A RIEMANN-HILBERT APPROACH TO SCATTERING ON A ONE-DIMENSIONAL SEMI-INFINITE CRYSTAL

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ABSTRACT

In this paper the scattering of a non-relativistic particle on a semi-infinite crystal is analyzed using the method of the Riemann-Hilbert Problem for analytic functions. We proceed in the framework of the limiting absorption principle. Our formulas allow to find the scattered field at any point of the crystal. In particular, we obtain an explicit formula for the reflection coefficient off the crystal. We discuss the limiting cases of the strong and weak potentials. For compactly supported potentials we present a general result regarding a relation between the reflection and transmission coefficients.

DEDICATION

This thesis is dedicated to family and to the memory of my Grandmother. My education owes much to their support and their nigh-infinite patience.

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CHAPTER I

INTRODUCTION

This paper is devoted to a particular explicitly solvable model from Quantum Mechanics. The general theory of the solvable models is described in [2]. We consider the scattering problem of a non-relativistic particle on a semi-infinite crystal. The general scattering theory is an exciting area of the modern Mathematical Physics. This branch of Mathematics studies diverse physical models with the help of a broad arsenal of mathematical methods. We only give two examples. (a) Spectral Analysis is used to study scattering from quite an arbitrary potential [11]. (b) The Wiener-Hopf technique [8] is used to study acoustic or electromagnetic scattering from the obstacles of the special form. This approach is based on the reduction of the scattering problem to the so-called Riemann-Hilbert problem for analytic functions [7]. We will use a modification of this method to our Quantum scattering problem.

In Section 2 we briefly describe Kronig-Penny model that was a motivation for the project. In Section 3 we formulate the scattering problem under consideration and reduce it to a linear algebraic system (LAS). In Section 4 we first of all formulate the limiting absorption principle that we use to guarantee the convergence of the infinite series that systematically appear in the project. We further reduce the algebraic system to a Riemann-Hilbert problem. We solve this problem in Section 5. In Section 6 we derive an explicit formula for the reflection coefficient. We also derive the asymptotic formulas for the reflection coefficient for a "strong" and "weak" crystals and give a brief remark on a possibility to solve Inverse Problem for our model. In Section 7 we give some remarks on the scattering from a finite crystal and prove a theorem that connects the reflection and transmission coefficients. In Section 8 we briefly discuss the Hamiltonian of a single delta potential. In Conclusion we summarize our results and outline the directions for future research.

CHAPTER II

KRONIG-PENNEY MODEL

In the Kronig-Penney model [5] an infinite one-dimensional crystal is considered. Two types of potentials are considered; (a) periodic piece-wise constant potential; (b) the series of equally spaced delta distributions. For instance

$$-\psi''(x) + \alpha \sum_{n=-\infty}^{\infty} \delta(x - nd)\psi(x) = k_0^2 \psi(x) \tag{II.1}$$

is the Schrödinger equation of a particle in a potential in the form of the delta functions of strength α spaced d units apart and energy k_0^2. The periodicity of the potential is exploited in the solution of the Schrödinger equation by using

Theorem II.0.1 (Bloch's Theorem). *The solution $\psi(x)$ to the Schrödinger equation with periodic potential with period d takes the form $\psi(x) = e^{ikx}u(x)$ with $u(x)$ also periodic with period d.*

■

Making the substitution into $\psi(x) = u(x)e^{ikx}$ into (II.1) we find that $u(x)$ solves the differential equation

$$-u''(x) - 2iku'(x) = (k_0^2 - k^2)u(x), \ 0 \le x \le d \tag{II.2}$$

subject to the boundary conditions $u(0) = u(d)$ and $u'(0+) = u'(d-) + \alpha u(0)$ with some constant α. We find that the solutions to this equation are of the form $u(x) = Ae^{i(k_0-k)x} + Be^{i(-k_0-k)x}$. Thus $\psi(x) = u(x)e^{ikx} = Ae^{ik_0x} + Be^{-ik_0x}$.

From the boundary conditions, we have the relations

$$\begin{aligned} A + B &= Ae^{i(k_0-k)d} + Be^{i(-k_0-k)d}\,, \\ i(k_0 - k)A + i(-k_0 - k)B + \alpha A + \alpha B &= \\ i(k_0 - k)Ae^{i(k_0-k)d} + i(-k_0 - k)Be^{i(-k_0-k)d}&. \end{aligned} \tag{II.3}$$

This system has a non-trivial solution when

$$\begin{vmatrix} 1 - e^{i(k_0-k)d} & 1 - e^{i(-k_0-k)d} \\ i(k_0 - k)(1 - e^{i(k_0-kd}) + \alpha & i(-k_0 - k)(1 - e^{i(-k_0-k)d}) + \alpha \end{vmatrix} = 0 \tag{II.4}$$

For the simplest case $\alpha = 0$ this gives the condition that $k_0 = 0$ or $k_0 = \pm(2\pi n/d + k)$, $n \in \mathbb{Z}$. We easily find a connection between A and B. We conclude that the spectrum of the problem is discrete and real.

CHAPTER III

SCATTERING OF SEMI-INFINITE CRYSTAL

The solution for the Kronig-Penney model relies on Bloch's theorem [4] which requires the periodicity of the potential. For a semi-infinite crystal that has evenly spaced delta distribution potentials for $x \geq 0$, we lose periodicity and hence we are unable to invoke Bloch's theorem. We must then approach the problem using a different strategy.

In the following discussion, we proceed at a formal level. Though we will see that all infinite series we are dealing with converge where appropriate, we leave many interesting questions unanswered. They may represent our future research.

The time-independent Schrödinger equation for a semi-infinite crystal of spacing d starting at 0 is

$$-\psi''(x) + \alpha \sum_{n=0}^{\infty} \delta(x - nd)\psi(x) = k_0^2 \psi(x). \tag{III.1}$$

III.1. Reduction to a Linear Algebraic System

The wave function ψ can be decomposed into the sum of two states, the incoming and outgoing states. We write these as $\psi = \psi_i + \psi_s$, where ψ_i is the incoming "incident" portion of the wave, and ψ_s is the outgoing "scattered" portion of the wave. We make the simplifying assumption that the incident wave is a plane wave approaching from the left, i.e., $\psi_i = e^{ik_0 x}$. Once this base case is solved, we may solve for other forms of the incident wave by Fourier analysis. Schrödinger's equation then becomes:

$$-\psi_s''(x) + k_0^2 e^{ik_0 x} + \sum_{n=0}^{\infty} \alpha\delta(x - nd) \left(\psi_s(x) + e^{ik_0 x}\right) = k_0^2 \psi_s + k_0^2 e^{ik_0 x}. \tag{III.2}$$

Canceling out the $k_0^2 e^{ik_0 x}$ from both sides yields

$$-\psi_s''(x) + \sum_{n=0}^{\infty} \alpha\delta(x - nd)\left(\psi_s(x) + e^{ik_0 x}\right) = k_0^2\psi. \tag{III.3}$$

We will use the following result.

Lemma III.1.1.

$$\frac{d^2}{dx^2}e^{ik|x|} = -k^2 e^{ik|x|} + 2ik\delta(x). \tag{III.4}$$

■

We omit the proof based on direct manipulations with distributions.

Applying this lemma to the equation (III.3) we find

$$\psi_s(x) = \frac{\alpha}{2ik_0}\sum_{n=0}^{\infty}\left(\psi_s(nd) + e^{ik_0 nd}\right)e^{ik_0|x-nd|} \tag{III.5}$$

yielding $\psi_s(x)$ as a function dependent on its values at an infinite number of points. Substituting in md for x for $m \in \mathbb{N} \cup \{0\}$ yields the infinite system of linear equations:

$$-\psi_s(md) + \sum_{n=0}^{\infty}\psi_s(nd)\frac{\alpha}{2ik_0}e^{ik_0|md-nd|} = -\sum_{n=0}^{\infty}e^{2ik_0 nd}\frac{\alpha}{2}ik_0 e^{ik_0|md-nd|}. \tag{III.6}$$

Thus, we have a nonhomogeneous LAS $A\vec{X} = \vec{\psi^0}$ where

$$A_{mn} = \frac{\alpha}{2ik_0}e^{ik_0|md-nd|} - \delta_{mn}\,,$$

$$X_m = \psi(md)\,,$$

and

$$\psi_m^0 = -\sum_{n=0}^{\infty}e^{ik_0 nd}\frac{\alpha}{2ik_0}e^{ik_0|md-nd|}\,. \tag{III.7}$$

We have reduced the scattering problem to a LAS. We note that for an arbitrary crystal with the potentials as above, not necessarily periodic and not necessarily of the equal strength, reduction to an algebraic system is also possible. For our specific model, the system is of the convolution type. That will allow us to use the Riemann-Hilbert problem approach and solve the problem explicitly.

CHAPTER IV

CONVERTING THE SYSTEM INTO A RIEMANN-HILBERT PROBLEM

In the following discussion, we will encounter many series whose convergence is non-trivial. We proceed according to the following principle [11].

IV.1. The Limiting Absorption Principle

The Limiting Absorption Principle is based on the idea that there is always a small positive damping in the physical system, so that the wave equation, with some potential V, should contain a damping term

$$u_{tt} + \gamma u_t = \triangle u + Vu.$$

The separation of variables

$$u(x,t) = e^{-ikt} v(x)$$

results in the stationary equation (Helmholtz equation) for $v(x)$. We denote its solution, in the presence of damping, as v_γ, so that

$$\triangle\, v_\gamma + V v_\gamma + (k^2 + ik\gamma) v_\delta = 0.$$

The solution of the problem with no damping is understood as the limit, in an appropriate functional space

$$v := \lim_{\delta \to 0+} v_\gamma.$$

The deep connection between this intuitive approach and the properties of the resolvent of the corresponding differential operators are discussed in many papers, starting with the classical paper [1] (see also the Ph.D. thesis [10] and further [9] which contain extensive literature). In these papers, the authors deal with a classical potential $V(x)$. In the following, we are considering the potential as a distribution/generalized function. The complete mathematical analysis of the corresponding resolvent would require to overcome obvious difficulties of working with the differential operators in a space of distributions, defining the corresponding resolvent, etc. So, we allow ourselves to proceed formally and set as our main goal to find an explicit formula for the reflection coefficient as the most important physical characteristic of scattering for our model.

IV.2. Reduction to the Riemann-Hilbert problem

We introduce the following parameters

$$\beta := \frac{\alpha}{2ik_0}, \ \gamma := k_0 d. \tag{IV.1}$$

We aslso let

$$\psi_m := \psi(md).$$

According to the limiting absorption principle,

$$\Im\gamma > 0, \ \text{so that } |e^{i\gamma}| < 1. \tag{IV.2}$$

The last inequality guarantees convergence of all series below in an appropriate domain of the complex plane.

Hence, we are tasked with solving the LAS in the class of bounded sequences:

$$-\psi_m + \beta \sum_{n=0}^{\infty} e^{i\gamma|n-m|}\psi_n = \psi_m^0, \tag{IV.3}$$

for $m \in \mathbb{N} \cup \{0\}$.

To solve the LAS, we use the method of the Riemann-Hilbert problem [7], see also [3].

Specifically, we will find that the above infinite system is equivalent to a Riemann-Hilbert problem over the contour of the unit circle. First, we expand the summation in (III.6) (or (IV.3)) to an infinite series from $-\infty$ to ∞. To do this, we make the definition:

$$\phi_m := \begin{cases} \psi(m) & , \ m \geq 0 \\ 0 & , \ m < 0. \end{cases} \tag{IV.4}$$

Under this definition, our LAS (IV.3) becomes

$$-\phi_m + \beta \sum_{n=-\infty}^{\infty} e^{i\gamma|n-m|}\phi_n = \begin{cases} \phi_m^0 & , \ m \geq 0, \\ \mu_m & , \ m < 0 \end{cases} \tag{IV.5}$$

where the quantities μ_m are unknown. We multiply both sides by z^m where z is an arbitrary complex number (the region for z is to be specified later). We get

$$-\phi_m z^m + \beta \sum_{n=-\infty}^{\infty} e^{i\gamma|n-m|}\phi_n z^m = \begin{cases} \phi_m^0 z^m & , m \geq 0, \\ \mu_m z^m & , m < 0. \end{cases} \tag{IV.6}$$

Define ϕ_m^0 to be equal to 0 when $m < 0$ and $\mu_m = 0$ when $m \geq 0$. If we sum equation (IV.6) from $-\infty$ to ∞, we get

$$-\sum_{n=-\infty}^{\infty} \phi_m z^m + \beta \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} e^{i\gamma|n-m|}\phi_n z^m = \sum_{m=-\infty}^{\infty} \phi_m^0 z^m + \sum_{m=-\infty}^{\infty} \mu_m z^m \ . \tag{IV.7}$$

We define the following functions on the complex plane

$$\Phi^+(z) = \sum_{m=-\infty}^{\infty} \phi_m z^m \,, \tag{IV.8}$$

$$\Phi^0(z) = \sum_{m=-\infty}^{\infty} \phi_m^0 z^m \,, \tag{IV.9}$$

$$\mu^-(z) = \sum_{m=-\infty}^{\infty} \mu_m z^m \,. \tag{IV.10}$$

Our equation (IV.7) then becomes:

$$-\Phi^+(z) + \beta \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} e^{i\gamma|n-m|} \phi_n z^m = \Phi^0(z) + \mu^-(z) \,. \tag{IV.11}$$

Here $\Phi^0(z)$ is a known function and $\mu^-(z)$ and $\Phi^+(z)$ are unknown functions we seek to find. We note that, because the ϕ_m are bounded, $\Phi^+(z)$ is an analytic function inside the unit circle. Similarly, $\mu^-(z)$ is analytic outside of the unit circle. Examining the double series in this equation we get

$$\sum_{m=-\infty}^{\infty} \left(\sum_{n=-\infty}^{\infty} e^{i\gamma|n-m|} \phi_n \right) z^m = \sum_{m=-\infty}^{\infty} \left(\sum_{n=-\infty}^{\infty} e^{i\gamma|n-m|} \phi_n \right) z^{(m-n)+n} \,. \tag{IV.12}$$

We further make the substitution $p := m - n$ and get

$$\begin{aligned} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \left(e^{i\gamma|n-m|} \phi_n z^{(m-n)+n} \right) &= \sum_{p=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \left(e^{i\gamma|p|} \phi_n z^{p+n} \right) \\ &= \left(\sum_{p=-\infty}^{\infty} e^{i\gamma|p|} z^p \right) \left(\sum_{n=-\infty}^{\infty} \phi_n z^n \right) \,. \end{aligned} \tag{IV.13}$$

We now introduce the function $G(z)$

$$G(z) = \beta \sum_{p=-\infty}^{\infty} e^{i\gamma|p|} z^p \,. \tag{IV.14}$$

This series may be represented as the sum of two geometric series

$$G(z) = \beta \sum_{p=-\infty}^{-1} e^{i\gamma|p|} z^p + \beta \sum_{p=0}^{\infty} e^{i\gamma|p|} z^p \tag{IV.15}$$

or

$$G(z) = \beta + \beta \sum_{p=1}^{\infty} e^{i\gamma p} z^p + \beta \sum_{p=1}^{\infty} e^{i\gamma p} z^{-p} \ . \tag{IV.16}$$

By the assumption of the limiting absorption principle, $\mathrm{Im}(\gamma) > 0$. Thus this series converges on the annulus $|e^{i\gamma}| < |z| < |e^{-i\gamma}|$. Hence, the sum above converges to

$$G(z) = \beta + \frac{\beta e^{i\gamma} z}{1 - e^{i\gamma} z} + \frac{\beta e^{i\gamma} z^{-1}}{1 - e^{i\gamma} z^{-1}} \ . \tag{IV.17}$$

After an elementary calculation

$$\begin{aligned} G(z) &= \frac{\beta - \beta e^{i2\gamma}}{(1 - e^{i\gamma} z)(1 - e^{i\gamma} z^{-1})} \\ &= -\beta \frac{2iz \sin\gamma}{z^2 - 2z\cos\gamma + 1}. \end{aligned} \tag{IV.18}$$

Looking back to equation (IV.11), we investigate the analyticity of the function $\mu^-(z)$. We note that for $|z| > 1$ the series

$$\mu^-(z) = \sum_{m<0} \mu_m z^m$$

is analytic.

Thus we have the equation

$$-\Phi^+(z) + G(z)\Phi^+(z) = \Phi^0(z) + \mu^-(z) \tag{IV.19}$$

on the annulus $|e^{i\gamma}| < |z| < |e^{-i\gamma}|$. Equivalently, we find

$$H(z)\Phi^+(z) = \Phi^0(z) + \mu^-(z)\,, \tag{IV.20}$$

where we define $H(z)$ as $G(z) - 1$.

We observe that G is invariant under the substitution $z \mapsto z^{-1}$, hence so is H. We will use this symmetry property in the sequel.

The explicit formula for $H(z)$ is

$$H(z) = G(z) - 1 = -\frac{z^2 - 2z(\cos\gamma + i\beta\sin\gamma) + 1}{z^2 - 2z\cos\gamma + 1}. \tag{IV.21}$$

We proceed according to the common strategy in the solution of the Riemann-Hilbert problem. Firstly, we factor $H(z)$ as a product of two functions $H^+(z) \cdot H^-(z)$, where $H^+(z)$ is analytic and zero-free inside the unit circle. Similarly, $H^-(z)$ is analytic and zero-free outside the unit circle. We calculate $H^+(z)$ and $H^-(z)$ in the following way.

Because $H(z)$ is invariant with respect to the transformation $z \mapsto z^{-1}$, we are able to factor the numerator of $H(z)$ as follows

$$z^2 - 2z(\cos\gamma + i\beta\sin\gamma) + 1 = (z - z_0)(z - z_0^{-1}), \tag{IV.22}$$

where we assume that $|z_0| > 1$.

We thus have that $H(z)$ can be represented by

$$H(z) = -\frac{(z - z_0)(z - z_0^{-1})}{(z - e^{-i\gamma})(z - e^{i\gamma})} = H^+(z) \cdot H^-(z), \tag{IV.23}$$

where

$$\begin{aligned} H^+(z) &= -\frac{z - z_0}{z - e^{-i\gamma}}, \\ H^-(z) &= \frac{z - z_0^{-1}}{z - e^{i\gamma}}. \end{aligned} \tag{IV.24}$$

Because $|z_0| > 1$, $H^+(z)$ is zero-free in the unit circle, and $H^-(z)$ zero-free outside the unit circle. Under the assumption of the limiting absorption principle, $\mathrm{Im}(\gamma) = \epsilon > 0$. Thus

$$|e^{i\gamma}| = |e^{i(\mathrm{Re}(\gamma)+i\epsilon)}| = |e^{-\epsilon}||e^{i\mathrm{Re}(\gamma)}| = e^{-\epsilon} < 1$$

and thus $H^+(z)$ is pole-free and zero-free inside and on the unit circle. Similarly, $H^-(z)$ is pole-free and zero-free outside and on the unit circle.

We observe that at this moment, we have completed one of the central problems in solving the Riemann-Hilbert problem, i.e. factoring $H(z)$. Our factoring is relatively simple because the function $H(z)$ is a rational function.

Equation (IV.20) then becomes:

$$H^+(z)H^-(z)\Phi^+(z) = \Phi^0(z) + \mu^-(z). \tag{IV.25}$$

Recalling our definition for $\Phi^0(z)$

$$\Phi^0(z) = -\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \beta e^{i\gamma n} e^{i\gamma|m-n|} z^m \ . \tag{IV.26}$$

If we make the substitution $p = m - n$, we get

$$\Phi^0(z) = -\sum_{n=0}^{\infty} e^{i\gamma n} z^n \sum_{p=-\infty}^{\infty} \beta e^{i\gamma|p|} z^p = -\sum_{n=-\infty}^{\infty} e^{i\gamma n} z^n G(z) \ . \tag{IV.27}$$

Because of the linearity of equation (IV.25), if we can find a solution $\Phi_n^+(z)$ with $z^n G(z)$ in place of $\Phi^0(z)$, we will find that our desired $\Phi^+(z)$ will be equal to

$$\Phi^+(z) = -\sum_{n=-\infty}^{\infty} e^{i\gamma n} \Phi_n^+(z) \ . \tag{IV.28}$$

Thus, the problem reduces to finding $\Phi_n^+(z)$ and $\mu_n^-(z)$ satisfying

$$H^+(z)H^-(z)\Phi_n^+(z) = z^n(H^+(z)H^-(z) + 1) + \mu_n^-(z) \ . \tag{IV.29}$$

CHAPTER V

SOLVING THE RIEMANN-HILBERT PROBLEM

In general, the solution of the Riemann-Hilbert problem may be expressed explicitly in terms of the Cauchy-type integrals. However, the form of these integrals are often intractable. In our particular case, we are able to omit the step of having to calculate the Cauchy integral.

In this section, we suppress the subscript n for the analytic functions $\Phi_n^+(z)$ and $\mu_n^-(z)$. We return the subscript at the end to find the complete formula for $\Phi^+(z)$ according to (IV.28).

We note that

$$\Phi^+(z) = \sum_{m=-\infty}^{\infty} \phi_m z^m = \sum_{m=0}^{\infty} \phi_m z^m \tag{V.1}$$

is analytic inside the unit circle. We also note that

$$\mu^-(z) = \sum_{m=-\infty}^{\infty} \mu_m z^m = \sum_{m=-\infty}^{-1} \mu_m z^m \tag{V.2}$$

decays as $1/z$ as $z \to \infty$ and is analytic outside the unit circle. On the boundary, we have equation (IV.29)

$$H^+(z)H^-(z)\Phi^+(z) = z^n(H^+(z)H^-(z) + 1) + \mu^-(z)\ . \tag{V.3}$$

Dividing by $H^-(z)$ and rearranging we find

$$H^+(z)\Phi^+(z) - z^n H^+(z) = z^n/H^-(z) + \mu^-(z)/H^-(z). \tag{V.4}$$

As it is common in the solution of the Riemann-Hilbert problem, we now proceed with analytic continuation. We reiterate that a relatively simple structure of the function $H(z)$ allows us to omit using the Cauchy integrals.

There are different ways of analytic continuation, and they result in two approaches to the solution of the Riemann-Hilbert problem.

V.1. Approach 1

We note that the left side of (V.4) is analytic inside the unit circle and the right side is analytic outside the unit circle, so both sides are equal to an entire function $P_n(z)$. We note, in particular, that $P_n(z)$ is a polynomial function because $(z^n + \mu^-(z))/H^-(z)$ only grows as fast as z^n, thus its Taylor expansion may only have non-zero coefficients up to n. Hence we find

$$H^+(z)\Phi^+(z) - z^n H^+(z) = P_n(z) = z^n/H^-(z) + \mu^-(z)/H^-(z) \; . \tag{V.5}$$

Rearranging, we conclude that

$$\Phi_n^+(z) = z^n + P_n(z)/H^+(z) \tag{V.6}$$

and

$$\mu^-(z) = H^-(z)P_n(z) - z^n \; . \tag{V.7}$$

Therefore, up to the unknown coefficients of the polynomial, the Riemann-Hilbert problem has been solved.

To find the coefficients, we examine the growth of both sides of equation (V.7) as $z \to \infty$. As stated earlier, $\mu^-(z)$ decays as z^{-1} as $z \to \infty$, so $\mu^-(z)$ can be represented as

$$\mu^-(z) = \sum_{m=-\infty}^{-1} \mu_m z^m \; . \tag{V.8}$$

Because the right side of equation (V.7) grows as z^n, we conclude that $H^-(z)P_n(z) - z^n$ can be represented as

$$H^-(z)P_n(z) - z^n = \sum_{m=-\infty}^{n} C_m z^m \; . \tag{V.9}$$

where C_m are the (unknown) Laurent coefficients of $H^-(z)P_n(z) - z^n$.

The right side of the above equation however represents the function $\mu^-(z)$ that decays as z^{-1} at infinity. But according to the previous equations, formally speaking, it grows as z^n. Thus, the $n + 1$ terms corresponding to the coefficients C_k from $k = 0$ to n, must all vanish. These $n + 1$ conditions are enough to determine $P_n(z)$ completely. After determining $P_n(z)$ we can determine $\Phi^+(z)$ and $\mu^-(z)$, hence solve the Riemann-Hilbert problem.

We further find for $H^-(z)$

$$H^-(z) = \frac{z - z_0^{-1}}{z - e^{i\gamma}} = \left(1 - \frac{1}{zz_0}\right) \sum_{\ell=0}^{\infty} \left(\frac{e^{i\gamma}}{z}\right)^{\ell} \; .$$

Letting $h := 1 - \frac{1}{z_0 e^{i\gamma}}$, we write out the Laurent series for $H^-(z)$ as follows

$$H^-(z) = \sum_{\ell=0}^{\infty} H_\ell^- z^{-\ell} \, ,$$

where $H_0 = 1$ and $H_\ell^- = he^{i\gamma\ell}$ for $\ell > 0$.

Letting $P_n(z) = \sum_{k=0}^{n} p_k z^k$, where p_k are the unknown coeffecients in the polynomial $P(x)$, we have the relation

$$\sum_{\ell=0}^{\infty} H_\ell^- z^{-\ell} \cdot \sum_{k=0}^{n} p_k z^k - z^n = \sum_{m=-\infty}^{-1} \mu_m^- z^m \; .$$

The coefficients of z^k on the left side, for $k \geq 0$ must vanish. Thus, we derive a system of $n + 1$ linear equations for the $n + 1$ unknown coefficients of the polynomial $P_n(z)$.

Finding the polynomial thus becomes equivalent to solving the LAS

$$\tilde{H}\tilde{p} = e_1 \; . \tag{V.10}$$

Here

$$\tilde{H} = \begin{bmatrix} H_0^- & & & & \\ H_1^- & H_0^- & & & \\ H_2^- & H_1^- & H_0^- & & \\ \vdots & & & \ddots & \\ H_n^- & & \dots & & H_0^-, \end{bmatrix} \tag{V.11}$$

$\tilde{p} = [p_n \; p_{n-1} \; p_{n-2} \; \dots p_0]^T$ and e_1 is the vector with 1 in the 1^{st} place and zeros elsewhere.

We note that we can rewrite the matrix $\tilde{H}$ as $\tilde{H} = I + hN$, where N is a nilpotent matrix and is equal to

$$N = \begin{bmatrix} 0 & & & & & \\ e^{i\gamma} & 0 & & & & \\ e^{i2\gamma} & e^{i\gamma} & 0 & & & \\ e^{i3\gamma} & e^{i2\gamma} & e^{i\gamma} & 0 & & \\ \vdots & & & & \ddots & \\ e^{i(n-1)\gamma} & e^{i(n-2)\gamma} & e^{i(n-3)\gamma} & \dots & e^{i\gamma} & 0 \end{bmatrix}.$$

In other words,

$$N_{pq} = \begin{cases} e^{i(p-q)\gamma}, & p - q > 1; \\ 0, & \text{otherwise.} \end{cases}$$

Our problem then becomes calculating $\tilde{p} = (I + hN)^{-1} e_1$. Because N is nilpotent, we get

$$\tilde{p} = \sum_{k=0}^{n} (-1)^k h^k N^k e_1 \; . \tag{V.12}$$

The form of N makes it particularly easy to calculate its powers explicitly. For $k \neq 0$ we find

$$N_{pq}^k = \binom{p - q - 1}{k - 1} e^{i\gamma(p-q)}.$$

We will prove this using induction. We note that this Toeplitz matrix satisfies the sufficient conditions needed for its powers to be Toeplitz, so it suffices to prove the result for $q = 1$. The proof for the other entries in the matrix follow from the fact that the matrix is Toeplitz.

Assuming the hypothesis holds for k, we calculate N_{p1}^{k+1}

$$N_{p1}^{k+1} = \sum_{s=1}^{n+1} N_{ps}^{k} N_{s1} = \sum_{s=2}^{p-k} \binom{p-s-1}{k-1} e^{i\gamma(p-s)} e^{i\gamma(s-1)} = \binom{p-2}{k} e^{i\gamma(p-1)} ,$$

and this completes the induction.

After finding the powers of N, we may calculate the coefficients of the polynomial. For $m = 1$ we find $p_n = 1$. Otherwise,

$$\begin{aligned} p_{(n+1-m)} &= \sum_{k=0}^{n} \binom{m-2}{k-1} (-1)^k h^k e^{i\gamma(m-1)} \\ &= -\, h e^{i\gamma(m-1)} \sum_{k=1}^{m-1} \binom{m-2}{k-1} (-1)^{k-1} h^{k-1}, \end{aligned} \tag{V.13}$$

which, by the binomial theorem, is equal to

$$p_{(n+1-m)} = -h e^{i\gamma(m-1)} (1-h)^{m-2} \, . \tag{V.14}$$

Re-indexing we get

$$p_k = \begin{cases} -h e^{i\gamma(n-k)} (1-h)^{n-1-k} & , k < n \\ 1 & , k = n \end{cases} \, . \tag{V.15}$$

The polynomial $P_n(z)$ is then equal to

$$P_n(z) = \sum_{k=0}^{n} p_k z^k = z^n - \sum_{k=0}^{n-1} h e^{i\gamma(n-k)} (1-h)^{n-1-k} z^k,$$

which we write as

$$P_n(z) = z^n - h e^{i\gamma} \frac{z^n - e^{in\gamma}(1-h)^n}{z - e^{i\gamma}(1-h)} \, . \tag{V.16}$$

Substituting our definition for h, this becomes

$$P_n(z) = z^n + (z_0^{-1} - e^{i\gamma})\frac{z^n - z_0^{-n}}{z - z_0^{-1}} \ . \tag{V.17}$$

Recall that

$$\Phi_n^+(z) = z^n + \frac{P_n(z)}{H^+(z)} \ .$$

Thus we find an explicit solution for $\Phi_n^+(z)$,

$$\Phi_n^+(z) = z^n + \frac{(z - e^{-i\gamma})\left(z^n + (z_0^{-1} - e^{i\gamma})\frac{z^n - z_0^{-n}}{z - z_0^{-1}}\right)}{z - z_0} \ , \tag{V.18}$$

which is equivalent to

$$\Phi_n^+(z) = z^n + \frac{(z - e^{-i\gamma})\left(-z_0^{-n}(z_0^{-1} - e^{i\gamma}) + z^n(z - e^{i\gamma})\right)}{(z - z_0)(z - z_0^{-1})} \ . \tag{V.19}$$

V.2. Approach 2

In the following argument, we return the index n to Φ_n^+. We recall that

$$H^+(z)\Phi_n^+(z) - z^n H^+(z) = z^n / H^-(z) + \mu_n^-(z)/H^-(z) \ . \tag{V.20}$$

Re-arranging the terms in this equation we get

$$H^+(z)\Phi_n^+(z) - z^n H^+(z) - z^n / H^-(z) = \mu_n^-(z)/H^-(z) \ . \tag{V.21}$$

The right side is analytic outside of the unit circle and approaches 0 as $z \to \infty$ and the left side is analytic inside except at the pole where $H^-(z) = 0$.

We recall that

$$H^-(z) = \frac{z - z_0^{-1}}{z - e^{i\gamma}} \ , \tag{V.22}$$

therefore the pole of the right side is at z_0^{-1}.

Because the left side of (V.21) is the unique analytic continuation of the right side, we find that

$$H^+(z)\Phi_n^+(z) - z^n H^+(z) - z^n/H^-(z) = \frac{C_n}{z - z_0^{-1}} = \mu_n^-(z)/H^-(z)\,, \tag{V.23}$$

for some unknown constant C_n. Up to this unknown constant, we have solved the Riemann-Hilbert problem. We now re-arrange the terms in (V.23) to find another form of the Riemann-Hilbert problem

$$H^+(z)\Phi_n^+(z) - z^n H^+(z) = \frac{C_n}{z - z_0^{-1}} + \frac{z^n}{H^-(z)}. \tag{V.24}$$

Here, the left side is analytic in the unit circle but the terms on the right side have a pole at z_0^{-1}. Thus

$$\mathrm{Res}_{z_0^{-1}}\left(\frac{C_n}{z - z_0^{-1}} + \frac{z^n}{H^-(z)}\right) = C_n + z_0^{-n}(z_0^{-1} - e^{i\gamma}) = 0 \tag{V.25}$$

Therefore

$$C_n = -z_0^{-n}(z_0^{-1} - e^{i\gamma})\,,$$

and this completes the solution of the Riemann-Hilbert problem. In particular, it may be shown that the representation for $\Phi_n^+(z)$ is the same as in (V.19) (see below).

CHAPTER VI

REFLECTION COEFFICIENT FOR THE SEMI-INFINITE CRYSTAL

We recall from equation (III.5) that for the semi-infinite crystal,

$$\psi(x) = \sum_{n=0}^{\infty} \psi(nd) e^{ik_0|x-nd|} + \sum_{n=0}^{\infty} e^{ik_0 nd} e^{ik_0|x-nd|}$$

or, if $x < 0$, we have

$$\psi(x) = e^{-ik_0 x} \left[\beta \sum_{n=0}^{\infty} \psi(nd) e^{ik_0 nd} + \beta \sum_{n=0}^{\infty} e^{2ik_0 nd} \right].$$

The expression in brackets is known as the *reflection coefficient*

$$R = \beta \sum_{n=0}^{\infty} \psi(nd) e^{ik_0 nd} + \beta \sum_{n=0}^{\infty} e^{2ik_0 nd} . \tag{VI.1}$$

According to the Born interpretation [6], the modulus squared of this quantity may be viewed as the probability that the particle will reflect off the potential.

We recall that, from the definition (IV.8) of $\Phi^+(z)$

$$\Phi^+(e^{i\gamma}) = \sum_{n=0}^{\infty} \psi(nd) e^{i\gamma n} .$$

We recall here that we proceed in the framework of the limiting absorption principle, so that $|e^{i\gamma}| < 1$.

So we have, by evaluating the geometric sum in (VI.1)

$$R = \beta\Phi^+(e^{i\gamma}) + \frac{\beta}{1 - e^{i2\gamma}} \; . \tag{VI.2}$$

Recalling our representation (IV.28) for $\Phi^+(z)$ in terms of $\Phi_n^+(z)$, we have

$$\Phi^+(e^{i\gamma}) = -\sum_{n=0}^{\infty} e^{i\gamma n}\Phi_n^+(e^{i\gamma}) \; . \tag{VI.3}$$

From our solution to the Riemann-Hilbert problem (V.24) we have

$$\Phi_n^+(e^{i\gamma}) = e^{i\gamma n} + \frac{1}{H^+(e^{i\gamma})}\left(\frac{C}{z - z_0^{-1}} + \frac{z^n}{H^-(z)}\right) \; . \tag{VI.4}$$

Using the formula for $H^-(z)$ and after some algebraic manipulation we get the final formula for $\Phi_n^+(z)$

$$\Phi_n^+(z) = z^n + \frac{(z - e^{-i\gamma})\left(-z_0^{-n}(z_0^{-1} - e^{i\gamma}) + z^n(z - e^{i\gamma})\right)}{(z - z_0)(z - z_0^{-1})} \; . \tag{VI.5}$$

It is easy to see that this coincides with the result (V.19) obtained by Approach 1.

Evaluating the above representation at $e^{i\gamma}$, we get

$$\Phi_n^+(e^{i\gamma}) = e^{i\gamma n} - \frac{2iz_0^{-n}\sin(\gamma)(z_0^{-1} - e^{i\gamma})}{(e^i\gamma - z_0)(e^{i\gamma} - z_0^{-1})} \; . \tag{VI.6}$$

Substituting the above into equation (VI.3) we get

$$\begin{aligned}\Phi^+(e^{i\gamma}) &= -\sum_{n=0}^{\infty} e^{i\gamma n}\left(e^{i\gamma n} - \frac{2iz_0^{-n}\sin(\gamma)(z_0^{-1} - e^{i\gamma})}{(e^i\gamma - z_0)(e^{i\gamma} - z_0^{-1})}\right)\\ &= -\frac{1}{1 - e^{i2\gamma}} + \frac{2i\sin(\gamma)(z_0^{-1} - e^{i\gamma})}{(e^i\gamma - z_0)(e^{i\gamma} - z_0^{-1})} \cdot \frac{1}{1 - z_0^{-1}e^{i\gamma}}.\end{aligned} \tag{VI.7}$$

From (IV.22) we conclude that

$$(e^{i\gamma} - z_0)(e^{i\gamma} - z_0^{-1}) = -2i\beta\sin(\gamma)e^{i\gamma}.$$

Representation (VI.2) for the reflection coefficient leads now to the formula

$$R = -\frac{z_0^{-1} - e^{i\gamma}}{e^{i\gamma}(1 - z_0^{-1}e^{i\gamma})}. \tag{VI.8}$$

This is the final formula that we set out to derive.

VI.1. Asymptotic formulas for the reflection coefficient. Inverse Problem

Our next goal is to derive the asymptotic formulas for the reflection coefficient for "strong" and "weak" crystals.

We recall the formula (IV.22) that defines z_0 and z_0^{-1}

$$z^2 - 2z(\cos\gamma + i\beta\sin\gamma) + 1 = (z - z_0)(z - z_0^{-1}),$$

where we assume that $|z_0| > 1$. We find

$$z_0,\ z_0^{-1} = \cos\gamma + i\beta\sin\gamma \pm \sqrt{-\sin^2\gamma + 2i\beta\sin\gamma\cos\gamma - \beta^2\sin^2\gamma}\,. \tag{VI.9}$$

A. As $\beta \to \infty$, we easily find

$$z_0^{-1} \sim 2i\beta\sin\gamma.$$

Formula (VI.8) now implies

$$\lim_{\beta\to\infty} |R| = 1, \tag{VI.10}$$

which is compatible with the physical notion that an infinitely rigid crystal would reflect the wave completely.

B. As $\beta \to 0$, we use the Taylor series for the square root in (VI.9) to find

$$z_0^{-1} \sim e^{i\gamma}(1 + \beta).$$

Formula (VI.8) now implies

$$R \sim -\frac{\beta}{1-e^{2i\gamma}}, \text{ so that } \lim_{\beta\to 0} R = 0, \tag{VI.11}$$

which is compatible with the physical notion that the crystal becomes “transparent”, i.e. does not reflect the wave at all.

The presence of the denominator $1 - e^{2i\gamma}$ in the last formula shows that the asymptotic representation is not uniform with respect to γ.

The study of the so-called Inverse Problem, i.e. reconstruction of the potential or obstacle, represents a branch of the modern Mathematical Physics. Formula (VI.8) allows to find either the strength of the potential α or the period of the structure d if the reflection coefficient is measured for the given energy k_0^2. We remind here that z_0 is a known function of the parameters γ and β and note the connection between the parameters of the problem

$$\beta := \frac{\alpha}{2ik_0}, \ \gamma := k_0 d. \tag{VI.12}$$

The complexity of the realization of this program though is that we may be able to measure the modulus of the reflection coefficient but not its argument. On the other side, R seems to be an analytic function of all participating parameters and the Cauchy-Riemann equations may be used to reconstruct the argument. Yet, this reconstruction may be ill-posed since we have to differentiate the experimental data. We leave this problem for the future research.

CHAPTER VII

SCATTERING COEFFICIENTS FROM A FINITE CRYSTAL

We believe that the technique of solving the Riemann Hilbert boundary value problem will prove efficacious in calculating the reflection and transmission coefficients for a finite system of equally spaced identical delta distribution potentials. We leave the solution of this problem to the future.

Here, we present only the following general result regarding any compactly supported potential.

Theorem VII.0.1. *(Energy Conservation Law). For any potential that is a compactly supported distribution,* $|R|^2 + |T|^2 = 1$.

Proof. Let $K = [a, b]$ be a closed interval that contains the support for the potential $V(x)$. We may rewrite the Schrödinger equation as

$$\psi''(x) = \left(V(x) - k_0^2\right)\psi(x). \qquad \text{(VII.1)}$$

Let U be a finite open interval containing K. We note that in $U \setminus K$, the Schrödinger equation takes the form

$$\psi''(x) = k_0^2\psi(x). \qquad \text{(VII.2)}$$

Hence, for $x < a$, the solutions to the equation are of the form:

$$\psi(x) = e^{ik_0x} + Re^{-ik_0x}, \qquad \text{(VII.3)}$$

where Re^{ik_0x} is the reflected portion of the incoming wave e^{ik_0x}.

For $x > b$, the solutions to the equation are of the form:

$$\psi(x) = Te^{ik_0 x}, \tag{VII.4}$$

which is the transmitted portion of the wave.

Consider the integral

$$\int_{\bar{U}} |\psi'(x)|^2 = \int_{\bar{U}} \overline{\psi'(x)}\psi'(x). \tag{VII.5}$$

Performing integration by parts yields

$$\int_{\bar{U}} \overline{\psi'(x)}\psi'(x) = \overline{\psi(x)}\psi'(x)\Big|_{\partial U} - \int_{\bar{U}} \overline{\psi(x)}\psi''(x). \tag{VII.6}$$

Substituting in solutions for $\psi(x)$ on U/K we get that the evaluation at the boundary is equal to

$$(\overline{T}e^{-ik_0 x})(ik_0 Te^{ik_0 x}) - (\overline{R}e^{ik_0 x} + e^{-ik_0 x})(-ik_0 Re^{-ik_0 x} + ik_0 e^{ik_0 x}). \tag{VII.7}$$

Simplifying we get

$$\overline{\psi(x)}\psi'(x)\Big|_{\partial U} = ik_0\left(|T|^2 + |R|^2 - 1\right) + ik_0\left(Re^{-ik_0 x} - \overline{R}e^{ik_0 x}\right). \tag{VII.8}$$

We note that the right term is equal to $ik_0(2i\Im Re^{-ik_0 x})$, and thus is real valued. Substituting (VII.1) into the integral we get

$$\int_{\bar{U}} \overline{\psi(x)}\psi''(x) = \int_{\bar{U}} \overline{\psi(x)}(V(x) - k_0^2)\psi(x) = \int_{\bar{U}} |\psi(x)|^2(V(x) - k_0^2), \tag{VII.9}$$

which is real valued. Thus, the only imaginary part of our integral is $ik_0(|R|^2 + |T|^2 - 1)$. But the entire integral must be real valued.

Thus

$$|R|^2 + |T|^2 = 1.$$

Which we set out to prove

□

■

CHAPTER VIII

HAMILTONIAN OF A DELTA POTENTIAL

Formally, the Hamiltonian in one dimension for a Dirac Delta potential of strength 1 located at 0 is given by

$$H = -\frac{\mathrm{d}^2}{\mathrm{dx}^2} + \delta(\cdot), \tag{VIII.1}$$

which we take to act on the space of test functions $C_0^\infty(\mathbb{R})$. Note that, on the restricted space of test functions $C_0^\infty(\mathbb{R} - 0)$, the space of functions vanishing outside some compact set not including 0, we have that the above differential operator becomes:

$$H|_{C_0^\infty(\mathbb{R}-0)} = -\frac{\mathrm{d}^2}{\mathrm{dx}^2}. \tag{VIII.2}$$

We now note that the $C_0^\infty(\mathbb{R} - 0)$ is dense in the Sobolev space $\{g \in H^2(\mathbb{R}) | g(0) = 0\}$. We can use this density to define the above Hamiltonian operator on the Sobolev space. We thus get the symmetric operator on $L^2(\mathbb{R})$ defined by:

$$\dot{H} = -\frac{\mathrm{d}^2}{\mathrm{dx}^2}, \qquad \mathscr{D}(\dot{H}) = \{g \in H^2(\mathbb{R}) | g(0) = 0\}. \tag{VIII.3}$$

The adjoint of $\dot{H}$ is:

$$\dot{H}^* = -\frac{\mathrm{d}^2}{\mathrm{dx}^2}, \qquad \mathscr{D}(\dot{H}^*) = H^2(\mathbb{R} - \{0\}) \cap H^1(\mathbb{R}).$$

The deficiency subspaces of H are

$$\mathscr{K}_{\pm} = \mathrm{Ker}(i \mp A^{*}) = \mathrm{Ker}\left(i \pm \frac{\mathrm{d}^2}{\mathrm{dx}^2}\right).$$

Further, $\mathrm{Ker}\left(i + \frac{\mathrm{d}^2}{\mathrm{dx}^2}\right)$ consists of functions of the form $\psi(x) = Ae^{\frac{-\sqrt{2}}{2}(i+1)|x|}$ where A is an arbitrary constant. We similarly have $\mathscr{K}_{-} = \{Ae^{-\frac{-\sqrt{2}}{2}(-i+1)}|A \in \mathbb{C}\}$. We thus find that the deficiency indices of $\dot{H}$ are $(1, 1)$, and thus $\dot{H}$ has self-adjoint extensions.

CHAPTER IX

CONCLUSION

We have constructed an explicit solution of the scattering problem from a one-dimensional semi-infinite crystal. Our method is based on two key facts. Firstly, for the evenly spaced delta potentials of equal strength, it is possible to reduce the scattering problem to a LAS of the convolution type. Secondly, the method of the Riemann-Hilbert problem allows to solve that system explicitly. It is important to note that the factoring required for the solution of the Riemann-Hilbert problem is relatively simple for our model since the corresponding function is a rational function on the complex plane of the auxiliary variable. We find the limit of the modulus of the reflection coefficient when the strength of the potentials approaches infinity or zero and discuss the physical meaning of the limiting values.

We may continue this project by solving the following problems.

(a) Scattering from a one-dimensional finite crystal of the equidistant delta potentials of the equal strength.

(b) Asymptotic study of the solution for a small damping coefficient and further understanding of the limit in the limiting absorption principle.

(c) Asymptotic study of the reflection coefficient for a "strong" and "weak" crystals (for a finite crystal).

(d) Inverse problem, i.e. finding the strength of the crystal and / or its period from the measurement of the reflection coefficient for a given energy (for both semi-infinite and finite crystal).

(e) The possibility of resonances (see the discussion of the asymptotic formula for the reflection coefficient).

(f) Placing the aforementioned scattering problems in the appropriate functional spaces. Construction of the resolvent for both semi-infinite and finite crystals and its study.

(g) Scattering problem for a vector potential and all aforementioned problems for this model. The Riemann-Hilbert problem in this case will be formulated for the unknown vectors $\vec{\Pi}_n^+(z)$ and $\vec{\mu}^-(z)$ and factoring of a matrix will be required. In general, this factoring may not be done explicitly except the case of a rational matrix.

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VITA

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