Transmission Properties of an Electron in One Dimensional Crystals with Periodic Potentials

David Boxi Hu(880304-6518), Dan von Martens (871013-7574)
bdhu@kth.se, dvm@kth.se
SA104X Degree Project in Engineering Physics, First Level
Department of Theoretical Physics
Royal Institute of Technology (KTH)
Supervisor: Patrik Henelius

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Abstract

In 2010, R. Olsen and G. Vignale, published a paper presenting a recursive method for calculating electron transmission probability for one dimensional periodic potentials. Based on their method, this thesis studies electron transmission in a one dimensional lattice of periodic potential barriers both using a classical and quantum mechanical description. The transmission is measured by the transmission probability of the system. The transmission probabilities are computed with regards to two separate variables, namely the number of potential barriers, i.e. the length of the lattice, and the wave number of the incident electron. These computations are made using rectangular and Dirac delta potential barriers respectively. Lastly, the paper expands on the area of disordered systems of periodic potentials by introducing irregularities in potential size and separation.
Abstract

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Chapter 1

Introduction

This thesis investigates the transmission properties of an electron incident on a one dimensional crystal. The crystal will be described using a regular one dimensional lattice, with potential barriers at each lattice point. In such a system, there are certain characteristics that reveal interesting properties pertaining to the transmission of the electron. To the extent of this thesis, these variables will be the shape and dimensions of the potential barriers, and the level of disorder in the one dimensional lattice. Additionally, given the sub atomic scale of the system and the wave particle duality of the electron, the transmission probabilities and properties are likely to differ depending on whether assessed from a classical or quantum mechanical viewpoint.

Formally, this thesis studies electron transmission in four different representations of a one dimensional crystal, analyzed both clasically and quantum mechanically:

1. A one dimensional lattice with periodical potential barriers in the shape of Dirac delta potentials
2. A one dimensional lattice with periodical rectangular potential barriers
3. A one dimensional lattice with non equidistanced rectangular potential barriers, thereby introducing a dimension of disorder to the system.
4. A one dimensional lattice with periodical equidistanced rectangular potential barriers, with differing widths.

These four systems represents crystals as one dimensional lattices endowed with potential barriers, and systems 1 and 2 in particular, also assume a perfect crystal structure, consistent with the crystal completely lacking any structural imperfections. System 3, is endowed with a level of impurity by relaxing the constraint of perfect potential barrier periodicity in terms of potential separation. System 4 assumes equidistance, but represents disorder in the differing shapes of the potential barriers. An implicit assumption to all four systems is that of zero temperature, so that every pure periodic potential barrier is a perfect conductor with zero resistance when assessed from quantum mechanical viewpoint.

Transmission is studied by computing the transmission probability of the electrons as a function of certain system variables. Pertaining to these relationship and to the extent of this thesis, these variables, will be the number of potential barriers, i.e. the length of the system and the wave number of the incident electron. It will be of interest to understand how transmission behaves as a function of the crystal length, especially in the upper limit of infinite length. Also, intuition tells us that the incoming energy of the electron should
affect the transmission of the same. The energy of the incident electron is contained in the wave number.

Following studies on perfect periodical potentials the thesis will also expand to cover imperfect periodicity by introducing disorder to the system. Disorder will be introduced by implementing randomness in the potential width, relevant to rectangular potentials, and the potential separation measure. The study on transmission in a disordered system will also be focused on the relation to the number of potentials and the wave number.

1.1 Concepts, History and Theories

The field of study in this thesis, while itself being rather narrow and specified, entails many different areas of physics that are essential for a complete understanding and description. Thus, we discuss some conceptual, historical and theoretical background that is of relevance. Readers familiar with the concepts of wave particle duality, the Schrödinger equation, potential barriers, Bloch's theorem and the occurrence and conditions for energy bands within the context of electron transmission, might skip this section.

Wave Particle Duality

The wave particle duality, postulates that matter has both the properties of waves and particles.

Historically, one can trace the debate of wave particle duality back to the 17th century when Sir Isaac Newton and Christian Huygens proposed competing theories of light. Huygens believed that light consisted of waves, while Newton claimed that it consisted of corpuscles. It was not until Young and Fresnel, in the early 19th century performed their double-slit experiment that evidence first emerged in favour of Huygen's wave theories. In the late 19th century, James Clerk Maxwell's Maxwell equations concluded that electromagnetic waves propagates at the speed of light, thus postulating that light displays wave-like properties. Young and Fresnel verified this notions through their double-slit experiment in 1887 fortifying the wave theory of light rendering it to become widely accepted. In 1905 Albert Einstein explained the photoelectric effect\cite{5}(pg. 75-78), thus proposing the existence of photons as quanta of light with particle properties. Einstein postulated that the energy of these quanta, the photons, was related to their frequency, $f$, by

$$E = hf,$$

where $h$ is Planck's constant. Thus, Einstein's notion of photons led to a wave particle duality for light. Adding to Einstein's discovery, Louis-Victor de Broglie, in 1924, formulated what is known as the de Broglie hypothesis\cite{5}(pg. 73, 87-90, 98-99), stating that all matter, not just light that, had wave-like properties. The de Broglie hypothesis related the wavelength, $\lambda$, a property of waves and momentum, $p$, a property of matter using the relation

$$\lambda = h/p,$$

using Planck's constant, $h$. There is debate as to who confirmed de Broglie's hypothesis experimentally, but the observation of electron diffraction in an experiment at Bell Labs by Clinton Joseph Davisson and Lester Halbert Germer is usually attributed that discovery\cite{1}. 


The Schrödinger Equation and Potential Barriers

Considered to be one of the most central concepts in quantum mechanics, the Schrödinger wave equation bears the same importance to quantum mechanics as does Newton’s laws for classical mechanics. It was following the discovery of the wave-particle duality and de Broglie’s hypothesis that Erwin Schrödinger decided to find a wave equation for the electron. The equation that he formulated was

\[ i\hbar \frac{\partial}{\partial t} \Psi(x,t) = -\frac{\hbar^2}{2m} \nabla^2 \Psi(x,t) + V(x)\Psi(x,t), \]

and is known as the time-dependent Schrödinger equation. Below the Schrödinger equation is stated using the Hamiltonian operator for a single particle in a potential \( V(x) \),

\[ \mathcal{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(x), \]

so that the Schrödinger equation above translates to

\[ i\hbar \frac{\partial}{\partial t} \Psi(x,t) = \mathcal{H}\Psi(x,t). \]

Here \( \Psi(x,t) \) represents the wave function, which strictly is to be interpreted as a probability amplitude\[5\](pg. 103), for it is the amplitude of the wave that, when squared, tells us the probability. In quantum mechanics, the probability amplitude is a complex number. It was from the double-slit experiment that Young and Fresnel found that only complex numbers could contain the information necessary to describe the notion of classic probability in a quantum mechanical system. The relation between the two reads that a probability can be obtained by squaring the modulus of the probability amplitude\[6\]. This distinction between probability in the classic realm and the probability amplitude in the quantum realm will be of central importance to the computations in our study. Furthermore, \( V(x) \), is a coefficient that describes the potential energy of the system. For example, when considering the interaction between an electron and a potential barrier, \( V(x) \), will represent the potential of the barrier.

Further to the Schrödinger equation, this section includes a treatment of an electron incident on a potential barrier. Essentially, this thesis is built around this particular phenomenon. However, for the sake of relevance we will not provide detailed derivations but rather state the formulas that are important to our study. Simply stated, these formulas pertain to a one dimensional time independent Schrödinger equation for a particle incident on a rectangular potential energy barrier. Our study focuses on the probability of the transmission of that particle, in our case an electron, which formally is given by a transmission coefficient. Analogously, the probability of reflection is contained in the reflection coefficient. By solving the Schrödinger equation for a given potential barrier function, \( V(x) \), these two coefficients can be computed. In the case of a single rectangular potential barrier the result is

\[ t = e^{-2i(k\kappa)} \frac{2k\kappa}{2k\kappa \cosh 2\kappa a - i(k^2 - \kappa^2) \sinh 2\kappa a}, \]  
(1.1)

\[ T = |t|^2 = \frac{(2k\kappa)^2}{(k^2 + \kappa^2)^2 \sinh^2(2\kappa a) + (2k\kappa)^2}, \]  
(1.2)
The value of $R$ is given by the conservation of probabilities.

In the above expressions,
- $t$ represent the probability amplitude for the transmitted part of the wave
- $r$ represent the probability amplitude for the reflected part of the wave
- $T$ represent the probability of transmission
- $R$ represent the probability of reflection
- $k$ represents the wave number for the incoming electron wave,
- $V_0$ is the potential energy deduced from the potential barrier,
- $E$ is the energy of the incident wave and
- $a$ is the width of the potential barrier.

The other potential barrier shape that is of interest to our study is the Dirac delta potential. The Dirac delta potential is formulated as

$$V(x) = \lambda \delta(x),$$

where $\delta(x)$ is the Dirac delta function. When $\lambda > 0$, the potential is a barrier. The transmission and reflection coefficient of the Dirac delta potential are derived by solving the one dimensional time-independent Schrödinger equation and subsequently evaluating the requirement of the wave function that its derivative is to be continuous at the barrier boundaries. The obtained expression for the transmission probability is

$$t = \frac{1}{1 - (\lambda/2ika)},$$

$$T = |t|^2 = \frac{1}{1 + (m\lambda/2\hbar^2E)},$$

$$r = t - 1,$$

$$R = 1 - T.$$

In the methodology section, we will describe how these formulas are applied to study the transmission of a wave associated with an electron.

**The Bloch Theorem**

Having explained the concept of matter waves, the Schrödinger equation and potential barriers, we now introduce a theorem that describes the wave function in the presence of periodic potentials. For the sake of the arguments below, we assume a crystal built around a perfect lattice, meaning that the ions are spaced equally and consist of identical potential barriers.
Going back to the Schrödinger equation, and the Hamiltonian operator, we first impose periodicity on the potentials requiring that

$$V(x + a) = V(x). \quad (1.8)$$

The kinetic component of the Hamiltonian, \(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2}\), is already invariant under lattice translation, i.e. the change \(x \to x + a\), which means that given the periodicity of the potential energy, the entire Hamiltonian becomes invariant under displacements by \(a\). From this periodicity of translation we can derive a result known as Bloch’s theorem. Such a derivation can be found in [3]. In one dimension the Bloch theorem states that

$$\Psi(x) = e^{iqx}u(x), \quad (1.9)$$

which is a restrictive condition of the Schrödinger wave function in the presence of periodic potentials. Here \(u(x)\) is a periodic function obeying \(u(x + a) = u(x)\) and the factor \(e^{iqx}\) represents a plane wave function. In this context the Schrödinger wave function is sometimes called a Bloch wave or Bloch state, named after Felix Bloch. Formally, Eq. (1.9) applies to the wave function for a particle placed in a periodic potential. For free electrons we have \(q = k\), whereas for the general case the relation between \(q\), which is a crystal property, and \(k\), the plane wave number, is much more complicated. We will arrive at such a relation when studying the propagation of an electron wave through periodic potentials.

**Quantum Mechanical Wave Propagation and Energy Bands**

In the classical mechanics case of an electron incident on periodic potential barriers, we should expect the transmission probability to decrease as the number of potentials increase until the electron is completely reflected. This kind of behaviour is somewhat inline with our intuition of how the world works.

However, considering quantum mechanical effects, meaning that we consider the electron a wave, with a wave number, \(k\), there are ranges for \(k\), there are certain energy bands for which the electron wave transmission is non zero for any given number of potentials. By combining the Bloch Theorem stated above with periodic boundary conditions on Dirac delta potentials, the condition for a wave to be inside a band is [6]

$$\frac{\cos(ka + \delta)}{|t|} = \cos qa \quad (1.10)$$

where \(t\) is the part of the wave that is transmitted through the barrier, \(t = |t| e^{i\theta}\). Here \(\delta\) is the relative phase gained by an electron by transmitting through a single barrier. \(ka\) is the geometric phase gained by an electron with wave vector \(k\) that travels a distance \(a\) between the barriers.

For readers familiar with the Kronig-Penney model, applying the same type of derivations, a very similar relation for the condition of being inside the barrier can be formulated. The below expression is, however, derived for only Dirac delta potentials[3]

$$\cos qa = \cos ka + \frac{\lambda \sin ka}{2ka} \quad (1.11)$$

Here \(\lambda\) is a parameter and not to be confused with wave length. \(q\) is the wave number associated with the crystal. From the energy wave number relation, \(E = \frac{\hbar^2 k^2}{2m}\), we see that
the constrictions on $k$ translates to constrictions on $E$, arriving at the notion of allowed energy bands for the indicent wave.

The band gap region represents the energies outside the band for an electron that is localized, which means that it most probably is limited to only a part of the crystal.

Having introduced the above concepts, we feel that we have prepared the reader sufficiently in being able to follow our reasoning and deductions expanding and tying together the various areas. With the purpose of this thesis to mainly examine electron wave propagation through periodic potentials, we will now take the reader through previous research made on the subject, and delve more into the specifics of our research topic.
Chapter 2

Previous Research and Background

2.1 Model

Our research on this topic is primarily based on the work of Raina Olsen & Giovanni Vignale in their 2010 paper “The Quantum Mechanics of Electric Conduction in Crystals”. In their article, Olsen and Vignale introduced an algorithm where the behaviour of an electron incident on a one dimensional crystal with periodic potentials can be described recursively. For $N+1$ potential barriers, the algorithm recursively describes the particle/wave potential barrier interaction in such a way that it can be described by a geometric sum that is simple to both interpret and implement. With adjustments for a quantum mechanical system, the recursive algorithm can be applied to both a classical interpretation and a quantum mechanical one.

For the sake of reader comprehension, we will limit this section to a conceptual description of the algorithm in Olsen and Vignale, presenting the idea behind the method, and also the final expressions used for computation. In the methodology section, the reader will find a more in depth description of the intuition behind the algorithm and the derivations behind the mathematical results of the same.

First their paper presents the interaction between the electrons and the potential barriers using classical mechanics. In classical mechanics, we assume that each potential is endowed with a known probability of transmission, $T$, and reflection, $R$. Conservation of probabilities imply that $T + R = 1$. To deduce the same probabilities for a system of $N$ potentials, Olsen & Vignale go about recursively, by computing the case for $N$ potentials, from the base case of $T$ and $R$ for each individual potential. When doing this, they find that for $N$ potentials the recursive algorithm for transmission and reflection converges to a geometrical sum

\[
T_{N+1} = \frac{T_N T}{1 - R_N R}, \quad (2.1)
\]

\[
R_{N+1} = 1 - T_{N+1}. \quad (2.2)
\]

For the quantum mechanical system the equations are similar but with a couple of adjustments. Firstly, we present the expressions for the transmitted and reflected parts for the wave. If we let $t$ denote the transmitted part of the wave and $r$, denote the reflected part of the wave, we can formulate the corresponding relations, for the quantum mechanical case

\[
t = |t| e^{i\theta}, \quad r = \pm i |r| e^{i\theta}, \quad (2.3)
\]
Here we see that there are two components to the probability amplitude in quantum mechanics, a magnitude and a phase. When, interacting with a potential barrier, the wave function describing the electron is coupled with a probability of being either transmitted or reflected.

However, when considering a wave propagating through a barrier, one has to make another adjustment. This adjustment accounts for the geometric phase gained by an electron with a wave vector, $k$, as it travels a distance $a$, between the barriers. In the case of Dirac delta potentials, $a$ is just the distance travelled, since the delta potential has a width close to zero. The expressions for total transmission and reflection are

$$\tilde{t} = |t| e^{ika} \text{ and } \tilde{r} = |r| e^{ika}. \quad (2.5)$$

Applying the recursive algorithm presented in the article we arrive at two recursive expressions for total transmission and reflection probability amplitudes for $N + 1$ barriers

$$\tilde{t}_{N+1} = \frac{\tilde{t}_N \tilde{t}}{1 - \tilde{r}_N \tilde{r}} \quad (2.6)$$

$$\tilde{r}_{N+1} = \tilde{r}_N - \frac{\tilde{t}_N^2 \tilde{r}}{1 - \tilde{r}_N \tilde{r}}. \quad (2.7)$$
Chapter 3

Methodology

3.1 Recursive Algorithm for the Transmission through an array of periodic potentials

In this section we will outline and explain the algorithm used to compute transmission probabilities for a one dimensional lattice of periodic potential barriers. The algorithm differs for the classical and quantum mechanical case, and thus both will be presented.

The Classical System and the Quantum Mechanical System

Classically, an electron incident upon a potential barrier is either transmitted or reflected. It is assumed that, within the system, the transmission and reflection are associated with known probabilities, $T$ for transmission and $R$ for reflection. For the sake of simplicity, we begin by describing the algorithms for two potential barriers, and then expand it to include an arbitrary number of barriers.

Consider, classically, the case in which an electron is incident upon two identical potential barriers endowed with known transmission and reflection probabilities, $T$ and $R$. The possible scenarios for the propagation of the electron are endless. For example, the electron might be transmitted through the first barrier, reflected back and forth between the two barriers any number of times before then transmitting through the second barrier. Classically, adding the probabilities for all the possible paths the electron can take before transmitting through the second barrier should provide the probability for final transmission. Mathematically, where the subscript indicates two barriers, the above reasoning is translated into

\[
T_2 = TT + TRRT + TRRRT + TRRRRRT + \cdots
\]

\[
= T^2 \left( 1 + R^2 + R^4 + \cdots \right) = \frac{T^2}{1 - R^2}.
\]

Essentially, the sum of the endless paths of transmission through two barriers converge into a geometric series, for which we know the expression.

Now, consider a periodic array consisting of $N$ identical periodic potential barriers. Again, let $T$ and $R$ denote transmission and reflection probability for each barrier. The total probability of transmission and reflection probability through $N$ barriers will be denoted $T_N$ and $R_N$. Based on the same reasoning as for the case of two potential barriers, the total probability of transmission through a barrier added at the end of the array can then be described mathematically as
Thus, we have obtained a recursive formula, that makes it possible to compute the transmission probability for any given number of identical potential barriers, when the transmission probability \( T \) and reflection probability \( R \) is known. From the conservation of probability it follows that

\[
R_N = 1 - T_N. \tag{3.2}
\]

In the quantum mechanical case, where instead, the probability amplitudes are complex numbers, the same reasoning for deducing Eq. (3.1) still holds, with the exception of the invalidity of Eq. (3.2). Thus, in formula, Eq. (3.1), one can exchange the coefficients \( T \) and \( R \) with the total transmission and reflection amplitudes, denoted \( \tilde{t} \) and \( \tilde{r} \), as in Eq. (2.6). However, the reflection coefficient will have to be calculated by adding together the probability of the incoming wave being reflected from the initial chain and all the paths of being transmitted through the initial chain, reflected back and forth within chain and an additional barrier, ultimately being transmitted through the initial chain. The formula reads,

\[
\tilde{r}_{N+1} = \tilde{r}_N + \tilde{t}_N^2 \tilde{r} + \tilde{r}_N^2 \tilde{r}_N + \cdots = \tilde{r}_N - \frac{\tilde{r}_N^2 \tilde{r}}{1 - \tilde{r}_N \tilde{r}}. \tag{3.3}
\]

### Disordered Systems

Due to disorder, in a quantum mechanical system, the reflection coefficient is no longer the same for an electron incident from the different sides of an chain of potential barriers. By adding a new potential barrier at the beginning of an array of \( N \) non identical potential barriers, we can again calculate the transmission and reflection coefficient for the extended chain by adding up the probability for all the possible paths the wave might travel. We have used the following formulation

\[
\tilde{t}_{N+1} = \tilde{h}_N + \tilde{t}_N \tilde{r}_{NI} \tilde{t} + \tilde{t}_N^2 \tilde{r}_{NI}^2 \tilde{t}_N + \cdots = \frac{\tilde{h}_N}{1 - \tilde{r}_N \tilde{r}_{NI}}, \tag{3.4}
\]

\[
\tilde{r}_{N+1} = \tilde{r} + \tilde{t}_N^2 \tilde{r}_{NI} \tilde{r} + \tilde{t}_N^2 \tilde{r}_{NI} \tilde{r} + \cdots = \tilde{r} + \frac{\tilde{r}_N^2 \tilde{r}_{NI}}{1 - \tilde{r}_N \tilde{r}_{NI}}, \tag{3.5}
\]

where \( \tilde{t} \) and \( \tilde{r} \) are the transmission and reflection coefficient for the added potential, and \( \tilde{r}_{NI} \) the total reflection coefficient for an electron incident on the left upon the array composed of the \( N \) potentials at the end.[6] The two above formulas are deduced using the same intuition as the above cases for completely ordered systems.

### 3.2 The Energy Eigenvalue Equation

The occurrence and specifications of energy bands and gaps, are essentially traced back to the energy eigenvalue equation Eq. (1.10), which provides a condition for the allowed and forbidden electron wave numbers. We have solved the energy eigenvalue equation numerically in order to arrive at what wave number should place the incident electron inside or outside the allowed energy band. However, below, is rather the more important deduction, not only describing the underlying intuition behind energy bands but adding a level of rigourosity to an important result that we have used.
Consider the one-dimensional periodic potential

\[ V(x) = \sum_{n=-\infty}^{\infty} v(x-na). \]  

(3.6)

Let \( v \) be an even function so that \( v(x) = v(-x) \). Let an electron with energy \( E = \frac{\hbar^2 k^2}{2m} \) be incident from the left on a single potential barrier \( v(x) \). Then the time-independent Schrödinger equation becomes

\[ \frac{d^2 \psi(x)}{dx^2} + (v(x) - k^2)\psi(x) = 0. \]

The corresponding solution for \( 0 < E < v \) in the region \( |x| > a \) reads

\[ \psi_l(x) = e^{ikx} + re^{-ikx}, x \leq -\frac{a}{2} \]

(3.7)

\[ = te^{ikx}, x \geq \frac{a}{2}. \]

(3.8)

Here \( r \) and \( t \) are the reflection and transmission coefficients that determine the probability amplitude that the electron will be transmitted or reflected by the potential barrier. \( \psi_l(x) \) with the subscript \( l \), indicates that the wave is incident from the left. Since, \( v(x) \) is an even function, it is implied that \( \psi_r(x) = \psi_l(-x) \) also is a solution to the Schrödinger equation. By superposition, so is any linear combination of \( \psi_l(x) \) and \( \psi_r(x) \): \( \psi(x) = A\psi_l(x) + B\psi_r(x) \). Thus, given that the Hamiltonian associated with the crystal is equal to that of a single potential barrier in the interval \( -\frac{a}{2} \leq x \leq \frac{a}{2} \), any solution to the Schrödinger equation for the entire system with energy \( E \) must be a linear combination of \( \psi_l \) and \( \psi_r \) in that region:

\[ \psi(x) = A\psi_l(x) + B\psi_r(x), -\frac{a}{2} \leq x \leq \frac{a}{2}. \]

Evaluating \( \psi(x) \) in the region \( |x| \geq \frac{a}{2} \) yields

\[ \psi(x) = Ae^{ikx} + Are^{-ikx} + Bte^{-ikx}, x \leq -\frac{a}{2} \]

\[ = Ae^{ikx} + Be^{-ikx} + Bre^{ikx}, x \geq \frac{a}{2}. \]

Because of the periodicity of the potentials we can apply Bloch’s theorem, Eq. (1.9) stating that

\[ \psi(x+a) = e^{iqa}u(x) = e^{iqa}\psi(x). \]  

(3.9)

When differentiating the last expression we obtain

\[ \frac{d\psi(a+x)}{dx} = e^{iqa}\frac{d\psi(x)}{dx}. \]  

(3.10)

Now we evaluate the last two conditions Eq. (3.9) and Eq. (3.10) at \( x = -\frac{a}{2} \),

\[ Ate^{ika} + Be^{-ika} + Bre^{ika} = e^{iqa} \left( Ae^{-ika} + Are^{ika} + Bte^{ika} \right) \]

\[ ik \left( Ate^{ika} - Be^{-ika} + Bre^{ika} \right) = e^{iqa} ik \left( Ae^{-ika} - Are^{ika} - Bte^{ika} \right). \]
Multiplying both equations with $e^{ikx}$ and gathering the coefficients of $A$ and $B$ respectively yields

$$\begin{align*}
A \left( e^{iqa} + e^{iqa} r e^{ika} - te^{ika} \right) + B \left( e^{iqa} t e^{ika} - re^{ika} - 1 \right) &= 0 \\
A \left( e^{iqa} - e^{iqa} r e^{ika} - te^{ika} \right) + B \left( -e^{iqa} t e^{ika} - re^{ika} + 1 \right) &= 0.
\end{align*}$$

By writing this system of equation on matrix form we must have the determinant of the system matrix equal to zero to find any non trivial solution. This translates into

$$0 = \left( e^{iqa} + e^{iqa} r e^{ika} - te^{ika} \right) \left( -e^{iqa} t e^{ika} - re^{ika} + 1 \right) - \left( e^{iqa} t e^{ika} - re^{ika} - 1 \right) \left( e^{iqa} - e^{iqa} r e^{ika} - te^{ika} \right) = 4 e^{iqa} e^{ika} \left( \frac{t^2 - r^2}{2} e^{ika} + \frac{e^{-ika}}{2} - t e^{ika} + e^{-ika} \right).$$

By using the identity $\cos \theta = \frac{e^{i\theta} + e^{-i\theta}}{2}$ we arrive at

$$\cos qa = \frac{t^2 - r^2}{2t} e^{ika} + \frac{1}{2t} e^{-ika}. \quad (3.11)$$

If we rewrite the transmission and reflection coefficient on polar form and use the fact that they are orthogonal (derived in the appendix of [6]) we obtain

$$\begin{align*}
t &= |t| e^{i\delta} \\
r &= \pm i |r| e^{i\delta}.
\end{align*} \quad (3.12)$$

From electron conservation it follows that

$$1 = |r|^2 + |t|^2. \quad (3.13)$$

Inserting the relations Eq. (3.12) and Eq. (3.13) into Eq. (3.11) yields

$$\cos qa = \frac{|t|^2 + |r|^2}{2 |t|} e^{i(ka + \delta)} + \frac{1}{2 |t|} e^{-i(ka + \delta)} = \frac{\cos (ka + \delta)}{|t|}.$$ 

Thus the condition for the energy eigenvalues reads

$$\cos qa = \frac{\cos \theta}{|t|}, \quad (3.14)$$

where we have introduced the total phase argument $\theta = ka + \delta$ which we can relate to Eq. (1.10). [?] 

### 3.3 Implementation

To calculate the probability of transmission as a function of the number or potential barriers, in the classical case, we applied the recursion formulas Eq. (2.1) and Eq. (2.2) and implemented them using Matlab.
In the quantum cases we instead applied the total probability amplitudes $\tilde{t} = te^{ikd}$, and $\tilde{r} = re^{ikd}$, where $d$ is the distance between the potentials. We implemented the recursion formulas Eq. (2.6) and Eq. (2.7) for the total transmission and reflection amplitude respectively. The probability of transmission for $N$ potential barriers was calculated as $T_N = |t_N|^2 = |\tilde{t}_N|^2$. The implementation was made in MatLab computing the total probability of transmission for the $N$:th barrier starting simply with the transmission and reflection coefficient for a single potential barrier.

For the special case of delta potentials we used Eq. (1.4) as the transmission coefficient along with Eq. (1.6) as a reflection coefficient for a single potential. Especially, we included the two cases choosing the wave number to be inside and outside the allowed band respectively. Next we considered a rectangular potential barrier and applied Eq. (1.1) as the transmission probability amplitude and Eq. (1.3) as the reflection probability amplitude for one potential. The transmission probability was calculated and plotted for a periodic array of 100 identical potentials for three different barrier widths.

Moreover, we aimed to look at how the probability of transmission depended on the wave vector of an electron incident on the different kinds of potential barriers. We implemented the same principles and formulas in Matlab as for computing transmission probability relative to the number of potentials, since the algorithm used to calculate the transmission probability for $N$ potentials is the same. The main difference was in using a fixed number of periodic potentials and instead determining the transmission probability, $T_n = |t_n(k)|^2$, over a certain range of the wave number. We decided to implement this computation on three systems of periodic potentials with different number of potentials, $N$, namely $N = 3$, $N = 6$ and $N = 1000$.

We further investigated the relationship between the energy of an electron propagating through a periodic potential composed of $N$ identical potentials and the crystal wave number An illustration of this was obtained by solving Eq. (1.10) numerically for a certain range in energy and subsequently plotting the real solutions for the crystal wave number.

Expanding from our first assumption of perfect crystal structures, we modified our previous model for certain types of disorder. By defining $\Delta w$ as a random disorder in the potential width and calibrating for this disorder in our previous model we produced new figures for transmission probability versus wave vector and transmission probability versus number of periodic potentials. The magnitude of $\Delta w$ was designed to be homogenously distributed and bounded. Thus in our model the potential width $a$ is made to be randomly fluctuating around an mean value $w$ according to:

$$w - \Delta w \leq a \leq w + \Delta w.$$

Also we introduced a random disorder in the potential separation while keeping the width of the potential barrier fixed. The location of each potential barrier fluctuates randomly around the potential barrier position in an equally spaced potential array. Formalizing this yields

$$l - \Delta l \leq d \leq l + \Delta l,$$

where $d$ is the potential separation, $l$ the mean separation and $\Delta l$ a uniformly distributed and bounded disorder such that $\Delta l \leq l$.

We used the Lyapunov exponent to measure the degree of localization[2],

$$\gamma = -\frac{\ln(T)}{2N}, \quad (3.15)$$
where $N$ is the number of potential barriers and $T$ is the transmission probability for the entire system of potentials. In addition, for our one-dimensional model, the $\gamma$ corresponds to the inverse of the localization length. We intend to illustrate how the degree of localization varies with potential width for an electron with a wave number inside and outside the band. This was done by calculating $\gamma$ as a function of the potential width, $a$, using Eq. (3.15) and plotting the value of $\gamma$ averaged over 100 samples. The potential width, $a$, is implicitly contained in the transmission probability, $T$. The transmission probability, $T$ in Eq. (3.15) was computed in the same recursive manner as previous studies for a fixed number of rectangular potentials, potential separation and wave number.
Chapter 4

Results and Discussion

In this section we will present our results and analysis. First, we present the results pertaining to the relations between transmission probability and the number of potentials. Then we present the results of our studies on the relationship between transmission probability and wave number. Lastly, we present our results on our studies of disorder.

4.1 Transmission and Number of Potentials

From the theory of quantum mechanics, we know that for certain energies, even for an infinite number of potential barriers, the transmission probability will be non zero. However, if the electron has an energy outside of the allowed band, quantum mechanics tells us that the incident electron will experience a decrease in transmission when the number of potential barriers increase. For the classical case, knowing that classical mechanics is an approximation of quantum mechanics for large scale objects, we would expect the electron to behave like a particle, and thus the transmission probability should decrease when increasing the number of potentials.

Figure 4.1: The transmission probability $T$ as a function of the number of potential barriers $N$ where three cases are depicted; wave number inside the allowed band, outside the allowed band and classical. The wave number to place the electron inside the band was $5 \times 10^8 m^{-1}$. To place it outside the allowed band we set the wave number to $3.3 \times 10^8 m^{-1}$. In figure a) Dirac delta potentials and b) rectangular potentials. For both figures the potential width was set to $2 \times 10^{-10} m$ and the potential separation to $10^{-8} m$. 

![Figure 4.1: Transmission probability T as a function of the number of potential barriers N.](image)
For both the case of Dirac delta potentials and rectangular potentials the above described expected behaviour should be similar. Analyzing the results from Fig. 4.1 we see that our recursive algorithms reproduce results that are in line with expectations from theory.

However, there are differences between applying Dirac delta functions or rectangular potentials. Our results show that the transmission on average is higher applying rectangular potentials. However, we do not think that that is a general result, meaning that for some rectangular potentials, the average transmission could well be lower applying rectangular potentials instead of Dirac delta potentials.

### 4.2 Transmission and Wave Number

When we analyze the relation between the transmission probability and the wave number of the incoming electron, we can see that the probability of transmission, on average, increase as the wave number increase. From the same figure, Fig. 4.2, we can observe the allowed energy bands and the restricted energy gaps in terms of electron wave numbers.

![Graph showing transmission probability as a function of wave number for different numbers of potentials (N=3, 6, 1000).](image)

Figure 4.2: The transmission probability $T$ as a function of the wave number $k$ for three different number of potentials, $N=3, 6, 1000$. Figure a) pertains to Dirac delta potentials and b) to rectangular potentials with the potential width $2 \times 10^{-10} m$. The potential separation was set to $10^{-8} m$.

We see that the energy bands widen and energy gaps tighten as the wave number is increased. This behaviour accounts for both the case of applying Dirac delta- and rectangular potentials. Comparing the two, we can, however, observe that the allowed energy bands are tighter for the case of rectangular potentials. We can also observe that the average transmission probability as a function of the wave number is lower for the case of rectangular potentials.

### 4.3 Rectangular Potentials with differing widths

Here we analyze the results pertaining to Fig. 4.3. In Fig. 4.3, we have plotted, for $N = 100$, the relation between the transmission probability and the wave number of the
incident electron for three widths of the rectangular potentials. A measure $K$ is introduced, where $K = Potential \times Width$, and is defined to be $3 \times 10^8 \text{Jm}$. Geometrically, in one dimension it is the area of the potential barrier. While changing the width, the barrier area remains constant. Thus, while increasing the width the potential is lowered.

Figure 4.3: The Transmission probability $T$ as a function of the wave number $k$ for three different rectangular potential sizes, with widths $1.9885 \times 10^{-10} \text{m, } 1.4609 \times 10^{-10} \text{m, } 1.1185 \times 10^{-10} \text{m}$. The potential separation is $10^{-8} \text{m}$.

From Fig. 4.3 we can understand that it is hard to draw any conclusions on the differences between the three widths. However, it appears that when the width is increasing the initial value for the wave number that allows for transmission is increased. Otherwise, the three graphs look very similar apart from that parallel shift. Therefore, it is reasonable to think that the relation between transmission behaviour and potential width is dominated by the size of the potential. However, it seems that the width creates a parallel shifts for the plots, implying that for a given transmission probability, the wave number must be higher for a wider potential barrier.

The relation between the transmission probability and the number of potentials is presented for different potential widths in Fig. 4.4.
Figure 4.4: a) The transmission probability $T$ as function of number of potentials $N$ for different widths; $1.9885 \times 10^{-10} m$, $1.4609 \times 10^{-10} m$, $1.1185 \times 10^{-10} m$ for an electron a) inside the allowed band, with a wave number of $5 \times 10^8 m^{-1}$ b) outside the allowed band, with a wave number of $3.3 \times 10^8 m^{-1}$ c) described classically. The potential separation is $10^{-8} m$ in all figures.

The three figures represent the three cases of an electron being inside the allowed band, outside the allowed band and being viewed classically as a particle. For the each case we can clearly observe that the average transmission decreases with increasing potential width. However, in neither case is the nature of the behaviour different. When the electron is inside the band, Fig. 4.4a), the transmission behaves oscillatory for all widths. When the electron is outside the band, the transmission drops off in an exponential manner, no matter potential width. The same type of exponential decrease is observed in the classical case for all three widths. When changing widths for the potentials, we have applied the same methodology as for Fig. 4.3.

The below figures relate to the study of how the energy bands/gaps change for different widths of the potential barriers.

Figure 4.5: Energy $E[meV]$ of an electron versus crystal wave number $q$ for three different potential widths $\alpha$: a) $1 \AA$ b) $5 \AA$ and c) $15 \AA$. For all figures the potential separation $d=100 \AA$. The dotted parabolas represent the free particle.

From Fig. 4.5 we see that at any non zero multiple of $\frac{2\pi}{\alpha}$ energy gaps occur. It is clear that these gaps are increasing with increasing potential width. In addition, the range of the energy bands decreases for wider potentials. Notice that as the width approach zero the solutions of Eq. (1.10) tends to those of the free electron.
4.4 Random Disturbance in Potential Width and Separation

Fig. 4.6 depicts the probability of transmission through a chain of 100 random potentials for three different levels of disorder; in Fig. 4.6a) it is applied to potential width and in Fig. 4.6b) to potential separation. In both figures, the transmission probability for the disordered systems inside the allowed energy band oscillates with a higher amplitude than for the completely ordered system (blue curve). In the band region, we observe that the average transmission probability decreases for a higher order of disorder in potential width and separation respectively. In Fig. 4.6a) the energy band corresponding to a higher disorder in potential width (red dotted line) are tighter, and located in right part of the energy band for the completely ordered system. From Fig. 4.6b) we see that the effect of an increasing disorder in the potential separation lowers the transmission probability in the band region and increases the minimum transmission probability in the gap region. Especially, in the third gap region a high disorder in potential separation (red dotted line) seems to result in an average transmission probability close to that of the subsequent band region.

Figure 4.6: The transmission probability $T$ as a function of the wave vector $k$ for three different disorders in a) potential width: $\Delta w = 0$ (blue curve), $\Delta w = 0.3w$ (green dashed curve) and $\Delta w = w$ (red dotted curve). The average width $w = 2A$ and the potential separation $d = 100A$.

b) potential separation: $\Delta l = 0$ (blue curve), $\Delta l = 0.2l$ (green dashed curve) and $\Delta l = 0.5l$ (red dotted curve). The mean potential separation $l = 100A$ and the potential width $d = 2A$. For figures a) and b) the number of potential barriers $N = 100$ the potential strength $V = 1.1E$. $E$ is given by $E = \frac{\hbar^2k^2}{2m}$.

It should be noted that the generality of these claims are hard to establish since the potential width and separation fluctuates randomly. For example, there is a probability, although small, that all the potential widths relevant to Fig. 4.6a) and potential separations relevant to Fig. 4.6b) are identical for a system intended to be disordered. Clearly this is not the case in Fig. 4.6. Also, it is mentionable that the system corresponding to a specific disorder is fixed for all the wave numbers.

Fig. 4.7 shows the probability of transmission for an electron inside the band versus the number of potential barriers averaged over 100 samples of disorder in potential width, Fig. 4.7a), and potential separation Fig. 4.7b). In the completely ordered system (blue curve) the transmission probability oscillates with an average value close to one. However, from both Fig. 4.7a) and Fig. 4.7b) we observe that the transmission probability for a disordered system decreases with an increase in the number of potentials.
Figure 4.7: The transmission probability $T$ as a function of the number of potential barriers $N$ for three different disorders in a) potential width: $\Delta w = 0$ (blue curve), $\Delta w = 0.5w$ (green curve) and $\Delta w = w$ (red curve). The mean width $w = 2\text{Å}$ and the potential separation $d = 100\text{Å}$. b) potential separation: $\Delta l = 0$ (blue curve), $\Delta l = 0.3l$ (green curve) and $\Delta l = l$ (red curve). The mean potential separation $l = 100\text{Å}$ and the potential width $d = 2\text{Å}$. For figures a) and b) the wave vector $k = 10 \times 10^8 \text{m}^{-1}$ and the potential strength $V = 1.1E$. $E$ is given by $E = \frac{\hbar^2 k^2}{2m}$.

In Fig. 4.8, we show by means of the Lyapunov exponent the effect of disorder in the potential width on the transmission probability. The result is an average of 100 samples. From Fig. 4.8a) we see that inside the energy band the degree of localization increases for an increasing degree of disorder. In contrast, in the energy gap region, Fig. 4.8b), shows that the degree of localization decreases for an increasing degree of disorder.

Figure 4.8: The Lyapunov exponent $\gamma$ as a function of the level of disorder $\Delta w$ for an electron a) inside the band ($k = 5 \times 10^8 \text{m}^{-1}$) b) in the gap ($k = 6.5 \times 10^8 \text{m}^{-1}$). The mean width $w = 2\text{Å}$, the potential separation $d = 100\text{Å}$, the number of potential barriers $N = 100$ and the potential strength $V = 1.1E$. 
Chapter 5

Conclusions

5.1 Classic Transmission

Classically, our results follow intuition. As the number of potential barriers increases the transmission probability strictly decreases. Also, it seems like the width of the potential barrier has the same effect. As the width of the potential barrier is increased, while holding the potential size constant, the transmission probability decreases on average.

5.2 Quantum Mechanical Transmission

While having no formal hypothesis, from theory we know that quantum mechanically, there is a presence of energy bands and gaps. We also know from energy band theory in conjunction with electron transmission probability, that the bands and gaps should provide completely different transmission behaviour. From our models, this is exactly what we have been able to confirm. Quantum mechanically, when the wave vector of the incident electron is within the allowed energy band, transmission probability is non zero for any number of potentials. In other words, one dimensional propagation through a perfect crystal with infinite length is possible, only contingent on the electron wave number. However, when the wave number of the incident electron is outside the allowed energy band the transmission probability decreases quickly, faster than in the classical case.

Another conclusion drawn from our computations is that the width of the allowed energy bands increase as the wave number increases. Based on our figures of the transmission probability as a function of the wave number with different widths we could not clearly draw any distinct conclusions. However, when we plotted the energy bands and gaps as a function of the crystal wave number, and introduced different widths, we could draw the conclusion that the energy gaps increased when the potential width increased. The opposite effect was seen on the energy bands that tightened for increasing potential widths. This was in line with expectations from theory, and also the energy band representation provided a clearer display of the behaviour, while being equivalent to plotting the transmission probability versus the wave number.
5.3 Disorder

Disorder in Potential Width

The way disorder was introduced in the potential width, by applying it randomly within an interval around an average width, enabled an implementation of disorder throughout the entire system. This not only provides more impact and change to the ordinary case, but also much better approximates that of a real crystal, endowed with random impurities. We executed two different computations for disorder, where we allowed for different magnitudes of variation of the width around its average. One computation was made for an interval of 50%, and one was made for an interval of 100%. Thus on average, the second computation potentially, and most probably imply a higher level of disorder. Comparing the two we were able to draw conclusions on how the transmission probability changes as a function of the level of disorder. In addition, by introducing a level of randomness to the variations, we were able to compute an expected value of the transmission coefficient approximated by an average over 100 iterations of the transmission computation. The average transmission probabilities of these 100 samples, provide a robust and generalized representation of the behaviour of the transmission probability, strengthening our conclusions. 

We found that the implementation of disorder in an array of rectangular potential barriers yields many interesting effects. Our results show that a disorder in potential width induces a localization of energy states. For higher degrees of disorder in potential width the energy band tighten and the minimum level of transmission probability in the gap increases. Also, we conclude that the average transmission probability inside the energy band is lower than for a completely ordered system and that inside the energy band the degree of localization increases for an increasing degree of disorder. This is indicated from our computations of the Lyapunov exponent as a measure of the degree of disorder. Finally, our results told us that for an energy in the energy gap region the degree of localization decreases for an increasing degree of disorder.

Disorder in Potential Separation

As for the disorder in the potential width, we let the potential separation vary randomly within a set interval around a fixed average value. Again, this representation provides not only a strong and widespread level of disorder, but also a closer approximation to a real crystal, endowed with random and natural impurities. We computed the transmission probability but rescaled it using \( \ln(T) \) because we found that due to the behaviour of the relation between the transmission probability and wave number, this rescaling provided smoother curves than the ordinary transmission probability, \( T \). This adjustment increased the level of clarity and simplified analysis. Again two levels of disorder was introduced in the potential separation, allowing for random variation around the average of 20% and 50%. As for the case of disorder in the potential width, we were able to perform 100 iterations for both levels of variation and compute the expected value for the transmission, obtaining a more robust and generalized behaviour. Our first conclusions drawn from these computations is that inside the band the average transmission probability decrease with increasing levels of disorder, as with the case of the potential widths. The second conclusion pertains to our plot of the disordered transmission behaviour as a function of the number of potentials, and we find that even though the incident electron wave number is within the energy band the transmission probability decreases as the number of potentials increase.
Bibliography


