Wave Transport and Chaos in Two-Dimensional Cavities

Björn Wahlstrand

Adviser: Karl-Fredrik Berggren
Theoretical Physics

Irina Yakimenko
Theoretical Physics

Examiner: Irina Yakimenko
Theoretical Physics

Linköping, 3 December, 2008
This thesis focuses on chaotic stationary waves, both quantum mechanical and classical. In particular we study different statistical properties regarding these waves, such as energy transport, intensity (or density) and stress tensor components. Also, the methods used to model these waves are investigated, and some limitations and specialities are pointed out.
To Natalia
Abstract

This thesis focuses on chaotic stationary waves, both quantum mechanical and classical. In particular we study different statistical properties regarding these waves, such as energy transport, intensity (or density) and stress tensor components. Also, the methods used to model these waves are investigated, and some limitations and specialities are pointed out.
Acknowledgements

I would like to thank my adviser, Karl-Fredrik Berggren and my examiner, Irina Yakimenko for providing me with a very interesting diploma work, and also for Your great knowledge in the field of quantum chaos. The discussions with You have been invaluable help to me. I would also like to thank John Wärnå for acting as my opponent, and also for discussions during the course of this work.
## Contents

1. **Introduction**  
   1.1 Chaos .......................... 1  
   1.2 Origins of Wave Chaos ...................... 1  
   1.3 Wave Chaos Today ...................... 1  
   1.4 The Aim of this Thesis ...................... 2

2. **Theory**  
   2.1 Quantum Mechanics ...................... 3  
      2.1.1 The Schrödinger and Helmholtz Equations  3  
      2.1.2 Normalization ...................... 4  
      2.1.3 Energy Transport ...................... 4  
      2.1.4 Quantum Mechanical Stress Tensor .......... 5  
      2.1.5 Continuity Equation ...................... 5  
      2.1.6 Bracket Notation ...................... 5

3. **Finite Difference Method**  
   3.1 Discretization ...................... 7  
      3.1.1 The Schrödinger Equation in FDM .......... 8  
   3.2 Boundary Conditions ...................... 9  
      3.2.1 Dirichlet Boundary Condition .......... 11  
      3.2.2 Neumann Boundary Condition .......... 11  
      3.2.3 Similarities between NBC and DBC .......... 12  
      3.2.4 Mixed Boundary Conditions .......... 13  
   3.3 The Matrix Eigenvalue Problem .......... 13  
      3.3.1 Setting Up the Matrix .......... 13  
      3.3.2 Normalization .......... 15

4. **Imaginary Potential**  
   4.1 Currents ...................... 18  
   4.2 Conservation of Probability Density .......... 18  
   4.3 Perturbation Theory .......... 20  
   4.4 Balanced Imaginary Potential .......... 21  
      4.4.1 Verification of the Balanced Potential Method .......... 22  
   4.5 Interaction between Wave Functions .......... 24
<table>
<thead>
<tr>
<th>Chapter</th>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>Accuracy</td>
<td>29</td>
</tr>
<tr>
<td>5.1</td>
<td>Theoretical Solution</td>
<td>29</td>
</tr>
<tr>
<td>5.2</td>
<td>Numerically Obtained Eigenvalues</td>
<td>29</td>
</tr>
<tr>
<td>5.3</td>
<td>Numerically Obtained Eigenfunctions</td>
<td>32</td>
</tr>
<tr>
<td>5.4</td>
<td>Perturbation Theory</td>
<td>32</td>
</tr>
<tr>
<td>6</td>
<td>Complexity</td>
<td>35</td>
</tr>
<tr>
<td>6.1</td>
<td>Data Complexity</td>
<td>35</td>
</tr>
<tr>
<td>6.2</td>
<td>Time Complexity</td>
<td>36</td>
</tr>
<tr>
<td>6.3</td>
<td>Exclusion of High Potential Grid Points</td>
<td>36</td>
</tr>
<tr>
<td>6.4</td>
<td>Using Symmetry</td>
<td>38</td>
</tr>
<tr>
<td>7</td>
<td>Statistical Distributions</td>
<td>41</td>
</tr>
<tr>
<td>7.1</td>
<td>Density Distributions</td>
<td>42</td>
</tr>
<tr>
<td>7.1.1</td>
<td>Numerically Obtained Density Distributions</td>
<td>43</td>
</tr>
<tr>
<td>7.2</td>
<td>Current Distributions</td>
<td>45</td>
</tr>
<tr>
<td>7.2.1</td>
<td>Numerically Obtained Current Distributions</td>
<td>45</td>
</tr>
<tr>
<td>7.3</td>
<td>Stress Tensor Distributions</td>
<td>48</td>
</tr>
<tr>
<td>7.3.1</td>
<td>Numerically Obtained Stress Tensor Distributions</td>
<td>48</td>
</tr>
<tr>
<td>8</td>
<td>Conclusions and Future Work</td>
<td>51</td>
</tr>
<tr>
<td>8.1</td>
<td>The Method</td>
<td>51</td>
</tr>
<tr>
<td>8.2</td>
<td>The Statistics</td>
<td>51</td>
</tr>
<tr>
<td>8.3</td>
<td>Future Work</td>
<td>52</td>
</tr>
<tr>
<td></td>
<td>Bibliography</td>
<td>53</td>
</tr>
<tr>
<td>A</td>
<td>Plots</td>
<td>55</td>
</tr>
<tr>
<td>A.1</td>
<td>Sample Plots</td>
<td>55</td>
</tr>
<tr>
<td>A.2</td>
<td>Density Distributions</td>
<td>60</td>
</tr>
<tr>
<td>A.3</td>
<td>Current Distributions</td>
<td>63</td>
</tr>
<tr>
<td>A.4</td>
<td>Stress Tensor Distributions</td>
<td>68</td>
</tr>
<tr>
<td>B</td>
<td>Derivations</td>
<td>73</td>
</tr>
<tr>
<td>B.1</td>
<td>Helmholtz Equation in a Quasi-Two-Dimensional Cavity</td>
<td>73</td>
</tr>
<tr>
<td>B.2</td>
<td>Derivation of the Continuity Equation</td>
<td>75</td>
</tr>
</tbody>
</table>
Chapter 1

Introduction

1.1 Chaos

In classical mechanics, chaos can be described as extreme sensitivity to change in initial conditions, but also as great disorder or even randomness \( \text{(or \[1\])} \) for a more popular description). For example, a particle bouncing around a very irregular domain can be seen as moving chaotically. After sufficiently long time evolution, it is impossible to guess where it is without looking. A chaotic system in classical mechanics can never be restarted without altering the results, nor can it be reversed. Wave chaos is in different in several ways. First, the systems can be restarted. Second, the systems can sometimes be time reversed, and returned to the initial state, something that is impossible classically. This is because a wave can be seen as propagating in all possible classical directions. In waves, chaotic behaviour can be seen in amplitude and other properties such as current and stress tensor components.

1.2 Origins of Wave Chaos

The field of wave chaos has long fascinated both artists and scientists. Its popular breakthrough was probably due to E. F. F. Chladni \([2][1]\). In the 18th century he placed dust on glass plates and made them vibrate with their eigenfrequency. By doing this, the dust on the plates positioned itself along the nodal lines of the vibration. This phenomena got many mathematicians and physicists interested in the subject, but also artists who saw the beauty of these patterns.

1.3 Wave Chaos Today

In later days, the topic still lives, and is more active than ever. Wave chaos is being studied both on microscopic level in quantum mechanics, and on macroscopic level in acoustics and electromagnetics. Because of the one-to-one correspondence between these areas, most measurements are done at macroscopic level. The
results can then be translated into quantum mechanics using simple rescaling techniques.

1.4 The Aim of this Thesis

In this thesis we seek to numerically simulate experiments concerning statistical distributions of density (intensity) \[6\], wave transport \[6\] and stress tensor components \[4\]. In particular, we want to investigate the effect of net wave transport that was found experimentally, and see if a higher energy (or frequency) dampens this effect. The same kind of cavity was used in all these experiments, and is also for calculations in this thesis. As numerical method we have chosen the finite difference method (FDM) \[9\] with an imaginary potential \[8\]. This choice was made for two reasons. First, this method is easy to implement, and the results can be used without much after-work. Second, the experiments were done using certain measurement techniques that coincide very well with how FDM handles the problem. The method of using an imaginary potential has its origin in modelling of inelastic scattering in nuclear physics \[3\], where it is used to absorb particles. In this thesis, it acts as a source and drain, creating a transport through the cavity, much like a battery. These methods are studied in detail in this thesis, both the accuracy of FDM and the limitations of the imaginary potential model.
Chapter 2

Theory

In order to understand this thesis, a very basic knowledge of quantum mechanics is needed. In this chapter the most fundamental ideas are discussed, and some quantities are defined. This should provide sufficient knowledge to read and understand the remainder of the thesis. In the following sections we restrict ourselves to a two-dimensional theory.

2.1 Quantum Mechanics

In quantum mechanics the state of a system is described by a wave function. Observables, such as the energy, can be extracted by applying operators to such functions. The most common interpretation of quantum mechanics is that the modulus square of the wave function is the probability density, the probability function regarding where a particle can be found.

2.1.1 The Schrödinger and Helmholtz Equations

The most fundamental equation of Quantum Mechanics is the Schrödinger equation. This equation describes the time evolution of a wave function. In this thesis we only need the time independent Schrödinger equation, seen in equation (2.1).

\[ H \phi = \left( -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right) \phi(r) = E \phi(r) \] (2.1)

This is an eigenvalue problem where the eigenvalue is the energy of the state, and the eigenfunction \( \phi \) is the wave function. \( V \) is the potential in which the particle (or wave) moves. If this potential is zero, we can re-arrange this equation to another form, seen in equation (2.2).

\[ \nabla^2 + \frac{2mE}{\hbar^2} \phi(x, y) = 0 \] (2.2)

Now, let’s compare this with another equation, used to describe the perpendicular \( E \)-field \( (E_z) \) in a quasi-two dimensional domain (see appendix B.1). This equation
Theory

is of the same form as the Helmholtz equation in a two-dimensional cavity, and can be seen in equation (2.3).

\[
\nabla^2 + k^2 E_z(x, y) = 0 \tag{2.3}
\]

As seen here, there is a one-to-one correspondence between the \( E_z \)-field and the wave function, \( \phi(x, y) \), in a quasi-two-dimensional region. The relation between the wave number, \( k \), and the energy, \( E \), is then (2.4).

\[
k = \sqrt{\frac{2mE}{\hbar^2}} \tag{2.4}
\]

This is a very convenient way to transform between the Schrödinger equation and the Helmholtz equation, because it is usually hard to do measurements at atomic level. Many experiments can be done at macroscopic level, and then translated into quantum mechanics using this relation [1].

### 2.1.2 Normalization

The most common interpretation of the wave function, \( \phi(\vec{r}) \) is that the modulus square, \( |\phi(\vec{r})|^2 \) is the probability density regarding where the particle can be found. This calls for normalization of the wave function, that the total probability to find the particle is 1. If we know that the wave function is completely contained in volume \( V \), then the condition for normalization is seen in equation (2.5).

\[
\int_V |\phi(\vec{r})|^2 dV = 1 \tag{2.5}
\]

This means that the probability \( P \) to find the particle in volume \( V' \subseteq V \) is equation (2.6).

\[
P = \frac{\int_{V'} |\phi(\vec{r})|^2 dV'}{\int_V |\phi(\vec{r})|^2 dV} = \frac{\int_{V'} |\phi(\vec{r})|^2 dV'}{\int_V |\phi(\vec{r})|^2 dV} \tag{2.6}
\]

### 2.1.3 Energy Transport

In quantum mechanics, the transport of probability density, called the probability density current, \( \mathbf{S} \), is defined as (2.7) [8].

\[
\mathbf{S} = \frac{\hbar}{2mi} (\phi^* \mathbf{\nabla} \phi - \phi \mathbf{\nabla} \phi^*) \tag{2.7}
\]

This expression has a one-to-one correspondence with the expression for the Poynting vector, \( \mathbf{P} \), seen in (2.8) [1].

\[
\mathbf{P} = \frac{c}{4\pi k} (\phi^* \mathbf{\nabla} \phi - \phi \mathbf{\nabla} \phi^*) \tag{2.8}
\]
2.1 Quantum Mechanics

2.1.4 Quantum Mechanical Stress Tensor

The quantum mechanical stress tensor (QST) is defined as (2.9).

\[ T_{\alpha,\beta} = \frac{\hbar^2}{4m} \left( -\phi^* \frac{\delta^2 \phi}{\delta x_\alpha \delta x_\beta} - \phi \frac{\delta^2 \phi^*}{\delta x_\alpha \delta x_\beta} + \frac{\delta \phi}{\delta x_\alpha} \frac{\delta \phi^*}{\delta x_\beta} + \frac{\delta \phi^*}{\delta x_\alpha} \frac{\delta \phi}{\delta x_\beta} \right) \] (2.9)

2.1.5 Continuity Equation

The continuity equation, (2.10), describes the process of creation and annihilation of the probability density, \(|\phi(\vec{r}, t)|^2\) [8]. Here is presented in an integrated form, seen in equation B.2.

\[ \frac{\delta}{\delta t} \int_A |\phi(\vec{r}, t)|^2 = - \int_{\alpha} S_n d\alpha + 2 \frac{\hbar}{i} \int_A V_i |\phi(\vec{r}, t)|^2 dA \] (2.10)

Here, \(A\) is some region and \(\alpha\) is the boundary of \(A\). \(S_n\) is the component of \(\vec{S}\) that is normal to the boundary and \(V_i\) is the imaginary part of the potential. It may seem strange to use the imaginary part of the potential, because traditionally potentials are assumed to be real. By not making this assumption, we find that an imaginary part can be used to model creation and annihilation of particles or waves. Even better, we can create waves in one region, and annihilate them in another, creating a flow between the regions!

2.1.6 Bracket Notation

In order to save space it is common to use a bracket notation when working with quantum mechanical states. The set of all quantum states \(\phi_n\) is often denoted \(|\phi\rangle\), and the set of all \(\phi^*_n\) is denoted \(\langle \phi |\). These are often called bra and ket vectors (from the word bracket, bra-ket). \(|n\rangle\) corresponds to \(\phi_n\) and \(\langle n|\) corresponds to \(\phi^*_n\). There is much to say about this notation, but the only thing needed to understand this thesis is the notation (2.11). For a more in detail description of this notation, see [8] or any other book in quantum mechanics.

\[ \langle m|K|n\rangle = \int_A \phi^*_m K \phi_n dA \] (2.11)
Chapter 3

Finite Difference Method

In order to solve the Schrödinger equation in a more complex region than, for example, a circle or rectangle, a numerical method is needed. One such method is the finite difference method (FDM) [9]. In FDM the problem is discretized — approximated by a finite number of points — with each point describing the problem (in this case the eigenfunction, \( \phi(x, y) \)) in a corresponding spatial coordinate. These points are chosen so that they span a rectangular grid, making it easy to approximate derivatives and to keep track of the correspondence between a point and its spatial coordinates. Once discretized, the Schrödinger equation becomes a matrix eigenvalue problem that can be solved by a computer. This chapter contains an introduction to FDM and its application to this problem. The accuracy of this method is studied, and some limitations are pointed out. FDM can of course be used to approximate a problem of arbitrary dimension, but here only the 2D-version is studied. The main reason why FDM has been used, and not the finite element method (FEM) or some other method, is that we want to stay close to experiments [1][3][9]. In these experiments, the sample points were placed as a rectangular grid, just like the grid points in FDM. Also, FDM is simple to setup, and it is easy to work with the results, something that can be tricky in FEM.

3.1 Discretization

As briefly explained above, the points are organized as a rectangular grid. For simplicity the grid’s axis are chosen so that they coincide with the x- and y-axis of the system. First, the width, \( W_x \), and the height, \( W_y \), of the grid must be defined. This is done in such a way that the rectangle completely covers the domain where the equation is to be solved. Note that the grid does not need to mimic the shape of the domain, boundary conditions, potential walls and/or defining a set of points as zero can deal with this. The rectangle is divided into \( N \) rows and \( K \) columns. The separation between rows is \( \alpha \), and between columns it is \( \beta \) according to equations (3.1) and (3.2).

\[
\alpha = \frac{W_x}{N - 1} \quad \text{(3.1)}
\]
\[ \beta = \frac{W_y}{K-1} \]  

The grid points are defined as the intersections between rows and columns. Let \( n \) be the index of the rows and \( k \) the index of the columns. \( \phi(x, y) \) (the eigenfunction) is then discretized into \( \phi_{n,k} \) according to equation (3.3).

\[ \phi_{n,k} = \phi(\alpha \cdot (n-1), \beta \cdot (k-1)) \quad 0 < n \leq N \quad 0 < k \leq K \]  

In addition to indices \( n \) and \( k \), each point is also given a single index which is needed for calculations later. For now let’s just make the definition according to (3.4).

\[ \phi_s = \phi_{n,k} \quad s = N(k-1) + n, \quad 0 < n \leq N \quad 0 < k \leq K \]  

An example of a \( 4 \times 4 \) grid can be seen in figure 3.1, where the number in parenthesis is the s-value corresponding to the n and k of each grid point.

![Figure 3.1. An example of a 4 x 4 grid.](image)

### 3.1.1 The Schrödinger Equation in FDM

The Schrödinger equation in cartesian coordinates is seen in equation (3.5).

\[ H \phi = \left( -\frac{\hbar^2}{2m} \left( \frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} \right) + V(x, y) \right) \phi(x, y) = E \phi(x, y) \]  

In order to solve this eigenvalue problem numerically, the second derivatives need to be approximated. This turns out to be very simple in FDM. The definition of derivative in the continuous case is seen in equation (3.6).

\[ \frac{\delta f(x, y)}{\delta x} = \frac{f(x + \delta x, y) - f(x - \delta x, y)}{2\delta x} \]
3.2 Boundary Conditions

And in the corresponding way for y. This equation, (3.6), applied to itself, gives the second derivative, (3.7).

\[ \frac{\delta^2 f(x, y)}{\delta x^2} = \frac{f(x + \delta x, y) - 2f(x, y) + f(x - \delta x, y)}{\delta x^2} \] (3.7)

From the definition of the grid we know that the rows are separated by a distance \( \alpha \), and the columns by a distance \( \beta \). Quite intuitively, a good approximation for (3.7) is equation (3.8)

\[ \frac{\delta^2 f(x, y)}{\delta x^2} = \frac{f(x + \alpha, y) - 2f(x, y) + f(x - \alpha, y)}{\alpha^2} \] (3.8)

for x and

\[ \frac{\delta^2 f(x, y)}{\delta y^2} = \frac{f(x, y + \beta) - 2f(x, y) + f(x, y - \beta)}{\beta^2} \] (3.9)

for y. By inserting the definition of discretazion, (3.3), into these derivatives, they become

\[ \frac{\delta^2 \phi_{n,k}}{\delta x^2} = \frac{\phi_{n+1,k} - 2\phi_{n,k} + \phi_{n-1,k}}{\alpha^2} \] (3.10)

and

\[ \frac{\delta^2 \phi_{n,k}}{\delta y^2} = \frac{\phi_{n,k+1} - 2\phi_{n,k} + \phi_{n,k-1}}{\beta^2} \] (3.11)

By applying equations (3.10) and (3.11) to the Schrödinger equation (with \( \frac{\hbar^2}{2m} = 1 \)) it becomes

\[ \left( 2\alpha^2 + \beta^2 \right) \phi_{n,k} - \beta^2 \left( \phi_{n+1,k} + \phi_{n-1,k} \right) - \alpha^2 \left( \phi_{n,k+1} + \phi_{n,k-1} \right) = E\phi_{n,k} \] (3.12)

Figure 3.2 shows the dependency of the wave function in point \( n, k \). In every point, the value of the wave function depends on the sum of the wave functions in the four closest neighbouring points. In the case that \( \alpha = \beta \), the value depends on the average wave function value in the four closest neighbouring points.

3.2 Boundary Conditions

There is one problem left before this equation can be solved. As stated in the previous section (and seen in (3.12)), the wave function in a point depends directly on its four closest neighbouring points (see figure 3.2). On the boundary of the grid however, there are not four neighbours available (see figure 3.3 for an example). In order to deal with this, proper boundary conditions must be defined. The boundary conditions tell something about how the wave function behaves outside the grid. It can be constant (Dirichlet boundary condition, DBC), have a constant derivative (Neumann boundary condition, NBC), or anything else that one may find appropriate. No matter what, a set of boundary conditions must be chosen in order for the problem to have a solution. In this section the most common boundary conditions are discussed and applied to equation (3.12).
Figure 3.2. The grid point indexed $n,k$ depends on its four closest neighbours.

Figure 3.3. There are one or more neighbours missing in the boundary. In this case there is one point missing on the left hand boundary.
3.2 Boundary Conditions

3.2.1 Dirichlet Boundary Condition

As stated in the previous section, a Dirichlet boundary condition means defining constant function value on the boundary. Although this constant can be chosen freely, the only meaningful value in this in this application is zero. If not chosen to zero, the eigenfunction stretches over all space in a uniform fashion, making normalization impossible and making the probability density interpretation of quantum mechanics unapplicable. If this constant is chosen to be zero, Dirichlet boundary condition can be used to describe a closed system, a system where the wave function is very well contained within potential walls, often called a hard wall potential. The solution to such a problem can easily be normalized and translated into probability density. It is very easy to apply DBC to (3.12). Simply define all references to points outside the grid to zero:

\[ \phi_{n,0} = 0 \] (3.13)

\[ \phi_{n,K+1} = 0 \] (3.14)

\[ \phi_{0,k} = 0 \] (3.15)

\[ \phi_{N+1,k} = 0 \] (3.16)

As an example, the left hand side of equation (3.12) corresponding to \( \phi_{1,1} \) (the top left corner point) becomes:

\[
\frac{(2(\alpha^2 + \beta^2) + \alpha^2 \beta^2 V_{1,1}) \phi_{1,1} - \beta^2 (\phi_{2,1} + \phi_{0,1}) - \alpha^2 (\phi_{1,2} + \phi_{1,0})}{\alpha^2 \beta^2} = 0
\]

\[
\frac{(2(\alpha^2 + \beta^2) + \alpha^2 \beta^2 V_{1,1}) \phi_{1,1} - \beta^2 \phi_{2,1} - \alpha^2 \phi_{1,2}}{\alpha^2 \beta^2} \]

So instead of depending on the average of its four closest neighbours, the value of the wave function in this point now depends on the average of its two closest neighbouring points within the grid. Points on the sides, but not in the corners, depend on its three closest neighbours.

3.2.2 Neumann Boundary Condition

A Neumann boundary condition means that the derivative of the wave function is constant on the boundary. If this constant is chosen to zero, this represents a neutral connection to the outside, the wave function (for example, the electron) is neither repelled nor attracted to the surroundings. One problem with NBC is that it breaks the absolute probability density interpretation of \( |\phi|^2 \). Instead it has to be treated as relative probability. Applying NBC to (3.12) is as easy as applying...
DBC. The definition of the discrete derivative, obtained by inserting (3.3) into (3.6), can be seen in (3.18).

\[
\frac{\delta \phi}{\delta x} = \frac{\phi_{n+1,k} - \phi_{n-1,k}}{2\alpha}
\]

(3.18)

Now, let’s look at what the derivative looks like on the upper boundary of the grid, i.e. when \( n = 1 \).

\[
\frac{\delta \phi_1}{\delta x} = \frac{\phi_{2,k} - \phi_{0,k}}{2\alpha}
\]

(3.19)

The term \( \phi_{2,k} \) is inside the grid, and should not be defined. The term \( \phi_{0,k} \), however, is just outside the grid and can be used to manipulate the derivative on the boundary. Trivially, choosing \( \phi_{2,k} = \phi_{0,k} \) will make the derivative zero. By doing the same study on all boundaries, the definitions (3.20), (3.21), (3.22) and (3.23) can be made in order to apply NBC to (3.12).

\[
\phi_{0,k} = \phi_{2,k}
\]

(3.20)

\[
\phi_{N+1,k} = \phi_{N-1,k}
\]

(3.21)

\[
\phi_{n,0} = \phi_{n,2}
\]

(3.22)

\[
\phi_{n,K+1} = \phi_{n,K-1}
\]

(3.23)

Let’s look at the equation corresponding to \( \phi_{1,1} \) once more, but with Neumann instead of Dirichlet boundary condition (compare with (3.17)). The left hand side of (3.12) corresponding to this point becomes (3.24).

\[
\frac{\alpha^2 \beta^2}{2(\alpha^2 + \beta^2) + \alpha^2 \beta^2 V_{1,1}} \phi_{1,1} - \beta^2 \left( \phi_{2,1} + \phi_{0,k} \right) - \alpha^2 \left( \phi_{1,2} + \phi_{0,0} \right) = \frac{\alpha^2 \beta^2}{2(\alpha^2 + \beta^2) + \alpha^2 \beta^2 V_{1,1}} \phi_{1,1} - 2\beta^2 \phi_{2,1} - 2\alpha^2 \phi_{1,2}
\]

(3.24)

### 3.2.3 Similarities between NBC and DBC

As seen by comparing equations (3.17) and (3.24), the difference between applying DBC and NBC is very little, in fact there is only a different constant appearing in front of the \( \phi_{1,2} \) and \( \phi_{2,1} \) terms. This makes it very easy to switch boundary conditions, from a programming point of view. The two examples, (3.17) and (3.24), can be rewritten as a common expression (including the right hand side of the equation this time), (3.25).

\[
\frac{2(\alpha^2 + \beta^2) + \alpha^2 \beta^2 V_{1,1}}{\alpha^2 \beta^2} \phi_{1,1} - C\beta^2 \phi_{2,1} - C\alpha^2 \phi_{1,2} = E\phi_{1,1}
\]

(3.25)

Here, \( C = 1 \) means applying DBC, and \( C = 2 \) means applying NBC.
3.2.4 Mixed Boundary Conditions

The Neumann, Dirichlet or any other boundary conditions can be mixed and applied to different boundaries of the grid. For example, one may want a Neumann boundary condition on the left and right boundaries, and Dirichlet on the upper and lower boundaries. To do this, simply mix the different definitions as required. In this case, definitions (3.13), (3.14), (3.22) and (3.23) should be used. It’s possible to have different boundary conditions on different parts of the boundary, there are no limitations here. As long as all to the grid adjacent points are defined, the problem can be solved. One can have alternating NBC and DBC along each boundary (although the physical meaning of this is questionable at best), NBC on upper five grid points on the left and right side and DBC on the rest, or anything else that one may find appropriate in order to adapt to a certain problem.

3.3 The Matrix Eigenvalue Problem

After choosing a set of boundary conditions and applying them to the problem, it is fully defined. As will be seen in this section, the set of equations can easily be organized as a matrix eigenvalue problem which can be solved numerically.

3.3.1 Setting Up the Matrix

In order to arrange this problem as a matrix eigenvalue problem, it’s convenient to use one index instead of the two used so far (n and k). By inserting (3.4) into equation (3.12) it becomes:

\[
\frac{(2(\alpha^2 + \beta^2) + \alpha^2 \beta^2 V_s)\phi_n - \beta^2(\phi_{n+N} + \phi_{n-N}) - \alpha^2(\phi_{n+1} + \phi_{n-1})}{\alpha^2 \beta^2} = E\phi_n \quad (3.26)
\]

This can easily be arranged as a matrix eigenvalue problem, as in (3.27).

\[
H \begin{pmatrix}
\phi_1 \\
\phi_2 \\
\vdots \\
\phi_{K-N}
\end{pmatrix} = E \begin{pmatrix}
\phi_1 \\
\phi_2 \\
\vdots \\
\phi_{K-N}
\end{pmatrix} \quad (3.27)
\]

Here, H has a rather interesting form, with some variations depending on boundary conditions. For example, let’s look at an example featuring DBC, a grid of size $4 \times 4$ ($N = K = 4$) with a potential $V = 4$ along the boundary, and $\alpha = \beta = 1$. The resulting matrix can be seen in Figure 3.4. To understand how this matrix is generated, let’s have a look at the first row. This row corresponds to the top left corner point, $n = k = 1 \leftrightarrow s = 1$ that has been studied before (DBC in (3.17) and NBC in (3.24)). In this case there’s a DBC, so the constants defined above inserted into (3.17) give (3.28).

\[
8\phi_1 - \phi_2 - \phi_5 = E\phi_1 \quad (3.28)
\]

This means that on row 1 in the matrix, there should be an 8 in column 1, and -1 in column 2 and 5. This is seen in Figure 3.4. Luckily, the matrix elements follow certain
patterns which make the matrix fairly easy to construct for an arbitrary NxK grid. The matrix changes slightly when applying Neumann boundary condition, as seen in figure 3.5. As pointed out in a previous section, the equations for NBC and DBC differ only by a constant that appears in front of the "neighbours". This time the equation on the first line becomes

$$8\phi_1 - 2\phi_2 - 2\phi_5 = E\phi_1$$  \hspace{1cm} (3.29)

This means that there is value -2 in columns 2 and 5, instead of -1 like it was for the DBC case. As expected, the rows 6, 7, 10 and 11 are identical in the NBC and the DBC case, the corresponding grid points are not on the boundary of the grid.
3.3 The Matrix Eigenvalue Problem

With the matrix set up, all that is left is to let a computer solve the eigenvalue problem. Matlab and many other software packages have built in routines for this.

3.3.2 Normalization

One has to be careful with the normalization of the eigenfunctions. In most cases the software normalizes the eigenfunction as if it was a vector in an ON-base, $\phi^\dagger \phi = 1$. However, the criteria for normalization is seen in equation (3.30), where $\alpha\beta$ is the area element corresponding to each grid point. Therefore the eigenfunctions often needs to be multiplied by a factor $\frac{1}{\sqrt{\alpha\beta}}$ in order to be normalized properly.

$$\alpha\beta \cdot \sum_{n,k} \phi^*_n \phi_{n,k} = \alpha\beta (\phi^\dagger \phi) = 1$$  \hspace{1cm} (3.30)
Finite Difference Method
Chapter 4

Imaginary Potential

As seen in the previous section, the solution to the Schrödinger equation depends on the potential and on boundary conditions. So far the potentials have been assumed to be real, but what about an imaginary potential? Does it have any physical relevance? As it turns out, an imaginary potential acts as source and drain in the cavity. This means that there is a resulting net current running through the cavity. As will be seen, this net current often starts internal currents in the cavity, creating vortices which do not contribute to the net flow.

Figure 4.1. A two dimensional cavity of size 11.109Åx11.638Å
4.1 Currents

Let’s study a solutions to the Schrödinger equation in a non-symmetrical cavity with a complex source and drain (constant positive imaginary part on the left hand side and constant negative imaginary part on the right hand side). This imaginary part is chosen to be $V_i = 1.34 \text{[eV]}$. The cavity, seen in figure 4.1, has been chosen similar to the one used in experiments [5][6][4]. These experiments are done at macroscopic level, but the solutions we obtain here can easily be rescaled and translated into microwaves using equation (2.4). The grid has been adjusted so that each grid point coincides with one experimental sample point. After the eigenvalue problem has been solved, the probability density current, $S$, can be calculated according to (2.7).

$|\phi|^2$, and $|S|$ for energy eigenvalue $(27.43 - 0.008i)$ [eV] can be seen in figures 4.2 and 4.3. As you can see, $|S|$ takes rather interesting form. Many vortices are created throughout the cavity. However, there seems to be a problem with the net flow through the cavity. The output (right hand side) seems much larger than the input. This clearly violates what a steady state stands for. This problem is linked to the imaginary part of the eigenvalue, and will be studied further in the next section.

4.2 Conservation of Probability Density

Recall the expression for the continuity equation, integrated over the region $A$, (2.10). For stationary states the left hand side of this equation is required to be zero, otherwise the probability density grows or shrinks over time, violating what a stationary state stands for. If $A$ is the two dimensional grid, then the first term on the right hand side (containing $S_n$) corresponds to the flow into the grid from outside. Since this is zero (at least for NBC and DBC), the only remaining term is the integral containing the imaginary potential. Now, let’s look at a wave of the form $\Phi^m(r,t) = \phi^m(\mathbf{r}) T^m(t)$ where the $m$ denotes a certain state. By inserting this into equation (2.10) it becomes (4.1)

$$\int_V |\phi^m(\mathbf{r})|^2 dV \cdot \frac{\delta |T^m(t)|^2}{\delta t} = \frac{2}{\hbar} \int_V V_i(\mathbf{r}) |\phi^m(\mathbf{r})|^2 dV \cdot |T^m(t)|^2 \quad (4.1)$$

If $\phi^m(\mathbf{r})$ is properly normalized, this first order differential equation in time has a solution of exponential form seen in (4.2).

$$|T^m(t)|^2 \propto e^{\frac{2}{\hbar} \int_V V_i(\mathbf{r}) |\phi^m(\mathbf{r})|^2 dV \cdot t} = e^{\frac{2}{\hbar} \langle m | V_i | m \rangle \cdot t} = e^{I^m \cdot t} \quad (4.2)$$

This means that for positive $\langle m | V_i | m \rangle$ the wave function grows exponentially larger over time, and for negative it grows exponentially smaller. The condition for conservation of probability for state $m$ is then (4.3).

$$I^m = \frac{2}{\hbar} \int_V V_i(\mathbf{r}) |\phi^m(\mathbf{r})|^2 dV = 0 \quad (4.3)$$
4.2 Conservation of Probability Density

Figure 4.2. $|\phi|^2$ for $E=(27.43 - 0.008i)$ [eV]

Figure 4.3. The absolute value of the probability density current, $|S|$, for $E=(27.43 - 0.008i)$ [eV]
The problem with this condition is that $\phi(r)$ must be known in order to choose a suitably $V_i(r)$. Also, even if this condition holds for one state, it does not mean it is does for other states; $I$ varies for different energies. For symmetrical problems however, this condition is easy to meet, at least if $V_i(r)$ is sufficiently small to only have a minor impact on $|\phi(r)|^2$. Since the wave functions in these systems are symmetrical or anti-symmetrical, the probability density, $|\phi(r)|^2$ is symmetrical. Thus, choosing an anti-symmetrical imaginary potential is enough to satisfy (4.3).

For non-symmetrical problems one must either aim on single states (first solving the equations without imaginary potential, then choosing a state, balance the imaginary potential with respect to this state and then re-solve using the balanced potential), or use complementary methods such as perturbation theory. A pure FDM-solution is only useful for real systems, or complex systems with symmetrical real part-potential. Of course one can find certain states where the input and output actually add up to zero, but full solutions will generally not be obtained.

### 4.3 Perturbation Theory

Perturbation theory is used to slightly change initial conditions without forcing a full re-calculation of a problem. In this case the solution to the Schrödinger equation in a real potential is easily obtained using the previously described method. The imaginary potential acting as source and drain is treated as a perturbation of the original system. The equation describing the perturbed system is

$$ (H_0 + iV_i)\phi^m = E^m \phi^m $$

(4.4)

where $H_0$ is the Hamiltonian of the real system, for which the solution is already known, $H_0\phi^m_0 = E^m_0 \phi^m_0$. $V_i$ is the imaginary part of the potential, the perturbation. Now, seek a solution of the form $E^m = E^m_0 + E^m$ and $\phi^m = \phi^m_0 + \phi^m$. For simplicity, let’s look at first order solutions ($E^m = E^m_0$, $\phi^m = \phi^m_0$) and expand $\phi^m_1$ in a base orthogonal to $\phi^m_0$, according to (4.5)

$$ \phi^m_1 = \sum_{n, n \neq m} a^n_0 \phi^n_0 $$

(4.5)

The solution to (4.4) is seen in equations (4.6) and (4.7).

$$ E^m = E^m_0 + i \langle m|V_i|m \rangle $$

(4.6)

$$ \phi^m = \phi^m_0 + \sum_{n, n \neq m} \frac{i \langle n|V_i|m \rangle}{E^m_0 - E^n_0} \phi^n_0 $$

(4.7)

Note that the correction term to the energy eigenvalue is purely imaginary as long as the unperturbed eigenfunctions are real. In the previous section where we found a condition for the conservation of probability, (4.3). Compare this with the expression for the perturbed energy, (4.6). As it turns out, the condition for conservation of the probability density is that the imaginary part of the eigenvalue
is zero, at least for first order perturbation theory. This can also be found by studying the time evolution of a stationary state with complex eigenvalue, seen in equation (4.8).

\[ \phi(t, \mathbf{r}) = \phi(\mathbf{r}) e^{-i \frac{E_m}{\hbar} t} \]  

For \( E^m = E^m_r + i E^m_i = E^m_0 + i \langle m| V_i |m \rangle \), the square of the absolute value of this expression becomes (4.9).

\[ |\phi(t, \mathbf{r})|^2 \propto \left( e^{E_i/\hbar} t \right)^2 = e^{2E_i/\hbar} \langle m| V_i |m \rangle \cdot t \]  

If the complex part of the eigenvalue is positive, the wave function grows exponentially stronger over time, and exponentially weaker for a negative eigenvalue. This is exactly what was found previously in (4.2) without using perturbation theory. This correspondance is important because it validates the use of first order perturbation theory. Also, this is a interesting expression because this lets us investigate the credibility of the wave functions obtained using full FDM solutions, simply by looking at the eigenvalues. The larger the imaginary part is, the less stationary it is. A very small imaginary part means that the system can remain under control for some time, while eigenvalues with large imaginary part causes the system to explode instantly. This conclusion is supported by the results obtained in figure 4.3. The imaginary part of the eigenvalue corresponding to this state is negative (and apparently pretty large in magnitude), creating a decaying wave function.

### 4.4 Balanced Imaginary Potential

Since the unperturbed wave functions are known, it is quite easy to fulfill condition (4.3) when \( V_i \) can be chosen freely. This can be done in many ways, and one way to do so is to first divide the imaginary potential into two parts, one positive and one negative according to \( V_i = V_+ - V_- \). Now, for each state \( m \), calculate the integrals (4.10) and (4.11).

\[ \int V_+ (\mathbf{r}) |\phi_0^m (\mathbf{r})|^2 dV \]  

and

\[ \int V_- (\mathbf{r}) |\phi_0^m (\mathbf{r})|^2 dV \]  

Here \( I \) is the input integral and \( O \) is the output integral. In a balanced situation, these two integrals are equal. Generally they are not however, and in order to balance them, replace \( V_i \) by \( V_i^m = V_+ - \frac{I^m}{O^m} V_- \). By doing this, the output is scaled to fit the current flowing into the system, ensuring a steady state. Note that the imaginary potential now depends on which state is being treated ("perturbed"). This means that the potential will be different for different states. This kind of balancing cannot be done while running full solutions because the potential cannot depend on the eigenfunctions, before they are known!
4.4.1 Verification of the Balanced Potential Method

Let’s study the same state as before (in the section called “Currents”), but this time with a balanced potential. By solving the integrals 4.10 and 4.11, the balancing factor is found to be 0.033. This means that the output from the system is made about thirty times weaker than it was previously. The new solution, obtained by perturbation of 1439 states, can be seen in figures 4.4 and 4.5. This time there is no visible unbalance between input and output. The eigenvalue becomes $(27.43 - 10^{-19}i)$ [eV], so the imaginary part of the eigenvalue is about $10^{-17}$ times smaller than it previously was. This small imaginary part is merely a calculation error, so the eigenvalue can be treated as real. This means that the state acquired with a balanced potential is much more resilient to time evolution, the wave function does not decay at all.
4.4 Balanced Imaginary Potential

Figure 4.4. $|\phi|^2$ for $E = 27.43$ [eV]

Figure 4.5. The absolute value of the probability density current, $|S|$, for $E = 27.43$ [eV]
4.5 Interaction between Wave Functions

We have noticed an interesting phenomena when increasing the imaginary potential \((V_i)\), i.e. increasing the strength of the input and output. As seen in figure 4.6, the two eigenfrequencies \(f_{28}\) and \(f_{29}\) between 5.5 and 5.6 [GHz] approach each other for increased \(V_i\), and become degenerate for some \(V_i = V_{bp}\). For larger \(V_i\) they separate again. Also the corresponding wave functions (or eigenfunctions), \(\phi_{28}\) and \(\phi_{29}\) show very interesting behavior when increasing \(V_i\). The case \(V_i = 0\) can be seen in figure 4.7. Here, the wave functions are real, just as expected. What’s interesting is what happens when the antennas are introduced. The case \(V_i = \pi^2 \cdot 0.05 [cm^{-2}]\) is seen in figure 4.8. This time the eigenfunctions have both real and imaginary part. The real parts are about the same as in the case \(V_i = 0\), but the wave functions seem to have picked each other up as imaginary part! Note that the absolute value of the real and imaginary part are being shown in order to make the mixing more clear. The mixing terms have to appear with different sign as can be found by studying perturbation theory; \(E_0^m - E_0^n\) changes sign depending on which wave function is being perturbed. The magnitude of these imaginary influences grows with \(V_i\), and in the region when the solutions separate again the two wave functions become almost purely imaginary, as seen in figure 4.9. This interaction between wave functions can be predicted by looking at perturbation theory. If we look at expression for the perturbed wave function, 4.14, we see that

**Figure 4.6.** Merging and splitting of energy levels as the imaginary potential grows in magnitude. The dots on the left hand sides are the energies for \(V_i = 0\), and the stars on the right hand side are the energies corresponding to a closed system, when \(V_i\) is replaced by a real potential \(V \rightarrow \infty\).
4.5 Interaction between Wave Functions

the correcting term \( \phi_{corr} \) is (4.12).

\[
\phi_{corr} = \sum_{n,n \neq m} \frac{i\langle n|V|m\rangle}{E^m - E^n} \phi_0^m
\]  (4.12)

This means that the change of wave function with increase \( V_i \) is a purely imaginary superposition of all other wave functions. We see that the more the energy levels are separated, the weaker is this interaction. \( f_{28} \) and \( f_{29} \) are indeed very close, which is one explanation why they interact so strongly. It’s worth noting that by studying equation (4.12) we find that the only interaction possible is between wave functions with opposite symmetry; symmetrical wave functions only interact with anti-symmetrical wave functions. No matter how close two states are, they will never interact if they share symmetry. Granted, perturbation theory should only be used to slightly change initial conditions, but to get a feeling for how things work it is still a good method. In the degenerate region, it seems like the wave functions \( \phi_{28,\text{deg}} \) and \( \phi_{29,\text{deg}} \) are a roughly a linear combination of the original states. The case when each wave appears with equal strength is seen in equations (4.13) and (4.14).

\[
\phi_{28,\text{deg}} \approx \frac{1}{\sqrt{2}} (\phi_{28} - i\phi_{29}) \quad (4.13)
\]

\[
\phi_{29,\text{deg}} \approx \frac{1}{\sqrt{2}} (\phi_{29} + i\phi_{28}) \quad (4.14)
\]

This means that \( \phi_{28,\text{deg}} \) and \( \phi_{29,\text{deg}} \) are almost linearly dependent according to equation (4.15).

\[
\phi_{29,\text{deg}} \approx i\phi_{28,\text{deg}} \quad (4.15)
\]

The phenomena of mixing of wave functions and energy level crossings are studied in detail in several articles, for example in \[10\][11][12].
Figure 4.7. The different parts of wave functions $\phi_{28}$ and $\phi_{29}$ for $V_i = 0$

Figure 4.8. The different parts of wave functions $\phi_{28}$ and $\phi_{29}$ for $V_i = 0.05 \cdot \pi^2 [cm^{-2}]$
Figure 4.9. The different parts of wave functions $\phi_{28}$ and $\phi_{29}$ for $V_i = 10 \cdot \pi^2 [cm^{-2}]$
Chapter 5

Accuracy

Like all other numerical methods, FDM needs to be evaluated in order to make sure that the solutions are credible. The best way to do this is to compare solutions acquired by FDM calculations with known theoretical solutions. Here, let’s focus on solutions to the Helmholtz equation, \([\Delta + k^2] \phi = 0\), rather than the Schrödinger equation. There are very few potentials where solutions to the Helmholtz equation can be found without using numerical methods, but one such potential is a rectangular potential.

5.1 Theoretical Solution

The solution to the Helmholtz equation in a hard wall ("infinite potential") two dimensional rectangular well (see figure 5.1) is known to be (5.1) and (5.2) (Normalized wave function).

\[
k^2 = \pi^2 \left( \frac{n}{W_x} \right)^2 + \left( \frac{m}{W_y} \right)^2
\]

(5.1)

\[
\phi^{m,n}(x,y) = \sqrt{\frac{4}{W_x W_y}} \sin \left( \frac{n \pi x}{W_x} \right) \sin \left( \frac{m \pi y}{W_y} \right)
\]

(5.2)

5.2 Numerically Obtained Eigenvalues

Let’s study the accuracy of the eigenvalue, \(k^2\), found using FDM. The size of the box is chosen to be \(W_x = W_y = 1\) [cm]. The dimension is of course completely arbitrary, the solutions can be rescaled to fit any square potential. The accuracy of the FDM calculations depend on the roughness on the grid, a more dense grid certainly makes the solutions more accurate. Let’s have a look at solutions to the Helmholtz equation in this cavity for three different grid qualities, \(30 \times 30\), \(50 \times 50\) and \(80 \times 80\) grid points. The different \(k^2\) obtained for these grids qualities, and the theoretical eigenvalues, are seen in figure 5.2. As we can see, all of these grids
provide accurate results for low energies, but for higher energies the density of the
grid plays a big role. For a more detailed view of how fast the solutions diverge,
see the relative error $k_2^{\text{numerical}} / k_2^{\text{theoretical}}$. The initial error is 0.1% for the $30 \times 30$ grid,
0.03% for the $50 \times 50$ grid and 0.01% for the $80 \times 80$ grid. The error grows in a
linear fashion until about half the eigenvalues are obtained.

In order to reach some kind of general test of confidence, let’s compare the
wavelength $\lambda = \frac{2\pi}{k}$ to the grid spacing at different accuracy levels. Table 5.1 shows
the different breakpoints for accuracy 90% and 80%. Here, $n_P$ is the number of
the highest eigenvalue with $P\%$ accuracy or better. The wavelength corresponding
to these eigenvalues are denoted $\lambda_P$ and $a$ is the grid spacing. What’s interesting
here is the ratio between the different $\lambda$ and $a$. Roughly, 90% or better accuracy
is held for $\lambda > 5.2a$ and 80% accuracy is held for $\lambda > 3.8a$. This is a good rule of
thumb when working on other cavities.

![Figure 5.1. A two dimensional hard wall potential well.](image-url)

<table>
<thead>
<tr>
<th>Grid</th>
<th>$n_{90}$</th>
<th>$n_{80}$</th>
<th>$\lambda_{90}[cm]$</th>
<th>$\lambda_{80}[cm]$</th>
<th>$a[cm]$</th>
<th>$\frac{\lambda_{90}}{a}$</th>
<th>$\frac{\lambda_{80}}{a}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$30 \times 30$</td>
<td>108</td>
<td>216</td>
<td>0.172</td>
<td>0.130</td>
<td>$\frac{\pi}{2}$</td>
<td>4.994</td>
<td>3.776</td>
</tr>
<tr>
<td>$50 \times 50$</td>
<td>306</td>
<td>626</td>
<td>0.100</td>
<td>0.077</td>
<td>$\frac{\pi}{2}$</td>
<td>5.084</td>
<td>3.792</td>
</tr>
<tr>
<td>$80 \times 80$</td>
<td>794</td>
<td>1656</td>
<td>0.065</td>
<td>0.048</td>
<td>$\frac{\pi}{2}$</td>
<td>5.139</td>
<td>3.793</td>
</tr>
</tbody>
</table>

Table 5.1. A table over the accuracy breakpoints.
5.2 Numerically Obtained Eigenvalues

Figure 5.2. The theoretically and numerically obtained eigenvalues.

Figure 5.3. The relative error of the numerically obtained eigenvalues.
5.3 Numerically Obtained Eigenfunctions

When studying the eigenfunctions (wave functions), it’s convenient to chose a slightly different cavity. This time, \( W_x = \sqrt{2} - 0.3 \) and \( W_y = 1 [\text{cm}] \). The reasoning behind this choice of dimension is that the well is almost square, and still has an irrational relation between the length and the width. This means that there are no degeneracies in the solution, which is convenient when comparing the wave functions to each other.

As a measure of accuracy, the integral (5.3) can be used to compare the theoretical eigenfunctions with the ones obtained numerically using FDM. Here \( \phi^m_t \) is the theoretical solution and \( \phi^m_n \) is the numerical solution. Smaller \( \Delta \) means better accuracy, and \( \Delta = 0 \) means exact agreement between the theoretical and the numerical solutions.

\[
\Delta^m = \int_A ||\phi^m_t|| - ||\phi^m_n|| dA 
\]

(5.3)

The solution to this integral for solutions obtained from an \( 80 \times 80 \) grid can be seen in figure 5.4. As seen in this graph, the error is very small even for higher energies (The integral of \( |\phi^m_t|^2 \) is of the order of \( 1 \)). The eigenfunction solutions are very stable, even if the eigenvalue has some error. The “spikes” seen in the graphs come from eigenfunctions that have almost degenerated eigenvalues. The closer to de-generated the eigenvalues are, the harder it is for the solver to separate the solutions from each other. Another problem that is not seen in these graphs is that the eigenfunctions switch positions as the energy goes up. The theoretical eigenfunction number 80 may very well be eigenfunction number 81 or 79 numerically, so the solutions are shuffled somewhat (This was accounted for when calculating the \( \Delta \) seen in the graphs.).

5.4 Perturbation Theory

There is no in-detail study of the accuracy of perturbation theory here, just a few pointers. The accuracy of perturbation theory depends mainly on two things; the size of the perturbing potential and the number of eigenfunctions in the sum of the perturbing term, \( t_n \). If the perturbing potential is too large, it can no longer be treated as a small change of initial conditions to the problem. Using higher order perturbation theory can somewhat compensate for this. Also, if the number of perturbing eigenfunctions is too small, \( \phi^m_t \) cannot be described accurately.
Figure 5.4. $\Delta m$ as a function of m for 80x80 grid.
Accuracy
Chapter 6

Complexity

As most numerical methods, FDM is limited by its time and data complexities as the grid grows in density. This chapter treats different methods to reduce the complexity, and to deal with problems that can occur when the data complexity grows too big.

6.1 Data Complexity

Full matrices are the standard way of storing matrices in the computer’s memory. Each field is stored separately and with a set accuracy, even if many elements share the same value. When using full matrices, the size of the Hamiltonian can be a problem for large grids. A grid consisting of \( n \) grid points results in a Hamiltonian of size \( nxn \). In Matlab, each matrix element takes up between 1 and 8 bytes of memory, and another 1 to 8 bytes if an imaginary part is used (even if only a single element has an imaginary part). This means that a \( 80 \times 80 \) grid with 16 byte representation (8 byte from the real part and 8 byte from the imaginary part) results in a \( 6400 \times 6400 \) matrix which has a data size of about 625 MB. A \( 160 \times 160 \) grid results in a \( 25600 \times 25600 \) matrix which is about 10 GB of data. This amount of data can rarely be handled by the RAM of normal desktop computers (as of 2008), which slows the calculations down a great deal. The calculations are already demanding, so this puts a limit on what matrices can be used in FDM. Since the Hamiltonian is mostly populated by zero elements, it can be convenient to use a sparse matrix notation to store it. Sparse matrices only save each non-zero value and its coordinate. On average there is close to 5 non-zero elements per row in the Hamiltonian. This means that for a Hamiltonian of size \( n \times n \) there are \( 5 \cdot n \) non-zero elements. Clearly, it is convenient to store \( 5 \cdot n \) instead of all \( n^2 \) elements. For the \( 80 \times 80 \) grid discussed earlier, the data size of the (real) Hamiltonian is reduced from about 320MB (real valued Hamiltonian) to 422kB, a reduction by about 99.9%. Sparse matrices should be used whenever memory is the issue.
6.2 Time Complexity

Theoretically, all problems can be solved as long as sufficient memory is available. However, the time complexity plays a big role for practical reasons. Therefore it’s important to investigate the time complexity of the methods used. For FDM, the complexity depends on if sparse or full matrices are used, and on the size of the grid. Let’s assume that the time complexity $t$ is of the type $t \propto A \cdot n^c$, where $c$ and $A$ are real constants depending on which method is used and $n$ is the number of grid points. The proportionality relation depends on the calculation power of the computer used. By running tests in Matlab using the built-in eigenvalue solvers for sparse and full matrices, the time complexity can be seen plotted against the number of grid points in figure 6.1. As seen, the sparse matrix solver is considerably slower. By running fitting tests, $c$ can be found, and also the relation between $A_{\text{sparse}}$ and $A_{\text{full}}$. These tests have found that $c_{\text{sparse}} = 3.26$ and $c_{\text{full}} = 3.11$. Also the relation between $A_{\text{sparse}}$ and $A_{\text{full}}$ is found to be $\frac{A_{\text{sparse}}}{A_{\text{full}}} = 2.43$. This means that the expressions for the time complexities are as seen in equations (6.1) and (6.2). Here $T$ is some constant depending on the computer’s calculation power (but independent on which matrix representation is used). These functions are also seen plotted in figure 6.1. The difference between the two exponents, $c_{\text{sparse}}$ and $c_{\text{full}}$ may seem small, but it has a huge impact for large $n$, as seen in this figure.

$$t_{\text{sparse}} = T \cdot 2.43 \cdot n^{3.26} \quad (6.1)$$

$$t_{\text{full}} = T \cdot n^{3.11} \quad (6.2)$$

6.3 Exclusion of High Potential Grid Points

Grid points with a high potential cause the wave function to shrink rapidly toward zero. In order to save calculation time, the wave function can be approximated to zero in grid points with a potential higher than a certain threshold. By doing this, grid points are removed from the eigenvalue problem, causing it to decrease in complexity. This method is very useful in cavities similar to the one used in chapter 3 (see figure 4.1). In this cavity, about one third of the points have a high potential. This means that the time complexity can reduced to about 25% when using a sparse matrix, and to about 30% when using a full matrix, by excluding high potential grid points. This method can be implemented in different ways. It can be taken into account when building the Hamiltonian in the first place, but there is another way which is a bit easier. When a point is assumed to be zero, all reference to this point is also zero. This means that if the wave function in gridpoint number $n$ is zero, column number $n$ can also be treated as zero. Also there is no need to solve the equation on line number $n$, as the solution to this equation is already known to be zero. This is the same as completely removing row and column $n$ from the matrix. When there are many high potential grid points, this shrinks the matrix considerably. Let’s return to the example in figure 3.4 but with a potential $V = 1000$ instead of $V = 4$ on the boundary. In order
to exclude these high potential grid points, rows and columns 1 to 5, 8 to 9 and 12 to 16 must be removed. The result is a 4 × 4 matrix, seen in figure 6.2. This is the same matrix that is obtained using a 2 × 2 grid of a hard wall potential. Now, let’s look at the eigenvalues obtained using this method. The eigenvalues for the full matrix, $E_{full}$, and the eigenvalues for the simplified matrix, $E_{simp}$ are seen in table 6.1. The error is of the order 0.1%. The time complexity is reduced to about 1.3% for a full matrix solution, and to about 1.1% for a sparse matrix solution. This decrease in complexity certainly makes up for the small error that has been introduced. Granted, the expressions for the time complexities (6.1) and (6.2) do not hold for such small matrices, but the decrease in complexity is great, no matter what. This method should always be used when simulating hard wall potentials in order to save time without affecting the results.

Table 6.1. Eigenvalues using the full matrix and using the reduced matrix.
6.4 Using Symmetry

For some cavities the time and data complexity can be greatly reduced by using symmetry. If a cavity is symmetrical, it can be cut into half along the symmetry line. Then two calculations are done on this half cavity, one with a Dirichlet boundary condition along the symmetry line, and one with a Neumann boundary condition (see figure 6.3). The solutions are then expanded as an odd function for Dirichlet, and an even function for Neumann (see figure 6.4). This effectively reduces a problem of time complexity $n^c$ (where $n$ is the number of grid points) into two problems with complexity $(\frac{n}{2})^c = 2^{-c}n^c$, for a total complexity $2^{1-c}n^c$. This is a reduction by a factor $2^{1-c}$, which is helpful as long as $c > 1$. For full matrix solutions $c_{\text{full}} \approx 3.11$ and for sparse matrices $c_{\text{sparse}} \approx 3.26$. This means that calculation time is reduced to about 21% when using a sparse matrix notation, and 23% when using a full matrix notation. Cavities may have more than one symmetry line, and these problems can be reduced even further. Generally, if a problem can be divided into $k$ parts because of symmetry, the solution time required is reduced to $k^{1-c}$ times the full solution time.

![Figure 6.3. The problem is divided into two parts, one with a Dirichlet boundary condition and one with a Neumann boundary condition.](image)
6.4 Using Symmetry

Figure 6.4. The full solution is obtained by expanding the functions obtained in half the cavity.
Chapter 7

Statistical Distributions

Chaotic quantum systems (and their equivalents) have been shown to follow certain statistical distributions regarding amplitude ($\phi$) [1], Area scaled density ($\rho = A|\phi|^2$) [2], currents ($j, j_\alpha$) [3] and stress tensor components ($T_{xx}$ and $T_{xy}$) [4]. These distributions are derived from an assumption that in each point the wave function can be described as a random superposition of monochromatic plane waves, as long as the point is sufficiently far from the boundary. In this chapter we will study the distributions of the densities, currents and stress tensor components for wave functions that are closed and open to the surroundings. As a measure of openness the parameter $\epsilon$ is used. $\epsilon \rightarrow 1$ means that the cavity is open and $\epsilon \rightarrow 0$ means that the cavity is closed. This parameter is calculated according to equation (7.1).

$$\epsilon = \sqrt{\frac{q^2}{p^2}}$$  (7.1)

Here, the wave function $\phi(\vec{r}) = p(\vec{r}) + iq(\vec{r})$ has been adjusted by some phase factor so that $q$ and $p$ are statistically uncorrelated, i.e. $\langle pq \rangle = 0$, and also $0 \leq \epsilon \leq 1$ [7]. Here we will focus on the cavity seen in figure 7.1 because it is similar to a cavity used in microwave experiments [1][2][3]. The dents on the sides of the cavity are there to prevent so called bouncing modes, which bring some order to the system. The grid used in the FDM model has been chosen so that the grid points coincide with the sample points in the experiments. We will restrict ourselves to a symmetrical cavity in order to do a full solution rather than using perturbation theory. Even if the experimental cavity is non-symmetrical, we believe that this has no major influence on the distributions obtained.
7.1 Density Distributions

The statistical distribution of the density, $|\phi|^2$, has been shown to be under the assumptions of a random superposition of plane waves. Here, $I_0$ is the modified Bessel function of zeroth order.

$$P(\rho, \epsilon) = \mu e^{(-\mu^2 \rho)} I_0(\mu \nu \rho)$$  \hspace{1cm} (7.2)

$$\mu = \frac{1}{2} \left( \frac{1}{\epsilon} + \epsilon \right) \quad , \quad \nu = \frac{1}{2} \left( \frac{1}{\epsilon} - \epsilon \right)$$

In the limit $\epsilon \to 0$ this expression becomes the Porter-Thomas distribution, which is the density distribution of wave function that is invariant under time reversal and that can be chosen real.

$$P(\rho) = \frac{1}{\sqrt{2\pi\rho}} e^{-\frac{\rho}{2}}$$  \hspace{1cm} (7.3)

On the other hand, in the limit $\epsilon \to 1$ (Time symmetry broken, $\phi$ must be complex), becomes the Rayleigh distribution.

$$P(\rho) = e^{-\rho}$$  \hspace{1cm} (7.4)

As seen in equation (7.4), the Porter-Thomas distribution is singular in $\rho = 0$, while the Rayleigh distribution is not. This is not strange at all.
7.1 Density Distributions

$|\phi|^2 = p^2$, thus only $p$ needs be zero in order to get a zero density. This occurs along nodal lines. In the complex case however, $|\phi|^2 = p^2 + q^2$. Now both the independent variables $p$ and $q$ must take value zero in order $|\phi|^2$ to be zero. This happens in points, the intersections between the nodal lines belonging to $p$ and $q$. For a completely chaotic case, $p^2$ and $q^2$ can be seen as individually following the Porter-Thomas distribution (if rescaled properly), and the sum $|\phi|^2 = p^2 + q^2$ following the Rayleigh distribution.

7.1.1 Numerically Obtained Density Distributions

The numerically obtained density distributions for eigenfrequencies 9.78 and 8.60 [GHz], corresponding to $\epsilon = 0.14$ and $\epsilon = 0.77$ can be seen in figure 7.2. Here, a sample of 1472 interior grid points (see figure 7.1) has been used. These graphs clearly show the transitions from an, in practice, closed system (following the Porter-Thomas distribution) to an open system (following the Rayleigh distribution). The reason why not all points are treated is that we want to avoid boundary effects, the theory states that the random superposition of plane waves only applies to points sufficiently far from the boundary. Also, we need to avoid the symmetry line along the central axis of the cavity, because some solutions are anti-symmetrical with respect to this axis. This forces the amplitudes to zero near the center of the cavity, effectively working as an invisible boundary. For a more detailed view on the density distributions (more than 1472 sample points), we need to look at a distribution over many eigenfunctions with similar energy. These distributions can be seen in the appendix for frequencies 4.80-5.92, 15.20-16.01 and 30.85-31.15 [GHz] in figures A.5, A.6 and A.7 correspondingly. What can be seen here is a slight dependence on energy, but the overall results are very good.
Figure 7.2. The numerically obtained density distribution (solid line) and the theoretically obtained distribution (dashed line). Top: The density distribution for frequency 9.78 [GHz], $\epsilon = 0.20$. Bottom: The density distribution for frequency 8.60 [GHz], $\epsilon = 0.77$. 
7.2 Current Distributions

Just like the density, the current flowing in the cavity follows certain statistical distributions. Also these distributions have been derived using the random superposition of monochrome plane waves approach \[7\]. Here we will study the distribution of \( j_\alpha \) and \( j = \langle j \rangle \). Theoretically, these quantities follow the distributions given in equations (7.6) and (7.5), where \( K \) is the modified Bessel function of the second kind. The distribution of the current components (for example \( j_x \) and \( j_y \)) is completely isotropic in theory, the current is not biased toward any direction.

\[
P(j_\alpha) = \frac{1}{\sqrt{2\langle j_\alpha^2 \rangle}} e^{-\frac{2\langle j_\alpha^2 \rangle}{\langle j_\alpha^2 \rangle}}
\]

(7.5)

\[
P(j) = \frac{4j}{\langle j^2 \rangle} K_0 \left( 2 \frac{j}{\sqrt{\langle j^2 \rangle}} \right)
\]

(7.6)

Here it is interesting to note that \( j \to 0 \Rightarrow P(j) \to 0 \). This means that the probability to find a zero current in a point is zero. There is a current flowing everywhere in the cavity, with the exception of some infinitesimally small areas (i.e. points). These points are the centers of the vortices created throughout the cavity. (For sample pictures, see Appendix A.1).

7.2.1 Numerically Obtained Current Distributions

The numerically obtained current distributions for eigenfrequencies \( f = 4.80 \) and \( f = 29.33 \) [GHz] can be seen in figures 7.3 and 7.4. Again, only the part of the cavity used in the previous section has been used for sampling. There is a clear difference between these distributions; the low energy solution shows very poor agreement with theory, while the higher energy solution shows a much more isotropic behavior. In order to get a more detailed view of the effect of this net current we need to look at a combined distribution over different eigenfunctions. Five such graphs have been put in the appendix A.3. These graphs show the different current distributions for different frequency ranges (4.80-5.92, 9.95-10.50, 15.20-16.01, 20.86-21.44 and 30.85-31.15 [GHz]). By comparing these plots we come to the conclusion that the frequency is the most important factor regarding the coincidence with the theoretically predicted distributions. The small shift in \( P(j_y) \) is an effect of the net current, an effect that seems negligible at least in the high energy region.
Figure 7.3. The numerical distributions (solid line) obtained for eigenfrequency 4.80 [GHz]. $\frac{\langle j^2 \rangle}{\langle j \rangle^2} = 0.178$. Also the theoretical distributions (dashed line). Top left: The distribution of $j_x\langle j \rangle$. Top right: A picture of $j$ in the sample area. Bottom left: The distribution of $j_x\sqrt{\langle j_x^2 \rangle}$. Bottom right: The distribution of $j_y\sqrt{\langle j_y^2 \rangle}$.
7.2 Current Distributions

Figure 7.4. The numerical distributions (solid line) obtained for eigenfrequency 29.33 [GHz]. $\frac{\langle j^2 \rangle}{\langle j \rangle} = 0.116$. Also the theoretical distributions (dashed line). Top left: The distribution of $\frac{j}{\langle j \rangle}$. Top right: A picture of $j$ in the sample area. Bottom left: The distribution of $\frac{j_x}{\sqrt{\langle j^2_x \rangle}}$. Bottom right: The distribution of $\frac{j_y}{\sqrt{\langle j^2_y \rangle}}$. 
7.3 Stress Tensor Distributions

Just like the previous quantities, the different components of the stress tensor, $T_{xx}$, $T_{yy}$ and $T_{xy}$ (see equation (2.9)) have been shown to follow certain distributions. Again, the distribution of these quantities have been derived using the approach of random waves. Just like for the current distributions, the distributions of the stress tensor components are isotropic, there is no preferred direction. Thus $T_{xx}$ and $T_{yy}$ follow the same distribution. Rather than some exponential function, the distribution of the stress tensor components is given as an integral, seen in equation (7.7).

$$P(T_{\alpha\beta}) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \theta_{\alpha\beta}(a)e^{-iaT_{\alpha\beta}} da$$  \hspace{1cm} (7.7)

Here, $\theta_{\alpha\beta}$ is the characteristic function for the different components. Because of symmetry, only two different $\theta_{\alpha\beta}$ are needed, one for $T_{xx}$ ($\theta_{xx}$) and one for $T_{xy}$ ($\theta_{xy}$). The expressions for these functions can be seen in equations (7.8) and (7.9) (These expressions have been corrected in the original article).

$$\theta_{xx}(a) = \frac{8}{\sqrt{(1 - ia)(1 - i\epsilon^2 a)[a - i(\sqrt{24} + 4)][\epsilon^2 a - i(\sqrt{24} + 4)]}} \cdot \frac{1}{\sqrt{[a + i(\sqrt{24} - 4)][\epsilon^2 a + i(\sqrt{24} - 4)]}}$$  \hspace{1cm} (7.8)

$$\theta_{xy}(a) = \frac{2}{\sqrt{[2 + (\frac{a}{2})^2][2 + (\frac{\epsilon^2 a}{2})^2][1 + (\frac{a}{2})^2][1 + (\frac{\epsilon^2 a}{2})^2]}}$$  \hspace{1cm} (7.9)

7.3.1 Numerically Obtained Stress Tensor Distributions

The numerically obtained stress tensor distributions for a low energy ($f = 7.318$ GHz) and high $\epsilon$ ($\epsilon \approx 0.93$) can be seen in figure 7.5. This is the lowest energy wave function with $\epsilon > 0.9$. This result displays very poor fitting to the theoretical distribution. Another numerically obtained distribution can be seen in figure 7.6. This is a wave function of similar $\epsilon$ value ($\epsilon \approx 0.94$) but a much higher frequency, $f = 28.17$ GHz. This time the results fit theory much better and the distributions certainly looks more isotropic. Several distributions over groups of states with similar energy have been put in the appendix (A.4). Each of these groups contain 11 states. The states have not been chosen using any selection other than that they have a similar frequency, and all the frequencies are in the region with predicted error less than 20% (As discussed in the "Accuracy" chapter). From these graphs we can clearly tell that the energy plays a big role regarding the agreement with the theoretical predictions.
7.3 Stress Tensor Distributions

Figure 7.5. The numerically obtained distributions of $T_{xx}$ (in units of $\langle T_{xx} \rangle$), $T_{yy}$ (in units of $\langle T_{yy} \rangle$) and $T_{xy}$ (in units of $\sqrt{\langle T_{xy}^2 \rangle}$) for frequency $f = 7.318$ [GHz], $\epsilon \approx 0.93$. *Top left:* The distribution of $T_{xx}$. *Top right:* The distribution of $T_{yy}$. *Bottom left:* The distribution of $T_{xy}$. *Bottom right:* The density, $|\phi|^2$. 
Figure 7.6. The numerically obtained distributions of $T_{xx}$ (in units of $\langle T_{xx} \rangle$), $T_{yy}$ (in units of $\langle T_{yy} \rangle$) and $T_{xy}$ (in units of $\sqrt{\langle T_{xy}^2 \rangle}$) for frequency $f = 28.169$ [GHz], $\epsilon \approx 0.94$. Top left: The distribution of $T_{xx}$. Top right: The distribution of $T_{yy}$. Bottom left: The distribution of $T_{xy}$. Bottom right: The density, $|\phi|^2$. 
Chapter 8
Conclusions and Future Work

This chapter presents the conclusions we have come to, both regarding the methods of modeling these systems, and regarding the different statistical distributions. Also some topics for future work are suggested.

8.1 The Method

The method of choice depends on the symmetry of the system that is being simulated. The full FDM solution is recommended for both symmetrical and non-symmetrical real problems and also for symmetrical complex problems. For non-symmetrical complex problems, perturbation theory is required to assure that the power input and output are consistent. Using FDM, 80% accuracy for $k^2$ (which means about 90% accuracy for the frequency) has been shown to hold for wavelengths larger than 3.8 times the grid spacing. 90% accuracy for $k^2$ (which means about 95% accuracy for the frequency) has been shown to hold for wavelengths larger than 5.2 times the grid spacing.

8.2 The Statistics

The density, $\rho$, has been shown to follow theory (based on the random wave approach) very good, with a slightly better result for higher energies. The different current distributions are mostly dependent on from what energy region the results are taken. Higher energy makes the distributions much more isotropic. There is always an effect of the net current, but this effect is dampened somewhat for higher energy. For the stress tensor components, it is the energy that is the most important factor. We find a perfect match between calculations and theory for high energies. For lower energies, the results are not very isotropic, there is a clear difference between $T_{xx}$ and $T_{yy}$. 

51
8.3 Future Work

Experiments in the higher energy region should be performed to confirm these results. These experiments could be done by rescaling the cavity instead of increasing the frequency of the transmitter. Also the effect of the antennas should be investigated, mainly to see the mixing effect that we have found numerically. Will the energy levels interact when the input is made stronger? Another topic could be to investigate the magnetic field induced by the current flow in the cavity.
Bibliography

Appendix A

Plots

A.1 Sample Plots

This section contains sample plots of the density, $|\phi|^2$, the current, $\vec{j}$ and the stress tensor components $T_{xx}$ and $T_{yy}$. 
Figure A.1. Plots for frequency 3.09 [GHz]. Top left: $|\phi|^2$. Top right: The current, $j$. Bottom left: The stress tensor component $T_{xx}$. Bottom right: The stress tensor component $T_{yy}$.
Figure A.2. Plots for frequency 6.87 [GHz]. Top left: \(|\phi|^2\). Top right: The current, \(j\). Bottom left: The stress tensor component \(T_{xx}\). Bottom right: The stress tensor component \(T_{yy}\).
Figure A.3. Plots for frequency 20.87 [GHz]. Top left: $|\phi|^2$. Top right: The current, $j$. Bottom left: The stress tensor component $T_{xx}$. Bottom right: The stress tensor component $T_{yy}$. 

\[ \rho = |\phi|^2 \]
Figure A.4. Plots for frequency 31.98 [GHz]. Top left: $|\phi|^2$. Top right: The current, $j$. Bottom left: The stress tensor component $T_{xx}$. Bottom right: The stress tensor component $T_{yy}$. 
A.2 Density Distributions

The following figures contain numerical distributions of the density.

Figure A.5. The numerical distributions (solid line) obtained as averages over 11 wavefunctions with frequency between 4.80 and 5.92 [GHz] and $\langle \epsilon \rangle = 0.124$. Also the theoretical prediction (dashed line).
Figure A.6. The numerical distributions (solid line) obtained as averages over 11 wavefunctions with frequency between 15.20 and 16.01 [GHz] and $\langle \epsilon \rangle = 0.489$. Also the theoretical prediction (dashed line).
Figure A.7. The numerical distributions (solid line) obtained as averages over 11 wavefunctions with frequency between 30.85 and 31.15 [GHz] and $\langle \epsilon \rangle = 0.640$. Also the theoretical prediction (dashed line).
A.3 Current Distributions

The following figures contain numerical distributions of the different current components, \( j_x, j_y \) and \( j = \sqrt{j_x^2 + j_y^2} \).

![Graphs showing numerical distributions of different current components.](image)

**Figure A.8.** The numerical distributions (solid line) obtained as an average over 11 wave functions between 4.80 and 5.92 [GHz] with \( \langle j_y \rangle = 0.149 \). Also the theoretical distributions (dashed line). **Top:** The distribution of \( \langle \frac{j_x}{\langle j_x^2 \rangle^{1/2}} \rangle \). **Bottom left:** The distribution of \( \langle \frac{j_x}{\langle j_x^2 \rangle^{1/2}} \rangle \). **Bottom right:** The distribution of \( \langle \frac{j_y}{\langle j_y^2 \rangle^{1/2}} \rangle \).
Figure A.9. The numerical distributions (solid line) obtained as an average over 11 wave functions between 9.95 and 10.50 [GHz] with $\langle j^2 \rangle^{1/2} = 0.075$. Also the theoretical distributions (dashed line). Top: The distribution of $j_{\langle j \rangle}$. Bottom left: The distribution of $j_{\langle j^2 \rangle}^{1/2}$. Bottom right: The distribution of $j_{\langle j^2 \rangle}^{1/2}$. 
Figure A.10. The numerical distributions (solid line) obtained as an average over 11 wave functions between 15.20 and 16.01 [GHz] with $\langle j_y \rangle \langle j \rangle = 0.110$. Also the theoretical distributions (dashed line). Top: The distribution of $j \langle j \rangle$. Bottom left: The distribution of $j_x \sqrt{\langle j_x^2 \rangle}$. Bottom right: The distribution of $j_y \sqrt{\langle j_y^2 \rangle}$.
Figure A.11. The numerical distributions (solid line) obtained as an average over 11 wave functions between 20.86 and 21.44 [GHz] with $\langle j_y \rangle = 0.09$. Also the theoretical distributions (dashed line). Top: The distribution of $|j|\langle |j| \rangle^{-1}$. Bottom left: The distribution of $|j_x|\langle |j_x|^2 \rangle^{-1/2}$. Bottom right: The distribution of $|j_y|\langle |j_y|^2 \rangle^{-1/2}$.
Figure A.12. The numerical distributions (solid line) obtained as an average over 11 wave functions between 30.85 and 31.15 [GHz] with \( \langle j_y \rangle / \langle j \rangle = 0.143 \). Also the theoretical distributions (dashed line). Top: The distribution of \( j \langle j \rangle \). Bottom left: The distribution of \( j_x / \sqrt{\langle j_x^2 \rangle} \). Bottom right: The distribution of \( j_y / \sqrt{\langle j_y^2 \rangle} \).
A.4 Stress Tensor Distributions

The following figures contain numerical distributions of the different stress tensor components, $T_{xx}$, $T_{yy}$ and $T_{xy}$.

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{stress_tensor_distributions}
\caption{The numerical distribution of the different stress tensor components (solid line) obtained as an average over 11 wave functions with frequency between 4.80 and 5.92 [GHz]. Also the theoretical prediction (dashed line). \textit{Top left}: The distribution of $T_{xx}$. \textit{Top right}: The distribution of $T_{yy}$. \textit{Bottom left}: The distribution of $T_{xy}$. }
\end{figure}
Figure A.14. The numerical distribution of the different stress tensor components (solid line) obtained as an average over 11 wave functions with frequency between 9.95 and 10.50 [GHz]. Also the theoretical prediction (dashed line). Top left: The distribution of $T_{xx}$. Top right: The distribution of $T_{yy}$. Bottom left: The distribution of $T_{xy}$. Bottom right: The distribution of $T_{xy}$. 

Figure A.15. The numerical distribution of the different stress tensor components (solid line) obtained as an average over 11 wave functions with frequency between 15.20 and 16.01 [GHz]. Also the theoretical prediction (dashed line). Top left: The distribution of $T_{xx}$. Top right: The distribution of $T_{yy}$. Bottom left: The distribution of $T_{xy}$. Bottom right: The distribution of $T_{xy}$. 
Figure A.16. The numerical distribution of the different stress tensor components (solid line) obtained as an average over 11 wave functions with frequency between 20.86 and 21.44 [GHz]. Also the theoretical prediction (dashed line). Top left: The distribution of $T_{xx}$. Top right: The distribution of $T_{yy}$. Bottom left: The distribution of $T_{xy}$. 
Figure A.17. The numerical distribution of the different stress tensor components (solid line) obtained as an average over 11 wave functions with frequency between 30.85 and 31.15 [GHz]. Also the theoretical prediction (dashed line). Top left: The distribution of $T_{xx}$. Top right: The distribution of $T_{yy}$. Bottom left: The distribution of $T_{xy}$. 
Appendix B

Derivations

This appendix contains some derivations that have been referred to in the theory chapter.

B.1 Helmholtz Equation in a Quasi-Two-Dimensional Cavity

Let’s say that we have a region that has a constant thickness \( d \) in \( \hat{z} \) direction, but is otherwise unspecified. The origin of our coordinate system is centered so that it is in the middle of the cavity with respect to the \( z \)-axis. For the electromagnetic field, \( \mathbf{E} \) we have

\[
\mathbf{E} = E_x \hat{y} + E_y \hat{y} + E_z \hat{z}
\]  
(B.1)

and the Helmholtz equation

\[
[\nabla^2 + k^2] \mathbf{E} = 0
\]

(B.2)

By inserting (B.1) into (B.2), and taking the \( z \)-component we get equation (B.3).

\[-\nabla^2 E_z = k^2 E_z
\]  
(B.3)

Now we assume that \( E_z \) is separable, i.e. \( E_z = Z(z)E(x, y) \). By inserting this into equation (B.3) we get three equations, equations (B.4), (B.5) and (B.6).

\[
-\delta^2 Z(z) \delta z^2 = \alpha^2 Z(z)
\]  
(B.4)

\[-\nabla^2 E(x, y) = \beta^2 E(x, y)
\]  
(B.5)

and

\[\alpha^2 + \beta^2 = k^2\]

(B.6)

By application of \( Z(\frac{d}{2}) = Z(\frac{-d}{2}) = 0 \), the solution to the first differential equation, (B.4), is (B.7).

\[Z(z) = \cos(\frac{n\pi z}{d})\]

(B.7)
This gives $\alpha^2 = \left(\frac{n\pi}{d}\right)^2$, which means $\beta^2 = k^2 - \left(\frac{n\pi}{d}\right)^2$. By inserting this into equation (B.5), it becomes equation (B.8):

$$\left(\nabla^2 + k^2 - \left(\frac{n\pi}{d}\right)^2\right)E(x, y) = 0$$

(B.8)

In the case $k^2 < \left(\frac{n\pi}{d}\right)^2 \Rightarrow |k| < \frac{\pi}{d}$, the only allowed $n$ is $n = 0 \Rightarrow Z(z) = C$. Thus, the equation for the perpendicular electromagnetic field, $E_z$ becomes (B.9):

$$[\nabla^2 + k^2]E(x, y) = 0$$

(B.9)
B.2 Derivation of the Continuity Equation

In order to derive the continuity equation \( \nabla \cdot \mathbf{S} \) we need the time-dependent Schrödinger equation, (B.10)
\[
\frac{i\hbar}{\delta t} \frac{\delta \phi}{\delta t} = \frac{-\hbar^2}{2m} \nabla^2 \phi + V \phi
\]
and the expression for probability density current \( \mathbf{S} \), (B.11).
\[
\mathbf{S} = -\frac{i\hbar}{2m} (\phi^* \nabla \phi - \phi \nabla \phi^*)
\]
Here \( V = V_r + iV_i \), where \( V_r \) and \( V_i \) are the real and imaginary part of the potential. Now, take the time derivative of the probability density, \( |\phi|^2 = \phi^* \phi \). By using the notation \( \frac{\delta \phi}{\delta t} = \phi_t \) we get equation (B.12).
\[
|\phi|^2_t = \phi^* \phi_t + \phi \phi_t^*
\]
Now, by re-arranging equation (B.10) and taking the complex conjugate, we get two equations, (B.13) and (B.14).
\[
\phi_t = \frac{i\hbar}{2m} \nabla^2 \phi - \frac{i}{\hbar} V \phi
\]
\[
\phi_t^* = -\frac{i\hbar}{2m} \nabla^2 \phi^* + \frac{i}{\hbar} V^* \phi^*
\]
By inserting this into equation (B.12) it becomes (B.15).
\[
|\phi|^2_t = \frac{i\hbar}{2m} (\phi^* \nabla^2 \phi - \phi \nabla^2 \phi^*) + \frac{2}{\hbar} V_i \phi^* \phi
\]
The first term on the right hand side is in fact \( \nabla \cdot \mathbf{S} \). By inserting this and integrating over \( A \) it becomes (B.16).
\[
\frac{\delta}{\delta t} \int_A |\phi|^2 dA = - \int_A \nabla \cdot \mathbf{S} dA + \frac{2}{\hbar} \int_A V_i |\phi|^2 dA
\]
By applying Gauss’ Theorem to the integral containing \( \mathbf{S} \) we arrive at the final expression, (B.17)
\[
\frac{\delta}{\delta t} \int_A |\phi|^2 dA = - \int_\alpha \mathbf{S} \cdot \mathbf{n} d\alpha + \frac{2}{\hbar} \int_A V_i |\phi|^2 dA
\]
Here, \( \alpha \) is the boundary of \( A \), and \( \mathbf{n} \) is the normal to the boundary.