

Studies of Time Dependent Behavior of Few Interacting  
Electrons in Quantum Transport Geometries

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Bachelor's Thesis

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# Studier av elektroners transport i små system

Nanosystem är väldigt intressanta att studera. Nya material kan skapas genom nanoteknik med otroliga egenskaper, och många forskare är sysselsatta med problemet hur sådana små system uppför sig. Dock är gränslandet mellan stora och små system ett svårt område. Makroskopiska objekt kan beskrivas med statistik, till exempel kan alla partiklars rörelseenergi i en gas beskrivas med en storhet, nämligen temperatur. Om man studerar väldigt många partiklar smatidigt så kan man strunta i enskilda partiklars rörelse, eftersom de ändå inte märks.

I det andra extrema fallet, då vi har ett fåtal partiklar, kan man istället beskriva alla partiklar var för sig, och studera deras rörelser.

Ett problem uppstår i gränslandet mellan dessa två urartningar, när vi har flera partiklar - mer än ett fåtal men mindre än väldigt många. Vi kan då inte längre uttala oss om storheter som temperatur och liknande, men vi kan ändå inte säga något om rörelserna hos varje enskild partikel, eftersom detta helt enkelt tar för lång tid (datortid). Speciellt är coulombkraften mellan elektroner ofta krävande.

Detta är ett område det forskas mycket inom eftersom väldigt små system, som bara består av ett fåtal atomer, är relativt välkända (kvantprickar, till exempel), men lite större system kräver mer finess för att låta sig beskrivas. Detta kan till exempel röra sig om beteendet hos långa nanotrådar.

Denna rapport försöker utforska detta gränsland, genom att modellera ett relativt stort antal atomer (mer än 20), och låta elektroner hoppa mellan dessa. I modellen kan också coulombrepulsionen mellan elektronerna studeras. Denna repulsion borde spela väldigt stor roll om de färdas i mycket smala system, och därför studerar vi vad som händer när elektroner rör sig i en smal kedja av atomer. Vi låter kedjan vara kopplad till två metallkontakter, och låter alla elektroner börja i den ena metallkontakten. Sedan studerar vi vad som händer då vi startar klockan och studerar hur transmissionen genom kedjan beror av olika parameterar.

Vad som vi kommer fram till i rapporten är, att om elektronerna tillåts känna av varandra i en tunn kedja av atomer, med en coulombkraft kommer de att åka igenom kedjan en och en, och de kommer inte att befinna sig på samma ställen samtidigt.

Dock kan man, genom att kompensera repulsionen med en spänning över systemet, få ett fenomen där man tvingar elektronerna att färdas genom kedjan kopplade, d.v.s.

de hoppar genom kedjan tillsammans, istället för att undvika varandra.

Detta är ett väldigt intressant fenomen; man kan få parade elektroner i en kedja från oparade elektroner i en metallkontakt. Om detta kan uppnås praktiskt är en obesvarad fråga, och mer simuleringar behövs. T.ex. kanske fononer (vibrationer) kommer att förstöra fenomenet av parade elektroner. Detta är frågor som är intressanta att studera i framtiden.

# Abstract

This thesis deals with the study of the motion of correlated electrons in a nano-scale lead-chain-lead geometry. Usually electrons repel each other, but by adding an electric bias which counteracts the repulsion from the interaction, one can achieve a situation where the electrons travel in pairs through a thin chain of atoms, instead of traveling one at a time.



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# Chapter 1

## Introduction

Quantum transport is a very interesting area of research. As its name suggests, quantum transport deals with transport, usually electron transport, when the quantum mechanical effects of nature become important. This is usually when the size of the system studied is comparable to the the de Broglie wave length of the electrons. This area of research is important in several modern applications. For example, an understanding of how the resistance changes if we reduce the length of a conductor to a few atoms is of great importance. This knowledge is used in computers, where billions of transistors are connected via conductors only a few hundred atoms long. These kinds of small systems can only be described correctly by quantum transport.

The length scale of these systems is a troublesome one, small enough that a macroscopic treatment (classical or semi classical) will produce large errors, but large enough that computers available today cannot simulate the system properly.

To be able to describe quantum transport theoretically, one can choose between two different approaches: 1) Make a realistic model and make extensive simulations from it, getting quantitative results. 2) Make the models simpler and less realistic, so that one can explore new concepts, ideas and get a qualitative understanding for the models.

Concerning 1), it is necessary to have a good understanding how to model a realistic system and make simulations on it. Even for a simple system, for example two clusters of atoms connected via a linear chain, one would need to describe several difficult things, including heat properties, local chemical bonding between the atoms and so on. Much work has been done in this area. However, in this approach the calculations become very complicated if the system is far away from equilibrium.

Concerning 2), the simplicity of the models makes it possible to study effects that are too complicated to be treated in 1). Two of these are electron-electron interaction and electron-phonon interaction. Interactions like these are very important in small systems, like nano devices. However, we are far from having a complete picture of this. Therefore, it would be useful to make a simple model, using a few number of electrons in a small system which has a fairly simple geometry.

This thesis describes an attempt to simulate systems according to approach 2), and

within this approach the time dependent behavior will be studied. A typical nano-scale experiment consists of two conducting bulk materials, called leads, connected with a nano device. Therefore the thesis will focus on systems which contain a number of electrons traveling from one lead to another which are connected by a linear chain. A computer code will be used in order to make simulations on the system.

The outline of the thesis is as follows: Chapter 2 will describe the methods used to numerically simulate these kinds of systems. Chapter 3 will present the simulation results and the analysis of them. Chapter 4 presents our conclusions and an outlook.

The purpose of these simulations is to gain fundamental knowledge of what effects the electron-electron correlation has on the time dependent behavior of the system.

## Chapter 2

# The Model

Here the model which is used in the computer simulations will be described. We first show how to obtain the Hamiltonian matrix of the system expressed in a localized basis set. After that we will look at time propagation, and then describe a method to do time evolution in an efficient way, namely with the Lanczos method. Finally there is a brief introduction to the concept of density of states DOS and the local density of states LDOS.

### 2.1 The Model Hamiltonian

We want to extract information from a system, which consists of a discrete number of atoms. We can do this by finding a basis set in which we can write the Hamiltonian matrix. The matrix can then be diagonalized, which gives the eigenenergies and eigenstates of the system. With this information, one can calculate the density of states, let the system evolve in time, and so on. The first obstacle is then, which basis set should be used?

The system is built up from two leads connected by a linear chain. Therefore a basis set of functions could be used, localized on the atoms that build up the leads and the chain. In other words, atomic orbitals could be used as a basis set. However, to simplify, an atom is modelled by an object which only has a single energy level. This object will be called a *site*, and the *i*:th site will be denoted  $R_i$ . The basis used will be the basis of the sites,  $\{R_i\}_{i=1}^N$

Now we have a discrete system consisting of sites. Let us use these sites as a basis for a 1-dimensional lattice, i.e. a linear chain. What does the Hamiltonian look like for this system? For one electron in the continuous  $x$  space, the time independent Schrödinger equation is

$$\hat{H}\psi(x) = \hat{T}\psi(x) + \hat{v}\psi(x) = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + v(x)\psi(x) = \epsilon\psi(x) \quad (2.1)$$

where the superscript  $\hat{\phantom{x}}$  specifies that the object is an operator, and  $\hat{v}$  is the potential at each site.

A quick way to derive the model Hamiltonian is to discretize Equation 2.1. The second derivative can be approximated with the central-difference formula for the second derivative, which is obtained by the fact that

$$\frac{\partial^2 \psi(x)}{\partial x^2} = \frac{\psi'(x+a) - \psi'(x)}{a} \quad (2.2)$$

$$= \frac{\psi(x+a) - 2\psi(x) + \psi(x-a)}{a^2} \quad (2.3)$$

where we have used  $\psi'(x+a) = (\psi(x+a) - \psi(x))/a$  and  $\psi'(x) = (\psi(x) - \psi(x-a))/a$ .

If we discretize, and at each spacial step  $ja$  there is a site  $R_j$ ,  $R_j = ja$ ,  $\psi(R_j) = \psi_j$ ,  $v(R_j) = v_j$ , the Schrödinger equation becomes:

$$-\left(\frac{\hbar^2}{2ma^2}\right)\psi_{j-1} + \left(-\frac{\hbar^2}{ma^2} + v_j\right)\psi_j - \left(\frac{\hbar^2}{2ma^2}\right)\psi_{j+1} = \epsilon\psi_j \quad (2.4)$$

Since Equation 2.4 holds for all  $j$ , we can write this as a matrix equation, and if we denote

$$-\frac{\hbar^2}{2ma^2} := W_{j+1,j} \quad (2.5)$$

$$-\frac{\hbar^2}{ma^2} + v_j := E_j \quad (2.6)$$

$$-\frac{\hbar^2}{2ma^2} := W_{j,j-1} \quad (2.7)$$

we will obtain the matrix as follows:

$$\bar{\mathbf{H}} = \begin{bmatrix} E_1 & W_{2,1} & 0 & 0 & \dots \\ W_{1,2} & E_2 & W_{3,2} & 0 & \dots \\ 0 & W_{2,3} & E_3 & W_{4,3} & \dots \\ 0 & 0 & W_{3,4} & E_4 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \quad (2.8)$$

$E_i$  is called the *on-site energy* for site  $R_i$ , and  $W_{i,j}$  is called the *hopping term* between site  $R_i$  and  $R_j$ , for reasons that shall become clear later. Note that it is only for linear chains that the Hamiltonian in this model is tridiagonal in the site basis. For more information, see [3].

For a more thorough procedure to obtain a tight-binding Hamiltonian (where, however, site labels denote localized, e.g. Wannier, orbitals) see references: [4] and [2].

This matrix can then be diagonalized, and we obtain the eigenvalues and eigenvectors of the system. Note that the on-site energies are always on the diagonal, independent of the geometry of the system.

## 2.2 Model for several electrons

To show the basic principles of diagonalization when more than one electron is present in the system, we discuss briefly such a case. The traditional way of formulating quantum mechanics is less convenient when dealing with many electrons. Instead, one constructs states with creation operators  $a^\dagger$  acting on a vacuum state. This is called the occupation number formalism, or second quantization. To see an example of this, we will consider a specific example, namely a two-site system with two electrons of opposite spins. In this model we consider the on site energy, hopping and a Coulomb repulsion between electrons at the same site. We name the sites 1, 2, and the Hamiltonian can be written in second quantization:

$$\hat{H} = \sum_{i,j,\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + \sum_i U_c n_{i\uparrow} n_{i\downarrow} \quad (2.9)$$

where the sites are  $i = 1, 2$ , the spin is  $\sigma = \uparrow, \downarrow$ , the on-site energies are  $t_{11} = t_{22} = E$ , the hopping term is  $t_{12} = t_{21} = W$  and  $U$  represents the on-site Coulomb repulsion term. Furthermore, we set  $E = 0$ , shifting the single particle energy levels to make the Hamiltonian simpler. As a basis for the system, we can use the states

$$|1\rangle = a_{1\uparrow}^\dagger a_{1\downarrow}^\dagger |0\rangle, \quad |2\rangle = a_{1\uparrow}^\dagger a_{2\downarrow}^\dagger |0\rangle, \quad (2.10)$$

$$|3\rangle = a_{2\uparrow}^\dagger a_{1\downarrow}^\dagger |0\rangle, \quad |4\rangle = a_{2\uparrow}^\dagger a_{2\downarrow}^\dagger |0\rangle \quad (2.11)$$

which describe the entire system. These four states describe the fact that the two electrons can either be on site 1, site 2, or one at each site. The Hamiltonian in this basis becomes

$$\hat{H} = \begin{pmatrix} U & W & W & 0 \\ W & 0 & 0 & W \\ W & 0 & 0 & W \\ 0 & W & W & U \end{pmatrix} \quad (2.12)$$

This Hamiltonian can then be diagonalized as usual.

Note that two electrons with opposite spin on two sites require 4 basis states, while one electron only demands two. This is general; one electron on  $L$  sites requires  $L$  basis states.  $N$  electrons with the same spin on  $L$  sites demands  $\binom{L}{N}$  basis states, where

$$\binom{L}{N} = \frac{L!}{N!(L-N)!} \quad (2.13)$$

In particular, given  $L$  sites, each of the sites can be in one of four states; The site has no electron, the site has an electron with spin up, the site has an electron with spin down, the site has two electrons of opposite spins. This means that in total,  $4^L$  basis states are needed to describe the system. Already for 10 sites, the number of basis states will be very large, and hence methods which do not require the diagonalization of the full Hamiltonian are very useful (e.g. the Lanczos method).

### 2.3 The Lanczos Method

The Lanczos procedure is a method which creates a tridiagonal matrix as a tool in order to get information about a system. One starts by choosing an initial, 'seed', state  $|\varphi_0\rangle$  at one's convenience, in other words the choice of  $|\varphi_0\rangle$  is dictated by the nature of the problem at hand. In general,  $|\varphi_0\rangle$  will be a linear combinations of the basis states in which the Hamiltonian is represented, but the procedure is entirely general. The objective here is to, from a seed state, create states  $|\varphi_m\rangle$  and find the matrix elements  $\langle\varphi_m|\hat{H}|\varphi_n\rangle$ , which means that we can represent the Hamiltonian as a matrix in the basis of these states.

We begin by applying the Hamiltonian to the seed state once. The result can be expressed as a linear combination of two states:  $|\varphi_0\rangle$  and a state  $|\varphi_1\rangle$  perpendicular to it, which we assume to be normalized. We also assume the the Hamiltonian is hermitian.

$$\hat{H}|\varphi_0\rangle = \alpha_0|\varphi_0\rangle + \beta_1|\varphi_1\rangle \quad (2.14)$$

By multiplying with  $\langle\varphi_{0,1}|$  we find that

$$\langle\varphi_0|\hat{H}|\varphi_0\rangle = \alpha_0 \quad \langle\varphi_1|\hat{H}|\varphi_0\rangle = \beta_1 \quad (2.15)$$

Note however, that  $\langle\varphi_1|\hat{H}|\varphi_0\rangle = \beta_1$  is an implicit relation. To calculate this explicitly, we use equation 2.14 to get

$$\langle\varphi_1| = \frac{\langle\varphi_0|\hat{H} - \langle\varphi_0|\hat{H}|\varphi_0\rangle}{\beta_1} \quad (2.16)$$

and inserting this in the implicit relation yields

$$|\beta_1|^2 = \langle\varphi_0|\hat{H}^2|\varphi_0\rangle - \bar{\alpha}_0\langle\varphi_0|\hat{H}|\varphi_0\rangle \quad (2.17)$$

$$= \langle\varphi_0|\hat{H}^2|\varphi_0\rangle - \langle\varphi_0|\hat{H}|\varphi_0\rangle^2 \quad (2.18)$$

$$= \langle\hat{H}^2\rangle - \langle\hat{H}\rangle^2 \quad (2.19)$$

$$= (\Delta\hat{H})^2 \quad (2.20)$$

For the next step in this procedure, we write

$$\hat{H}|\varphi_1\rangle = a|\varphi_0\rangle + \alpha_1|\varphi_1\rangle + \beta_2|\varphi_2\rangle \quad (2.21)$$

where  $|\varphi_2\rangle$  is orthogonal to  $|\varphi_{0,1}\rangle$  and normalized. By multiplying with  $\langle\varphi_{0,1,2}|$  we find that

$$\langle\varphi_0|\hat{H}|\varphi_1\rangle = a \quad \langle\varphi_1|\hat{H}|\varphi_1\rangle = \alpha_1 \quad \langle\varphi_2|\hat{H}|\varphi_1\rangle = \beta_2 \quad (2.22)$$

We see here that  $a = \bar{\beta}_1$  if we compare with Equation 2.22.

For the next step in this procedure, we have that

$$\hat{H}|\varphi_2\rangle = \gamma|\varphi_0\rangle + b|\varphi_1\rangle + \alpha_2|\varphi_2\rangle + \beta_3|\varphi_3\rangle \quad (2.23)$$

Now it seems like we could proceed as usual, but first let us check a specific matrix element,  $\langle\varphi_0|\hat{H}|\varphi_2\rangle$ . On one hand, using Equation 2.23, we see that  $\langle\varphi_0|\hat{H}|\varphi_2\rangle = \gamma$ . On the other hand, using Equation 2.14, we find that  $\langle\varphi_0|\hat{H} = \bar{\beta}_1\langle\varphi_1| + \alpha_0\langle\varphi_0|$  ( $\alpha_0$  is real). This gives that  $\langle\varphi_0|\hat{H}|\varphi_2\rangle = 0$ , which means that  $\gamma = 0$ . This is true even for higher powers,  $\langle\varphi_0|\hat{H}|\varphi_n\rangle = 0$  when  $n \geq 2$ , a fact which is crucial for the entire procedure which will become evident below.

Now, as before, we get the constants as

$$\langle\varphi_1|\hat{H}|\varphi_2\rangle = \bar{\beta}_2 \quad \langle\varphi_2|\hat{H}|\varphi_2\rangle = \alpha_2 \quad \langle\varphi_3|\hat{H}|\varphi_2\rangle = \beta_3 \quad (2.24)$$

Since  $\gamma = 0$ , the expression in 2.23 has three terms only. This will hold for all steps in the procedure. The general formula for this is

$$\hat{H}|\varphi_n\rangle = \bar{\beta}_{n-1}|\varphi_{n-1}\rangle + \alpha_n|\varphi_n\rangle + \beta_{n+1}|\varphi_{n+1}\rangle \quad (2.25)$$

and the matrix elements is given by

$$\langle\varphi_n|\hat{H}|\varphi_{n-1}\rangle = \bar{\beta}_n \quad \langle\varphi_n|\hat{H}|\varphi_n\rangle = \alpha_n \quad (2.26)$$

We have therefore derived all the matrix elements for the Hamiltonian in this basis, so we can write the Hamiltonian as

$$\bar{\mathbf{H}} = \begin{bmatrix} \alpha_0 & \beta_1 & 0 & 0 & \dots \\ \bar{\beta}_1 & \alpha_1 & \beta_2 & 0 & \dots \\ 0 & \bar{\beta}_2 & \alpha_2 & \beta_3 & \dots \\ 0 & 0 & \bar{\beta}_3 & \alpha_3 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \quad (2.27)$$

This matrix is tridiagonal, which is the reason for doing this procedure. A tridiagonal matrix can be diagonalized much quicker than many other matrices, and this is crucial for many purposes, including time evolution, as can be seen in the next section.

### 2.3.1 Time Evolution with the Lanczos method

If, at a time  $t$ , the state of a system is known,  $|\psi(t)\rangle$ , and a basis of size  $N$  has been chosen, the system can be calculated at a later time  $t + \Delta t$ , with the use of the time evolution operator:

$$|\psi(t + \Delta t)\rangle = e^{-\frac{i}{\hbar}\hat{H}(t+\frac{\Delta t}{2})\Delta t}|\psi(t)\rangle \quad (2.28)$$

Note that the Hamiltonian is evaluated at a time  $t + \Delta t/2$ , and not  $t + \Delta t$ . This gives a numerically better result, see [5]

The simplest method to calculate the time evolution is to use the completeness relation for the eigenstates of  $\hat{H}$ ,  $\hat{1} = \sum_{i=1}^N |\lambda_i\rangle\langle\lambda_i|$ . Inserting this directly after the exponential leads to

$$|\psi(t + \Delta t)\rangle = \sum_{\lambda} |\lambda\rangle e^{-\frac{i}{\hbar} E_{\lambda}(t + \frac{\Delta t}{2})} \langle\lambda|\psi(t)\rangle \quad (2.29)$$

thereby calculating  $|\psi(t + \Delta t)\rangle$  by diagonalizing the full Hamiltonian in our original basis. This approach is usable only if the size of the system studied is very small, and if the number of time steps is small. Because the Hamiltonian is time dependent, the Hamiltonian has to be diagonalized in every time step.

Another way to do the time evolution is to make use of the properties of the tridiagonal matrix obtained with the Lanczos procedure. We first obtain  $|\varphi_0(t)\rangle, |\varphi_1(t)\rangle \cdots |\varphi_N(t)\rangle$  from the procedure above, a total of  $N$  states. Then, in this basis, we write

$$|\psi(t + \Delta t)\rangle = e^{-\frac{i}{\hbar} \hat{H}_{\kappa}(t + \frac{\Delta t}{2}) \Delta t} |\psi(t)\rangle \quad (2.30)$$

Now  $\hat{H}$  is a tridiagonal matrix in this basis, of size  $N \times N$ . To handle this better, we look at a truncated space instead, of dimension  $M \leq N$ . The size of this space will be referred to as the size of the Krylov space,  $k_{size}$ .

We then diagonalize the truncated Hamiltonian, by using  $\hat{H} = \hat{Z} \hat{D} \hat{Z}^\dagger$ , where  $\hat{Z}$  is a transformation matrix. Inserting this gives

$$|\psi(t + \Delta t)\rangle = e^{-\frac{i}{\hbar} \hat{Z} \hat{D} \hat{Z}^\dagger \Delta t} |\psi(t)\rangle = \quad (2.31)$$

$$\hat{Z} e^{-\frac{i}{\hbar} \hat{D} \Delta t} \hat{Z}^\dagger |\psi(t)\rangle \quad (2.32)$$

Here all the matrices are time dependent, and we evaluate them at the time  $t + \Delta t/2$ . Now we have diagonalized the Hamiltonian in the truncated Krylov basis, thereby using the tridiagonal structure.

Now we can find the state at a later time  $t + \Delta t$ , and to find the wave function in the basis of our choice. Taking two electrons with opposite spins as an example, the basis is,  $|ij\rangle = a_{i\uparrow}^\dagger a_{j\downarrow}^\dagger |0\rangle$ , whereas the total wave function can be written as  $\sum_{ij} c_{ij} a_{i\uparrow}^\dagger a_{j\downarrow}^\dagger |0\rangle$

By using the tridiagonal structure of the Hamiltonian in the Krylov space, we have been able to truncate and diagonalize the Hamiltonian efficiently. This procedure makes it possible to look at larger systems than simpler methods allow for.

## 2.4 Density of states

The concept of density of states will be used in the simulations. This density is often written  $D(E) = \sum_{i=1}^N \delta(E - E_i)$  where  $E_i$  is an eigenenergy.  $D(E)$  gives peaks when  $E = E_i$ , and  $\int D(E) dE = N$ , the number of states. The function  $D(E)$  shows all the energy states for the system. This means that  $D(E)$  is the *total* density of states.

However, one can also look at the density of states at a certain position. In this context, a certain position is a certain site. The density of states at a certain site can

be written as

$$\sum_n |\langle R_i | \lambda_n \rangle|^2 \delta(E - E_n) \quad (2.33)$$

This equation takes the peaks from the delta function, and kills off the peaks which site  $R_i$  does not see. For example, if  $|R_i\rangle = |\lambda_n\rangle$ , an eigenket, we get only one peak in the local density of states, and the peak is at  $E = E_n$ . This means that the only state that  $|R_i\rangle$  feels is its own state. Also, since the system is in an eigenstate, the electron does not move anywhere. In general, the more peaks an electron sees at a site, the more places it can jump to.

Numerically, one can calculate the density of states by diagonalizing the Hamiltonian to get the energy eigenvalues and eigenstates, and then replacing the delta function with a Lorentzian.

## 2.5 Small systems solved analytically

Here we will look at small chains in one dimension, which will be studied analytically.

### 2.5.1 One site

This is a linear chain consisting of one site, which is not much of a chain. The basis set is just  $|R_1\rangle$ , and the Hamiltonian in this basis is  $[E]$ . The on-site energy equals the energy eigenvalue, and the ground state is  $|R_1\rangle$ .

### 2.5.2 Two sites

Let us assume that these two sites have different on site energies,  $E_1$  and  $E_2$ , but equal hopping parameters,  $W$ . The latter condition means that it is equally probable for an electron to travel from  $R_1$  to  $R_2$ , as it is to travel from  $R_2$  to  $R_1$ . This results in the following matrix representation for the Hamiltonian in the R-basis:

$$\bar{H} = \begin{bmatrix} E_1 & W \\ W & E_2 \end{bmatrix} \quad (2.34)$$

We find the eigenenergies  $\lambda$  from the characteristic equation  $0 = \det(\bar{H} - \bar{I}\lambda)$ , which gives

$$\lambda_{\pm} = \frac{E_1 + E_2}{2} \pm \sqrt{\frac{(E_1 - E_2)^2}{4} + W^2} \quad (2.35)$$

We can look at two limiting cases in equation 2.35. One is when the difference in the on site energies is much larger than the hopping parameter. This will give the energy eigenvalues  $\lambda_{\pm} = \frac{E_1 + E_2}{2} \pm \frac{(E_1 - E_2)}{2}$ , giving  $\lambda_+ = E_1$  and  $\lambda_- = E_2$ . The eigenstates resulting from this are  $|\mu_1\rangle = |R_1\rangle$  and  $|\mu_2\rangle = |R_2\rangle$ . This is the same situation as when we had only 1 site. If the electron is placed at one of the sites initially, then the electron will not move because it is in an eigenstate.

The other case is when  $E_1 = E_2 = E$ . The two eigenenergies will be  $\lambda_+ = E + W$  and  $\lambda_- = E - W$ . If  $W$  were very small, we would get almost degenerate eigenvalues but, as  $W$  increases, the energy levels split up. This is exactly what happens when two atoms are brought together. The parameter  $W$  can be thought of as a measure of the inverse distance between the sites, or how much the electron feels the other site.

As we shall see, the hopping parameter also determines how fast the electron moves from one site to another. If the system is in a state  $|\psi(t)\rangle$ , which is not an eigenstate, then we can write

$$|\psi(t)\rangle = c_1 e^{-\frac{i}{\hbar}\lambda_1 t} |\mu_1\rangle + c_2 e^{-\frac{i}{\hbar}\lambda_2 t} |\mu_2\rangle \quad (2.36)$$

The amplitude of the wave function at site  $R_1$  is  $\psi(R_1, t) = \langle R_1 | \psi(t) \rangle$ . The probability density at site  $R_1$  is  $|\psi(R_1, t)|^2$ . This gives

$$|\psi(R_1, t)|^2 = |c_1 \langle R_1 | \mu_1 \rangle + c_2 \langle R_1 | \mu_2 \rangle e^{-\frac{i}{\hbar}(\lambda_1 - \lambda_2)t}|^2 \quad (2.37)$$

and, according to 2.35,

$$\lambda_1 - \lambda_2 = 2\sqrt{\frac{(E_1 - E_2)^2}{2} + W^2} \quad (2.38)$$

This means that two things provide the movement of the electron; the difference between the on site energies and the hopping term. This explains the name hopping term, a large value give rise to a fast change in the probability density.

One final remark, if one only looks at equation 2.38, one would be led to think that large on site differences means fast changes. However, recall the first limiting case, when the large separation meant that the states could not communicate at all. In other words, too large an energy separation between the on site energies means that the electron does not move at all. The energy separation is not the all determining, one also needs to look at the state coefficients  $\langle R_i | \mu_i \rangle$  to determine how fast the electron will move.

## Chapter 3

# Simulations

The code which was used in the simulations makes use of the tridiagonal nature of the Hamiltonian written in the Lanczos basis. By diagonalizing the Hamiltonian in this basis, one can do time evolution on larger systems than if one had used a more direct way. To use the program, one specifies the following parameters:

- The total number  $N_{el}$  of electrons in the system.
- The spin  $\sigma = \uparrow, \downarrow$  of each electron
- The total number  $N$  of sites  $\{R_i\}$  in the system.
- The on-site energy  $E$  for every site.
- The hopping parameters  $W_{R_i R_j} = W_{ij}$  between the sites.
- The strength of the electron-electron interaction  $U_{ij}$  when one electron is at  $R_i$  and the other at  $R_j$ .
- The geometry of the system
- The external bias  $V_{R_i}(t) = V_i(t)$
- The size  $k_{size}$  of the Krylov space

The following results are calculated from this:

- The eigenenergies and eigenstates of the system
- The development in time of the one-electron density  $\langle n_{i\sigma} \rangle$
- The development in time of the correlation function  $\langle n_{i\sigma} n_{j-\sigma} \rangle$

The correlation function for two electrons is the probability to find a electron at  $R_i$  provided that the other electron is at  $R_j$ . If there is a repulsive interaction, the correlation function will generally decrease when the electrons are close to each other.

The hopping parameters determine the connections between the different sites in the system. A large hopping parameter between two sites correspond to a short distance between the sites, and vice versa. This means that the hopping parameter should decrease if the sites are far apart. To make things more simple, the nearest neighbor tight-binding approximation is used. The approximation states that electrons can only hop to neighboring sites, so  $\langle R_i | \hat{H} | R_i \rangle = W$  if the sites are next to each other, and 0 otherwise. A site in a linear chain in 1D has two nearest neighbors, whereas a site in a fcc lattice has 12 nearest neighbors. This means that one electron in a linear chain geometry is described by a tridiagonal Hamiltonian (see 2.8), while a fcc geometry, for example, is described with a more complicated Hamiltonian. In this way, the geometry of the system is reflected in the Hamiltonian.

We start the simulations by first looking at one electron hopping along a small chain of 7 sites in 1D, and then we continue by looking at one electron on a 2D chain. After that, we move to 3D, and start to look at a more complicated system consisting of two simple cubic leads connected by a linear chain. The first simulations will only take one electron into account, followed by two electrons where we study the effect of the electron-electron interaction. Finally, we look at four electrons hopping on smaller leads.

## 3.1 One Electron

### 3.1.1 Chain of 7 sites

In this section, we look at one electron which can hop on a linear chain composed of 7 sites, see Figure 3.1. The box contains the parameters used in the simulations. See page 11 for an explanation of the parameters.

$N_{el} = 1$ $E = 0$ $W = 1$
------------------------------------



Figure 3.1: Linear chain of 7 atoms

We have already seen the Hamiltonian for the linear chain, see equation 2.8.

As a simplification, we make the sites identical. This means that all on-site energies  $E$  are equal, and all hopping terms  $W$  as well. The Hamiltonian becomes

$$\bar{H} = \begin{bmatrix} E & W & 0 & 0 & 0 & 0 & 0 \\ W & E & W & 0 & 0 & 0 & 0 \\ 0 & W & E & W & 0 & 0 & 0 \\ 0 & 0 & W & E & W & 0 & 0 \\ 0 & 0 & 0 & W & E & W & 0 \\ 0 & 0 & 0 & 0 & W & E & W \\ 0 & 0 & 0 & 0 & 0 & W & E \end{bmatrix} \quad (3.1)$$

Now, we want to place one electron at a starting site and start the simulation. For simplicity, we choose the starting point to be to the left, i.e. at  $R_1$ . This means that  $|\psi(t=0)\rangle = |R_1\rangle$ .

The results of the simulation are shown below. We see that the wave packet, which is the electron, moves from the starting point to the left to the end of the chain, to the right. We also see that the wave packet appears to move just like a free particle would. This is because of the constant potential that the electron sees.

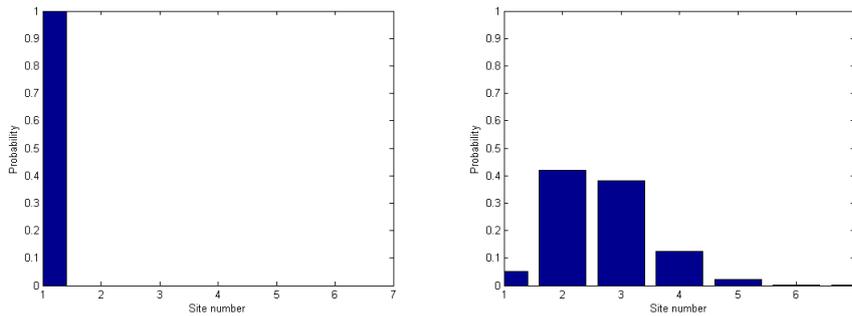


Figure 3.2: To the left:  $t = 0$ ; To the right:  $t = 1.5$

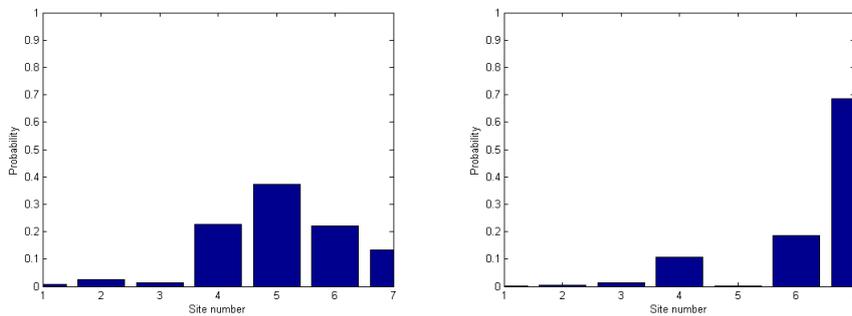


Figure 3.3: To the left:  $t = 3$ ; To the right:  $t = 5$

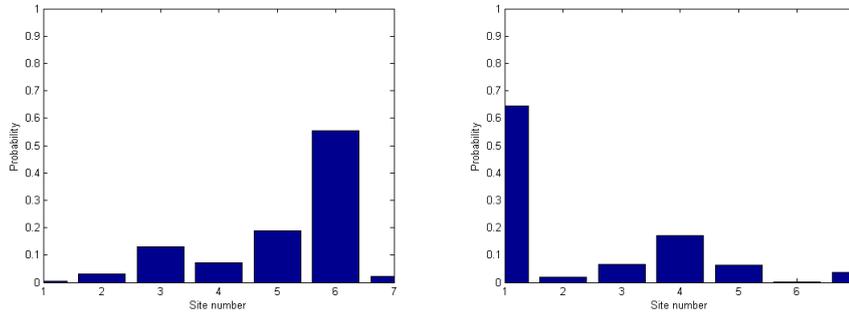


Figure 3.4: To the left:  $t = 6$ ; To the right:  $t = 9$

Testing different values of the on-site energy  $E$ , it is found that shifting all the on-site energies by a constant value does not change the time evolution of the system. This means that there is no difference in choosing  $E = 0$  than any other number in this simulation. Another point to be made is that increasing  $W$  increases the speed of the wave packet, which is also understandable, because  $W$  is a measure how easy it is to hop to neighboring sites.

### 3.1.2 Chain of 9 sites

In this section we will make our system two-dimensional. The new system is our previous linear chain, but now supplemented by two extra sites sticking out perpendicularly from the central site, see Figure 3.5. We let these two new sites to have different on-site energies  $\langle R_8|H|R_8 \rangle = \langle R_9|H|R_9 \rangle = e$  and hopping parameters  $\langle R_4|H|R_8 \rangle = \langle R_4|H|R_9 \rangle = w$  than the rest of the chain.

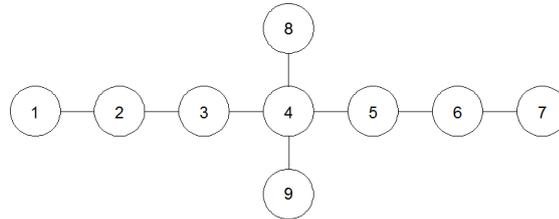


Figure 3.5: Chain of 9 atoms

Since we have 9 sites in this system, the Hamiltonian becomes a  $9 \times 9$  matrix. However, since the problem is no longer one-dimensional, the Hamiltonian matrix is no longer tridiagonal.

$$\bar{H} = \begin{bmatrix} E & W & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ W & E & W & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & W & E & W & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & W & E & W & 0 & 0 & w & w \\ 0 & 0 & 0 & W & E & W & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & W & E & W & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & W & E & 0 & 0 \\ 0 & 0 & 0 & w & 0 & 0 & 0 & e & 0 \\ 0 & 0 & 0 & w & 0 & 0 & 0 & 0 & e \end{bmatrix} \quad (3.2)$$

In this system we can vary four different parameters. However, if we just plug in random values of  $E$ ,  $W$ ,  $w$  and  $e$  we get complicated movements of the electron. Therefore, we simplify by looking at what happens if  $E = e$ .

The first thing to notice is that when  $w \rightarrow 0$  the problem should reduce to the 7-atom problem. This can be seen physically, as the electron can not travel to atom 8 or 9, trapping the electron inside the chain. Another way to see it is to look at equation 3.2; the matrix can be diagonalized first as a  $7 \times 7$  matrix, then as two  $1 \times 1$  matrices.

Running the simulation, we see that this is indeed the case. The electrons do not feel the added sites. If  $w$  is increased, the electron should feel the added sites more and more.

To see how much the electron can interact with the added sites, we can look at the density of states at  $R_8$  and  $R_9$ , the local density of states. As discussed in the theory section, if there are many and large peaks in the local density of states, then the electron will hop between sites quickly, and the other way around. The local density of states at  $R_8$  was calculated and plotted in Figure 3.6.

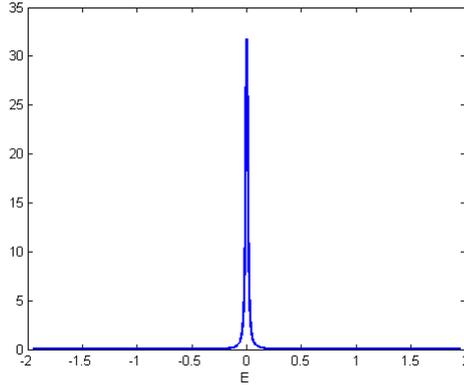


Figure 3.6: LDOS at site  $R_8$  when  $w = 0$ ,  $e = E = 0$ . The units on the  $y$ -axis are arbitrary.

In Figure 3.6, we see that there is only one peak. This means that if the electron is placed at  $R_8$ , the electron will only see site  $R_8$  and no other, which means that the

electron will not hop to any other sites in the system. If  $w$  is increased, we should see an increase of the number of peaks in the local density of states. This will let the sites  $R_8$  and  $R_9$  communicate with  $R_4$ , spreading out the local density of states. The results are plotted in Figure 3.7

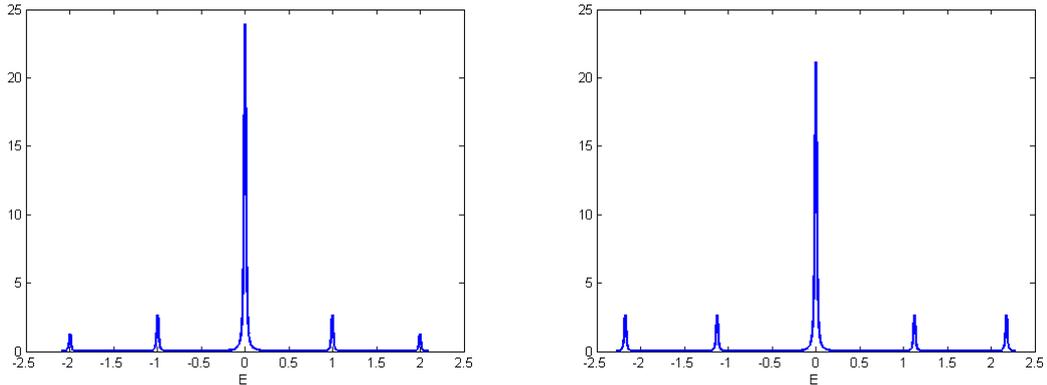


Figure 3.7: LDOS at  $R_9$ . To the left:  $w = 0.7$ ; To the right:  $w = 1$

The isolation is now broken, and any electron which is initially placed at  $R_8$  will begin to travel to other sites in the system.

## 3.2 Cubic leads with a linear chain

So far we have only studied the behavior of a chain. Now, let us make a more complicated system, consisting of two cubic structures with a linear chain in between (the cubic structures are a finite size model of the so called leads of the system). The leads in the computer simulation represent the metallic conductors in a nano-scale experiment. In a typical experiment, there are usually two connectors with a nano device connecting them. This nano device is the only means of transportation for the electrons, so all electrons must go through the device to get to the other lead. This nano device is modelled by the linear chain. See Figure 3.8 for a schematic view of the system. For each lead, we use a simple cubic lattice, which is built up by 8 sites. The chain is 10 sites long. The structure we study represents the central and nearby region of a molecular wire-like nano-device.

### 3.2.1 Simulation setup for the cubic leads

In all of these simulations, we want to place our electron(s) in the left lead. The starting conditions are described below.

The on-site energies  $E$  of the sites in the left lead is changed to a low value compared to the rest of the system. Thus, when the ground state of this system is calculated, the

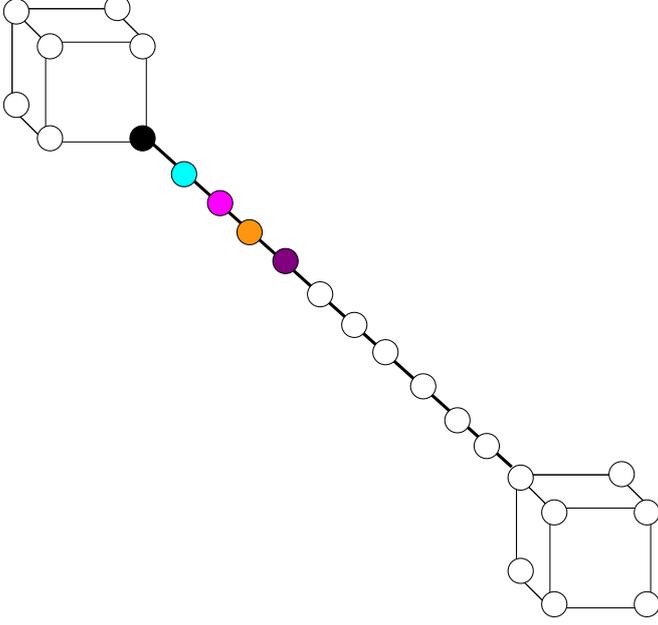


Figure 3.8: Schematic overview of the system. The color codes in the figure are used in the graphs below to denote curves pertaining to different sites.

electronic wave function is (almost) zero in the chain and the right lead, but not in the left lead. This means that the electron(s) is located in the left lead. If we start the simulations in this system, we have an isolated lead, where nothing happens because of the large energy gap between the left lead and the chain.

In these simulations, we have put  $E_{left\ lead} = E_{ll} = -10$ , whereas the rest of the system has  $E_{chain} = E_c = 0$  and  $E_{Rlead} = 0$ . The hopping parameter in the leads is set to  $W_l = -0.5$ , and in the chain  $W_c = -0.1$ . This results in a calculated ground state energy of  $E_{gs} = -11.5001$ .

In order to make the electron(s) move, we must raise their energy. This is made by applying a bias to the sites of the left lead, raising the electrons which have energy  $E_{gs}$  to the rest of the system. The bias used in the simulations has the form

$$V_{ll} = \sum_{i \in left\ lead} \frac{V_0}{2} \left( 1 + \tanh \frac{t - t_0}{\tau} \right) \hat{n}_i \quad (3.3)$$

Since  $-1 < \tanh(x) < 1$ , we have that  $0 < (1 + \tanh(x))/2 < 1$ , which means that this function can be used as a step function, whose slope is controlled by  $\tau$ , and the strength is determined by  $V_0$ . A large  $\tau$  means that the change in bias happens slowly, while a small value means that it happens instantaneously. The parameter  $t_0$  determines when the bias is switched on; at  $t = t_0$  the bias is at  $V_0/2$ . The bias acts on each site in the left lead, effectively changing the on site energy.

The magnitude of the hopping parameter in the leads is larger than in the chain, because the electrons should hop more easily inside the (metallic) lead. As before, only relative magnitudes have significance, not absolute magnitudes.

A first question one could raise is: what strength of the bias gives for the maximum transmission of electrons? We see the results for three different bias strengths in Figure 3.9. We remind the reader that the color description for the curves can be found in Figure 3.8.

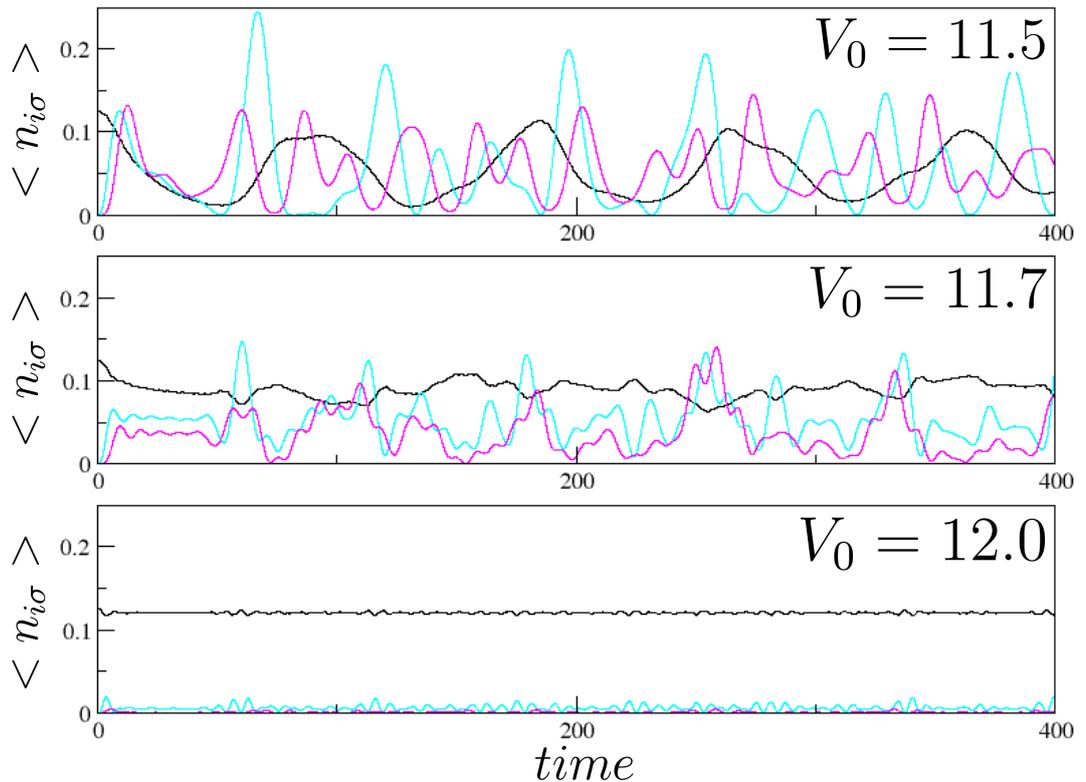


Figure 3.9: The result in simulations for one electron when the bias of the left lead  $V_0$  is changed. The energy window in which transmission occurs is relatively thin. See Figure 3.8 for color codes.

Here we see that if the strength of the bias corresponds to the ground state energy of the electron, then we have most of our movement. We can also see that the energy window of electron transmission is rather small; a small change in bias means much less transmission rates. This energy window seems to shrink with the size of the system.

These results are qualitatively in line which one would obtain from an analytical calculation for a two-site system, with a Hamiltonian according to 2.9 on page 5.

### 3.3 Two Electrons with Opposite Spins

In this section, we still have the same system, two cubic leads with structure  $2 \times 2 \times 2$  connected with a linear chain. However, we add one more electron to the system, and we choose its spin so that the two electrons have opposite spins. Now things get more complicated because electrons repel each other. We can model this by saying that, if two electrons are on the same site in the chain, there is an energy penalty of  $U_c$ . If they are on different sites, there is no penalty. We can also include an off-site interaction, and see what happens.

First, let us start with the non-interacting case ( $U_c = 0$ ). The parameters used are in the box above.

$N_{el} = 2$
$U_c = 0$
$E_{ll} = -10$
$E_c = 0$
$W_l = -0.5$
$W_c = -0.1$
$k_{size} = 10$
$\tau = 0.2$
$t_0 = 5$
$E_{gs} = -11.5$

#### Without Interaction

If the electrons are non-interacting the electrons will move independently because they have opposite spins. This means that the one-electron density per spin channel will look like the one in Figure 3.9. This is confirmed by the simulation as shown in Figure 3.10. If we compare this figure with Figure 3.9 we see that they are identical.

#### Adding on-site Interaction

Now, let us add an on site electron-electron interaction  $U_c$ . We can include it in our Hamiltonian by adding the terms (in second quantization)

$$\hat{H}_{interaction} = \sum_{i \in chain} U_c n_{i\downarrow} n_{i\uparrow} \quad , \quad (3.4)$$

where the summation runs over the chain only, i.e. we only have an electron-electron interaction in the chain. This is motivated by the fact that the chain is much smaller than the lead, and therefore the electrons should feel the repulsive interaction more there since they are more localized. Furthermore, if we assume that the leads are metallic the electrons are screened more efficiently in the leads than in the chain.

Figure 3.11 show what happens if we increase  $U_c$ . There is a change in the transmission when  $U_c$  is increased from 0 to 1; we go from un-correlated electrons to correlated ones.

An interesting feature is when we increase  $U_c$  further. We see that the transmission is relatively unchanged if the interaction is increased to large values of  $U_c$ . In other words, increasing the interaction further does not have any effect on the transmission. An explanation to this can be that the electrons travel through the chain one at a time, and thus the electrons do not suffer from this energy penalty. To be sure of this, we must look at the correlation function, denoted as  $\langle n_{i\sigma} n_{i-\sigma} \rangle$ . We see in Figure 3.12 that, if the interaction term  $U_c$  is large, the correlation function is much lower than the single-electron density in the chain, meaning that the electrons simply travel through the chain one by one.

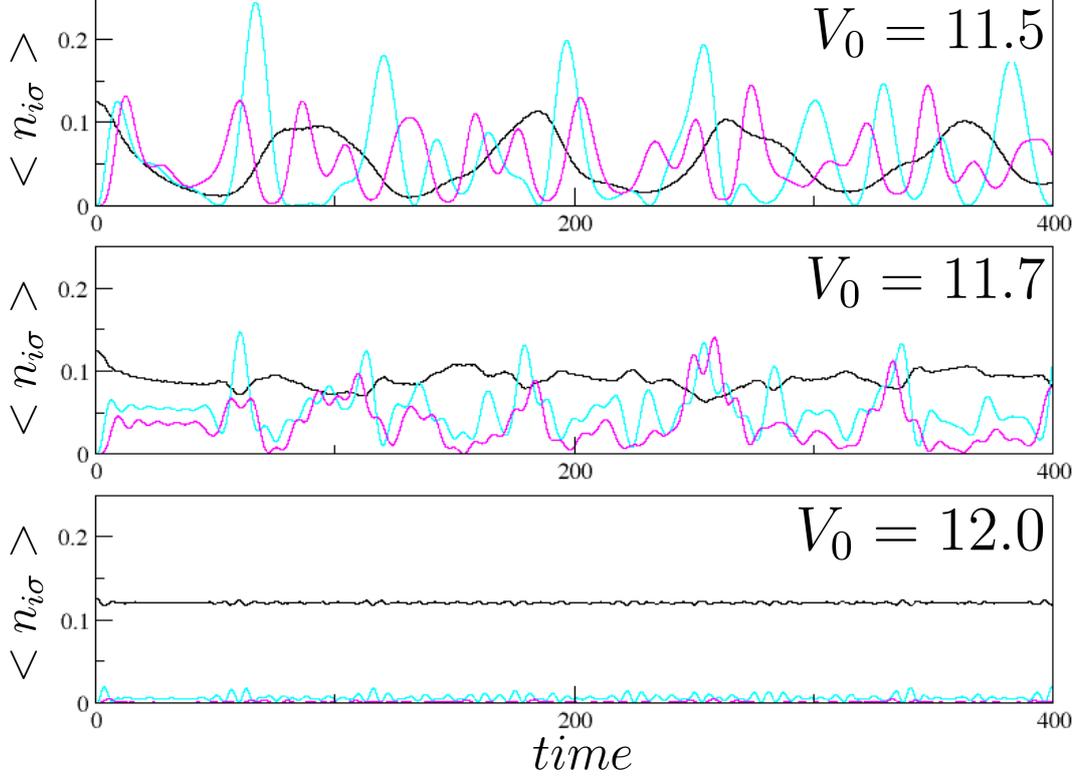


Figure 3.10: The result in simulations for two electrons when the bias of the left lead  $V_0$  is changed. These results are the same as for the one-electron case, see Figure 3.9

We can also study what happens when the bias of the left lead is increased, to compensate for the energy penalty from the electron-electron interaction.

The compensation should be such that there is no difference in energy for the electrons at the lead or at the chain. The total energy at the lead is the sum of the ground state energy and the bias energy,  $E_{gs} + N_{el} \cdot V_0$ . The total energy in the chain is the sum of the on-site energy for each electron, and the energy gain from the interaction term,  $N_{el}E_c + U_c \cdot N_{el}/2$ . This means that the resonance energy condition is

$$E_{gs} + N_{el} \cdot V_0 = \frac{N_{el}}{2}(2E_c + U_c) \quad (3.5)$$

If we choose  $U_c = 10$ , we find that  $V_0 = 16.5$  is the anticipated resonance. Figure 3.13 shows what happens in this case. This means that if we match the energy of the electrons in the lead, with the energy of the electrons in the chain, we get correlated electron motion; the electrons travel through the chain in pairs. This means that, starting from completely de-localized electrons in a lead, we have created concerted motion.

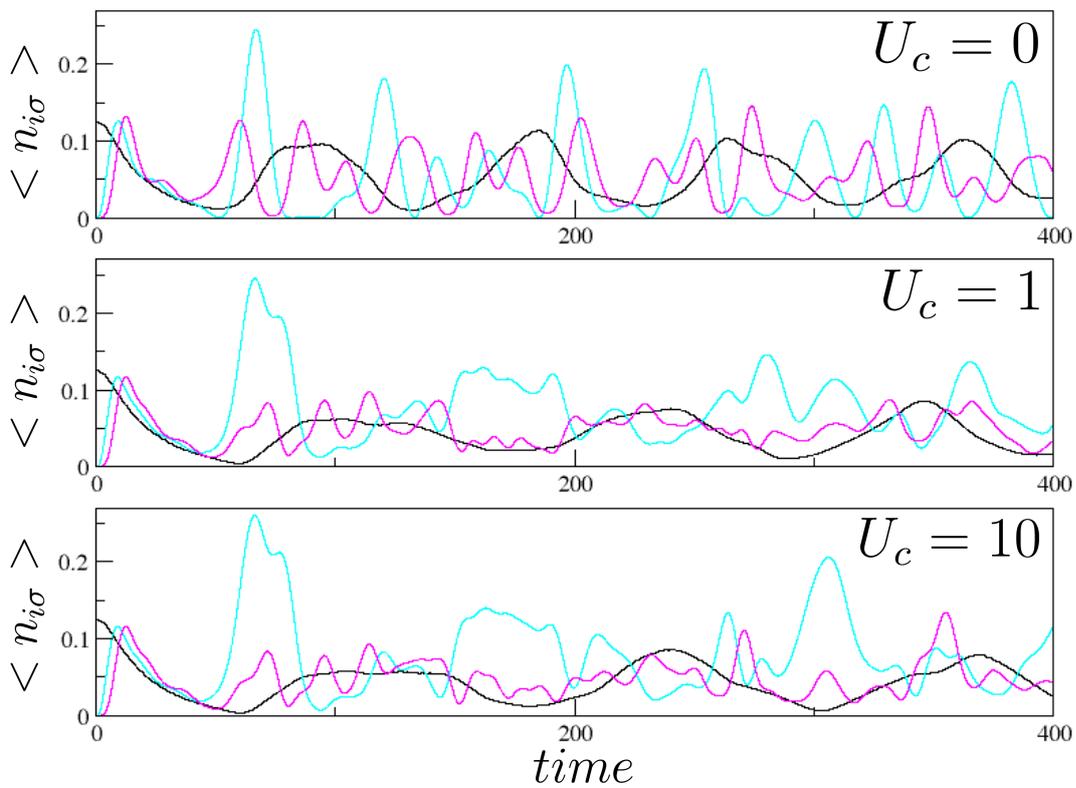


Figure 3.11: Two electrons when  $V_0 = 11.5$ . Here we change the electron-electron interaction term  $U_c$ . The difference, when going from  $U_c = 1$  to  $U_c = 10$ , is small.

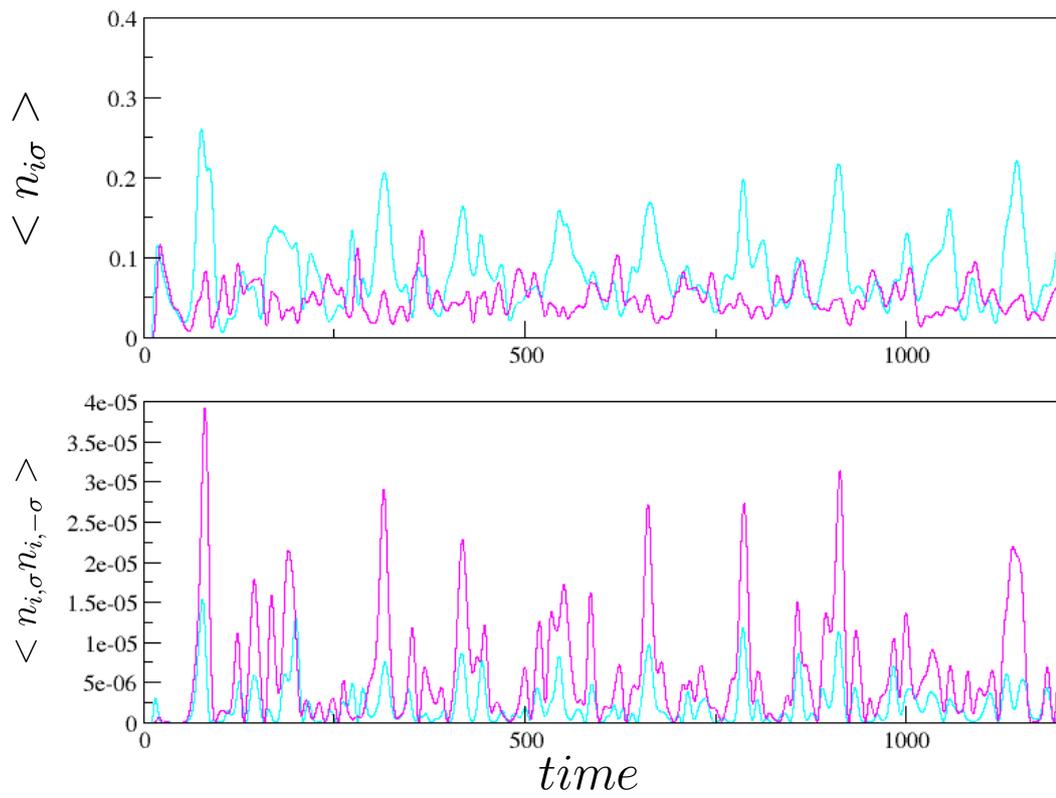


Figure 3.12: Two electrons off resonance, at energy  $V_0 = 11.5$ . Note the different scales. This means that no electrons travel through the chain coupled.

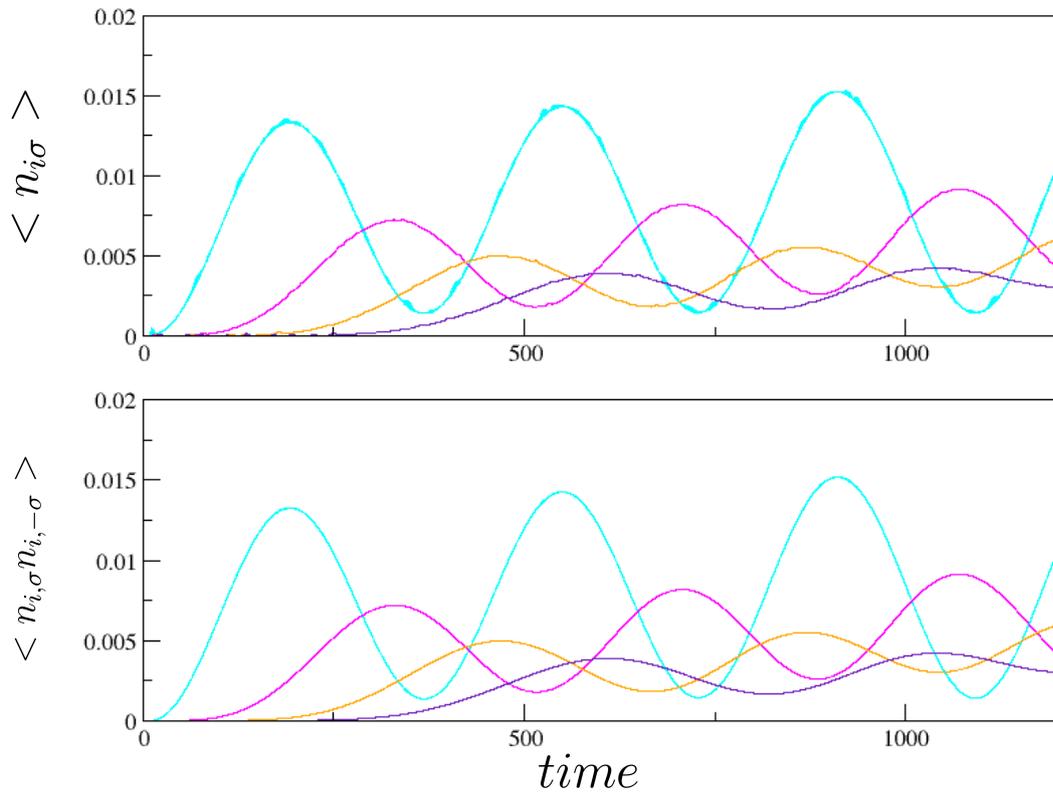


Figure 3.13: Two electrons at resonance, when the bias  $V_0 = 16.5$  and  $U_c = 10$ . The 1-electron density equals the double occupancy. This means that the entire transmission is happening through double hopping.

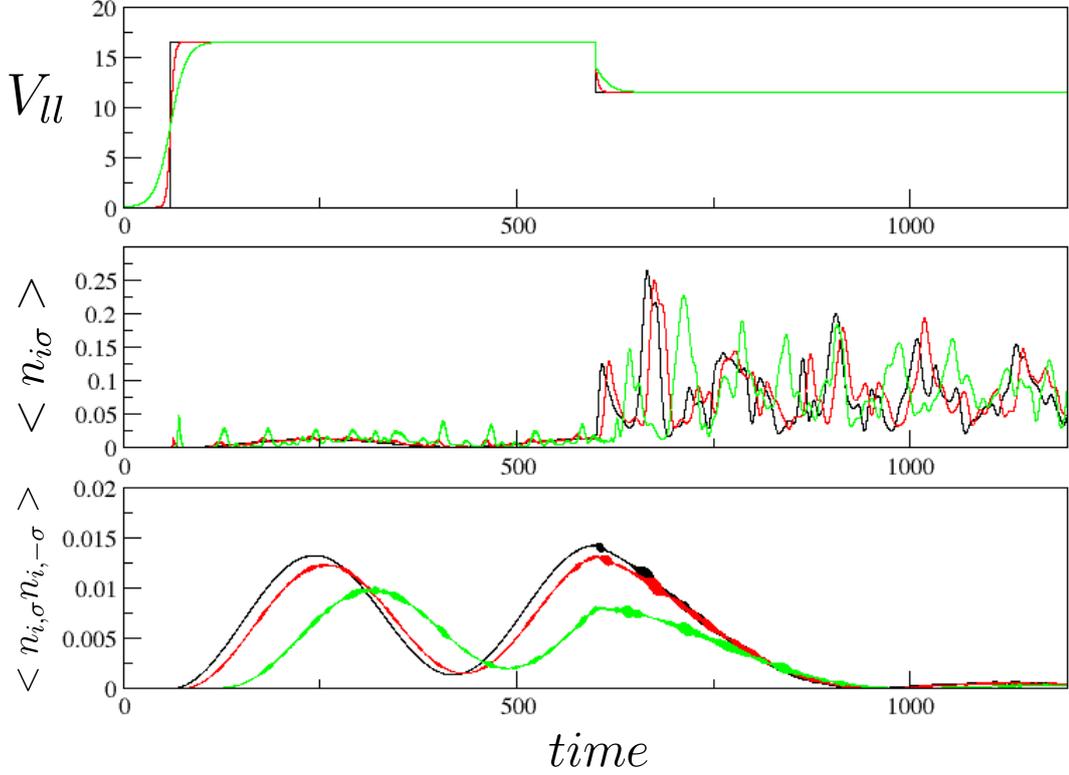


Figure 3.14: Three different kinds of biases; fast (black,  $\tau = 1$ ), intermediate (red,  $\tau = 50$ ), slow (green,  $\tau = 200$ ). The coupled motion fades out after some time has passed, if we lower the bias from the resonance channel to the off-resonance channel. The first site in the chain is shown, directly after the lead.

### Comparing with slowly varying biases at resonance

This is a quick look into what happens if the bias is raised to match the energy condition, not as a step function, but adiabatically. Because there are two channels of transmission, one off-resonance at  $V_{ll} = 11.5$  and one on-resonance at  $V_{ll} = 16.5$ , a part of the electron cloud should go through the off-resonance channel if the bias is raised sufficiently slow up to 16.5, effectively decreasing the double occupancy.

The speed of which the bias was raised depends on the parameter  $\tau$  in Equation 3.3. Three different speeds were used,  $\tau = 1$ ,  $\tau = 50$  and  $\tau = 200$ . The results are shown in Figure 3.14.

As Figure 3.14 shows, there is a difference in having a fast bias in comparison for a slow one; if the bias is slow, then the electrons can pass through the chain one by one at the time  $t'$  when  $V_{ll}(t') \approx 11.5$ . The electrons do not have this chance if the speed of the bias is fast, and this yields a lower combined motion as compared to the faster biases.

Furthermore, when the bias goes from resonance condition to off-resonance, the single particle density goes up and the correlated motion goes to zero.

### Adding off-site interactions

The simulations so far have been made with an on-site interaction only. The question is, if an interaction of longer range will destroy the correlated motion between the electrons. We study this by adding an interaction term of the form  $U_{off}n_{i\sigma}n_{i+1,\sigma}$  to the Hamiltonian, where  $U_{off} < U_c$  because the coulomb interaction diminishes with distance. With terms like these, the range of the interaction extends to the nearest neighbors only. We only include effects from nearest neighbors, i.e. the electrons get an energy penalty of size  $U_{off}$  if they are one site apart from each other, and no penalty if they are further apart. We put  $U_{off} = U_c/3 = 3.33$  in these simulations.

To show whether there is an increased probability for the electrons to be one site apart from each other, we make use of the correlation function  $\langle n_i, \sigma n_{i+1}, -\sigma \rangle$  which is the probability that an electron is at  $R_{i+1}$  provided that another electron is located at  $R_i$ .

Simulations were done at three different biases;  $V_0 = 11.5$ , corresponding to the usual off-resonance condition,  $V_0 = 13.166$ , which should be a resonance condition for the off-site interaction, and  $V_0 = 16.5$ , the resonance condition for the on-site interaction. These values were obtained by using the resonance formula,

$$E_{gs} + N_{el} \cdot V_0 = \frac{N_{el}}{2}(2E_c + U_c) \quad , \quad (3.6)$$

and by putting in our values,  $E_{gs} = -23.0$ ,  $N_{el} = 2$ ,  $E_c = 0$ , we get  $V_0 = \frac{U_c - E_{gs}}{2}$ . By inserting  $U_c = 0$ , which is the condition when the electrons travel one by one, we get  $V_0 = 11.5$ . The on-site resonance is given by  $U_c = 10$ , yielding  $V_0 = 16.5$ , and the off-site resonance is given by  $U_c = 10/3$ , giving  $V_0 = 13.1664$ .

The results are shown in the figures below, Figure 3.15, Figure 3.16 and Figure 3.17.

Figure 3.15 shows that, if off-site interaction is added, the electrons tend to keep themselves at a distance from each other, usually more than one site apart. This means that there should be less transmission through the chain, than if the off-site interaction would be absent. A comparison with Figure 3.12 tells us that this is indeed the case; the 1-electron density is lower in presence of an off-site interaction.

Figure 3.16 shows that in a similar way as coupled motion occurred in the case of only an on-site interaction, we also get coupled motion when we match the bias with the off-site interaction. Now the electrons are coupled one site apart, however.

Figure 3.17 shows, that even if we add an off-site interaction, the resonance channel for the on-site is not destroyed.

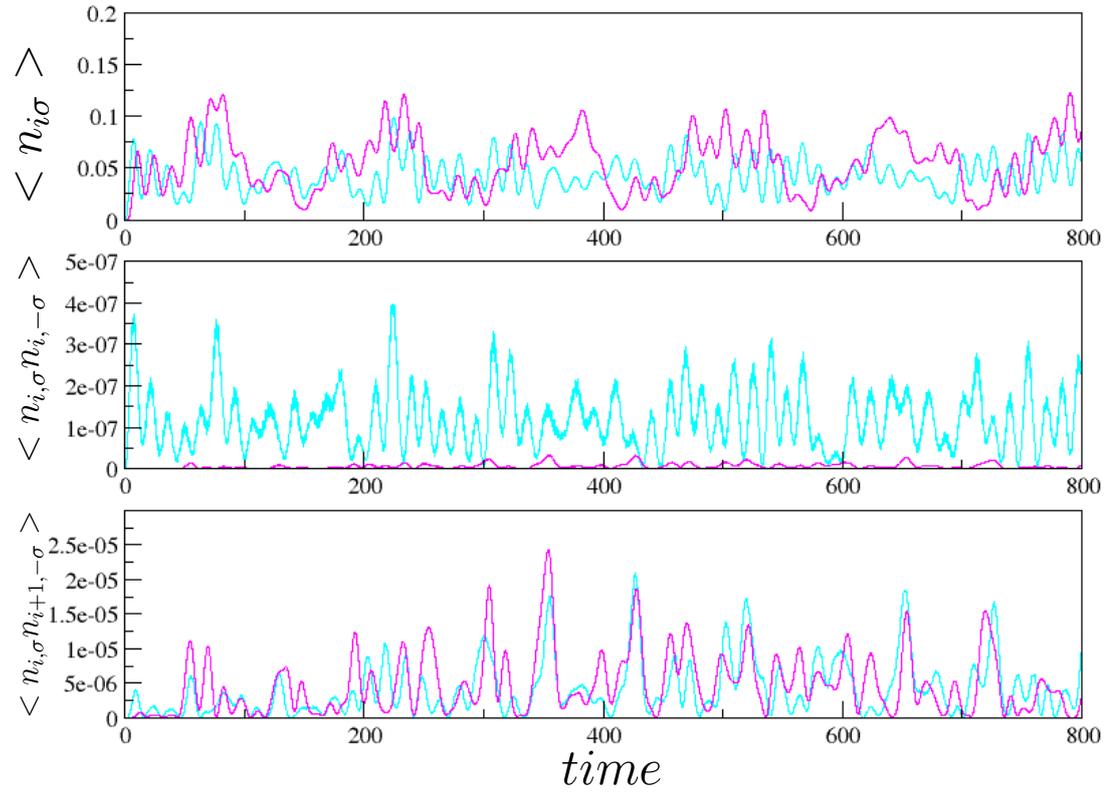


Figure 3.15:  $V_0 = 11, 5$ , meaning that we are off-resonance. We see similar results to the previous cases, the electrons go through the chain one by one. However, we also see that it is unusual for the electrons to be one site apart. This lowers the total transmission, as compared to the case when we only had on-site interaction, Figure 3.12 as well.

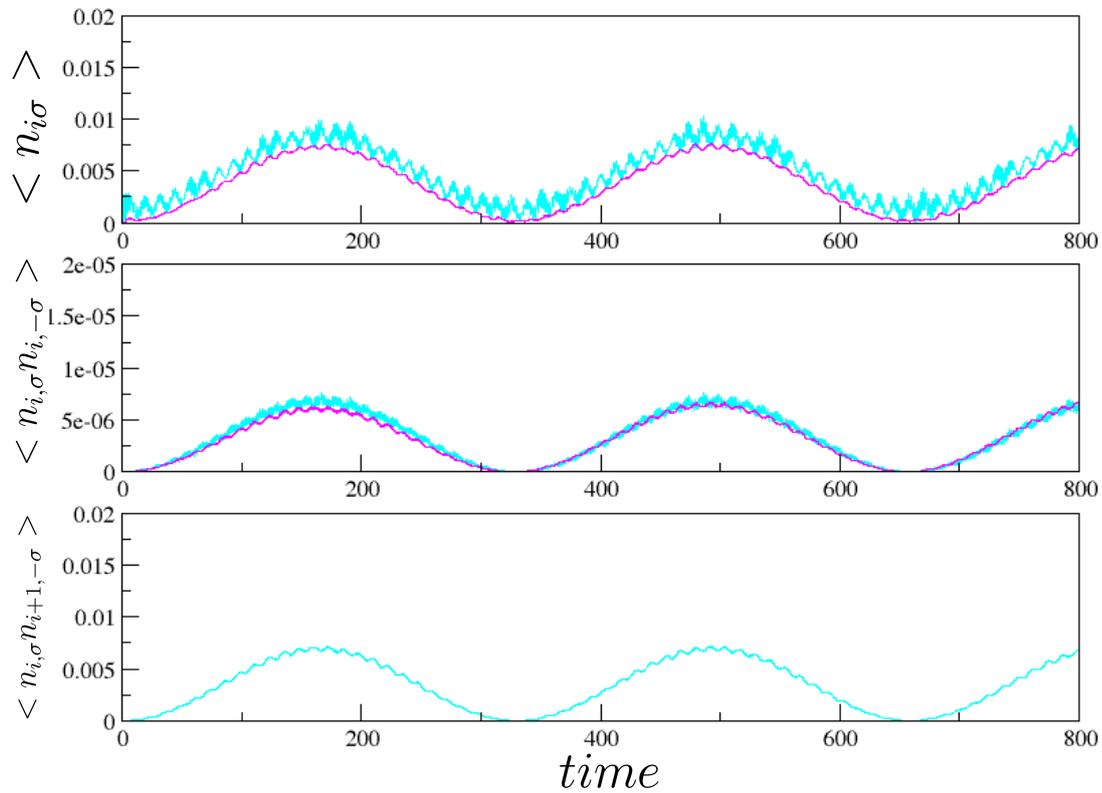


Figure 3.16:  $V_0 = 13.1666$ , which means that the bias matches the energy penalty the electrons get when they are one site apart from each other. We see that we get paired electrons, as in the previous cases, but now the electrons are at a distance from each other.

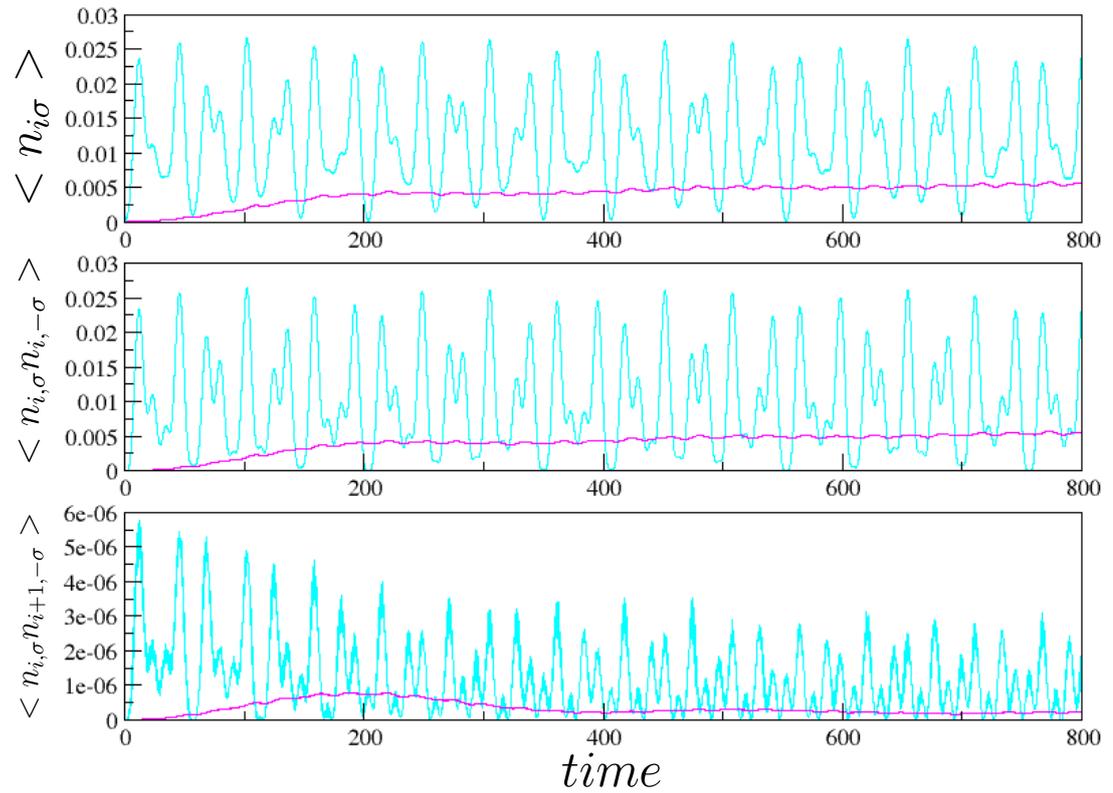


Figure 3.17:  $V_0 = 16.5$ , which means that we are at resonance with the on-site interaction. We see that the largest part of the transmission occurs through coupled motion, just as in the case when we only included the on-site interaction. Hence, it seems that adding an off-site interaction does not affect the mechanism that couples the electrons close together.

### 3.4 Four electrons

In this section we will look at 4 electrons. This will of course be much more demanding computationally, so to make the calculations somewhat faster, the complexity of the leads was reduced. Three different types of leads were used:

In Figure 3.18 the lead consists simply of a linear chain of 4 sites.

In Figure 3.19 the lead consists of a square of sites connected to the chain. There are 4 sites in this lead.

In Figure 3.20 the lead consists of a tetrahedron with 4 sites in it.

$N_{el} = 4$
$U_c = 10$
$E_{ll} = -10$
$E_c = 0$
$W_l = -0.3$
$W_c = -0.1$
$k_{size} = 10$

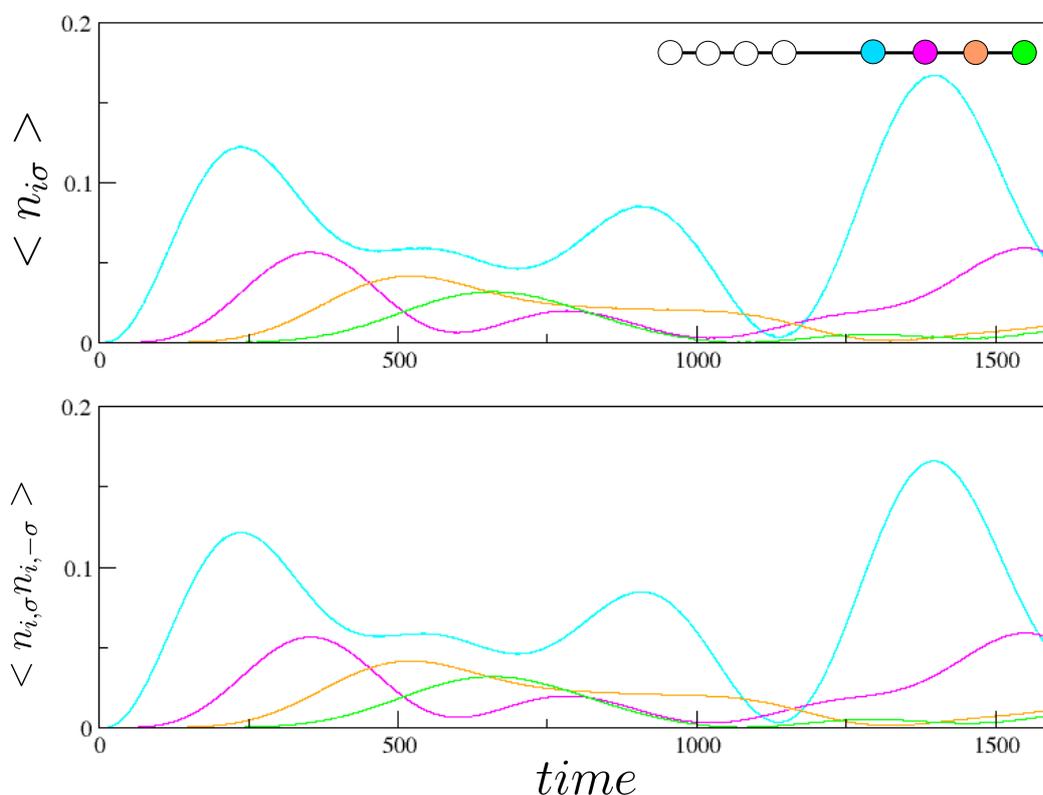


Figure 3.18: Chain as a lead. The lead consists of 4 sites.

In all of these results, in Figure 3.18, Figure 3.19 and Figure 3.20, we see that we obtain the same results as in the two-electron case. Adding two more electrons to the system does not seem to change the behavior of the travelling electrons, since the resonance condition for this is fulfilled, i.e. the bias is chosen so that the condition  $E_{gs} + N_{el} \cdot V_0 = \frac{N_{el}}{2}(2E_c + U_c)$  is fulfilled. For many particles, the condition can be rewritten as

$$\frac{E_{gs}}{N_{pairs}} + 2V_0 = 2E_c + U_c \quad (3.7)$$

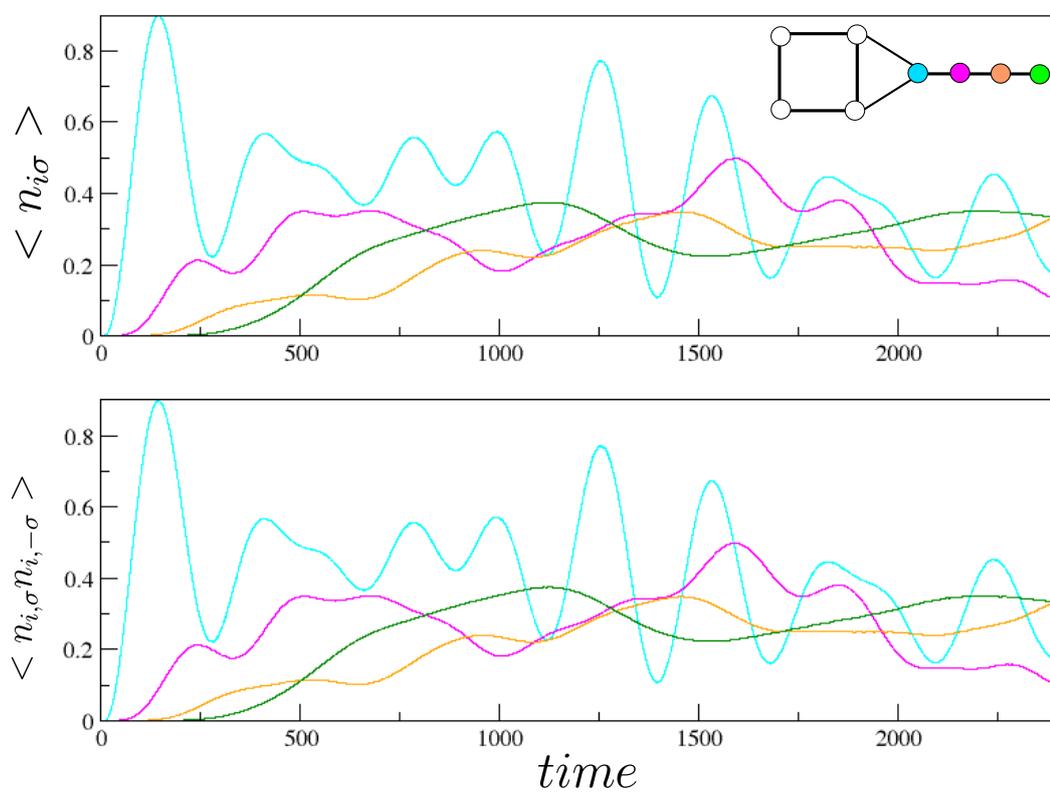


Figure 3.19: A square as a lead. The lead consists of 4 sites.

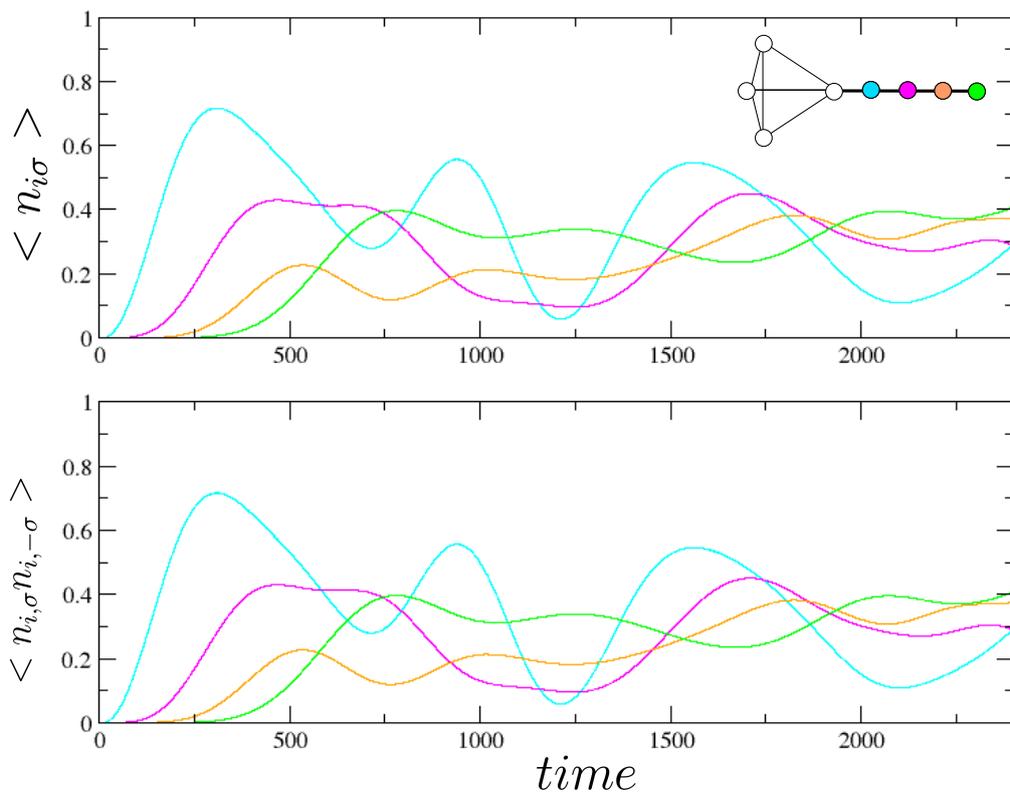


Figure 3.20: A tetrahedron as a lead. The lead consists of 4 sites.



## Chapter 4

# Conclusions and Outlook

In this thesis we have studied model systems and looked at the time evolution without further approximations. We first examined the properties of a linear chain and then moved on to a chain in 2D. After that we added leads, shaped as cubes to the system. From this we found that the electrons move more slowly in larger systems. We also saw that if there is a large energy difference between the lead and the chain, the transmission rate is essentially zero. The width of this energy window was narrow.

We then studied two-electron systems and again looked at how the system evolved in time. We saw that if we did not have any electron-electron interaction the system evolved in time in exactly the same way as if we had only one electron.

We also added an electron-electron repulsion term  $U$  which had a very small effect on the transmission through the chain. By increasing the bias to compensate for  $U$ , the electrons started to travel paired through the chain. This was confirmed by further simulations, and similar results were obtained in a four-electron system.

In the preceding chapter, we have seen several interesting properties of this model. One is the speed at which things happen, which scales with the size of the system; the linear chain had to be evolved for short times only to see the properties, whereas the lead-chain-lead system needed much longer simulation times. This will probably also hold for even larger systems, meaning that the simulation time would need to be very large for large systems.

We have also seen that even if we have an electron-electron interaction  $U_c$ , the difference in transmission through the chain is not large, see Figure 3.11. This was because of the tendency for the electrons to travel through the chain one by one, as shown by the small correlation function in this figure. If one counter this by raising the bias further, so that the energy condition  $E_{gs} + N_{el} \cdot V_0 = \frac{N_{el}}{2}(2E_c + U_c)$  is fulfilled, concerted motion was achieved. This is shown in Figure 3.13, where the correlation function is equal to the single particle density, indicating that all motion is concerted.

By applying a suitable bias, the uncorrelated motion of the electrons in the lead will change into a correlated motion in the chain. In other words, we build electron-electron pairs from random movements of electrons. The concerted motion was also

demonstrated to exist also in the presence of a Coulomb interaction with a longer range, although the resonance condition was somewhat different.

Future investigations could be made to include the effects of electron-phonon interaction, multiple orbital effects, magnetic effects, etc. More in general, by resorting to many-body theoretical methods, which we plan to address next, one could investigate systems larger in size and with different geometries.

For the phonons, one of the primary aspects to investigate would be to see if correlated motion is hindered by electron-phonon interaction, or if concerted motion is still possible.

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