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DIVISION OF MATHEMATICAL PHYSICS
FACULTY OF SCIENCE

LUND UNIVERSITY, SWEDEN

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DOCTOR OF PHILOSOPHY

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Abstract

Cutting-edge technology needs small, ultrafast devices, operational in a wide range of regimes. This calls for solids with novel, unconventional and tailorable properties. Great progress is expected from materials in which electron-electron and electron-phonon correlations strongly affect the dynamics (i.e. "unforeseen" useful properties are expected to be most likely found in systems with complex behavior). In spite of the potentially huge technological pay-off, our understanding of these systems is rather incomplete, especially in non-equilibrium. Often, with knowledge of systems or phenomena at an early stage, it is rewarding to resort to model, simplified descriptions. This strategy is used in this thesis, where we study several models lattice systems via density-functional theory. The latter is a well established approach (in fact, it is the current method of choice) for investigations of real materials. In our research, we focussed on little understood properties of interacting many-particle systems, such as the time-dependent conduction properties of electronic devices in the presence of interactions, disorder, and lattice vibrations, or the expansion of ultracold fermion clouds in 3D optical lattices. All these systems were described in terms of Hubbard-type interactions for the electrons, and Holstein-type electron-phonon interactions. Our results show interesting features due to the interactions which depend on dimensionality; they also show a dynamical crossover for several properties, due to the competition between disorder and interaction. Finally, when lattice vibrations are included, we showed how it is possible to manipulate in a controlled way the nuclear dynamics of molecular device via fast electronic external fields, of potential interest for technologies employing nanomolecular motors. We include four papers in the thesis:

In paper I, we study the competition between disorder and interactions in 1D chains attached to leads.

In paper II, we study the expansion properties of a cloud of ultracold Fermions in a 3D optical lattice.

In paper III, we show how ultrafast fields affect the limit cycles of the nuclei in a molecular device.

In paper IV, we present a compendium of original, unpublished results from work in progress.

Key words: Time dependent density functional theory, quantum transport, ultracold atoms in optical lattices, Hubbard model, disorder, strongly correlated systems, electron-phonon interactions

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I devote my final acknowledgements to Sven Åberg for a creative organization of the academic process and solid management of daily challenges and tasks of our department.

These new justifications are termed "scientific". But by the term "scientific" is understood just what was formerly understood by the term "religious": just as formerly everything called "religious" was held to be unquestionable simply because it was called religious, so now all that is called "scientific" is held to be unquestionable.

Leo Tolstoy

Popular Science Summary

Nowadays, cutting-edge technologies require devices to be small, ultrafast, and operational in a wide range of regimes. To fulfill these requirements we need to go beyond the traditional materials, i.e. to solids with novel, unconventional and tailorable properties. Great progress in this direction is conjectured to stem from materials in which the effect of inter-particle interactions (e.g. among electrons or between electrons and atomic vibrations) strongly affects the dynamical behavior. In other words, the expectation is that "unforeseen" useful properties are most likely to be found in systems exhibiting a complex behavior, which cannot be reduced to a picture where particles act if they were mutually independent.

A theoretical description of these systems is not easy; thus, in spite of the potentially huge technological pay-off, our current understanding is far from complete, especially in the out-of-equilibrium regime. This challenging state of affairs is what motivates the strong ongoing effort in the scientific community to develop theories for systems out of equilibrium.

Often, when knowledge is at an early stage, simplified descriptions are rewarding for preliminary insight. This strategy is used in this thesis, where we investigate several simple models lattice systems via density-functional theory. The latter is a well established theoretical technique (in fact, it is the current method of choice) for investigations of real materials, which is used here in a rather novel way. The model used by us here is the Hubbard model (see Figure). It is one of the simplest pictures of interacting fermions on a discrete lattice, and yet it exhibits a fascinating and rich physical behavior, useful for deep qualitative insight into the properties of real materials where the independent-particle picture fails (materials where electron-electron interactions make an independent-particle picture not possible, are commonly referred to as strongly correlated materials/systems).

This thesis concern some intriguing and little-understood properties and

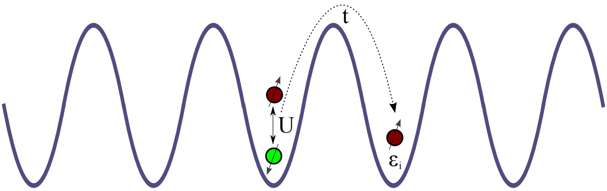

Figure 0.1: Ultracold atoms moving (confined) in an optical lattice produced by optical standing waves. For deep confinement, an effective description of this systems can be given in terms of the Hubbard model. In this case, fermions can tunnel between nearest-neighbor lattice sites with a tunneling energy t. According to the Pauli principle of quantum mechanics, tunneling for a particle with a given spin projection is possible only if the final lattice site is empty or occupied with an atom of a different spin projection. Fermions on the same lattice site and with opposite spin projections have an interaction energy U, which can be tuned to be either repulsive or attractive. The interplay between t and U, the particle density, and possibly the underlying confining potential ε_i determine the physical properties of the system.

behavior of nonequilibrium fermions.

One of them is clouds of cold atoms expanding in a disordered environment. Within density-functional theory, we studied the the so-called *melting of the Mott insulator*, a dynamical process due to a complicated interplay among many-body interactions, kinetic energy, and spatial confinement. We simulated large 3D systems (47^3 lattice sites, with disorder also taken into account), and also considered collisions between atomic clouds. Our results showed interesting features, which depend on dimensionality of the system and the strength of interactions and/or disorder.

We also investigated the electronic conduction in model nanodevices with disorder, interactions and lattice vibrations. Our main finding was a robust evidence of a competing behavior between interactions and disorder. By including lattice vibrations in the picture, we showed how it is possible to manipulate in a controlled way the nuclear dynamics of a molecular device via fast electronic external fields, a result of potential interest for technologies employing mechanical motors at the nanoscale.

These brief remarks give an idea of the contents and the scope of this thesis. As an outlook, if our work is of any help to improve the understanding of nonequilibrium fermions in general, it is not for us to decide, and not at this stage. In any case, we vividly hope that it will stimulate further investigations in this beautiful and challenging field of physics research.

Популярное введение

Понимание природы явлений конденсированного состояния является нетривиальной задачей. В частности, изучение неравновесных процессов – одно из важнейших направлений в физике конденсированного состояния, как и с фундаментальной точки зрения, так и с позиции применения этих знаний на практике. Современные теоретические исследования могут дать ответ на многие важнейшие вопросы теории неравновесных систем и внести огромный вклад в ее понимание.

Достаточно часто полная картина взаимодействия большого числа электронов может быть приближённо описана с помощью более простой модели, приимуществом которой является возможность пренебречь несущественными эффектами. В свою очередь акцент в данной модели делается на описании ключевых физических процессов. Модель Хаббарда – одна из широко используемых моделей в современной физике конденсированного состояния, которая используется для описания сильно коррелированных систем. Это одна из простейших моделей рассматривающих взаимодействующие фермионы на дискретной решетке, гамильтониан которой содержит только два члена: кинетическую энергию и Кулоновское взаимодействие между электронами на узле. С помощью данной модели возможно объяснить переход между проводящим и диэлектрическим состояниями.

Одной из целей данной диссертационной работы является теоретическое изучение процессов, происходящих в экзотических многочастичных системах, так называемых ультрахолодных атомах. В рамках метода функционала плотности был изучен процесс плавления Моттовского изолятора в трехмерной оптической решетке, в том числе для случае присутствия разупорядочения. Были проведены параллельные компьютерные вычисления для достаточно большой системы, Хаббардовского кластера, содержащего порядка 47^3 узлов. Размеры этой системы практически сравнимы с теми, которых возможно достичь в современных экспериментах.

Еще одним важным аспектом, затроннутым в данной работе, является разупорядочение, связанным с квантовым транспортом в сильно коррелированных разупорядоченных Хаббардовских кластерах. Полученные результаты позволяют лучше понять взаимосвязь между взаимодействием и разупорядочением и их влиянием на свойства реальных материалов. В последней части данной работы было проведено исследование роли сил атомных ядер в квантовом транспорте, что имеет огромный потенциал для развития нано технологий.

Contents

List of publications and author's contribution

The thesis is based on the following publications and manuscripts:

Paper I

Interacting fermions in 1D disordered lattices: Exploring localization and transport properties with lattice density-functional theories
V. Vettchinkina, A. Kartsev, D. Karlsson and C. Verdozzi
Physical Review B **87**, 115117 (2013)

In this paper, we analyzed how the interplay of interactions and disorder affects the conduction properties of short Hubbard chains contacted to semi-infinite leads. The investigation was done within the framework of (TD)DFT in its lattice formulation. To perform real-time dynamics, we used a lead-embedding technique from the literature; however, the efficiency of this scheme was considerably augmented by introducing a modification based on the recursive Lanczos method. As a side issue, we also tested merits and shortcomings of a popular treatment of disordered systems, the coherent potential approximation. The degree of localization induced by disorder was estimated in terms of a novel expression for the inverse participation ratio. We also benchmarked the TDDFT description in the adiabatic local density approximation (ALDA) against exact results in finite systems, finding that the TDDFT-ALDA provides a good qualitative account of the dynamics. The central result of this work is is that, compared to the disordered but noninteracting case, localization from disorder is diminished by the presence of interactions. This outcome was primarily obtained looking at arithmetic averages but, due to the large sample-to-sample fluctuations, we also performed an analysis based of full statistical distributions, typical values and geometrical averages, reaching the same conclusion.

In this project, in order to deal with a 1D LDA functional, I wrote an extra module for a previously developed (TD)DFT code. To obtain the LDA exchange-correlation energy and thus construct the XC potential, I also developed a separate code for solving the self-consistent Bethe-Ansatz equations, and performed all the necessary testing and benchmarking. I was actively involved in all the scientific discussions, and in the writing of the paper.

Paper II

Three-dimensional dynamics of a fermionic Mott wedding-cake in clean and disordered optical lattices
A. Kartsev, D. Karlsson, A. Privitera and C. Verdozzi
Submitted to Scientific Reports (Nature Publishing Group)

This paper provides a detailed theoretical description of the non-equilibrium behavior of the inhomogeneous Hubbard model in three dimensions, in terms of a method which combines lattice TDDFT and dynamical mean-field theory. We were able to address different interaction regimes for a a realistic three-dimensional setup, namely time-of-flight experiments on ultracold Fermi gases in optical lattices. We considered interactions strength above and below the Mott threshold and also the presence of disorder. Our results underline the striking consequences of Mott physics on the system dynamics at strong-coupling and the qualitative differences with the metallic regime. We observed many interesting effects including the stabilization of the Mott plateau at the expenses of the metallic domain in the earlier times of the expansion (that is, we observe multiple timescales in the dynamic melting of the Mott wedding-cake, as the Mott plateau persist orders of magnitude longer than the band insulating core), and a dynamic crossover in the cloud localization degree in presence of disorder and strong interactions.

Apart from taking part in the results interpretation and writing of the paper, I developed part of the theoretical formulation, most of the computer codes needed to produce the results and the post-processing, and performed all the numerical simulations.

Paper III

Title: Nonadiabatic Van der Pol oscillations in molecular transport
A. Kartsev, C. Verdozzi and G. Stefanucci
Submitted to Physical Review B, arXiv:1305.1811v1

Quantum transport in the presence of electron-phonon interactions is currently a very active area of research in condensed matter. Most of the available studies consider the case of steady state dynamics, and indeed much less attention has been so far devoted to time-dependent phenomena. However, the interest of describing/understanding the real-time dynamics of these systems has been recently increased due to interesting evidence of negative friction in nuclear forces, responsible for van der Pol-type oscillations of the nuclear coordinates. I have studied the robustness of the van der Pol oscillations against high-frequency bias and gate voltage. This has made necessary to improve over the adiabatic approximation and perform full time-dependent simulations based on the Ehrenfest dynamics scheme. Our results show that the fast electron dynamics can have remarkable effects on the van der Pol-like dynamics of the nuclei. Namely, the phase-space trajectories of the nuclei are distorted, and the period of the oscillations can also been altered. Another interesting finding of our study is that, even while staying in the adiabatic regime, the period of the oscillation as emerging from the full Ehrenfest dynamics is different from the one obtained within an adiabatic framework. Finally, by switching the high-frequency fields off at different times, cycles of different amplitudes can be obtained, which attain the limit cycle only after considerably long times, i.e. for practical purposes they can be considered as quasi-stable limit cycles. Thus, the outcome of our work can be summarized by saying that ultrafast fields acting on the electrons can constitute an important knob to manipulate such nuclear cycles, something of great potential interest for nanomechanical engines.

For the project presented in this paper, I performed all the necessary computer simulations for the nonadiabatic dynamics, actively participated in theoretical development, the interpretation of the results, and the writing of the paper.

Paper IV

Title: Lattice Density Functional Theory for Cold Atoms and Quantum Transport
A. Kartsev
Internal Report at the Division of Mathematical Physics, Lund-MPh-13/03

This paper is an internal report on work in progress, which describes several projects that I have been involved in during my PhD studies, and that are not finalized yet. The material presented concerns original, unpublished research. The only exception is represented by the first part of the report, where the concepts and practicalities behind the construction of an exchange-correlation potential for 1D systems are exposed in some detail. In fact, the construction of such potential has been performed for the first time by others. However, such XC potentials are very central to much of the original research in our thesis work, hence the considerable space devoted to the subject. Coming to the original research projects described in the manuscript, some of them are at a rather early stage, and thus they need to be pursued considerably further. Others, instead, are in a very advanced state: for example, we anticipate the submission of a paper in the near future, dealing with collisions between two ultracold fermionic clouds. The focus of this work will be a comparative study of collisions in 1D and 3D systems, which will rely on the results preliminarily presented in the report. Looking further ahead, we also anticipate the completion of a project inherent the time-dependent spin-dynamics in transport using the spin-dependent methodology, which is briefly illustrated in the report in terms of very preliminary results. In summary, this report is a compendium of original results from work in progress on transport and cold atom phenomena, performed within the TDDFT framework.

For the all the projects presented in this report, I performed all the necessary computer simulations, and substantially contributed to the necessary theoretical (both analytical and computational) developments, and to all the inherent scientific discussions. The report was entirely written by me.

Part I

Background and Methods

Chapter 1

Introduction

This thesis is about the properties of Fermions out of equilibrium. In its entirety, this is a very broad subject, which certainly cannot fit into the scope of a PhD thesis (it can be easily argued that the topic would not even fit into a book of reasonable size); thus, as already done in the thesis title, a specification is in order: we study the dynamical properties of Fermions within two fairly well defined areas, namely the time-dependent flow of electrons in devices at the quantum (molecular) scale, and the time dependent behavior of ultracold fermionic atoms in optical lattices.

On the surface (and not only), these two topics look quite different. So, what do they have in common? Our answer is on three distinct levels:

i) In both these fields, many interesting open issues are related to the correlated motion of the basic constituents, where standard independent-particle approaches fail.

ii) When inter-particle correlations are important, a considerable fraction of the theoretical treatments for quantum transport or ultracold atom systems makes use of model Hamiltonians: a notable example is the Hubbard Hamiltonian, one of the paradigmatic model systems in condensed matter research, which is the “bare minimum” description for the competition between itinerant and localized behavior of electrons. In this thesis, the Hubbard model is used for the description of both quantum transport and cold-atom phenomena.

iii) A third common denominator, specific to our work here, is the methodology adopted, namely density-functional theory. It is perhaps worth to offer few preliminary considerations about this method. In condensed matter systems, to achieve a quantitative description, one is required to apply first principles techniques. We have to deal with systems which contain 6x10^{23} particles per mole of the substance or more. This is a large number. It forces us to find alternative theories which permit to investigate the electronic structure of many-body systems. One of these theories was offered by Hohenberg, Kohn and Sham [1, 2] and it is called Density-Functional Theory. Nowadays it is one of the most reliable and computationally tractable tools in condensed matter physics. Particularly in combination with the so-called local density approximation, it has now impacted every area of material science. Three decades ago, a time-dependent version of this approach, namely Time-Dependent Density-Functional Theory, was also proposed. This method is rapidly gaining favor to describe the dynamical properties of realistic systems. Here we use its adaptation for lattice model systems out of equilibrium.

So far, we have not specified if we are considering only fermionic species. This is no accident, since part of the thesis is devoted to the study of how manipulating the flow of electrons in a molecular device affects the nuclear dynamics in the device. In this case, the emphasis is on the response of the nuclei in the harmonic regime, but the nonequilibrium behavior of the electrons plays a key role. Thus, this somewhat distinct topic is actually not defying the main scope (and the implications of the title) of this thesis.

Finally, a few words about Part A ("Background and Methods") of this thesis. Its aim is not to provide a coherent (and consequently very limited for reasons of space) review of the the field of Fermions out of equilibrium. Rather, we cover in a somewhat scattered way a few topics that, in our view, constitute useful pre-knowledge to the papers of Part B. The hope is that between Part A and Part B the reader is offered all the material necessary to become acquainted with the contents of the papers, and with the scope of this thesis more in general.

2 DFT and TDDFT Basics

The main goal of condensed matter physics and materials science is to understand the properties of systems which normally contain a macroscopic number of particles (electrons and nuclei). This leads to a quantum-mechanical many-body problem of enormous size involving $\sim N$ interacting particles where N is typically of the order Avogadro's number $\sim 10^{23}$! Important early attempts to cope which this difficult problem include mean-field approximations in which each particle is considered moving in the static average field from all other particles such as the Hartree and Hartree-Fock approximations. The system is described by a many-body wave function Ψ depending on $3N$ coordinates, one for each particle. In the mean-field methods the N-body problem is replaced by N one-body problems, which is in itself an enormous simplification. Density-functional theory (DFT) involves an even more dramatic simplification, and all physical properties are described in terms of the particle density $n(\mathbf{r})$. In this way, the key role is played by a function of three space variables rather than a many-body wave function depending on $3N$ variables.

DFT in its modern form was founded by Hohenberg and Kohn [1] as a formally exact reformulation of quantum mechanics for ground states. They proved that the ground-state properties of any electron system can be obtained from a density functional $F[n(\mathbf{r})]$. This functional is exactly defined but only approximately known. It may be decomposed into kinetic and potential energy parts which are both quite large. In 1965, Kohn and Sham [2] invented a method whereby the major independent-electron part $T_0[n]$ of the kinetic energy in F may be obtained exactly via self-consistent one-electron equations. In the potential energy part, the classical Coulomb energy

$$E_H[n] = \frac{1}{2} \int n(\mathbf{r}) n(\mathbf{r}') u(\mathbf{r} - \mathbf{r}') d^3r d^3r', \tag{2.1}$$

is explicitly known. Here, u is the two-body inter-particle interaction, normally the Coulomb interaction[1]

$$u(\mathbf{r}) = \frac{1}{r}. \tag{2.2}$$

Thus, only a much smaller part E_{xc} from exchange and correlation needs to be approximated, and already the simplest so-called local-density approximation (LDA) has proved very successful and goes far beyond earlier density-functional methods such as the Thomas-Fermi approximation [3,4].

In 1984, Runge and Gross [5] extended density-functional theory to time-dependent phenomena and thereby to excited states and to systems out of equilibrium. The main ingredient is an action functional $A[n(\mathbf{r}, t)]$ depending on the time-dependent density. Again, self-consistent one-particle-like equations can be derived which treat the independent-electron kinetic action functional exactly. The time-dependent density-functional theory (TDDFT) is much less developed than its counterpart for ground states, but already the simplest ”adiabatic local-density approximation” (ALDA) local in both space and time has proved very useful.

In the following two subsections I will describe the main ideas behind DFT and TDDFT. For more detailed information the reader is referred to the reviews in Refs [6–8].

2.1 Ground-State DFT

2.1.1 The Hohenberg-Kohn Theorem

Let us consider different many-fermion systems with the same inter-particle interaction. The different systems are however shaped by different external potentials v. Different external potentials will correspond to different ground-state energies (E_0) and different ground-state density profiles (n). The ground-state energy and density profile are thus functionals of v, $E_0 \equiv E_0[v], n(\mathbf{r}) \equiv n[v; \mathbf{r}]$. Hohenberg and Kohn [1] proved that if the densities of two systems are equal then the corresponding potentials are equal up to a constant. If we normalize v in some way, for instance by requiring that it tends to zero at far distances, the mapping from v to n is invertible, and v may be considered as a functional of the corresponding ground-state density,

$$v(\mathbf{r}) \equiv v[n; \mathbf{r}]. \tag{2.3}$$

---

[1] we use atomic units such that $e^2 = m = \hbar = 1$ in this section

With a given interaction, the ground state and all ground-state properties depend functionally on v, and from the Hohenberg-Kohn theorem, on n. Thus, it seems probable that v and $E_0[v]$ may be obtained from some underlying functional depending only on n. We first note that $E_0[v[n]]$ is not suitable. In fact, from first-order perturbation theory we have

$$\frac{\delta E_0}{\delta v(\mathbf{r})} = n(\mathbf{r}),$$

and by considering E_0 as a functional of its derivative n we would lose integration constants. Hohenberg and Kohn therefore used the Legendre transform

$$F[n] = E_0 - \int \frac{\delta E_0}{\delta v(\mathbf{r})} v(\mathbf{r}) d^3r = E_0 - \int n(\mathbf{r}) v(\mathbf{r}) d^3r, \tag{2.4}$$

as the basic density functional. We then have

$$v[n;\mathbf{r}] = -\frac{\delta F}{\delta n(\mathbf{r})}. \tag{2.5}$$

The ground-state energy may in principle be obtained via a Legendre transform on F back to E_0, but Hohenberg and Kohn use a different, self-consistent method and introduce an auxiliary functional

$$E_v[n] = F[n] + \int n(\mathbf{r}) v(\mathbf{r}) d^3r \tag{2.6}$$

with two independent variables v and n. They show that $E_0[v]$ may be obtained by minimizing $E_v[n]$ with respect to n while keeping v fixed,

$$E_0[v] = \min_n E_v[n]. \tag{2.7}$$

The minimizing density is the ground-state density corresponding to v. In this way, both the ground-state density and energy may be obtained without reference to the wave-function provided the basic density functional $F[n]$ is known.

2.1.2 The Kohn-Sham one-particle scheme

The density functional $F[n]$ contains energy contributions from the kinetic energy T and the inter-particle interaction U. By subtracting the explicitly known classical Hartree energy in Eq. (2.1) only a much smaller contribution from exchange and correlation remains. Unfortunately, the kinetic energy T is not known as an explicit functional of n, not even for independent particles. However, in 1965 Kohn and Sham invented a one-particle scheme that evaluates the major, independent-electron part T_0 of the kinetic energy exactly. In this way, only the exchange-correlation contribution E_{xc} to the kinetic and potential energies needs to be approximated.

Kohn and Sham thus rewrite the density functional in terms of three contributions,

$$F[n] = T_0[n] + E_H[n] + E_{xc}[n]. \tag{2.8}$$

Instead of minimizing E_v under constraint $N = \int n d^3\mathbf{r}$ we may introduce a Lagrange parameter μ and do free minimization of $E_v - \mu N$. This leads to

$$\frac{\delta T_0}{\delta n(\mathbf{r})} + V_H(\mathbf{r}) + v_{xc}(\mathbf{r}) + v(\mathbf{r}) = \mu. \tag{2.9}$$

Here,

$$V_H(\mathbf{r}) = \frac{\delta E_H[n]}{\delta n(\mathbf{r})} = \int d^3r\ n(\mathbf{r}')u(\mathbf{r} - \mathbf{r}') \tag{2.10}$$

is the classical ‘Hartree’ potential from the density n, and

$$v_{xc}(\mathbf{r}) = \frac{\delta E_{xc}[n]}{\delta n(\mathbf{r})}. \tag{2.11}$$

If we would density-functionalize the problem of N non-interacting electrons subject to a one-body potential V_{eff}, the density functional would be $F_0 = T_0$, and the Euler equation for the minimum

$$\frac{\delta T_0}{\delta n(\mathbf{r})} + V_{eff}(\mathbf{r}) = \mu. \tag{2.12}$$

When the one-body potential (in this case V_{eff}) is known, T_0 may be obtained via the one-particle orbitals φ_k as

$$T_0[V_{eff}] = \sum_k^{occ} |\langle \varphi_k[V_{eff}]| - \frac{\nabla^2}{2} |\varphi_k[V_{eff}]\rangle \tag{2.13}$$

If we now combine these two results and construct a self-consistency sequence in which we at each iteration ‘i’ solve one-particle orbitals in the potential

$$V_{eff}(\mathbf{r}) = v(\mathbf{r}) + V_H[\mathbf{r}; n_i] + v_{xc}[\mathbf{r}; n_i], \tag{2.14}$$

$$\left[-\frac{\nabla^2}{2} + V_{eff}(\mathbf{r})\right]\varphi_k(\mathbf{r}) = e_k\varphi_k(\mathbf{r}), \tag{2.15}$$

recompute the density from the one-particle expression

$$n_{i+1} = \sum_k^{occ} |\varphi_k(\mathbf{r})|^2 \tag{2.16}$$

and continue until self-consistency has been achieved, *i*.e., until the difference between input (n_i) and output (n_{i+1}) density is smaller than some suitable tolerance, the full problem in Eq. (2.9) has been solved. At self-consistency, V_{eff} has become the potential that forces a fictitious system of non-interacting particles to have the same density as the interacting system subject to the potential v. One can say the the self-consistency cycles construct the functional $V_{eff}[\mathbf{r}; n]$, and once V_{eff} has been obtained, T_0 at this particular density can be obtained from Eq. (2.13). The method is illustrated in Fig. (2.1).

The energy eigenvalues (e_k) which appear in Eq. (2.15) have no particular meaning except the highest occupied one (which gives the ionization energy), they are just ingredient which are needed in order to form the total energy.

In order to to treat real systems like solids, solid surfaces, adsorbates etc the development of efficient one-electron methods has been extremely important. In one class of methods, the tightly bound core electrons and the valence electrons are treated on the same footing, and here the linearized muffin-tin (LMTO) and augmented plane wave (LAPW) methods developed by O.K. Andersen and collaborators [9] have played a central role. In an other class of methods, the core electrons are transformed away [10], leading to much weaker pseudopotentials. This transformation makes it possible to use plane waves in basis-set-based calculations. In order to speed the convergence of the self-consistency cycles, methods from non-linear optimization by Broyden and by others [11–13] are often used.

A large part of current works is based on the simplest local-density approximation (LDA) in which E_{xc} is approximated by

$$E_{xc}^{LDA} = \int d^3r\; n(\mathbf{r})\epsilon_{xc}(n(\mathbf{r})). \tag{2.17}$$

Despite its simplicity the LDA gives useful semiquantitative or even quantitative results for a large class of systems such as molecules, solids, adsorbates etc. During the last three decades more accurate approximations

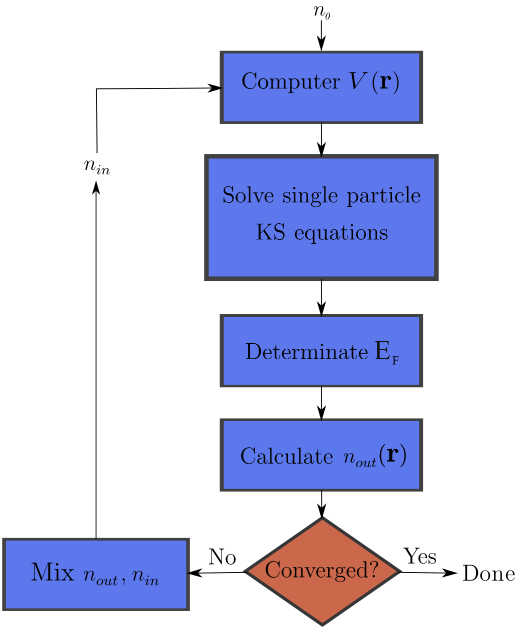

Figure 2.1: A self-consistent charge density-functional based scheme of Kohn-Sham equation solution.

have been developed by Langreth, Perdew, Becke and by others; for a comprehensive review see e.g. Ref. [14]

2.2 Spin-polarized systems

Density-functional theory may be generalized to account for spin-magnetic effects. This was first done by von Barth and Hedin [15], and shortly afterwards Rajagopal and Callaway described how spin-orbit effects from the orbital motion may be handled [16]. In order to cover the case of non-collinear magnetism, one has to use the full spin-dependent density

$$n_{\alpha\beta}(\mathbf{r}) = \langle \psi_\alpha^\dagger(\mathbf{r}) \psi_\beta(\mathbf{r}) \rangle \tag{2.18}$$

($\psi_\alpha^\dagger$ and ψ_β are the usual Fermi field operators and α and β are spin indices). The spin-dependent density introduces a non-locality in spin space, and as shown by von Barth and Hedin this makes the mapping from spin-dependent densities to spin-dependent potentials non-unique. However, a well-defined density functional $F[n_{\alpha\beta}]$ can still be defined, and a Kohn-Sham one-particle scheme can be established with a spin-dependent effective potential. In the case of collinear magnetism, the up/down-spin densities $n_{+,-}$ contain sufficient information, and the Kohn-Sham equations reduce to separate equations for the two spin channels, coupled only via the self-consistency requirement.

2.3 Time-dependent density-functional theory

Density-functional theory is quite powerful but has the drawback that only ground-state properties can rigorously be obtained. In 1984, Runge and Gross [5] laid down the foundation of a time-dependent counterpart to DFT, TDDFT, by proving a uniqueness theorem for time-dependent phenomena analogous to the Hohenberg-Kohn theorem for ground states. Via the time dependence, excitation properties which can be related to time-dependent densities become accessible, such as optical absorption and charge transport. Runge and Gross studied how interacting systems evolve when exposed to different local but time-dependent potentials $v(\mathbf{r},t)$. They prove that if two systems start from the same initial state (usually but not necessarily the ground state) at time $t=0$ and have the same density profile $n(\mathbf{r},t)$ for $t>0$, then the corresponding time-dependent potentials are equal up to a time-dependent constant $C(t)$. Ground-state DFT is based on the HK theorem and the minimal properties of the expectation value of the Hamiltonian. IN TDDFT, however, the basic action functional

$$B[\Psi] = \int_{t_0}^{t_f} dt \langle \Psi(t)|\hat{T} + \hat{U} + \hat{V}(t) - i\frac{\partial}{\partial t}|\Psi(t)\rangle \tag{2.19}$$

is only stationary but not in general minimal for the actual trajectory $\Psi_{solution}(t)$. ($\hat{T}$ and $\hat{U}$ are the kinetic and interaction energy parts of the Hamiltonian, and $\hat{V}(t)$ the interaction energy with the external time-dependent field.) However, an action functional $A[n]$ depending on only the time-dependent density (and the chosen initial state) can still be defined, and then actual time-dependent density $n(\mathbf{r},t)$ corresponding to a given potential potential $v(\mathbf{r},t)$ is the stationary trajectory of the functional

$$A_v[n] = A[n] + \int_{t_0}^{t} dt' \int d^3r v(\mathbf{r},t')n(\mathbf{r},t'). \tag{2.20}$$

The time-dependent density may thus be obtained from the action functional A without any reference to the underlying time-dependent wave function.

As is ground-state DFT we may split A in an independent-electron part A_0, a classical Hartree energy part A_H, and a remainder A_{xc} describing exchange and correlation. In much the same way as in ground-state DFT this leads to an equivalent one-particle scheme. In this time-dependent Kohn-Sham scheme, one-electron orbitals are evolved in an effective potential

$$V_{eff}(\mathbf{r},t) = v(\mathbf{r},t) + V_H(\mathbf{r},t) + v_{xc}(\mathbf{r},t), \tag{2.21}$$

$$i\frac{\partial\varphi(\mathbf{r},t)}{\partial t} = \left[-\frac{1}{2}\nabla^2 + V_{eff}(\mathbf{r},t)\right]\varphi(\mathbf{r},t)r. \tag{2.22}$$

Here,

$$v_{xc}(\mathbf{r},t) = \frac{\delta A_{xc}}{\delta n(\mathbf{r},t)}. \tag{2.23}$$

The time-dependent density is given by

$$n(\mathbf{r},t) = \sum_i^{occ} |\varphi_i(\mathbf{r},t)|^2 \tag{2.24}$$

All effects of exchange and correlation have now been encapsulated in the exchange-correlation function A_{xc} and its variational derivative v_{xc}. As in ground-state DFT, these functionals are exactly defined but only approximately known. They are non-local in both space and time and are thus history dependent. The most widely used approximation is the “adiabatic local density approximation” ALDA, in which v_{xc} is approximated by the ground-state LDA potential for the instantaneous density,

$$v_{xc}^{ALDA}(\mathbf{r},t) = v_{xc}^{LDA}(n(\mathbf{r},t)). \tag{2.25}$$

2.4 Lattice (TD)DFT

2.4.1 General aspects

Static density-functional theories for lattice models were introduced about thirty years ago [17, 18], but it is only in the last decade that they have received considerable attention [19–22]. Conversely, lattice TDDFT for Hubbard-like models out of equilibrium is a more recent topic [23]. While studies of lattice v_0-representability (concerning the existence of a Kohn-Sham image system) have been been available for a few years, [23–26], a rigorous uniqueness proof when the density is the basic variable was given only very recently [27]. The type of lattice systems one considers with these approaches are described by a Hubbard-type Hamiltonian:

$$H = -\sum_{ij,\sigma} h_{ij} a^{\dagger}_{i\sigma} a_{j\sigma} + \sum_{\sigma}\sum_{i}\left[w_i(\tau) + \frac{U_i}{2}\hat{n}_{i-\sigma}\right]\hat{n}_{i\sigma}, \tag{2.26}$$

where the time-dependent onsite energies $w_l(\tau)$ are split as $w_l(\tau) = \epsilon_l + v_l(\tau)$, to distinguish a static and time-dependent part. In this way, $\hat{\mathcal{V}}(\tau) \equiv \sum_{l\sigma} v_l(\tau)\hat{n}_{l\sigma}$ describes a local (in space and time), time-dependent perturbation. In some cases the systems in question can be small clusters connected to macroscopic contacts, as in the case of Paper I; or, in other cases, the one-body diagonal terms may be distributed according to some disorder distribution (as in Paper I and II). However, to find suitable XC potentials, we will consider infinite homogeneous system (specifically for the 1D and 3D case, Paper I and II, respectively).

2.4.2 Formulation

Here, for simplicity, we consider spin-independent (TD)DFT (for a full discussion of the spin-dependent case, see Paper IV). The ground-state energy [28, 29] is

$$E[n, v_{ext}] \equiv T_0[n] + E_H[n] + E_{xc}[n] + \sum_i v_{ext}(i) n_i, \tag{2.27}$$

with $v_{ext}(i) \equiv \epsilon_i$, $T_0[n]$ and $E_H = \frac{1}{4}\sum_i U_i n_i^2$ the static external field, the non-interacting kinetic energy and the Hartree energy, respectively. Also, $n_i = \sum_\sigma n_{i\sigma}$. Using the Hubbard model as the homogeneous reference system,

$$E_{xc} = E - T_0 - E_H \ . \tag{2.28}$$

Defining $e_{xc} \equiv E_{xc}/V$, v_{xc} is obtained as

$$v_{xc} = \frac{\partial e_{xc}(n, U)}{\partial n} \ . \tag{2.29}$$

Finally, a local-density approximation is introduced: $v_{xc}(i) = v_{xc}(n_i)$. This is then used to to solve self-consistently the static Kohn-Sham (KS) equations

$$(\hat{t} + \hat{v}_{KS})\varphi_\kappa = \varepsilon_\kappa \varphi_\kappa. \tag{2.30}$$

The effective potential matrix $\hat{v}_{KS}$ is diagonal in the site indexes, and we write $v_{KS}(i) = v_H(i) + v_{xc}(i) + v_{ext}(i)$, where $v_H(i) = \frac{1}{2}U_i n_i$ is the Hartree potential. Moving to lattice TDDFT, the KS equations similarly become

$$\left(\hat{t} + \hat{v}_{KS}(\tau)\right) \varphi_\kappa(\tau) = i\partial_\tau \varphi_\kappa(\tau) \ , \tag{2.31}$$

In general, $v_{KS}(i,\tau) = v_H(i,\tau) + v_{xc}(i,\tau) + v_{ext}(i,\tau)$ depends non-locally on the density via v_{xc}. The adiabatic local density approximation (ALDA) [30] to the XC potential is then obtained with the prescription $v_{xc}^{ALDA}(i,\tau) \equiv v_{xc}^{LDA}(n_i(\tau))$. According to recent benchmarks in terms of Kadanoff-Baym dynamics and exact diagonalization, [31], the ALDA often performs well, but is inadequate for fast fields and/or very strong interactions.

2.4.3 One-dimensional case: v_{xc} from a Bethe Ansatz solution of the 1D Hubbard model

The LDA based on the Bethe-Ansatz was introduced in Ref. [29], an analytical interpolating expression for the XC functional was given [19], and used practically to investigate different inhomogeneous Hubbard-type models. Constructing a LDA in 1D requires [19, 29, 32, 33] solving the coupled Bethe-Ansatz equations for the charge and spin distribution functions [34] (see also Paper IV). An ALDA is then obtained [23] when v_{xc} becomes a function of the instantaneous local density. The entire procedure is described in detail in Paper IV.

2.4.4 Three-dimensional case: v_{xc} from a Dynamical Mean-Field Theory of the 3D Hubbard model

In Ref. [35], a connection was initially established between (TD)DFT and DMFT. The dynamical mean-field theory (DMFT) is a non-perturbative approach which has been developed during the nineties in the context of strongly correlated electron systems and nowadays is quite successfully employed to describe many physical features of strongly correlated systems, mainly in connection with the Mott transition and high-T_c superconductivity. The original idea stemmed from a paper from Metzner and Vollhardt [36], showing that in the limit of infinite dimensions $d \to \infty$ (i.e. very large connectivity $z \to \infty$), the physics of a quantum system is much richer than the one of a classical system. In fact, by suitably rescaling the hopping parameter t (so that both entropy and internal energy per site remains finite in the $d = \infty$ limit), the spatial fluctuation from site to

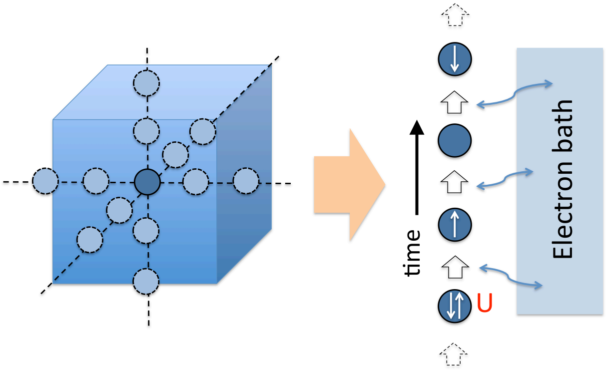

Figure 2.2: A cartoon of the impurity scheme of DMFT. A homogeneous Hubbard model (left) is described in terms of an impurity level in the presence of a bath, which accounts for particle-fluctuations at the impurity, and which is determined self-consistently (right).

site are frozen while local quantum fluctuation in time are not. Therefore the same limit is intrinsically much richer for a quantum system compared to a classical system. In this limit the self-energy $\Sigma(k,\omega)$ becomes local, $\Sigma(k,\omega) \equiv \Sigma(\omega)$, but fully retains a non-trivial dependence on the frequency. Outside the $d = \infty$ limit, DMFT can be thought as an approximation with local self-energy for quantum systems in three-dimensional space, exactly like the static mean-field theory provides an (approximate) description of a classical system in $d = 3$.

We briefly illustrate the DMFT approach focussing on Mott physics, i.e. we confine the discussion to paramagnetic solutions where there is no explicit dependence on the spin index. In the limit that the number of nearest neighbors goes to infinity, DMFT exactly remaps the infinite lattice into a local problem, represented through an Anderson impurity model [37], where the rest of the lattice is treated as a reservoir of non-interacting electrons (Fig. 2.2):

$$\begin{aligned} H_{AIM} = &\sum_{\sigma=\uparrow,\downarrow} \epsilon_0 c^\dagger_\sigma c_\sigma + U c^\dagger_\uparrow c_\uparrow c^\dagger_\downarrow c_\downarrow + \sum_{\nu\sigma} \epsilon^{bath}_\nu n^{bath}_{\nu\sigma} \\ &+ \sum_{\nu\sigma} \left[V_\nu c^\dagger_{0,\sigma} a^{bath}_{\nu,\sigma} + V^\dagger_\nu a^{\dagger,bath}_{\nu,\sigma} c_{0,\sigma} \right]. \end{aligned} \tag{2.32}$$

The impurity system contains the effective parameters ϵ_ν^{bath} (the energy of the bath), and V_ν (the probability amplitude for adding/removing an electron to/from the bath), to be determined self-consistently.

In $d = \infty$, the many-body self-energy Σ has no dispersion in k. A local, k-independent Σ is also employed in finite (e.g. $d = 3$) dimensions, only this time as an (often excellent) approximation (so-called single-site DMFT). In this case, for a paramagnetic, homogeneous system, the local Green function is

$$G_H(\omega) = \int_{-\infty}^{\infty} d\omega' \frac{\rho_0(\omega')}{\omega - \omega' - \Sigma_H(\omega')} \tag{2.33}$$

On the other hand, for the effective impurity system of Eq.(2.33), one has

$$G_{imp}(\omega) = \frac{1}{\omega - \epsilon_0 - \Delta(\omega) - \Sigma_{imp}(\omega)} \tag{2.34}$$

where Δ is the frequency-dependent (hence the attribute "dynamical" in the acronym DMFT) hybridisation function

$$\Delta(\omega) = \sum_\nu \frac{|V_\nu|^2}{\omega - \epsilon_\nu^{bath}}, \tag{2.35}$$

where all details of the lattice are encapsulated. DMFT crucially relies on the fact that Σ_{imp} and Σ_H have the same functional dependence on the propagator. Thus the parameters $\epsilon_\nu^{bath}, V_\nu$ can be determined within the DMFT self-consistency condition:

$$\Delta(\omega) = \omega - \epsilon_0 - \Sigma_{imp}(\omega) - G_H^{-1}(\omega) \tag{2.36}$$

corresponding to

$$G_{imp}(\omega) = G_H(\omega) \tag{2.37}$$

or

$$\Sigma_{imp}(\omega) = \Sigma_H(\omega). \tag{2.38}$$

The mapping scheme is amenable to a self-consistent iterative procedure: a) An initial Σ_H is considered; b) G_H is then calculated; c) the hybridization term $\Delta(\omega)$ is then determined via Eqs (2.36,2.37); d) the parameters $\epsilon_\nu^{bath}, V_\nu$ of the AIM bath are obtained; e) the AIM is solved non-perturbatively, and a new self-energy is obtained; f) the loop b-e) is repeated until self-consistency is attained.

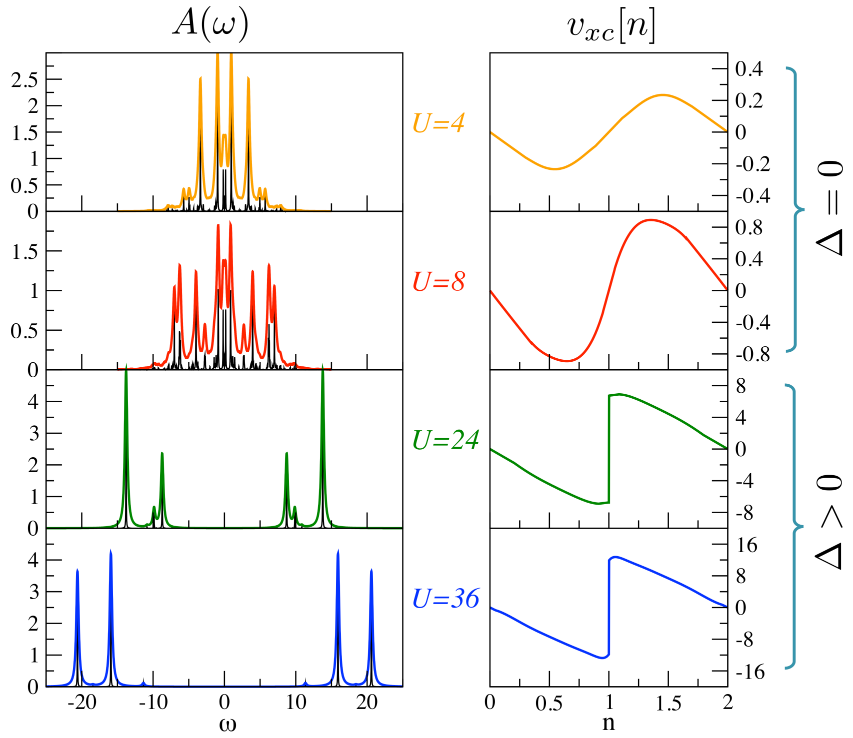

Figure 2.3: Spectral functions (left) and corresponding XC potentials (right), as a function of the Hubbard onsite interaction U.

DMFT and (TD) DFT. Once the total energy of the systems is determined, one can extract, with a procedure similar to the one described for the 1D case, the XC potential for the 3D homogenous case (for a detailed discussion, the refer the reader to Ref. [35]. The behavior of v_{xc} for the 3D Hubbard model is illustrated in Fig. 2.3. Compared to the 1D, the crucial novel feature is that the discontinuity Δ in v_{xc} occurs only above a critical value U_{crit}, which reflects the Mott-Hubbard metal-insulator transition. The latter manifests clearly in the many-body spectral function (Fig. 2.3, left). This behavior should be contrasted with the 1D case, where $\Delta > 0$ for any $U > 0$ (however, the size of Δ decreases exponentially when $U \to 0$). The XC potential for $U = 8$ and $U = 24$ shown in Fig. 2.3 are those used in Paper II and the Paper IV.

Chapter 3

Hubbard model, disorder, phonons

3.1 The Hubbard Model

We have already considered the Hubbard model [38] in connection with lattice density-functional theory in the previous Chapter. Here, we wish to offer a short historical and conceptual background to the model, which arguably provides the simplest way to describe the competition between itinerant and localized behavior in condensed matter and ultracold-atom systems. In standard notation, the Hubbard model is described by the following Hamiltonian:

$$H_{Hub} = -t \sum_{\langle ij \rangle, \sigma} a^{\dagger}_{i\sigma} a_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \tag{3.1}$$

and pertains to electrons moving in a lattice which can accommodate two electrons/site with opposite spin. The interaction term $U \sum_i n_{i\uparrow} n_{i\downarrow}$ is local, since it only concerns electrons with opposite spin, and only when they are at the same site. The original motivation to introduce the Hubbard model was the study of the magnetic properties of materials with narrow-band materials, such as d-bands. Starting from the general Hamiltonian describing electrons and nuclei in a solid, a number of steps is to be taken in order to arrive to the Hubbard model. First, the nuclear positions are kept fixed. Then, one expresses the electronic Hamiltonian in the basis of the Wannier functions. The latter, being quite localized in character and centered at the lattice sites, offer a natural way to select/neglect different contributions based on interatomic distance. Then the original argument by J. Hubbard is that the most important (i.e. the largest) contributions to the Hamiltonian come from the site-diagonal terms for the interactions, and kinetic terms which connect orbitals centered at nearest-neighbor lattice sites. As just said, this is because the overlap of Wannier functions decays fast with distance. Finally, in spite of band-degeneracy one assumes that different degenerate bands can be treated separately, and thus the model of Eq. (3.1) is recovered.

In some cases, the drastic simplifications made to obtain the Hubbard model must be released. For example, in studies of complex magnetic ordering, the usually neglected off-site interaction terms ($\sim n_i n_j$, with $i \neq j$) are often reinstated (by their inclusion one speaks of Extended Hubbard Model). Similarly, one may need to take into account band-degeneracy, for example in comparisons between theory and experimental spectroscopic data. This requires a substantial modification of Eq. (1) (in particular, the term U becomes a matrix in spin-orbital indexes).

At arbitrary band filling and dimensionality $D > 1$, no general exact solution for the Hubbard model is known, even for the single band case. For this reason, the formal treatment of the Hubbard model has been approached in several ways, such as Quantum Monte Carlo techniques, the density-matrix renormalization group, dynamical mean-field theory, the Gutzwiller approximation, to mention a few (and, as done in this thesis, density-functional theory). The situation becomes even more complicated when the model is further generalized in two other different directions: disorder or electron-phonon interactions. When disorder is added, the generalized Hamiltonian is called the Anderson-Hubbard Hamiltonian:

$$H_{AH} = -t \sum_{\langle ij \rangle,\sigma} a^{\dagger}_{i\sigma} a_{j\sigma} + \sum_{i\sigma} \epsilon_i n_{i\sigma} + \sum_i U_i n_{i\uparrow} n_{i\downarrow}. \qquad (3.2)$$

In many studies in the literature, U_i is kept site-independent, and disorder only enters through the onsite energies $\{\epsilon_i\}$. On the other hand, if phonons are included, we arrive at the Hubbard-Holstein Hamiltonian:

$$H_{HH} = -t \sum_{\langle ij \rangle,\sigma} a^{\dagger}_{i\sigma} a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \omega \sum_i \beta^{+}_i \beta_i + g \sum_{i\sigma} (\beta^{+}_i + \beta_i) a^{+}_{i\sigma} a_{i\sigma}, \qquad (3.3)$$

where $\beta_i, \beta^{\dagger}_i$ are phonon operators, and ω and g denote the phonon frequency and the electron phonon-coupling, respectively (see Sect.3 below).

It goes without saying that solving any of these generalized models constitutes a considerably more difficult problem than solving the original Hubbard Hamiltonian.

3.2 The role of disorder

Disorder appears everywhere in Nature. Not surprisingly, understanding the role of disorder in condensed matter systems has been one of the high-priority topics for the past five decades of theoretical research. Possibly, the single most important concept in the physics of disordered condensed matter systems is Anderson localization [39], which corresponds to the lack of wave-propagation in inhomogeneous systems. Nowadays, Anderson localization has became a central conceptual paradigm in several areas of physics. Of relevance to this thesis, Anderson localization, and even more the interplay of disorder and strong correlations (the so-called Mott-Anderson scenario), are topics of extreme interest within the ultracold-atom community [40–42]. This interest has received even further momentum since the first experimental observation of Anderson localization of matter in ultracold gases experiments analogous to the 3D setup we describe in Papers II and IV (the dimensionality is crucial in this case, since only in 3D one can observe a metal-insulator transition induced by disorder according to Anderson's paradigm [42]).

There are several ways to theoretically address the role of disorder, and reviewing them is beyond the scopes of this Section. Here we take a more practical perspective and provide few simple remarks about the way disorder is taken into account in Paper I and II.

Our approach is essentially numerical in character and based on two strategies (we also use at some point the Coherent Potential Approximation [43], as discussed in Paper I and not considered any further here).

The first strategy corresponds to perform statistical averages over several, randomly selected, disorder configurations. However, for small samples, as in Paper I, fluctuations of "measurable" quantities (e.g. the current in Paper I), can be large. If the fluctuations are of the same order of magnitude as the current itself, what is then the physical meaning of the average of an observable? While this question is addressed in detail in Paper I, the argument can be summarized as follows: in lack of self-averaging, one can analyze the data directly in terms of probability distributions, and/or consider the "typical" value of the statistical quantity (e.g. the current) corresponding to the maximum of the (current) distribution.

A second route is followed in Paper II where, due to the large size of the system investigated, considering a large number of disorder configurations is numerically very challenging, if not prohibitive. In this case we choose only one disorder configuration via the *special quasi-random structure* approach. This procedure effectively describes the random arrangements of sites at short range [44], thus providing a single disorder realization with several "typical" features [45].

3.3 The Holstein Model for phonons

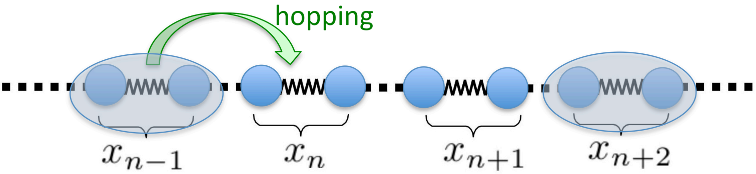

Figure 3.1: The Holstein model for one electron moving in a 1D tight-binding chain. The molecular units are schematically represented by the shaded shapes.

Another situation we discuss briefly here is when the Hamiltonian describes an interacting fermion-boson system. In Paper III, we analyze the effect of ultrafast electron dynamics on the nuclear motion in a current-carrying molecular junction. We do this in the harmonic approximation for the nuclear coordinates. In particular, we study the robustness of the cycles attained by the nuclear coordinates in phase space, when time-dependent AC biases and square-pulse gate voltages are applied. This is done using a two-site model junction where the electron-nuclei interaction is modeled via the following term in the Hamiltonian:

$$V_{e-ph} = \lambda(\hat{n_1} - \hat{n_2})\ \hat{X}\ . \tag{3.4}$$

The interaction in Eq.(3.4) is of the so-called Holstein-phonon type, which introduces a coupling between the electron density (in this case, at sites 1 and 2 in the junction) and the phonon coordinate. Originally conceived for the motion of a slow electron in a polar crystal, the Holstein model [46] has become a popular choice for theoretical investigations of electron-phonon interactions. A simple way to look at the model is to consider an electron hopping along a diatomic molecular chain, with intra-molecular harmonic vibrations. The key ingredient in a tight-binding picture is that the electron onsite energy is taken linear in the atomic displacement, as shown in Fig.3.1. Considering that for a nuclear oscillator, $\hat{x} = \sqrt{\frac{\hbar}{2m\omega_0}}(\beta + \beta^+)$, the Holstein Hamiltonian, in obvious notation, takes the following expression:

$$H_{Holstein} = -V \sum_{\langle ij \rangle} a_i^+ a_j + \omega_0 \sum_i \beta_i^+ \beta_i + g_0 \sum_i (\beta_i^+ + \beta_i) a_i^+ a_i, \qquad (3.5)$$

where ω_0 and g_0 denote the intramolecular frequency and the electron phonon-coupling, respectively. In general, approximations are introduced to solve this model (achieving an accurate solution is already a challenging task in the equilibrium case, and even for one electron). The strategy that we use in Paper III was to adopt a mixed quantum-classical dynamical scheme, the so-called Ehrenfest Dynamics, which is discussed in the rest of this Chapter.

3.4 Propagators for real-time dynamics

In our work we have dealt with purely electronic systems, but also with systems with both electrons and nuclei. In all cases, we had to numerically solve the time-dependent Schrödinger equation, and we wish to provide here details of the time-propagators we used. For the more complex case of electrons and nuclei (Paper III), we used a method originally introduced in [47]. This algorithm, suitable for mixed quantum-classical dynamics in quantum transport, is based of the Ehrenfest's dynamics [48] for the mixed electron-nuclear dynamics, and combines an exact electronic algorithm in the presence of embedding [49] and a classical Verlet-type algorithm for the classical nuclear motion [50]. All these aspects are considered in turn below, where further information for the case of purely electronic systems can also be found. For further details, we defer the reader to Paper I and III.

3.4.1 Ehrenfest's dynamics

We start by briefly reviewing the Ehrenfest's dynamics, closely following the discussion in Ref. [51]. In the presence of electrons and nuclei, the

Schrödinger equation (expressed in the space-coordinates picture) reads

$$i\hbar\frac{\partial\Psi(\mathbf{r},\mathbf{R};t)}{\partial t} = \mathcal{H}\Psi(\mathbf{r},\mathbf{R};t), \tag{3.6}$$

where $\mathbf{r}$ ($\mathbf{R}$) collectively denote the electron (nuclear) coordinates. The Hamiltonian in Eq. (3.6) has the following form:

$$\begin{aligned}\mathcal{H} = & -\sum_{\mathbf{R}}\frac{\hbar^2}{2M}\nabla^2_{\mathbf{R}} - \sum_{\mathbf{r}}\frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}} + V_{ee}(\mathbf{r},\mathbf{r}') + V_{nn}(\mathbf{R},\mathbf{R}') + V_{en}(\mathbf{r},\mathbf{R}) = \\ & -\sum_{\mathbf{R}}\frac{\hbar^2}{2M}\nabla^2_{\mathbf{R}} + \mathcal{H}_e(\mathbf{r},\mathbf{R}), \qquad (3.7)\end{aligned}$$

where the part $\mathcal{H}_e(\mathbf{r},\mathbf{R})$ can be interpreted as the Hamiltonian for the electrons when the nuclear coordinates are fixed (the subscripts ee, en, nn in the potential term $W \equiv V_{ee} + V_{nn} + V_{en}$ refer to the electron-electron, electron-nuclei, and nuclei-nuclei interaction terms, respectively). A simple product-ansatz is now introduced, to separate electrons and nuclei:

$$\Psi(\mathbf{r},\mathbf{R};t) \approx \Psi_{approx}(\mathbf{r},\mathbf{R};t) = \psi(\mathbf{r},t)\chi(\mathbf{R},t)e^{i\epsilon(t)}, \tag{3.8}$$

$$\epsilon(t) = \frac{1}{\hbar}\int_{t_0}^{t} dt' \int d\mathbf{r} \int d\mathbf{R}\; \psi^*(\mathbf{r},t')\chi^*(\mathbf{R},t')\mathcal{H}_e(\mathbf{r},\mathbf{R})\psi(\mathbf{r},t')\chi(\mathbf{R},t'), \tag{3.9}$$

where the explicit phase factor is introduced give the equations below a more compact form. After i) Eq.(3.8) is inserted in Eqs. (3.6,3.7), ii) we multiply from the left by ψ^* (χ^*) and integrate over $\mathbf{r}$ ($\mathbf{R}$) and iii) requiring the energy to be conserved (i.e. $d\langle\mathcal{H}\rangle/dt = 0$), we obtain separate equations for each part in Eq.(3.8):

$$\begin{aligned}
i\hbar\frac{\partial\psi}{\partial t} &= \left[-\sum_{\mathbf{r}}\frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}} + W_{\chi\chi}\right]\psi, && (3.10)\\
i\hbar\frac{\partial\chi}{\partial t} &= \left[-\sum_{\mathbf{R}}\frac{\hbar^2}{2M}\nabla^2_{\mathbf{R}} + \mathcal{H}_{\psi\psi}\right]\chi, && (3.11)\\
W_{\chi\chi}(\mathbf{r},t) &= \int d\mathbf{R}\; \chi^*(\mathbf{R},t)[V_{ee}(\mathbf{r},\mathbf{r}') \\
&\quad + V_{nn}(\mathbf{R},\mathbf{R}') + V_{en}(\mathbf{r},\mathbf{R})]\chi(\mathbf{R},t), && (3.12)\\
H_{\psi\psi}(\mathbf{R},t) &= \int d\mathbf{r}\; \psi^*(\mathbf{r},t)\mathcal{H}_e(\mathbf{r},\mathbf{R})\psi(\mathbf{r},t). && (3.13)
\end{aligned}$$

These equations represent the electron-nuclear dynamics in terms of two coupled, time-dependent, equations, where electrons and nuclei mutually provide effective fields to each other. It is at this point convenient to use an "amplitude-phase" representation for χ:

$$\chi(\mathbf{R},t) = A(\mathbf{R},t)e^{\frac{i}{\hbar}S(\mathbf{R},t)}, \tag{3.14}$$

which permits to express Eq.(3.11) as two coupled equations:

$$\begin{aligned}
\frac{\partial S}{\partial t} &+ \sum_{\mathbf{R}} \frac{(\nabla_{\mathbf{R}} S)^2}{2M} + \int d\mathbf{r}\psi^* \mathcal{H}_e \psi = \hbar^2 \sum_{\mathbf{R}} \frac{1}{2M} \frac{\nabla^2_{\mathbf{R}} A}{A} && (3.15)\\
\frac{\partial A}{\partial t} &+ \sum_{\mathbf{R}} \frac{(\nabla_{\mathbf{R}} A)(\nabla_{\mathbf{R}} S)}{M} + \sum_{\mathbf{R}} \frac{1}{2M} A(\nabla^2_{\mathbf{R}} S) = 0. && (3.16)
\end{aligned}$$

One can see [51] that Eq.(3.16) represents the continuity equation for $A^2 \equiv |\chi|^2$ (one simply rewrites the equation as $\partial A^2/\partial t + M^{-1}\sum_{\mathbf{R}} \nabla_{\mathbf{R}}[A^2 \nabla_{\mathbf{R}} S] = 0$ and makes the identification $\mathbf{P}_{\mathbf{R}} = \nabla_{\mathbf{R}} S$). At the same time, when $\hbar \to 0$, Eq. (3.15) becomes formally identical to the Hamilton-Jacobi equation of classical mechanics, with Hamilton function $\mathcal{H}_{cl}(\mathbf{R},\mathbf{P}) \equiv \sum_{\mathbf{R}} \frac{(\nabla_{\mathbf{R}} S)^2}{2M} + \int d\mathbf{r}\psi^* \mathcal{H}_e \psi$. By applying $\nabla_{\mathbf{r}'}$ to Eq.(3.15), we then get

$$\frac{\partial \nabla_{\mathbf{R}'} S}{\partial t} \equiv \frac{\partial \mathbf{P}'}{\partial t} = -\nabla_{\mathbf{R}'} \mathcal{H}_{cl}(\mathbf{R},\mathbf{P}). \tag{3.17}$$

Thus, the connecting transformation $\mathbf{P}_{\mathbf{R}} = \nabla_{\mathbf{R}} S$ permits to arrive to the final expression

$$M\ddot{\mathbf{R}}(t) = -\nabla_{\mathbf{R}} \int d\mathbf{r}\psi^* \mathcal{H}_e \psi \equiv -\nabla_{\mathbf{R}} V_e^E[\mathbf{R}(t)]. \tag{3.18}$$

The classical limit of the nuclear dynamics must also be taken into account into the electron dynamics, Eqs. (3.10,3.12). This is achieved by performing the replacement $|\chi(\mathbf{R},t)|^2 \to \delta(\mathbf{R} - \mathbf{R}(t))$ in these equations, where $\mathbf{R}(t)$ are the instantaneous classical nuclear positions as given by Eq. (3.18). One thus finally arrives to the coupled equations for the Ehrenfest dynamics,

$$\begin{aligned}
M\ddot{\mathbf{R}}(t) &= -\nabla_{\mathbf{R}} V_e^E[\mathbf{R}(t)], && (3.19)\\
i\hbar\frac{\partial \psi}{\partial t} &= -\sum_{\mathbf{r}} \frac{\hbar^2}{2m} \nabla^2_{\mathbf{r}} \psi + W_{\chi\chi}[(\mathbf{r},\mathbf{R}(t)]\psi, && (3.20)
\end{aligned}$$

where ψ depends parametrically on $\mathbf{R}(t)$ through $W_{\chi\chi}[(\mathbf{r}, \mathbf{R}(t)]$. Ehrenfest's dynamics is a two-component mean field approach, but includes inter-electronic transitions. At the same time, it is an "asymmetric" formulation, because of the different nature (classical vs quantum) of the two constituents which can e.g. prevent an accurate description of the heat-exchange between electrons and nuclei [52]. Also, the lack of correlation between classical and quantum motions can affect microscopic reversibility, and can give an inadequate account of reaction channels [51], as they e.g. occur in chemical reactions, especially those with low weight.

3.4.2 Time evolution for the electrons

In Papers I, II and IV, the time evolution of the electronic wavefunction for isolated systems is performed according to the Lanczos algorithm. For systems contacted to leads (i.e. for quantum transport, Papers III and IV), the time-evolution algorithm we use was originally introduced in Ref. [49]. A concise and detailed exposition of such algorithms for non-magnetic systems can be found in Paper I of this thesis, where an adaptation to include a short-iterative Lanczos solver for quantum transport is also discussed. A generalization to magnetic systems, as used in Paper IV, is not discussed here, and requires a formulation based on spinors [53].

3.4.3 Classical time evolution: the Verlet's algorithm

Consider the expansion for the classical coordinate

$$\mathbf{r}(t \pm \delta) = \mathbf{r}(t) \pm \mathbf{v}(t)\delta + \frac{1}{2}\mathbf{a}(t)\delta^2 \pm \cdots \; . \tag{3.21}$$

Adding $\mathbf{r}(t+\delta)$ and $\mathbf{r}(t-\delta)$ results in

$$\mathbf{r}(t+\delta) = 2\mathbf{r}(t) - \mathbf{r}(t+\delta) + \mathbf{a}(t)\delta^2 + O(\delta^4) \tag{3.22}$$

This integration algorithm is known as the coordinate-Verlet algorithm [50]; however, in paper III, its is used in a slightly modified form, known as the symmetric velocity-Verlet algorithm [54]:

$$\begin{aligned} \mathbf{p}(t+\delta/2) &= \mathbf{p}(t) + \mathbf{F}(t)\delta/2 \\ \mathbf{r}(t+\delta) &= \mathbf{r}(t) + \mathbf{p}(t+\delta/2)\;\delta/m \\ \mathbf{p}(t+\delta) &= \mathbf{p}(t+\delta/2) + \mathbf{F}(t+\delta)\delta/2 \; . \end{aligned} \tag{3.23}$$

For details of how it is combined with the time-evolution of the electronic wavefunctions in Paper III, we defer to the original work [47]. Here we wish to add that the algorithm of Eq. (3.23) is time-reversible, symplectic (i.e. area conserving in phase space) and energy conserving. These features can be traced back to the fact that a Verlet-type algorithm is exact for a pseudo-system (so-called ghost-system) described by a Hamiltonian H_{pseudo}, with exhibits oscillating small deviations around the true one, but without any systematic drift.

Chapter 4

Ultracold Fermions in Optical Lattices

Undisputedly, ultracold gases currently are one of most active research areas in physics. In this sizzling research field, the experimental side is clearly leading the way, and the need for new theoretical approaches to side with the experimental data is extreme and even explicitly declared by the experimentalists themselves[1]. Furthermore, looking for trends in the field, it soon becomes very clear that the top entries are non-equilibrium dynamics [56], strong-correlations [57], and disorder effects [58]. Here, we briefly describe the physics of ultracold atoms, with no pretense of detail or exhaustiveness. Excellent reviews exist on this topic (see e.g. Refs [59,60]), which cover the field from different perspectives. Rather, the aim of this very superficial and concise exposition to introduce some the notions and nomenclature used in Papers II and IV, and to motivate and locate our research work in this area.

4.1 General aspects of ultracold-atom physics

Ultra-cold atoms in optical lattices exhibit a rich and interesting physics. The high-parameter tunability of these systems makes them ideal candidates to investigate open issues in condensed matter, since simplified model

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[1] "Therefore, it is likely that progress on the theory of dynamics and thermalization in strongly correlated systems will have a strong impact on guiding experiments to cool into new regimes", excerpt from Ref. [55]

Hamiltonians, like e.g. the Hubbard model, can provide a very accurate description of ultra-cold atom physics. Looking for a possible date of birth of this field, one can point to 1995, when Bose-Einstein condensation (BEC) was experimentally observed [61,62]. However, a decisive contributing factor to this breakthrough was the availability of sophisticated laser cooling techniques, which started to be developed in the sixties. Thus, the combination of two eminent areas of physics, atomic physics and quantum optics, was essential in providing a fertile soil for the establishment of ultra-cold-atom physics, as recognized by the the Nobel Foundation in 1997 with an award for the development of methods to cool and trap atoms with laser light. Although major focus in ultracold-atom research was initially in bosonic condensates (thus, for atoms which obey Bose-Einstein statistics), later on it became possible to apply improved cooling techniques also to the case of atoms with Fermi statistics (the statistics being determined, in neutral atoms, by the number of neutrons). This has induced a steadily rising interest in Fermi systems, since they exhibit interesting features due to the Pauli principle (for example, at low temperature, in a dilute Fermi gas which is fully polarized, the dominant s-wave scattering is quenched by the Pauli principle - i.e. the gas is non-interacting).

4.2 Fano-Feshbach resonances

We come now to a concept, the Fano-Feshbach resonance, which plays a central role in cold-atom physics. The Fano-Feshbach resonance was originally considered within the realm of nuclear and atomic phenomena [63,64]. In cold-atom systems its occurrence is related to the existence of two two-body states (*closed* and *open* channel, see Fig. 4.1) with distinct magnetic moments. During an interatomic collision, transitions between these two states can occur, an thus a coupling between the channels occurs, with the coupling strength depending on the energy separation between the channels (i.e. bound state vs. continuum). This energy separation, and even the relative energetic ordering of the channels can be tailored by a magnetic field and, where applicable, allows for an effective one-channel description, where the scattering length a_s turns out to be dependent on the external magnetic field B:

$$a_s(B) = a_s^0(1 - \frac{\alpha}{B - B_{cr}}). \tag{4.1}$$

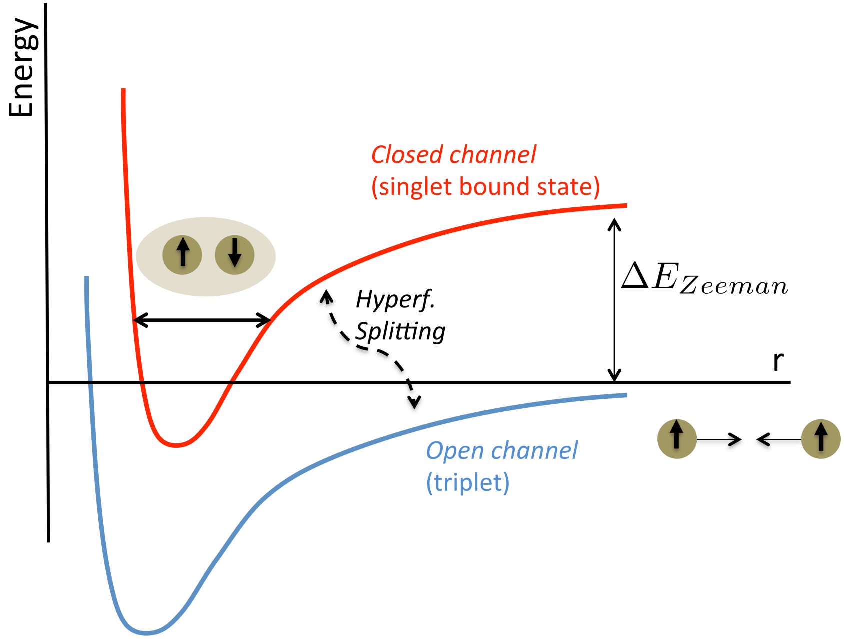

Figure 4.1: Schematic view of a Fano-Feshbach resonance.

Here, a_s^0 is the off-resonance scattering length for the open channel, while B_{cr} is the field at which the channel crossing occurs, and α is the resonance width, for which B is such that $a_s(B) = 0$. This behavior near resonance permits to consider an ultracold-atom system on equal footing with an ordinary condensed matter system, since the system can now be seen as a fermion system with spins (the two hyperfine states) interacting through a potential with a tunable scattering length (thus, experimentally observing ultracold Fermi gases with interaction requires trapping and cooling two or more hyperfine states).

Tuning the Feshbach resonances permits to access a broad range of parameters in Fermi systems. This should be contrasted to conventional condensed matter systems, where the phenomenon/feature under observation must often be disentangled by many concomitant other effects. With these possibilities, several potential applications are in principle within reach, such as, e.g., quantum information systems, the so-called atomtronics, and an accurate description of paradigmatic condensed matter model systems (i.e. one accurately prepares and manipulates an experimental ultracold-atom system to study another type of system). One should also include in this list Hamiltonian quenches, which by sudden changes of Hamiltonian parameters, permit to study important non-equilibrium aspects of many-body physics, like phase- (spin-) separation, entanglement distillation, thermalization, collisions between atomic clouds, etc.

4.3 The experimental side

An important feature of ultracold cases is their intrinsic nonhomogeneous nature, due to the trapping potential. This can complicate the direct interpretation of experiments aiming to elucidate issues in extended condensed matter systems. Another hurdle in experiments is the fragility of cold atoms against temperature: maintaining the system cooled requires isolation. In fact, one of the standard measurement techniques is to observe the gas expansion after the removal of the trapping potential. This measurement protocol is studied via numerical simulations in Paper II and IV.

4.4 Features of the inter-particle interaction

A key aspect of ultracold gases is their diluteness, i.e. the range of potential among particles is usually much smaller the average distance between the particles. A very attractive feature of this state of affairs is that diluteness reflects in the system manifesting in several respect a universal behavior. Indeed for dilute gases, it is the s-wave scattering length (see below) that encompasses all the information about the interaction properties. As a simple illustrative argument, for the relative motion of two particles scattering against each-other in a generic, spherical-symmetric short-ranged potential, the wavefunction in the asymptotic region can be written as

$$\psi_k^+ = e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{f(k,\theta)}{r} e^{ikr}, \tag{4.2}$$

where $f(k,\theta)$ can be decomposed in partial-waves contribution, each relative to an angular momentum value [65]. At small momentum k, the centrifugal barrier, proportional to $l(l+1)$, hampers the penetration of the high-l components, and only the s-wave component to scattering remains relevant. Thus, for small k,

$$f(k,\theta) \to -\frac{1}{(1/a_s) + ik + \text{subleading terms}}, \tag{4.3}$$

i.e. scattering becomes expressible in terms of the scattering length. The main conclusion, and of general validity, is that for short ranged potentials in the dilute, low-energy limit, the scattering process has generic (universal) features, which permit to consider/use theoretically the most convenient potential description which gives the same scattering length as the experimental one.

4.5 Optical lattices

With the advent of ultracold atom physics, and the high degree of parameter control attainable with them, it has become perfectly viable to realize experimental versions of paradigmatic models of condensed matter physics. The most notable example is given by the Hubbard model [66], either in the fermion or boson flavor. Here, the degree of control of Fano-Feshbach resonances in experiments is such that the strength and even the sign of the Hubbard interaction U can be changed within the same experiment. How to mimic the lattice potential of condensed matter systems? Experimentally, this is done resorting to laser optics. As an example in 1D, an oscillating laser beams far away from resonance, can interact with an atom; this i) induces a dipole moment on the atom and ii) there is an interaction between the (electric) field $\mathbf{E}$ and the induced atomic dipole:

$$v_{Laser}(\mathbf{r}) = -\mathbf{d} \cdot \mathbf{E}_{Laser}(\mathbf{r}). \tag{4.4}$$

By counterpropagating two laser beams of this kind, one can develop a optical standing-wave which produces a periodic potential in which the atom can be trapped. The laser intensity is responsible for the potential height, and the laser wavelength for the lattice spacing. At the same time, the hyperfine structure can be exploited to simulate Fermions with spin moving in virtually any type of optical lattice structure. An additional asset of this setup is that “side-effects” such as lattice vibrations and disorder can be made absent, or re-introduced in a controlled way when desired. Accordingly, theoretical treatments used for specific situations in condensed matter systems can be tested without ambiguity. In short, optical lattices offer outstanding potential to establish deep connections between ultracold atoms and condensed matter systems.

In spite of the exceptional advances, many open, crucial issues still lay on the table. Experimentally, to reach some interesting regimes for condensed matter, far lower temperatures are needed. Furthermore, from the theoretical point of view, the question of non-equilibrium properties has been vividly addressed in low dimensions (especially d=1, where powerful techniques such as the Density-Matrix Renormalization Group (DMRG) are available. However, much less is known for Fermions out of equilibrium in higher dimensions. Here, the presence of a Mott metal-insulator transition at a finite, critical value U_{crit} of the Hubbard interaction plays a crucial role already in the ground state of trapped Fermions (see Fig. 4.2), and its importance becomes even greater in the out-of-equilibrium regime. This is the topic of Paper II and part of Paper IV of this thesis.

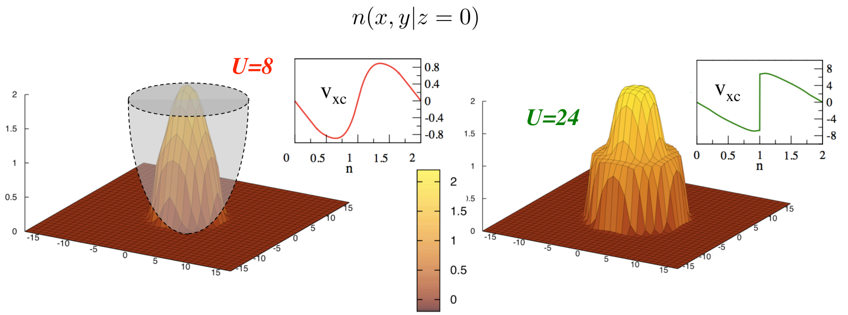

Figure 4.2: DFT density profiles in the z=0 plane for metallic and insulating regimes of trapped fermions. The inherent shape of the exchange-correlation potential is also shown.

Bibliography

[1] P. Hohenberg and W. Kohn, *Phys. Rev.* **136**, B864 (1964).

[2] W. Kohn and L. J. Sham, *Phys. Rev.* **140**, A1133 (1965).

[3] L. H. Thomas, *Proc. Cambridge Phil. Soc.* **23**, 542 (1927).

[4] E. Fermi, *Rend. Accad. Naz. Lincei* **6**, 602 (1927).

[5] E. Runge and E. Gross, *Phys. Rev. Lett.* **52**, 997 (1984).

[6] E. K. U. Gross and D. M. Dreizler, editors, *Density Functional Theory*, Plenum Press, New York, 1995.

[7] W. Kohn, *Rev. Mod. Phys.* **71**, 1253 (1999).

[8] M. A. L. Marques, C. Ullrich, F. Nogueira, A. Rubio, K. Burke, and E. K. U. Gross, editors, *Time-Dependent Density-Functional Theory*, Springer, Berlin, 2006.

[9] O. K. Andersen, *Phys. Rev. B* **12**, 3060 (1975).

[10] D. R. Hamann, M. Schlüter, , and C. Chiang, *Phys. Rev. Lett* **43**, 1497 (1979).

[11] C. G. Broyden, *Mathematics of Computation* **19**, pp. 577 (1965).

[12] D. G. Anderson, *J. ACM* **12**, 547 (1965).

[13] D. Singh, *Phys. Rev. B* **40**, 5428 (1989).

[14] U. von Barth, *Phys. Scr.* **T 109**, 9 (2004).

[15] U. von Barth and L. Hedin, *J. Phys. C* **5**, 1629 (1972).

[16] A. K. Rajagopal and J. Callaway, *Phys. Rev. B* **7**, 1912 (1973).

[17] O. Gunnarsson and K. Schönhammer, *Phys. Rev. Lett.* **56**, 1968 (1986).

[18] O. Gunnarsson and K. Schönhammer, *J. Phys. C: Solid State Phys.* **20**, 3675 (1987).

[19] N. A. Lima, M. F. Silva, L. N. Oliveira, and K. Capelle, *Phys. Rev. Lett.* **90**, 146402 (2003).

[20] N. Lima, L. Oliveira, and K. Capelle, *Europhys. Lett.* **60**, 601 (2002).

[21] V. L. Campo, K. Capelle, C. Hooley, J. Quintanilla, and V. W. Scarola, *Phys. Rev. A* **85**, 033644 (2012).

[22] X. L. Gao, A. Chen, I. V. Tokatly, and S. Kurth, *Phys. Rev. B* **86**, 235139 (2012).

[23] C. Verdozzi, *Phys. Rev. Lett.* **90**, 166401 (2008).

[24] R. Baer, *J. Chem. Phys.* **128**, 044103 (2008).

[25] Y. Li and C. A. Ullrich, *J. Chem. Phys.* **129**, 044105 (2008).

[26] W. Li, G. Xianlong, C. Kollath, , and M. Polini, *Phys. Rev. B* **78**, 195109 (2008).

[27] M. Farzanehpour and I. V. Tokatly, *Phys. Rev. B* **86**, 125130 (2012).

[28] K. Schönhammer and O. Gunnarsson, *Phys. Rev. B* **37**, 3128 (1988).

[29] K. Schönhammer, O. Gunnarsson, and R. Noack, *Phys. Rev. B* **52**, 2504 (1995).

[30] A. Zangwill and P. Soven, *Phys. Rev. A* **21**, 1561 (1980).

[31] C. Verdozzi, D. Karlsson, M. P. von Friesen, C.-O. Almbladh, and U. von Barth, *Chemical Physics* **391**, 37 (2011).

[32] G. Xianlong, M. Polini, M. Tosi, V. Campo, K. Capelle, and M. Rigoli, *Phys. Rev. B* **73**, 165120 (2006).

[33] A. Akande and S. Sanvito, *Phys. Rev. B* **82**, 245114 (2010).

[34] E. Lieb and F. Wu, *Phys. Rev. Lett.* **20**, 1445 (1968).

[35] D. Karlsson, A. Privitera, and C. Verdozzi, *Phys. Rev. Lett.* **106**, 116401 (2011).

[36] W. Metzner and D. Vollhardt, *Phys. Rev. Lett.* **62**, 324 (1989).

[37] A. Georges, G. Kotliar, W. Krauth, and M. Rozenberg, *Rev. Mod. Phys.* **68**, 13 (1996).

[38] J. Hubbard, *Proc. R. Soc. Lond. A* **276**, 238 (1963).

[39] P. W. Anderson, *Phys. Rev.* **109**, 1492 (1958).

[40] J. Billy, V. Josse, Z. Zuo, A. Bernard, B. Hambrecht, P. Lugan, D. Clment, L. Sanchez-Palencia, P. Bouyer, and A. Aspect, *Nature* **453**, 891 (2008).

[41] F. Jendrzejewski, A. Bernard, K. Möller, P. Cheinet, V. Josse, M. Piraud, L. Pezz, L. Sanchez-Palencia, A. Aspect, and P. Bouyer, *Nature Physics* **8**, 398 (2012).

[42] R. Kaiser, *Nature Physics* **8**, 363 (2012).

[43] R. J. Elliott, J. A. Krumhansl, and P. Leath, *Rev. Mod. Phys.* **45**, 465 (1974).

[44] A. Zunger, S.-H. Wei, L. G. Ferreira, and J. E. Bernard, *Phys. Rev. Lett.* **65**, 353 (1990).

[45] C. Verdozzi, P. J. Durham, R. J. Cole, and P. Weightman, *Phys. Rev. B* **55**, 16143 (1997).

[46] T. Holstein, *Ann. Phys.* **8**, 325 (1959).

[47] C. Verdozzi, G. Stefanucci, and C.-O. Almbladh, *Phys. Rev. Lett.* **97**, 046603 (2006).

[48] P. Ehrenfest, *Z. Phys.* **46**, 455 (1927).

[49] S. Kurth, G. Stefanucci, C.-O. Almbladh, A. Rubio, and E. K. U. Gross, *Phys. Rev. B* **72**, 035308 (2005).

[50] L. Verlet, *Phys. Rev.* **159**, 98 (1967).

[51] J. C. Tully, *Faraday Discuss.* **110**, 407 (1998).

[52] A. P. Horsfield, D. R. Bowler, A. J. Fisher, T. Todorov, and M. Montgomery, *J. Phys. Cond. Mat.* **16**, 3609 (2004).

[53] G. Stefanucci, E. Perfetto, , and M. Cini, *Phys. Rev. B* **78**, 075425 (2008).

[54] M. P. Allen and D. Tildesley, *Computer simulation of liquids*, Oxford University Press, Oxford, 1989.

[55] D. C. McKay and B. D. Marco, *Rep. Prog. Phys.* **74**, 054401 (2011).

[56] C. J. M. Mathy, M. B. Zvonarev, and E. Demler, *Nature Physics* **8**, 881 (2012).

[57] C. Wu, *Nature Physics* **8**, 784 (2012).

[58] F. Jendrzejewski, A. Bernard, K. Möller, P. Cheinet, V. Josse, M. Piraud, L. Pezz, L. Sanchez-Palencia, A. Aspect, and P. Bouyer, *Nature Physics* **8**, 398 (2012).

[59] I. Bloch, *Nature Physics* **1**, 23 (2005).

[60] C. J. Pethick and H. Smith, *Bose-Einstein condensation in dilute gases*, Cambridge University Press, Cambridge, 2nd edition edition, 2008.

[61] K. Davis, M. Mewes, M. Andrews, N. van Druten, D. Durfee, D. Kurn, and W. Ketterle, *Phys. Rev. Lett.* **75**, 3969 (1995).

[62] M. Anderson, J. Ensher, M. Matthews, C. Wieman, , and E. Cornell, *Science* **269**, 5221 (1995).

[63] U. Fano, *Nuovo Cimento* **12:156+**, 11 (1935).

[64] H. Feshbach, *Annals of Physics* **19**, 11 (1962).

[65] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics - Non relativistic theory*, Pergamon Press, London, 1958.

[66] J. Hubbard, *Proc. Roy. Soc. London, Series A* **276**, 238 (1963).

Part II

The Papers