Electron-phonon dynamics in Hubbard rings and chains

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Abstract

Electron-phonon interactions play a central role in the behaviour of matter in the condensed phase. Physicists' interest in this subject can be traced back to the early days of quantum mechanics, when key concepts like vibration quanta in the theory of specific heat or the Born-Oppenheimer approximation in molecular electronic structure, to mention a few, were first introduced.

The controlled manufacturing of nanoscale systems has ushered a renewed interest in the basic aspects of electron-phonon interactions since the spatial confinement in nano-structures can enhance the effect of specific vibrational modes, leading to concrete manifestations of interesting concepts such as, local temperature and heating. It is also expected that in an another area of physics, namely ultracold-atoms, the study of the interaction between itinerant fermions and phonon-like excitations can be successfully undertaken due to the possibility of controlled and accurate manipulation of experimental setups and selective inclusion of physical effects.

This thesis investigates some elementary aspects of the electron-phonon interactions in small open and closed 1D chains. Using an exact numerical method, the time-behaviour of 1) quantum rings in magnetic fields, and 2) parabolically trapped systems has been addressed when electron-phonon and/or electron-electron interaction are present.

A first outcome of this thesis is the implementation *ex-novo* of a computer code to describe the non-equilibrium dynamics of these aforementioned model systems. Using such numerical capability, we performed several numerical simulations. As a second outcome of our work, we have obtained a set of results which illustrates the complex interplay among fermion-fermion and fermion-phonon interactions in the presence of magnetic time-varying fields, and how such interplay depends on the i) non/adiabatic and ii) non/resonant character of the external perturbation.

Our work only touches the very superficial aspects of these very interesting topics, and we hope it will provide inspiration for further investigations.

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Chapter 1

Introduction

Richard Feynman claimed in a famous quote that nobody can understand quantum physics. The reason for his statement was probably the counterintuitive nature of quantum mechanics, and depending on how you define understanding you could say that Feynman was either right or wrong.

However what we can say most certainly is that we do have some knowledge of what goes on behind the curtain, in the world of probability waves. At least this is what experiments suggest.

Until the end of the 19th century, the world as we knew it could be satisfactory described in the language of classical physics. Of course nobody knew at the time the truly microscopic and probabilistic nature of the basic constituents of solid materials. One could just state that the building blocks of a solid material were in themselves solid, and at a very small scale, indivisible units existed, called atoms. Now we know that, to be able to know what really goes on, it is necessary to "peek behind the curtain".

Without the knowledge of quantum mechanics, society would be very different. Almost every piece of modern electronics has in it components that would have never been realized if it was not for ground-breaking theoretical work in the field of quantum mechanics.

With ever decreasing size of electrical components, quantum phenomena have become a limiting factor and the study of electronic behaviour in small quantum systems is nowadays a research topic of central importance. Important phenomena in such systems are the effects of phonons on the dynamics of the electrons, as well as the interaction amongst the electrons themselves.

This thesis investigates how the time evolution of one-dimensional quantum systems in presence of time varying electric and magnetic fields are affected by electron-phonon (and, at the same time, by electron-electron) interactions.

1.1 Electron-phonon and electron-electron interactions

In solids, atoms are arranged in regular lattice structures. Of course, there can be imperfections, vacancies, etc., since disordered or "defective" structures (e.g. amorphous solids) are a common occurrence in nature. However, the very existence of regular patterns for the atom equilibrium positions and their displacement around such positions, are at the origin of many physical and chemical properties exhibited by materials.

This simple fact has been recognized for a long time by material scientist, chemists, and physicists, with statistical or macroscopical theories for sound or heat or electrical conduction (e.g. in terms of equations for wave propagation in continuous media, or the Drude's model for metals), but it was only with the introduction of quantum mechanics and the quantization of lattice (or atomic) vibrations (e.g. Einstein's and Debye's theories of specific heat [1] [2]), that quantitative agreement between theory and experiment was possible in situations precluded to a classical description.

The key concept/entity in the quantum theory of lattice vibrations is the phonon (this notion was introduced by Igor Tamm in 1932 [3]), the quantum of a vibration mode, which corresponds to a coherent motion of atoms in a solid. Different types of phonons exist, corresponding to vibrations of different frequency and wavelength, and also to different patterns of relative motion of the atoms. In the following we assume that the reader is familiar with the phonon concept, and defer to the literature [4] for a simple introduction to the subject.

Phonons affect conductivity at high temperatures. This is simply because the scattering rate of the electrons increases as the lattice is deformed by the vibrations. But even at low temperatures, where the lattice vibrations are at a minimum, the electron-phonon interaction can significantly affect the properties of quantum systems.

For example, at low temperatures electrons can form pairs through indirect interaction through lattice deformations i.e. electrons interact through electron-phonon interaction. The bound electrons pairs, which are called Cooper pairs [5], are bosonic and hence not a subject to the Pauli exclusion principle; this is the core aspect in the explanation of superconductivity, one of the more spectacular examples of phenomena caused by electron-phonon interactions, *h.c.* refers to the hermitian conjugate.

The systems considered in this thesis are strongly correlated one dimensional systems. A simplified model for the description of these systems is the Hubbard

model [6]. The corresponding Hamiltonian (the so-called Hubbard Hamiltonian), written in the formalism of second quantization, reads as follows:

$$\mathrm{H} = -t \sum_{\langle i,j\rangle,\sigma} (c^{\dagger}_{i,\sigma} c_{j,\sigma} + h.c.) + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} + \sum_{i} \epsilon_i n_i \tag{1.1}$$

The Hamiltonian is made up of three parts: a kinetic part, a part which accounts for the electron-electron interaction and a part for the on-site energies. The creation (annihilation) of and electron with spin σ at site i is described by the creation (annihilation) operator $c^{\dagger}_{i,\sigma}$ ($c_{i,\sigma}$), t is the hopping amplitude (taken to be $t = 1$ in our simulations), U the electron-electron coupling, $n_{i,\sigma} = c^{\dagger}_{i,\sigma} c_{i,\sigma}$ the number operator for electrons of spin σ on site i (the site occupation operator is $n_i = n_{i,\uparrow} + n_{i,\downarrow}$) and ϵ_i the on-site energy of site i.

In the expression for the kinetic energy, $\langle i, j\rangle$ stands for the sites i, j that the electrons are allowed to hop between. In most cases this would be the adjacent sites.

Approximations made in the model are that the electrons only can exist spatially at given sites and that the Coulomb repulsion only affects electrons that occupy the same site and that the electrons only are allowed to hop between adjacent sites.

It should be noted that the Hubbard model is just an extension of the tight binding model with added electron-electron interaction, because of this the term $U \sum_i (n_{i,\uparrow} n_{i,\downarrow})$ is referred to as the Hubbard term.

The Hubbard Hamiltonian does however not take phonons into account. A popular model which is the analogous of the Hubbard model but with electron-phonon (instead of electron-electron) interactions is the Holstein model [7], first introduced to describe system where every "site" consisted of two atoms vibrating with respect to each other. With the atoms closer to each other the overlap of the potentials would be larger and thus the on site energy would lower.

In terms of energy operators the vibration between the atoms at one site i is described by a quantum oscillator $\omega_0 b^{\dagger}_i b_i$ with $b^{\dagger}$ (b) being the phonon creation (annihilation) operator. The term $\omega \frac{1}{2}$ is left out since it just shifts the overall energy by an amount and hence does not affect the dynamics. The shifting of the site energy is accounted by the term $\lambda(b^{\dagger}_i + b_i)$ which, multiplied by the electron density accounts for the electron-phonon interaction.

When electron-phonon (electron-electron) interactions are introduced in the Holstein (Hubbard) model, one then arrives to the so-called Hubbard-Holstein model. This model is very popular and has proven successful in many situations involving

strongly correlated systems in the presence of phonons [8], and it will be the model used in this thesis.

In more detail, the whole Hubbard Holstein Hamiltonian is a sum of a electronic part, a phononic part and an electron-phonon part:

$$\begin{aligned} \mathrm{H} &= \mathrm{H}_{el} + \mathrm{H}_{ph} + \mathrm{H}_{el-ph} && (1.2)\\ \mathrm{H}_{el} &= -t \sum_{\langle i,j\rangle,\sigma} (c^{\dagger}_{i,\sigma} c_{j,\sigma} + h.c.) + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} + \sum_{i} \epsilon_i n_i && (1.3)\\ \mathrm{H}_{ph} &= \omega_0 \sum_{i} b^{\dagger}_{i} b_i && (1.4)\\ \mathrm{H}_{el-ph} &= \lambda \sum_{i} n_i \cdot (b^{\dagger}_{i} + b_i) && (1.5) \end{aligned}$$

The Holstein Hamiltonian is obtained from Eq.(1.2) when $U = 0$.

In another, equally important way to invoke the electron-lattice interaction, the phonons, instead of being coupled to the density at one or more sites, can affect the hopping between sites. The hopping amplitude would then change in time, which could be seen as the distance between nearest neighbour sites is oscillating. i.e. almost as if the lattice was "breathing", see Eq. (1.6). With this type of coupling Eq. (1.5) is removed and the kinetic energy term in the Hamiltonian changes into:

$$\mathrm{H}_{kin} = -\left(t + \lambda \cdot (b^{\dagger} + b)\right) \sum_{\langle i,j\rangle,\sigma} (c^{\dagger}_{i,\sigma} c_{j,\sigma} + h.c.) \qquad (1.6)$$

In this thesis the effect of such a phonon mode is investigated for quantum-ring systems.

1.2 Quantum rings

An interesting class of 1D systems is quantum rings. The study of quantum rings is a very popular topic for research and the manufacturing of rings has gone through a vast development and today it is at a stage where it is possible to create quantum rings with only nanometres in circumference [9] and with only a few electrons. Furthermore, cold atom experiments can be used to simulate ring systems with the advantage of tuning the parameters with high precision.

One can also pierce a quantum ring with a magnetic flux and then the Lorenz force will act upon all of the charged particles in the ring. This is also possible to do with quantum rings.

This is most often done by a magnetic flux that is zero at the perimeter of the ring. This kind of flux is known as Aharonov-Bohm flux after the Aharonov-Bohm effect which is a quantum phenomenon where charged particles are affected by a electromagnetic field despite not being in the field. Using the Aharonov-Bohm flux also means that one doesn't have to account for on-site energy splitting due to the Zeeman effect which would instead occur if the magnetic field was non-zero at the perimeter of the ring. The Lorentz force will act upon the electrons in a uniform manner, such that the force on every electron would be equal and in the same direction in the ring (clockwise or counter clockwise). This force can be implemented as a complex phase in the hopping terms of the Hamiltonian. [10]

$$\mathrm{H}_{kin} = -t \sum_{i,\sigma} (c^{\dagger}_{i+1,\sigma} c_{i,\sigma} e^{\phi(t)/L} + h.c.). \tag{1.7}$$

Here L is the number of sites in the system.

By this kind of manipulation of the magnetic flux it is possible to create persistent currents. This is one of the most studied subject related to quantum rings. It has for example been proposed that this prescription could be used for memory bits in a quantum computer (qubits). [11]

It has also been proposed that a quantum motor could be driven by an alternating magnetic field [12]. The manufacturing of such a device is still in the future, but thanks to the continuous advances in cold atom physics, it is expected that these types of systems can be eventually simulated and evaluated.

For a non-interacting system without impurities a constant change of the magnetic flux ($\dot{\phi}(t) = c \neq 0$) will result in an oscillating current with average zero, for this reason most people study cases where the magnetic flux is changed from an initial value ϕ_i to a final value ϕ_f. An example of this kind of investigations is offered by the work of Mierzejewski *et al.* [13], where the focus is on how the persistent current in a ring is influenced by the way the magnetic flux is ramped up.

In this thesis we reproduce and build on the results of Mierzejewski *et al.*: after reproducing the results of Ref. [13], we then study the case where the ring is coupled to a breathing phonon mode, and we look at how the current changes with different strengths of the electron-electron interaction.

1.3 Cold atoms and optical potentials

Lasers have been a great asset in many areas of physics. Since the 90's the use of lasers to cool and trap atoms has gone through a vast improvement. Today it is

possible to tune optical potentials for both bosonic and fermionic atoms to a very high degree of precision. [14–16]

Using fermionic atoms it is possible to simulate systems with electrons in a way that would be impossible otherwise. The ability to tune all of the parameters makes cold atoms a great playground for testing new ideas and models.

In dealing with a many-particle problem (this is the typical situation one has to face when working with condensed matter systems), both analytical and numerical approaches are at a limit where the dynamics only can be calculated through severe approximations. Here cold atom physics can play a role in simulating systems. By directly comparing the experiments to simulations, the effect of the approximations can be evaluated and thus the theoretical work can be pointed in the right direction.

In this work we investigate a one-dimensional system with a few electrons trapped in a parabolic potential. The middle site, which is least affected by the parabola, has a localized Holstein phonon attached. We examine the time evolution in this system when the parabola is shaken.

To summarize, this thesis investigates one-dimensional quantum systems through computer simulations, using the Hubbard and Hubbard-Holstein-like models. Our work is limited to small systems with up to four electrons and one phonon mode at most.

Since the models we have used in this study are based on simplifying approximations, this will of course affect the results when compared to specific realistic situations or materials. Therefore it should be stressed that all the results in this thesis are purely theoretical and that they rest upon the assumption that the model is applicable to the systems investigated (an assumption often justified in the case of cold atoms). At the same time, it is hoped that some of the qualitative aspects of our findings are relevant to the understanding of more realistic situations.

The aim of this thesis is to produce results that will be used in a future publication and, through this, contribute to the scientific advancements in the field of condensed matter physics.

Chapter 2

Method

The results produced in this thesis are the output of several simulations done with two distinct computer programs. While quite different in structure and range of applicability, the two computer codes rest of the same basic methodology, namely the exact diagonalization solution of the static and time-dependent Schrödinger equation for a finite number of particle/orbital in a full configuration-interaction scheme. [17]

Input to the programs are parameters like the number of sites and electrons in the system, on-site interaction etc. From the input parameters the Hamiltonian is created. The Hamiltonian is diagonalized by a routine which returns the eigenvalues and the eigenstates in a pre-assigned order. The lowest eigenvalue is the groundstate energy and the corresponding eigenvector is the groundstate.

After this, the program calculates the time evolution, starting from the ground-state. If nothing in the system is changed, the state will remain in the groundstate. With the system disturbed, the state will change in time. The integration in time will be made by discretizing the time-axis in terms of small "time-steps".

For every time step the program will apply a number of operators which calculate the expectation values of the respective physical quantities and save the data so that they can be analysed at a later time.

The program used for the ring systems was coded from scratch as part of the bachelor project. Thus, this chapter will be used to explain the theory and the methodological principle behind building such a program.

2.1 Creating the Hamiltonian.

2.1.1 Basis set and assembly

To create the Hamiltonian one has to decide which basis will be used throughout the simulation. Furthermore, the system needs to be described within a finite Hilbert space, so that it can be implemented in a computer with a finite memory.

Take the example of a system with two sites and one electron: a simple basis set would be $\{|1\rangle, |2\rangle\}$ with $|i\rangle$ being the state with the electron being on site i. This written in second quantization formalism would be $\left\{c_i^\dagger |0\rangle : i \in sites\right\}$ with $|0\rangle$ being the vacuum state.

The mathematical requirements for the basis is that it should be complete within the Hilbert space and that the basis state vectors should be orthogonal. This means that one could use any linear combination of the basis vectors above that fulfils these mathematical requirements. However, for the construction of the Hamiltonian another requirement one should add is that the basis set should be relevant for the given Hamiltonian.

This is not only important for aesthetic reasons. If a good basis set is used the Hamiltonian matrix will be sparse, i.e. it will have many zero elements, and sparse matrices are in general easier to diagonalize. Some approximative methods of diagonalization only work on sparse matrices. In our case we have a Hubbard model (and extensions), where all the interactions are on-site or between adjacent sites and therefore a basis like the one suggested for the two site system is advantageous in most instances.

For one spin up and one spin down electron the Hilbert space becomes the product space of two single electron subspaces and the space dimension is just L^2, where L is the number of orbitals. However for systems with electrons of the same spin it gets a bit more complicated. Since the electrons aren't allowed to occupy the site, the Hilbert space dimension becomes $\binom{L}{N_\sigma}$ where N_σ is the number of electrons in the spin σ channel. With both spin up and spin down systems the Hilbert space will be the product space of the spin up and the spin down subspaces.

To incorporate a phonon mode, the Hilbert space becomes the product space of the phonon mode subspace and the electronic subspace. The only problem is that the phonon mode which is described by a harmonic oscillator has an infinite number of energy levels, i.e. an infinite number of phonons. But since the energy within the system is finite, the amount of phonons that can be created is limited and thus one sets a limit of how many phonons are practically allowed in the system. This

is something that can cause trouble in some situations: to make sure this doesn't happen, one can do tests to see if the results are converged in terms of maximum phonon number, (see the Ehrenfest's theorem in section 2.4.5).

The basis set which was used during the bachelor project was in the most complex case made of two spin up and two spin down electrons and one phonon mode $\{|i<j;k<l,p\rangle\}$ with $i,j,k,l \in Sites$ and $p \in \{0,1,2,\ldots,P_{max}\}$. Here the basis vector is labelled with five letters: i,j are the spin up electrons, and k,l are the spin down electrons; p is the number of phonons in the phonon mode. The Hilbert space dimension in this problem is $\binom{L}{N_\uparrow}\binom{L}{N_\downarrow}\cdot(P_{max}+1)$.

With the basis fixed one has to assemble the Hamiltonian matrix, i.e. the matrix elements $H_{\alpha\beta}=\langle\alpha|H|\beta\rangle$ have to be calculated. For the phononic part of the Hamiltonian this becomes:

$$H_{ph-ij}=\langle\alpha|\omega_0 b^\dagger b|\beta\rangle=\omega_0\cdot p_\beta\cdot\delta_{\alpha,\beta} \tag{2.1}$$

With p_β being the number of phonons in the state the basis vector $|\beta\rangle$, and $\delta_{\alpha,\beta}$ being the Kronecker delta. To assemble the Hamiltonian matrix all the parts of the Hamiltonian should be expressed in a similar way. This is a bit harder for the kinetic part in a many-electron systems, but the approach, while requiring tedious algebra, remains completely straightforward.

2.2 Diagonalization and groundstates

To determine the groundstate of the system defined by a Hamiltonian matrix one has to diagonalize the Hamiltonian. This can be done with many different specialized routines. In our case, we used full-diagonalization techniques for the case of quantum rings, and the Lanczos algorithm [18] for the system modelling ultracold fermion-atoms in a 1D chain and a localized phonon at the middle site.

The diagonalization method can either be based on i) full diagonalization of the Hamiltonian, or ii) the calculation of only the few lowest eigenvalues/eigenvectors (including of course the ground state). With i), one can reach highly excited states, but the method can only be used for relatively small matrices; with ii) much less information is available, but considerably larger systems can be tackled than those accessible with i). In any case, for the program build, it is expedient to use properties such as hermiticity, spin and translational symmetries, fixed number of particles, etc., to reduce the numerical effort, since this permits to block-diagonalize the Hamiltonian at the analytical level.

The diagonalization method returns eigenvalues (the lowest of them is the ground-state energy) with their respective eigenvectors. Trouble can arise if not all relevant symmetries are taken into account, since undesired degeneracies may occur, which may affect the expectation value of some observables. For example, this is something that we expected and numerically experienced for 4 non-interacting electrons (2 up, 2 down) in a 6 site ring. By performing the calculation in a straightforward way (no translational symmetry taken into account), the density was not uniform. This is because of degeneracy. In the basis of Bloch states, states with wave number k and $-k$ have the same energy, and thus the resulting state will be an arbitrary linear combination of these states. There are different ways to address this. The slightest change in one parameter can make the groundstate non-degenerate, which solves the issue. In our case this could be done by calculating the groundstate of a very weakly interacting system. This sort of trick can affect the accuracy of the results and is most certainly not always possible. The rigorous way is to enforce the required symmetry in the basis set, or for the Lanczos technique, to start with a "seed" state which has the symmetry in question. When $U = 0$, for the simple case at hand (a six sites ring, four two up and two down electrons), we used a shortcut, since the ground state can be easily determined analytically (here expressed in the basis of Bloch states):

$$|\Psi_{in}\rangle = c^\dagger_{k_0,\uparrow} c^\dagger_{k_0,\downarrow} \frac{c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow} + c^\dagger_{-k,\uparrow} c^\dagger_{k,\downarrow}}{\sqrt{2}} |0\rangle \,, \quad k_0 = 0, k = \frac{\pi}{3a} \tag{2.2}$$

With a in the formula referring to the lattice constant.

This state has uniform spin-up/down densities, zero charge- and spin-currents, and is a singlet ($S = 0$) state.

2.3 Time evolution

If the Hamiltonian used when doing the time evolution is the same as the one used to calculate the ground state the system will not change in time, apart from an obvious phase factor. Thus, to be able to see any non-equilibrium dynamics, the Hamiltonian must be changed at at least once (for example, suddenly at some time t_0).

It is of course possible to set by hand the initial state of the system. For example if the system was consisting of six sites with one electron one could put the electron in on the first site and then look at what happens when "the clock starts". Having the possibility to do this via a computer program is a huge asset, as seeing the dynamics in the simplest cases helps to understanding the more complex ones.

2.3.1 Time-independent Hamiltonian

To do time evolution one has to solve the Schrödinger equation. According to the discussion made earlier, one can express the solution of the Schrödinger equation in the following way:

$$|\Psi(t)\rangle = \exp(-iHt) \cdot |\Psi(0)\rangle \,. \tag{2.3}$$

By inserting the completeness relation in the basis of the eigenvectors one gets an expression of the wave function without any operators.

$$|\Psi(t)\rangle = \exp(-iHt) \cdot \sum_i |\lambda_i\rangle \langle\lambda_i| \cdot |\Psi(0)\rangle = \sum_i \exp(-iE_i t) \cdot \langle\lambda_i|\Psi(0)\rangle \, |\lambda_i\rangle \tag{2.4}$$

It is easy to see that if the initial state would be an eigenstate of the Hamiltonian, the state would only change by a phase factor, i.e. the system would not change.

2.3.2 Time-dependent Hamiltonian

To be able to look at systems affected by time-changing external fields (which is the purpose of this bachelor project) the Hamiltonian itself becomes time dependent and Eq. (2.4) as it is does not work.

However, one can use Eq. (2.4) recursively [19]

$$|\Psi(t + \Delta t)\rangle = \sum_i \exp(-iH(t + \frac{\Delta t}{2}) \cdot \Delta t) \cdot \langle\lambda_i|\Psi(t)\rangle \,. \, |\lambda_i\rangle \tag{2.5}$$

The downside of dealing with time-dependent Hamiltonians via Eq. (2.5) is that for every time step one is calculating, the new altered Hamiltonian will need to be diagonalized, and diagonalization time easily becomes the bottleneck of the program. For larger systems, other methods (e.g. the Lanczos method) are the necessary choice.

For quantum rings, for which the code just described was developed and used, the Hamiltonian is complex, and to diagonalize it will be even more expensive computation-wise. To diagonalize a 1500 by 1500 complex matrix for 4000 time steps took about one week using exact diagonalization. This time would have been reduced by orders of magnitude using, for example, the Lanczos algorithm (this procedure is followed in the code used for 1D chains in presence of localized phonons).

2.4 Operators

The state vectors contain all of the information about the system and it is useful to look at them sometimes; however, in most cases, it is much better to directly deal with

expectation values of physical observables using $\langle\Psi|\hat{O}|\Psi\rangle$, where $\hat{O}$ is the operator for the physical quantity of interest. If this is done for each time step, one can obtain the temporal behaviour of $\langle\hat{O}\rangle(t) = \langle\Psi(t)|\hat{O}|\Psi(t)\rangle$.

2.4.1 Energy

To get the total energy of the system, the operator needed is of course the Hamiltonian. It can however in many cases be interesting to see where the system deposits its energy, for instance, looking at the electronic energy versus the phonon energy in a Holstein system, or just looking at the kinetic energy. For all different cases one just uses different parts of the Hamiltonian operator.

2.4.2 Density

The quantity that in most cases probably best explains what is going on in the system is the density distribution of the electrons. It gives an intuitive picture of what is happening. The density operator is calculated for each site and the results are most often presented as the electron distribution over the sites.

In second quantization, the electron density on one site is described by the sum of the number operators for spin up and spin down electrons:

$$n_i = n_{i,\uparrow} + n_{i,\downarrow} = c^\dagger_{i,\uparrow}c_{i,\uparrow} + c^\dagger_{i,\downarrow}c_{i,\downarrow}. \tag{2.6}$$

In strongly correlated systems, electrons can pair together and bind to each other, although their interaction is repulsive. This is one of the reasons why it sometimes is relevant to look at the electron pair density (or "doublon" density). The operator is just the product of the spin up and spin down densities:

$$n_{d,i} = n_{i,\uparrow}n_{i,\downarrow} = c^\dagger_{i,\uparrow}c_{i,\uparrow}c^\dagger_{i,\downarrow}c_{i,\downarrow}, \tag{2.7}$$

and was used to monitor the degree of local correlations.

2.4.3 Current density

In general, the density current J is derived from the continuity equation:

$$\frac{\partial\rho}{\partial t} + \nabla J = 0 \tag{2.8}$$

Here ρ is the density and ∇J the flow of the current. On the lattice, the density is defined only at the sites, and this simplifies the expression. The density change at

site i is simply the amount of density that flows into the site, minus the amount of density that flows out.

$$\frac{\partial n_i}{\partial t} = J_i - J_{i+1} \tag{2.9}$$

Using the Ehrenfest theorem on the left hand side gives us for the Hubbard Hamiltonian:

$$\frac{\partial n_i}{\partial t} = i\left[H, n_i\right] = -it((c_i^\dagger c_{i-1} - h.c.) - (c_{i+1}^\dagger c_i - h.c.)) = J_i - J_{i+1} \tag{2.10}$$

Notice that the density operator commutes with all parts of the Hamiltonian except for the kinetic energy term.

Identifying J_i and taking the average of all the sites we get an expression for the mean current in the system.

$$J = -i\frac{t}{L}\sum_{i,\sigma}(c_{i+1,\sigma}^\dagger c_{i,\sigma} - h.c.) \tag{2.11}$$

To get the electrical current one just multiplies the density current with, in this case, minus the elementary charge, which in our units is $-e = -1$.

When the ring is pierced by the magnetic flux and/or breathing phonons are present, we can follow a similar strategy to determine J. This is possible because the density operator commutes with all phonon operators, and the magnetic field is just represented by a phase factor in the hopping amplitude. Thus, the expressions for the charge current in the most general case of interest in this thesis becomes:

$$J = (t + \lambda(b^\dagger + b))\frac{1}{L}\sum_{i,\sigma}(c_{i+1,\sigma}^\dagger c_{i,\sigma} e^{\phi(t)/L} - h.c.). \tag{2.12}$$

2.4.4 Phonon operators

Even if one is only interested in the purely electrical quantities in a system, like charge densities, doublon densities, etc., it is good to know what the phononic part of the system does.

The simplest example is the number operator which gives the number of phonons in the system. This is simply $b^\dagger b$ and is found in the Hamiltonian in the expression for the phonon energy which is $\omega b^\dagger b$, with ω being the frequency of the phonon mode.

Other interesting operators are the position and the momentum operators:

$$x = \sqrt{\frac{1}{2\omega}}(b^\dagger + b), \tag{2.13}$$

$$p = \sqrt{\frac{\omega}{2}}(b^\dagger - b). \tag{2.14}$$

These two operators can also be used as an asset in developing the program to test if the phonon mode was correctly implemented and if the results are converged with respect to the highest amount of phonons allowed P_{max} (in the following, we will occasionally refer to P_{max} as the "phonon-roof"). The computer program that was built in this project uses the Ehrenfest theorem for the momentum operator to perform these checks.

2.4.5 Ehrenfest's test

The Ehrenfest theorem [20] states that

$$\frac{\partial}{\partial t}\langle A\rangle = i\langle[H, A]\rangle + \left\langle \frac{\partial A}{\partial t} \right\rangle. \tag{2.15}$$

In our case we will apply Eq. (2.15) to the phonon momentum for two reasons: i) the time-derivative of $\langle p\rangle$ is the force, which in itself could be an interesting quantity to look at; ii) the theorem can be used to check the accuracy of the numerical calculation. In more detail, the left and right hand side of Eq. (2.15) are calculated independently, and their difference is monitored at all time steps. If the mean error is close to zero then the calculations are correct and have converged, otherwise P_{max} and/or the time-step needs to be corrected.

To have a function that to some extent tests the results qualitatively is a huge asset when developing the program. The phonon-roof convergence is here just a bonus.

2.5 Limitations

First of all, there are limitations in the physical model. The Hubbard model assumes that the effects of density distributions between the sites, the tunnelling between non-adjacent sites and Coulomb interactions between electrons outside the sites are negligible. One can easily imagine situations where this is not the case.

Besides limitations in the model, we also have technical limitations related to the numerical implementation of the model, for example effects related to the truncation of the phonon subspace. With time dependent Hamiltonians, the time step also becomes an issue. By making the time step small, one reduces the error that comes with the making the time dimension discrete, but this means that the amount of time it takes to do a simulation is increased.

We also have limitations in the kind of calculations that can be performed with today's computers. With full diagonalization, the limit in size of the viable matrices is about ≈ 25000. With indirect methods such as Lanczos diagonalization, and using parallel architectures, the dimension of the matrices can be increased up to hundreds of millions, which may sound large; however, when considering many particles and phonon modes one realizes that this is in fact quite small, especially when looking at systems in higher spatial dimensions.

Chapter 3

Simulations

In this chapter the results produced by the computer simulations will be presented with relevant figures and analysis. The two kinds of systems we considered will be discussed separately, in two sections. For every run the input parameters will be specified and also a qualitative analysis of what causes the effects seen will be given.

3.1 Ring system

The program used to produce the results in this section was developed during the bachelor project. Because of this, some previous results already published [13] were reproduced to check the validity of the program, and they are presented here for the sake of comparison to our results with rings in presence of a breathing mode (see 3.1.2). It should also be stated that the currents in the plots are relative currents, i.e. the quantity presented as the current is equal to $\langle J \rangle / J_0$ with $J_0 = \frac{2\pi t}{L\Phi_0}$ (this is $\frac{t}{L}$ in our units and the prefactor in the expression of the current operator, see Eq. (2.11)) with $\Phi_0 = h/e$ being the flux quantum.

In all cases, the magnetic flux will be ramped up from zero to Φ_0 in a finite time T, as seen in figure 3.1. By looking at different ramping times we observe the difference in the charge density current.

3.1.1 Four electrons in systems with different electron-electron interactions

In the four-electron case without phonons we reproduce the results of M. Mierzejewski, J. Dajka and J. Luczka [13]. Although we use a smoother ramping shape, the differences in the results are very small. The results are

$L = 6$
$N_\uparrow = 2$
$N_\downarrow = 2$
$U \in \{0, 1, 4, 16\}$
$T \in \{1, 25\}$

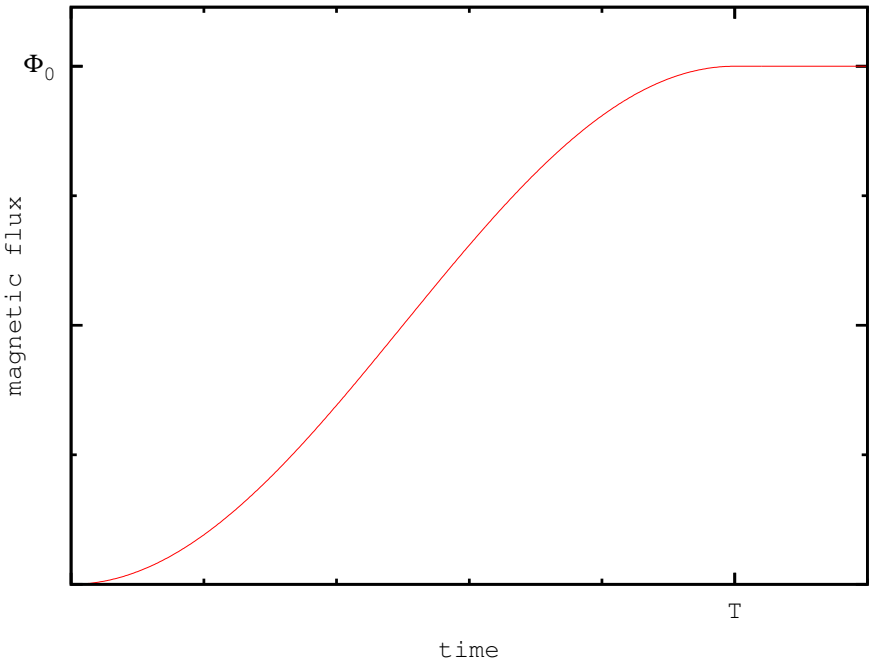

Figure 3.1: In this figure we see the shape of ramping up the magnetic flux. For the parameters used, see main text.

presented in figure 3.2. (When we use the exact same ramping as M. Mierzejewski *et al.* the differences are indistinguishable in the way the results are presented.)

We can see that the final value of the current does not depend on the ramping when the electron-electron interaction is 0 and when it tends to infinity. For $U = 0$ the current is much larger than for $U = 16$: in fact, this is is a general trend, i.e. the DC component of the final current decreases with U. The decrease in current, even for intermediate electron-electron interaction, can be seen as increased viscosity in the electrons as the effect of collisions increases.

For the intermediate electron-electron interactions, the effect of different ramping speeds becomes apparent. The oscillation amplitude of the final current is larger when the magnetic field is ramped up fast, and the DC component of the current becomes larger for longer ramping times.

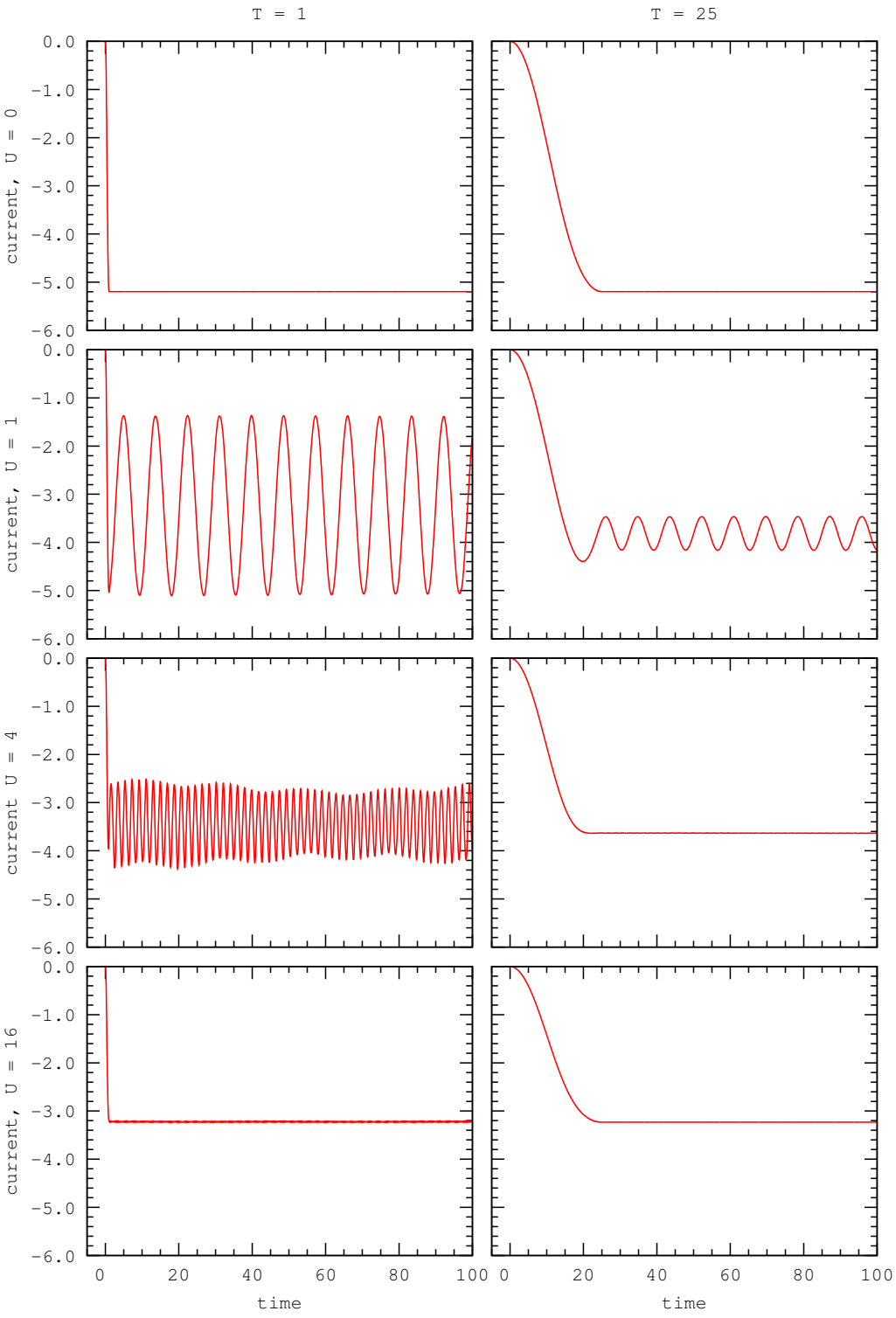

Figure 3.2: Ring, 6 sites, 4 electrons, ramping from 0 up to Φ_0 in T unit times.

3.1.2 Two electrons in presence of a breathing mode

$L = 6$
$n_\uparrow = 1$
$n_\downarrow = 1$
$U \in \{0, 1, 4\}$
$T \in \{5, 25\}$
$\omega_0 = 0.5$
$\lambda = 0.2$

In the presence of phonons, we again ramp up the magnetic flux at different speeds and consider the current for different strengths of the electron-electron interaction. This time, we choose a system with two spin-compensated electrons instead of four, to reduce the computational effort in the presence of phonons. The results are shown in Fig. 3.3. As an aid to the discussion, we also include the case of two electrons with opposite spins and no electron-phonon coupling.
Looking at Fig. 3.3, we can see a superficial similarity with the case of four particles without phonons (namely, the current carries in general both DC and AC components).

However, a closer look reveals a crucial difference: in the presence of the phonon mode (red curves), the oscillations are exclusively due to the phonon mode (they in fact always have the same frequency, the phonon frequency). Conversely, oscillations induced from the interactions are visible in the absence of phonons (blue curves), at frequencies other than ω_0. However, these are much weaker than in Fig. 3.2. Thus, it appears that one simple reason why we see strongly reduced (or no-) oscillations related to the electron-electron interaction is that there are fewer particles (two instead of four) in the ring, and they produce less AC and DC currents.

A second and less obvious reason (for a reduction of the oscillations when phonons are present) is the increased effective hopping due to the presence of the phonon mode, which contributes to an increased delocalization of the electrons (i.e. the system is effectively less correlated): for the ground state with phonons, the average displacement $\langle b^\dagger + b \rangle = 3.2$, meaning that the the module of the effective hopping parameter has increased. This makes the system less correlated, and at the same time increases the prefactor for the current operator. We are currently performing a systematic scan of the parameters to test a broader validity of these conjectures.

Turning to the oscillations induced by the phonon mode (these are the only oscillations visible in the red curves of Fig. 3.3), we observe a smaller DC component with higher U, and the oscillations of the AC component are larger for the faster ramping times. Comparing the plots with equal T and different U, the differences in the shapes of the current are now much smaller than in the no-phonon case, and only the magnitude of the DC component appears to be affected.

By changing the magnetic field slowly the amplitude of the oscillations tends to zero, but this appears to require a much slower rate of change of the magnetic

field than for the four-electron case without phonons. Most likely, this behaviour is strongly dependent on the frequency of the phonon and the number of particles in the system, and it deserves further scrutiny (additional simulations are under way).

As a conclusion to this section, electron-phonon interactions and their competition with electron-electron interactions can affect in a non-trivial way the currents in a quantum ring threaded by a magnetic flux. We have just begun to grasp few simple aspects of the dynamics, and additional investigations, currently under way, are expected to provide additional features and more comprehensive scenario for the behaviour of ring currents.

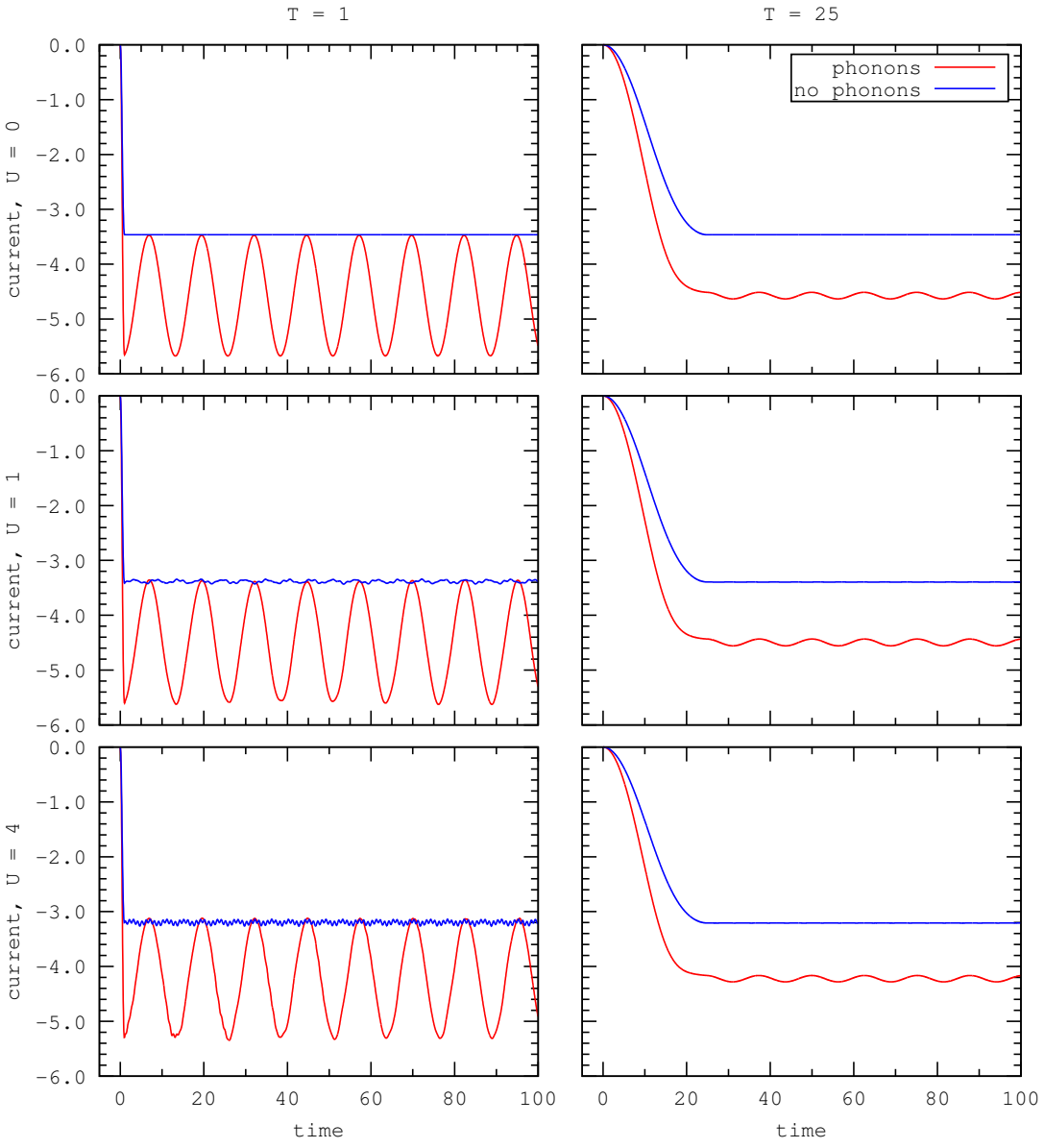

Figure 3.3: Ring coupled to a breathing phonon mode, 6 sites, 2 electrons, ramping from 0 up to Φ_0 in T unit times.

3.2 A 1D chain in an oscillating trapping potential

One of the most used experimental set-up in ultracold-atom physics consists in trapping an atomic cloud in a confining (usually parabolic) potential, and then release the trap (usually suddenly), to observe the cloud expansion, and to infer characteristic features (correlation functions, entanglement, ballistic vs diffusive behaviour) of the cloud. This setup has been also used for ultracold atoms loaded into optical lattices, providing the motivation for our investigation here. The novel element in our analysis is the presence of phonon-like vibrations in the optical lattice.

More specifically, we will present our results for a system consisting of a one dimensional chain of 11 sites. The middle site is interacting with a Holstein phonon mode. The whole system is disturbed (and at the same time trapped) by an external potential in the form of a parabola. The parabola strength, whose strength is oscillating in time, is introduced as a change in the on-site energies of the system. We label the sites i with $i \in \{-5, -4, -3, -2, -1, 0, 1, 2, 3, 4, 5\}$ and 0 being the middle site. The parabola potential is then

$$\epsilon_i(t) = \frac{i^2}{2} \cdot (1 + \frac{\sin \omega_{par} t}{4}) \tag{3.1}$$

We look at fermion density, total energy and energy deposited in the phonon mode and we observe the differences in the dynamical behaviour of the system when varying the oscillation frequency ω_{par}.

3.2.1 Two fermions

To start with, we look at the results for two fermions and with interaction strength of $U = 10$ (figure 3.4). In the first case (leftmost column) we consider, the parabola frequency is $\omega_{par} = 0.1$, which is very slow compared to the electronic time-scale. Because of this we see almost perfect periodic behaviour of the fermion densities. The phonon has very little energy, but one can see that it creates overtones on the densities, especially prominent at site 0.

$L = 11$
$n_\uparrow = 1$
$n_\downarrow = 1$
$U = 10$
$\lambda = 0.1$
$\omega_0 = 0.5$
$\omega_{par} \in$
$\{0.1, 0.5, 0.6, 2.5\}$

Looking at the energy temporal profile, one can see quite big oscillations in the total energy. These oscillations coincide with the oscillations of the parabola and thus should be interpreted as an effect of the change in on-site-energy (of course, in reality some energy is also deposited as kinetic energy and interaction energy (for example, the particles tend to pile on top of each other when the parabola is narrowed.)

The case with $\omega_{par} = \omega_0$ is probably the most interesting one among those considered. Starting with the energy curves, we see a great deal of difference from the previous case (note however that the amplitude of the oscillations in the total energy is the same as for $\omega_{par} = 0.1$. On the other hand, and as expected, the frequency of the oscillations is changed as the latter now are in sync with the parabola oscillation.

What is especially interesting in this case is that the phonon energy and the total energy both increase in time. This suggests that the change in fermion density at the phonon site gives the phonon an energy boost and excites the phonon mode, but the latter does not have time to de-excite completely before the next pulse of energy. In this way the parabola increases the total energy of the system by pumping energy into the phonon mode. .

In the third case we have $\omega_{par} = 0.6$, which is slightly off the resonance condition $\omega_{par} = \omega_0$. For this value of ω_{par}, we obtain a picture similar to the $\omega_{par} = 0.1$ case. However, here we don't see the same smoothness in the particle densities. We also note some oscillations in the phonon energy. In fact, there is a beating frequency in the phonon energy (see figure 3.4), useful to estimate how far are we from the resonance condition.

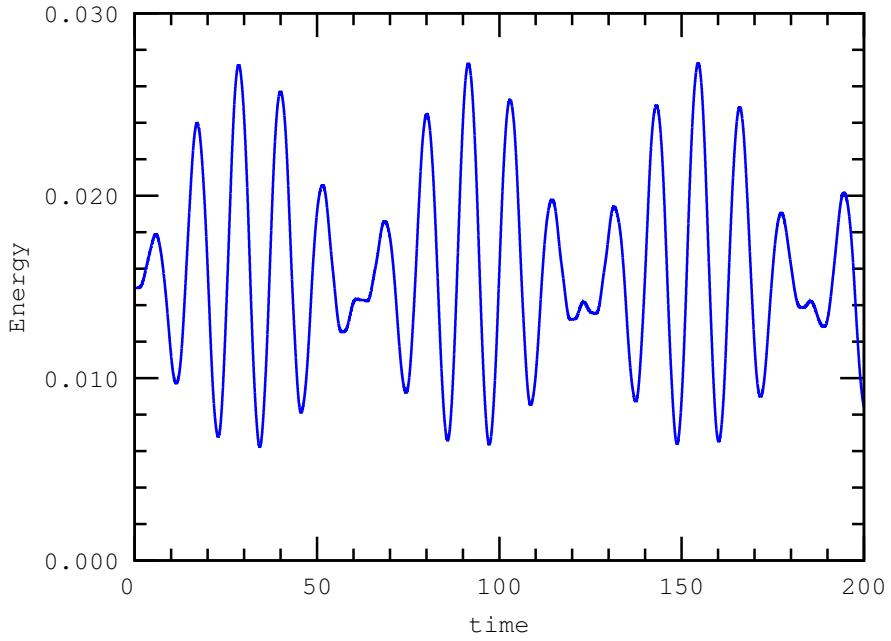

Figure 3.4: In this figure we see the phonon energy for the case with two fermions, $U = 10$ and $\omega_{par} = 0.6$.

For two sinusoidal waves with similar but not equal frequencies (here, $\omega_{par} = 0.6$ and $\omega_0 = 0.5$), we get a beating frequency ω_{beat}:

$$\omega_{beat} = |\omega_{par} - \omega_0|/2. \tag{3.2}$$

Changing ω_{par} in an experiment, and observing the beats in the phonon energy, would permit to establish the resonant frequency, and thus determine ω_0.

In the fourth case of Fig. 3.5, we have $\omega_{par} = 2.5$, which is much larger than the phonon frequency. We see that the energy of the system has oscillations induced by the parabola movement, but we also note big irregular changes in the energy curves. Qualitatively, this is understood by observing that the speed of the parabola is well into the nonadiabatic regime. Consequently, the fermions are knocked around a lot. Sometimes the parabola speeds them up, and sometimes slows them down. The change in density at the phonon site is too fast, and the phonon mode cannot keep up; therefore, it never goes into a highly excited state.

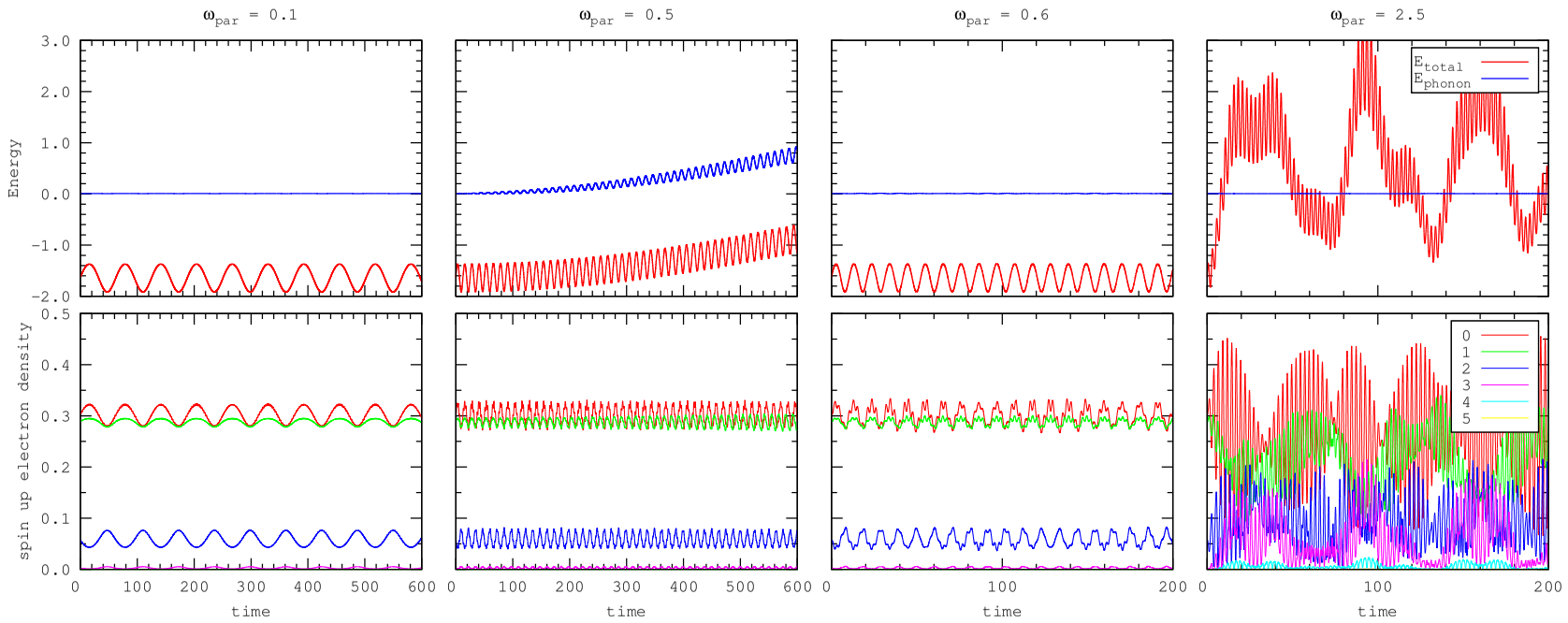

Figure 3.5: Two fermions. Total energy, phonon energy and spin-up density as a function of time. Different columns represent different parabola frequencies. The phonon frequency is $\omega_0 = 0.5$. Note that the time scales in the two last columns is different.

3.2.2 The $\omega_{par} = \omega_0$ resonance at different fermion-fermion interactions: the two-particle case

$L = 11$
$N_\uparrow = 1$
$N_\downarrow = 1$
$U \in \{0, 1, 4, 10\}$
$\lambda = 0.1$
$\omega_0 = 0.5$
$\omega_{par} = 0.5$

In this case we look at what happens when the resonance condition is fulfilled in systems with different strengths of the fermion-fermion interaction.

Looking at general trends Fig. 3.6, the oscillation amplitude of the total energy increases with U, while the phonon energy oscillations decreases in amplitude. This change of the amplitudes can be attributed to the increased fermion-fermion interaction, which forces the particles to be closer to the parabola edges, where the on-site energy is larger, see Eq. (3.1). This is easily seen in the plots of the particle density, where site 1 and 2 and even site 3 are increased substantially in density.

At the same time, when U increases, the amplitude of the density oscillations at site 0 decreases, since a larger inter-particle interaction enhances the viscosity of the fermion system. This also reflects in a smaller oscillation of the phonon energy, i.e. the energy exchange between the phonon and the fermion density is reduced (at least at the time scales we are looking at).

This decrease in energy exchange affects the rate at which energy is pumped into the phonon (seen, in figure 3.6, as a decrease in the steepness of the average phonon energy for higher values of U).

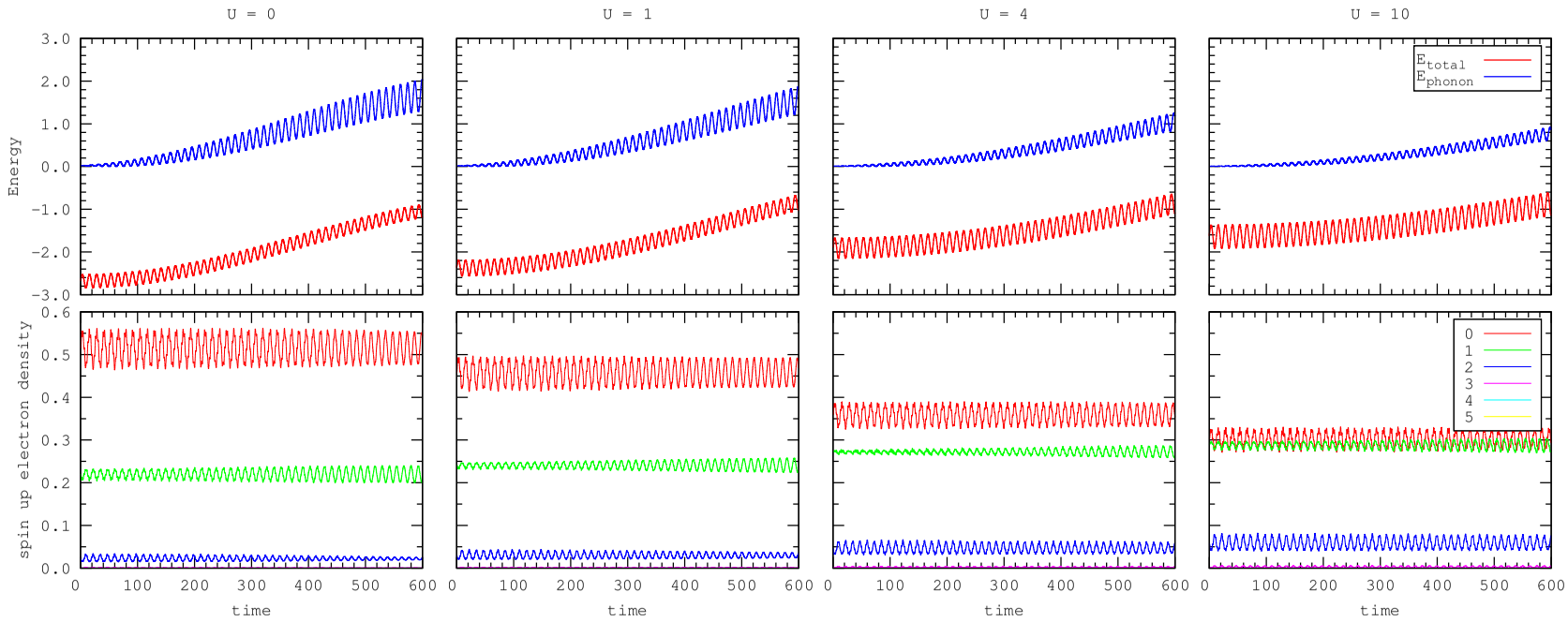

Figure 3.6: Two fermions. Total energy, phonon energy and spin-up density as a function of time. Different columns represent different fermion-fermion interaction strengths. The phonon frequency and the parabola frequency is $\omega_0 = \omega_{par} = 0.5$ i.e. the resonance condition is fulfilled in all cases.

3.2.3 Four fermions when $\omega_{par} = \omega_0$.

$L = 11$
$n_\uparrow = 2$
$n_\downarrow = 2$
$U \in \{1, 4, 10\}$
$\lambda = 0.1$
$\omega_0 = 0.5$
$\omega_{par} = 0.5$

With four particles, Fig. (3.7), and for increasing interaction strength U, the system exhibits the same qualitative behaviour in terms of total energy, phonon energy and fermion density as we have illustrated in the two-particle case. Some specific trends, though, are more easily seen with four particles, for instance the change in fermion densities at the outer sites.

One new feature, absent in the two-fermion cases we examined, is that, on increasing U and in the long-time limit, the oscillations in densities for site 0 and site 1 seem to tend to very regular, smooth shapes, with very little of the overtones we observe in the case of two fermions (see figure (3.6)).

It seems almost that this is happening for the other sites as well. The effect is prominent with higher U. On speculative grounds, this behaviour could depend on the oscillator being able to slow down the speed at which the particles are released/accepted from/into the center when the parabola is opened/closed. The slowing down of the fermionic dynamics is greater at higher U, and it makes the fermions behave more adiabatically relative to the parabola oscillations.

To briefly summarize our discussion, the system considered in this Section exhibits a rich and very structured behaviour, quite sensitive to the parameter values, and we have just given a superficial glance at its dynamical properties. We plan to perform more investigations to put our findings on a firmer ground.

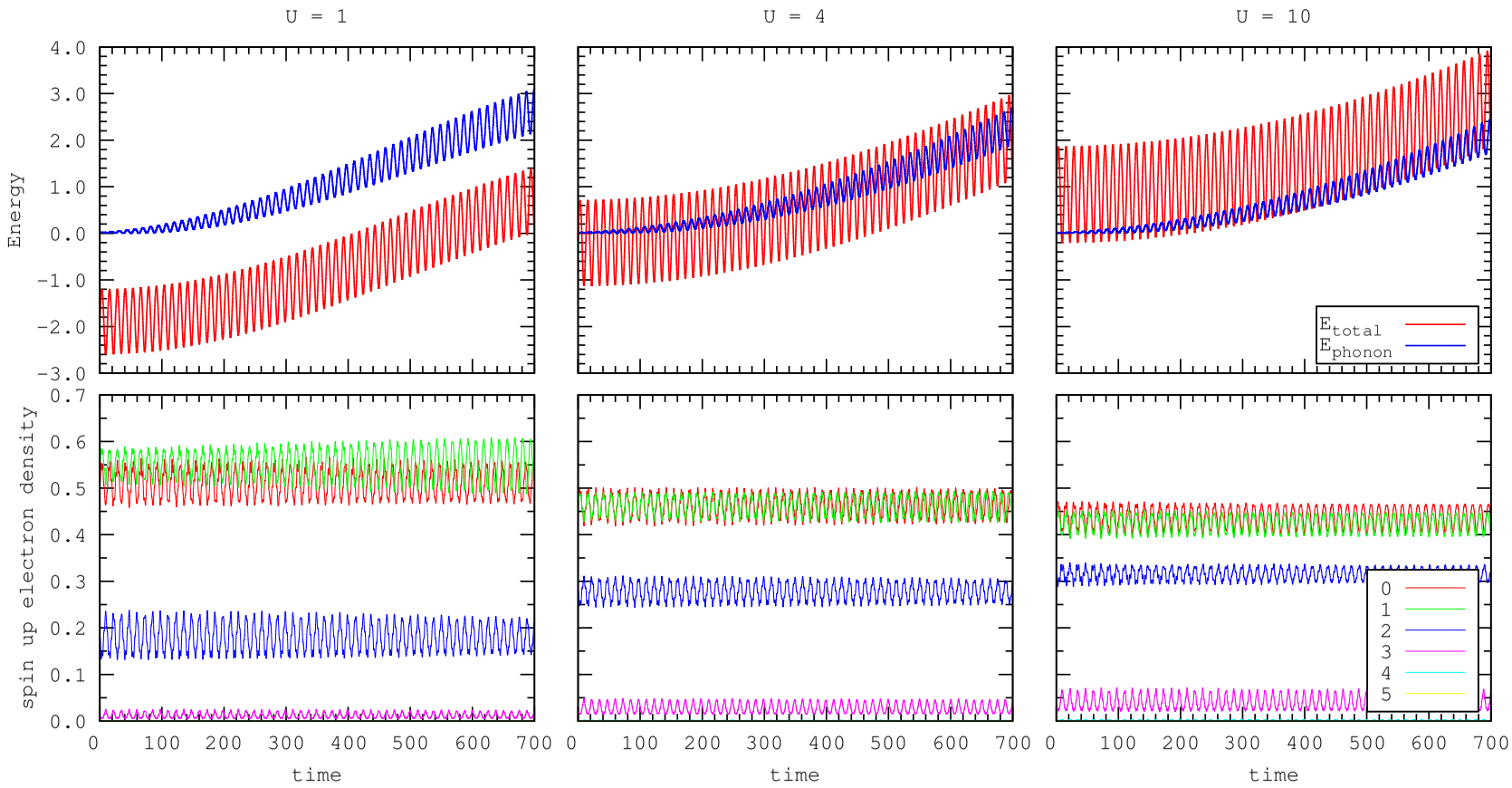

Figure 3.7: Four particles. Total energy, phonon energy and spin up density as a function of time. Different columns represent different fermion-fermion interaction strengths. The phonon frequency and the parabola frequency is $\omega_0 = \omega_{par} = 0.5$ i.e. the resonance condition is fulfilled in all cases.

Chapter 4

Conclusion and outlook

In this thesis we have investigated the role of the fermion-phonon interaction in simple finite systems such as nanorings or parabolically confined fermions. Both types of systems were studied in- and out-of equilibrium, and the the effect of fermion-fermion interactions was also considered.

To perform this task, and as part of the learning process, we have built a computer program from scratch, which has been successfully benchmarked against a pre-existing code, and that has subsequently been applied to the system(s) of interest.

In more detail, the first system we looked at was a ring with six sites and four electrons (two spin up, two spin down) which was pierced by a magnetic flux. We saw that, when the electron-electron interaction is zero or very large, the final current induced by the change in the magnetic field is independent of the speed at which the magnetic flux is ramped up. Conversely, in the intermediate coupling regimes we saw that the value of the current after the ramping had both a DC and AC part. With slower ramping, the DC component is bigger and the oscillations in the current have smaller amplitudes; the opposite is true for faster ramping.

We finally looked at a ring system in the presence of breathing phonons. We showed that the oscillations in the final current were dependent on the speed at which the magnetic field is ramped up.

The second system we looked at is a one-dimensional open-ended chain where the fermion particles are in a parabolic potential. The parabolic field oscillates (and thus it is at the same time responsible for the trapping of the particles and for their non-equilibrium dynamics), and the middle site in the chain is coupled to a local phonon mode. We have investigated the dynamical behaviour of this system for different ratios of the frequency of the parabola oscillations to the phonon frequency, i. e. for on- and off-resonance regimes.

We have found that if the parabola frequency is equal to the frequency of the phonon, more phonons are excited than de-excited, i.e. energy is injected in the phonon mode at faster rate than it can be released. For parabola frequencies close to the phonon frequency, we observed a beating pattern in the phonon energy which might be practically used to "zoom in" on the correct phonon frequency. Far away from resonance, the phonon mode is hardly excited, and practically decoupled from the electronic system.

As possible future work, it would certainly be interesting to see how the dynamical behaviour of these nanoring and chain systems changes when more particles are present. Additionally,

i) For the ring system, it would be interesting to see what would happen when the fermions in the ring are coupled to a distinct mode at each site.

ii) For the parabola system, one could see what happens with the pumped up phonon mode if the parabola frequency is changed slightly or if the oscillation completely stops. Another direction would be to go into higher dimension and see if the dynamics changes.

Chapter 5

Self-reflection

In the months that I have spent working on my bachelor project, I have learned a great deal about how scientific work is carried out. I have also learned a lot in terms of physics in general, and gained some detailed knowledge in the field of strongly correlated systems which I have studied in detail.

As part of the project, I have built a computer program from scratch. Through this process, I have not only increased my programming ability, but also learnt how to solve and work around countless obstacles in varying sizes.

During the time spent producing and analysing results, I have learnt the amount of patience and stubbornness that is needed to go through all of the "bad" results, before finding anything of interest.

Perhaps due to somewhat failing to stick with the time plan, I have learnt the importance of good time estimates. In future work I will be aware of the amount of time that can go into solving unexpected problems, and I will be less of a time optimist when it comes to planning ahead.

Furthermore, I have learnt a great deal about writing scientific text, how to present results in a convincing manner without jumping to conclusions, etc.

To summarize, this project has been a great experience and there is a lot more that I will take with me from it than I can fit into this page.

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