice of k. Then (6.61) becomes

$$\widehat{\Gamma}_+(\vec{p},\vec{p}_0) \approx \frac{e^{i(l_1+l_3)}\sqrt{\mathscr{V}_2}}{il_2\sqrt{\mathscr{V}_2}-2}\tilde{\phi}^*_{1,1}(\vec{p}_0)\tilde{\phi}_{1,1}(\vec{p}) \tag{6.64}$$

and

$$\widehat{\Gamma}_-(\vec{p},\vec{p}_0) \approx \frac{e^{2il_1|\mathscr{V}_2|}}{1+\frac{i}{l_2\sqrt{\mathscr{V}_2}}}\tilde{\phi}^*_{1,1}(\vec{p}_0)\tilde{\phi}_{1,1}(\vec{p}) + \sum_{a=1}^{d_2}\tilde{\phi}^*_{2,a}(\boldsymbol{p}_0)\tilde{\phi}_{2,a}(\vec{p}) \tag{6.65}$$

Negative Potential

If $\mathscr{V}_2 < 0$, (6.52) and (6.53) can be expressed as

$$\begin{aligned} T_{22}^{-1}(\vec{p},\vec{p}_0) &= \sum_{n=1}^{m_*}\sum_{a=1}^{d_n} r_n^+\tilde{\phi}^*_{n,a}(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}) \\ &+ \sum_{n=m_*+1}^{n_*}\sum_{a=1}^{d_n} v_n^+\tilde{\phi}^*_{n,a}(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}) + \sum_{n=n_*+1}^{\infty}\sum_{a=1}^{d_n} s_n^+\tilde{\phi}^*_{n,a}(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}), \end{aligned} \tag{6.66}$$

and

$$\begin{aligned} (T_{12}T_{22}^{-1})(\vec{p},\vec{p}_0) &= \sum_{n=1}^{m_*}\sum_{a=1}^{d_n} r_n^-\tilde{\phi}^*_{n,a}(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}) \\ &+ \sum_{n=m_*+1}^{n_*}\sum_{a=1}^{d_n} v_n^-\tilde{\phi}^*_{n,a}(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}) + \sum_{n=n_*+1}^{\infty}\sum_{a=1}^{d_n} s_n^-\tilde{\phi}^*_{n,a}(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}), \end{aligned} \tag{6.67}$$

where

$$v_n^+ = \frac{2i|\varpi_n||w_{n,2}|e^{-(l_1+l_3)|\varpi_n|}e^{il_2|w_n|}}{d_{2,n}^+}, \qquad v_n^- = -\frac{e^{-2l_3|\varpi_n|}o_{2,n}}{d_{2,n}^+}, \tag{6.68}$$

and $r^{\pm}$ and $s^{\pm}$ are defined by (6.55) and (6.57) respectively.

Now, we assume $l_2 \gg L_x$ and $l_1, l_3 \sim L_x$. If $k < \mathscr{E}_{n_*}$, (6.50) and (6.51) reduce to

$$T_{22}^{-1}(\vec{p},\vec{p}_0) \approx \sum_{n=1}^{m_*}\sum_{a=1}^{d_n} r_n^+\tilde{\phi}^*_{n,a}(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}) + \sum_{n=m_*+1}^{n_*}\sum_{a=1}^{d_n} v_n^+\tilde{\phi}^*_{n,a}(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}), \tag{6.69}$$

$$(T_{21}T_{22}^{-1})(\vec{p},\vec{p}_0) \approx \sum_{n=1}^{m_*}\sum_{a=1}^{d_n} r_n^{\pm}\tilde{\phi}_{n,a}^*(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}) + \sum_{n=m_*+1}^{n_*}\sum_{a=1}^{d_n} v_n^{\pm}\tilde{\phi}_{n,a}^*(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}). \quad (6.70)$$

which implies that the transmission and reflection are determined with the first n_*. As the positive potential filled waveguide, the reflection transmission is determined by a finite number of $\tilde{\phi}_{n,a}$.

Let the wavenumber be the lth exceptional wavenumber of the filled waveguide, i.e, $k^2 = \mathcal{E}_l + \mathscr{V}_2$, $\mathscr{V}_2 = \mathcal{E}_j - \mathcal{E}_l$ for some positive integer $j < l$, then the wavenumber is also equal to the jth exceptional wavenumber of the empty waveguides, i.e, $k^2 = \mathcal{E}_j$. Then we get $\varpi_j = 0$ and $w_{2,l} = 0$. Then using (6.55) and (6.68), we find

$$v_l^+ = \frac{ie^{-(l_1+l_3)|\varpi|_l}}{2 - l_2\sqrt{|\mathscr{V}|}} \qquad v_l^- = \frac{e^{-2l_3|\mathscr{V}_2|}}{2i + \frac{1}{l_2\sqrt{\mathscr{V}_2}}} \quad (6.71)$$

$$r_j^+ = 0 \qquad r_j^- = 1, \quad (6.72)$$

where we used the L'Hospitals rule to calculate $v_l^{\pm}$ and the fact that $|\varpi_l| = i\sqrt{|\mathscr{V}|}$. This shows that, the transmission is determined by the Fourier transform of $\phi_{n,a}$ that corresponds to the first j energy levels except l.

If $\mathscr{V}_2 = \mathcal{E}_2 - \mathcal{E}_3$, and $k^2 = \mathcal{E}_3 + \mathscr{V}_2 = \mathcal{E}_2$, (6.69) becomes

$$T_{22}^{-1}(\vec{p},\vec{p}_0) \approx r_1^+\tilde{\phi}_{1,1}^*(\vec{p}_0)\tilde{\phi}_{1,1} + \sum_{a=1}^{d_3} v_3^+\tilde{\phi}_{3,a}^*(\vec{p}_0)\tilde{\phi}_{3,a}(\vec{p}). \quad (6.73)$$

The transmission of this waveguide is determined by the Fourier transform of the first and the third $\phi_{n,a}$. For a two-dimensional there is always one ϕ_3. However, in three-dimensions we can choose the height to width ratio of the waveguide, so that there is one or two $\phi_{3,a}$.

If $\mathscr{V}_2 = \mathcal{E}_1 - \mathcal{E}_2$ and $k^2 = \mathcal{E}_2 + \mathscr{V}_2 = \mathcal{E}_1$, (6.78) becomes

$$T_{22}^{-1}(\vec{p},\vec{p}_0) \approx \sum_{a=1}^{d_2} \frac{ie^{(l_1+l_3)\sqrt{|\mathcal{V}_2|}}}{2 - l_2\sqrt{|\mathcal{V}_2|}}\tilde{\phi}_{2,a}^*(\vec{p}_0)\tilde{\phi}_{2,a}(\vec{p}), \quad (6.74)$$

where we used (6.71). This shows that we can choose the wavenumber, the potential and the lengths of the each waveguide such that the transmission of a left-incident wave is determined by just the Fourier transform of ϕ that corresponds to the second energy level. If these waveguides are tow-dimensional of three-dimensional with height to width ratio other than one, this is only one function. If these are three-dimensional waveguides have equal height and width, (6.74) has two terms in the summations. This is another difference that can be observed only in three-dimensional cases.

Now, consider the right reflection coefficient. We can choose $\mathscr{V}_2$ and k such that $k = \mathcal{E}_1 < \mathcal{E}_2 + \mathscr{V}_2$. Then (6.70) reduces to

$$(T_{21}T_{22}^{-1})(\vec{p}_0, \vec{p}) \approx \tilde{\phi}_1^*(\vec{p}_0)\tilde{\phi}_1(\vec{p}) \tag{6.75}$$

which is independent of lengths l_1, l_2, l_3 of the system provided that $l2 \gg L_x$, that is, the part filled with negative potential is long. This is another result of exceptional points in real potential scattering and a multiple finite waveguide system.

6.3 Non-adjecent waveguides

Consider two waveguides with the same size parameters that are not adjacent which means $a_{2-} \neq a_{1+}$. Then the operator $\widehat{\mathbf{T}}$ becomes

$$\widehat{\mathbf{T}} = e^{-il_2\widehat{\mathbf{H}}_2} e^{ia_{2-}\widehat{\varpi}\boldsymbol{\sigma}_3} e^{-ia_{1+}\widehat{\varpi}\boldsymbol{\sigma}_3} e^{-il_1\widehat{\mathbf{H}}_1} = e^{-il_2\widehat{\mathbf{H}}_2} e^{ia\widehat{\varpi}\boldsymbol{\sigma}_3} e^{-il_1\widehat{\mathbf{H}}_1} \tag{6.76}$$

where $a := a_{2-} - a_{1+}$. Using (6.38), we arrive at

$$\begin{aligned}\widehat{\mathbf{T}} &= \frac{e^{-il_2\widehat{W}_2} e^{-il_1\widehat{W}_1}}{4\widehat{W}_1\widehat{W}_2\widehat{\varpi}^2} \begin{bmatrix} \widehat{d}_2^- & -\widehat{o}_2 \\ \widehat{o}_2 & \widehat{d}_2^+ \end{bmatrix} \begin{bmatrix} e^{ia\widehat{\varpi}} & 0 \\ 0 & e^{-ia\widehat{\varpi}} \end{bmatrix} \begin{bmatrix} \widehat{d}_1^- & -\widehat{o}_1 \\ \widehat{o}_1 & \widehat{d}_1^+ \end{bmatrix} \\ &= \frac{e^{-il_2\widehat{W}_2} e^{-il_1\widehat{W}_1}}{4\widehat{W}_1\widehat{W}_2\widehat{\varpi}^2} \begin{bmatrix} e^{ia\widehat{\varpi}}\widehat{d}_2^-\widehat{d}_1^- - e^{-ia\widehat{\varpi}}\widehat{o}_2\widehat{o}_1 & -e^{ia\widehat{\varpi}}\widehat{d}_2^-\widehat{o}_1 - e^{-ia\widehat{\varpi}}\widehat{o}_2\widehat{d}_1^+ \\ e^{ia\widehat{\varpi}}\widehat{d}_1^-\widehat{o}_2 + e^{-ia\widehat{\varpi}}\widehat{d}_2^+\widehat{o}_1 & -e^{ia\widehat{\varpi}}\widehat{o}_2\widehat{o}_1 + e^{-ia\widehat{\varpi}}\widehat{d}_2^+\widehat{d}_1^+ \end{bmatrix}\end{aligned} \tag{6.77}$$

$$\widehat{T}_{22}^{-1} = \frac{4e^{il_2\widehat{W}_2}e^{il_2\widehat{W}_1}\widehat{W}_1\widehat{W}_2\widehat{\varpi}^2}{-e^{ia\widehat{\varpi}}\widehat{o}_2\widehat{o}_1 + e^{-ia\widehat{\varpi}}\widehat{d}_2^+\widehat{d}_1^+} = \frac{4e^{il_2\widehat{W}_2}e^{il_2\widehat{W}_1}e^{ia\widehat{\varpi}}\widehat{W}_1\widehat{W}_2\widehat{\varpi}^2}{\widehat{d}_2^+\widehat{d}_1^+ - e^{2ia\widehat{\varpi}}\widehat{o}_2\widehat{o}_1} \tag{6.78}$$

$$\widehat{T}_{12}\widehat{T}_{22}^{-1} = -\frac{e^{2ia\widehat{\varpi}}\widehat{d}_2^-\widehat{o}_1 + \widehat{d}^+1\widehat{o}_2}{\widehat{d}_2^+\widehat{d}_1^+ - e^{2ia\widehat{\varpi}}\widehat{o}_2\widehat{o}_1} \tag{6.79}$$

Since the size parameters are the same for all waveguides considered here, we can define $\varpi := \varpi_1 = \varpi_2$.

Nonadjacent waveguides filled with equal positive potentials

If the potentials of the waveguides are equal we get, $\widehat{W}_1 = \widehat{W}_2 =: \widehat{W}$, then $\widehat{d}_1^{\pm} = \widehat{d}_2^{\pm} =: \widehat{d}^{\pm}$ and $\widehat{o}_1 = \widehat{o}_2 =: \widehat{o}$, then $\widehat{\mathbf{T}}$ becomes

$$\widehat{\mathbf{T}} = \frac{e^{-i(l_1+l_2)\widehat{W}}}{4\widehat{W}^2\widehat{\varpi}^2}\begin{bmatrix} e^{ia\widehat{\varpi}}(\widehat{d}^-)^2 - e^{-ia\widehat{\varpi}}\widehat{o}^2 & -e^{ia\widehat{\varpi}}\widehat{d}^-\widehat{o} - e^{-ia\widehat{\varpi}}\widehat{o}\widehat{d}^+ \\ e^{ia\widehat{\varpi}}\widehat{d}^-\widehat{o} + e^{-ia\widehat{\varpi}}\widehat{d}^+\widehat{o} & -e^{ia\widehat{\varpi}}\widehat{o}^2 + e^{-ia\widehat{\varpi}}(\widehat{d}^+)^2 \end{bmatrix} \tag{6.80}$$

and T_{22}^{-1} becomes

$$\widehat{T}_{22}^{-1} = \frac{4\widehat{W}^2\widehat{\varpi}^2 e^{i(l_1+l_2)\widehat{W}} e^{ia\widehat{\varpi}}}{e^{-2ia\widehat{\varpi}}(\widehat{d}^+)^2 - \widehat{o}^2} \tag{6.81}$$

Let n_*, m_* be the largest positive integers that makes w_n and ϖ_n are real respectively. Additionally, if we assume $\mathscr{V} > 0$, we can use (6.81) to write

$$\begin{aligned}\widehat{T}_{22}^{-1}(\boldsymbol{p}, \boldsymbol{p}_0) = \sum_{n=1}^{n_*}\sum_{n=a}^{d_n} r_n \tilde{\phi}_{n,a}^*(\boldsymbol{p}_0)\tilde{\phi}_{n,a}(\boldsymbol{p}) + \sum_{n=n^*+1}^{m_*}\sum_{n=a}^{d_n} u_n \tilde{\phi}_{n,a}^*(\boldsymbol{p}_0)\tilde{\phi}_{n,a}(\boldsymbol{p}) \\ + \sum_{n=m^*+1}^{\infty}\sum_{n=a}^{d_n} s_n \tilde{\phi}_{n,a}^*(\boldsymbol{p}_0)\tilde{\phi}_{n,a}(\boldsymbol{p})\end{aligned} \tag{6.82}$$

where

$$r_n = \frac{4|w_n|^2|\varpi_n|^2 e^{2il|w_n|} e^{ia|\varpi_n|}}{e^{-2ia|\varpi_n|}(d^+)^2 - o^2}, \tag{6.83}$$

$$u_n = \frac{4i|w_n|^2|\varpi_n|^2 e^{-2l|w_n|} e^{ia|\varpi_n|}}{e^{-2ia|\varpi_n|}(d^+)^2 - o^2}, \tag{6.84}$$

$$s_n = \frac{-4|w_n|^2|\varpi_n|^2 e^{-2l|w_n|} e^{-a|\varpi_n|}}{e^{-2a|\varpi_n|}(d^+)^2 - o^2}, \tag{6.85}$$

If we let $a \gg L_x$ and $l_1, l_2 \sim L_x$, we have $a|w_n| \gg 1$ for all $n > m_*$ and (6.82) can be written as

$$\widehat{T}_{22}^{-1}(\vec{p}, \vec{p}_0) \approx \sum_{n=1}^{n_*}\sum_{n=a}^{d_n} r_n \tilde{\phi}_{n,a}^*(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}) + \sum_{n=n^*+1}^{m_*}\sum_{n=a}^{d_n} u_n \tilde{\phi}_{n,a}^*(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}). \tag{6.86}$$

This shows that the transmission is determined by the Fourier transform of $\phi_{n,a}$ that corresponds to the first m_* energy levels. This result is similar to what we found in chapter 5 for a single finite waveguide. However, note that for this result to hold the length of the single waveguide must be larger than its height. If there is two finite waveguides filled with positive and equal potentials, the lenght of the waveguides must be similar to their height, however, the length of the empty space between the them must be larger than their height. Moreover, unlike a single waveguide, the number of $\tilde{\phi}_{n,a}$ is not independent of the potential. This is because m_*, which appears in the second summation of (6.86), is determined by the wavenumber and size parameters of the waveguides.

Nonadjacent waveguides filled with equal negative potentials

If $\mathscr{V} < 0$, we get $m_* < n_*$. Here n_* and m_* are defined as previously. Then (6.82) implies

$$\begin{aligned}\widehat{T}_{22}^{-1}(\vec{p},\vec{p}_0) = &\sum_{n=1}^{n_*}\sum_{n=a}^{d_n} r_n\tilde{\phi}_{n,a}^*(\vec{p}_0)\tilde{\phi}_{n,a}(\vec{p}) + \sum_{n=n^*+1}^{m_*}\sum_{n=a}^{d_n} v_n\tilde{\phi}_{n,a}^*(\vec{p}_0)\tilde{\phi}_{n,a}(\boldsymbol{p})\\ &+\sum_{n=m^*+1}^{\infty}\sum_{n=a}^{d_n} s_n\tilde{\phi}_{n,a}^*(\boldsymbol{p}_0)\tilde{\phi}_{n,a}(\vec{p}),\end{aligned} \tag{6.87}$$

where

$$r_n = \frac{4|w_n|^2|\varpi_n|^2 e^{2il|w_n|}e^{ia|\varpi_n|}}{e^{2ia|\varpi_n|}(d^+)^2 - o^2}, \tag{6.88}$$

$$v_n = \frac{4i|w_n|^2|\varpi_n|^2 e^{2il|w_n|}e^{-a|\varpi_n|}}{e^{-2a|\varpi_n|}(d^+)^2 - o^2}, \tag{6.89}$$

$$s_n = \frac{-4|w_n|^2|\varpi_n|^2 e^{-2l|w_n|}e^{-a|\varpi_n|}}{e^{-2a|\varpi_n|}(d^+)^2 - o^2}, \tag{6.90}$$

Moreover, let $l := l_1 = l_2$, $l \gg L_x$ and $a \sim L_x$. Then (6.87) becomes

$$\widehat{T}_{22}^{-1}(\vec{p},\vec{p}_0) \approx \sum_{n=1}^{m_*}\sum_{n=a}^{d_n} r_n\tilde{\phi}_{n,a}^*(\boldsymbol{p}_0)\tilde{\phi}_{n,a}(\vec{p}) + \sum_{n=m^*+1}^{n_*}\sum_{n=a}^{d_n} v_n\tilde{\phi}_{n,a}^*(\vec{p}_0)\tilde{\phi}_{n,a}(\boldsymbol{p}). \tag{6.91}$$

The transmission is determined by the Fourier transform of $\phi_{n,a}$ corresponding to the first m_* energy levels. However, these waveguides must have much larger length compared to the their positive potential filled counterparts. Let $k^2 = \mathcal{E}_l$ and $\mathscr{V} = \mathcal{E}_l - \mathcal{E}_j$ for some positive integer $j > l$. Then the wavenumber is equal to the jth exceptional wavenumber of the waveguides. Moreover we have,

$$\varpi_l = 0, \qquad w_l = \sqrt{-\mathscr{V}} \tag{6.92}$$

$$\varpi_j = i\sqrt{-\mathscr{V}}, \qquad w_j = 0. \tag{6.93}$$

These imply

$$r_l = 0, \qquad v_j = \frac{-4i\mathscr{V}e^{-a\sqrt{-\mathscr{V}}}}{e^{-2a\sqrt{-\mathscr{V}}}(2il\mathscr{V} - 4i\sqrt{-\mathscr{V}})^2 - (2il\mathscr{V})^2} \tag{6.94}$$

Here, we found the second equality by calculation the limit of (6.89) as $|w_j| \to 0$ and used the L'Hospitals rule twice. Then the transmission is determined by the Fourier transform of $\phi_{n,a}$ corresponding to the first j energy levels except the jth energy level.

Let $k = \mathcal{E}_2$ and $\mathscr{V} = \mathcal{E}_2 - \mathcal{E}_3$, then (6.91) becomes

$$\widehat{T}_{22}^{-1}(\vec{p}, \vec{p}_0) \approx r_1 \tilde{\phi}_{1,a}^*(\vec{p}_0)\tilde{\phi}_{1,a}(\vec{p}) + \sum_{n=a}^{d_2} v_2 \tilde{\phi}_{2,a}^*(\vec{p}_0)\tilde{\phi}_{2,a}(\vec{p}). \tag{6.95}$$

Here we dropped the summation in the first term because the first energy level is always nondegenerate.

Let $k = \mathcal{E}_1$ and $\mathscr{V} = \mathcal{E}_1 - \mathcal{E}_2$, then (6.91) becomes

$$\widehat{T}_{22}^{-1}(\vec{p}, \vec{p}_0) \approx \sum_{n=a}^{d_2} v_2 \tilde{\phi}_{2,a}^*(\vec{p}_0)\tilde{\phi}_{2,a}(\vec{p}). \tag{6.96}$$

The transmitted wave from this system is determined by just the second energy level and corresponding eigenfunctions of particle in *box*. This result cannot be obtained by a single finite waveguide. This is a result existence exceptional point in our systems. The nonadjecent two finite waveguides filled with negative potential can be used to filter the effects all eigenfunctions except the second. Moreover, we can see the effects of existence of degenerate energy levels in the three-dimensional case. It is possible to choose the height to witdh ratio of the waveguide so that there is Fourier transforms one or two $\phi_{2,a}$ appear in (6.96). However, for a two-dimensional waveguide there is always one.

6.4 Waveguides with different size parameters

Consider three empty two-dimensional waveguides, such that $L_{x,i}^- = 0$, $L^x := L_{x,1}^+ = L_{x,3}^+ < L_{x,2}^+ =: b$ for all $i, j \in \{1, 2, 3\}$. Since the waveguides are empty $\widehat{W}_i = \widehat{\varpi}_i$ for

$i \in \{1,2,3\}$. The operator $\widehat{\mathbf{T}}$ becomes

$$\widehat{\mathbf{T}} = e^{-il_3\widehat{\mathbf{H}}_3}e^{-il_2\widehat{\mathbf{H}}_2}e^{-il_1\widehat{\mathbf{H}}_1} = e^{il_3\widehat{\varpi}_3\boldsymbol{\sigma}_3}e^{il_2\widehat{\varpi}_2\boldsymbol{\sigma}_3}e^{il_1\widehat{\varpi}_1\boldsymbol{\sigma}_3}$$
$$= \begin{bmatrix} e^{il_3\widehat{\varpi}_3}e^{il_2\widehat{\varpi}_2}e^{il_1\widehat{\varpi}_1} & 0 \\ 0 & e^{-il_3\widehat{\varpi}_3}e^{-il_2\widehat{\varpi}_2}e^{-il_1\widehat{\varpi}_1} \end{bmatrix} \tag{6.97}$$

The operators $\widehat{\varpi}_1$ and $\widehat{\varpi}_2$ commute with each other, however do not commute with $\widehat{\varpi}_3$, which makes calculation more complicated compared to previous examples.

Notice that we can write

$$e^{\pm il_j\widehat{\varpi}_j} = \sum_{n=1}^{\infty}\sum_{a=1}^{d_n} e^{\pm il_j\varpi_{j,n}}|\phi_{n,a}^{(j)}\rangle\langle\phi_{n,a}^{(j)}|, \tag{6.98}$$

which implies

$$e^{\pm il_3\widehat{\varpi}_3}e^{\pm il_2\widehat{\varpi}_2}e^{\pm il_1\widehat{\varpi}_1} =$$
$$\Big(\sum_{n=1}^{\infty}\sum_{a=1}^{d_n} e^{\pm il_3\varpi_{3,n}}|\phi_{n,a}^{(1)}\rangle\langle\phi_{n,a}^{(1)}|\Big)\Big(\sum_{m=1}^{\infty}\sum_{b=1}^{d_m} e^{\pm il_2\varpi_{2,m}}|\phi_{m,a}^{(2)}\rangle\langle\phi_{m,a}^{(2)}|\Big)\Big(\sum_{t=1}^{\infty}\sum_{c=1}^{d_t} e^{\pm il_1\varpi_{1,t}}|\phi_{t,a}^{(1)}\rangle\langle\phi_{t,a}^{(1)}|\Big)$$
$$= \sum_{n,m,t=1}^{\infty} e^{\pm il_3\varpi_{3,n}}e^{\pm il_2\varpi_{2,m}}e^{\pm il_1\varpi_{1,t}}|\phi_{n,a}^{(1)}\rangle(\langle\phi_{n,a}^{(1)}|\phi_{m,b}^{(2)}\rangle)(\langle\phi_{m,b}^{(2)}|\phi_{t,c}^{(1)}\rangle)\langle\phi_{t,c}^{(1)}|$$
$$= \sum_{n,m,t=1}^{\infty} e^{\pm il_3\varpi_{3,n}}e^{\pm il_2\varpi_{2,m}}e^{\pm il_1\varpi_{1,p}}(\langle\phi_{n,a}^{(1)}|\phi_{m,b}^{(2)}\rangle)\langle\phi_{m,b}^{(2)}|\phi_{t,c}^{(1)}\rangle)|\phi_{n,a}^{(1)}\rangle\langle\phi_{t,c}^{(1)}|, \tag{6.99}$$

Inserting this to (6.97) we get

$$T_{11}(\vec{p},\vec{p_0}) = T_{22}^{-1}(\boldsymbol{p},\boldsymbol{p}_0) = \sum_{n,m,t=1}^{\infty} e^{il_3\varpi_{3,n}}e^{il_2\varpi_{2,m}}e^{il_1\varpi_{1,t}}C_{n,m}^{1,2}C_{m,t}^{2,1}\tilde{\phi}_{n,a}^{(1)*}(\vec{p}_0)\tilde{\phi}_{t,b}^{(1)}(\vec{p}) \tag{6.100}$$

where $C_{nm}^{jk} := \langle\phi_{n,a}^{(j)}|\phi_{m,b}^{(k)}\rangle$, which can be found with the following integral.

$$\int_{-\infty}^{\infty} dx\langle\phi_n^{(j)}|x\rangle\langle x|\phi_m^{(k)}\rangle = \frac{2}{\sqrt{bL_x}}\int_0^{L_x} dx\sin(\frac{\pi nx}{L_x})\sin(\frac{\pi mx}{b})$$
$$= \frac{1}{\sqrt{L_x b}}\int_0^{L_x} dx\Big[\cos(\frac{\pi nx}{L_x} - \frac{\pi mx}{b}) - \cos(\frac{\pi nx}{L_x} + \frac{\pi mx}{b})\Big] \tag{6.101}$$
$$= \frac{1}{\sqrt{L_x b}}\int_0^{L_x} dx\Big[\cos(\frac{\pi x}{bL_x}(nb - mL_x)) - \cos(\frac{\pi x}{bL_x}(nb + mL_x))\Big]$$

Consider the integrals separately,

$$\int_0^{L_x} dx \cos\big(\frac{\pi x}{bL_x}(nb+mL_x)\big) = -\frac{bL_x \sin\big(\frac{\pi x}{bL_x}(nb+mL_x)\big)}{\pi(nb+mLx)}\Bigg|_0^{L_x}$$
$$= \frac{(-1)^{n+1}bL_x}{\pi(nb+mL_x)}\sin(\pi m L_x/b)$$

If $nb = mL_x$

$$\int_0^{L_x} dx \cos\big(\frac{\pi x}{bL_x}(nb-mL_x)\big) = \int_0^{L_x} dx \cos 0 = L_x$$

otherwise

$$\int_0^{L_x} dx \cos\big(\frac{\pi x}{bL_x}(nb-mL_x)\big) = -\frac{bL_x \sin\big(\frac{\pi x}{bL_x}(nb-mL_x)\big)}{\pi(nb-mLx)}\Bigg|_0^{L_x}$$
$$= \frac{(-1)^{n}bL_x}{\pi(nb-mL_x)}\sin(\pi m L_x/b),$$

Inserting these into (6.101), we get the following expression for C^{jk}_{nm}.

$$C^{jk}_{nm} = \begin{cases} \sqrt{\frac{L_x}{b}} + \frac{(-1)^n\sqrt{bL_x}}{\pi(nb+mL_x)}\sin(\pi m L_x/b) & \text{if } nb = mL_x, \\ \frac{(-1)^n 4b\sqrt{bL_x}}{\pi\big((nb)^2-(mL_x)^2\big)}\sin(\pi m L_x/b) & \text{if } nb \neq mL_x, \end{cases} \tag{6.102}$$

Note that if $b = L_x$, $C^{jk}_{nm} = \delta_{nm}$ as expected.

Let n_*, m_* be the largest integers such that $\varpi_{1,n}$ and $\varpi_{2,n}$ are real respectively. Since $b > L_x$, we have $\mathcal{E}_{1,n} > \mathcal{E}_{2,n}$, which implies $m_* > n_*$. Then (6.99) can be written as

$$\begin{aligned} T^{-1}_{22}(\vec{p},\vec{p}_0) = &\sum_{n,m,t=1}^{n_*} e^{i(l_1|\varpi_{1,n}|+l_2|\varpi_{1,p}|)} e^{il_2|\varpi_{2,m}|} C^{1,2}_{n,m} C^{2,1}_{m,t} \tilde{\phi}^*_n(\vec{p}_0)\tilde{\phi}_t(\vec{p}) \\ &+ \sum_{n,m,t=n_*+1}^{m_*} e^{-(l_1|\varpi_{1,n}|+l_3|\varpi_{1,p}|)} e^{il_2|\varpi_{2,m}|} C^{1,2}_{n,m} C^{2,1}_{m,p} \tilde{\phi}^*_n(\vec{p}_0)\tilde{\phi}_t(\vec{p}) \\ &+ \sum_{n,m,t=m_*+1}^{\infty} e^{-(l_1|\varpi_{1,n}|+l_2|\varpi_{1,p}|)} e^{-l_2|\varpi_{2,m}|} C^{1,2}_{n,m} C^{2,1}_{m,p} \tilde{\phi}^*_n(\vec{p}_0)\tilde{\phi}_t(\vec{p}) \end{aligned} \tag{6.103}$$

Let $l := l_1 = l_3 \gg L_x$, then $(l_1|\varpi_{1,n}| + l_3|\varpi_{1,p}|) \gg 1$ for $n, p > n_*$, and the equation (6.103) becomes

$$T^{-1}_{22}(\vec{p},\vec{p}_0) \approx \sum_{n,m,t=1}^{n_*} e^{il(|\varpi_{1,n}|+|\varpi_{1,t}|)} e^{il_2|\varpi_{2,m}|} C^{1,2}_{n,m} C^{2,1}_{m,t} \tilde{\phi}^*_n(\vec{p}_0)\tilde{\phi}_t(\vec{p}) \tag{6.104}$$

which can be rearranged as

$$T_{22}^{-1}(\vec{p},\vec{p}_0) \approx \sum_{t=1}^{n_*}\left(\sum_{n,m=1}^{n_*} e^{i(l\varpi_{1,n}+l_2\varpi_{2,n})}C_{n,m}^{1,2}C_{m,t}^{2,1}\tilde{\phi}_n^*(\vec{p}_0)\right)e^{il|\varpi_{1,t}|}\tilde{\phi}_t(\vec{p}). \tag{6.105}$$

Compared to T_{22}^{-1} for a single empty waveguide of length $l_{tot} = l_1 + l_2 + l_3$ and height L_x. We can use equations and find

$$T_{22}^{-1}(\vec{p},\vec{p}_0) \approx \sum_{t=1}^{n_*} e^{iL\varpi_{1,t}}\tilde{\phi}_t^*(\vec{p}_0)\tilde{\phi}_t(\vec{p}). \tag{6.106}$$

The coefficient of $\tilde{\phi}_t(\vec{p})$ that appears in T_{22}^{-1} for these waveguides are different. In order to observe the effects of this difference we let the incident angle $\theta_0 = 0$. Then (4.35) implies $p_0 = 0$, and

$$\tilde{\phi}_m^*(\vec{p}_0) = i\sqrt{\frac{L_x}{2}} \tag{6.107}$$

Here we used (5.51). The coefficient of $\tilde{\phi}_t(\vec{p})$ for a single waveguide becomes

$$e^{iL\varpi_{1,t}}\tilde{\phi}_t^*(\vec{p}_0) = i\sqrt{\frac{L_x}{2}}e^{il_{tot}k\sqrt{1-\pi^2t^2/L_x^2}} \tag{6.108}$$

and the coefficient of $\tilde{\phi}_t(\vec{p})$ for the three waveguide system we considered in this subsection is

$$\begin{aligned}&\sum_{n,m=1}^{n_*} e^{i(l\varpi_{1,n}+l_2\varpi_{2,m})}C_{n,m}^{1,2}C_{m,t}^{2,1}\tilde{\phi}_n^*(\vec{p}_0)\\ &\quad = i\sqrt{\frac{L_x}{2}}\sum_{n,m=1}^{n_*} e^{ik(l\sqrt{1-\pi^2n^2/k^2L_x^2}+l_2\sqrt{1-\pi^2m^2/k^2b^2})}C_{n,m}^{1,2}C_{m,t}^{2,1}.\end{aligned} \tag{6.109}$$

Chapter 7

CONCLUSIONS

Exceptional points are kind of isolated singularities that can appear in non-Hermitian operators that have significant physical consequences. At these points, two or more eigenvalues and the corresponding eigenvectors coalesce, rendering the operator non-diagonalizable. In chapter 2, we examine a parameter dependent eigenvalue problem and the behaviour of the Jordan Normal form of an linear operator at certain kinds points, one of which is defined as exceptional points. Chapter 2, shows how an analytical function of an almost everywhere diagonalizable behaves at an exceptional point.

Exceptional points can be observed exclusively in non-Hermitian operators. The fact that closed systems considered in standard quantum mechanics require Hermitian Hamiltonian operators, lead to the idea that exceptional points are irrelevant to quantum mechanics of such systems. The paper [23], proves the contrary by showing that exceptional points can be relevant to stationary scattering from a real potential, which is a closed system. In this paper, scattering from a two-dimensional finite waveguide filled with some non-active, homogeneous material is examined using the dynamical formulation of two-dimensional stationary scattering. This formulation, allows a generalization of the transfer matrix to higher dimensions, which was previously restricted to one-dimensional scattering, by associating the transfer matrix with the time-evaluation operator for a non-Hermitian effective Hamiltonian. The non-Herminicity of this effective Hamiltonian, makes it possible to observe exceptional points, even for real potential scattering problems. The significant results found in this paper are, In this thesis, we extend this scattering problem to three-dimensions by examining the stationary scattering from a finite three-dimensional waveguide filled homogeneously with non-active and lossless material. Chapter 3, provides the DFSS in one dimensions, which is first introduced by [26], [27]. In chapter 4, we extend this formulation for higher-dimensional stationary scattering problems and define a higher-dimensional counterpart of the transfer matrix, which [24] and [25] showed previously for two- and three-dimensional systems. In particular, we showed the composition property for higher-dimensional transfer matrix and find an expression for the transfer matrix for a potential that is bounded in its scattering axis and is a confining potential in the axes that are perpendicular to the scattering axis. The latter property of the potential, the effective Hamiltonian of the system has a discrete spectrum which in turn allows us to find an explicit formula for the transfer matrix. Moreover, for real potential, the effective Hamiltonian turns out to be a pseudo-Hermitian operator, and as discussed in chapter 2, it has a spectrum consists of real and complex conjugate pairs numbers. In particular, the spectrum of the effective Hamiltonian for the

Chapter 5 uses the machinary developed in chapter 4 to solve the scattering problem for finite waveguides for two-and three-dimensions, and analyzes the reflection and transmission of the the incident wave for different cases of waveguides and find an excplicit expression for the transfer matrix. This choise of potential reduces the calculation of the transfer matrix to the exponential of the effective Hamiltonian. This is an eigenvalue problem that is dependent to the wavenumber of the incident wave.

Section 5.4 discusses the similarities and differences of two-and three-dimensional finite waveguides. For both two and three-dimensional waveguides, we can choose the length of the waveguide such that the transmission is determined by the first n energy levels of a particle in a box and the Fourier transforms of the eigenfunctions corresponding to these energy levels. Moreover, we can choose the size parameters of an empty waveguide such that the transmission is determined by the Fourier transform of the first eigenfunction and the transmission is independent of the length of the waveguide. The difference of the three-dimensional case over its two-dimensional counterpart are that the energy levels can be degenerate and in addition to the length and the height of the waveguide, the width is an additional parameter. By changing the width parameter and keeping the height same, the number of Fourier transforms of eigenfunctions that determined the transmission amplitude becomes more sensitive to the change of the wavenumber of the incident wave. In particular, if the width of a three-dimensional waveguide increases the number of this number increases. However, it is possible make use of the possible degeneracy of the spectrum, and choose the wavenumber such that a waveguide of smaller waveguide is equal to the the number for the wider waveguide. These properties cannot be observed in a two-dimensional waveguide.

In chapter 6, we made use of the composition property of the transfer matrix to examine the scattering problem of a system that consists of multiple finite waveguide in both two- and three-dimensions. First we consider waveguides such that the height, and the width if the waveguide is three-dimensional, are equal. This restriction makes the calculations simpler. We showed that for two filled waveguides separated by an empty waveguide, we can choose the sizes of the waveguides, the potential that describes the material inside the filled waveguides and such that the incident wavenumber is equal to the first and the third exceptional wavenumber of the filled and empty waveguides respectively. In this case, transmission is determined by the Fourier transform of the second eigenvalue and the corresponding eigenfunctions. For the two-dimensional case there is one wavefunction, however for the three-dimensional case we can choose the height to width ratio of the waveguide such that the second energy level is doubly degenerate, that is, there is two eigenfunctions corresponding to the second energy level and the transmission from this waveguide is determined by the Fourier transform of these eigenfunctions. This is an another difference of the two- and three-dimensional waveguides. Additionally, we showed that it is possible to choose the potential and the sizes of the waveguides such that, the transmission is determined by the first n Fourier transform except one. The combination of the the different waveguides, allows us to set up a system such that the reflection is determined by the first n Fourier transforms, this property does not exist for one finite waveguide.

BIBLIOGRAPHY

[1] Tosio Kato. *Perturbation theory for linear operators*, volume 132. Springer Science & Business Media, 2013.

[2] MV Berry and DHJ O'Dell. Diffraction by volume gratings with imaginary potentials. *Journal of Physics A: Mathematical and General*, 31(8):2093, 1998.

[3] WD Heiss. Phases of wave functions and level repulsion. *The European Physical Journal D-Atomic, Molecular, Optical and Plasma Physics*, 7:1–4, 1999.

[4] E Persson, Ingrid Rotter, H-J Stöckmann, and M Barth. Observation of resonance trapping in an open microwave cavity. *Physical review letters*, 85(12):2478, 2000.

[5] C Dembowski, H-D Gräf, HL Harney, A Heine, WD Heiss, H Rehfeld, and A Richter. Experimental observation of the topological structure of exceptional points. *Physical review letters*, 86(5):787, 2001.

[6] Carl M Bender and Stefan Boettcher. Real spectra in non-hermitian hamiltonians having p t symmetry. *Physical review letters*, 80(24):5243, 1998.

[7] Patrick Dorey, Clare Dunning, and Roberto Tateo. Spectral equivalences, bethe ansatz equations, and reality properties in p t-symmetric quantum mechanics. *Journal of Physics A: Mathematical and General*, 34(28):5679, 2001.

[8] Uwe Günther, Ingrid Rotter, and Boris F Samsonov. Projective hilbert space structures at exceptional points. *Journal of Physics A: Mathematical and Theoretical*, 40(30):8815, 2007.

[9] Eva Maria Graefe, Uwe Günther, HJ Korsch, and AE Niederle. A non-hermitian symmetric bose–hubbard model: eigenvalue rings from unfolding

higher-order exceptional points. *Journal of Physics A: Mathematical and Theoretical*, 41(25):255206, 2008.

[10] Patrick Dorey, Clare Dunning, Anna Lishman, and Roberto Tateo. symmetry breaking and exceptional points for a class of inhomogeneous complex potentials. *Journal of Physics A: Mathematical and Theoretical*, 42(46):465302, 2009.

[11] Hossein Hodaei, Absar U Hassan, Steffen Wittek, Hipolito Garcia-Gracia, Ramy El-Ganainy, Demetrios N Christodoulides, and Mercedeh Khajavikhan. Enhanced sensitivity at higher-order exceptional points. *Nature*, 548(7666):187–191, 2017.

[12] Jan Wiersig. Enhancing the sensitivity of frequency and energy splitting detection by using exceptional points: application to microcavity sensors for single-particle detection. *Physical review letters*, 112(20):203901, 2014.

[13] Weijian Chen, Şahin Kaya Özdemir, Guangming Zhao, Jan Wiersig, and Lan Yang. Exceptional points enhance sensing in an optical microcavity. *Nature*, 548(7666):192–196, 2017.

[14] Matthias Liertzer, Li Ge, Alex Cerjan, A Douglas Stone, Hakan E Türeci, and Stefan Rotter. Pump-induced exceptional points in lasers. *Physical Review Letters*, 108(17):173901, 2012.

[15] Jan Wiersig. Sensors operating at exceptional points: General theory. *Physical review A*, 93(3):033809, 2016.

[16] Mohammad-Ali Miri and Andrea Alù. Exceptional points in optics and photonics. *Science*, 363(6422):eaar7709, 2019.

[17] R El-Ganainy, KG Makris, DN Christodoulides, and Ziad H Musslimani. Theory of coupled optical pt-symmetric structures. *Optics letters*, 32(17):2632–2634, 2007.

[18] Konstantinos G Makris, R El-Ganainy, DN Christodoulides, and Ziad H Musslimani. Beam dynamics in p t symmetric optical lattices. *Physical Review Letters*, 100(10):103904, 2008.

[19] Shachar Klaiman, Uwe Günther, and Nimrod Moiseyev. Visualization of branch points in p t-symmetric waveguides. *Physical review letters*, 101(8):080402, 2008.

[20] Stefano Longhi. Bloch oscillations in complex crystals with p t symmetry. *Physical review letters*, 103(12):123601, 2009.

[21] Massimo Moccia, Giuseppe Castaldi, Francesco Monticone, and Vincenzo Galdi. Exceptional points in flat optics: A non-hermitian line-wave scenario. *Physical Review Applied*, 15(6):064067, 2021.

[22] Alex J Grede, Nina Krainova, and Noel C Giebink. Exceptional point magneto-optic isolators. *Optics Express*, 29(14):22614–22622, 2021.

[23] Farhang Loran and Ali Mostafazadeh. Exceptional points and pseudo-hermiticity in real potential scattering. *SciPost Physics*, 12(3):109, 2022.

[24] Farhang Loran and Ali Mostafazadeh. Transfer matrix formulation of scattering theory in two and three dimensions. *Physical Review A*, 93(4):042707, 2016.

[25] Farhang Loran and Ali Mostafazadeh. Fundamental transfer matrix and dynamical formulation of stationary scattering in two and three dimensions. *Physical Review A*, 104(3):032222, 2021.

[26] Ali Mostafazadeh. A dynamical formulation of one-dimensional scattering theory and its applications in optics. *Annals of Physics*, 341:77–85, 2014.

[27] Ali Mostafazadeh. Transfer matrices as nonunitary s matrices, multimode unidirectional invisibility, and perturbative inverse scattering. *Physical Review A*, 89(1):012709, 2014.

[28] Ali Mostafazadeh. Pseudo-hermitian representation of quantum mechanics. *International Journal of Geometric Methods in Modern Physics*, 7(07):1191–1306, 2010.

[29] Sheldon Axler. *Linear algebra done right*. Springer Science & Business Media, 1997.

[30] Israel Gohberg and Kreĭ. *Introduction to the theory of linear nonselfadjoint operators*.

[31] Konrad Knopp. *Theory of functions, Parts I and II*. Courier Corporation, 2013.

[32] Nimrod Moiseyev. *Non-Hermitian quantum mechanics*. Cambridge University Press, 2011.

[33] Ali Mostafazadeh. Transfer matrix in scattering theory: A survey of basic properties and recent developments. *Turkish Journal of Physics*, 44(6):472–527, 2020.

[34] R Clark Jones. A new calculus for the treatment of optical systemsi. description and discussion of the calculus. *Josa*, 31(7):488–493, 1941.

[35] Farhang Loran and Ali Mostafazadeh. Composition of transfer matrices for potentials with overlapping support. *Annals of Physics*, 359:230–242, 2015.

[36] JB Pendry and A MacKinnon. Calculation of photon dispersion relations. *Physical Review Letters*, 69(19):2772, 1992.

[37] P Markoš and CM Soukoulis. Numerical studies of left-handed materials and arrays of split ring resonators. *Physical Review E*, 65(3):036622, 2002.

[38] Pochi Yeh and Michael Hendry. Optical waves in layered media. *Physics Today*, 43(1):77, 1990.

[39] CC Wan, Tiago De Jesus, and Hong Guo. Magnetoconductance of a quantum wire with several antidots: A transfer-matrix study. *Physical Review B*, 57(19):11907, 1998.

[40] D R Smith, S Schultz, P Markoš, and CM Soukoulis. Determination of effective permittivity and permeability of metamaterials from reflection and transmission coefficients. *Physical review B*, 65(19):195104, 2002.

[41] Peter Markos. Numerical analysis of the anderson localization. *arXiv preprint cond-mat/0609580*, 2006.

[42] Daniel Lévesque and Luc Piché. A robust transfer matrix formulation for the ultrasonic response of multilayered absorbing media. *The Journal of the Acoustical Society of America*, 92(1):452–467, 1992.

[43] William T Thomson. Transmission of elastic waves through a stratified solid medium. *Journal of applied Physics*, 21(2):89–93, 1950.

[44] Bernard Hosten and Michel Castaings. Transfer matrix of multilayered absorbing and anisotropic media. measurements and simulations of ultrasonic wave propagation through composite materials. *The Journal of the Acoustical Society of America*, 94(3):1488–1495, 1993.

[45] JG Muga, JP Palao, B Navarro, and IL Egusquiza. Complex absorbing potentials. *Physics Reports*, 395(6):357–426, 2004.

[46] Luis L Sánchez-Soto, Juan J Monzón, Alberto G Barriuso, and José F Cariñena. The transfer matrix: A geometrical perspective. *Physics Reports*, 513(4):191–227, 2012.

[47] Steven Weinberg. *The quantum theory of fields*, volume 2. Cambridge university press, 1995.

Appendix A

DYNAMICS OF A TWO-LEVEL QUANTUM SYSTEM

Consider a two level quantum system with a Hilbert space $\mathscr{H}$ that is isomorphic to $\mathbb{C}^2$. Every vector $\psi \in \mathscr{H}$ and linear operator $O : \mathscr{H} \to \mathscr{H}$, can be expressed int he following form,

$$\mathbf{\Psi} = \begin{bmatrix} \mathbf{\Psi}_1 \\ \mathbf{\Psi}_2 \end{bmatrix}. \tag{A.1}$$

The Hamiltonian $\mathbf{H} = \mathbf{H}_0 + \mathbf{V}$, where $\mathbf{H}_0$ is called the free Hamiltonian and $\mathbf{V}$ is the interaction Hamiltonian The dynamics of this system is given by the time-dependent Schrödinger equation,

$$i\partial_t \mathbf{\Phi}(t) = \mathbf{H}(t)\mathbf{\Phi}(t). \tag{A.2}$$

The time-evolution operator $\mathbf{U}(t, t_0)$ is defined as,

$$\mathbf{\Phi}(t) = \mathbf{U}(t, t_0)\mathbf{\Phi}(t). \tag{A.3}$$

It must satisfy,

$$i\partial_t \mathbf{U}(t, t_0) = \mathbf{H}(t)\mathbf{U}(t, t_0), \qquad U(t_0, t_0) = \mathbf{I}, \tag{A.4}$$

where $\mathbf{I}$ is the identity operator defined on $\mathscr{H}$.

The time evolution operator has the composition property, i.e,

$$\mathbf{U}(t_2, t_1)\mathbf{U}(t_1, t_0) = \mathbf{U}(t_2, t_0), \tag{A.5}$$

where t_0, t_1 and t_2 are real parameters that satisfy. This also implies,

$$\mathbf{U}(t, t_0)^{-1} = \mathbf{U}(t_0, t). \tag{A.6}$$

Now, we define the interaction picture of this system. The interaction picture Hamiltonian $\boldsymbol{\mathcal{H}}(t)$, state-vector $\mathbf{\Psi}(t)$ and evolution operator $\boldsymbol{\mathcal{U}}(t, t_0)$ are related to

$\mathbf{H}(t)$,$\mathbf{\Psi}(t)$ and $\mathbf{U}(t, t_0)$ as follows.

$$\boldsymbol{\mathcal{H}}(t) = e^{i(t-t_0)\mathbf{H}_0}\mathbf{H}(t)e^{-i(t-t_0)\mathbf{H}_0} - \mathbf{H}_0, \tag{A.7}$$

$$\mathbf{\Psi}(t) = e^{i(t-t_0)\mathbf{H}_0}\mathbf{\Phi}(t), \tag{A.8}$$

$$\boldsymbol{\mathcal{U}}(t, t_0) = e^{i(t-t_0)\mathbf{H}_0}\mathbf{U}(t_1, t_0). \tag{A.9}$$