Theoretical investigation of correlated fermions on optical lattice with spin-dependent disorder

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Abstract

The aim of this thesis is to investigate the properties of correlated fermions on optical lattice with spin-dependent disorder. The system is modeled by an Anderson-Hubbard Hamiltonian on a bipartite Bethe lattice with the on-site potential treated as a random variable drawn from the spin-dependent probability distribution function. The solution of this model is obtained within the dynamical mean-field theory with geometric average over the disorder realization. This method treats disorder and interaction on equal footing and is sensitive to the Anderson localization on single-particle level. In the thesis two scenarios are discussed: (i) paramagnetic case, where the instability towards forming a magnetic long-range order is blocked, and (ii) staggered magnetic case, where this instability is enabled.

In case (i) the paramagnetism is imposed by forcing the equivalence of the solution on both sublattices. Thanks to this one can focus solely on the competition between the disorder ($\Delta$) and interaction ($U$). The obtained phase diagram for this case shows the existence of three phases: metal, disordered Mott insulator and spin-selective localized phase. Oppose to the conventional disorder case where the interaction and randomness competed, in the spin-dependent case these two factors cooperate in order to drive the system into the insulating phase. The reason being that breaking the spin symmetry affects directly the efficiency of the process that leads to the quasiparticle resonance formation. This is why the transition lines on the $U - \Delta$ phase diagram are tilted towards the lower interaction strengths. Because of the spin-dependence of the disorder a novel spin-selective localized phase has been observed at high disorder strengths. It is characterized by the coexistence of itinerant fermions in the spin channel not directly affected by the randomness and localized carriers in the other spin channel. This phase is separated form the insulating phase by a disorder strength independent line of transition points, which reflects the Falicov-Kimball-like nature of the spin-selective localized phase.

In case (ii) the possibility of forming an magnetic long-range order was included in the model by treating the sublattices separately. The resulting phase diagram shows five distinct phases with four different spin ordering. Starting at small $\Delta$ the system is an insulator with anti-parallel ordered spins, which reflects the natural tendency of the half-filled Hubbard model to form an insulator with an antiferromagnetic order. Due to the spin-dependence of the disorder the magnetization on the subalttices does not have the same absolute value, but becomes reduced in case when the majority spin is directly affected by the disorder. At higher $\Delta$ and small $U$ first the gap in one spin channel is closed (spin-selective localized phase of type I) and at even higher disorder strengths the system becomes a ferromagnetic metal. Finally, at large enough $\Delta$ the system turns into a spin-selective localized phase of type II. It is a counterpart of the spin-selective localized phase in paramagnetic case but with a magnetic order. As in previous case this phase boarders with insulator (insulator of type II) on a $\Delta$-independent line of transition points. Lastly, when $\Delta$ and $U$ is large the system becomes an insulator of type II. Which is characterize by a broad spectral gap and a SDW ferromagnetic order.
Contents

1 Introduction 9

2 Experiments in cold atoms 13
  2.1 Experimental setup ........................................ 14
  2.2 Disordered optical lattice .................................. 17
  2.3 Spin-dependent optical lattice ............................. 17

3 Model and method 19
  3.1 The one-band Hubbard model ................................. 19
    3.1.1 Non-interacting and non-hopping limit ............... 20
    3.1.2 AF insulator ............................................ 21
  3.2 The Dynamical Mean-Field Theory ........................... 23
    3.2.1 Infinite dimension limit .............................. 24
    3.2.2 Locality of self-energy in $d \to \infty$ limit .......... 25
  3.3 The single impurity Anderson model ......................... 27
    3.3.1 Non-interacting limit (U=0) ......................... 29
    3.3.2 Atomic limit ($V_{\vec{k},\sigma} = 0$) ................ 30
    3.3.3 Schrieffer-Wolf transformation ...................... 31
    3.3.4 Poor-man’s scaling ................................... 32
  3.4 DMFT loop ................................................. 33
  3.5 Numerical Renormalization Group ........................... 35
    3.5.1 Calculation of thermodynamic properties ............. 37
  3.6 The Coherent Potential Approximation ........................ 39
  3.7 The Typical Medium Approximation .......................... 41
  3.8 The Bethe lattice ......................................... 42
  3.9 The Falicov-Kimball model ................................ 46

4 Results 49
  4.1 Paramagnetic Case ....................................... 51
    4.1.1 Metallic phase ....................................... 52
    4.1.2 Mott-Hubbard MIT and the coexistence regime .......... 52
    4.1.3 Spin-selective Anderson localized phase ............. 53
    4.1.4 Disordered Mott insulator ............................ 56
  4.2 Staggered magnetic case .................................. 59
4.2.1 Ferrimagnetic insulator of type I (Ins-I) ........................................ 60
4.2.2 Ferrimagnetic spin-selective localized phase of type I 
(SSLP-I) ........................................................................................................ 62
4.2.3 Ferromagnetic metal (FM) ................................................................. 63
4.2.4 Ferromagnetic SDW spin-selective localized phase of type II (SSLP-II) 64
4.2.5 Ferromagnetic SDW insulator (Ins-II) .............................................. 67

5 Summary ..................................................................................................... 70

Appendix A Derivation of the Hubbard model ............................................. 73
Appendix B Green’s function properties ....................................................... 75
## List of abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Full form</th>
</tr>
</thead>
<tbody>
<tr>
<td>AF-LRO</td>
<td>antiferromagnetic long-range order</td>
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<td>CPA</td>
<td>coherent potential approximation</td>
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<td>DMFT</td>
<td>dynamical mean-field theory</td>
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<td>EOM</td>
<td>equation of motion</td>
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<tr>
<td>FM</td>
<td>ferromagnetic metal</td>
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<tr>
<td>Ins-I</td>
<td>ferromagnetic insulator of type I</td>
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<tr>
<td>Ins-II</td>
<td>ferromagnetic SDW insulator of type II</td>
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<tr>
<td>LDOS</td>
<td>local density of states</td>
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<td>MIT</td>
<td>metal-insulator transition</td>
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<td>NRG</td>
<td>numerical renormalization group</td>
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<tr>
<td>PDF</td>
<td>probability distribution function</td>
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<td>SDW</td>
<td>spin density wave</td>
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<td>SIAM</td>
<td>single impurity Anderson model</td>
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<tr>
<td>SSLP-I</td>
<td>ferromagnetic spin-selective localized phase of type I</td>
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<tr>
<td>SSLP-II</td>
<td>ferromagnetic SDW spin-selective localized phase of type II</td>
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<td>TMT</td>
<td>typical medium theory</td>
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Chapter 1

Introduction

Since the early days of solid state physics the question of why some materials are conducting and others are insulating has been the central issue. The first attempt to solve this problem was a propose made by F. Bloch in 1928 [1]. The idea behind this theory was that ions placed in a periodic structure create a potential for valence electrons that restricts their movement. As a result this electrons form bands of allowed energies separated by gaps. In the zero temperature limit electrons, being fermions, occupy the lowest energy levels. The energy of the highest occupied level is called the Fermi energy. Depending on the chemical composition (number of valence electrons) the Fermi energy can be located within either the band or in the gap. If the Fermi energy is located within the band the applied infinitesimal voltage can promote an electron to a higher energy level and create a positively charged hole below the Fermi energy. As a result this system is a conductor. On the other hand, if the Fermi level is placed in the gap one has to apply a large enough voltage that the electron could overcome the energy gap. Otherwise the excitation is prohibited and this system is an insulator.

Although band theory was very successful in explaining electronic properties of a large number of materials, there were also cases where it failed. Historically the first class of materials in which the band theory failed to work was the transition metal oxides [2]. According to the band theory they should be metallic but experiments showed the insulating behavior. The first one who understood the reason for this discrepancy was Sir N. Mott, who pointed out in his seminal paper [3] the importance of the Coulomb interaction between the electrons. In the Bloch theory the inter electron interaction was completely neglected. As a result the electrons were treated as independent fermions. This is the reason why Bloch theory is referred to as a single particle theory. What Mott has showed is that when the interactions are taken into account the picture changes drastically. His line of reasoning was that since the excitation in the system is an electron-hole pair, it is kept together by the Coulomb interaction. To delocalize the excitation one has to create more excitations which will mutually screen the interaction between the constituents of the pair. Holes will screen the electron charge and electrons will screen the hole charge. Because the screening strongly relies on the density of electrons, if it is insufficient, the screening is too weak and the excitations remain localized to their ions. Thus the system is insulating. The crucial factor in this scenario is the interplay between the interaction
CHAPTER 1. INTRODUCTION

and the electron density. The change of the electronic state of the system caused by increasing role of interaction is called a many-body metal-insulator transition (MIT) or just Mott transition. The idea of Mott was later reformulated by J. Hubbard when he introduced the Hubbard model [42] in 1963. This model has become the paradigm for studying strongly correlated electronic system. An in-depth analysis of this model showed that the Mott transition can be tied to the appearance of a magnetic order. A major role in understanding of the physics described by the Hubbard model was played by the high dimension limit introduced to this problem by Metzner and Vollhard [54]. Their study has lead to the construction of the Dynamical Mean-Field Theory (DMFT) [62]. A method that captures the complex behavior of electrons described by the Hubbard model when they undergo the transition from a metallic phase to an insulating phase upon increasing the interaction strength. The results obtained within this method become exact in the limit of infinite spatial dimensions.

At the time when the idea of Mott was crystallizing and physicists started to acknowledge the importance of electron interaction in different surprising discoveries an unexpected observation was made. In 1958 P. W. Anderson showed that disorder can also play a major role in the electronic properties of solids [4]. The disorder was understood as randomly distributed (local) potentials on a lattice. What was earlier believed to be a simple scattering problem that could only weakly affect the system properties has turned out to have tremendous repercussions. Anderson showed that if the spread of energies of the random potentials (disorder strength) on a lattice is large enough the single particle wave function will change its spatial character from extended to localized. As a consequence of this change the diffusion in the system would disappear [5]. Later it was rigorously shown, using the scaling theory introduced by Abraham, Anderson, Ricardello and Ramakrishnan in 1979 [6], that in dimensions lower or equal to two localization will always take place at zero temperatures, no matter what the disorder strength is. This phenomenon of localizing the wave function due to scattering from randomly distributed impurities is called the Anderson localization. The fact that localization appears when the character of wave function changes has inspired Mott [7] to introduce the concept of the “mobility edge” in dimensions higher then two. He introduced it as the energy separating the localized from the delocalized states. The reasoning was based on Ioffe-Regel [8] criterion which states that the in order for the scattering off the impurities to take place the mean free path (average distance between scattering centers) cannot be shorter then the particle (de Broglie) wavelength. Otherwise the particle will become localized. Particles with energies around to the band center have the wavelength comparable with lattice spacing (shortest possible distance), whereas the one with energies closer to the band edge have a longer wavelength. Increasing the disorder reduces the mean free path. From the Ioffe-Regel criterion this means that first the particles with energies away from the band center will be affected, due to their longer wavelength. Thus there must exist an energy that separates this two cases and its value should depend on the strength of the disorder and the dimensionality. Although the Anderson localization is a non-interacting phenomenon it is far from being simple. The complications in theoretical treatment originate from the scattering triggered by the randomness. This is the reason why in
dimensions larger than two still not much exact results were obtain. The central question being how does the mobility edge behaves with disorder strength in three dimensional systems. Thanks to the numerical calculations a lot of insight has been gained concerning this problem [9, 10], such as the re-entrance of the mobility edge.

The discoveries made by Mott and Anderson have showed how diverse the mechanisms for the metal-insulator transition can be. This posed another question: How these mechanisms affect each other if they both exist in the same system?. The question is of big importance, since in real materials both correlations and disorder are present. This problem motivated a large group of scientists to develop a theory that treats both the Coulomb interaction and the randomness on equal footing.

Studying effects of the interaction and the disorder poses a major problem not only from the theoretical point of view but also from the experimental side. Precise control over the interaction and the disorder is impossible in standard solid state systems. Very often one effect is connected to the other and separating them seems hopeless. This is why ultracold atoms in optical lattices has become such an important tool in condensed matter physics. They enable one to directly study models and tune their parameters in a broad range. One of such model, studied using cold atoms, is the Anderson-Hubbard model, an extension of the Hubbard model to a random on-site potential. But current experimental setups also can enable one to explore physics that go beyond the standard solid state physics. One interesting outlook is the Hubbard-Anderson model with a spin-dependent disorder. Although not yet realized, the development in the past years on spin-dependent lattices and disorder lets one believe that it could be brought to life in the near future. Since this model has not yet been a subject of theoretical investigation it is important to learn its properties before it will be realized in a cold atom laboratory. This is why this thesis is devoted to study of interacting fermions in presence of the spin-dependent disorder.

The first Chapter of this dissertation is an introduction to the field of cold atoms, with special emphasis on the development that can lead to creation of the spin-dependent disorder. It begins with the description of how ultracold atomic gases and optical lattices are obtained. Later it is described how disorder is imprinted onto the optical lattice. Finally, examples of experiments with the spin-dependent optical lattices are described.

The second Chapter is devoted to the description of the model and method used to obtain the results presented later in this dissertation. It begins with a description of the one-band Hubbard model with basic intuitions about the physics encoded in it. Later the limit of the infinite dimensions and its implications in a context of the Hubbard model is discussed. Special emphasis is put to show the mapping of the model onto the single impurity Anderson model (SIAM). Then it is followed by the introduction to the physics of SIAM. This part is crucial for further understanding of physical results. Finally the complete DMFT self-consistent equations are introduced, followed by a short presentation of the Numerical Renormalization Group (NRG) as a method for solving the SIAM. Later the extension of standard DMFT approach to disordered systems is presented, with discussions of the Coherent Potential Approximation (CPA) and the Typical Medium Theory (TMT). Finally the second Chapter concludes with a short introduction to the
Bethe lattice and the Falicov-Kimball model.

The third Chapter is dedicated to present the results of the theoretical investigation of the interacting fermions on a lattice with spin-dependent disorder. It is divided into two parts: a paramagnetic case and a staggered magnetic case. Both parts are centered around the ground state phase diagrams for the corresponding situations. In the a paramagnetic case the magnetic instability not allowed and the determined phase diagram is the result of only charge instabilities triggered by the interplay of interaction and the spin-dependent disorder. The main concern in the second case is how the magnetic instability affects the previously calculated phase diagram.
Chapter 2

Experiments in cold atoms

The past 22 years has been a period of rapid development in physics of ultracold atomic gases. What started as a narrow field focused on experimental study of fundamental concepts in quantum mechanics has rapidly transformed into a broad field that not only extends our understanding of atomic physics but is also used as a testbed for models in the condensed matter physics [11] or in applications of a quantum information processing [12]. The first milestone in the history of experiments with cold atomic gases was reached in 1995 in the group of professor Eric Cornell at the University of Colorado [13]. By cooling a gas of $^{87}\text{Rb}$, with $2.5 \cdot 10^{22}$ particles per cubic centimeter, down to 170 nK they have observed a Bose-Einstein condensation (BEC). The BEC phenomenon is observable only at low enough temperatures, when a large fraction of particles with integer spin (bosons) starts to occupy the lowest energy state. For this historic experiment, which confirmed the prediction made more than seventy years earlier by S. N. Bose [14] and A. Einstein [15], E. Cornell together with C. Wiemann were awarded a Nobel prize in 2001. Reaching even lower temperatures and exploring the physical phenomena at this extreme conditions has remained an important direction in this field of research. Just three years later after Cornell’s achievement, a new direction of study was started with the seminal paper by Jaksch, et al. [16]. The aim of this paper was to propose that using laser beams one can crate an artificial crystal-like lattice, and that dynamics of the Bose gas placed in such an optical confinement can be described by the Bose-Hubbard Hamiltonian with the repulsive interaction [17]. This Hamiltonian is a bosonic version of the Hubbard Hamiltonian for fermions described in details in Section 3.1. The suggestion in Ref. [16] meant that using an optical lattice one would be able to observe the phase transition from a superfluid to a Mott insulator. In the first phase atoms are collectively spread out over the whole lattice with a long-range phase coherence. In the Mott insulating phase atoms are much more localized and the long-range phase coherence is lost. Jaksch, et al. predictions where confirmed four years later by the group of W. T. Hänsch in Munich [18], and the transitions between these two phases were measured. A further development in this field has lead to observation of the fermionic analog of the superfluid-Mott insulator transition. In 2008 the group of T. Esslinger in Zurich studied the dynamics of the Hubbard model using a two component ultracold fermionic gas loaded into an optical lattice [19]. High tunability of the experimental setup enables one to sample a wide range of parameters in this models.
CHAPTER 2. EXPERIMENTS IN COLD ATOMS

The techniques used in the two mentioned above papers have paved the way for further investigations of various models from the condensed matter physics. The number of such reports has grown rapidly since the year 2008. To mention a few, ultracold atomic gases have been used to simulate the spin Hall effect [20], to show fractional statistics [21] or to prove the existence of the mobility edge in the disordered systems [22]. What was also recognized, is the ability of cold atomic experiments to study models that go beyond the standard condensed matter problems. For example it is possible to manipulate with a lattice type for different spin species separately [28, 29]. The aim of this Chapter is twofold. The first one is to discuss the necessary steps to create an atomic gas whose dynamics is governed by the Hubbard Hamiltonian. The second aim is to show how the development of the field has enabled one to explore the behavior of exotic models of correlated systems that exceeds what has been studied in the past. This possibility was the motivation behind the study of the Hubbard model on a spin-dependent disordered lattice which is the topic of this Thesis.

2.1 Experimental setup

The route to simulate the Hubbard model with a cold atom gas on an optical lattice consist of three steps. Firstly, one has to optically cool and trap the gas in order to obtain the limit in which its dynamics is governed by quantum mechanics. This happens, when the thermal de Broglie wave length of particles becomes comparable with the average distance between them. The second step is to turn on the optical lattice, to confine the atoms around periodic minima of the electric field, which are called the lattice sites. This confinement restricts the movement of particles mainly to tunneling processes between the neighboring lattice sites. Finally the local interactions between particles is tuned by means of the Feshbach resonance [23].

Although the details of this process depend on the atomic gas used in the experiment, the general scheme is very similar. The schematic plot of an experimental set up is shown in Fig. 2.1. At the beginning the gas of a given element is created by heating up the source of atoms above the temperature at which the evaporation starts. Then the vapor is transported through the so-called Zeeman slower [24] to the vacuum chamber where the experiment is conducted. During the transport the initial cooling is performed in order to decrease the velocity of atoms in the vapor from few hundred meters per second to around ten meters per second. It is obtained by illuminating the moving vapor with the counter propagating laser light with frequency tune to maximize the absorption by the atoms in the gas. The photons which are absorbed by the atoms have had only one direction of momenta in contrast to the isotropically emitted photons due to the spontaneous relaxation. Because of the momentum conservation most of the emission processes will decrease the particles velocities along the laser light direction. As the average velocity is reduced, the laser light frequency experienced by the particles is also changed due to the Doppler effect. In order to overcome it and keep the resonant absorption a spatially varying magnetic field is applied along the path from the source to the vacuum chamber. The role of the magnetic field is to split the hyperfine states of the atom and to control the
2.1. EXPERIMENTAL SETUP

Figure 2.1: Schematic plot of experimental setup used to obtain an ultracold atomic gas.

distance between them using the Zeeman effect. This is why this part of the experimental setup is called the Zeeman slower.

Once the gas enters the vacuum chamber it is subjected to the magneto-optical trap (MOT). The MOT uses the same principles as the Zeeman slower, but the magnetic field is spherically symmetric with radially increasing strength. In this configuration only the atoms that move outwards from the trap are slowed down. This results in a spatial confinement of atoms around the center of the chamber. The final step of the cooling process is the so called evaporating cooling. At this step the atoms with energies above some threshold are enabled to leave the trap. In the end a hot vapor created from the source at temperature around few hundred Kelvin is cooled down to few hundred nanokelvins and confined to the area of the order of centimeters in diameter. At this stage the atoms form a degenerate quantum gas. Using procedures based on this scheme the following atomic fermionic species have been cooled down to a quantum regime: $^{40}\text{K}$ [30], $^{6}\text{Li}$ [31], $^{173}\text{Yb}$ [32]

After cooling down the quantum gas is loaded into an optical lattice. The optical lattice is created by shining pairs of counter propagating laser lights to create a standing wave. Depending on the lattice dimension one can use one, two or three such pairs. The light acting on an atom induces a varying in time dipole moment by shifting the negatively charged electronic cloud with respect to the positively charged nuclei. This induced dipole moment interacts with the external electric field coming from the laser light. The effective potential felt by each atom can be described by

$$V_{dip}(\vec{r}) = -\vec{d} \cdot \vec{E}(\vec{r}) \propto \alpha(\omega_L)|\vec{E}(\vec{r})|^2,$$
where $\vec{d}$ is the vector of electric dipole, $\vec{E}(\vec{r})$ is the space dependent electric field, and $\alpha(\omega_L)$ is the frequency dependent polarizability constant of the atom. Polarizability relates the induced dipole moment to the external field. Depending on its sign the atoms may favor places with low intensity (low-field seekers) or high intensity of light (high field-seekers).

By crating interference between the laser beams the spatial dependence of the potential can be approximately written as

$$V_{dip}(\vec{r}) \propto V_x \cos^2(k_x x) + V_y \cos^2(k_y y) + V_z \cos^2(k_z z), \quad (2.1)$$

where $k_i = \frac{\lambda_i}{2\pi}$ is the i-th Cartesian coefficient of the wave vector and $\lambda_i$ is the laser wavelength in the i-th direction. The potential in Eq. 2.1 has periodicity of half of the wave length and depth controlled by the intensity of light and the polarizability constant. The mixed terms in the potential that should appear in the calculation of $|\vec{E}(\vec{r})|^2$ can be canceled by choosing the proper relative polarization and frequency offset of the laser beams. Since the lasers can be controlled to a very large extend one can create multiple types of lattices, from simple chains [25] to much more complicated structures such as triangular [25] or cubic lattices [26]. What is also important is that optical lattices, unlike solid state crystals, are free of defects such as distortions or vacancies. This fact enables one to perform measurements on really pristine lattices.

The final step in creating a system modeled by the Hubbard Hamiltonian is to control the interaction. Although atoms are neutral, when they collide with each other the electromagnetic (Coulomb) interaction between their elementary constituents becomes important giving rise to scattering processes. Since the temperature is low and the de Broglie wavelength associated with the atoms is large, the s-wave scattering a dominates. The corresponding parameter $U$, describing the interaction strength in Hubbard model, can be approximated by

$$U = g \int d^3r |\psi(\vec{r})|^4,$$

where $\psi(\vec{r})$ is the wave function of an atom residing at a given lattice site. The parameter $g = \frac{4\pi a}{m}$ depends on the mass $m$ of the atoms and on the scattering length $a$. The value of $a$ can be changed from negative to positive values by changing the external magnetic field. This is a consequence of the Feshbach resonance [27], which is a process of mixing between the pure scattering states and a virtual bound stated formed between the pair of atoms. The role of the magnetic field is to control the relative energy of this bound state with respect to the energy of the scattered particle. As a result the s-wave scattering length close to the Feshbach resonance is given by

$$a(B) = a_0 \left(1 - \frac{\Delta}{B - B_0}\right),$$

where $a_0$ is a scattering length without considering the virtual bound state, $B$ is the external magnetic field, $B_0$ is the resonant value of the magnetic filed and $\Delta$ is the width of the resonance [33]. Since $a$ is proportional to $g$, hence also to $U$, the interaction strength can be controlled in a broad range.
2.2 Disordered optical lattice

Introducing a disorder into the optical lattices may sound like an unnecessary step since the investigation of Hubbard-like models in ideal periodic potential has been one of the driving forces behind the development of this field. Indeed, it was later realized that the control over different parameters of the atoms in optical lattices opens a great opportunity to investigate the Anderson model [4]. By producing a system of non-interacting particles in a randomly distributed potential one can experimentally validate the most profound effect of disorder, the Anderson localization. Such a situation could not be rigorously realized in solid state materials due to the inevitable Coulomb repulsion that can potentially mask the single particle effect, that is the Anderson localization. The first such experiments with cold atoms were reported in 2008 [34, 35]. Both groups have investigated localization in one dimensional bosonic condensates. Later, the Anderson localization was studied in three dimensional ultracold fermionic gases [36]. Although there has been a number of different studies of this phenomena, they all used one of two available methods to create the disorder. First one, introduced by the group of Aspect [34], used a speckle potential created by shining a laser light through a ground-glass diffusing plate. Light passing through such a plate encounters many scattering centers and when it reaches the optical lattice is an interfering sum of many scattered waves created in the plate. This results in an additional potential for cold atoms, which shape consists of many randomly distributed intensity peaks. Although the spatial positions of the peaks are not under experimental control, the height of them can be tuned by changing the intensity of the laser. This scheme was used in the study of three dimensional Anderson localization conducted by the group of de Marco [36]. The second method, used by the group of Inguscio [35], relies on creating a second optical lattice on top of the one used to simulate the tight-binding model. The key point is to choose the laser wavelength in such a way that the resulting additional optical lattice is incommensurate with the initial one. This can be achieved by choosing the ratio of the wavelengths of this two lasers to be an irrational number. As a result of the interferences the effective potential loses periodicity and each lattice site is shifted by a quasi-random offset. Because of using of two optical lattices, it is called a bichromatic lattice method. Although less popular, this method enables one to continuously turn on the disorder strength. It also create an opportunity to study quasi-periodic systems described by Aubry-Andre model [37], that have also been a subject of vast theoretical interest.

2.3 Spin-dependent optical lattice

The possibilities of optical lattices are not limited to reproducing the models known form the condensed matter theory. By properly engineering the interference pattern of laser beams one can form optical lattices that go beyond solid state crystals. One of such cases was studied by the group of DeMarco in 2010 [38]. Namely, they created a spin-dependent optical lattice. The main idea is to introduce an additional external magnetic field and to tune the angle between this field and the polarizations of the laser beams.
beams used to create the optical lattice. As a result the potential, apart from spin-independent periodic structure, would have a spatially varying local spin-dependent on-site component. This new potential can effectively be described by a site-dependent magnetic field. Initially DeMarco and McKay used this setup to investigate effects of turning on the lattice potential on the systems temperature. Because the spin-dependent lattice does not affect the $m_F = 0$ magnetic component of the gas, it can play a role of a thermometer.

The concept of spin-dependent optical lattices was explored further in experiments done by Soltan-Panahi and co-workers [29] a year later. They created a spin-dependent hexagonal optical lattice using the same principles as in [38]. Their experiment was conducted using a quantum gas formed by cooling the $^{87}$Rb atoms in a single hyperfine state with $F=1$. This hyperfine state were later split by external magnetic field into three $m_F = 1, 0, -1$ states. Then by intersecting three linearly polarized laser beams at 120° angle they created a hexagonal lattice. Interestingly the angle between the polarization was chosen such that the resulting interference pattern had opposite light polarization in neighboring sites. As a result the lattice could be viewed as a combination of a spin-independent hexagonal lattice and a triangular spin-dependent superlattice. Using this setup they explored the influence of such a lattice on a superfluid-Mott insulator transition.

This intriguing possibility of creating spin-dependent lattices in cold atomic systems has been a driving force behind this work. Especially the question of what would be the effect of spin-dependent disorder on a metal-insulator transition. This scenario has not been a subject of theoretical investigation yet because of impossibilities to realize it in solid state materials.
Chapter 3
Model and method

3.1 The one-band Hubbard model

The Hubbard model is one of the most important models in condensed matter theory. It was introduced independently by M. Gutzwiller [40], J. Kanamori [41], and J. Hubbard [42] in 1963. The name Hubbard model remained because of the series of six papers [42, 43, 44, 45, 46, 47] by Hubbard that have largely influenced our understanding of it. Hubbard model was introduced to investigate correlation effects in d-band electrons in transition metals ferromagnets. As it was pointed out in first paper [42] the free-electron gas approach, being exploited at that time, was insufficient to characterize the narrow band electrons even at quantitative level and one should use theory that “takes into account adequately the atomistic nature of the solid” [42]. The Hamiltonian of the Hubbard model is given by

\[ H = -t \sum_{<i,j>,\sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + \sum_{i,\sigma} \epsilon_{i,\sigma} n_{i,\sigma} + \frac{U}{2} \sum_{i,\sigma} n_{i,\sigma} n_{i,\bar{\sigma}} = H_{\text{hop}} + H_{\text{int}}, \]  

(3.1)

where \( c_{i,\sigma} (c_{i,\sigma}^\dagger) \) is the annihilation (creation) operator of an electron in a Wannier state centered at the \( i \)-th site of the lattice with spin \( \sigma \) and \( n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma} \) is the corresponding particle number operator. The \( <i,j> \) in the first sum denotes summation only over the neighboring sites. The first term describes the hopping of an electron from site \( i \) to \( j \) with the amplitude \( t \). Because this process lowers the total energy due to the delocalization of particles traditionally one puts the minus sign in front keeping \( t > 0 \). The second terms corresponds to the on-site energy \( \epsilon_{i,\sigma} \) at a given lattice site \( i \). The last term describes the local interaction between the electrons with opposite spins. Full derivation of the Hamiltonian 3.1, with the discussions of the used approximations can be found in Appendix A. The Hubbard model is the minimal model that takes into account propagation of the electrons through the lattice and their mutual interaction. Because of two non-commuting parts, namely the hopping term \( H_{\text{hop}} \) and the interaction term \( H_{\text{int}} \), finding a solution to this model has been a challenging problem for over 50 years. More interestingly, although its simple form the Hubbard model is believed to exhibit a
plethora of interesting physical phenomena such as the Mott metal-insulator transition, an antiferromagnetism, a ferromagnetism or a Tomonaga-Luttinger liquid behavior.

3.1.1 Non-interacting and non-hopping limit

When the Hubbard interaction $U$ is set to zero, the Hamiltonian from Eq. 3.1 becomes quadratic in fermionic operators. It follows that there always exists a basis in which this Hamiltonian is diagonal. In case of Eq. 3.1 with $\epsilon_{i,\sigma} = \epsilon_{\sigma}$ this basis is formed by Bloch wave functions and can be introduced by the discrete Fourier transform

$$c_{j,\sigma} = \frac{1}{\sqrt{N}} \sum_{k} e^{i k \cdot R_{i}} c_{k,\sigma}$$

Once the Wannier states are transformed into the reciprocal (quasimomentum) space the Hamiltonian 3.1 becomes

$$\mathcal{H}_{U=0} = \sum_{k,\sigma} \epsilon_{k,\sigma} n_{k,\sigma},$$

(3.2)

where

$$\epsilon_{k,\sigma} = \epsilon_{\sigma} - 2 t \sum_{i=1}^{d} \cos(k_{i} a_{i}),$$

(3.3)

where $d$ represents the number of dimensions, $k_{i}$ is the $i$-th coefficient of the crystal wave vector, and $a_{i}$ is the length of a primitive translation in the $i$-th direction of the lattice. The fact that the Hamiltonian is diagonal in the reciprocal space reflects the translation invariance of the system. The result 3.2 means that the eigenstates of the Hamiltonian are waves with a dispersion given by Eq. 3.3, highlighting the wave-like nature of particles in this limit. The ground state is build by filling each energy state with two (in case of spin degeneracy) electrons and forming a Fermi sea. The energy of the highest occupied state is called the Fermi energy.

Another important limit is obtained by setting the hopping amplitude to zero ($t = 0$). The Hubbard Hamiltonian becomes

$$\mathcal{H}_{t=0} = \sum_{i,\sigma} \epsilon_{i,\sigma} n_{i,\sigma} + \sum_{i,\sigma} U n_{i,\sigma} n_{i,\bar{\sigma}}.$$  

In this case the Hamiltonian is diagonal in the Wannier state basis and particles can be thought of as being localized at the lattice sites. The ground-state is formed by filling the localized states. Since adding two particles at the same site costs extra energy, which is controlled by $U$, the lowest energy is obtained by avoiding a double occupancy at any site.

The two limits described above are the most extreme cases from which later one can try to understand physics of the full Hamiltonian. When both terms in Eq. 3.1 are present the competition between the particle-like and the wave-like nature takes place. This leads to many interesting behaviors depending on the $t/U$ ratio and the density of particles.
3.1.2 AF insulator

To get a glimpse of what can happen if both terms in the Hamiltonian Eq.3.1 are kept, let us consider two scenarios. In the first one the interaction will be considered on the basis of the $U = 0$ limit by using the mean-field (Hartree-Fock) approximation. In the second scenario the hopping will be accounted for in the non-hopping limit by using second order perturbation theory. In both cases a half-filled hypercubic lattice will be considered. The term half-filled means that the average number of particles per lattice site is one and the hypercubic means that the lattice is a generalization of a square lattice to any natural $d$ dimensions. The key reason behind choosing a hypercubic lattice is that it possesses a property called bipartitness. It means that this lattice can be decomposed into two sublattices $A$ and $B$ with all nearest neighbors of any site form the sublattice $A$ belonging to the sublattice $B$.

The Hartree-Fock (HF) approximation in the context of Hubbard model is equivalent to neglecting the fluctuations in the local number of particles. Then the interaction term can be rewritten as

$$
\mathcal{H}_{\text{int}} = \frac{U}{2} \sum_{i,\sigma} n_{i,\sigma} n_{i,\bar{\sigma}} \approx \frac{U}{2} \sum_{i,\sigma} \langle n_{i,\sigma} \rangle n_{i,\bar{\sigma}} + \frac{U}{2} \sum_{i,\sigma} n_{i,\sigma} \langle n_{i,\bar{\sigma}} \rangle - \frac{U}{2} \sum_{i,\sigma} \langle n_{i,\sigma} \rangle \langle n_{i,\bar{\sigma}} \rangle,
$$

(3.4)

where $\langle \ldots \rangle$ denotes the thermodynamic average of a given quantity. The average is taken with respect to the grand canonical ensemble. The HF approximation enables one to include the interaction as an effective on-site potential (static mean-field). In this way the Hamiltonian becomes quadratic in fermionic operators, which makes it in principle exactly solvable. Since fluctuations are neglected one can assume that the lattice sites belonging to the same sublattice are equivalent. Because one considers a two sublattice problem the primitive shift in this case is twice the lattice spacing. Finally the problem can be diagonalized in the plane wave basis but with a half of the initial Brillouin zone due to doubling of the unit cell. The dispersion relation is given by

$$
\varepsilon_{k_{\sigma}}^{\pm} = \pm \frac{U}{2} \left[ \langle n_{A\sigma} \rangle - \langle n_{B\bar{\sigma}} \rangle \right]^2 + 4 \left( \frac{d}{2} \sum_{j=1}^{d} 2 t U \cos(k_{j}a_{j}) \right)^2
$$

(3.5)

where $A, B$ distinguish the sublattices, and $k$ from the reduced (magnetic) Brillouin zone. The superscript $\pm$ reflects the fact that bonding and anti-bounding bands are formed. If the band is half-filled then

$$
\sum_{\sigma} \langle n_{A\sigma} \rangle = 1 \quad \text{and} \quad \sum_{\sigma} \langle n_{B\sigma} \rangle = 1,
$$

(3.6)

where $\langle n_{A\sigma} \rangle, \langle n_{B\sigma} \rangle$ are the average occupancy of particles with a given spin projection $\sigma$ on sublattices $A$ and $B$ correspondingly. Due to the spin symmetry of Hamiltonian, Eq. 3.4, increasing the average concentration of particles with one spin projection on the sublattice $A$ must trigger a corresponding decrease on the sublattice $B$. To keep a half-filling condition (Eq. 3.6) the opposite redistribution must happen in the other spin
channel. This discrepancy between the local occupations on the two sublattices leads to opening of a band gap at the Fermi level, as is seen from Eq. 3.5. The band gap is caused by lowering the energy of one band and increasing the energy of the other, as depicted in Fig. 3.1. By opening the gap the spin-symmetry is broken, which means that $\langle n_{i,\sigma}^A \rangle \neq \langle n_{i,\sigma}^B \rangle$. The difference in the local occupation of particles with spin up and spin down is proportional to the magnetization. In this case the magnetization on the sites from the sublattice A is exactly opposite to the magnetization on the sites from the sublattice B. This is called an antiferromagnetic order and the mechanism described above is known as the Slater instability [48]. Since this instability appears in the plane wave picture it is also referred to as the itinerant antiferromagnetism or the spin density wave (SDW) with a period equal to twice the lattice spacing.

Figure 3.1: Change in the dispersion relation of the one dimensional tight-binding Hamiltonian. Left panel show the dispersion relation for homogeneous system. Right panel shows the dispersion relation of the same Hamiltonian but represented in a two site basis. In the right panel the effect of redistribution of particles between the sublattices on dispersion relation is shown.

In the second scenario the Hubbard Hamiltonian will be approached form the opposite side, namely from the non-hopping limit. In this case the kinetic term is included in a second order in the perturbation theory. The discussion here will be limited only to the case where the average number of particles per site remains one. Then the first order perturbation term vanishes. In the second order of perturbation the correction to the
atomic limit is given by

\[ H_{\text{pert}} = - \sum_{i,j,\sigma} \frac{2t^2}{U} \left( \tilde{c}^\dagger_{i,\sigma} \tilde{c}_{j,\sigma} \tilde{c}^\dagger_{i,\sigma} \tilde{c}_{j,\sigma} + \tilde{c}^\dagger_{i,\sigma} \tilde{c}_{j,\sigma} \tilde{c}^\dagger_{j,\sigma} \tilde{c}_{i,\sigma} \right) \] (3.7)

where

\[ \tilde{c}_{i,\sigma} = c_{i,\sigma} (1 - n_{\hat{\sigma},i}) \]

are the fermionic operators projected onto the singly occupied subspace [50]. Physically Eq. 3.7 takes into account the virtual process where the electrons hop back and forth from a given site . The formula above can be rewritten in the following compact form, as shown by J. Spałek et. al [50],

\[ H_{\text{pert}} = \sum_{<i,j>} \frac{4t^2}{U} \left( S_i \cdot S_j - \frac{1}{4} \right), \] (3.8)

where \( S_i \) is the spin operator in second quantization representation [50]. The Hamiltonian Eq. 3.8 is the so called the Heisenberg Hamiltonian with an antiferromagnetic coupling \( J = 4t^2/U \) between the neighboring spins. In this case the antiferromagnetic coupling means that the lower energy state is when neighboring spins point in the opposite directions. The process described by \( H_{\text{pert}} \) is called the kinetic exchange [51, 50] and it leads to the localized antiferromagnetism (opposed to the Slater instability). This observation was first made by P.W. Anderson in 1959 [49].

This two examples have shown that the Hubbard model, although its simple form, can exhibit as complex behavior as antiferromagnetism. Which breaks one of the symmetries of the Hamiltonian, in this case the spin symmetry. Moreover the above examples show that the antiferromagnetism can be triggered by different physical processes. In the first case it was due to the appearance of static magnetization modulation and in the second example it was because of the virtual exchange.

### 3.2 The Dynamical Mean-Field Theory

Over the past 50 years there has been many theoretical approaches to solve the Hubbard model. Because of the complexity coming from the two non-commuting terms most of them have failed to give exact statements. The approaches fall into two categories, each failing for a different reason. In the first category are methods based on a Greens function formalism. They can be based either on the perturbation theory or on solving the equation of motion. Although there are honorable mentions such as the Hartree-Fock approximation or Random Phase Approximation [60] that paved the way we understand the weakly interacting regime, most often this methods suffer from uncontrolled approximations. In the one using the equation of motion (e.g. Hubbard in [44]) problem appears at the level of truncating the equations connecting the higher order Greens functions. In methods using perturbation theory the unphysical results can originate from incorrect treatment of a given subset of Feynman diagrams. The second category of methods to solve the
Hubbard model are based on direct numerical calculations such as an exact diagonalisation. These methods most often fail to reproduce the complexity of behaviors in the Hubbard model due to the exponential growth of the dimension of the Hilbert space. It makes the investigation of thermodynamical limit, at which true phase transitions appear, out of reach for the conventional computers. Therefore not many exact statements were made about the Hubbard model in dimensions higher then one by the end of 1980s. The one dimensional case turned out be exactly solvable by means of the Bethe ansatz [52]. In the higher dimensions only few results were discovered, such as the theorem that the total spin of the ground state of the system on a bipartite lattice is equal to the difference in lattice sites numbers in each sublattice [53]. The exact statements play a crucial role in studying the Hubbard model. They supply benchmarks which new approximate methods have to fulfill in order to be validated. For this reason the pioneering works of Metzner and Vollhardt [54] and Müller-Hartmann [55] in 1989 are so important. They extend our understanding of the Hubbard model by introducing the limit of infinite dimensions \( d \to \infty \). In \( d \to \infty \) new exact statements can be made, which have led to formulation of the Dynamical Mean-Field Theory (DMFT). An approximate method to solve the Hubbard model, that is exact in the infinite dimensions.

### 3.2.1 Infinite dimension limit

Taking the limit of \( d \to \infty \) has been a well-know method in classical statistical mechanics for constructing a mean filed approximation for spin models. For example the partition function of the Ising model in the infinite dimension limit becomes exactly the same as partition function of the mean-field solution of the Ising model obtained using the Weiss molecular field [57]. The reason behind this is that fluctuations in the environment of a given spin in this limit become negligible due to the large number of neighbors. Enabling one to fully describe the coupling of each spin to its environment by a single parameter. The observation that \( d \to \infty \) is useful in constructing a mean-field has inspired Metzner and Vollhardt to apply the same idea to the interacting lattice fermions. In order for the problem to remain non-trivial as the dimensionality is increased one has to rescale the hopping amplitudes. Otherwise the width of the density of states, which controls the kinetic energy, will become infinite [58] whilst the interaction energy would remain finite. As a result the problem will always become non-interacting. They found that on the hypercubic lattice the rescaling of the hopping amplitude is given by

\[
t = \frac{t^*}{\sqrt{2d}},
\]

where \( 2d = Z \) is the coordination number (number of neighbors). The kinetic energy per lattice site in the non-interacting system is given by the expectation value

\[
\frac{E_{\text{kin}}}{N_L} = \frac{1}{N_L} \langle H_{\text{kin}} \rangle = -t \sum_{j, \sigma} \langle c_{i, \sigma}^\dagger c_{j, \sigma} \rangle_{\text{non}},
\]

where \( N_L \) is the number of sites, the primed sum means summation over all neighbors of site \( i \) and \( \langle \ldots \rangle_{\text{non}} \) is the expectation value in grand canonical ensemble with the non-
3.2. THE DYNAMICAL MEAN-FIELD THEORY

interacting Hamiltonian. From this one can conclude that in order for the kinetic energy
to remain finite the following must be obeyed

\[ \left\langle c_i^{\dagger}c_j^{\sigma}\right\rangle_{\text{non}} = O\left(\frac{1}{\sqrt{d}}\right), \ i \neq j. \]

Since this correlation function is proportional to the non-interacting Green function the
latter should also obey the same scaling

\[ G_{i,j,\sigma}^{(0)} = O\left(\frac{1}{\sqrt{d}}\right), \ i \neq j. \] (3.10)

Even though the off-diagonal element of Green function scales as inverse of the dimension
it does not mean the particles become localized in \( d \to \infty \). The reason is that the number
of neighbors is growing as well. To see this one can consider how the probability amplitude
of a particle leaving the \( i \)-th site scales with \( d \):

\[ \sum_{j,\sigma}^t G_{i,j,\sigma}^{(0)} \sim d \frac{t^*}{\sqrt{2d}} O\left(\frac{1}{\sqrt{d}}\right) < \infty. \] (3.11)

This scaling considerations can be generalize to Green function for any lattice sites \( i, j \)
[59] and the final result yields

\[ G_{i,j,\sigma}^{(0)} \sim O\left(\frac{1}{d^{||R_i - R_j||}}\right), \] (3.12)

where \( ||R_i - R_j|| \) is the distance in the so-called “New York mertic”.

3.2.2 Locality of self-energy in \( d \to \infty \) limit

The result 3.12 have tremendous implications on the perturbation expansion around the
weak-coupling regime of the Hubbard model. By considering the skeleton diagrams [60]
for the self-energy one can see that although the first order diagram is not effected by
\( d \to \infty \) limit, due to its local nature (Hartree term),

\[ \Sigma_{i,i,\sigma}^{(1)}(\omega) = \frac{U}{2} n_{i,\bar{\sigma}}, \]

for the higher order diagrams scaling becomes relevant. For example, diagrams in the
second order of the perturbation theory have three propagators, c.f. right panel of Fig.
3.2. As shown in [56] taking the limit of infinite dimensions causes the following behavior

\[ G_{i,j,\sigma}^{(0)}(\omega)G_{i,j,\bar{\sigma}}^{(0)}(\omega)G_{j,i,\bar{\sigma}}^{(0)}(-\omega) = O\left(\frac{1}{d^{||R_i - R_j||}}\right)^3 \xrightarrow{d=\infty} \begin{cases} 0 & \text{if } j \neq i \\ \text{non-zero} & \text{if } j = i \end{cases} \]
Figure 3.2: Skeleton diagrams contributing to the self energy in the first order (a) and in the second order (b). Solid lines represent the Green function and the wave connecting the vertices corresponds to the local Hubbard interaction.

From the above one can see that only the local part of the self-energy remains. The same takes place in higher order diagrams [55]. Thus in the limit of infinite dimensions

$$\Sigma_{i,j,\sigma}(\omega) \xrightarrow{d=\infty} \Sigma_{i,i,\sigma}(\omega)\delta_{i,j}.$$  (3.13)

The following fact triggers a huge simplification of the Dyson equation [60], which in $d = \infty$ reads

$$G_{i,i,\sigma}(\omega) = G^{(0)}_{i,i,\sigma}(\omega) + \sum_j G^{(0)}_{i,j,\sigma}(\omega)\Sigma_{j,j,\sigma}(\omega)G_{j,i,\sigma}(\omega)$$  (3.14)

This form of the Dyson equation was used in the literature as an approximate equation even before the scaling was introduced. But owing to the investigation of $d \to \infty$ limit this approximation gained a range of validity.

An important consequence of the locality of the self-energy comes from the following consideration. Eq. 3.14 can be reformulated in the following way

$$G_{i,i,\sigma}(\omega) = F_{i,i,\sigma}(\omega) + \sum_j' F_{i,j,\sigma}(\omega)\Sigma_{j,j,\sigma}(\omega)F_{j,i,\sigma}(\omega),$$  (3.15)

where a new function $F_{i,i,\sigma}(\omega)$ was defined as

$$F_{i,i,\sigma}(\omega) = G^{(0)}_{i,i,\sigma}(\omega) + \sum_j' G^{(0)}_{i,j,\sigma}(\omega)\Sigma_{j,j,\sigma}(\omega)F_{j,i,\sigma}(\omega).$$  (3.16)

As introduced in Eq. 3.11 the $\sum'$ indicates sum over all nearest neighbors of a given site $i$. Physically the function $F_{i,i,\sigma}(\omega)$ contains all non-local effects of the interaction on the non-interacting Green function. Even though the Hubbard interaction is purely local the non-local terms are caused by processes such as the following. The particle hops to a neighboring site, where it interacts, and hops back to the initial site. Other processes are constructed as a higher order products of the one previously described. All of them are encapsulated in $F_{i,i,\sigma}(\omega)$. On the other hand this function can be viewed as the Green function of a lattice without the $i$-th site but with dynamic potential $\Sigma_{\sigma}(\omega)$. From the Eq.
3.3. THE SINGLE IMPURITY ANDERSON MODEL

3.15 one can conclude that the self-energy of the Hubbard model in the limit of infinite dimension is a functional of \( F_{i,i,\sigma}(\omega) \). If we now consider a completely new situation in which the interaction is at one site only, the same form of functional would appear, but instead of \( F_{i,i,\sigma}(\omega) \) it would only depend on the non-interacting Greens function \( G_{i,i,\sigma}^{(0)}(\omega) \) (cf. Eq. 3.25 and Eq. 3.26) [61].

This means that due to the scaling in \( d = \infty \) the Hubbard model can be mapped onto the Anderson single impurity model, described in details below, with properly chosen \( G_{i,i,\sigma}^{(0)}(\omega) \). This fact lays in the hart of the Dynamical Mean-Field Theory [62]. A self-consistent method for solving the Hubbard model can be summarized in the following five steps:

1. Start with an initial (guessed) \( F_{i,i,\sigma}(\omega) \),
2. Solve the single impurity problem (SIAM),
3. Calculate the (local) self-energy \( \Sigma_{i,i,\sigma}(\omega) \),
4. Update the function \( F_{i,i,\sigma}(\omega) \),
5. Go back to step two and proceed until the functions \( F_{i,i,\sigma}(\omega) \) from two consecutive iterations meet a convergence criterion.

Before looking into technical details of how each step is made, one should first take a look at the Anderson single impurity model to understand what kind of behaviors can be expected. Because of the mapping these behaviors are suppose to be seen also in the solution of the Hubbard model.

3.3 The single impurity Anderson model

The single impurity Anderson model was first introduced by P. W. Anderson [39] in 1961 as an attempt to grasp the physics behind the local magnetic moment formation in iron-group ions dissolved in metals. Intrigued by the experimental reports by B. Matthias’s group showing that the magnetic moment formation mainly depends on the type of metallic environment, he proposed this simplified model. It consisted of a one d-type or f-type orbital ion embedded in a non-interacting metallic bath. Because of its constituents the name single impurity model was later adopted. Anderson believed that the moment formation is indeed a many-body phenomena thus the Hamiltonian was given in the second quantization form by

\[
H = \sum_\sigma \epsilon_{d\sigma} d^\dagger_{\sigma} d^\sigma + \sum_{k\sigma} \epsilon_{k\sigma} c^\dagger_{k\sigma} c_{k\sigma} + U d^\dagger_{\uparrow} d^\dagger_{\downarrow} d_{\uparrow} + \sum_{k\sigma} \left( V_{k\sigma} c^\dagger_{k\sigma} d^\sigma + V^*_k d^\dagger_{\sigma} c_{k\sigma} \right). \tag{3.17}
\]

The fermionic operators \( d^\dagger_{\sigma} \) and \( c^\dagger_{k\sigma} \) create an electron with spin \( \sigma \) at the impurity and an electron in Bloch state with crystal momentum \( k \) and spin \( \sigma \), respectively. Hamiltonian 3.17 is composed of four terms. First two terms correspond to the bare energy of an
electron at the ion (first term) and the metallic bath (second term) characterized by the dispersion $\epsilon_{k,\sigma}$. Third term describes the repulsive local Coulomb interaction among the electrons at the ion. The interaction among the electrons in the metallic bath is neglected due to much more extended nature of their wave functions with respect to the extension of the impurity orbitals. The last term, called the hybridization term, describes the process of mixing between the electronic states of the metal and those of the impurity, which comes from the non-zero hopping matrix elements between these wave functions.

In the analysis of the single impurity problem it is convenient to introduce two fermionic retarded Green functions, similar to those defined in Eq. B.1 in the Appendix B,

$$G^R_{dd,\sigma}(t) := -i\theta(t) \langle \{ d_\sigma(t), d^\dagger_\sigma(0) \} \rangle,$$

(3.18)

$$G^R_{kd,\sigma}(t) := -i\theta(t) \langle \{ c_{k\sigma}(t), d^\dagger_\sigma(0) \} \rangle.$$  

(3.19)

Also an important correlation function is $D^R_{d,\sigma}(z)$ given by

$$D^R_{d,\sigma}(z) = -i \int dt e^{itz} \langle \{ n_{d,\sigma}(t)d_\sigma(t), d^\dagger_\sigma(0) \} \rangle,$$

(3.20)

where $z = \omega + i\eta$ is the frequency shifted by infinitesimal complex element to ensure the convergence of the integral in $D^R_{d,\sigma}(z)$. By following Eq. B.4 one arrives at the following set of equations of motion

$$\hbar z G^R_{dd,\sigma}(z) = 1 + \epsilon_{d,\sigma} G^R_{dd,\sigma}(z) + \sum_k V^*_k G^R_{kd,\sigma}(z) + U D^R_{d,\sigma}(z),$$

(3.21)

$$\hbar z G^R_{kd,\sigma}(z) = \epsilon_{k,\sigma} G^R_{kd,\sigma}(z) + V_{k,\sigma} G^R_{dd,\sigma}(z).$$

(3.22)

From the second equation of motion Eq. 3.22, one can extract the relation between $G^R_{kd,\sigma}(z)$ and $G^R_{dd,\sigma}(z)$, which is

$$G^R_{kd,\sigma}(z) = \frac{V_{k,\sigma}}{\hbar z - \epsilon_{k,\sigma}} G^R_{dd,\sigma}(z).$$

(3.23)

After plugging this relation to the Eq. 3.21 one obtains

$$\left( \hbar z - \epsilon_{d,\sigma} - \sum_k \frac{|V_{k,\sigma}|^2}{\hbar z - \epsilon_{k,\sigma}} \right) G^R_{dd,\sigma}(z) = 1 + U D^R_{d,\sigma}(z).$$

(3.24)

The term in the bracket on the left hand side of the Eq. 3.24 is the inverse of the non-interacting Greens function $(G^R_{dd,\sigma}(z))^{-1}$. That is a resolvent of the Hamiltonian from Eq. 3.17 with $U = 0$. Multiplying this equation of motion by the inverse of $G^R_{dd,\sigma}(z)$ and subtracting this inverse from both sides of the Eq. 3.24 one obtains

$$\left( G^R_{dd,\sigma}(z) \right)^{-1} - \left( G^R_{dd,\sigma}(z) \right)^{-1} = U \frac{D^R_{d,\sigma}(z)}{G^R_{dd,\sigma}(z)}.$$

(3.25)
3.3. THE SINGLE IMPURITY ANDERSON MODEL

Comparison with the Dyson equation yields the following definition of the self-energy

$$\Sigma_\sigma(z) = U \frac{P_{d,\sigma}(z)}{G_{dd,\sigma}^R(z)}. \quad (3.26)$$

The self-energy only exists for the d-orbital electrons because the metallic bath is non-interacting. This is the reason for the formal mapping described in previous section. Before considering the full problem it is important to analyze two limiting cases. As in previous analysis of the Hubbard model these limits are: 1) the non-interacting limit, and 2) the atomic limit (vanishing hybridization).

3.3.1 Non-interacting limit \((U=0)\)

In the non-interacting limit, when \(U\) is set to zero, Eqs. 3.21 and 3.22 form a closed set of equations. The resulting non-interacting Green function for the impurity is given by

$$G_{dd,\sigma}^{R, \text{non-int}}(z) = \frac{1}{hz - \epsilon_{d,\sigma} - \Delta_\sigma(z)}, \quad (3.27)$$

where the hybridization function \(\Delta_\sigma(z)\) was introduced. Comparing with 3.24, one can see that it is given by

$$\Delta_\sigma(z) = \sum_k |V_{k,\sigma}|^2 \frac{hz - \epsilon_{k,\sigma}}{\hbar z - \epsilon_{k,\sigma}}. \quad (3.28)$$

Hybridization function describes the dynamical process in which the number of d-orbital electrons is not conserved due to the coupling to the bath. To understand the effect of this process on the spectral function at the impurity it is convenient to decompose hybridization function into a real and an imaginary part, namely,

$$\Delta_\sigma(z) = \mathcal{R}_\sigma(z) - i \Gamma_\sigma(z). \quad (3.29)$$

Then, the Cauchy principal value decomposition of the Green function gives

$$\lim_{\eta \to 0^+} \frac{1}{hz - \epsilon_{d,\sigma} - \Delta_\sigma(z)} = \mathcal{P} \frac{1}{h\omega - \epsilon_{d,\sigma} - \mathcal{R}_\sigma(\omega)} - \frac{\Gamma_\sigma(\omega) + \eta}{(h\omega - \epsilon_{d,\sigma} - \mathcal{R}_\sigma(\omega))^2 + (\Gamma_\sigma(\omega) + \eta)^2}, \quad (3.30)$$

where \(\mathcal{P}\) denotes participial value. Assuming frequency independence of \(\Delta_\sigma\) one can see that the spectral function at the impurity \((\rho_{d,\sigma}(\omega) = -\frac{1}{\pi} \text{Im} \left[G_{dd,\sigma}^R(\omega)\right])\) evolves from one delta peak at \(h\omega = \epsilon_{d,\sigma}\), in case of no hybridization, to a Lorenzian peak centered at \(\omega_0\) such that \(h\omega = \epsilon_{d,\sigma} + \mathcal{R}(\omega_0)\) (cf. Fig. 3.3). The width of the Lorentzian function is controlled by the imaginary part of the hybridization function.
3.3.2 Atomic limit \((V_{k,\sigma} = 0)\)

In the atomic limit the hybridization term vanishes leading to the separation of
the impurity and the bath quantum states. In order to close the set of equation in
this limit one can calculate the EOM for the two particle Green function

\[
\hbar z D^R_{d,\sigma}(z) = \langle n_{d\bar{\sigma}} \rangle + (\epsilon_{d,\sigma} + U) D^R_{d,\sigma}(z),
\]

where \(\langle n_{d\bar{\sigma}} \rangle\) is the average number of particles with spin \(\bar{\sigma}\) at the
impurity. Substituting the resulting formula for the two particle Green function
into Eq. 3.21 one obtains

\[
\hbar z G^R_{d\bar{d},\sigma}(z) = 1 + \epsilon_{d,\sigma} G^R_{d\bar{d},\sigma}(z) + U \frac{\langle n_{d\bar{\sigma}} \rangle}{\hbar z - \epsilon_{d,\sigma} - U}.
\]

After recasting terms one ends up with the following formula

\[
G^R_{d\bar{d},\sigma}(z) = \frac{1 - \langle n_{d\bar{\sigma}} \rangle}{\hbar z - \epsilon_{d,\sigma}} + \frac{\langle n_{d\bar{\sigma}} \rangle}{\hbar z - \epsilon_{d,\sigma} - U}.
\]

In this limit the impurity Greens function becomes equivalent to the Greens
function of the Hubbard model at \(t = 0\) and with the chemical potential \(\mu = -\epsilon_{d,\sigma}\). Taking
the imaginary part of this formula one can find a two peaked structure of the spectral
function:

\[
\rho_{d,\sigma}(\omega) = \frac{1}{\pi} \lim_{\eta \rightarrow 0^+} \left( \frac{1 - \langle n_{d\bar{\sigma}} \rangle}{(\hbar \omega - \epsilon_{d,\sigma})^2 + \eta^2} + \frac{\langle n_{d\bar{\sigma}} \rangle}{(\hbar \omega - \epsilon_{d,\sigma} - U)^2 + \eta^2} \right) =
\]

\[
= (1 - \langle n_{d\bar{\sigma}} \rangle) \delta(\hbar \omega - \epsilon_{d,\sigma}) + \langle n_{d\bar{\sigma}} \rangle \delta(\hbar \omega - \epsilon_{d,\sigma} - U).
\]

This two peaked structure physically means that due to the Coulomb repulsion placing
at the impurity a particle with a spin \(\sigma\) cost extra energy \(U\) in case when there is a particle
with an opposite spin \((\langle n_{d,\bar{\sigma}} \rangle = 1)\).
3.3. **THE SINGLE IMPURITY ANDERSON MODEL**

### 3.3.3 Schrieffer-Wolf transformation

Apart from the limits discussed above to obtain a solution to SIAM with non-zero interaction and non-zero hybridization is a much more complicated problem. Especially in the limit when the interaction exceeds the hybridization. The reason is that due to the interaction at the impurity the Wick theorem is not applicable and hence construction of a perturbation theory around the atomic limit highly non-trivial [60]. In 1966 J. R. Schrieffer and P.A. Wolf showed the equivalence between the spin symmetric SIAM in the limit of weak hybridization and the Kondo model. The Schrieffer-Wolf transformation is a method to obtain a low-energy effective Hamiltonian from a full Hamiltonian by constructing a unitary transformation which decouples high and low-energy subspaces [64]. The effective dynamics in one particle subspace, obtained via this transformation is governed by the Kondo Hamiltonian [65] given by

\[
H_{ex} = -\frac{1}{\hbar^2} \sum_{k,k'} J_{k,k'} \left( \psi_k^\dagger S \psi_{k'} \right) \cdot \left( \psi_{d}^\dagger S \psi_d \right),
\]

where \(\psi_k\) and \(\psi_d\) denotes spinors defined in the following way:

\[
\begin{align*}
\psi_k &= \begin{pmatrix} c_{k,\uparrow} \\ c_{k,\downarrow} \end{pmatrix}, \\
\psi_d &= \begin{pmatrix} d_\uparrow \\ d_\downarrow \end{pmatrix}.
\end{align*}
\]

The spin 1/2 operator \(S\) is given by

\[
S = \vec{\sigma} = \frac{\hbar}{2} \begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{pmatrix}
\]

with \(\sigma_x, \sigma_y, \sigma_z\) being Pauli matrices. The coupling between the spinors is given by

\[
J_{k,k'} = V_k V_{k'} \left[ \frac{1}{\epsilon_k - \epsilon_d - U} + \frac{1}{\epsilon_{k'} - \epsilon_d - U} - \frac{1}{\epsilon_k - \epsilon_d + U} + \frac{1}{\epsilon_{k'} - \epsilon_d + U} \right] =
\]

\[
V_k V_{k'} \left[ U \left( \frac{\epsilon_k - \epsilon_d - U}{(\epsilon_k - \epsilon_d)(\epsilon_{k'} - \epsilon_d)} + \frac{\epsilon_{k'} - \epsilon_d - U}{(\epsilon_k - \epsilon_d)(\epsilon_{k'} - \epsilon_d)} \right) \right]
\]

What is worth to notice is that for \(\epsilon_d < \epsilon_{k,f} < \epsilon_d + U\) this coupling becomes negative and the interaction between spins turns out to be antiferromagnetic. Also also it is worth to notice the similarity of this result to the effective Hamiltonian form Eq. 3.8 where the spins where coupled by \(J = -\frac{t^2}{\tau}\).

This mapping from the single impurity model onto the Kondo Hamiltonian shone a new light on the initial problem. At the time when Schrieffer-Wolf transformation was introduced it was already known that the solution of the Kondo model have a peculiar behavior at low temperatures. It was discovered by Juan Kondo in 1964 [65]. It appears in the third order of the perturbation theory calculation that the scattering rate \(1/\tau\) of the electrons on the impurity spin behaves as

\[
\frac{1}{\tau} \propto J \rho \left[ 1 + 2 J \rho \frac{D}{T} \right]^2,
\]

(3.36)
where $T$ is the temperature and $\rho$ is the density of states of the electrons at the Fermi level, and bandwidth is equal to $D$. From the above formula one can see that there exists a temperature, called the Kondo temperature,

$$T_k = D e^{-\frac{1}{\rho}}.$$

at which this scattering rate becomes zero. This means that the impurity and the bath particles form a correlated resonant state. Unfortunately at this energy scale ($T_k$) perturbative corrections become comparable to the bare interaction, leading to the breakdown of the perturbation theory. Nevertheless the calculations of Kondo showed that there exist a new energy scale, the Kondo temperature, below which the system becomes strongly coupled. This behavior gives rise to a resistance minimum observed in disordered gold wires by de Haas and co-workers in 1934 [66]. This effect was not understood for over 30 years. When the coupling $J$ is positive by lowering the temperature the magnetic scattering rate increases, Eq. 3.36. Simultaneously the usual phonon scattering becomes less important. Once the first scattering process dominates the second one the minimum in resistance appears. This phenomenon gained the name a Kondo effect. Although Kondo paper [65] pointed out the reason for the formation of the resistance minimum, the explanation how a new energy scale emerges and how the physics below this energy scale looks like remained an open question. These questions gained a formal name of ”Kondo problem”. Now turning back to the initial problem, due to the mapping of SIAM onto the Kondo model, the SIAM has to exhibit a similar behavior.

### 3.3.4 Poor-man’s scaling

Large improvement in understanding of the Kondo problem came at the beginning of 1970. Around that time few authors have taken a new way to approach it. Although methods used by Fowler-Zawadowski [67], Abrikosov-Migdal [68] or Anderson [69] differed in details, the main idea was the same. To redefine the problem at a given energy scale in terms of a similar problem, but at lower energy scales with changing the values of the model parameters. Using this procedure the authors were able to show the equivalence between a whole class of problems and obtained the equations governing the behavior of the coupling parameters once the energy scale is reduced. These equations are called the scaling equations. Methods used by those authors were the first implementations of the renormalization group in solid state physics. The most intuitive line of approach was taken by Anderson in his paper from 1970 [69], where he used the ”poor-man’s scaling” method. He started by considering the Kondo problem with different couplings between spins in plane and along the $z$-axis

$$\mathcal{H} = \sum_{k,\sigma} \epsilon_{k,\sigma} n_{k,\sigma} + J_z S_z s_z + \frac{J_z}{2} (S_+ s_- + S_- s_+),$$

where $S_+$ ($S_-$) is the rising (lowering) spin operator at the impurity and $s_+$ ($s_-$) is the rising (lowering) spin operator of the electrons from the bath, characterized by the dispersion relation $\epsilon_k$. Anderson was reducing the bare bandwidth by including scattering from
the band edges into the couplings constants. By comparing the initial and the renormalized Hamiltonians he wrote down the scaling equations and concluded that the following relation must hold

$$J_z^2 - J_\pm^2 = \text{const.}$$

The Fig. 3.4 shows the regions of different couplings in Kondo model and curves obtained from the scaling equations. Arrows on the curves are pointing towards the direction in which couplings change as the energy scale is decreased. From this figure one can see why any earlier attempt to solve Kondo problem have failed, when the coupling was antiferromagnetic (right hand side of Fig. 3.4). Namely, no matter how small the initial couplings $J_z$ and $J_\pm$ between the spins are, there exist an energy scale above which the couplings become arbitrarily large. This means that no matter how weakly the spins are coupled at the beginning there exist an energy scale at which they become strongly coupled. As a result the Kondo problem misses a characteristic energy scale which would enable one to construct the perturbation theory around it. To solve the problem one has to find a non-perturbative approach. Again, because of the equivalence, the Anderson model must behave in a similar manner. This observation done by Anderson, although does not solve the problem, has helped to develop the full solution of the Kondo problem by means of the numerical renormalization group [70].

### 3.4 DMFT loop

The Dynamical Mean-Field Theory is a self-consistent method of obtaining an approximate solution to the Hubbard model which becomes exact in the limit of infinite dimension. It relies on the mapping of the more complicated Hubbard model onto a simpler
but still complicated single impurity model. The central role in this method plays the so-called DMFT loop. In terms of a single impurity model it is a procedure aiming to correct the baths Green function by including the effects of the interaction. As it was shown in Eq. 3.15 the Dyson equation for the Hubbard model in infinite dimension can be recast into a Dyson equation for SIAM by introducing the function $F_{i,i,\sigma}(\omega)$. This quantity is referred to as the bath Green's function since it describes a lattice with the $i$-th site removed Eq. 3.16. The $F_{i,i,\sigma}(\omega)$ can be obtained from the Hilbert transform [62]:

$$F_{i,i,\sigma}(z) = \int d\epsilon \frac{\rho_{\sigma}(\epsilon)}{z - \epsilon - \Sigma_{\sigma}(z)}, \quad (3.37)$$

where $\rho_{\sigma}(\epsilon)$ is the density of states for the non-interacting lattice problem. Physically this step represents the fact that the local effects of the interaction at the impurity are imprinted onto the rest of the lattice. This step closes the DMFT loop because by updating a bath Green function sets up a new single impurity problem.

To sum up, the loop starts with the mapping of Hubbard Hamiltonian onto a single impurity model. In case of the first iteration it is done by using a guessed bath Green's function ($F_{i,i,\sigma}(\omega)$). Then the single impurity problem is solved by some means and the impurity Green function is obtained ($G_{i,i,\sigma}(z)$). From the Eq. 3.15 one can extract the self energy

$$\Sigma_{\sigma}(z) = \mathcal{F}_{i,i,\sigma}^{-1}(z) - \mathcal{G}_{i,i,\sigma}^{-1}(z)$$

Then the self-energy is used to update the baths Green function ($\mathcal{F}_{i,i,\sigma}(z)$) by means of the Hilbert transform (Eq. 3.37). The DMFT loop is terminated when $\mathcal{F}_{i,i,\sigma}(z)$ from two
consecutive loops coincide within a convergence criterion. The name Dynamical Mean-Field comes from the fact that the local self-energy acts as a frequency dependent and complex one particle potential. So the interaction is encoded into a local potential as in the standard mean-field approximation but this potential is frequency dependent. Thus it is a dynamical quantity.

The most demanding (in terms of computational methods) part in the DMFT loop is to solve the single impurity model. As mentioned this problem does not have any characteristic energy scale, which would make perturbation based approach reliable for a broad energy range. There are only a few methods developed up to now to deal with this kind of problems. One of them is the Numerical Renormalization Group technique (NGR) which will be discussed next.

3.5 Numerical Renormalization Group

The NRG was developed in the early 1970’s by K. G. Wilson, as a first non-perturbative approach to calculate the thermodynamic properties of the Kondo Hamiltonian. It enabled Wilson to determine, among other quantities, the magnetic susceptibility. He used it to find the critical exponent at the transition from a weakly coupled (local moment) to a strongly coupled regime. For this development he was awarded Nobel prize in 1982. The existence of this transition was known from the Kondo work but due to the breakdown of the perturbation theory nothing more could have been said about it. Thanks to the ingenious idea of Wilson a renormalization procedure suitable to deal with Kondo problem was invented. The applicability of NRG extends to a broader range of models called in general “the impurity problems”. They consist of two coupled subsystems. One is described by a small number of quantum degrees of freedom whereas the second one is composed of a large number, often a continuum, of states. Any perturbative treatment of such impurity problems leads to a divergences, as in the case of the Kondo problem. An example of problems that falls into this category, apart from Kondo problem, is the single impurity Anderson problem or tunneling through a quantum dot. Although the method was invented to calculate thermodynamic properties, over the past 40 years the development has been made to calculate also dynamical quantities such as spectral functions, conductivity etc.

The aim of any renormalization group (RG) approach is to analyze the evolution of the parameters characterizing the effective Hamiltonian upon the mapping from one scale of the problem to another. The origin of this mapping is either a changing of a length scale as in Kadanoff approach [71], or a changing of an energy scale, as for example, in the poor-man’s scaling [69]. In the Numerical Renormalization Group scheme the latter is used. As the iterative mappings are applied the key point in the RG analysis is to find which parameters flow becomes more important or irrelevant. Whether this flow is unbounded or if it reaches a certain fixed point. The mapping is composed of a successive application of the same steps, each time by infinitesimally reducing the energy scale.

Any numerical renormalization group procedure follows along the five steps laid out first by Wilson and depicted in Fig. 3.6:
CHAPTER 3. MODEL AND METHOD

Figure 3.6: Depiction of NRG steps from [72]. On the left hand side steps (1)-(3) are shown. On the right hand side the iterative diagonalization is depicted.

1. Division of energy domain of a subsystem described by large number of states (bath) into logarithmic intervals

2. Reduction of this energy spectrum into to a set of states, one for each interval,

3. Mapping of the problem onto a semi-infinite chain,

4. Iterative diagonalisation of the chain,

5. Analysis of many-particle energy spectra, matrix elements etc. to calculate static and dynamic properties of the impurity model.

The fixed point is reached when the spectrum of the impurity does not change from iteration to iteration.

The idea behind introducing the logarithmic discretization was guided by the observation that excitations at each energy scale contribute equally. This is due to the fact that although the energy intervals are becoming smaller with reducing the energy, the coupling at these scales are getting larger. The important energy scales in the impurity models (e.g. Kondo temperature) are often orders of magnitude smaller then the energy scales of the initial Hamiltonians. This means that obtaining energy resolution on the important scale using linear discretization would demand introducing huge amount of energy intervals in the discretization. On the other hand, the logarithmic discretization introduces the low energy resolution which exponentially depend on the number of energy intervals. It is characterized by a parameter Λ, which sets the discretization points at $\pm \Lambda^{-n}$ at the n-th discretization step. Two consecutive points define an interval, which in the limit $\Lambda \to 1$ becomes of unity length. This is how the continuum limit is recovered.

After the discretization a Fourier transformation on each interval is made and only the long wavelength ($k = 0$) state is retained. This approximation is motivated by the fact that in the limit $\Lambda \to 1$ this mode dominates over the others [70]. After this step the
bath terms in the SIAM Hamiltonian are rewritten by using the retained states from the Fourier transform on each energy interval. Since a single state at each energy interval is kept the hybridization term in the new basis is given as a sum of terms each describing the coupling of the impurity to a different energy scale of the bath band. Finally, a new orthonormal basis is introduced to rewrite the Hamiltonian in tridiagonal form. This step is called the mapping on the semi-infinite chain since first site is the impurity and, in principle, there is no last site. In numerical calculation the chain has to be finite and the last site dictates the lowest energy scale reached during the calculations. The exact form of the off-diagonal terms are only known analytically for some special cases [72] but, interestingly, they always have the same asymptotic behavior. For \( n \) being the chain site the hoppings behave as

\[
t_{n \to \infty} \propto \frac{1}{2} (1 + \Lambda^{-1})\Lambda^{-\frac{n}{2}}.\]

The further a chain site from the impurity is the weaker the coupling becomes. Moreover, this decay is exponential. In this procedure the bath is always considered in the one dimensional energy representation. This is possible because in the single impurity problem bath can be fully represented by the hybridization function, Eq. 3.27. To make the connection to the standard renormalization group procedure, the logarithmic discretization and the tridiagonalization has an interpretation of introducing the energy shells around the impurity. Once the mapping on the semi-infinite chain is made the renormalization group nature of this procedure becomes clearly visible. The relation between Hamiltonian on the chain with \( N + 1 \) and \( N \) sites is given by

\[
H_{N+1} = \sqrt{\Lambda} H_N + \Lambda^{\frac{N+1}{2}} \frac{\sum_{\sigma} \epsilon_{N+1} c^\dagger_{N+1,\sigma} c_{N+1,\sigma}}{\sum_{\sigma} t_N} + \Lambda^{\frac{N+1}{2}} t_N \left( c^\dagger_{N,\sigma} c_{N+1,\sigma} + c^\dagger_{N+1,\sigma} c_{N,\sigma} \right).
\]

Each site in Eq. 3.38 represents a different energy scale. Thus there exists an explicit transformation from one energy scale to another.

In general a clear representation in which the Hamiltonian at each step is characterized by a fixed set of parameters does not have to exist. That is why in the Numerical Renormalization Group approach, as opposed to the standard RG, each Hamiltonian \( H_N \) is represented by its many-body spectrum rather than the coupling parameters. This quantity is then analyzed at a fixed point. Hence the final step is the iterative diagonalization of the chain. Starting from the impurity site consecutive sites are added by using the prescription given by Eq. 3.38. Then each sub-chain is diagonalized and the spectrum is analyzed. Later the eigenbasis is used in the next step. This corresponds to the iterative application of the renormalization group transformation in the standard approach. Since the diagonalization is done numerically thus the name “numerical renormalization group”.

### 3.5.1 Calculation of thermodynamic properties

Static thermodynamic properties can be simply calculated by simply approximating the spectrum of full the Hamiltonian by the spectrum of the effective Hamiltonian at a chosen
NRG step, which corresponds to the energy scale proportional to the temperature. The thermodynamic properties at temperature $T$ are determined by transitions between the energy levels spaced by $k_B T$. The probability of creating a high energy excitation of the ground state vanishes quickly due to the Boltzman weight in the expectation vale. On the other hand excitations, with lower energies become smeared out due to the thermal fluctuations. The spacing between the lowest laying energy levels in the semi-infinite chain is controlled by the smallest hopping amplitude. Thus the energy resolution $T_N$ at the step $N$ is

$$T_N \sim \Lambda^{-\frac{N}{2}},$$

due to the recursion in Eq. 3.38. This is the reason why using eignesystem of the effective Hamiltonian at the N-th iteration ($T_N = O(T)$) it is suitable for determining thermodynamic properties of the full system.

Calculation of dynamical properties, such as a Green function, poses a much more difficult problem. In this case excitations on different energy scales are important. Thus approximating the true spectrum by the effective one at some NRG step is insufficient. The traditional approach was to calculate at each NRG step $N$ the excitation in the energy interval $\omega_N \leq \omega \leq \Lambda \omega_N$. In general the form of $\omega_N$ depends on details of the discretization procedure but asymptotically is given by

$$\omega_N \sim \Lambda^{-\frac{N-1}{2}}.$$

After the excitations in a given energy window are obtained the results were combined by using the so-called patching procedure. This patching was the source of double-counting ambiguities because the way to combine data from different steps is not uniquely defined. Few schemes for the patching has been developed but they all involve arbitrariness and frequently lead to a breaking of the respective sum rules. Important development has been made in 2007, when the so-called “Full Density Matrix” approach was introduced by Weichselbaum and von Delft [73]. The idea was build upon the “Anders-Schiller basis” [74], which is a complete basis of a Fock space $\mathcal{F}_N$ of a Wilson chain with $N$ sites build from the discarded states during the NRG iterations. As mentioned before the NRG procedure relies on the iterative diagonalization of a chain which is extended by one site at each iteration step. Since the Hilbert space of a chain grows exponentially, one has to reject states to keep the calculations manageable for standard computers. The rejected states are the one with the highest energy. This discarded states, for example, at the step $m$ are then supplemented by a set of $d^{N-m}$ states of the “environment” to form a state belonging to $\mathcal{F}_N$. Such states have two very special properties. Firstly the discarded states at a chosen step of the NRG are orthogonal to the discarded states at any other step. Moreover they are also orthogonal to the kept states at all later steps. This two properties enable one to construct a complete base that spans $\mathcal{F}_N$. This is the “Anders-Schiller basis”. As it was shown in [73] using this base has few advantages over the standard patching procedure. The most important is that it enables one to get rid of the double counting problem. It is possible because the density matrix of the full $N$ site Wilson chain can be rewritten as a sum of properly normalized density matrices for the discarded states at each iteration step (energy shell). Since in this representation the
density matrix has contributions from all energy shells one does not have to use a “single shell approximation”. Thus the patching is not needed, which enables one to calculate thermal averages accurately. Also, by construction, the relevant sum rules for spectral functions are fulfilled. The details of constructing the “Anders-Schiller basis” will not be discussed here due to their complexity.

## 3.6 The Coherent Potential Approximation

The DMFT loop described so far had an assumption that the system under consideration is homogeneous. Only then the self-energy obtained from the solution of the single impurity problem can be used to update the local Green function at each lattice site. This poses a question, how one can introduce a disordered local potential into the DMFT scheme and treat the disorder and the interaction on the same footing. It was achieved by combining the DMFT with the Coherent Potential Approximation (CPA) [89, 90].

The CPA was developed as a self-consistent method for solving approximately the Anderson model. Mathematically this model is defined by

\[
H = \sum_i \epsilon_i n_i - t \sum_{<i,j>} (c_i^\dagger c_j + h.c.),
\]

where the on-site energies \(\epsilon_i\) are random variables drawn from a given probability distribution function. Despite of the simple form of the Hamiltonian in Eq. 3.39 it defines a very complicated problem. Indeed, the complexity follows from the random character of the on-site energies. Each site is a different scattering center for the particle propagating through the lattice. Because of the randomness present in the model a solution is expressed by the averaging the physical quantities over a different on-site energies realization. This averaging introduce the correlations between different possible scattering events and makes, in general, the problem unsolvable. The aim of CPA is to construct such approximation that focus on treating exactly the scatterings events from a single site. The general scheme of CPA approach can be best summarized in the following two steps. First one assumes that the disordered potential can be exactly replaced by a complex, frequency dependent effective potential and expressed by a certain self-energy. Second, at a given site one replaces the effective medium by a true potential and demand that after averaging over the disorder realization the change in the propagator caused by this substitution have to vanish. This condition is used to self-consistently determine the self-energy of the effective medium by the following condition

\[
\left\langle \frac{\epsilon_\sigma - \Sigma_\sigma(z)}{1 - (\epsilon_\sigma - \Sigma_\sigma(z)) \bar{G}_\sigma(z)} \right\rangle_{\text{dis}} = 0,
\]

where \(\epsilon_\sigma\) is the matrix of on-site potentials, \(\Sigma_\sigma(z)\) is the self-energy matrix, \(\bar{G}_\sigma(z)\) is the averaged Greens function and \(z\) is the complex frequency. The angle brackets represent the average over a disorder probability distribution function. Exact solution of
CHAPTER 3. MODEL AND METHOD

This equation, apart from the Lloyd model [91], is not possible. In CPA one makes another assumption, namely that the self-energy should be site-diagonal and homogeneous to restore the translation invariance, i.e.

\[ \Sigma_{i,j,\sigma}(z) = \Sigma_{\sigma}(z)\delta_{i,j}. \]  

(3.41)

The indexes \( i, j \) enumerate the lattice sites. This drastically simplifies the condition 3.40, which now reads

\[ \left\langle \frac{\epsilon_{i\sigma} - \Sigma_{\sigma}(z)}{1 - (\epsilon_{i\sigma} - \Sigma_{\sigma}(z)) G^0_{\sigma}(i, i; z - \Sigma_{\sigma}(z))} \right\rangle_{\text{dis}} = 0, \]  

(3.42)

where

\[ G^0_{\sigma}(i, i; z) = \int d\epsilon \frac{\rho(\epsilon)}{z - \epsilon}. \]  

(3.43)

The results obtained by using the Coherent Potential Approximation have shown very good agreement with experiments both qualitative and even quantitative. In particular, in three dimensional systems a good agreement remained even in the parameter regime where concentration of impurities was quite high. In this case the two impurity scattering should start to play an important role. The understanding of this fact came in 1992. By applying the \( d \to \infty \) scaling of hopping, introduced by Metzner and Vollhardt, to the renormalized perturbation expansion of the scattering series Vlaming and Vollhardt [94] showed that the CPA solution becomes exact in \( Z = \infty \). Moreover, they have shown that by increasing coordination number the scattering events become less correlated and derived the corrections to the \( Z = \infty \) limit that scales as \( 1/Z \). This discovery has proven once again how important is the rescaling of the hopping amplitude in lattice problems.

Important step towards formulating a method that treats interactions and disorder was made by Janiš in late 1980’s [92] and early 1990’s [93]. Using the functional integral technique he reformulated the CPA in terms of the effective propagator \( G \) given by

\[ G^{-1}_{\text{eff}}(i, i, z) = \langle G(i, i, z) \rangle_{\text{dis}}^{-1} + \Sigma(z). \]  

(3.44)

In this formula the assumption about the locality of self-energy, thus \( \langle G(i, i, z) \rangle_{\text{dis}} = G^0_0(i, i, z - \Sigma(z)) \) is made. Using the effective propagator the CPA condition is now given by

\[ \left\langle \frac{1}{G^{-1}_{\text{eff}}(i, i, z) - \epsilon_i} \right\rangle_{\text{dis}} = \frac{1}{G^{-1}_{\text{eff}}(i, i, z) - \Sigma(z)} \]  

(3.45)

By using the Eqs. 3.44 and 3.43 the above condition can be rewritten as

\[ \int d\epsilon \frac{\rho(\epsilon)}{z - \Sigma(z) - \epsilon} = \left\langle \frac{1}{\langle G(i, i, z) \rangle_{\text{dis}}^{-1} + \Sigma(z) - \epsilon_i} \right\rangle_{\text{dis}}. \]  

(3.46)

This form resembles the DMFT condition that connects the local Green function at the impurity to the local Green function of the bath. The difference being that the “impurity”
Green function has to be averaged now over disorder realizations before equating it to the bath Green function. This reformulation of CPA enables one to easily include interactions and to develop a mean-field theory of interacting fermions in a disordered potential. In addition this method becomes exact in the limit of infinite dimensions. The difference between the DMFT loop for the disorder and the homogeneous cases is that instead of solving one single impurity problem, one has to solve a set of single impurity problems for each disorder realization. Then average of the local Green functions is performed to extract the approximation for \( \langle G(i, i, z) \rangle_{\text{dis}} \). Then, this function is used to calculate the self-energy, which now encapsulates both the effects of disorder and interaction. This merge of the DMFT and the CPA was possible because both approaches relay the same assumption that the effect of interactions or disorder can be described by a local self-energy.

### 3.7 The Typical Medium Approximation

Although CPA is very successful, especially in the description of real materials, it is unable to describe the Anderson localization, as proved by Wegner in 1981 [95]. He derived the upper and the lower bounds for the value of averaged over disorder realization density of states. Thus proving that in this quantity neither appearance of delta peaks nor a complete disappearance of spectral weight is possible inside the bandwidth. These were the two features that would indicate the Anderson localization transition on a single particle level. Because of the bounds introduced by Wegner it was believed for a long time that the Anderson localization can only be captured by calculating the conductivity, which is a two-particle quantity.

This has changed in 2003 when the typical medium theory (TMT) was introduced by Dobrosavljević et. al. [98]. They took the local single site point of view natural for DMFT and CPA. Here important is the hybridization function \( \Delta_i(\omega) = \sum_{<i,j>} t^2_{i,j} G_{j,j}(\omega) \) at a given site. It is a random complex function, whose imaginary part is inversely proportional to the life-time of a particle with energy \( \hbar \omega \) at a given site. Close to the Anderson transition this quantity should start to change its behavior from being a continuous function to being represented by a dense set of delta peaks. The former case describes a conducting band with a continuous distribution of energies, whereas the latter describe the localized states with a discrete set of energies. In real systems this quantity will start to display large spatial fluctuations because of the inhomogeneous nature of the disordered system. In the CPA+DMFT treatment the simple averaged hybridization function is used because of the homogeneity of the self-energy. It is proportional to the effective Green function Eq. 3.45 obtained by averaging over all disorder realizations. This means that even if sharp peaks start to develop averaging will smear them out. This observation has lead Dobrosavljević and coworkers to the idea of substituting the simple average value of the hybridization function at a given energy by the quantity that corresponds to its most probable (typical) value. Unlike the probability distribution of local potentials, which is a property of the model, the probability distribution function of hybridization (Green) functions in random media is not known. This makes finding the typical value of
hybridization function an ambiguous procedure. The outcome may strongly depend on
the method chosen to estimate the typical value. The choice made by Dobrosavljević was
an educated guess. He opted for the geometric average because the results from the exact
diagonalization studies of Anderson model were showing that the probability distribution
of spectral functions close to the Anderson transition approaches log-normal distribution
[97]. In this case the typical value of this particular distribution is given by the geometric
average

$$\rho(\omega) = \exp\left\{ \int d\epsilon \mathcal{P}(\epsilon) \ln \rho(\omega, \epsilon) \right\},$$

(3.47)

where \( \mathcal{P}(\epsilon) \) is the probability distribution function (PDF) of the on-site potentials and
\( \rho(\omega, \epsilon) \) is the spectral function for the on-site potential equal to \( \epsilon \). In case of the Anderson
transition the \( \rho(\omega_F) \) goes to zero. In the local point of view this implies that the imaginary
part of the effective hybridization function at Fermi level goes to zero, thus particles
with Fermi energy cannot leave the site. This gives a simple criterion for the Anderson
transition, which is based on a one-particle quantity. The use of the geometric average
has opened a possibility to study the Anderson transition within the effective medium
description. But this comes with a price. Namely, from the form of the geometric average
one can see that it is bias towards localization. Indeed, whenever \( \rho(\omega, \epsilon) \) goes to zero the
logarithm explodes and produces the exponential decay of the spectral weight in \( \rho(\omega) \). As
an effect the geometrically averaged spectral function loses the normalization condition

$$\int d\omega \rho(\omega) \neq 1.$$  

(3.48)

Physically this means that the geometric average reproduces only the continuous part of
the spectrum. The localized part is lost during this averaging. This effect makes the
typical medium approach not suitable for calculating the thermodynamic properties, but
it is a very good method for identification of localization transition. Moreover, since it is
build on the effective medium theory it can be very easily incorporated into the DMFT
scheme. This gives the method that treats both the disorder and the interaction on equal
footing and sensitive to the Anderson transition and the Mott transition as well. At
weak disorder the typical medium approach reproduces results obtained within the CPA.
The spectral functions at given energies are distributed normally and for the Gaussian
distribution the typical and the average value coincide.

Over the past thirteen years the TMT method has been extensively used in studying
various interacting models. For example disordered Hubbard model [99], [100], [101],
Fallov-Kimball model [102, 103], or a charge-transfer model [104]. The results obtained in
[99] about the behavior of the transition line between a disordered metal and an Anderson
insulator where confirmed by the experiments in cold atom system [105].

3.8 The Bethe lattice

In theoretical physics the exactly solvable models are rare. However, having an exact
solution enables one to completely understand the physics of a given model. This knowl-
edge can serve as a starting point for studying approximately more complicated models. Although some cases where an exact solution is known might seem unrealistic, they are found to be a good starting point capturing the right physics on a qualitative level of related but unsolvable models. This was the case, for example, with the infinite coordination number limit that becomes crucial for understanding the metal-insulator transition in materials such as vanadium oxides. For interacting particle or spin systems the Bethe lattice is a tool for obtaining an exact solution. It is an infinite set of sites placed in the vertices of a tree graph, each connected to Z neighbors along the edges of the graph. The finite subset of Bethe lattice is a Cayley tree, cf. Fig. 3.8. A tree graph structure means that the Bethe lattice has no closed loops (retracted paths), which is origin of its usefulness. The name “Bethe lattice” is deceiving for two reasons. Firstly it is not a Bravis lattice in a traditional sense. Although it is a certain ordered structure, one cannot construct it using primitive shifts in Euclidian space because of the fast growing tree-like structure. Therefore, it is referred to as a pseudo-lattice. Second reason is that it was not introduced by Bethe. First report on simplifications arising from considering such a peculiar arrangement of sites came from Kurata, Kikuchi and Watari [75]. These authors have recognized that on this pseudo-lattice the Bethe-Peierls approximation [76, 77] becomes exact. This has been the origin of the Bethe name in context of Bethe lattice. The Bethe-Peierls approximation is a mean-field approximation first used for the Ising model to determine the ferromagnetic transition. The underlying assumption in this approximation was that the full lattice can be described by a cluster of Z+1 sites, described by the following Hamiltonian $H_{c1}$,

$$H_{c1} = -J \sum_{i=1}^{Z} \sigma_0 \sigma_i - h_0 \sigma_0 - h_1 \sum_{i=1}^{Z} \sigma_i, \quad (3.49)$$

where $\sigma_0$ is the spin at the central site in the cluster, $\sigma_i$ are the surrounding Z spins, $J$ is the coupling between the spins, and $h$ is the external magnetic filed. Field $h_1$ is the

---

**Figure 3.7:** Evolution of spectral function on Bethe lattice with on-site disordered drawn from the box-shaped probability distribution function of with $\Delta$ from [98]
field that simulates the environmental effects on the cluster and is determined during the calculations. Indeed, on a tree-like lattice structure the effect of the environment can be mimicked by a local effective magnetic field, as shown in [75]. The approach of Bethe and Peierls has shown that apart form \( Z=2 \), when Bethe lattice reduces to 1D chain, the transition temperature to a ferromagnetic state in the Ising model is non-zero.

The tight binding Hamiltonian can also be solved on the Bethe lattice. In order to do that one can directly use the approach used by Bethe and consider the effects of the environment as a local potential. Then the cluster Hamiltonian can be written as

\[
\mathcal{H}_c = -t \sum_{i=0,\sigma}^{Z} a^\dagger_{i,\sigma} a_{i,\sigma} + h \sum_{i=1,\sigma}^{Z} n_{i,\sigma},
\]

where \( h \) is the field mimicking the presence of the rest of the lattice, \( t \) is the hopping amplitude, \( a^\dagger_{j,\sigma}(a_{j,\sigma}) \) is the fermionic or bosonic creation (annihilation) operator in site \( j \) with spin \( \sigma \). For such a Hamiltonian one can write a set of equations of motion for the retarded Greens functions.

\[
\begin{align*}
(\omega + i\eta)G_{0,0,\sigma}(\omega + i\eta) &= 1 - tZG_{i,0,\sigma}(\omega + i\eta), \\
(\omega + i\eta - h)G_{i,0,\sigma}(\omega + i\eta) &= -tG_{0,0,\sigma}(\omega + i\eta), \\
(\omega + i\eta - h)G_{i,i,\sigma}(\omega + i\eta) &= 1 - tG_{i,0,\sigma}(\omega + i\eta).
\end{align*}
\]

In this set of equations \( i \) denotes the nearest neighbors of the site 0 and the equivalence between the different sites of the Bethe lattice is assumed. This leads to the following
solution

\[
\begin{align*}
\mathcal{G}_{0,0,\sigma}(\omega + i\eta) &= \frac{1}{\omega + i\eta - \frac{\epsilon^2 Z}{\omega + i\eta - h}}, \\
\mathcal{G}_{i,i,\sigma}(\omega + i\eta) &= \frac{\left(\omega + i\eta - \frac{\epsilon^2 (Z-1)}{\omega + i\eta - h}\right) \left(\frac{1}{\omega + i\eta - h}\right)}{\omega + i\eta - \frac{\epsilon^2 Z}{\omega + i\eta - h}}.
\end{align*}
\tag{3.52}
\]

Because of the homogeneity of the Bethe lattice the two Green functions have to be equal

\[
\mathcal{G}_{0,0,\sigma}(\omega + i\eta) = \mathcal{G}_{i,i,\sigma}(\omega + i\eta)
\]

Finally this leads to the condition on \(h\) [75], i.e.

\[
2h = (\omega + i\eta) \pm \sqrt{(\omega + i\eta)^2 - 4(Z-1)t^2}.
\tag{3.53}
\]

Substituting this formula into Eq. 3.52 the local Green function becomes

\[
\mathcal{G}_{0,0,\sigma}(\omega + i\eta) = \frac{2(Z-1)}{(Z-2)(\omega + i\eta) \mp Z\sqrt{(\omega + i\eta)^2 - 4(Z-1)t^2}}
\tag{3.54}
\]

From the local Greens function one can extract the density of states

\[
\rho_\sigma(\omega + i\eta) = \frac{Z}{2\pi} \frac{\sqrt{(Z-1)t^2 - (\omega + i\eta)^2}}{(Z\epsilon^2 - (\omega + i\eta)^2)},
\tag{3.55}
\]

where the positive branch of square root was chosen in order to have the positive valued density of state. The density of state has a finite support bounded by \(\omega = \pm 2\sqrt{Z-1}t\).

In the limit of \(Z \to \infty\) it becomes semi-circular shape [62], i.e.

\[
\rho_\sigma(\omega + i\eta) = \frac{1}{\pi t^*} \sqrt{1 - \left(\frac{\omega + i\eta}{2t^*}\right)^2},
\tag{3.56}
\]

where \(t^*\) is the rescaled hopping as in Eq. 3.9.

Another interesting feature of the Bethe lattice is a direct connection to the DMFT procedure. One of the steps in the DMFT loop is to calculate the Green function of the lattice with the impurity site removed, i.e. \(F_{i,i,\sigma}(z)\). For general lattice it is given by the Hilbert transform of the lattice Green function with frequency shifted by the self-energy. Later this function is used to calculate the hybridization function. On the Bethe lattice this procedure is simplified. Because of the characteristic geometry of the Bethe lattice, removing one site completely disconnects all the branches of the graph originating form this site. Thus the hybridization function can be expressed in a compact form

\[
\Delta_{i,\sigma}(z) = t^2 \sum_{j=1}^{Z} F_{j,j,\sigma}(z) = Z t^2 F_{j,j,\sigma}(z).
\tag{3.57}
\]

The last equality comes form the fact that each branch is equivalent. Now in the \(Z \to \infty\) limit removing one site does not influence the local propagator since there infinite other branches. Thus \(F_{i,i,\sigma}(z) = G_{i,i,\sigma}(z)\) and the hybridization function is given by

\[
\Delta_{i,\sigma}(z) = (t^*)^2 G_{i,i,\sigma}(z).
\tag{3.58}
\]
The Bethe lattice has the bipartite property. Hence if one distinguishes two sublattices then the hoppings takes place only between them. In this case the Eq. 3.58 becomes modified because each site of the sublattice A is surrounded by the sites belonging to the sublattice B and vice versa. If one follows similar steps, the hybridization function for a sublattice \( s \) will be given by

\[
\Delta_{i,s,\sigma}(z) = (t^*)^2 G_{i,i,\bar{s},\sigma}(z),
\]

where \( \bar{s} \) represents the other sublattice.

### 3.9 The Falicov-Kimball model

Another important model from the point of view of the results presented in this thesis is the Falicov-Kimball model. It is a simplified model for studying metal-insulator transition consisting of two types of particles: itinerant electrons that form bands and localized electrons residing on ions. Formally it was introduced in 1969, but first considerations of similar model were already done by Hubbard and Gutzwiller. In Wannier basis the Hamiltonian proposed by Falicov and Kimball \(^{[107]}\) has the following form

\[
\mathcal{H} = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j + h.c.) + U \sum_i a_i^\dagger a_i d_i^\dagger d_i,
\]

where \( a_i \) is an annihilation operator of itinerant electron, and \( b_i \) is the annihilation operator of localized electron. The parameter \( U \) controls the interaction between this two species. In Hubbards and Gutzwillers considerations this model appeared as an approximation of Hubbard model, obtained by immobilizing particles with given only one spin projection. The paper by Falicov and Kimball was focused on thermodynamic properties of the metal-insulator transition in the static mean-field approximation. The occupation of immobile particles was fixed and could have a non-integer value. Using this approximation they were able to show that the nature of the phase transition changes from continuous to discontinuous upon changing the temperature. Their results seemed to coincide with measurements on VO and V\(_2\)O\(_3\) compounds. The interest in the model was renewed in 80’s when it was realized that the model exhibits long-range order \(^{[79]}\) and that the static problem becomes exactly solvable in large spatial dimensions \(^{[80]}\) thanks to simplifications introduced by Metzner and Vollhardt and the development of DMFT.

What was quickly realized is that immobilizing one particle species changes the the electronic behavior close to the MIT, with respect to the Mott scenario. The Kondo type resonance which would appear in Hubbard model is not possible due to the complete freezing of one type of particles. In the Falicov-Kimabll model interaction forces the band formed by mobile particles to split into two sub-bands. This is shown Fig. 3.9 where the spectral function for various \( U \) values and for the Bethe lattice are presented. It can be seen, that the the system evolves into a gaped phase by splitting the non-interacting band into two subbands. On the other hand in the Hubbard model a narrow peak at Fermi level is present until the critical interaction strength is reached. This peak is originates from the previously discussed Kondo resonance formation.
Figure 3.9: The LDOS of itinerant particles for Falicov-Kimball model on Bethe lattice for various U. The plot shows the evolution of the gap as the metal-insulator transition is approached (from [111])
Chapter 4

Results

This chapter is devoted to presenting the result on the Anderson-Hubbard model on a Bethe lattice with spin-dependent disorder. The Hamiltonian of this model for the case of a half-filled lattice can be written as

\[
H = -t \sum_{<i,j> \sigma} c_i^\dagger c_j + \sum_{i \sigma} \epsilon_i n_i + U \sum_i \left( n_{i\uparrow} - \frac{1}{2} \right) \left( n_{i\downarrow} - \frac{1}{2} \right),
\]

where \( c_i \) (\( c_i^\dagger \)) is the fermionic annihilation (creation) operator of an electron at site \( i \) and spin projection \( \sigma = \pm \frac{1}{2} = (\uparrow, \downarrow) \), \( n_i = c_i^\dagger c_i \) is the particle number operator, and \( U \) is the on-site repulsion. Since the hopping amplitude \( t \) is non-zero only between nearest-neighbor (NN) sites \( i \) and \( j \) the considered lattice is bipartite. The on-site energy \( \epsilon_i \) is treated as a random variable drawn from a given probability distribution function. The results were obtained using the DMFT method with the NRG solver. The NRG calculations where done using an open source NRGLjubljana code [81]. In the case studied here the disorder acts directly on particles with spin up and the probability distribution function (PDF) is described by

\[
P_{\sigma}(x) = \frac{1 + 2\sigma}{2\Delta} \theta\left(\frac{\Delta}{2} - |x|\right),
\]

where \( x \) is the on-site energy, \( \sigma \) is the spin projection and \( \Delta \) is the disorder strength. The \( \theta(\frac{\Delta}{2} - |x|) \) denotes the Heaviside step function which is zero when the argument is negative and one when the argument is positive. The results are devised into two parts. In the first part the paramagnetic case is considered. This means that the magnetic instability is frozen by equating the two sublattices. The aim of this part is focus only on the charge fluctuations caused by the competition between the disorder and interaction. In the second part the magnetic instability will be included by enabling the two sublattices to be non-equivalent. This will be refereed to as staggered magnetic case.

In the paramagnetic case the DMFT loop consist of the following steps. First, the set of single impurity models is solved with initial hybridization function. Each considered SIAM has a different local potential \( (\epsilon_d) \) drawn from the PDF \( P_{\sigma}(\epsilon_d) \), given by Eq. 4.1. To decrease the calculation time solving the set of SIAMS using NRGLjubljana code
has been parallelized. From the solutions of SIAMs the spin-dependent local densities of states are computed $\rho_\sigma(\omega, \epsilon, d_{\delta})$, which are used to determine the disorder averaged LDOS. In case of CPA (arithmetic average) it is given by

$$\overline{\rho_{\sigma}}(\omega) = \int d\epsilon p_{\sigma}(\epsilon) \rho_{\sigma}(\omega, \epsilon)$$

and in the case of TMT (disorder average) it is given by

$$\overline{\rho_{\sigma}}(\omega) = \exp \left\{ \int d\epsilon p_{\sigma}(\epsilon) \log \rho_{\sigma}(\omega, \epsilon) \right\}.$$

The averaged LDOS is then used to calculate the disorder averaged Green function by using the Hilbert transformation

$$G_{\sigma}(\omega) = \int d\omega' \frac{\rho_{\sigma}(\omega')}{\omega - \omega'}.$$

This step is crucial in order to ensure the causality of the Green function even after averaging. Next the averaged Green function $G_{\sigma}(\omega)$ is used to calculate the hybridization function, which in the paramagnetic case is given by

$$\Delta_{\sigma}(\omega) = t^2 G_{\sigma}(\omega).$$

This concludes a single DMFT loop since later the hybridization function from the equation above is used to define the new set of SIAM.

As discussed before, to account for a staggered magnetic ordering within the DMFT scheme one has to consider the two sublattices as being non-equivalent. This is why, in addition to spin and site indices, a sublattice index $s = A, B$ will be introduced. The PDF will remain sublattice independent. The DMFT loop in magnetic case consists of the following steps. First, for each sublattice a set of SIAMs is solved. Similarly to the paramagnetic case, each SIAM corresponds to a different local potential. Later from the solution of the two sets of SIAMs, each for one sublattice, the averaged LDOS $\overline{\rho_{s,\sigma}}(\omega)$ is calculated, as described above. The difference being, that now the local density of states depends also the sublattice index $s$. Then using the Hilbert transformation the full spin and sublattice dependent averaged Green function is calculated. The final step in the DMFT loop is to calculate the hybridization function for each sublattice $s$ using Eq. 3.59, which reads

$$\Delta_{s,\sigma}(\omega) = t^2 G_{s,\sigma}(\omega),$$

where $\overline{s}$ denotes the opposite sublattice to $s$.

In both, paramagnetic and magnetic, cases the convergence is achieved once the difference at any frequency between Green functions from two consecutive DMFT loops is smaller than $10^{-6}$. 
4.1 Paramagnetic Case

The main result of this section is the ground state phase diagram of the Anderson-Hubbard model with spin-dependent disorder shown in Fig. 4.1. The corresponding phase diagram for conventional disorder, as obtained in [99], is shown in Fig. 4.2. It will serve as a reference point and the crucial differences between the two will be pointed out. In the system under consideration three different phase transitions take place:

(i) a Mott-Hubbard type MIT for weak disorder $\Delta$, where the correlation gap at the Fermi level opens in the LDOS for spin up and down,

(ii) an Anderson MIT for weak interaction $U$, where the LDOS for spin up vanishes, and

(iii) a Falicov-Kimball type MIT, where the DOS for spin down acquires a correlation gap.

This three phase transitions define the three distinct phases. The correlated, disordered metallic phase which borders on the Mott insulator and the spin-selective localized phase. In the latter the spin-up particles are localized while those with spin down are still itinerant. This phenomenon will be referred to as ”spin-selective localization“. The spin-selective localized phase originates from the spin dependence of the disorder. In the following the properties of these three phases and characterize the transitions between them will be discussed in details.

Figure 4.1: Nonmagnetic ground state phase diagram of the Anderson-Hubbard model at half filling with spin-dependent disorder determined by DMFT with the typical local density of states (LDOS). The inset shows the phase diagram obtained from the arithmetically averaged LDOS.
4.1.1 Metallic phase

The correlated metallic phase is defined by a non-zero value of the geometrically averaged LDOS at the Fermi level, $\rho_\sigma(0) \neq 0$, for both spin channels. In the metallic phase without disorder ($\Delta = 0$) $\rho_\sigma(0)$ corresponds to the non-interacting DOS $N_0(0)$ for both spins and arbitrary $U$. In this case the Luttinger theorem is obeyed [60] and Landau quasiparticles at the Fermi level are well defined [62]. In the presence of spin-dependent disorder, $\rho_\sigma(0)$ is reduced for particles in both spin channels, but differently depending on the spin direction. Only for $U = 0$ are the spin down particles not affected by the disorder at all. The reduction of $\rho_\sigma(0)$ due to an increase of $\Delta$ or $U$ is shown in Fig. 4.3. In contrast to the case of conventional disorder [99] where a sufficiently strong interaction was found to protect the quasiparticles from decaying due to impurity scattering 4.2, $\rho_\sigma(0)$ now always decreases with $U$ for any finite $\Delta$. Spin-dependent disorder violates the Luttinger pinning condition at any $U$, and the local interaction cannot restore the Landau quasiparticle picture. This originates from the SU(2) spin symmetry breaking by the considered type of disorder.

4.1.2 Mott-Hubbard MIT and the coexistence regime

In the Mott insulating phase the LDOS vanishes at the Fermi level in both spin channels, $\rho_\sigma(0) = 0$. This is seen in the upper panel in Fig. 4.3, which leads to Hubbard subbands for stronger interactions $U$, cf. Fig. 4.4. The MIT at weak disorder, $\Delta \lesssim 0.8$, is accompanied with hysteresis (upper panel in Fig. 4.3), and the transition lines $\Delta_{c1}^{MH}(U)$ and $\Delta_{c2}^{MH}(U)$ are tilted to the left (Fig. 4.1). These transition lines terminate at a single critical point close to $U \approx 0.6$ and $\Delta \approx 0.8$. In contrast to conventional disorder [99], where the critical point is located at $\Delta \approx 1.8$, the coexistence regime is found to be significantly smaller.
4.1. PARAMAGNETIC CASE

and a crossover regime does not occur at all. These differences must be attributed to the reduced spin-symmetry in the present problem. Namely, the quasiparticle central peak between the Hubbard subbands, which originates from spin-flip scatterings leading to the Kondo resonance, is destroyed when a Zeeman magnetic field is applied [82, 83, 84, 85, 86, 87, 88]. The induced finite magnetization reduces the number of scattering states at the Fermi level in different spin channels. Although in the present problem the magnetization is zero [108], the density of states in the two spin bands differ and the central (Kondo) peak is not developed, cf. Fig. 4.4. The spin asymmetry of the bands, which is induced by spin dependent disorder, leads to an unequal population of particles with different spin in extended states. This is seen in Figs. 4.5-4.8, which illustrates the dependence of the density \( n_\sigma \) of fermions with spins \( \sigma \) (upper insets) and of the polarization \( p \equiv |(n_\uparrow - n_\downarrow)/(n_\uparrow + n_\downarrow)| \) (lower insets) on the disorder strength \( \Delta \) for different interactions \( U \). Without interaction only the spin-up band is affected by the disorder. Due to the interaction between up and down particles the effect of the disorder is transmitted to the spin down band. The difference in the occupation of extended states is reduced by the interaction \( U \), which leads to a decrease of the polarization. Altogether, spin-dependent disorder reduces the metallicity, forcing the interacting system into an insulating state, in contrast to the spin-independent case.

4.1.3 Spin-selective Anderson localized phase

In the weakly interacting case, \( U \lesssim 0.55 \), a spin-selective Anderson localization is found for \( \Delta \geq \Delta_A^\uparrow(U) \), as shown in Fig. 4.1. Interestingly, only the particles with spin up become
Figure 4.4: Local density of states for different values of the interaction $U$ at disorder strength $\Delta = 0.5$. Upper panel: disordered metallic phase away from the transition line $\Delta_{c2}^{MH}$; middle panel: disordered metallic phase close to the transition line $\Delta_{c2}^{MH}$; lower panel: disordered Mott insulator at the critical interaction strength $U = 0.6$.

Figure 4.5: Upper panel: Density of particles with spin up and spin down, respectively, in extended states at $U = 0.25$ as a function of disorder strength $\Delta$. Lower panel: Polarization of extended states at $U = 0.25$ as a function of disorder.
4.1. PARAMAGNETIC CASE

Figure 4.6: Upper panel: Density of particles with spin up and spin down, respectively, in extended states at \( U = 0.5 \) as a function of disorder strength \( \Delta \). Lower panel: Polarization of extended states at \( U = 0.5 \) as a function of disorder.

Figure 4.7: Upper panel: Density of particles with spin up and spin down, respectively, in extended states at \( U = 0.75 \) as a function of disorder strength \( \Delta \). Lower panel: Polarization of extended states at \( U = 0.75 \) as a function of disorder.
localized when $\Delta \geq \Delta_{c1}^A(U)$, cf. Fig. 4.1, whereas the particles with spin down are still itinerant. The LDOS at the Fermi level is zero in the former case and non-zero in the latter, as shown in the lower panel of Fig. 4.3 by the blue and green lines, respectively. On physical grounds this spin-selective localized phase may be effectively interpreted within a Falicov-Kimball model, [107] where spinless lattice fermions interact with immobile particles. In the present case, the particles with spin up are localized due to the disorder $\Delta$ and form an immobile subsystem on which the particles with spin down are scattered due to the interaction $U$. This spin-selective localization implies the absence of spin-up quasiparticle states around the Fermi level. However, Hubbard subbands are formed in the LDOS for both spins at higher energies, as is shown in the middle panel of Fig. 4.9. Again, although the disorder acts only on spin-up particles, the interaction transfers the effect of the disorder also to the spin-down particles. This is evident from Figs. 4.3 and 4.9, where it is seen that some states with spin down become localized. Indeed, by setting the hybridization function for particles with spin up to zero, one can show that the DMFT action for the Hubbard model reduces to that for the Falicov-Kimball model [111]. This justifies the interpretation of the spin-selective Anderson localized phase in terms of the Falicov-Kimball model.

### 4.1.4 Disordered Mott insulator

For strong disorder, $\Delta \gtrsim 0.8$, a transition from the spin-selective Anderson localized phase to a disordered Mott insulator can be found upon increasing $U$ ("Falicov-Kimball
4.1. PARAMAGNETIC CASE

Figure 4.9: LDOS at disorder strength $\Delta = 1$ for different values of the interaction $U$. Upper panel: disordered metallic phase; middle panel: transition point from the disordered metallic to the spin-selective Anderson localized phase; lower panel: disordered Mott insulator.

There is no hysteresis and the spin-down band is completely split off for $U_c \gtrsim 0.55$. Above this value the LDOS at the Fermi level for spin down particles vanishes, cf. Fig. 4.3. The transition line $\Delta_{cH}^{\uparrow \downarrow}(U)$ is seen to be vertical for disorder $\Delta \gtrsim 0.8$. This means that the localized spin-up fermions now play the role of the immobile particles in the Falicov-Kimball model. By further increasing $U$ for a fixed $\Delta$ a Mott gap proportional to $U$ develops, cf. the lower panel in Fig. 4.9. On the insulating side the integral over the LDOS changes with $U$ although $\Delta$ is held constant. This is due to the Hubbard type coupling between spin up and down particles, leading to changes in both hybridization functions $\Delta_{\sigma}(\omega)$. Therefore, one can conclude that although the MIT above $\Delta \approx 0.8$ is of the Falicov-Kimball type, the phase on the right hand side of the phase boundary in Fig. 4.1 is still a disordered Mott insulator. In other words, there is no phase boundary between weakly and strongly disordered Mott insulators.
CHAPTER 4. RESULTS

Figure 4.10: Comparison of LDOS obtained using geometric and arithmetic average for various interaction strengths and $\Delta = 0.5$.

Figure 4.11: Comparison of LDOS obtained using geometric and arithmetic average for various disorder strengths and $U=0.5$. 
4.2 Staggered magnetic case

Now the influence of magnetic ordering on the previously described scenario will be exploited. In this case the ground state is determined by the competition of three factors: the strengths of the disorder and of the local repulsion, respectively, and the possible existence of AF-LRO. They lead to the emergence of four different types of spin ordering, which are depicted schematically in panels (a)-(d) in Fig. 4.12. The first pattern, (a), is the usual Néel AF-LRO, where the averaged spins are of equal length, but are oriented anti-parallel on neighbouring sites. The second pattern, (b), is a ferrimagnet, where the averaged spins on all sites are directed anti-parallel but their lengths on neighbouring sites differ. The third pattern, (c), is a ferromagnetic spin-density wave (SDW), where on neighbouring sites the averaged spins are oriented parallel but have different lengths. The last type of spin ordering, (d), is the usual ferromagnet, which is characterized by the same length and direction of the averaged spins on every lattice site.

To fully characterize the observed phases four different quantities are computed:
1) the geometrically averaged LDOS \( \rho_{\sigma,s}(\omega) \) for spin \( \sigma \) and sublattice \( s \),
2) the local magnetization \( m_s \), i.e. the averaged value of the spin, defined on a site belonging to sublattice \( s \)
   \[
   m_s = \frac{n_{s,\uparrow} - n_{s,\downarrow}}{2},
   \tag{4.2}
   \]
   where \( n_{\sigma,s} = \int_{-\infty}^{0} \rho_{\sigma,s}(\omega)d\omega \) is the density of particles with spin \( \sigma \) on sublattice \( s \) (here the energy scale is chosen such that \( \omega = 0 \) corresponds to the Fermi energy),
3) the ferrimagnetic order parameter, i.e., the difference between the local magnetizations on neighbouring sites
   \[
   m_{\text{Ferri}} = \frac{|m_A - m_B|}{2}\Theta\left(-\frac{m_A}{m_B}\right),
   \tag{4.3}
   \]
   and
4) the ferromagnetic spin-density wave order parameter, i.e., the difference between the parallel local magnetizations on neighbouring sites
   \[
   m_{\text{SDW}} = |m_A - m_B|\Theta\left(\frac{m_A}{m_B}\right).
   \tag{4.4}
   \]

The order parameters and the magnitude of the local magnetization, \( |m_s| \), change between zero and 1/2.

With these quantities one may identify the following five different phases:

i) *ferromagnetic metal (FM)* if \( \rho_{\sigma,s}(0) \neq 0 \) and \( m_A = m_B \neq 0 \) (and consequently \( m_{\text{Ferri}} = 0 \) and \( m_{\text{SDW}} = 0 \)),

ii) *ferrimagnetic insulator of type I (Ins-I)* if \( \rho_{\sigma,s}(0) = 0 \), \( m_{\text{Ferri}} \neq 0 \), and \( m_{\text{SDW}} = 0 \),

iii) *ferromagnetic SDW insulator of type II (Ins-II)* if \( \rho_{\sigma,s}(0) = 0 \), \( m_{\text{Ferri}} = 0 \), and \( m_{\text{SDW}} \neq 0 \),

iv) *ferrimagnetic spin-selective localized phase of type I (SSLP-I)* if \( \rho_{\sigma,s}(0) \neq 0 \), \( \rho_{\downarrow,s}(0) = 0 \), \( m_{\text{Ferri}} \neq 0 \), and \( m_{\text{SDW}} = 0 \)

v) *ferromagnetic SDW spin-selective localized phase of type II (SSLP-II)* if \( \rho_{\downarrow,s}(0) = 0 \) and
Figure 4.12: Panels (a)-(d) show different spin patterns found in the Anderson-Hubbard model with spin dependent disorder: (a) antiferromagnet, (b) ferrimagnet, (c) ferromagnetic spin-density wave, and (d) ferromagnet.

\[ \rho_{\downarrow s}(0) \neq 0 \text{ when } m_{\text{Ferri}} = 0, \text{ and } m_{\text{SDW}} \neq 0. \]

Within DMFT, a dynamical but local approximation, there are no other phases on a bipartite lattice.

The magnetic ground state phase diagram of the Anderson-Hubbard model with spin-dependent disorder obtained in this way is shown in Fig. 4.13 and is the main result of our investigation. It will now be discussed in detail.

### 4.2.1 Ferrimagnetic insulator of type I (Ins-I)

This ferrimagnetic insulating phase is characterized by AF-LRO where the magnetization alternates in sign and magnitude on neighbouring sites, and the geometrically averaged LDOS vanishes at the Fermi energy in both spin channels and on every lattice site. In the absence of disorder (\( \Delta = 0 \)) this phase becomes an AF insulator (AFI), which is the only stable DMFT solution for the half-filled Hubbard model on a bipartite lattice at \( T = 0 \) and any \( U > 0 \), due to particle-hole and spin symmetries. The ferrimagnetic insulator exists only at weak disorder \( \Delta \), i.e., in the regimes with \( \Delta \lesssim U/3 \) for \( U \lesssim 0.6 \) and \( \Delta \lesssim 0.25 \) for \( U \gtrsim 0.6 \). Upon increasing the disorder the ferrimagnetic order parameter \( m_{\text{Ferri}} \) goes to zero in both interaction regimes as is seen in the upper panel of Fig. 4.14. The vanishing of \( m_{\text{Ferri}} \) signals a possible transition to a different spin pattern. At the same time, by turning up \( U \) the ferrimagnetic order parameter increases and the system tends toward the saturated Néel antiferromagnet with \( m_{\text{Ferri}} = 1/2 \), as shown by the
Figure 4.13: The magnetic ground state phase diagram of the Anderson-Hubbard model on a bipartite lattice at half filling with spin-dependent disorder determined by DMFT with the geometrically averaged local density of states (LDOS). Five phases are distinguished: FM (Ferromagnetic metal), Ins-I (insulator of type I), Ins-II (insulator of type II), SSLP-I (spin-selective localized phase of type I), and SSLP-II (spin-selective localized phase of type II). At the point \( \Delta = 0, U = 0 \) the system is a paramagnet (Fermi gas) while on the horizontal line \( (\Delta = 0, U > 0) \) it is a Néel antiferromagnet. For details see text.
Figure 4.14: Ferrimagnetic order parameter $m_{\text{Ferri}}$ as a function of disorder strength $\Delta$ for different interaction strengths $U$ (upper panel), and as a function of interaction strength $U$ for various disorder strengths $\Delta$ (lower panel).

Curves for $\Delta = 0.05$ and 0.2 in the lower panel of Fig. 4.14.

The geometrically averaged LDOS for the ferrimagnetic insulator for $U \lesssim 0.6$ exhibits a narrow spectral gap and a pronounced asymmetric peak (cf. the upper panel in Fig. 4.15) similar to the $\Delta = 0$ case [106]. Due to the staggered (Néel) spin order the lattice unit cell is doubled in the ferrimagnetic insulator. The existence of LRO in this phase is caused by the interaction, while the ferrimagnetic modulation of the local magnetization is an effect of the spin-dependent disorder. This type of disorder reduces the band-width of fermions with spin up in extended states. Since the interaction is weak here, the LDOS for spin down particles is not strongly modified by spin-dependent disorder and almost remains the same as in the $\Delta = 0$ case. This altogether leads to staggered, but different in magnitude, local magnetizations $|m_A| \neq |m_B|$ and ferrimagnetic order.

### 4.2.2 Ferrimagnetic spin-selective localized phase of type I (SSLP-I)

In the weakly interacting regime with $U \lesssim 0.6$ the ferrimagnetic insulator undergoes a transition to the ferrimagnetic spin-selective localized phase upon increase of the disorder $\Delta$. This phase is shown as a narrow orange area in the phase diagram in Fig. 4.13. The SSLP-I phase is characterized by small values of $m_{\text{Ferri}}$ as is seen in Fig. 4.14 and a non-vanishing geometrically averaged LDOS at the Fermi energy in only one spin channel, as is illustrated in the middle panel of Fig. 4.15. This means that particles with spin up, which are directly influenced by the disorder, are now in the metallic phase because the
disorder redistributes their spectral weight, thereby closing the gap for these fermions. By contrast, the spin down particles remain in the insulating state. In other words, particles with spin down, which are not directly affected by the spin-dependent disorder, sustain the gap in the geometrically averaged LDOS due to the existence of AF-LRO. Although the gap is closed in $\rho_{\uparrow}(\omega)$, the asymmetry of the geometrically averaged LDOS in the two spin channels remains, giving rise to different local magnetizations $|m_A| \neq |m_B|$ and a finite value of $m_{\text{Ferri}}$.

### 4.2.3 Ferromagnetic metal (FM)

Upon increasing the disorder strength further the FM becomes stable with finite and equal local magnetizations $m_s$ on both sublattices. This phase does not possess a spontaneous LRO since the uniform spin polarization is driven solely by the spin-dependent disorder. This phase is characterized by $m_{\text{Ferri}} = 0$ and $m_{\text{SDW}} = 0$ (c.f., Figs. 4.14, and 4.16) whereas the geometrically averaged LDOS at the Fermi energy for both spin species becomes non-zero, as is seen in Fig. 4.17.

In this ferromagnetic metallic phase spin-dependent disorder plays a dominant role. Indeed, it closes the gaps in the geometrically averaged LDOS in the two spin channels and leads to an equal distribution of spectral weights below and above the Fermi level, as is shown in the lower panel of Fig. 4.15. Since disorder reduces the spectral weight of spin up particles, c.f., the lower panel of Fig. 4.15, the system becomes spin polarized with
Figure 4.16: Ferromagnetic SDW order parameter as a function of disorder strength $\Delta$ for different interaction strengths $U$ (upper panel), and as a function of interaction strength $U$ for various disorder strengths $\Delta$ (lower panel).

$|m_A| = |m_B| \neq 0$. The interaction (repulsion) thereby plays a minor role here: namely, it mediates the influence of the disorder also to the spin down particles. As a result, both spin up and spin down particles are distributed uniformly on both sublattices, which leads to the absence of LRO ($m_{\text{Ferri}} = 0$ and $m_{\text{SDW}} = 0$).

### 4.2.4 Ferromagnetic SDW spin-selective localized phase of type II (SSLP-II)

When the disorder strength is increased even further a transition from the FM phase to the ferromagnetic SDW spin-selective localized phase takes place at $U \lesssim 0.5$. In the SSLP-II the spin-up particles, which are influenced directly by spin-dependent disorder, have a vanishing geometrically averaged LDOS at Fermi level on both sublattices: $\rho_{\uparrow,s}(0) = 0$, i.e., they are in an insulating state. By contrast, the spin-down particles have $\rho_{\downarrow,s}(0) \neq 0$ on both sublattices, and hence are metallic. At the same time the ferromagnetic SDW is stabilized, with $m_{\text{SDW}}$ being relatively small, as seen in Fig. 4.16. This SSLP-II is a magnetic counterpart to the spin-selective localized phase found in the paramagnetic ground state phase diagram in Ref. [110].

The origin of this phase can be explained as follows: strong spin-dependent disorder renormalizes the geometrically averaged LDOS of the spin-up particles and opens a gap at the Fermi level due to the disorder-driven localization transition, thus forming two narrow, continuous subbands. The changes of the geometrically averaged LDOS, and the spin-selective opening of the gap when $U$ is increased at fixed $\Delta = 1$, is shown in
4.2. STAGGERED MAGNETIC CASE

![Graph showing LDOS vs Interaction](image)

Figure 4.17: Geometrically averaged LDOS on sublattice $A$ at the Fermi level as a function of interaction $U$ for different values of the disorder $\Delta$. Spin-up particles: upper panel, spin-down particles: lower panel.

the panels of Fig. 4.18. The properties of SSLP-II can be effectively understood within a Falicov-Kimball model [107, 111] where spinless fermions on a lattice interact with immobile particles. Indeed, the spin up particles are localized due to spin-dependent disorder and act as scatterers for the spin down particles due to the Hubbard interaction $U$. In contrast to the paramagnetic case studied in Ref. [110] here the parallel oriented local magnetic moments have different values on different sublattices, yielding a small but finite ferromagnetic SDW order parameter $m_{SDW}$. Spin-selective localization together with ferromagnetic SDW LRO implies the absence of spin up quasiparticles at the Fermi level. They are, however, present for spin-down particles as seen for $U = 0.35$ and $0.45$ in Fig. 4.18. We also see in Fig. 4.18 that Hubbard subbands at higher energies are formed in the geometrically averaged LDOS for both spins.

At the interaction $U \approx 0.5$ the SSLP-II turns into a ferromagnetic SDW insulator (Ins-II) as is seen in Fig. 4.13, and the geometrically averaged LDOS shows a gap for both spin particles, cf. the lower panel of Fig. 4.18. Similar to the paramagnetic case discussed before [110], the critical interaction $U_c$, at which the transition from SSLP-II to Ins-II takes place, is independent of the disorder strength $\Delta$ as shown in Fig. 4.13. We conclude that the transition from SSLP-II to Ins-II is of the Falicov-Kimball type because the geometrically averaged LDOS for spin-down particles splits in a similar way as in the case of binary-alloy disorder, where particles with spin-up provide localized scattering centers [111]. The slight reduction of the critical interaction from $U_c \approx 0.55$ for the paramagnetic ground state discussed in Ref. [110], to $U_c \approx 0.5$ in the case studied here, is caused by the presence of the ferromagnetic SDW LRO which naturally tends to form
Figure 4.18: Geometrically averaged LDOS on sublattice $A$ for different values of the interaction $U$ at disorder strength $\Delta = 1$. Top panel: FM; second panel from the top: border between FM and SSLP-II; third panel from the top: SSL-II; bottom panel: border between SSLP-II and AFI.
4.2. STAGGERED MAGNETIC CASE

a gap and subbands, as in the Slater theory of AF [106]. Indeed, this is seen in Fig. 4.19, where we compare the geometrically averaged LDOS at $\Delta = 1$ and $U = 0.5$ obtained from the uniform and bipartite lattice DMFT solutions, respectively. The ferromagnetic SDW LRO leads to an asymmetric transfer of the spectral weight away from the Fermi level and an opening of the gap at smaller $U$ as compared with the uniform case. We also note that for the disorder values considered here $m_{SDW}$ is almost independent of $\Delta$, which we can see in Fig. 4.16. Therefore the $U_c(\Delta)$ line is vertical in the phase diagram Fig. 4.13.

4.2.5 Ferromagnetic SDW insulator (Ins-II)

Once the interaction strength exceeds $U \approx 0.6$ for $\Delta \gtrsim 0.2$, the system makes a transition from the ferrimagnetic insulator (Ins-I) with $m_{Ferri} \neq 0$ to the ferromagnetic SDW insulator (Ins-II) with $m_{SDW} \neq 0$. Due to the spin-dependent bandwidth renormalization caused by the localization transition, the density of spin up particles is reduced when the disorder strength is increased. Above $\Delta \approx 0.2$ the reduction is so strong that, although there is an interaction driven tendency toward formation of AF-LRO in the system, the spin-dependent disorder together with the localization transition of spin up particles drives the system into the ferromagnetic SDW order, e.g. the left and right panel of Fig. 4.20. Thereby this type of disorder reduces the role of virtual exchange processes responsible for AF magnetic LRO at large $U$ [112]. On the other hand, unequal but parallel local magnetization on two sublattices keeps the system in the insulating phase with $m_{SDW} \neq 0$. In the case of disorder acting equally on both spin directions, this part of the phase diagram would be an antiferromagnetic insulator and the interaction would play a dominant role,
Figure 4.20: Comparison of geometrically averaged LDOS on sublattice A and sublattice B for Ins-I (left-hand side) and Ins-II (right-hand side) at the same $U = 0.7$.

generating AF-LRO [100].
Chapter 5

Summary

The aim of this thesis was to present the result on interacting lattice fermions in presence of spin-dependent disorder. This problem is interesting for two reasons. First, it provides a new insight into the metal-insulator transition in systems with interaction and disorder. A topic that has drawn the attention of condensed matter physicists for over fifty years. Introducing the randomness acting only on one spin channel enables one to directly investigate the importance of the spin symmetry for MIT. It does so without braking the particle-hole symmetry that would happen in presence of a magnetic field. Secondly, due to the development in cold atom physics this model could be realized in experiments. Thus it is important to know theoretical predictions for future comparison.

The system was modeled by the Anderson-Hubbard Hamiltonian, Eq. 4.1, with spin dependent probability distributions of on-site energies. To solve it a combination of dynamical mean-field theory (DMFT) and typical medium theory (TMT) has been used. Results obtained within this approach were compared with the other method often used in this kind of problems, i.e. DMFT+CPA (coherent potential approximation). A method that becomes exact in the infinite dimensions. Both methods are based on Green function formalism and assume that all the effects of interaction and disorder can be encapsulated in a local frequency dependent potential. But they differ in treatment of the disorder. In CPA the Green function is arithmetically averaged over the disorder realization, whereas in TMT a geometric average is used. The advantage of using a geometric average over the arithmetic one is that the former enables one to capture the Anderson transition. On the down side geometrically averaged Greens function gives a spectral function that does not conserve the normalization. This is why DMFT+TMT is a good method for constructing a phase diagram but not for calculating thermodynamic properties of the system.

The results presented in the thesis where obtained for the Bethe lattice and at zero temperature. They are divided into two categories: the paramagnetic case and the magnetic case. Due to the bipartite nature of the lattice the considered system has a natural tendency to form a staggered magnetic long-range order for non-zero interactions. In the paramagnetic case this tendencies where blocked by assuming a sublattice independent solution of the model Hamiltonian. It was done to focus solely on the effects of the spin-dependent disorder on the charge degree of freedom. Later in the calculations for the magnetic case the two sublattices where distinguished enabling the system to exhibit a
magnetic long-range order. The results for both cases where compared with the results for the spin-independent (conventional) disorder obtained by using the same methods.

In the paramagnetic case the spin dependence of the disorder has proven to have a drastically different effect as compared to the conventional disorder. In the latter the interaction and randomness where two competing factors, whose interplay stabilized the metallic phase. Once the disorder becomes spin dependent the two factors start to cooperate and drive the system into an insulating phase. As a result the binodal region on the phase diagram becomes narrow and tilts towards lower interaction strengths. Moreover in the region where disorder becomes dominant a spin-selective localization takes place and the system enters a spin-selective localized phase. Because in this phase particles in a single spin channel becomes immobilized the MIT becomes Falicov-Kimball-like.

In the staggered magnetic case the phase diagram is richer due to the long-range order. In this case any finite amount of disorder destroys the antiferromagnetic order. As a result ferrimagnetic orders appear, characterize by unequal absolute values of magnetization at each sublattice. Thus the antiferromagnetic insulator, a natural phase for an interacting fermionic system on a bipartite lattice, becomes the insulator of type I (Ins-I). At weak interactions the system undergoes three phase transitions as the disorder is increased. First Ins-I becomes a spin-selective localized phase of type I. The phase where particles that are not directly effected by the disorder are localized, as opposed to particles in the other spin state that are mobile due to scattering. This phase turns into a ferromagnetic metal phase upon the increase of the disorder. In this phase both sublattice equivalent and the gap in spectral function is closed irrespective of spin direction. Because of the localization effects the system becomes spin imbalanced. As the disorder is increased further the system enters the spin-selective localized phase of type II. An analogon of the spin-selective localized phase obtained in the paramagnetic case. Due to the tendency of the system to form a long-range order this phase have slightly different magnetization on two sublattices. Finally at strong interaction system exhibits only one phase transition from Ins-I to insulator of type II. In this phase spectral functions for particles in both spin channels are gaped but due to the action of the disorder the the magnetizations on sublattice have the same sign.

The above presented study shows that including the spin-dependent disorder opens a possibility for controlled spin symmetry breaking without effecting any other symmetry in the system. This shows to have a profound effect on the shape of phase diagram in both paramagnetic and staggered magnetic cases. Most importantly tuning the disorder strength enables one to change the behavior from governed by the Hubbard Hamiltonian to the one described by the Falicov-Kimball model. This unprecedented possibility alone shows the importance of further experimental study of this model for deepening the knowledge about the metal-insulator transition.

The results presented in this thesis also pose a number of interesting questions which could be a future research directions. Firstly, since this study was done at T=0 a natural thing would be to investigate the influence that thermal fluctuations will have on both the paramagnetic case and the staggered magnetic case. A second possible direction of research would be to extend this study by introducing the non-local correlations using
cluster extension of DMFT [113]. This would be especially important for the staggered magnetic case, since antiferromagnetic order on a bipartite lattice is known to be even stronger stabilized by including the non-local effects. The third research direction would be to make calculations for a model which is directly connected to the experimental setups. This can be achieved either by considering more realistic lattices or by studying more experimentally relevant on-site potential PDF. An example of a more realistic lattice would be a square or a cubic lattice. As far as the on-site potential PDF is concerned to have a more experimentally relevant results in stead of the rectangular-shaped PDF, studied in this thesis, a speckle-like PDF should be used.
Appendix A

Derivation of the Hubbard model

In this appendix the Hubbard Hamiltonian will be derived. As a starting point one consider the following Hamiltonian in the second quantization formulation

\[ \mathcal{H} = \sum_{\sigma} \int d^3 r \, \psi_{\sigma}^\dagger(\mathbf{r}) \left( \frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{r}) \right) \psi_{\sigma}(\mathbf{r}) + \frac{1}{2} \sum_{\sigma, \sigma'} \int d^3 r d^3 r' \, \psi_{\sigma}^\dagger(\mathbf{r}) \psi_{\sigma'}^\dagger(\mathbf{r}') U(\mathbf{r} - \mathbf{r}') \psi_{\sigma'}(\mathbf{r}') \psi_{\sigma}(\mathbf{r}) \]  

(A.1)

where \( \psi(\mathbf{r}) \) is the fermionic field operator, \( \hat{\mathbf{p}} \) is the momentum operator, \( \sigma \) represents the spin projection, and \( U(\mathbf{r} - \mathbf{r}') \) is the Coulomb interaction

\[ U(\mathbf{r} - \mathbf{r}') = \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \]

with \( e \) being the electronic charge. The potential \( V(\mathbf{r}) \) in the first term of Eq. A.1 is a periodic function of \( \mathbf{r} \) describing the lattice. The period of this function defines the lattice spacing. The Hubbard model was introduced to capture the key physics of the so-called narrow band materials. In any lattice problem the band width is directly related to the overlap of electronic wave functions. Which means that in case of small bandwidths the lattice spacing is large as compared to the spread of the wave functions. As a result the electrons are more localized in space then in the wide band materials. In order to reflect that, rather then using Bloch states, it is more convenient to write the field operators in the Wannier function basis. They are defined as

\[ W_l(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_k e^{-i\mathbf{k} \cdot \mathbf{R}_l} u_k(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}}, \]  

(A.2)

where \( \mathbf{k} \) is the reciprocal lattice vector, vector \( \mathbf{R}_l \) points at \( l \)-th lattices site, \( u_k e^{i\mathbf{k} \cdot \mathbf{r}} \) is a Bloch wave function for the corresponding \( \mathbf{k} \), and the summation runs over all vectors from the Brouillion zone. The normalization factor is a square root of the number of lattice sites \( N \). The Wannier functions form an orthonormal basis of wave functions centered on lattice sites

\[ \int d^3 r W_l(\mathbf{r}) W_m(\mathbf{r}) = \delta_{l,m}. \]
In the Wannier function basis the field operators are given by
\[ \hat{\psi}_{i,\sigma}(\mathbf{r}) = \sum W_i(\mathbf{r}) c_i,\sigma, \]
\[ \hat{\psi}^\dagger_{i,\sigma}(\mathbf{r}) = \sum W_i(\mathbf{r}) c_i,\sigma^\dagger, \]
where \( c_{i,\sigma} \) (\( c_{i,\sigma}^\dagger \)) is the fermionic annihilation (creation) operator of particle with spin \( \sigma \) on the \( i \)-th site. After rewriting the field operators in Wannier function basis the Hamiltonian (A.1) reads
\[ H = \sum_{i,j,\sigma} t_{ij} c^\dagger_{i,\sigma} c_{j,\sigma} + \frac{1}{2} \sum_{i,j,k,l,\sigma,\sigma'} U_{ijkl} c^\dagger_{i,\sigma} c^\dagger_{j,\sigma'} c_{k,\sigma'} c_{l,\sigma}, \]
where \( t_{ij} \) and \( U_{ijkl} \) are matrix elements given by:
\[ t_{ij} = \int d^3r W_i^*(\mathbf{r}) \left( \frac{\hbar^2}{2m} + V(\mathbf{r}) \right) W_j(\mathbf{r}) \]
\[ U_{ijkl} = \int d^3r \int d^3r' W_i^*(\mathbf{r}) W_j^*(\mathbf{r}') U(\mathbf{r} - \mathbf{r}') W_k(\mathbf{r}') W_l(\mathbf{r}). \]
The first term in A.4 is called the hopping term and the second term is the interaction term. Because of the strong localization of the Wannier functions around a given lattice site two approximations can be made. First approximation is to neglect all contributions to the interaction term in Eq. A.4 apart from the \( i = j = k = l \) term. Following Hubbard reasoning [42] if one assumes the s-wave nature of the electronic wave functions this would be the dominant contribution. To simplify the notation one introduces the so called Hubbard \( U \) parameter
\[ U = \int d^3r W_i^*(\mathbf{r}) W_j^*(\mathbf{r}) U(\mathbf{r} - \mathbf{r}') W_i(\mathbf{r}) W_j(\mathbf{r}). \]
and using the described approximations the Hamiltonian from Eq. A.4 can be rewritten as
\[ H = \sum_{i,j,\sigma} t_{ij} c^\dagger_{i,\sigma} c_{j,\sigma} + \frac{U}{2} \sum_{i,\sigma,\sigma'} c^\dagger_{i,\sigma} c^\dagger_{i,\sigma'} c_{i,\sigma'} c_{i,\sigma}. \]
Due to the fact that the fermionic particles obey Pauli exclusion principle the only contribution to the interaction term comes from \( \sigma \neq \sigma' \). Thus this term can be rewritten as \( \frac{U}{2} \sum_{i,\sigma} n_{i,\sigma} n_{i,\bar{\sigma}} \). Where the shorthand notation \( \bar{\sigma} = -\sigma \) was introduced. The second approximation used to obtain the Hubbard model is to keep the only the hopping elements which couple the same or the adjacent lattice sites. This approximation is also supported by the localized nature of the Wannier functions. The summation over hoppings between the nearest neighboring sites will be denoted as \( \sum_{<i,j>} \). The last step before obtaining the final form of the Hubbard Hamiltonian 3.1 is to extract from the hopping term elements coupling the same Wannier functions and introduce parameter \( \epsilon_i = t_{ii} \). This terms will be called on-site energies. Finally introducing \( t_{ij} = -t \) one ends up with the following Hamiltonian:
\[ H = \sum_{i,\sigma} \epsilon_i n_{i,\sigma} - t \sum_{<i,j>,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + \frac{U}{2} \sum_{i,\sigma} n_{i,\sigma} n_{i,\bar{\sigma}}, \]
which was introduced in Eq. 3.1.
Appendix B

Green’s function properties

The central object used in calculations conducted in this thesis is a retarded Green’s function. It is defined in the following way

\[ G^R_{i,j}(t) := -i \theta(t) \left\langle \{a_i(t), a_j^\dagger(0)\} \right\rangle, \tag{B.1} \]

where \(a_i, (a_j^\dagger)\) are annihilation (creation) operators of a fermionic field in basis characterized by a set of quantum numbers \(i, j\). Brackets denote thermodynamic average, which in this thesis is calculated using grand canonical ensemble and is given by

\[ \{ \ldots \} = \frac{1}{Z} Tr \left\{ e^{-\beta (H - \mu N)} \ldots \right\}. \]

Trace is calculated over all states in a chosen basis, \(Z = Tr \left\{ e^{-\beta (H - \mu N)} \right\}\) is the partition function for Hamiltonian \(H\) with fixed chemical potential \(\mu\). Operators used in definition B.1 are in Heisenberg picture

\[ a_i(t) = e^{\frac{i}{\hbar} H t} a_i e^{-\frac{i}{\hbar} H t}. \]

Using the Fourier transform in time domain

\[ \psi_\sigma(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} a_i(t) \tag{B.2} \]

one can define Green’s function in frequency domain

\[ G^R_{i,j}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} G^R_{i,j}(t). \]

Important feature of the retarded Green’s function can be seen by introducing a unity operator

\[ 1 = \sum_n |n\rangle \langle n| \]

written in the eigenbasis of the Hamiltonian with \(n\) particles

\[ H |n\rangle = E_n |n\rangle, \]

74
in between the operators in the Green’s function definition B.1. Then one ends up with
the following formula

\[
\mathcal{G}_{i,j}^R(\omega) = -i \int_0^\infty \frac{dt}{\mathcal{Z}} \sum_{n,m} \left( e^{-\beta(E_n-\mu_n)} + e^{-\beta(E_m-\mu_n)} \right) \langle n | a_i | m \rangle \langle m | a_j^\dagger | n \rangle \ e^{-\frac{\hbar}{\eta}(E_n-E_m-\omega)t} =
\]

\[
= \frac{\hbar}{\mathcal{Z}} \sum_{n,m} e^{-\beta(E_n-\mu_n)} + e^{-\beta(E_m-\mu_n)} \langle n | a_i | m \rangle \langle m | a_j^\dagger | n \rangle .
\]

The last equation is called the Lehmann representation of the Green’s function. It
highlights the crucial property of this object, namely that poles of Green’s function coincide
with the exact energy of the excitations in the system under consideration. Thus making
theoretical calculations of Green’s function directly connected to observable quantities.

A very useful staring point in Green’s function calculation is the equation of motion.
If one divide the initial Hamiltonian \( \mathcal{H} \) into part which is easily diagonalizable
\( \mathcal{H}_0 \) and perturbation \( \mathcal{V} \) then by differentiation of the Green’s function over time, the following
result can be obtained

\[
\frac{\partial}{\partial t} \mathcal{G}_{i,j}^R(t) = -i\delta(t) - E_i \mathcal{G}_{i,j}^R(t) - i\theta(t) \left\langle \left\{ [\mathcal{V}, a_i(t)], a_j^\dagger \right\} \right\rangle .
\]

In the above formula it was assumed that \( a_i \) is the eigenstate of \( \mathcal{H}_0 \). This can be translated
into a frequency domain by Fourier transformation

\[
\lim_{\eta \to 0^+} (\omega + i\eta) \mathcal{G}_{i,j}^R(\omega + i\eta) = 1 + E_i \mathcal{G}_{i,j}^R(\omega) - \lim_{\eta \to 0^+} \int_{-\infty}^{\infty} dt e^{i(\omega+i\eta)t} \left( -i\theta(t) \left\langle \left\{ [\mathcal{V}, a_i(t)], a_j^\dagger \right\} \right\rangle \right) ,
\]

where the integration by parts was used on the left hand side. This formula is known as
the equation of motion. For shorthand notation \( z = \omega + i\eta \) was introduced and whenever it appears the limit of \( \eta \to 0^+ \) is assumed. Finally equation of motion can be written as

\[
(z + E_i) \mathcal{G}_{i,j}^R(z) = 1 - \int_{-\infty}^{\infty} dt e^{i(\omega+i\eta)t} \left( -i\theta(t) \left\langle \left\{ [\mathcal{V}, a_i(t)], a_j^\dagger \right\} \right\rangle \right) .
\]

From this formula one can see that it is in fact a beginning of hierarchy of equations for
higher Green’s functions. By plugging the full expression for \( \mathcal{V} \) into the term with integral
a higher order Green’s function is generated.
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