Screening and Friedel oscillations in inhomogeneous systems with correlated fermions

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“I firmly believe that love [of a subject or hobby] is a better teacher than a sense of duty- at least for me.” Albert Einstein

This thesis is dedicated to my beloved parents who always keep the fire of ambition burning in me.
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<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
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<tbody>
<tr>
<td>( r )</td>
<td>Relative distance from the impurity</td>
</tr>
<tr>
<td>( n(r) )</td>
<td>Local electronic occupation for continuous system</td>
</tr>
<tr>
<td>( A )</td>
<td>Amplitude of Friedel oscillations</td>
</tr>
<tr>
<td>( k_F )</td>
<td>Fermi momentum</td>
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<tr>
<td>( \delta )</td>
<td>Scattering phase-shift</td>
</tr>
<tr>
<td>( d )</td>
<td>Dimension of the lattice</td>
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<tr>
<td>( H )</td>
<td>Hamiltonian</td>
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<tr>
<td>( p_i )</td>
<td>Momentum of the ( i^{th} ) electron</td>
</tr>
<tr>
<td>( m )</td>
<td>Mass of the electron</td>
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<tr>
<td>( U(r_i) )</td>
<td>Effective one-body potential</td>
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<tr>
<td>( V(r_i - r_j) )</td>
<td>Two-body interaction</td>
</tr>
<tr>
<td>( e )</td>
<td>Electronic charge</td>
</tr>
<tr>
<td>( \hat{\psi}<em>\sigma(r), \hat{\psi}^{\dagger}</em>\sigma(r) )</td>
<td>Annihilation (creation) field operator</td>
</tr>
<tr>
<td>( \delta_{\sigma\sigma'} )</td>
<td>Kronecker delta</td>
</tr>
<tr>
<td>( \delta(r - r') )</td>
<td>Dirac delta function</td>
</tr>
<tr>
<td>( W_i(r) )</td>
<td>Wannier function</td>
</tr>
<tr>
<td>( a_{i\sigma}, (a_{i\sigma}^\dagger) )</td>
<td>Fermionic annihilation (creation) operator</td>
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<tr>
<td>( t_{ij} )</td>
<td>Hopping amplitude</td>
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<tr>
<td>( U )</td>
<td>Hubbard interaction</td>
</tr>
<tr>
<td>( V_i )</td>
<td>External inhomogeneous potential</td>
</tr>
<tr>
<td>( n_{i\downarrow}, n_{i\uparrow} )</td>
<td>Particle number operator for spin down and spin up electrons</td>
</tr>
<tr>
<td>( \varepsilon_0 )</td>
<td>Ground state energy</td>
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<tr>
<td>( Z )</td>
<td>Partition function</td>
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<td>( \beta )</td>
<td>Inverse temperature</td>
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<tr>
<td>( \mu )</td>
<td>Chemical potential</td>
</tr>
<tr>
<td>( N_L )</td>
<td>Number of lattice sites</td>
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<tr>
<td>( \varepsilon_k )</td>
<td>Dispersion relation</td>
</tr>
<tr>
<td>( \tau )</td>
<td>Imaginary time</td>
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<tr>
<td>( G_{ij\sigma}(\tau) )</td>
<td>Matsubara Green’s function in tau-space</td>
</tr>
<tr>
<td>( T_\tau )</td>
<td>Chronological operator</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
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<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>$a_{i\sigma}(\tau)$</td>
<td>Time-dependent fermionic operator</td>
</tr>
<tr>
<td>$i\omega_n$</td>
<td>Matsubara frequency</td>
</tr>
<tr>
<td>$C_{AB}^R$</td>
<td>Retarded Green’s function</td>
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<td>$\omega$</td>
<td>Real frequency</td>
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<tr>
<td>$A_{i\sigma}(\omega)$</td>
<td>Spectral function at $i^{th}$ lattice site</td>
</tr>
<tr>
<td>$n_i$</td>
<td>Local electronic occupation at $i^{th}$ lattice site</td>
</tr>
<tr>
<td>$F_{ij}(\tau)$</td>
<td>Two particle Green’s function</td>
</tr>
<tr>
<td>$\Sigma$</td>
<td>Self-energy of the system</td>
</tr>
<tr>
<td>$\Sigma^{model}$</td>
<td>Phenomenological model self-energy</td>
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<tr>
<td>$\Sigma^{Hubb}$</td>
<td>Self-energy from Hubbard I approximation</td>
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<tr>
<td>$\Sigma^{NRG}$</td>
<td>Self-energy from Numerical Renormalization Group</td>
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<tr>
<td>$g, c, b$</td>
<td>Parameters of model self-energy</td>
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<tr>
<td>$G$</td>
<td>Green’s function matrix</td>
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<td>$t$</td>
<td>Hopping matrix</td>
</tr>
<tr>
<td>$\Sigma$</td>
<td>Self-energy matrix</td>
</tr>
<tr>
<td>$V$</td>
<td>External impurity potential matrix</td>
</tr>
<tr>
<td>$\mathbb{1}$</td>
<td>Unit matrix</td>
</tr>
<tr>
<td>$S_{loc}^l$</td>
<td>DMFT local action for $l^{th}$ site</td>
</tr>
<tr>
<td>$\tilde{G}_\sigma$</td>
<td>Weiss mean-field operator</td>
</tr>
<tr>
<td>$\Delta_{i\sigma}(i\omega_n)$</td>
<td>Hybridization function</td>
</tr>
<tr>
<td>$\Omega[G]$</td>
<td>Free energy functional</td>
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<tr>
<td>$\Phi[G]$</td>
<td>Luttinger-ward functional</td>
</tr>
<tr>
<td>$\langle O\rangle_{local}$</td>
<td>Average of the operator</td>
</tr>
<tr>
<td>$Z$</td>
<td>Screening charge</td>
</tr>
<tr>
<td>$Z_{sc}$</td>
<td>Neighbourhood screening charge (N-screening charge)</td>
</tr>
<tr>
<td>$Z_F$</td>
<td>Fermi renormalization factor</td>
</tr>
<tr>
<td>$z$</td>
<td>Coordination number</td>
</tr>
<tr>
<td>$V_0$</td>
<td>Single impurity potential</td>
</tr>
<tr>
<td>$D_{FSR}$</td>
<td>Relative percentage error between scattering phase-shift and N-screening charge</td>
</tr>
<tr>
<td>$V_1, V_2$</td>
<td>First and second impurity</td>
</tr>
<tr>
<td>$Z_{par}$</td>
<td>Partial screening charge in between the two impurities</td>
</tr>
<tr>
<td>$h$</td>
<td>Magnitude of the step polarization</td>
</tr>
<tr>
<td>$m$</td>
<td>Polarization parameter</td>
</tr>
<tr>
<td>$L$</td>
<td>Difference between the average occupation of spin up and spin down electrons</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>--------------------------------------------------</td>
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<tr>
<td>$\xi$</td>
<td>Characteristic length over which a smooth potential varies</td>
</tr>
<tr>
<td>$\eta$</td>
<td>Broadening parameter</td>
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<tr>
<td>$W$</td>
<td>Band-width</td>
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<tr>
<td>$a_0$</td>
<td>Scattering length</td>
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<tr>
<td>$f^+$</td>
<td>Scattering amplitude</td>
</tr>
<tr>
<td>$\tau_v$</td>
<td>Volume of the unit cell</td>
</tr>
<tr>
<td>$</td>
<td>n\mathbf{k}\rangle$</td>
</tr>
</tbody>
</table>
## Abbreviations

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>FO</td>
<td>Friedel Oscillations</td>
</tr>
<tr>
<td>R-DMFT</td>
<td>Real space Dynamical Mean-Field Theory</td>
</tr>
<tr>
<td>CT-QMC</td>
<td>Continuous Time Quantum Monte Carlo</td>
</tr>
<tr>
<td>NRG</td>
<td>Numerical Renormalization Group</td>
</tr>
<tr>
<td>1D</td>
<td>One-dimensional</td>
</tr>
<tr>
<td>2D</td>
<td>Two-dimensional</td>
</tr>
<tr>
<td>3D</td>
<td>Three-dimensional</td>
</tr>
<tr>
<td>FSR</td>
<td>Friedel Sum Rule</td>
</tr>
<tr>
<td>N- screening charge</td>
<td>Neighbourhood screening charge</td>
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</table>
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Banhi Chatterjee
Abstract

The thesis presents theoretical and numerical studies on electronic screening and Friedel Oscillations (FO) in correlated fermionic systems in the presence of external inhomogeneity. These spatial oscillations in the electronic densities appear in the neighbourhood of the impurity due to quantum scattering from the impurity. They are observed in metals at low temperatures. The interacting system has been modeled by the Hubbard Hamiltonian which has been further solved numerically using the Real space Dynamical Mean-Field Theory (R-DMFT). We study one-, two-, and three-dimensional finite lattice systems with periodic boundary conditions. The inhomogeneous potential has been modeled by a single impurity, two impurities and an extended inhomogeneity. Different approximations accounting for the electronic correlations have also been discussed in the course of the thesis. The effects of electronic correlations, particularly at the Mott metal to insulator transition, on the behaviour of FO have been explored. According to our numerical studies, the oscillations are damped with the interactions, disappear at the Mott transition and completely beyond it. At finite temperature the oscillations are damped and slowly disappear as we increase the temperature of the system. At half-filling the period and phase of the oscillations remain unaltered by the interactions. The Friedel sum rule for the interacting system has been investigated. The variation of the screening charge around the neighbourhood of the impurity called "Neighbourhood screening charge" or "N-screening charge" with interaction, temperature is studied for different impurity potentials. It is further seen that the interactions weaken the screening effects. The spectral functions in the presence of an external inhomogeneity and electronic interactions have been studied at different lattice sites. In the presence of the interaction a sign of resonance appears in the spectral function at the impurity site. In the presence of two impurities interaction weakens the interference effects on the oscillations. Finally the one-body scattering formalism is modified to describe analytically the effects of correlations in many body systems modeled by a momentum independent self-energy with semi circular density of states. Effects of electronic correlations in the scattering phase-shift and spectral functions are obtained in our calculations. The thesis provides predictive numerical results which can motivate future experiments.
Chapter 1

Introduction

Screening of electrons in the presence of a charged impurity in a metallic host is a well-known phenomenon in solid state physics. Electrons are fermions as they obey the Fermi-Dirac statistics. If we place a charged ion in a metal at very low temperatures, i.e. around 0-5 K there is a modulation in the electronic density in the neighbourhood of the impurity as a result of electronic scattering. This gives rise to a spatial oscillation of charge density known as the Friedel oscillations (FO) named after the French physicist J. Friedel who first predicted it in 1952 [1]. Later in 1982 these oscillations were experimentally observed by H. Rohrer and G. Binnig in quantum corals using Scanning Tunneling Microscopy [2, 3]. FO is a purely quantum mechanical phenomenon and the finite wavelength of the electron is attributed as the cause of FO. As we raise the temperature of the system the oscillations slowly disappear. The current state of art exhibits both theoretical and experimental studies of FO for the non-interacting and weakly interacting systems.

The goal of this thesis is to theoretically study the behaviour of the oscillations in systems where the electronic interactions are strong and play a significant role. Such systems are known as strongly correlated systems and consist of a special class of compounds with partially filled d or f orbitals. Among several novel phenomena these class of compounds frequently exhibit the Mott metal to insulator phase transition. This work aims to theoretically address the question if the interaction between electrons affects the amplitude, the period, and the phase of FO, and how. The behaviour of FO in the Fermi liquid phase, Mott insulating phase and at the Mott metal to insulator transition have been investigated for one, two and three dimensional (1D, 2D, 3D) finite lattice systems in the presence of different impurity potentials, e.g. single impurity, two impurities, extended inhomogeneity, etc. The effect of dimensionality of the system on the oscillations has been observed. An estimate of the maximum temperature has been made beyond which the oscillations lose their significance. The interplay of finite temperature and the electronic correlations have been studied. The characteristics of the spectral functions at different lattice sites including the impurity site have also been studied. The influence of interaction, strength of the impurity potential, and temperature on the overall screening effect of the system has been explored.

The interacting lattice system is modeled by the Hubbard Hamiltonian which is also the most popular theoretical model to describe strongly correlated electron systems. The Hubbard model has been solved using the Real Space Dynamical Mean-Field Theory (R-DMFT) which is the best known method to solve it particularly in the regime of the Mott transition. We have primarily studied the problem using numerical simulations but some semi-analytical studies to explain our numerical results have also been conducted.

The thesis presents numerical results on the significant effects of electronic interactions on FO. It can serve as a motivation for similar experimental studies on real strongly correlated electronic systems, e.g. heavy fermionic compounds in the future.

The chapters in the thesis are organized in the following way:
CHAPTER 1. INTRODUCTION

- The first chapter introduces the reader to the problem, explains the motivation behind solving the problem, and highlights the significant conclusions from our work.

- The second chapter provides a historical background of the phenomenon of the FO. The origin of FO starting from the scattering theory in continuous system is explained. A brief literature review on both theoretical and experimental works on FO are presented. The significance of the problem addressed in the thesis is justified in context of the previous works.

- The third chapter introduces strongly correlated systems, briefly discusses on the classification of such compounds and highlights the unique properties exhibited by them.

- The fourth chapter introduces the inhomogeneous Hubbard model, which is the most popular theoretical model to represent a many-body electron system on lattices. Solution of the inhomogeneous Hubbard model in different limits is presented.

- The fifth chapter presents technical details of the many-body formalism. Detailed derivations of the equations of the Real-space Dynamical Mean-Field Theory approximation and the different methods to solve them are presented.

- In the sixth chapter numerical results from the simulation works in studying FO in presence of a single impurity potential is presented. The specific model details and the different methods used to account for the electronic interactions is discussed.

- The seventh chapter presents the numerical results of FO in presence of two impurities, multiple impurities.

- The eighth chapter presents the numerical results of FO in the presence of extended inhomogeneity.

- The ninth chapter presents some analytical studies of spectral functions using the Bethe Density Of States.

- The tenth chapter presents a conclusive summary of all the results.

- The eleventh chapter presents the future outlook and significance of the results obtained in this thesis for the future.
Chapter 2

Friedel Oscillations

The intent of this chapter is to present a historical background on how Friedel oscillations entered the field of condensed matter physics. An attempt has been made to highlight the important works concerning Friedel oscillations both in theory and experiment. The reader is introduced to the general behaviour of these oscillations. Finally, we present the relevance of these oscillations in today's physics and justify the motivation of the problem studied in this thesis.

2.1 A brief historical background

Friedel oscillations were theoretically predicted by the French physicist J. Friedel nearly 40 years ago, in 1952 [1]. In 1940, Friedel as a student, performed some experimental work in understanding the influence of defects on the metallurgical properties of disordered aluminium alloys [4]. Later on he switched to theoretical studies of the electronic distribution in metals such as copper, silver, and gold in the neighbourhood of substitutional impurities of different valencies like Ni, Zn, Ga, Sn, As, etc. being motivated by his first work. He studied the case of non-interacting systems under the Hartree-Fock approximation. He further calculated the bound-state energy, phase-shift in monovalent metals. He used the obtained results to study the absorption and emission of X-rays by monovalent metals. Emile Daniel illustrates on how Friedel oscillations historically became an essential component of the metallic alloys in the article “How the Friedel oscillations entered the physics of metallic alloys” [5]. The article describes how the phenomenon of Friedel oscillations together with the concept of the Friedel sum rule relating the screening effect and scattering phase-shifts could explain the peculiar experimental behaviour of the Knight shift in the Nuclear Magnetic Resonance spectra of AgCd alloys during 1957-58. Much later, in 1981 Rohrer and Binnig observed FO experimentally for the first time in quantum corals using Scanning Tunnel Microscopy (STM) [2, 3]. The reader is referred to Friedel's work on screening in metal alloys and the consequent oscillations for further historical references [6].

2.2 FO in continuous non-interacting systems from the scattering theory

If an atom or an ion (defect) is inserted into a metal then the electrons in the conducting band get distorted by the change in the local potential. Electrons near the Fermi-surface are scattered from the impurity potential. The sharp Fermi edge, even for $T > 0$ as long as $T/T_F \ll 1$, where $T_F$ is the Fermi temperature yields a spatial oscillation of the electronic charge density in the neighbourhood of the defect. These oscillations are called Friedel oscillations as shown in Fig. 2.1.

Mathematically, the electronic density modulation around a spherically symmetric impurity
in the asymptotic limit for non-interacting continuous systems can be formally derived from
the formal scattering theory for free electrons using the partial wave analysis and are obtained
as
\[ n(r) = n(0) + An \frac{\cos(2k_F r + \delta)}{r^d}, \]
where \( n(0) \) is the non-oscillatory term which gives the average background density, \( A \) is the
amplitude of oscillation, \( \delta \) is the scattering phase shift, \( k_F \) is the Fermi vector, \( d \) is the
dimension of space, and \( r \) measures the relative distance from the impurity. We would discuss
FO in a non-interacting finite lattice system in Chp. 5 after introducing the requisite formal
concepts. We now summarize the following basic characteristics of Friedel oscillation from the
present state of knowledge.

- FO is a quantum mechanical phenomenon. It can be perceived as a quantum analog of
  the classical phenomenon, screening of potential due to a charged impurity [7]. Classi-
  cally no oscillations are observed. Thus, these quantum ripples are the manifestations
  of the finite wavelength of the electrons.

- FO is a low temperature phenomenon and smoothly vanishes beyond a certain tempera-
  ture. At zero temperature there are no thermal fluctuations in the system and the
  oscillations are mostly visible. Thermal fluctuations increase with the temperature and
  FO disappears.

- The study of FO requires a quasi-particle or scattering formalism and it depicts a char-
  acteristic power law decay in the fermionic density near the impurity (perturbation)
  followed by on-going sinusoidal oscillations.


2.3 Experimental survey on FO

The density modulation can be observed in real materials by probing the surface of real materials using Scanning Tunneling Microscopy (STM). STM is a popular technique used for surface imaging at the atomic level. The working principle of STM is based on the concept of quantum tunneling. When a conducting tip is brought very near to the surface to be examined, a bias (voltage difference) applied between the two can allow electrons to tunnel through the vacuum between them. The resulting tunneling current is a function of tip position, applied voltage, and the local density of states (LDOS) of the sample.

FO has been observed at the surface of Cu(111) in quantum corrals in the presence of Fe ad atom in the famous experiment of M. Cromie et al. around 4 K, (see Fig. 2.2) [8].

Several experimental studies have been conducted on FO since the late nineties. In 1990 D. Eigler and E. Schweizer observed FO in quantum corrals in Cu(111) surface [9]. Y. Hasegawa et al. [10] observed FO at 5K on Si(111)Ag surface due to screening of Coulomb potential by a two dimensional electronic system. Friedel oscillations of the two-dimensional electron gas in the semi-conductor surface accumulation layer produced certain wave features around the point defects in the local density of states of epitaxially grown InAs surface on GaAs(111)A substrate. These were experimentally observed using low-temperature STM at 5.3 K [11].

2.4 Theoretical studies

The present literature provides us with the basic knowledge on the phenomenon of FO. Here we present a brief literature review on FO.

Studies till now have been mostly conducted in continuous systems where the electronic interactions have been either neglected or accounted for by some approximations [12, 13, 14, 15, 16]. The problem of FO in an one-dimensional non-interacting gas in presence of a static impurity has been analysed by G. Giuliani et al. [17]. E. Andrade et al. showed that the Friedel oscillations are suppressed in strongly renormalized Fermi liquids with stadt-DMFT implemented using a slave-boson impurity solver as shown in Fig. 2.3 [18].

G. Beduerflig et al. studied FO for the density and magnetization in a one-dimensional open Hubbard chain using density-matrix renormalization-group technique [19]. W. Ziegler studied the interplay of correlations and disorder using an unrestricted slave-boson technique in a real space in the presence of a nonmagnetic impurity [20].

K. Matveev et al. analytically studied the problem of scattering on an impurity in a weakly...
interacting 1D electron gas using renormalization group approach [21]. They showed that the scattering on the impurity is renormalized by the electron-electron interaction due to the formation of FO near the barrier. Thus, we see in the present literature that FO has been studied mostly in the presence of a single impurity. Recently M. Bouhassoune et al. observed spin-dependent FO in thin films of Fe in the presence of an oxygen impurity using density functional theory as shown in Fig. 2.4 [22]. D. Torre et al. analyzed the signatures of FO in cuprates superconductors to access the fermionic excitations in strongly correlated materials [23] using Lindhard theory. D. Torre further shows how FO can serve as a probe to understand different properties (e.g. effective mass, band structure) of quasi-particles in interacting electronic systems. Mross and Senthil have studied the phenomenon of charge Friedel oscillations in spin liquids at the Mott transition using linear response theory [24]. FO has been seen to produce an asymmetry in the quantum transport at the interface of mono-layer and bi-layer graphene which can be used as an application in a novel quantum switching [25]. Charge induced Friedel oscillations in spin densities have been shown in hole-doped semi-conductor using a Luttinger model [26].

Thus, we see that these oscillations are not only interesting from a historical point of view but also play a significant role in modern condensed matter physics as illustrated in a series of articles [27, 28, 12, 14, 29, 30]. A. Gerorges et al. illustrates how the virtual bound state and the concept of Friedel sum rule as formulated by Friedel revives in explaining the suppression of the Coulomb blockade in quantum dots in the presence of Kondo impurities [31]. Moreover, the current literature does not have sufficient quantitative analysis on the characteristics of these oscillations, screening effects due to the impurities in correlated systems around the Mott transition which is introduced in the next chapter. Hence, the choice of our problem in this thesis is novel and interesting.
CHAPTER 2. FRIEDEL OSCILLATIONS

Figure 2.4: Charge density oscillations induced around an oxygen impurity implanted in a Fe film surface using STM techniques. (a) Shows the basic experimental set-up of STM, (b) Shows the measured charge density of states using the STM tip, (c) presents the theoretically calculated charge density oscillations using DFT for the majority spin channel (d) shows the comparative studies of charge density using STM measurements for the majority spin channel (e) and (f) shows the theoretical and experimental results of the charge densities respectively around the minority spin channels [22].
Chapter 3

Strongly correlated systems

The goal of this chapter is to present about the special class of compounds called “Strongly Correlated Electronic Systems” (SCES). Starting from explaining the term electronic correlations, we discuss about the different types of SCES and mention the novel phenomena exhibited by them. Among the rest we focus our discussion on the Mott transition from a qualitative perspective since it is a significant topic in context of this thesis. The literature presenting description of the SCES together with its emergent phenomenon is exhaustive. Covering even a small portion of it is beyond any realizable scope of this chapter. A simple, comprehensive review discussing the studies of such systems both theoretically and experimental is presented in the review article of Vollhardt and Kotliar [32], which has been referred to for a larger content of this chapter.

3.1 Historical background of Mott transition

The band theory of solids despite its success in explaining a wide class of materials faced experimental challenges around the mid-nineties. Around 1940, a discovery revealed that NiO, MnO, and other similar magnetic oxides with an odd number of electrons per unit cell behave as electrical insulators. However, the band theory predicted them to be metals instead. In 1937 R. Pierls made a remark on the paper of Boer and Verway explaining the insulating nature of NiO. According to R. Pierls the repulsive energy of the two Ni^{++} d-electrons in NiO is larger than the kinetic energy which might be gained if the d-electrons formed a band. This prefers the d-shell occupancy at each site to remain Ni^{++} and is responsible for the insulating behaviour of the material. R. Pierls remark was formally established in two papers of N. F. Mott in 1949 and 1956. Since then these insulators came to be known as the Mott insulators. A first order Mott metal to insulator transition was initially observed in V_{2}O_{3} due to its unique structure. We stop with our historical discussion at this point and direct the reader to the article of P. W. Anderson which describes the journey of 50 years of Mott phenomena [33].

3.2 Strongly correlated systems

The phenomenon of the Mott transition from metal to insulator is exhibited by a special class of compounds known as SCES. First we try to introduce the quantitative concept of electronic correlations to illustrate about the nomenclature of these compounds.

Quantitative concept of electronic correlations

The term “correlations” originate from the Latin “con + relatio” which means “with relation”. The general concept of “correlations” is not only confined in physics but has a versatile scope of application. Even in English grammar there are certain words or expressions which should follow the other, e.g. either-or; neither-nor, etc, and thus the word pair are said to depend on each other or are correlated. In natural and mathematical sciences the idea of correlation
CHAPTER 3. STRONGLY CORRELATED SYSTEMS

refers to the “statistical dependence” between multiple quantities. Mathematically, it means that the average or expectation values of a product of random quantities is not equal to the product of averages of the individual quantities:

\[ \langle AB \rangle \neq \langle A \rangle \langle B \rangle. \]  

(3.1)

Also, in case of electronic density-density correlation function the above definition holds, i.e.

\[ \langle n(r)n(r') \rangle \neq \langle n(r) \rangle \langle n(r') \rangle. \]  

(3.2)

In a wide class of elements and compounds these correlation effects can be neglected and yet all their physical behaviour is understood. This is not the case for the compounds which belong to SCES. In case of transitional metals the electrons occupy narrow d or f-orbitals. Thus, the spatial confinement enhances the effect of the Coulomb interactions between the electrons and hence the “electronic correlations” become highly significant. This effect is known as “strong correlation” in many-body physics and the corresponding materials are called SCES. In SCES compounds the electrons are neither fully itinerant nor completely localized on their atomic site. Effective Hamiltonian approaches are used to calculate different quantities and effective phase diagrams of SCES. The celebrated Hubbard model is the most popular theoretical model based on such approach and is presented in Chp. 4. Mott transition is also discussed in light of the Hubbard model in Chp. 4. The effects of electronic correlations lead to profound quantitative and qualitative changes in the physical properties of the system compared to the non-interacting particles. Apart from Mott transition these materials show interesting properties like high-temperature superconductivity, colossal magneto-resistance, magnetic ordering, orbital ordering, Kondo effect, etc.

SCES compounds can be classified into different categories:

- **Transitional metal oxides and perovskites**
  These materials have partially-filled d-electron shells and include 3d metals like Nickel, Vanadium (V), and their oxides (e.g. V2O3) or 4f-rare earth metals such as Cerium (Ce), Plutonium (Pu). Plutonium and Cerium suffer itinerant magnetism and a large change in the crystal volume at the Mott transition [32]. Examples of perovskite structure include titanate systems like La1-xSrxCaTiO3, Y1-xCaxTiO3 etc.

- **Heavy fermionic compounds**
  These inter metallic compounds at low temperatures have an effective electron mass thousand times greater than the free electronic mass and hence are named so. The heavy fermionic behaviour was originally discovered in CeAL3 by K. Andres, J. E. Graebner and H. R. Ott [34]. Heavy fermions contain rare-earth ions and have partially filled f-orbitals. They can be useful for understanding the interaction between magnetic and electronic quantum fluctuations. Certain properties of heavy fermionic materials change qualitatively with the temperature, especially below the characteristic Kondo temperature [35]. Hence, they are also known as “Kondo lattices”. Popular examples of heavy fermionic compounds include CeCu6, CeCoIn5, Y3Rh2Si2 to mention a few. A discussion on heavy fermionic systems is presented in [36, 37].

- **High-\( T_c \) super-conductors and super-conducting organics**
  These types of materials include cuprates, layered organic super-conductors, pnictides etc which cannot be explained by the BCS theory of superconductivity. The normal phase of these superconductors are not simple Fermi liquids. These unconventional superconductors exhibit novel superconducting properties and can have different origins: a) superconductors arising from a doped Mott insulator, b) superconductors arising from doping an itinerant anti-ferromagnet. A detailed description of high \( T_c \) superconductors is presented in [38, 39].
3.2.1 Experimental realization of the Mott transition in fermionic optical lattices

Fermionic atoms trapped in a harmonic potential in an optical lattice provides an experimental implementation of the theoretical fermionic Hubbard model used to describe the Mott transition in SCES as shown in Fig. 3.1 [40]. A periodic potential for the atoms is realized in an optical lattice via three mutually standing laser waves. Tunneling rate of atoms between the neighboring lattice sites determine their kinetics while the interactions are attributed to the interatomic collisions when two atoms are on the same site. Collision interactions can be further tuned through Feshbach resonances without having any atomic losses. Formation of a Mott insulator in a repulsively interacting two-component Fermi gas in an optical lattice has been experimentally realized and reported by R. Jordens et al. [40]. In their experiment, a quantum degenerate gas of fermionic $^{40}$K atom prepared in a balanced mixture of two magnetic sub-levels was subjected to the potential of a three dimensional optical lattice of simple cubic symmetry. Other signatures of the Mott metal insulator transition in optical lattice are found in [41, 42, 43, 44].
Chapter 4

The Hubbard model with inhomogeneous potentials

The electrons in a solid are described by an interacting many-body fermionic system. Since our motivation is to study effects of electronic correlations on Friedel oscillations, the many-body system cannot be reduced to a one-particle problem using “the single electron approximation”. Moreover, with the rich development in the field of correlated electron physics in the last decades it is a well-established fact now that the local interactions between the different electrons give rise to a host of new interesting phenomena in many materials. In this chapter the reader is introduced to the elementary concepts of solving the many-body problem in the presence of electronic interactions.

4.1 From general many-body Hamiltonian to inhomogeneous Hubbard Hamiltonian

The Hamiltonian of a N body system in the first-quantized notation is given by

\[ H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \sum_{i=1}^{N} U(r_i) + \frac{1}{2} \sum_{i \neq j} V(r_i - r_j), \]  

(4.1)

where \( m \) is the mass and \( r_i \) is the position vector of the \( i^{th} \) electron, \( N \) is the total number of particles, \( \mathbf{p}_i = -i\hbar \nabla \) is the momentum operator of the \( i^{th} \) particle. In the above Hamiltonian the first term accounts for the kinetic energy of the electrons. The second term \( U(r_i) \) corresponds to an effective one-body potential which includes the interactions of the electrons with the ions of the lattice, impurities or defects present in the lattice, and influence of any external surrounding potential, e.g. gravity. We can divide the one-body potential term into,

\[ U(r_i) = U_{\text{per}}(r_i) + U_{\text{ext}}(r_i), \]  

(4.2)

where \( U_{\text{per}}(r_i + \mathbf{R}) = U_{\text{per}}(r_i) \) is the translationally invariant, periodic, inherent part of the potential and \( \mathbf{R} \) is the translation vector of the lattice. \( U_{\text{ext}}(r_i) \) corresponds to the external inhomogeneity which also breaks the ideal lattice symmetry.

The third term \( V(r_i - r_j) \) corresponds to the two body interaction between the electrons via the Coulomb potential given by \( e^2/4\pi\varepsilon_0|\mathbf{r}_i - \mathbf{r}_j| \) in SI units where \( e \) is the electronic charge and \( \varepsilon_0 \) is the free space permittivity. The constraint on the sum in the third term ensures that we sum over pairs of particles. The factor 1/2 is included to avoid counting the same interaction twice.

In general a many-body interacting Hamiltonian given by Eq. 4.1 is impossible to solve exactly for any dimensions, and situations which are interesting in the context of the real materials. As a first step of simplification one constructs effective model Hamiltonians, e.g. Ising model
CHAPTER 4. THE HUBBARD MODEL WITH INHOMOGENEOUS POTENTIALS

or a Hubbard model which can still significantly capture the physics of real system within some well-justified approximations. The simplest microscopic model describing interacting itinerant electrons in a solid is the one-band, spin-1/2 fermionic Hubbard model where the interaction between the electrons is assumed to be so strongly screened that it is purely local. This model was introduced independently by J. Hubbard, M. C. Gutzwiller and J. Kanamori in 1963 [45, 46, 47]. We present in the following how the inhomogeneous Hubbard Hamiltonian can be constructed from the general many-body hamiltonian presented in Eq. 4.1.

Many-body Hamiltonian in second quantized notation

Since we are dealing with fermionic systems the many-body wave-function always needs to be anti-symmetrized upon exchange of orbitals. In order to avoid any problem due to anti-symmetry we switch from the first quantization to the second quantization representation, which is also the standard method for many-body physics. In this representation the many-body wave-function is replaced by a field-operator and the Hamiltonian takes the form

$$H = \sum_{\sigma} \int \frac{d^3r}{2m} \left( \frac{\hat{p}_r^2}{2m} + U_{\text{per}}(r) + U_{\text{ext}}(r) \right) \hat{\psi}(r)$$

$$+ \frac{1}{2} \sum_{\sigma \sigma'} \int \frac{d^3r}{d^3r'} \hat{\psi}_\sigma^\dagger(r) \hat{\psi}_{\sigma'}(r') V(r-r') \hat{\psi}_\sigma(r) \hat{\psi}_{\sigma'}(r').$$

(4.3)

Here \(\hat{\psi}_\sigma(r)(\hat{\psi}_\sigma^\dagger(r))\) are annihilation (creation) field operators obeying anti-commutation relation given by,

$$\{\hat{\psi}_\sigma(r)\hat{\psi}_\sigma^\dagger(r')\} = \delta_{\sigma \sigma'} \delta(r - r'),$$

(4.4)

where \(\{a, b\} = ab + ba\), \(\delta_{\sigma \sigma'}\) is a Kronecker delta, whereas \(\delta(r - r')\) is a Dirac delta function.

Wannier Function Representation

Let us now introduce the concept of Wannier Functions (WF). WF are localized wave-functions represented by \(W_i(r) = W(r - R_i)\). The lattice site index is \(i = 1, \ldots, N_L\), where \(N_L\) is the total number of lattice sites [48]. \(R_i\) is any vector pointing to the \(i^{th}\) lattice site. The basic properties of WF are as follows:

1. Bloch functions may be expanded in terms of WF.

2. WF about different lattice points are ortho-normal, i. e.

$$\int d^3r W_i^\dagger(r) W_j(r) = \delta_{ij}.$$  

(4.5)

3. WF tend to be peaked and centered around the individual lattice sites i.

4. WF form a complete one-particle base

$$\sum_{i=1}^{N_L} W_i^\dagger(r) W_i(r') = \delta(r - r').$$  

(4.6)

The field operators can be expanded in the Wannier function basis using the creation and annihilation operators as:

$$\hat{\psi}(r) = \sum_i W_i(r) a_i^\sigma,$$  

(4.7)

$$\hat{\psi}^\dagger(r) = \sum_i W_i^\dagger(r) a_i^\dagger \sigma,$$  

(4.8)
where \( a_{i\sigma} \) is the fermionic annihilation (creation) operators of the electrons with spin \( \sigma = \pm 1/2 \) at the \( i^{th} \) lattice site.

In case of fermions the creation and annihilation operators anti-commute following the relations:

\[
\{a_{i\sigma}, a_{i'\sigma'}^\dagger\} = \delta_{\sigma\sigma'}\delta_{i'i'}, \quad (4.9) \\
\{a_{i\sigma}, a_{i'\sigma'}\} = 0, \quad (4.10) \\
\{a_{i\sigma}^\dagger, a_{i'\sigma'}^\dagger\} = 0. \quad (4.11)
\]

The Pauli exclusion principle due to which the maximum occupation at a particular lattice site with a given spin is one, follows as a direct consequence of the anti-commutation relations. Using Eq. 4.3, 4.7, 4.8 we obtain the many-body Hamiltonian as:

\[
H = \sum_{ijkl} \int d^3r W^*_i(r) \left[ \frac{p_i^2}{2m} + U_{\text{per}}(r) + U_{\text{ext}}(r) \right] W_j(r)a_{i\sigma}^\dagger a_{j\sigma} \\
+ \sum_{\sigma\sigma'} \sum_{ijkl} \int d^3r \int d^3r' W^*_i(r)W^*_j(r')V(r-r')W_k(r')W_l(r)a_{i\sigma}^\dagger a_{j\sigma'}^\dagger a_{l\sigma} a_{k\sigma'}. \quad (4.12)
\]

The non-interacting part of the Hamiltonian corresponds to

\[
\langle i|H_0|j \rangle = \int d^3r W^*_i(r) \left[ \frac{p_i^2}{2m} + U_{\text{per}}(r) + U_{\text{ext}}(r) \right] W_j(r) \quad (4.13)
\]

We define

\[
t_{ij} = \int d^3r W^*_i(r) \left( \frac{p_i^2}{2m} + U_{\text{const}}(r) \right) W_j(r). \quad (4.14)
\]

\( t_{ij} \) which accounts for the kinetic energy and the periodic part of the one-body potential. When \( i = j \) the electron stays on-site with ground state energy \( e_0 \), while for \( i \neq j \) the electron hops from the \( i^{th} \) site to the \( j^{th} \) site. Thus \( t_{ij} \) is also called the hopping term. It is translationally invariant, i.e. \( t_{ij} = t(|R_i - R_j|) \).

Next we define

\[
V_{ij} = \int d^3r W^*_i(r) (U_{\text{ext}}(r)) W_j(r). \quad (4.15)
\]

It accounts for the external non-periodic part of the potential which is not translationally invariant, i.e. \( V_{ij}(R_i, R_j) \). We use various models to account for the external potential, e.g. \( U_{\text{ext}}(r) = V_0 \delta(r - R_i) \) corresponds to a single impurity potential. In this model we get

\[
V_{ij} = W^*_i(R_i) V_0 W_j(R_i), \\
\approx V_0 |W_{i\text{imp}}(R_{i\text{imp}})|^2 \cdot \delta_{i\text{imp},i} \delta_{ij}, \quad (4.16)
\]

where \( i_{\text{imp}} \) is the site containing the impurity. Other models of the external impurity potential include two impurities, step potential which has been discussed in this thesis.

The term accounting for the two-body interaction is defined as

\[
U_{ijkl} = \int d^3r \int d^3r' W^*_i(r)W^*_j(r')V(r-r')(W_k(r')W_l(r)). \quad (4.17)
\]

Using the above definitions in Eq. 4.12 the many-body Hamiltonian is written as

\[
H = \sum_{ij,\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + \sum_{ij,\sigma} V_{ij} a_{i\sigma}^\dagger a_{j\sigma} + \sum_i \sum_{jkl} U_{ijkl} a_{i\sigma}^\dagger a_{j\sigma}^\dagger a_{l\sigma} a_{k\sigma'}. \quad (4.18)
\]
At this point we assume that the largest contribution from the interaction comes if all the
Wannier functions are on the same lattice site i.e. $i = j = k = l$.

Using this assumption Eq. 4.18 reduces to the inhomogeneous Hubbard Hamiltonian given by

$$H = \sum_{ij,\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + \sum_{i,\sigma} V_i a_{i\sigma}^\dagger a_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow},$$

where $n_{i\sigma} = a_{i\sigma}^\dagger a_{i\sigma}$ is the particle number operator with eigen values 0 and 1. We once more
remind the reader about the different terms of the Hubbard Hamiltonian. The first term in
the Hamiltonian describes the annihilation of the electron with spin $\sigma$ at the $j^{th}$ site and its
creation on the $i^{th}$ site where $t_{ij}$ gives the probability amplitude of an electron to hop from
lattice site $i$ to $j$. These hopping amplitudes also determine the average kinetic energy and
the total band-width ($W$) of the electron. In case of a uniform hopping for nearest neighbours
$t_{ij} \equiv t$, where $t$ is a parameter.

The second term corresponds to the additional external inhomogeneity which breaks the ideal
lattice symmetry and makes the system inhomogeneous. For homogeneous systems we have
$V_i = \varepsilon_0$, where $\varepsilon_0$ accounts for the ground state atomic energy which is usually set to zero.

The first and second term are the one-particle terms in the Hamiltonian. The third term
is a two-body term due to which two electrons with opposite spins on the same lattice site
interact via the Coulomb force and increase the system energy by $U > 0$. This model uses
the simplification that only a local part of the Coulomb interaction is included and other
longer-range terms are neglected. We also assumed that there is a single 1S orbital on each
lattice site.

**Mott transition in the Hubbard model**

Here we describe how the phenomenon of Mott transition presented in Chp. 3 can be described
from the point of view of the Hubbard model. There is a competition between the hopping
and interaction terms in Hamiltonian Eq. 4.19 since they do not commute which gives rise to
the phenomenon of Mott transition. Particularly, in case of a half-filled lattice where there is
already one electron per lattice site, an electron can only move to another site which is already
occupied at the cost of interaction energy $U$. Thus, unlike a nearly empty lattice in the half-
filled case the energy cost to add an electron to a pre-occupied site jumps by $U$ which is also
referred as the “Mott gap”. The kinetic energy term prompts the electron to hop from one
lattice to the other while the interaction term does not favour double occupation. In case of
low $U$, i.e. $U/t \ll 1$, it is more favorable for the electrons to hop to the next neighboring side.
Thus, the itinerant wave nature of electrons dominate and the system is metallic. However,
with the increase in $U$ it is more favorable for the electrons to stay on-site. Thus, the particle
nature of electrons pre-dominate, electrons locally freeze and the system goes to an insulator.
The Mott transition can be interpreted as a correlation-induced localization-delocalization
phase-transition.

**4.2 Inhomogeneous Hubbard model in different limits**

Though the simplification from Eq. 4.3 to Eq. 4.19 may give us an optimistic vision that the
solution of the simple Hubbard model henceforth would be trivial, yet it is not at all the case.
In this section we would like to discuss the inhomogeneous Hubbard Hamiltonian in different
limits to obtain a first insight. We discuss about the thermodynamic properties of the system
(e. g. partition function, free energy) in each case.

**Derivation of the partition function for the free fermions**

We consider the system to be in a thermodynamic equilibrium at some temperature $T$ (zero
or finite) such that it can be statistically represented by the grand-canonical ensemble. In
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this case the system can exchange both particles and energy with the reservoir. The partition function of the system is defined as

\[ Z = \text{Tr}e^{-\beta(H - \mu N)}, \quad (4.20) \]

where \( \beta = 1/k_B T \) is the inverse of the absolute temperature \( T \) of the system with \( k_B \) as the Boltzmann constant, \( \mu \) is the chemical potential which determines the average number of particles in the system and \( N \) is the number operator which counts the total number of particles in the system. \( T \) gives the trace over all the states.

The partition function can be explicitly written in the occupation number Hilbert space, using the eigen state basis as

\[
Z = \sum_{n_{k_1} n_{k_2} \ldots n_{k_\infty}} \langle n_{k_1} n_{k_2} \ldots n_{k_\infty} | e^{-\beta(\sum_{k_\sigma} \epsilon_{k_\sigma} \hat{n}_{k_\sigma} - \mu \sum_{k_\sigma} \hat{n}_{k_\sigma})} | n_{k_1} n_{k_2} \ldots n_{k_\infty} \rangle
\]

\[
= \sum_{n_{k_1}} \langle n_{k_1} | e^{-\beta(\epsilon_{k_1} \hat{n}_{k_1} - \mu \hat{n}_{k_1})} | n_{k_1} \rangle \sum_{n_{k_\infty}} \langle n_{k_\infty} | e^{-\beta(\epsilon_{k_\infty} \hat{n}_{k_\infty} - \mu \hat{n}_{k_\infty})} | n_{k_\infty} \rangle
\]

\[
= \prod_{k=1}^{\infty} \sum_{n_k=0}^{\infty} e^{-\beta(\epsilon_k - \mu)n_k},
\]

where \( n_{k,\sigma} \) are the number of particles in state \( k \) with spin \( \sigma \) [49]. The occupation number basis states are the direct product of the number operator for each mode, i.e. \( \{ n_{k_1} n_{k_2} \ldots n_{k_\infty} \} = \{|n_{k_1}\rangle |n_{k_2}\rangle \ldots |n_{k_\infty}\rangle \} \). Since these states are also the eigen states of the Hamiltonian and number operator we replaced the operators by their respective eigen values; \( \hat{H}|n_k\rangle = \epsilon_k |n_k\rangle, \hat{n}_{k,\sigma}|n_k\rangle = n_{k,\sigma} |n_k\rangle \). Due to the above properties we can equivalently simplify the exponential in the partition function as a product of traces, each referring to the \( k^{th} \) mode. We know that in case of fermions the occupation number \( (n_k) \) can be either 0 or 1. Thus, performing the summation we obtain the final expression of partition function as,

\[
Z = \prod_{k=1}^{\infty} [1 + e^{-\beta(\epsilon_k - \mu)}],
\]

(4.22)

Note that the partition function is always positive since the eigen values are real numbers and the exponential of real numbers is always positive.

Once we know the partition function the free energy of the system is obtained as,

\[
F = -\frac{1}{\beta} \ln(Z) = -k_B T \sum_{k,\sigma} \ln[1 + e^{-\beta(\epsilon_k - \mu)}].
\]

(4.23)

Now we would use Eq. 4.22 and Eq. 4.23 to calculate the partition function and free energy for different cases of the Hubbard model in the following subsections.

4.2.1 Homogeneous case

This corresponds to the homogeneous Hamiltonian in the absence of any external impurity given by

\[
H = \sum_{i,j,\sigma} t_{ij} \ a_{i\sigma}^{\dagger} a_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}.
\]

(4.24)

In case of a homogeneous system all the lattice sites are equivalent.

Non-interacting limit of homogeneous case

The homogeneous Hamiltonian can be further simplified by neglecting the Coulomb interaction between the electrons, i.e. \( U = 0 \), which is an extreme non-interacting limit of the Hubbard
model as

$$H = \sum_{ij,\sigma} t_{ij} \hat{a}_{i\sigma}^\dagger \hat{a}_{j\sigma}. \quad (4.25)$$

Since the system is homogeneous and translationally invariant it is more convenient to obtain the solution in the momentum space (k-space). The Fourier transform of the operators in position space on a discreet lattice is given by

$$\hat{a}_{i\sigma} = \frac{1}{\sqrt{N_L}} \sum_{k,\sigma} e^{i\mathbf{k} \cdot \mathbf{R}_i} \hat{a}_{k\sigma}, \quad (4.26)$$

$$\hat{a}_{i\sigma}^\dagger = \frac{1}{\sqrt{N_L}} \sum_{k,\sigma} e^{-i\mathbf{k} \cdot \mathbf{R}_i} \hat{a}_{k\sigma}^\dagger, \quad (4.27)$$

where $\mathbf{k}$ is the reciprocal lattice vector which has discretized values, (e.g. $2\pi n/N_L$) in case of 1D. Since Fourier transform is an unitarity transformation the anti-commutation relation of Eq. 4.9 is preserved and given by

$$\{\hat{a}_{k\sigma}, \hat{a}_{k'\sigma}'\} = \delta_{kk'} \delta_{\sigma\sigma'}. \quad (4.28)$$

The Hamiltonian in terms of new creation and annihilation operators in the momentum space is given by

$$H_{\text{nonint}}^k = \sum_{k,\sigma} \epsilon_k \hat{a}_{k\sigma}^\dagger \hat{a}_{k\sigma}, \quad (4.29)$$

where $\epsilon_k$ is the dispersion relation given by

$$\epsilon_k = \sum_{ij} t_{ij} e^{i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)}, \quad (4.30)$$

where the restricted summation only runs over the nearest neighbours. Thus, in case of tight binding approximation with nearest neighbour hopping the dispersion relation then simplifies to

$$\epsilon_k = -2t \sum_{\gamma=1}^d \cos(\mathbf{k}_\gamma a) \quad (4.31)$$

where $\gamma$ corresponds to the index of dimension of the system and $t$ is uniform hopping amplitude.

The dispersion relation depends on the structure of the lattice and hopping amplitudes. Thus, in this case the non-interacting Hamiltonian is quadratic in the fermionic creation and annihilation operators. It is a trivial problem to solve it by exact diagonalization of $H_{\text{nonint}}^k$ and calculate the exact eigen values $\epsilon_k$. The partition function and free energy can be calculated using Eq. 4.22 and Eq. 4.23.

**Atomic limit for the homogeneous case**

This is another extreme limit where we neglect hopping setting, $t = 0$ and thus have a collection of independent equivalent sites. It is enough to consider just a single-site in this case and this one site model can be easily solved.

This particular site has four possibilities of occupations corresponding to the site being a) empty ($|0\rangle$), b) singly occupied by a spin up/spin down electron ($|\uparrow\rangle$, $|\downarrow\rangle$), or c) doubly occupied by both spin up and spin down electrons ($|\uparrow\downarrow\rangle$). The corresponding eigen values of these eigen states are given by 0, $(\epsilon_0 - \mu)$, $(\epsilon_0 - \mu)$, $(2\epsilon_0 - \mu + U)$ respectively.

The partition function can be calculated from Eq. 4.22 as,

$$Z = [1 + 2e^{-\beta(\epsilon_0 - \mu)} + e^{-\beta(2\epsilon_0 - \mu + U)}] \quad (4.32)$$

Note that here again we use the fact that the occupation number basis states are the direct product of the number operator for each mode.
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Figure 4.1: The occupation of electronic states at the $i^{th}$ site with time corresponding to the Hubbard model. The “In” and “Out” represents the hopping of the electrons from one site to the other [50].

The free energy of the system can be calculated using Eq. 4.23 as,

$$F = -k_B T \sum_i \ln(1 + 2e^{-\beta(\varepsilon_0 - \mu)} + e^{-\beta(2\varepsilon_0 - \mu + U)}).$$

(4.33)

4.2.2 Inhomogeneous case

In this case the external impurity potential $V_i$ is non-zero, the system is inhomogeneous and the different lattice sites are non-equivalent. Also the non-interacting part of the Hamiltonian is not diagonal in the momentum space. Thus it is not useful to take a Fourier transform in the momentum space like in the homogeneous case. Hence we treat the problem in the real space.

**Atomic limit for inhomogeneous case**

The solution for the inhomogeneous case follows the same treatment as the homogeneous case with $\varepsilon_0 = V_i$. Thus, the partition function and free-energy can be calculated using Eq. 4.22, Eq. 4.23 as

$$Z = \prod_i \left[ 1 + 2e^{-\beta(V_i - \mu)} + e^{-\beta(2V_i - \mu + U)} \right],$$

(4.34)

$$F = -k_B T \sum_i \ln(1 + 2e^{-\beta(V_i - \mu)} + e^{-\beta(2V_i - \mu + U)}).$$

(4.35)

4.2.3 Inhomogeneous case with finite hopping and interaction

We presented the solution of the Hubbard model in the limits of $t = 0$ and $U = 0$. However, when both the kinetic energy and the interaction terms are finite, the occupation of a single site fluctuates in time. At a given time each lattice site still has four possibilities of occupation as illustrated in Fig. 4.1. The time evolution depends on the ratio $U/t$ and on the average number of electrons per site. It is not possible to solve the Hubbard model exactly in this case except for the one-dimensional systems using the Bethe Ansatz [51]. In higher dimensional systems e. g. $d = 2, 3$ which are important in the context of real-materials we have no other choice than to revert to numerical techniques to solve the Hubbard model. Still, it is not enough to employ a huge computational power to directly solve it. We need to choose approximate methods which still can capture the interesting physical information contained in the Hubbard model. The Real Space Dynamical Mean-Field Theory (R-DMFT) is the best approximate...
method known till date to solve the inhomogeneous Hubbard model as it keeps this local dynamics exactly at each lattice site, which is a key point for describing Mott insulators and Mott-Hubbard Metal to Insulator Transition (MIT). R-DMFT is introduced and discussed in details in the next chapter. Various studies with the Hubbard model with different physical systems can be found in [52, 53, 54, 55, 56, 57, 58] to mention a few.
Chapter 5

Many-body Formalism and Real-space Dynamical Mean-Field Theory approximation

The intent of this chapter is to introduce the Green’s function technique used for solving the many-body problem [59, 60, 61, 62]. We further present the Real Space Dynamical Mean-field Theory (R-DMFT) formalism in context of the inhomogeneous Hubbard model. Finally the many-body scattering formalism and generalised Friedel Sum Rule is presented using R-DMFT and T-matrix approach.

5.1 One-particle Green’s function

Matsubara formalism

The one particle Green’s function in Matsubara notation is given by

\begin{equation}
G_{ij\sigma}(\tau) = -\langle T_\tau a_{i\sigma}(\tau)a^\dagger_{j\sigma}(0) \rangle \\
= -\theta(\tau)a_{i\sigma}(\tau)a^\dagger_{j\sigma}(0) + \theta(-\tau)(a^\dagger_{i\sigma}(0)a_{j\sigma}(\tau)),
\end{equation}

(5.1)

where \(T_\tau\) is the chronological operator which orders the time with the earliest times furthest to the right according to the following prescription:

\begin{equation}
T_\tau a_{i\sigma}(\tau)a^\dagger_{j\sigma}(0) =
\begin{cases}
  a_{i\sigma}(\tau)a^\dagger_{j\sigma}(0) & \text{if } \tau > 0, \\
  -a^\dagger_{j\sigma}(0)a_{i\sigma}(\tau) & \text{if } \tau < 0.
\end{cases}
\end{equation}

(5.2)

\begin{equation}
\theta(\tau) =
\begin{cases}
  1 & \text{if } \tau > 0, \\
  0 & \text{if } \tau < 0.
\end{cases}
\end{equation}

(5.3)

Note that in case of fermions a minus sign appears on interchanging the order of operators. \(a_{i\sigma}(\tau)\) is the time-dependent fermionic operator in the Heisenberg picture given by

\begin{equation}
a_{i\sigma}(\tau) = e^{-\tau H}a_{i\sigma}e^{\tau H},
\end{equation}

(5.4)

where \(\tau\) is the imaginary time which runs from \((0, \beta)\).

\(\langle...\rangle\) represents both thermal and quantum averages in the grand-canonical ensemble [60].

The Matsubara Green’s functions in case of fermions obey the anti-periodicity relation given by

\begin{equation}
G_{ij\sigma}(\tau + \beta) = -G_{ij\sigma}(\tau).
\end{equation}

(5.5)

Owing to the periodicity they can be expanded in standard Fourier series in the interval
\( \tau \epsilon (-\beta, \beta) \). The Fourier transform from Matsubara frequency space to the time space is given by

\[
G_{ij\sigma}(\tau) = \frac{1}{\beta} \sum_{\omega_n} e^{i\omega_n \tau} G_{ij\sigma}(i\omega_n).
\]

(5.6)

The inverse Fourier transform is given by

\[
G_{ij\sigma}(i\omega_n) = \frac{1}{\beta} \int_{0}^{\beta} e^{-i\omega_n \tau} G_{ij\sigma}(ij\tau),
\]

(5.7)

where \( \omega_n = (2n + 1)\pi/\beta \) are the fermionic Matsubara frequencies. \( n \) is any integer and thus the fermionic Matsubara frequencies are real, odd, temperature dependent, discrete in finite temperature and become continuous in the limit of zero temperature \((\beta \to 0)\). They are symmetric, i.e. there is equal number of positive and negative Matsubara frequencies. The indices \( i = j \) correspond to the local diagonal Green’s functions \( G_{ii\sigma}(i\omega_n) \), while for \( i \neq j \) the Green’s functions are off-diagonal.

5.1.1 Relation to the retarded Green’s function

Physical observables can be related to the retarded Green’s function which gives the present state of the system defined by

\[
G_{ij\sigma}^{R} = -i\theta(t - t')\langle [a_{i\sigma}(t), a_{j\sigma}^{\dagger}(t')] \rangle.
\]

(5.8)

Physically, they can be interpreted as propagators since they give the amplitude of a particle inserted at the time \( t' \) for propagating to the time \( t \). It is called retarded since \( t > t' \). At this point we also mention that though the name is single-particle Green’s function these are actually many-body objects which describe the propagation of single particles governed by the full many-body Hamiltonian including all correlation effects \([60]\).

The imaginary time formalism is a mathematical method to compute the retarded Green’s function and has no physical meaning. It uses a mapping to a more general Green’s function where the time and frequencies are imaginary quantities. The retarded Green’s function is obtained from the corresponding Matsubara Green’s function \( G_{ij\sigma}(i\omega_n) \) as an analytical continuation in the real space by a substitution \( i\omega_n \to (\omega + i0^+) \). A formal derivation establishing the connection between the retarded Green’s function and Matsubara Green’s function using the Lehmann representation can be found in \([59]\). Once we know the one-particle Green’s functions all local single particle properties of the system can be calculated, few of which are presented below.

Spectral function

The local spectral function can be obtained from the local retarded Green’s function in real space as

\[
A_{i\sigma}(\omega) = \frac{1}{\pi} \text{Im} \ G_{i\sigma\sigma}(\omega + i0^+).
\]

(5.9)

The spectral function is given by

\[
A_{\sigma}(\omega) = \frac{1}{N_L} \sum_{i=1}^{N_L} A_{i\sigma}(\omega).
\]

(5.10)

The spectral function obeys a sum rule

\[
\int_{-\infty}^{\infty} A_{\sigma}(\omega) = 1
\]

(5.11)
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In the non-interacting limit the spectral function is equivalent to the Local Density of States (LDOS) and gives the probability that an electron with the energy $\omega$ will occupy the $i^{th}$ site given by

$$A_{i\sigma}(\omega) = \sum_k \delta(\omega - \epsilon_k).$$

(5.12)

The corresponding total density of states (DOS) is given by

$$A_\sigma(\omega) = \frac{1}{N_L} \sum_{i=1}^{N_L} \sum_k \delta(\omega - \epsilon_k).$$

(5.13)

Local occupation

The local electronic occupation can be obtained from the Green’s function as

$$n_i = \sum_\sigma \langle a_i^\dagger \sigma a_i \sigma \rangle = -\lim_{\tau \to 0^-} G_{ii\sigma}(\tau) = -\lim_{\tau \to 0^-} \sum_{i\omega_n} e^{i\omega_n \tau} G_{ii\sigma}(i\omega_n).$$

(5.14)

We now present an alternative expression for electronic occupation in terms of the spectral function and Fermi-Dirac distribution function [63]. Let us define a Matsubara sum

$$S_1(\nu, \tau) = \frac{1}{\beta} \sum_{i\omega_n} G_{ij}(i, i\omega_n) e^{i\omega_n \tau}.$$

(5.15)

This sum can be evaluated, re-writing it as a contour integral over a complex variable $z$ using residue theory. It turns out that the integrand function $n_F(z)$ which has poles at $z = i\omega_n$ is a Fermi-Dirac distribution function in case of fermions given by

$$f(\omega) = \frac{1}{1 + e^{\beta \omega}}.$$

(5.16)

The contour runs parallel to the real axis shifted by an infinitesimally small positive quantity $\eta$ away on either side. Thus, we get

$$S^F = -\int \frac{dz}{2\pi i} n_F(z) g(z) e^{zt}.$$

(5.17)

Following the analytical continuation in real axis using Eq. 5.15 we get

$$S_1(\nu, \tau) = -\frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega n_F(\omega) [G_{ii\sigma}(\omega + i\eta) - G_{ii\sigma}(\omega - i\eta)]$$

$$= -\frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega n_F(\omega) 2i \text{Im } G_{ii\sigma}(\omega)$$

$$= \int_{-\infty}^{\infty} d\omega n_F(\omega) A_{i\sigma}(\omega).$$

(5.18)
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Now we show how can this sum be related to the local occupation in the following as

\[
\langle a_i^\dagger \sigma a_i \sigma \rangle = - \lim_{\tau \to 0^-} G_{ij\sigma}(\tau) = \frac{1}{\beta} \sum_{\omega_n} G_{ij}(i, i\omega_n) e^{i\omega_n \delta} = S_1(\nu, 0^+) = \int d\omega n_F(\omega) A_{i\sigma}(\omega).
\]

Equation of motion for the inhomogeneous Hubbard model

Now we would derive the equation of motion for the inhomogeneous Hubbard Hamiltonian in Eq. 4.19. As a first step we need to evaluate the commutator \([H, a_{i\sigma}(\tau)]\) in Eq. 5.22.

\[
[H, a_{i\sigma}(\tau)] = \sum_{k, j, \sigma} t_{kj} [a_k^\dagger \sigma a_j \sigma, a_{i\sigma}(\tau)] + \sum_{k, \sigma} V_k [a_k^\dagger \sigma a_k \sigma, a_{i\sigma}] + U \sum_{k} [n_k n_k^\dagger, a_{i\sigma}] (5.23)
\]

Finally we have

\[
n_{i\sigma} = \int_{-\infty}^{+\infty} A_{i\sigma}(\omega) f(\omega) d\omega.
\]

The physical interpretation of Eq. 6.12 is that the occupation of the site \(|i\rangle\) is an energy integral of the spectral density of single particle states projected onto the site \(|i\rangle\) and weighted by the occupation at the given energy. The total occupation is given by

\[
N = \sum_{\sigma} \sum_{i=1}^{N_L} n_{i\sigma}.
\]
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The first two terms have the same commutator which can be evaluated using the fermionic anti-commutation relation as follows:
\[
[a_{i\sigma}^+ a_{j\sigma}, a_{i\sigma}] = a_{i\sigma}^+ a_{j\sigma} a_{i\sigma} - (\delta_{ik} - a_{k\sigma}^+ a_{i\sigma}) a_{j\sigma} \\
= a_{i\sigma}^+ a_{j\sigma} a_{i\sigma} - a_{k\sigma}^+ a_{i\sigma} a_{j\sigma} - \delta_{ik} a_{j\sigma} \\
= -\delta_{ik} a_{j\sigma}.
\] (5.24)

The third commutator can be re-written using the anti-commutation relations as
\[
U \left[ \sum_i n_{i\uparrow} n_{i'\sigma'}, a_{i'\sigma'}^+ \right] = U \sum_i (n_{i\uparrow} [n_{i\uparrow}, a_{i'\sigma'}^+] + [n_{i\uparrow}, a_{i'\sigma'}^+] n_{i\downarrow}).
\] (5.25)

Now, in general
\[
[n_{i\sigma}, a_{i'\sigma'}^+] = a_{i'\sigma'}^+ a_{i\sigma} a_{i'\sigma'} - a_{i'\sigma'}^+ a_{i'\sigma'} a_{i\sigma} \\
= a_{i'\sigma'}^+ a_{i\sigma} a_{i'\sigma'} - [\delta_{ii'} \delta_{\sigma'\sigma} - a_{i'\sigma'}^+ a_{i'\sigma'}] a_{i\sigma} \\
= -\delta_{ii'} \delta_{\sigma'\sigma} a_{i\sigma}.
\] (5.26)

Substituting Eq. 5.26 in Eq. 5.25 for the respective spins we get
\[
U \left[ \sum_i n_{i\uparrow} n_{i'\uparrow}, a_{i'\sigma'}^+ \right] = U \sum_i (n_{i\uparrow} (-\delta_{ii'} \delta_{\sigma'\sigma} a_{i\downarrow}) + (-\delta_{ii'} \delta_{\sigma'\sigma} a_{i\uparrow}) n_{i\downarrow}) \\
= -U (n_{i\uparrow} a_{i\downarrow} \delta_{\sigma'\uparrow} + n_{i\downarrow} a_{i\uparrow} \delta_{\sigma'\downarrow}).
\] (5.27)

Following the Pauli exclusion principle the contribution from the above terms is non-zero only when \( n_{i} \) and \( a_{i} \) have opposite spin indices, e. g., \( \sigma' = \uparrow \), then the commutator is 
\[-U (n_{i\uparrow} a_{i\downarrow} \delta_{\sigma'\uparrow} + n_{i\downarrow} a_{i\uparrow} \delta_{\sigma'\downarrow}).
\]
Thus, we can write the generalized expression for the third commutator as
\[
U \left[ \sum_i n_{i\uparrow} n_{i'\uparrow}, a_{i'\sigma'}^+ \right] = -U a_{i\sigma} n_{i\sigma}.
\] (5.28)

Using the values of the commutators from Eq. 5.24, Eq. 5.28 in Eq. 5.23 we finally have
\[
[H, a_{i\sigma}(\tau)] = -\sum_{k,j,\sigma} t_{kj} \delta_{ik} a_{j\sigma} - \sum_{k,\sigma} V_k \delta_{ik} a_{i\sigma} - U a_{i\sigma} n_{i\sigma} \\
= -\sum_{l,\sigma} U a_{i\sigma} - V a_{i\sigma} - U a_{i\sigma} n_{i\sigma}.
\] (5.29)

Finally from Eq. 5.29, and Eq. 5.22 we obtain the equation of motion in the \( \tau \)-space for the inhomogeneous Hubbard model as
\[
-\partial_{\tau} G_{i\sigma}(\tau) = \delta(\tau) \delta_{ij} - \sum_{l} t_{li}(T_{\tau} a_{i\sigma}(\tau) a_{i\sigma}^+(0)) - V_l(T_{\tau} a_{i\sigma}(\tau) a_{i\sigma}^+(0)) - U(T_{\tau} a_{i\sigma}(\tau) n_{i\sigma}(\tau) a_{i\sigma}^+(0)) \\
= \delta(\tau) \delta_{ij} + \sum_{l} t_{li} G_{i\sigma}(\tau) + V_l G_{i\sigma}(\tau) + U F_{ij}(\tau).
\] (5.30)

where,
\[
F_{ij}(\tau) = -\theta(\tau)(a_{i\sigma}(\tau) a_{i\sigma}^+(\tau) a_{i\sigma}(\tau) a_{i\sigma}(\tau)) + \theta(-\tau)(a_{i\sigma}^+(\tau) a_{i\sigma}^+(\tau) a_{i\sigma}(\tau) a_{i\sigma}(\tau))
\] (5.31)
is the two particle Green’s function.
$G_{ii}$ is the single particle Matsubara Green’s function given by Eq. 5.1. The equation of motion can be written in the Matsubara space using Eq. 5.6 as

$$i\omega_n G_{ii\sigma}(i\omega_n) = \delta_{ij} + \sum_l t_{il} G_{li\sigma}(i\omega_n) + V_i G_{ii}(i\omega_n) + UF_{ij}(i\omega_n).$$  \hspace{1cm} (5.32)$$

We can re-write Eq. 5.32 as follows:

$$i\omega_n G_{ii\sigma}(i\omega_n) = \delta_{ij} + \sum_l t_{il} G_{li\sigma}(i\omega_n) + V_i G_{ii}(i\omega_n) + \sum_k \Sigma_{ik\sigma}(i\omega_n) G_{kj\sigma}(i\omega_n).$$  \hspace{1cm} (5.33)$$

Comparing Eq. 5.32 and Eq. 5.33 we define

$$\Sigma_{ik\sigma}(i\omega_n) = \frac{UF_{ik\sigma}(i\omega_n)}{G_{ik\sigma}(i\omega_n)}$$  \hspace{1cm} (5.34)$$

as the self-energy of the system which accounts for all the electronic interactions.

### 5.2.1 Matrix notation

We now introduce the matrix notation for the different quantities:

- $G = (G_{ij})$ denotes the Green’s function matrix,
- $t = (t_{ij})$ denotes the hopping matrix, which is translationally invariant,
- $\Sigma = (\Sigma_{ij})$ denotes the self-energy matrix,
- $V = (V_{ij})$ correspond to the external impurity potential,
- $\mathbb{1}$ is the unit matrix.

Eq. 5.33 can be re-written in the matrix notation as

$$(i\omega_n)\mathbb{1} G_{\sigma}(i\omega_n) = \mathbb{1} + t G_{\sigma}(i\omega_n) + V G_{\sigma}(i\omega_n) + \Sigma(i\omega_n) G_{\sigma}(i\omega_n).$$  \hspace{1cm} (5.35)$$

The Green’s function for the non-interacting ($\Sigma = 0$), inhomogeneous system in the Matsubara frequency space is given by

$$G_{\sigma}^0(i\omega_n) = [(i\omega_n + \mu)\mathbb{1} - t - V]^{-1}.$$  \hspace{1cm} (5.36)$$

The interacting Green’s function in the Matsubara space can be obtained from the Dyson equation as

$$G_{\sigma}(i\omega_n) = [G_{\sigma}^0(i\omega_n) - \Sigma_{\sigma}(i\omega_n)]^{-1}.$$  \hspace{1cm} (5.37)$$

The analytical continuation ($i\omega_n \rightarrow \omega + i\delta^+$) of Eq. 5.37 and Eq. 5.36 gives us the corresponding interacting and non-interacting retarded Green’s function in the real space as

$$G_{\sigma}^0(\omega) = [(\omega + \mu)\mathbb{1} - t - V]^{-1},$$  \hspace{1cm} (5.38)$$
$$G_{\sigma}(\omega) = [G_{\sigma}^0(\omega) - \Sigma_{\sigma}(\omega)]^{-1}.$$  \hspace{1cm} (5.39)$$

### 5.3 Special cases for the Hubbard model

In this section we discuss about the Green’s function and spectral function obtained from the theory of equation of motion for the different cases of the Hubbard model.

#### Non-interacting homogeneous case

In case of homogeneous system the Hamiltonian is translationally invariant and it is convenient to perform a Fourier transform from the position space to the momentum space.

$$G_{ij\sigma}(i\omega_n) = \frac{1}{N L} \sum_k e^{i k \cdot (R_i - R_j)} G_{kj\sigma}(\omega_n),$$  \hspace{1cm} (5.40)$$
where,

$$G_{k\sigma}(\omega_n) = \frac{1}{i\omega_n - \epsilon_k}. \tag{5.41}$$

The spectral function obtained from Eq. 5.41 and Eq. 5.9 is same as the local density of states given by Eq. 5.12.

**Interacting, homogeneous case**

In case of interacting systems the Green’s function additionally has the self-energy term and is given by

$$G_{k\sigma}(\omega) = \frac{1}{\omega - \epsilon_k - \Sigma_k(\omega)}. \tag{5.42}$$

The spectral function is obtained from Eq. 5.9 and also contains the effect of self-energy.

**Atomic limit, inhomogeneous case**

In this case the Green’s function in the real space is given by

$$G_{ij}(\omega) = \left[1 - n_{i\sigma} \frac{\delta}{\omega - V_i} + \frac{n_{i\sigma}}{\omega - V_i - U}\right] \delta_{ij}. \tag{5.43}$$

Eq. 5.43 can also be expressed as,

$$G_{ij}(\omega) = \frac{1}{\omega_n - V_i - \Sigma_{Hubl}(\omega)} \tag{5.44}$$

where

$$\Sigma_{Hubl}(\omega) = U n_{i\sigma} - \frac{U^2 n_{i\sigma}(1 - n_{i\sigma})}{\omega - V_i - U(1 - n_{i\sigma})}. \tag{5.45}$$

\(\Sigma_{Hubl}\) is the self-energy for Hubbard I approximation which is purely real [65]. The spectral function in this case is given by

$$A_{i\sigma}(\omega) = (1 - n_{i\sigma})\delta(\omega - V_i) + n_{i\sigma}\delta(\omega - V_i - U). \tag{5.46}$$

**Atomic limit, homogeneous case**

It follows all the definitions of the inhomogeneous case with \(V_i = \epsilon_0\), where \(\epsilon_0\) is the ground state atomic energy.

### 5.4 Real-space DMFT (R-DMFT)

DMFT introduced by Vollhardt and Metzner is the best known method to solve the fermionic Hubbard model in the intermediate coupling regime where the Mott transition takes place and has been used in several works [50, 66, 67, 32, 68, 69, 70, 71, 72, 73, 74, 75]. It consists of a set of self-consistent equations. The main approximation of DMFT is that the self-energy is local, i.e. diagonal in the lattice site indices

$$\Sigma_{i\sigma}(i\omega_n) = \Sigma_{i\sigma}(i\omega_n)\delta_{ij}, \tag{5.47}$$

where \(\delta_{ij}\) is the Kronecker delta. The self-energy is site dependent for inhomogeneous systems while for homogeneous systems all lattice sites are equivalent having the same self-energy \(\Sigma_{i\sigma} = \Sigma_{\sigma}(\omega)\) in real space, or \(\Sigma_{k\sigma} = \Sigma_{\sigma}(\omega)\) in k-space.
5.4.1 Derivation of DMFT equations using cavity method

The method

There are various approaches to derive the DMFT equations. The basic idea behind all these approaches is that at \( d = \infty \), the Hubbard type of lattice models with a local interaction reduce to a dynamical single site problem. Here we present the derivation of the self-consistent DMFT equations for the inhomogeneous Hubbard model following closely the presentation of A. Georges, G. Kotliar, W. Krauth, and M. Rozenberg using the so-called “cavity method” for a homogeneous system which is also the most popular approach [76, 50, 77]. Generalization of the self-consistent DMFT equations for the inhomogeneous Hubbard model is also discussed in [78, 79, 80]. The general procedure is outlined as follows and also presented schematically in Fig. 5.71.

1. We remove one site together with its bonds from the lattice and denote this site by \( l \).

2. The rest of the lattice containing the cavity (site \( l \)) can be replaced by a particle bath which plays the role of a dynamical mean-field and accounts for the effects of all other sites \( i \neq l \).

3. The bath is then coupled with the cavity via a hybridization function.

4. The resulting problem is equivalent to solving an effective Single Impurity Anderson Model (SIAM) where the degrees of freedom of the bath given by an appropriate hybridization function which needs to be determined self-consistently.

For a homogeneous lattice system all the lattice sites are equivalent and it is enough to perform step 1 to 4 for a “single-site” only and the method is called “single site” DMFT. However, in the presence of external inhomogeneity, the translational invariance is broken and the lattice sites are non-equivalent and we need to perform step 1 to step 4 for every lattice site \( l = 1, 2, \ldots, N_L \). In other words, each lattice site is separately mapped into the single impurity problem and thus \( N_L \) number of impurity problems need to be solved. However, the number of non-equivalent sites and hence the impurity problem can be reduced taking into account the symmetry of the lattice. Thus, R-DMFT used for solving inhomogeneous systems is nothing but a real-space extension of the standard “single-site” DMFT used for solving homogeneous systems. The use of R-DMFT is also found in other works like [78, 79, 80].
Mathematical derivation

The partition function of the grand canonical ensemble in path integral representation is given by

$$Z = \int \prod_{i} Da_{i\sigma}^{*} Da_{i\sigma} \exp[-S_{i}].$$  \hspace{1cm} (5.48)

The action $S_{i}$ for the inhomogeneous Hubbard model which explicitly depends on the lattice index $i$ is given as a path integral of Grassmann variables $a_{i\sigma}^{*}$, $a_{i\sigma}$ as

$$S_{i} = \int_{0}^{\beta} d\tau \left[ \sum_{\sigma} a_{i\sigma}^{*}(\tau) \left( \frac{\partial}{\partial \tau_{i\sigma}} - \mu \right) a_{i\sigma}(\tau) + \sum_{ij\sigma} t_{ij} a_{i\sigma}^{*}(\tau) a_{j\sigma}(\tau) + \sum_{i\sigma} V_{i} a_{i\sigma}^{*}(\tau) a_{i\sigma}(\tau) + U \sum_{i} a_{i\uparrow}^{*}(\tau) a_{i\uparrow}(\tau) a_{i\downarrow}^{*}(\tau) a_{i\downarrow}(\tau) \right].$$  \hspace{1cm} (5.49)

We split the action into three parts,

$$S = S_{l} + \Delta S^{l} + S^{(l)},$$  \hspace{1cm} (5.50)

where $S_{l}$ is the part containing only the local variables on site $l$ which is removed, and given by

$$S_{l} = \int_{0}^{\beta} d\tau \left[ \sum_{\sigma} a_{i\sigma}^{*}(\tau) \left( \frac{\partial}{\partial \tau_{i\sigma}} - \mu \right) a_{i\sigma}(\tau) + \sum_{ij\sigma} t_{ij} a_{i\sigma}^{*}(\tau) a_{j\sigma}(\tau) + V_{i} a_{i\sigma}^{*}(\tau) a_{i\sigma}(\tau) + U \sum_{i} a_{i\uparrow}^{*}(\tau) a_{i\uparrow}(\tau) a_{i\downarrow}^{*}(\tau) a_{i\downarrow}(\tau) \right].$$  \hspace{1cm} (5.51)

$\Delta S^{l}$ accounts for the hopping terms between site $l$ and the remaining sites of the lattice where $i \neq l$ such that

$$\Delta S^{l} = \int_{0}^{\beta} d\tau \sum_{i\sigma} [t_{il} a_{i\sigma}^{*}(\tau) a_{l\sigma}(\tau) + t_{li} a_{i\sigma}^{*}(\tau) a_{i\sigma}(\tau)].$$  \hspace{1cm} (5.52)

The remaining part of the action excluding site $l$ together with its bonds is given by,

$$S^{(l)} = \int_{0}^{\beta} d\tau \left[ \sum_{i \neq l, \sigma} a_{i\sigma}^{*}(\tau) \left( \frac{\partial}{\partial \tau_{i\sigma}} - \mu - V_{i} \right) a_{i\sigma}(\tau) + \sum_{ij \neq l, \sigma} t_{ij} a_{i\sigma}^{*}(\tau) a_{j\sigma}(\tau) \right. \left. + U \sum_{i \neq l} a_{i\uparrow}^{*}(\tau) a_{i\uparrow}(\tau) a_{i\downarrow}^{*}(\tau) a_{i\downarrow}(\tau) \right].$$  \hspace{1cm} (5.53)

We define,

$$\Delta S^{l}(\tau) = \sum_{i\sigma} [t_{il} a_{i\sigma}^{*}(\tau) a_{l\sigma}(\tau) + t_{li} a_{i\sigma}^{*}(\tau) a_{i\sigma}(\tau)],$$  \hspace{1cm} (5.54)

such that the partition function in Eq. 5.48 can be written as,

$$Z = \int \prod_{\sigma} Da_{i\sigma}^{*} a_{i\sigma} \exp[-S_{i}] \int \prod_{i \neq l, \sigma} Da_{i\sigma}^{*} a_{i\sigma} \exp[-S^{l} - \int_{0}^{\beta} d\tau \Delta S(\tau)].$$  \hspace{1cm} (5.55)
Expanding Eq. 5.55 w.r.t. integral over $\Delta S(\tau)$ we obtain,

$$Z = \int \prod_{\sigma} \mathcal{D}a_{l\sigma}^* \mathcal{D}a_{l\sigma} \exp[-S^l]$$

$$\times \left(1 - \int_{0}^{\beta} d\tau \Delta S(\tau) + \frac{1}{2!} \int_{0}^{\beta} d\tau_{1} \int_{0}^{\beta} d\tau_{2} T_{T} \Delta S(\tau_{1}) \Delta S(\tau_{2}) + .... \right). \quad (5.56)$$

We introduce the ensemble average w.r.t. the cavity action $S^l$ as

$$\langle X \rangle_{(l)} = \frac{1}{Z^l} \int \prod_{\sigma \neq l} \mathcal{D}a_{l\sigma} \mathcal{D}a_{l\sigma} \exp[-S^l]. \quad (5.57)$$

where

$$Z^l = \int \prod_{\sigma \neq l} \mathcal{D}a_{l\sigma} \mathcal{D}a_{l\sigma} \exp[-S^l]. \quad (5.58)$$

Using Eq. 5.57, and Eq. 5.58 in Eq. 5.56 the partition function becomes

$$Z = \int \prod_{\sigma} \mathcal{D}a_{l\sigma}^* \mathcal{D}a_{l\sigma} \exp[-S^l] Z^l \left(1 - \int_{0}^{\beta} d\tau \langle \Delta S(\tau) \rangle_{l} \right)$$

$$+ \frac{1}{2!} \int_{0}^{\beta} d\tau_{1} \int_{0}^{\beta} d\tau_{2} T_{T} \Delta S(\tau_{1}) \Delta S(\tau_{2}) \langle \rangle_{l} + .... \right). \quad (5.59)$$

The odd terms in Eq. 5.59 vanish due to the particle number conservation as we are dealing with fermions. The lowest non-trivial term in Eq. 5.59 reads

$$\frac{1}{2!} \int_{0}^{\beta} d\tau_{1} \int_{0}^{\beta} d\tau_{2} \sum_{\sigma} a_{l\sigma}^* (\tau_{1}) \sum_{ij} t_{ij} t_{ij} (T_{T} a_{l\sigma} (\tau_{1}) a_{l\sigma}^*(\tau_{2}) \langle \rangle_{l}). \quad (5.60)$$

Using Eq. 5.1 we can rewrite the lowest order term in Eq. 5.60 in terms of the two-point cavity Green’s function as

$$\frac{1}{2!} \int_{0}^{\beta} d\tau_{1} \int_{0}^{\beta} d\tau_{2} \sum_{\sigma} a_{l\sigma}^* (\tau_{1}) \sum_{ij} t_{ij} t_{ij} (T_{T} a_{l\sigma} (\tau_{1}) a_{l\sigma}^*(\tau_{2}) \langle G_{ij\sigma} (\tau_{2}) \rangle_{l}). \quad (5.61)$$

Other higher-order terms appearing in Eq. 5.59 can be written as a 2n-point unconnected cavity Green’s functions. Till now we just reformulated the partition function without any approximation. In order to map the problem onto an impurity problem we integrate out the bath

$$\frac{1}{Z_{loc}} e^{-S_{loc}^l [a_{l\sigma}^* a_{l\sigma}]} = \frac{1}{Z} \int \prod_{\sigma \neq l} \mathcal{D}a_{l\sigma} a_{l\sigma} e^{-S^l} \quad (5.62)$$

The effective local action $S_{loc}^l$ allows us to access all correlation effects at the lattice site $l$ in an exact manner. Now employing the linked cluster theorem, the effective action can be expressed in terms of cavity Green’s function yielding an infinite series of many-body correlation functions as
\[ S_{loc}^l = S_l + \text{const} + \sum_{n=1}^{\infty} \sum_{i_1,\ldots,i_n} \int d\tau_{i_1} \ldots d\tau_{i_n} t_{i_1 j_1} \ldots t_{i_n j_n} \times a^*(\tau_{i_1}) \ldots a^*(\tau_{i_n}) G_{i_1 \ldots j_n}(\tau_{i_1}, \ldots, \tau_{i_n}, \tau_{j_1}, \ldots, \tau_{j_n}) a(\tau_{j_1}) \ldots a(\tau_{j_n}). \] 

(5.63)

The constant part which gives the overall normalization constant is neglected. The effective local action is still exact at this stage. At \( d \to \infty \) limit we need to rescale the hopping amplitudes as

\[ t_{ij} = \frac{t_{ij}^*}{\sqrt{z|i-j|}}, \] 

(5.64)

where, \( z \) is the co-ordination number of the system. \( |i-j| \) gives the “Manhattan distance” between the sites \( i \) and \( j \) and takes the value 1 for nearest neighbour hopping. As a consequence of this rescaling the problem is remarkably simplified as only \( n = 1 \) in the expansion of Eq. 5.63 survives. The local action on the \( l^{th} \) site is given by,

\[ S_{loc}^l = \beta \int_0^\beta d\tau \sum_\sigma a_{l\sigma}^*(\tau) \left( \frac{\partial}{\partial \tau} - \mu \right) a_{l\sigma}(\tau) + V_l \int_0^\beta d\tau a_{l\uparrow}^*(\tau) a_{l\downarrow}(\tau) + U \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \sum_\sigma \sum_{ij} t_{ij} t_{kl} G_{ij\sigma}(\tau_1 - \tau_2) a_{i\sigma}(\tau_1) a_{k\sigma}(\tau_2). \] 

(5.65)

Next we define the hybridization function in the imaginary time space in terms of the cavity Green’s function (where site \( l \) is removed) and rescaled hopping amplitudes as

\[ \Delta_{l\sigma}(\tau_1 - \tau_2) = - \sum_{ij} t_{ij} G_{ij\sigma}^l(\tau_1 - \tau_2) t_{ji}. \] 

(5.66)

The hybridization function can be defined in the frequency space taking a Fourier transform of Eq. 5.66 as

\[ \Delta_{l\sigma}(i\omega_n) = \sum_{ij} t_{ij} G_{ij\sigma}^l(i\omega_n) t_{ji}. \] 

(5.67)

Then, we define the Weiss’ dynamical mean-filed propagator which accounts for the effects of all lattice sites as

\[ G_{l\sigma}^{-1}(\tau_1 - \tau_2) = - \left( \frac{\partial}{\partial \tau_1} - \mu + V_l \right) \delta_{\tau_1 \tau_2} - \Delta_{l\sigma}(\tau_1 - \tau_2). \] 

(5.68)

It is dynamical as it depends on the imaginary time \( \tau \) and hence this theory is called the Dynamical Mean-Field Theory.

Again the representation in frequency space using Fourier transform is given by

\[ G_{l\sigma}^{-1}(i\omega_n) = (i\omega_n) + \mu - V_l) - \Delta_{l\sigma}(i\omega_n). \] 

(5.69)

Using Eq. 5.66, and Eq. 5.68 in Eq. 5.65 we obtain the final expression for the local action as
\[
S_{loc}^l = -\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \sum_\sigma a_\sigma^*(\tau_1) G_{\sigma}^{-1}(\tau_1 - \tau_2) a_\sigma(\tau_2) + U \int_0^\beta d\tau a_\uparrow^*(\tau) a_\uparrow(\tau) a_\downarrow^*(\tau) a_\downarrow(\tau).
\]

(5.70)

Note from Eq. 5.66, Eq. 5.68 and Eq. 5.70 that the hybridization function, Weiss' mean-field propagator and subsequently the local action has explicitly dependence on the lattice site \(l\) due to the local external potential term \(V_l\).

The relation between the cavity Green's function and the full lattice Green's function is given by

\[
G_{ij\sigma}(i\omega_n) = G_{i\sigma}(i\omega_n) - \frac{G_{i\sigma}(i\omega_n) G_{i\sigma}(i\omega_n)}{G_{i\sigma}(i\omega_n)}.
\]

(5.71)

Plugging in Eq. 5.71 in to Eq. 5.67 we get

\[
\Delta_{i\sigma}(i\omega_n) = \left\{ \mathbb{1} \cdot \mathbb{G}_\sigma(i\omega_n) \cdot \mathbb{1} \right\}_H - \frac{\left\{ \mathbb{1} \cdot \mathbb{G}_\sigma(i\omega_n) \cdot \mathbb{1} \right\}_H \left\{ \mathbb{1} \cdot \mathbb{G}_\sigma(i\omega_n) \cdot \mathbb{1} \right\}_H}{G_{i\sigma}(i\omega_n)}.
\]

(5.72)

The lattice Green's function can be expressed in form of the Dyson equation as,

\[
\mathbb{G}_\sigma(i\omega_n) = \left[ \xi(i\omega_n) - \mathbb{t} - \Sigma_\sigma(i\omega_n) \right]^{-1},
\]

(5.73)

where \(\xi_{ij}(i\omega_n) = (i\omega_n + \mu - V_i)\delta_{ij}\). The self-energy \(\Sigma_\sigma\) is obtained from DMFT approximation and is purely local and diagonal in lattice site indices.

In case of homogeneous systems the lattice Green's function can be obtained by Fourier transform in the momentum space and subsequent Hilbert transform. However, in the presence of inhomogeneity the translational invariance of the system is broken. Hence, the lattice Green's function is obtained via the matrix inversion of Eq. 5.73 in real space due to which this method is named as Real space DMFT. Finally we show the derivation of the local Dyson equation using the above equations with the help of some matrix algebra. Taking an inverse of Eq. 5.73 and re-arranging the terms we obtain,

\[
\mathbb{t} = \xi - \Sigma_\sigma - \mathbb{G}_\sigma^{-1}.
\]

(5.74)

(Note that we drop the argument \((i\omega_n)\) in these intermediate steps for notational simplicity.) Multiplying Eq. 5.74 with \(\mathbb{G}_\sigma\) from right we get,

\[
\mathbb{t} \cdot \mathbb{G}_\sigma = (\xi - \Sigma_\sigma) \cdot \mathbb{G}_\sigma - \mathbb{1}.
\]

(5.75)

Similarly, multiplying Eq. 5.74 with \(\mathbb{1}\) from left we get,

\[
\mathbb{G}_\sigma \cdot \mathbb{t} = \mathbb{G}_\sigma \cdot (\xi - \Sigma_\sigma) - \mathbb{1}.
\]

(5.76)

Again multiplying Eq. 5.74 with \(\mathbb{1} \cdot \mathbb{G}_\sigma\) we get

\[
\mathbb{1} \cdot \mathbb{G}_\sigma \cdot \mathbb{t} = \mathbb{1} \cdot \mathbb{G}_\sigma (\xi - \Sigma_\sigma) - \mathbb{t}.
\]

(5.77)
CHAPTER 5. MANY-BODY FORMALISM AND REAL-SPACE DYNAMICAL MEAN-FIELD THEORY APPROXIMATION

Using the relations Eq. 5.75, Eq. 5.76, Eq. 5.77 and Eq. 5.72

$$\Delta_l = \frac{[\langle \xi - \Sigma_\sigma \rangle \cdot G_\sigma - 1] \langle \xi - \Sigma_\sigma \rangle - 1]{ll} - \frac{[\langle \xi - \Sigma_\sigma \rangle \cdot G_\sigma - 1]{ll} \cdot [G_\sigma \cdot (\xi - \Sigma_\sigma) - 1]{ll}}{\Omega_{l\sigma}}$$

$$= \frac{[\langle \xi - \Sigma_\sigma \rangle \cdot G_\sigma \cdot (\xi - \Sigma_\sigma)_{ll} - (\xi - \Sigma_\sigma)_{ll} - \xi_{ll} - \frac{[\langle \xi - \Sigma_\sigma \rangle \cdot G_\sigma \cdot (\xi - \Sigma_\sigma) - G_\sigma \cdot (\xi - \Sigma_\sigma) + 1]{ll}}{\Omega_{l\sigma}}}{(\xi - \Sigma_\sigma)_{ll} - \frac{1}{\Omega_{l\sigma}}.}$$

(5.78)

Using Eq. 5.78 in Eq. 5.69 we finally obtain the local Dyson equation

$$G_{l\sigma}^{-1}(i\omega_n) = \Sigma_{l\sigma}(i\omega_n) + \frac{1}{\Omega_{l\sigma}(i\omega_n)}.$$  

(5.79)

The above equation also takes into account the self-consistency condition such that the Green’s function of the effective single site must coincide with the Green’s function of the original lattice. Finally, the functional integral determining the local propagator is given by

$$G_{\sigma}(i\omega_n) = -\frac{1}{\mathcal{Z}} \int \prod_{\sigma} Da_{\sigma}^* Da_{\sigma} [a_{l\sigma}(i\omega_n)a_{l\sigma}^*(i\omega_n)] \exp[-S_{\text{loc}}].$$  

(5.80)

together with the Dyson equation, Eq. 5.73, Eq. 5.69, Eq. 5.70, and Eq. 5.79 form a closed set of equations for the local propagator and self-energy. These equations are then solved iteratively.

5.4.2 Equivalence to the Single Impurity Anderson Model (SIAM)

We first show that the effective local action of DMFT is equivalent to SIAM using path integral formalism before presenting the algorithm to solve the self-consistent DMFT. The Hamiltonian for SIAM is given by

$$H_{\text{SIAM}} = \varepsilon \sum_{\sigma} a_{\sigma}^\dagger a_{\sigma} + U \sum_{\sigma} n_{\sigma\uparrow} n_{\sigma\downarrow} + \sum_{k\sigma} \left( \epsilon_k \cd_{\sigma}^\dagger c_{k\sigma} + \text{h.c.} \right) + \sum_{k\sigma} c_{\sigma}^\dagger c_{\sigma},$$  

(5.81)

where the first term represents the local single site with energy $\varepsilon$, the second term corresponds to the local Coulomb interactions. The third term describes the coupling between the impurity and the non-interacting fermionic bath given by the fourth term. h.c. implies hermitian conjugate. The partition function for SIAM in path integral formalism is given by

$$Z_{\text{SIAM}} = \int Da^* \int D[c^\dagger c] \exp[\int_{\sigma} a_{\sigma n}^* (i\omega_n + \mu + \varepsilon_\sigma) a_{\sigma n} - U \int_0^\beta d\tau n_\tau(\tau) \sum_{k\sigma} \cd_{\sigma n}(\cd_{k\sigma})^\dagger c_{k\sigma}] - \sum_{k\sigma} \nu_k a_{\sigma n}^* c_{k\sigma} - \sum_{k\sigma} \nu_k^* c_{k\sigma} a_{\sigma n} + \sum_{k\sigma} (i\omega_n - \epsilon_k) c_{\sigma n}^\dagger c_{\sigma n}. $$  

(5.82)

We perform a change of variables in Eq. 5.82 as, $c_{k\sigma} \rightarrow \cd_{k\sigma} - \eta_{k\sigma}$ and similarly for the hermitian conjugate term. Considering the c-terms only the condition for extremum demands

$$\sum_{k\sigma} (\nu_k) a_{\sigma n}^* c_{k\sigma} - \eta_{k\sigma} (i\omega_n - \epsilon_k) c_{k\sigma} = 0,$$  

(5.83)

which gives

$$\eta_{k\sigma}^* = \frac{-\nu_k}{i\omega_n - \epsilon_k} a_{\sigma n}^*.$$  

(5.84)
Similarly, from the conjugate term we get
\[ \eta_{\kappa \sigma n} = -\frac{v_k^*}{\omega_n - \varepsilon_k} a_{\sigma n}. \] (5.85)

The partition function from Eq. 5.82 can now be rewritten as
\[ Z_{\text{SIAM}} = \int D[a^* a] \exp \left[ \sum_{\sigma n} a_{\sigma n}^*(i\omega_n + \mu + \varepsilon_i) - \sum_k \frac{|v_k|^2}{\omega_n - \varepsilon_k} a_{\sigma n} \right. \\
- \left. U \int_0^\beta d\tau_\uparrow(\tau)n_\uparrow(\tau) \cdot \int D[\tilde{c}^* \tilde{c}] \exp \left[ \sum_{k, \sigma n} \tilde{c}_{\kappa \sigma n}^*(i\omega_n - \varepsilon_k) \tilde{c}_{\kappa \sigma n} \right]. \] (5.86)

Thus, we separate all the local impurity terms and the bath terms and the partition function is a product of two partition functions. The action in Eq. 5.86 is similar to the DMFT local action in Eq. 5.70. In order to establish an equivalence between the two problems the term coupling the bath with the impurity in Eq. 5.86 should be equal to the hybridization function in Eq. 5.70 as
\[ \Delta_{\sigma n} = \sum_k \frac{|v_k|^2}{\omega_n - \varepsilon_k}. \] (5.87)

### 5.4.3 DMFT self-consistency loop

The DMFT self-consistent equations are solved as follows:

- We start with an arbitrary initial self-energy with the properties obeyed as described in [76].
- The local Green’s function is determined using the Dyson equation, Eq. 5.73.
- The hybridization function is obtained using Eq. 5.69 and Eq. 5.79, the local Dyson equation.
- This hybridization function is used to calculate the effective local action using Eq. 5.70 and Eq. 5.69.
- The effective local action or equivalently SIAM is solved and the new local Green’s function is obtained from Eq. 5.80.
- Finally we use the new Green’s function to determine new self-energy using Eq. 5.70 and Eq. 5.69, which is again used as an input for the Dyson equation.

The solution scheme is presented schematically in Fig. 5.2. Depending on the method the equations can be solved either in real or Matsubara frequency space.

### 5.4.4 Methods of solving \( H_{\text{SIAM}} \)

Among the different self-consistent equations in the DMFT loop it is the most difficult to solve the auxiliary problem of SIAM, especially over a wide range of energy scales. Different techniques, so called "impurity solvers" have been developed to solve it over the years. A review discussing the developments of different methods used to solve the general quantum impurity problem including the SIAM is presented in [81]. Here we just mention about a few popular methods and categorize them based on their working principles. These methods are either numerically exact methods or approximate semi-analytical approaches. The numerical methods can be sub-divided into: i) methods based on exact diagonalization introduced by Caffarel and Krauth in 1994 [82], and ii) methods based on stochastic sampling and thermal averages i.e. Quantum Monte Carlo techniques (QMC). Apart from the numerical methods different analytical and phenomenological approaches are also adopted. Methods based on the exact diagonalization include:
Figure 5.2: Schematic representation of the DMFT self-consistency loop. We start with an initial self-energy $\Sigma_{ii}$, calculate the local Green’s function $G_{ii}$; then the hybridization function $\Delta_i$. For each lattice site we solve the effective SIAM to calculate the effective local DMFT action $S_{ii}^{eff}$ from which new set of Green’s functions is calculated. These Green’s functions are again used to generate a new set of self-energy and this is how the self-consistency loop works.

- Exact Diagonalization (ED),
- Numerical Renormalization Group Method (NRG) [83],
- Density Matrix Renormalization Group (DMRG) [84].

QMC based methods include:

- Hirsch Fye QMC algorithm [85]. This method employs the principle of equispaced time discretization.
- Continuous Time Quantum Monte-Carlo (CT-QMC) is the most popular method used by the practitioners these days [81, 86]. As the name suggests it avoids time-discretization and its subsequent problems. Instead, it uses stochastic Metropolis sampling for summing up the diagrams obtained in the Taylor series expansion of the impurity partition function. In case of SIAM we can have a further classification based on the expansion as a) CT-HYB (expansion about the hybridization function), b) CT-INT (expansion about local interaction).

The analytical approaches include,

- Hubbard I approximation [65].
- Hubbard III approximation [65].
- Equation of motions techniques [65, 59].
- Iterative perturbation theory [78, 87].
- Local moment approach [88].
- Phenomenological approaches [89, 90].

In this thesis NRG, CTQMC (CT-HYB) and the phenomenological approaches have been adopted for solving the DMFT equations. We present a short discussion of these methods in Chap. 6, Sec. 6.1.
5.4.5 Exactness and virtues of DMFT

In the absence of electronic interactions the Hubbard model corresponds to a pure metal which can be solved using the conventional band theory of solids. Once the interaction is turned on, for a weak coupling i.e. \( U/t \ll 1 \) the system can be treated using the Fermi liquid theory replacing the free electrons by Landau quasi-particles [91, 92]. In the strong coupling limit, i.e. \( U/t \gg 1 \) we approach the insulating regime which can be solved analytically using, e.g. the Hubbard I approximation. Thus, though several methods are known to exist to solve the Hubbard model in the extreme limits there is a lack of it in the intermediate regime where the Mott transition happens. Hence an approximate mean-field method is needed. A reliable, controlled approximate method should yield an exact solution of the Hubbard model at infinite dimensions with the following properties:

1. The solution should be non-perturbative and should be valid for all arbitrary values of the input parameters (e.g. particle density, interaction strength, temperature, magnetic field etc.),
2. It should obey all the conservation laws in physics,
3. It should be thermodynamically consistent,
4. There should be an existing limit where the theory becomes exact.

DMFT is the only method which meets the above four condition and gives a numerically exact solution of the Hubbard model at infinite dimensions for any arbitrary coupling. In the DMFT approximation, the hopping term is rescaled according to the quantum scale i.e. \( t \rightarrow \frac{t}{\sqrt{z}} \), where \( z \) is the co-ordination number of the system. In a perfect crystalline solid each lattice site has the same number of nearest neighbours and hence the co-ordination number \( z \) directly describes the dimensionality of the system, i.e. \( d = \infty \) implies \( z = \infty \). The large \( z \) limit corresponds to a small dimensionless parameter \( 1/z \) which vanishes when \( z = \infty \). However, the large \( z \) limit is approached already at lower dimensions \( (d = 2, 3) \) for real finite lattice systems since \( z = 4 \) for a two-dimensional cubic lattice, \( z = 6 \) for three dimensional simple cubic, \( z = 8 \) for 3D body-centered cubic, \( z = 12 \) for 3D face-centered cubic where DMFT is a good approximation [68].

Extensions of DMFT

Presently, several extensions of the single-site DMFT have been popularized in order to make its application more generic and versatile. In this thesis we already use such an extension called R-DMFT useful for solving inhomogeneous systems. Among the other extensions, cluster DMFT accounts for the short-range non-local correlations to study the problem of Mott transition in the Hubbard model [93]. “Nano-dmft” can be used for studying the Mott-localization process in generic nano-scale devices such as large molecules, quantum dot arrays, nanostructures implanted with magnetic impurities etc [94]. The bosonic Dynamical Mean-Field Theory has been developed to study interesting problems like superfluid Mott transition of cold bosons in an optical lattice [95, 96]. The extended DMFT takes into account the non-local part of the Coulomb interactions and is used to study phenomena like e.g. charge ordering, Wigner Mott transition etc [97].

5.5 Scattering formalism for R-DMFT

In this section we present the many-body scattering formalism for interacting electronic systems using the R-DMFT formalism. Many-body scattering theory in-case of a non-interacting continuous system is presented in [98]. The Dyson equation in real space in the presence of an external potential is given by

\[
G_\sigma(i\omega_n)^{-1} = [(i\omega_n + \mu)\mathbb{1} - \xi - \mathbb{V}]^{-1} = \Sigma_\sigma(i\omega_n),
\]  

(5.88)
where the matrix $V \in \mathbb{R}$ with real elements denotes the static external impurity potential applied to the lattice.

The Dyson equation for a homogeneous system in absence of any external potential is given by

$$G_{\text{hom } \sigma}(\omega_n) = \left[ (\omega_n + \mu)1 - \xi \right]^{-1} - \Sigma_{0 \sigma}(\omega_n)$$  \tag{5.89}

where $\Sigma_{0 \sigma}(i\omega_n)$ is the diagonal homogeneous part of the self-energy due to the interaction $U$ and it is in accordance to the R-DMFT approximation in Eq. 5.47. Thus, for inhomogeneous systems where $V \neq 0$ the full self-energy in Eq. 5.88 can be split into two parts as follows,

$$\Sigma_{\sigma}(\omega_n) = \Sigma_{0 \sigma}(\omega_n) + \Delta\Sigma_{\sigma}(\omega_n)$$  \tag{5.90}

The first term accounts for the homogeneous part of self-energy due to the electron-electron correlations while the second term accounts for the inhomogeneous part due to the external impurity potential and other effects.

Using Eq. 5.88, Eq. 5.89 and Eq. 5.90, we obtain

$$G_{\sigma}(\omega_n) = \left[ G_{\text{hom } \sigma}(\omega_n) - 1 - V(\omega_n) \right]^{-1}, \tag{5.91}$$

where we define the diagonal dynamical potential $V(\omega) = V - \Delta\Sigma(\omega_n)$.

We can define the Local Density of States (LDOS) for the inhomogeneous and homogeneous using the corresponding retarded Green’s functions using Eq. 5.9 as,

$$A_{\sigma}(\omega) = \frac{1}{\pi} \text{Im} \, G_{\sigma}(\omega)$$ \tag{5.92}

$$A_{\text{hom } \sigma}(\omega) = \frac{1}{\pi} \text{Im} \, G_{\text{hom } \sigma}(\omega) = -\frac{1}{\pi} \text{Im} \left( \frac{1}{\omega + \mu - \xi} - \Sigma_{0 \sigma} \right)$$ \tag{5.93}

### 5.5.1 Friedel Sum Rule

Friedel Sum Rule (FSR) plays a central role in studying the effect of impurities in a metallic host and is a consequence of charge neutrality in the system. The FSR appears due to the modulation in the local occupation given by Eq. 6.12 in presence of an impurity potential $V_i \neq 0$.

In accordance to the principle of charge neutrality the change in the local occupation at the impurity site must be compensated by commensurate changes in the potential of the neighbouring sites of the system. Formally the condition of charge neutrality is stated as, “If a cluster of impurities has a net charge $Z$ compared to the ion in the host lattice, then a screening charge equal to $Z$ electrons will be drawn to the defect to eliminate long-range Coulomb fields” [99]. FSR is given by

$$Z = \delta(\epsilon_f)$$  \tag{5.94}

where $\delta(\epsilon_f)$ is the scattering phase-shift at the Fermi energy, $\epsilon_f = \mu$ and $Z$ is the screening charge defined by

$$Z = \Delta n_{\sigma} = \sum_{i \sigma} \Delta n_{i \sigma}, \tag{5.95}$$

where $\Delta n_{i \sigma} = n_{i \sigma} - n_{i \sigma}^{\text{hom}}, n_{i \sigma}^{\text{hom}}$ is the local occupation for a homogeneous system in the absence of impurity. Physically this quantity gives us a measure how the local occupation of each lattice site deviates from that of a homogeneous system due to the presence of this additional impurity.

The FSR has been derived by G. D. Mahan for a non-interacting square lattice system using the tight-binding model of solid [99]. Langer first showed in 1961 that the FSR is obeyed even for a system of interacting electrons in a periodic potential at zero temperature using techniques devised by J. M. Luttinger and J. C. Ward. [100, 101, 102]. He considered a
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The general form of electron-electron interaction and assumed that the single particle-like state at the Fermi surface does not decay. Later, FSR has been derived and shown to be valid for the Anderson’s model of localized impurity states in metals, interacting multi-orbital quantum dot, when all many-body correlation effects are taken into account [103, 104, 105].

Derivation of generalised FSR using T-matrix

We now derive the FSR considering the electronic interactions in the framework of R-DMFT. The Friedel sum rule for $V_i \neq 0, U \neq 0$ can be hence obtained as follows.

For finite temperature we have

$$\Delta n_{i\sigma} = \int_{-\infty}^{+\infty} \Delta A_{i\sigma}(\omega) f(\omega) \, d\omega. \quad (5.96)$$

where $f(\omega)$ is the Fermi-Dirac distribution function given by Eq. 6.26, and

$$\Delta A_{i\sigma}(\omega) = A_{i\sigma}(\omega) - A_{i\sigma}^{\text{hom}}(\omega). \quad (5.97)$$

For $T = 0$, we have

$$\Delta n_{i\sigma} = \int_{-\mu}^{\mu} \Delta A_{i\sigma}(\omega) \, d\omega. \quad (5.98)$$

We would now calculate $\Delta n_{i\sigma}$ at $T = 0$ starting from Eq. 5.98 to obtain the general FSR in terms of the scattering $T_{\sigma}$-matrix.

We would use the following identity,

$$G_{i\sigma}(\omega) = \left( \frac{\partial}{\partial \omega} \ln \frac{1}{G_{\sigma}^{-1}(\omega)} \right)_{ii} + \left( G_{\sigma} \frac{\partial}{\partial \omega} \Sigma_{\sigma} \right)_{ii}. \quad (5.99)$$

Now using Eq. 5.99, Eq. 5.92, and Eq. 5.93 in Eq. 5.97 we get,

$$\Delta A_{i\sigma}(\omega) = -\frac{1}{\pi} \text{Im} \left[ \frac{\partial}{\partial \omega} \ln \left( \frac{1}{G_{\sigma}^{-1}(\omega)} G_{\text{hom} \sigma}(\omega) \right) + G_{\sigma}(\omega) \frac{\partial}{\partial \omega} \Sigma_{\sigma}(\omega) - G_{\text{hom} \sigma}(\omega) \frac{\partial}{\partial \omega} \Sigma_{0 \sigma}(\omega) \right]_{ii}. \quad (5.100)$$

Again using Eq. 5.91 it is seen that

$$G_{\sigma}^{-1}(\omega) G_{\text{hom} \sigma}(\omega) = \mathbb{1} - \mathcal{V}(\omega) G_{\text{hom} \sigma}(\omega). \quad (5.101)$$

Using Eq. 5.101 in Eq. 5.100, we get

$$\Delta A_{i\sigma}(\omega) = -\frac{1}{\pi} \text{Im} \left[ \frac{\partial}{\partial \omega} \ln \left( \mathbb{1} - \mathcal{V}(\omega) G_{\text{hom} \sigma}(\omega) \right) + G_{\sigma}(\omega) \frac{\partial}{\partial \omega} \Sigma_{\sigma}(\omega) - G_{\text{hom} \sigma}(\omega) \frac{\partial}{\partial \omega} \Sigma_{0 \sigma}(\omega) \right]_{ii}. \quad (5.102)$$

The Dyson equation in Eq. 5.91 can be represented as,

$$G_{\sigma}(\omega) = G_{\text{hom} \sigma}(\omega) + G_{\text{hom} \sigma} \mathcal{V}(\omega) G_{\sigma}(\omega). \quad (5.103)$$

$$G_{\sigma}(\omega) = G_{0 \sigma}(\omega) + G_{0 \sigma} \mathcal{T}(\omega) G_{0 \sigma}(\omega). \quad (5.104)$$

In context of the many-body scattering theory, introducing the $\mathcal{T}(\omega)$ matrix the Green’s function can be expressed as,

$$G_{\sigma}(\omega) = G_{\text{hom} \sigma}(\omega) + G_{\text{hom} \sigma} \mathcal{T}(\omega) G_{\text{hom} \sigma}(\omega). \quad (5.105)$$

Drawing an analogy between Eq. 5.104, and Eq. 5.105 we get,

$$G_{\text{hom} \sigma}(\omega) \mathcal{T}(\omega) G_{\text{hom} \sigma}(\omega) = G_{\text{hom} \sigma}(\omega) \mathcal{V}(\omega) G_{\sigma}(\omega) = G_{\sigma}(\omega) \mathcal{V}(\omega) G_{\text{hom} \sigma}(\omega). \quad (5.106)$$
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Using Eq. 5.106 we can define the scattering $\mathbb{T}$ matrix as

$$\mathbb{T}_\sigma(\omega) = \mathbb{V}(\omega) [1 - \mathbb{G}_{\text{hom } \sigma}(\omega)\mathbb{V}(\omega)]^{-1}. \quad (5.107)$$

It follows from Eq. 5.107,

$$[\mathbb{T}_\sigma(\omega)\mathbb{V}(\omega)^{-1}]^{-1} = [\mathbb{I} - \mathbb{V}(\omega)\mathbb{G}_{\text{hom } \sigma}(\omega)]. \quad (5.108)$$

Substituting Eq. 5.108 in Eq. 5.102 we get,

$$\Delta A_{\sigma}(\omega) = \frac{1}{\pi} \text{Im} \left[ \frac{\partial}{\partial \omega} \ln (\mathbb{T}_\sigma(\omega)\mathbb{V}(\omega)^{-1}) \right]_{ii} - \frac{1}{\pi} \text{Im} \left[ \mathbb{G}_\sigma(\omega) \frac{\partial}{\partial \omega} \mathbb{S}_\sigma(\omega) - \mathbb{G}_{\text{hom } \sigma}(\omega) \frac{\partial}{\partial \omega} \mathbb{S}_0(\omega) \right]_{ii}. \quad (5.109)$$

We now define the scattering phase-shift matrix as,

$$\delta_\sigma(\omega) = \text{Im} \ln (\mathbb{T}_\sigma(\omega)\mathbb{V}(\omega)^{-1}) = \text{Arg} (\mathbb{T}_\sigma(\omega)\mathbb{V}(\omega)^{-1}). \quad (5.110)$$

In absence of any interaction the phase-shift is equivalent to the formal definition obtained using the partial-wave analysis. Thus, with regard to the non-interacting system it can be physically understood as the difference between the states of the incident wave and the scattered wave in presence of impurity. However, it is not possible to have such a simple physical interpretation of phase-shift when the interaction is switched on as then the wave-function is a many-body object. The equivalent single electron picture fails.

Putting the definition of phase-shift Eq. 5.110 in Eq. 5.109 we get,

$$\Delta A_{\sigma}(\omega) = \frac{1}{\pi} \frac{\partial}{\partial \omega} \delta_\sigma(\omega)_{ii} - \frac{1}{\pi} \text{Im} \left[ \mathbb{G}_\sigma(\omega) \frac{\partial}{\partial \omega} \mathbb{S}_\sigma(\omega) - \mathbb{G}_{\text{hom } \sigma}(\omega) \frac{\partial}{\partial \omega} \mathbb{S}_0(\omega) \right]_{ii}. \quad (5.111)$$

Putting Eq. 5.111 in Eq. 5.98 we get

$$\Delta n_\sigma = \int_{-\infty}^{\mu} \frac{1}{\pi} \frac{\partial}{\partial \omega} \delta_\sigma(\omega)_{ii} d\omega - \frac{1}{\pi} \text{Im} \left[ \int_{-\infty}^{\mu} \mathbb{G}_\sigma(\omega) \frac{\partial}{\partial \omega} \mathbb{S}_\sigma(\omega) d\omega - \int_{-\infty}^{\mu} \mathbb{G}_{\text{hom } \sigma}(\omega) \frac{\partial}{\partial \omega} \mathbb{S}_0(\omega) d\omega \right]_{ii}. \quad (5.112)$$

The first integral gives $\delta_\sigma(\mu)_{ii}$. In order to evaluate the other two integrals we first briefly introduce the concept of the Luttinger-Ward functional [106]. The free-functional energy for the many-body interacting system can be approximately obtained from renormalized perturbation expansion as

$$\Omega[\mathbb{G}] = \Phi[\mathbb{G}] - \text{Tr} [\mathbb{S}(\omega)\mathbb{G}(\omega)] - \text{Tr} [\mathbb{G}_0^{-1}(\omega) - \mathbb{S}], \quad (5.113)$$

where $\Phi[\mathbb{G}]$ is the so-called Luttinger-Ward functional which is defined as a sum over closed linked Feynmann diagrams. In DMFT approximation, $\Phi[\mathbb{G}]$ contains contribution only from the local diagrams. In order to ensure this approximation would conserve the energy of the system we need to have a condition of extrema given by

$$\frac{\delta \Omega[\mathbb{G}_\sigma]}{\delta \mathbb{G}_\sigma} = 0. \quad (5.114)$$

The condition in Eq. 5.114 is satisfied if

$$\frac{\delta \Phi[\mathbb{G}_\sigma]}{\delta \mathbb{G}_\sigma} = \mathbb{S}_\sigma, \quad (5.115)$$

where $\delta \mathbb{G}_\sigma = \mathbb{G}_\sigma(i\omega + \delta \lambda) - \mathbb{G}_\sigma(i\omega)$ gives the frequency-shift. If the functional exists in a perturbative way, it is invariant under frequency shift, i.e. $\delta \Phi[\mathbb{G}] = 0$. Using the above mentioned concepts, it can be shown that the second and third integral in Eq. 5.112 are each equal to zero as follows
\[ \int_{-\infty}^{\mu} G_\sigma(\omega) \frac{\partial \Sigma_\sigma(\omega)}{\partial \omega} d\omega = G_\sigma(\omega) \Sigma_\sigma(\omega) - \int_{-\infty}^{\mu} \Sigma_\sigma(\omega) \frac{\partial G_\sigma(\omega)}{\partial \omega} d\omega \]

\[ = - \int_{-\infty}^{\mu} \frac{\partial G_\sigma(\omega)}{\partial \omega} \frac{\delta \Phi}{\delta G_\sigma} d\omega \]

\[ = \delta \Phi[G_\sigma] = 0. \]

Thus,

\[ \Delta n_\sigma = \frac{1}{\pi} \left( \sum_i \delta_\sigma(\mu)_{ii} \right) = \frac{1}{\pi} \text{Tr} \delta_\sigma(\mu). \] (5.117)

Note that the summation/partial trace is taken excluding the impurity site/sites. Finally using Eq. 5.117, Eq. 5.95, the FSR in presence of interaction is written in the most generalised form as

\[ Z = \frac{2}{\pi} \text{Tr} \delta_\sigma(\mu). \] (5.118)

More simplified form of the Eq. 5.118 can be obtained for specific types of external potential e.g., i) uniform perturbation, where all diagonal lattice sites have the uniform potential V ii) Point like impurity where only one particular lattice site has an on-site potential V.

We comment on the scattering problem in infinite energy limit where \( \omega \rightarrow \pm \infty \). \( G_{\text{hom} \sigma}(\omega) \), and \( G(\omega) \) which behaves as \( 1/\omega \) in the asymptotic limit thus approach zero when \( \omega \rightarrow \pm \infty \). It subsequently follows from Eq. 5.88, Eq. 5.89, and Eq. 5.90 that \( \Sigma_\sigma(\omega) \), \( \Sigma(\omega) \), and \( \Delta \Sigma(\omega_n) \) approaches zero in this limit. Thus, the dynamical potential reduces to the static part of the potential i.e. \( \Sigma(\omega \rightarrow \pm \infty) \approx \Sigma \) and the scattering matrix Eq. 5.107, \( \Sigma(\omega \rightarrow \pm \infty) \approx \Sigma \) in this limit.

5.5.2 T-matrix analysis for a point-like (single) impurity

In this sub-section we present the T-matrix analysis due to scattering from a single point-like impurity.

Friedel Sum Rule for point-like impurity

First we present the FSR in this case starting from the general expression in Eq. 5.118. In this case the impurity matrix \( \mathbb{V} \) is explicitly given by,

\[ \mathbb{V} = \begin{pmatrix} V & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \] (5.119)

Rewriting the definition of \( \Delta n_{i\sigma} \) using Eq. 5.112, Eq. 5.108 and Eq. 5.110 we have,

\[ \Delta n_{i\sigma} = -\frac{1}{\pi} \text{Im} \left[ \ln(1 - \mathbb{V}(\mu) G_{\text{hom} \sigma}(\mu)) \right]_{ii} \] (5.120)

In case of single impurity for non-interacting systems (\( \Sigma_\sigma(\mu) = 0 \)) we have,

\[ 1 - \mathbb{V}(\mu) G_{\text{hom} \sigma}(\mu) = \begin{pmatrix} 1 - VG_{11\sigma} & -VG_{12\sigma} & -VG_{13\sigma} & \cdots \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \] (5.121)
Consequently, for $\Delta n_\sigma = \sum_i \Delta n_i \sigma$, only the first non-zero diagonal element contribute to the trace and we have

$$\Delta n_\sigma = -\frac{1}{\pi} \text{Im} \ln(1 - VG_{11\sigma}(\mu))$$

$$= -\frac{1}{\pi} \text{Arg}(1 - VG_{11}(\mu))$$

$$= \text{Arctan} \left[ \frac{\pi G'_{11\sigma}(\mu)}{G''_{11\sigma}(\mu) - \frac{1}{\pi}} \right],$$

where $G'_{11\sigma}(\mu)$ and $G''_{11\sigma}(\mu)$ correspond to the real and imaginary parts of the complex non-interacting Green’s function. Thus, the FSR for the non-interacting system is given by

$$Z = \text{Arctan} \left[ \frac{\pi G''_{11\sigma}(\mu)}{G'_{11\sigma}(\mu) - \frac{1}{\pi}} \right].$$

(5.123)

If we turn on interaction, i.e. $\Sigma(\mu) \neq 0$, then it follows from Eq. 5.88 that effective energy is renormalized by the self-energy, i.e. $\mu \rightarrow \mu - \Sigma(\mu)$. Thus, we can derive the the FSR in the same way as the non-interacting system and,

$$Z = \text{Arctan} \left[ \frac{\pi G''_{11\sigma}(\mu - \Sigma_\sigma(\mu))}{G'_{11\sigma}(\mu - \Sigma_\sigma(\mu)) - \frac{1}{\pi}} \right],$$

(5.124)

where $G'_{11\sigma}(\mu - \Sigma_\sigma(\mu))$ and $G''_{11\sigma}(\mu - \Sigma_\sigma(\mu))$ correspond to the real and imaginary parts of the complex interacting Green’s function. Thus, we see that the FSR is ideally conserved even for the interacting systems.

**Friedel oscillations in interacting system in presence of a point impurity**

In case of a point impurity the T-matrix is given by

$$T_\sigma = \frac{V}{1 - G'_{11\sigma} V} \begin{pmatrix} 1 & 0 & 0 & \cdots & \cdots \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

(5.125)

Thus, the Green’s function $G = G_0 \mathbb{1} G_0$ can be explicitly written as multiplication of matrices as

$$G_\sigma = \frac{V}{1 - G'_{11\sigma} V} \begin{pmatrix} G_{11\sigma} & G_{12\sigma} & G_{13\sigma} & \cdots & \cdots \\ G_{21\sigma} & G_{22\sigma} & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & \cdots & \cdots \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix} \begin{pmatrix} G_{11\sigma} & G_{12\sigma} & G_{13\sigma} & \cdots & \cdots \\ G_{21\sigma} & G_{22\sigma} & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}$$

(5.126)

Performing the above matrix multiplication we have the difference between the homogeneous and inhomogeneous Green’s function as

$$\Delta G_{11\sigma}(\omega) = \frac{V}{1 - G'_{11\sigma}(\omega) V} G'_{11\sigma}(\omega) G'_{11\sigma}(\omega).$$

(5.127)
Consequently, following equation Eq. 6.12 and Eq. 5.127, the local occupation is given by

\[ \Delta n_{i\sigma} = -\frac{1}{\pi} \int_{-\infty}^{\mu} \frac{V}{1 - C_{i1\sigma}(\omega)V} C_{11\sigma}^{0}(\omega) d\omega. \]  

(5.128)

In Eq. 5.128 we see $\frac{V}{1 - C_{i1\sigma}(\omega)V}$ is the constant scattering term while $C_{11\sigma}^{0}$ gives the oscillatory part. However, solving the above integral analytically for the interacting Green’s function is not straight-forward and hence we revert to numerical methods for solving this problem in this thesis.

### 5.5.3 FO in non-interacting finite lattice system in the presence of a localized impurity potential

We can obtain an analytical formula for the local occupation in case of non-interacting electrons in the presence of a localized impurity potential. In Chp. 2 we mentioned that in case of a non-interacting continuous system the density modulation around the impurity is described by Eq. 2.1 which can be obtained using the formal scattering theory for free electrons. Under the free electron approximation the picture is rather simple where we consider one incoming particle scattered by one scattering centre. We assume that the individual scatterers contained in the target are dilute and do not interfere with each other. However the phenomenon cannot be described so simply when we move from the continuous system to a finite crystal lattice. We would conclude this chapter deriving the expression for local occupation and hence explaining the behaviour of FO in a finite non-interacting lattice in the presence of a localized impurity potential. A comprehensive discussion on the theory of scattering in real crystalline solids is presented in [107]. Here we would first remind the reader only about the essential background concepts relevant to the derivation before presenting it.

#### Bloch electrons

We know from elementary solid state physics that electrons in the solid are confined in a periodic crystal potential and described by the Bloch states with discrete translational invariance. We denote the Bloch state for the $n^{th}$ band and restricted wave-vector $\mathbf{k}$ for the first Brillouin zone by $|n\mathbf{k}\rangle$ such that

\[ \langle \mathbf{r}|n\mathbf{k}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}), \]  

(5.129)

\[ \langle n\mathbf{k}|n'\mathbf{k}'\rangle = \delta_{nn'} \delta(\mathbf{k} - \mathbf{k'}). \]  

(5.130)

The resolvent given by

\[ \hat{G}(\omega) = \sum_{n} \int d\mathbf{k} |n\mathbf{k}\rangle \langle n\mathbf{k}| \frac{1}{\omega - \epsilon_{\mathbf{k}}}, \]  

(5.131)

have the following matrix elements in the Bloch representation as

\[ \langle n\mathbf{k}|\hat{G}(\omega)|n'\mathbf{k}'\rangle = \delta_{nn'} \frac{\delta(\mathbf{k} - \mathbf{k}')}{\omega - \epsilon_{\mathbf{k}}}. \]  

(5.132)

The DOS per unit volume can be obtained from the resolvent in the Bloch basis as

\[ A(\omega) = \sum_{n} \int d\mathbf{k} \frac{\delta(\omega - \epsilon_{\mathbf{k}})}{2\pi^{d}}. \]  

(5.133)

In contrast to the free electron case for Eq. 5.133 instead of the free electron energy we have the energy obtained from a band structure calculation. Also the integral extends over the first Brillouin zone and the summation runs over the $n$ different bands.
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The transformation of the Bloch states to the Wannier representation and vice versa is given by

\begin{align}
a_n(r - R_i) &= \frac{1}{\sqrt{N}} \sum_k e^{-i k \cdot R_i} \varphi_{nk}(r), \\
\varphi_{nk}(r) &= \frac{1}{\sqrt{N}} \sum_i e^{i k \cdot R_i} a_n(r - R_i),
\end{align}

where \( N \to (2\pi^3/\tau_v) \), \( \tau_v \) is the volume of the unit cell and \( \tau_v = a^3 \).

The resolution in Wannier representation is given by

\begin{equation}
\langle n i | \hat{G}(\omega) | m j \rangle = \frac{1}{\sqrt{N}} \sum_k e^{i k \cdot (R_i - R_j)} \frac{\omega - \epsilon_k}{\omega - \epsilon_m}.
\end{equation}

DOS in the \( n^{th} \) band can be obtained in the Wannier representation as

\begin{equation}
A^{(n)}(\omega) = -\frac{1}{N \tau_v \pi} \text{Im} \sum_i \langle n i | \hat{G}(\omega^+) | n i \rangle.
\end{equation}

**Formal theory of scattering for Bloch electrons**

Having presented the basic formulae we now discuss the formal scattering theory for the Bloch electrons. In case of the Bloch states \( |n k \rangle \) the scattering solutions satisfy the integral equation

\begin{equation}
|\psi^\pm_{nk}\rangle = |nk\rangle + \hat{G}(\epsilon_{nk}^\pm) |V| \psi^\pm_{nk}\rangle
= |nk\rangle + \sum_m \int d_q \langle m q | \langle m q | V | \psi^\pm_{nk}\rangle \frac{\epsilon_{nk}^\pm - \epsilon_{mq}}{\epsilon_{nk}^\pm - \epsilon_{mq}}.
\end{equation}

In the above equation the scattering potential is \( V \) and \( \hat{G} \) is the resolvent given by Eq. 5.136

The essential difference of Eq. 5.150 with the formula for scattering of free electrons is in the summation over the inter-band terms \( (m \neq n) \). In order to simplify the problem it is common to make a one-band approximation, i.e. the potential has no inter-band matrix elements and retain only those terms with \( m = n \). Absence of scattering in between the bands factorizes the Fredholm determinant as

\begin{equation}
D(\omega) = \prod_n \text{det}(1 - G_n V_n) = \prod_n D_n(\omega).[107]
\end{equation}

Thus the one-band approximation factorizes out the entire problem such that we can study the effect of \( V_n \) on the Bloch states of the \( n^{th} \) band one at a time. In case of a perfect crystal the local occupation at the \( i^{th} \) site can be calculated using the resolvent as

\begin{equation}
n_i = \text{Tr} \hat{\rho}^i = -\frac{2}{\pi} \int d\omega \ f(\omega) \text{Im} \sum_n \langle n_i | \hat{G}^+ | n_i \rangle.
\end{equation}

Introducing the general concept we now study the scattering problem in the presence of a localized point-like impurity potential under one-band approximation. The one-band and the one-site containing the impurity are labelled by 0. In the Wannier representation we then have

\begin{equation}
\langle n i | V | m j \rangle = \delta_{nm} \delta_{m0} \delta_{ij} \delta_{j0} V_0.
\end{equation}

This is also the well-known Koster-Slater model.

The scattering solution then satisfies

\begin{equation}
\langle i | \psi^\pm_{nk}\rangle = \langle i | Bk\rangle + \langle i | G(\epsilon_{nk}^+) | V_0(0) | \psi^\pm_{nk}\rangle.
\end{equation}
For the outgoing solution taking arguments of Eq. 5.143 we get

\[\langle i | B_k \rangle = \frac{1}{\sqrt{N}} e^{i k \cdot R_i} . \tag{5.143}\]

Using Eq. 5.137 we get

\[G_{00}^{\pm} = \langle 0 | G(\epsilon_k^+) | 0 \rangle \equiv \text{Re} \ G_{00} \mp i \pi \tau_e A(\epsilon_k). \tag{5.144}\]

In the unit cell containing the impurity \(i = 0\) and we have

\[\langle 0 | \psi_{i n k}^+ \rangle = \frac{\sqrt{\tau_e}}{(2\pi)^{d/2}} \frac{1}{1 - \text{Re} \ G_{00} \mp i \pi \tau_e N(\epsilon_k) V_0} . \tag{5.145}\]

For the outgoing solution taking arguments of Eq. 5.143 we get

\[\text{arg} \ \langle 0 | \psi_{i n k}^+ \rangle = \text{arg} \ \langle 0 | B_k \rangle - \text{arg} \ (1 - G_{00}^{+} V_0) , \tag{5.146}\]

i.e. the impurity creates a phase-shift

\[\delta(\epsilon_k) = \text{Arctan} \frac{\pi \tau_e A(\epsilon_k) V_0}{1 - \text{Re} \ G_{00} V_0} . \tag{5.147}\]

Using Eq. 5.145 in Eq. 5.142 we describe the effect away from the impurity center and obtain

\[\langle i | \psi_{i n k}^+ \rangle = \langle i | B_k \rangle \frac{\langle i | G(\epsilon_k^+) | 0 \rangle V_0 \langle 0 | B_k \rangle}{1 - G_{00}^{+} V_0} . \tag{5.148}\]

Thus we need to calculate

\[I = \langle i | G(\epsilon_k^+) | 0 \rangle = \frac{\tau_e}{(2\pi)^d} \int d_3 k' \frac{e^{i k' \cdot R_i}}{\epsilon_k' - \epsilon_k} \tag{5.149}\]

which is extremely difficult. Even in the asymptotic limit, i.e. \(kR_i \gg 1\) it is non-trivial to calculate Eq. 5.149 for a model of band-structure. The easiest choice of model in this case is the nearly-free electron model where \(\epsilon_k = \alpha k^2\) with \(\alpha = h^2/2m^*\) and \(m^*\) is the effective mass of the electron in the crystal field. We now use this dispersion relation to evaluate \(I\) in Eq. 5.149 for a \(d = 3\) volume element.

\[I = \frac{\tau_e}{2\pi^3} \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta \int_0^\infty dk' k'^2 \frac{e^{i k' \cdot R_i}}{\epsilon_k' - \epsilon_k} \frac{\epsilon_k' R_{i \cos \theta}}{\epsilon_k'^2 - \alpha k'^2 - i\eta} \tag{5.150}\]

\[I = \frac{\tau_e}{4\pi^4 R_i} \int_{-\infty}^\infty dk' \frac{e^{i k' \cdot R_i}}{\alpha k'^2 - \alpha k^2 - i\eta} \tag{5.150}\]

\[I = \frac{\tau_e}{4\pi^4 R_i} \frac{e^{i k \cdot R_i}}{4\pi \alpha R_i} \tag{5.150}\]

Now we get the scattering state as

\[\langle i | \psi_{i n k}^+ \rangle = \frac{\sqrt{\tau_e}}{(2\pi)^{3/2}} \left[ e^{i k \cdot R_i} - \frac{\tau_e}{4\pi \alpha} \frac{V_0}{1 - G_{00}^{+} V_0} e^{i k \cdot R_i} \right] . \tag{5.151}\]

We define the scattering amplitude from Eq. 5.151 as,

\[f^+ = \frac{\tau_e}{4\pi \alpha} \frac{V_0}{1 - G_{00}^{+} V_0} \tag{5.152}\]

\[f^+ = \frac{\tau_e V_0}{4\pi \alpha (1 - G_{00}^{+} V_0)} \left[ 1 - \text{Re} G_{00}^{+} V_0 - i \pi A(\epsilon_k) V_0 \tau_e \right] \tag{5.152}\]

\[f^+ = \frac{\tau_e V_0}{4\pi \alpha (1 - \text{Re} G_{00}^{+} V_0)^2 + \pi^2 N^2(\epsilon_k) V_0^2 \tau_e^2} . \tag{5.152}\]
CHAPTER 5. MANY-BODY FORMALISM AND REAL-SPACE DYNAMICAL MEAN-FIELD THEORY APPROXIMATION

In our model $N(\alpha k^2) = k/4\pi^2\alpha$ and the scattering amplitude reduces to $f^+ = -1/k \, e^{ik\sin \delta}$ which is the same as the standard free electron case. At the impurity site the probability density of the electrons with energy $\epsilon_k$ is given by

$$
|\langle 0|\psi_{\epsilon_k}^+ \rangle| = \frac{\tau_v}{(2\pi)^3} \frac{1}{(1 - \text{Re} \, G_{00}^{(0)} + (\pi \tau V_0 A(\epsilon_k))^2)}.
$$

Away from the impurity charge in the asymptotic limit for $T = 0$ the local site occupation can be derived as follows:

$$
\delta n_l = -2 \frac{2}{\pi} \int_{-\infty}^{\infty} d\omega \ Im \frac{\langle i|G^+|0\rangle V_0 (0|G^+|i)}{1 - G_{00}^+ V_0} = \frac{\tau_v}{2\pi^2 a R_i} \int_{-\infty}^{\infty} d\omega \ Im [f^+ e^{2ikR_i}] .
$$

$k$ is purely imaginary for negative energies and $\text{exp}(-2ikR_i)$ is negligibly small for asymptotic distance and hence we change the lower limit of the integral to zero. In this range the scattering amplitude behaves smoothly in absence of resonances while $\text{exp}(2ikR_i)$ term oscillates quickly.

We can now extract the factor called the “scattering length” from the integrand of Eq. 5.154 defined as

$$
a_0 = -\lim_{k \to 0} f^+ .
$$

Eq. 5.154 can be further simplified using the definition of scattering length as follows:

$$
\delta n_l = \frac{\tau_v}{2\pi^2 a R_i^2} a_0 \int_{0}^{k_F} \frac{dk}{k} \frac{k^2}{2\alpha} e^{2ikR_i} \ Im \frac{[(2ikF R_i - 1)e^{2ikF R_i} + 1]}{[2kF R_i + i \sin (2kF R_i)]} = \frac{a_0 \tau_v}{4\pi^2 R_i^4} \frac{k_F^4}{R_i^4} \left[ (2kF R_i + i \sin (2kF R_i)) - \sin (2kF R_i) \right] .
$$

In the final expression of Eq. 5.156 we see that the local occupation has a constant part and oscillatory part which primarily decays as $1/R_i^3$. In comparison to Eq. 2.1 we see that we have an additional $1/R_i^3$ decay term in this case.

In case of interacting system we need to include the self-energy term in the resolvent and then evaluating the integral of Eq. 5.149 analytically is a complicated problem. It is an interesting problem to analytically study how interaction renormalizes the local occupation in Eq. 5.156 using the concepts of Landau Fermi liquid theory. The electronic correlations are expected to renormalize the scattering length $a_0$ in Eq. 5.156 and $k_F$ would remain unaltered by virtue of the Luttinger theorem. However, these propositions are intuitive while a rigorous analytical derivation to account for the effects of interactions on FO is beyond the scope of this thesis.
Chapter 6

Single Impurity

In this chapter we present our numerical results describing the behaviour of the Friedel oscillations, N-screening charge and spectral function in the presence of a single site impurity potential. We have performed our studies for finite lattice systems and accounted for the electronic interactions using different methods. This chapter has been organised as follows: In each section we present the behaviour of each physical quantity using the different methods. The behaviour for the different dimensions are further divided into subsections. In this way the reader gets a good comparative picture of the results from the different methods and can judge if they are consistent. Also, the effect of dimensionality on the behaviour of these quantities becomes clearly understood.

6.1 Model and methods

6.1.1 Model specification

- We consider one, two and three-dimensional finite lattice systems modeled by the inhomogeneous Hubbard Hamiltonian in Eq. 4.19. The external inhomogeneity is modeled by \( V_i = V_0 \delta_{i, \text{imp}} \), where \( i_{\text{imp}} \) is the impurity site and it corresponds to a single impurity potential. Both attractive \( (V_0 > 0) \) and repulsive \( (V_0 < 0) \) are considered.
- We consider uniform nearest neighbour hopping parametrized by \( t = 1 \) which also scales the energy units.
- We need to define boundary conditions since our system should be finite. We largely use Periodic Boundary Conditions (PBC) for our studies in which the electrons can hop from the last site to the first site. We have also performed some tests with open boundary conditions (where electrons do not move from the last site to the first site), natural boundary conditions (where we put infinite potential walls at the system boundaries) and would also present those results. Nevertheless, unless any additional comments are made on the boundary conditions of the system, all the cases are by default studied with PBC.
- We choose spin independent paramagnetic systems such that \( n_{i\sigma} = n_i/2 \) (number of spin up and spin down particles are equal).
- We choose the chemical potential such that the system is at half-filling, far away from the impurity.

Our model systems for 1D and 3D are presented in Fig. 6.1(a) and Fig. 6.1(c). It is desirable to have a considerably large number of lattice sites to study the decay of FO with the relative distance from the impurity. In case of smaller system sizes the range of oscillation is also small for studying the decay. Moreover additional oscillations due to the reflections from the boundary of the finite system become dominant. However, it demands
CHAPTER 6. SINGLE IMPURITY

Figure 6.1: Finite lattice models with a single impurity potential. (a) 1D lattice chain, (b) 2D lattice, (c) 3D lattice. In each case the single impurity potential placed on the $i^{th}$ site is indicated by a different colour. The arrows correspond to the nearest neighbour hopping and periodic boundary conditions.

huge computational time and memory to study large systems in higher dimensions using our method. Hence a compromise on the system size was required as we increased the dimensions.

6.1.2 Methods used

RDMFT+CTQMC

Electronic correlations are accounted for solving the R-DMFT equations self-consistently using the CTQMC method. As already mentioned, we have used CT-HYB, i.e. an expansion about the hybridization function for our work. Henceforth in the rest of the thesis CTQMC implicitly refers to CT-HYB. Werner first presented the CT-HYB algorithm for solving SIAM [108]. In our work, the CTQMC algorithm has been developed by Dr. K. Makuch using Fortran 90/95 language based on the approach of Haule [109].

CTQMC solver

We briefly outline the principle of CTQMC as used in our code following the description of Haule [109]. A detailed description including a comparative study of different CTQMC algorithm, Monte Carlo basics like sampling error, Markov chain, Metropolis algorithm is presented in [81]. It also discusses the different merits and demerits of CT-HYB. The computational time grows as the cube of inverse temperature in CT-HYB [109].

We start our description defining the Green’s function in the tau-space using Feynman path integral formalism as

$$G(\tau, \tau') = \frac{1}{Z} \int D[a^* a] a(\tau) a^*(\tau') e^{-S},$$

(6.1)
where the action $S$ can be split into non-interacting and interacting part as $S = S_0 + \Delta S$. The interacting part of the action $\Delta S$ is obtained from the hybridization function as

$$\Delta S = \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\tau' \sum_{a\alpha a'\alpha'} a^*_a(\tau) \Delta_{a\alpha a'\alpha'}(\tau - \tau') a_{a'}(\tau'),$$  \hspace{1cm} (6.2)$$

where $\alpha$ is the spin index.

The partition function of the system is

$$Z = \int D[a^* a] e^{-S_0}$$

is the spin index.

The self-energies obtained from this method include all the inhomogeneities from the external impurities and are thus numerically exact. Particularly CT-HYB works easily for any arbitrary interactions as long as the Hilbert space is not too large. In case of CT-HYB the average order of expansion for a typical problem around the Mott transition is much smaller as compared to CT-INT [81]. Hence, one can access low temperature which is one primary requirement for our studies in FO. However, still it works only for finite temperatures and the time of computation proportionally increases with increasing $\beta$. Hence, it

**Key features of RDMFT+CTQMC**

Finally, we sum up the key features of this method. The problem is solved in the Matsubara frequency space. The self-energies obtained from this method include all the inhomogeneities from the external impurities and are thus numerically exact. Particularly CT-HYB works easily for any arbitrary interactions as long as the Hilbert space is not too large. In case of CT-HYB the average order of expansion for a typical problem around the Mott transition is much smaller as compared to CT-INT [81]. Hence, one can access low temperature which is one primary requirement for our studies in FO. However, still it works only for finite temperatures and the time of computation proportionally increases with increasing $\beta$. Hence, it
Figure 6.2: Self-energy scheme for the approximate methods. All lattice sites are assumed to have the same homogeneous self-energy which is then transferred into the real-space Dyson equation containing the impurity potential as indicated by the arrows. Thus the Green's function are different for different lattice sites.

is computationally extremely time-consuming to obtain low temperatures using this method. Still we have reached temperatures low enough to observe the effect of interactions on F.O. Moreover, in this method SIAM is solved on every non-equivalent lattice site which adds to the computational difficulties (e.g. time factor, memory issues). Some further technical details used in our computational program have been presented in Appendix C.

Owing to the complications of RDMFT+CTQMC we at first use some approximate methods to obtain initial insights about the behaviour of F.O in presence of interactions in the limit of zero temperature. We intend to study FO in the asymptotic limit as in Eq. 2.1 in which $|r_i - \mathbf{r}_\text{imp}| \gg a$, $a$ being the lattice constant of the system. At so far away from the impurity the effect of the impurity is considered weak enough and the inhomogeneous part of the self-energy can be neglected. Thus it is a good approximation to consider only the homogeneous part of the self-energy and it introduces very small errors. All the lattice sites have the same self-energy. We use the approximation that the presence of the external impurity at a particular lattice site does not affect the self-energy at that site. The homogeneous part of the self-energy can be accounted for solving DMFT equations using Numerical Renormalization Group, or using some phenomenological model self-energy, Hubbard I approximations denoted by, $\Sigma_{\text{hom}} \approx \Sigma^{NRG}$ or $\Sigma^{\text{HubbardI}}$, or $\Sigma^{\text{model}}$. However, the homogeneous self-energy is transferred into the real space Dyson equation for computing the GF as shown in Fig. 6.2. Thus though the self-energy at different lattice site are same, but the GF still contains the effect of the impurity and is different for the different lattice site. We now begin with the discussion of these approximate methods.

**Approximation A**

The homogeneous part of the self-energy is modeled using Eq. 6.8 (model self-energy). It obeys Fermi liquid properties and has proper asymptotic behaviour in $\omega$. It is momentum independent, local i.e. diagonal in lattice site indices which is the same approximation as in R-DMFT [89, 90]. It is given by,

$$\Sigma(\omega) = g \frac{c\omega}{\omega + i(c \omega + ib)}$$

(6.8)

where $c, b, g$ are model parameters and $g$ accounts for the electronic interactions. $c$ and $b$ have dimensions of energy while $g$ is dimensionless and rescales the self-energy. Inoue et al. used the model self-energy to give a phenomenological description of the single-particle density of states of metallic perovskite $Ca_{1-x}Sr_xVO_3$ as observed experimentally in the photo-emission spectra [89]. In their work, the model parameters were adjusted to obtain the best fit to the experimental data. It stated that the model parameters may be related to the Hubbard interaction $U$ and the band-width $W$ of the system using second-order perturbation theory [110]. It further obeys the Luttinger theorem for Fermi liquids which states that the volume of the Fermi sphere does not change as the interaction is switched on [111, 112]. In our work, the parameters are fixed at $c = 0.2$, $b = 0.3$, and $g$ is tuned to account for the electronic correlations.
CHAPTER 6. SINGLE IMPURITY

Approximation B

The homogeneous part of the self-energy is modeled using self-energy under Hubbard I approximation given by

$$\Sigma_{HubI}(\omega) = Un_i\bar{\sigma} - \frac{U^2 n_i\bar{\sigma}}{\omega - V_i - U(1 - n_i\bar{\sigma})}. \quad (6.9)$$

The chemical potential $\mu = U/2$ corresponds to a half-filled band in this case.

Approximation C

In this method we solve the DMFT self-consistency equations for a homogeneous system using the NRG method to obtain the homogeneous self-energies. These self-energies have been calculated by my collaborator mgr J. Skolimowski using the “NRG Lubljana” code, which is a series of interrelated computer programs used to solve quantum impurity problems. It makes use of Fortran LAPACK library, block algorithm using C and Mathematica programming languages [113]. We briefly outline the NRG method in the following.

NRG solver

Numerical Renormalization Group is a numerical non-perturbative approach to solve the SIAM taking into account all possible energy scales which can contribute to the solution. It was invented by Wilson in 1975 and was originally designed to study the thermodynamical properties of the Kondo model. Eventually it was extended to study the SIAM for $T = 0$ and $T > 0$ [114, 115, 116, 117, 118]. SIAM can be derived from the Kondo model by including charge fluctuations at the impurity site. A brief and comprehensive discussion on NRG in the context of Anderson impurity model is presented in [78]. A further detailed description on NRG formulation can be found in [83]. Here we would outline the main components of the numerical techniques used for the computation of the self-energy using the “NRG Lubljana” code.

As discussed in subsection 5.4.2, the influence of the bath on the impurity is determined by the hybridization function in Eq. 5.87. Thus it is justified to reformulate the Hamiltonian in order to describe the physics of the impurity as long as it does not change the form of the hybridization function. The Hamiltonian can be reformulated using a one-dimensional representation of the conduction band as

$$H = H_{imp} + \sum_{\sigma} \int_{-1}^{1} d\varepsilon g(\varepsilon) a^\dagger_{\varepsilon\sigma} a_{\varepsilon\sigma} + \sum_{\sigma} \int_{-1}^{1} d\varepsilon h(\varepsilon)(c^\dagger_{\varepsilon\sigma} a_{\varepsilon\sigma} + a^\dagger_{\varepsilon\sigma} c_{\varepsilon\sigma}), \quad (6.10)$$

where the band cut-offs are chosen at energies $\pm 1$ [83]. The two functions $g(\varepsilon)$ and $h(\varepsilon)$ are related to the hybridization function via

$$\Delta(\omega) = \pi \frac{d\varepsilon(\omega)}{d\omega} h[\varepsilon(\omega)]^2, \quad (6.11)$$

where $\varepsilon(\omega)$ is the inverse function to the dispersion $g(\varepsilon)$. The effective one-dimensional band in Eq. 6.10 has infinite degrees of freedom which cannot be handled numerically. Hence, in NRG as a next step the continuous band is reduced to a discreet set of states via a logarithmic discretization where $\lambda$ is the discretization parameter and $\lambda > 1$. Next the the discretized model is mapped onto a semi-infinite chain where the impurity is the first site. A further iterative diagonalization of this chain is performed to finally obtain the many particle eigen energies. During the diagonalization process, after each iteration one lattice site is added and coupled to the energy eigen state of the previous NRG iterations. Addition of each site grows the number of states by a factor of four. In order to optimize the size of the Hilbert space, the number of states are truncated after each iteration based on a chosen cut-off energy. Once we obtain the energy eigen values, they can be used to calculate the spectral function from the...
Lehmann representation and hence the Green’s function. The self-energy is calculated using the Green’s function by the division of two correlation functions following Eq. 5.34 [119]. This is the rough sketch of the principle employed in the “NRG Lubljana” code to compute the self-energies self-consistently.

In each of these approximations the homogeneous self-energy is transferred into the real space Dyson equation to obtain the Green’s function. The problem is solved in the real frequency space, \( \omega + i\eta \) where the broadening parameter is set as \( \eta = 0.01 \).

The dense matrix inversion in order to obtain the Green’s function is done numerically using the Fortran NAG library. It uses the principle of Bunch-Kaumann pivoting method to factorize the matrix followed by a symmetrization to calculate the inverse [120]. This is the most time consuming part of the code and the time increases with the dimension of matrix. All these approximations work in the limit of zero temperature and we set \( \beta = 10000 \). Since all the lattice sites are assumed to have the same homogeneous self-energy the computational time is a lot less as compared to RDMFT+CTQMC. In Approximation C the SIAM is solved only once using NRG which takes orders of hours, in our present computational set up with a processor of 1.2 GHz and 16 GB RAM. In Approximation A and B the self-energy has a simple analytical form and hence the computational time is in the order of minutes for 1D systems. However increase in the computational time with increase in the dimensionality of the lattice still persists.

We always study the system for half-filling given by \( \bar{n} = 1 \), in all the methods. In Approximation A we need to self-consistently determine the chemical potential to obtain half-filling. In Approximation B, Approximation C and RDMFT+CTQMC \( \mu = U/2 \) corresponds to half-filling.

### 6.1.3 Choice of dimensionality of the lattice

The use of DMFT to study the behaviour of the FO around Mott transitions in a one-dimensional Hubbard model raises a couple of obvious contradictions. DMFT gives a numerically exact solution for infinite dimensions and requires the system to be a Fermi liquid. In case of 1D the charge fluctuations become significant, Fermi liquid picture breaks and the system is a Luttinger liquid instead. Again, according to the exact solution of Lieb and Wu using the Bethe Anstasz, there is no Mott transition in a 1D Hubbard model for any finite \( U > 0 \) [51]. So is it physically justified to study the problem in 1D system using our method? The arguments in favor of choosing 1D as the starting point of our calculations are as follows. It is computationally simple and fast to study 1D systems even for a large number of lattice sites using our method. Particularly for R-DMFT+CTQMC in which the SIAM needs to be solved for every non-equivalent lattice 1D systems are particularly useful to get initial insights regarding the behaviour of the system. DMFT approximates the self-energy to be momentum independent and hence reproduces features of higher dimensions even in 1D. Thus as an artifact of DMFT it is possible to see Mott transition even in 1D. The behaviour of FO around Mott transition in 1D has been used to speculate the behaviour in the higher dimensional systems. Hence, we choose the 1D system as a “Toy-Model” for initial studies and later repeat the same calculations for two and three-dimensions. It would be revealed in the results section that all the behaviour of FO predicted by the 1D model was actually reproduced for 2D and 3D and hence we considered it worthy also to present the 1D results.

### 6.2 Physical quantities calculated

We calculate:

1. Local spectral function \( A_{\sigma}(\omega) \) using Eq. 5.9.

   In case of Approximation A, B and C the Green’s function is already calculated in the real space which is required to calculate \( A_{\sigma}(\omega) \). However, in case of R-DMFT+CTQMC the Green’s function is calculated in the Matsubara (imaginary) frequency space and it is not so straight-forward to calculate the spectral function. We need to perform an
analytical continuation of the Green’s function from the Matsubara (imaginary) space to the real space using the Maximum Entropy (MaxEnt) method. MaxEnt is a statistical approach based on Bayesian logic or conditional probability which is used to extract information from the noisy Monte Carlo data. Discussions on the details of the working principle and the implementation of the algorithm of Maxent are available in [121, 122, 123].

2. Local occupation of electrons per lattice site or the electronic density is the most important quantity for studying FO. In case of RDMFT+CTQMC it is directly calculated from Eq. 5.19, where the average of the operators are calculated using Monte Carlo following Eq. 6.5 and Eq. 6.7. Since this method is based on stochastic sampling the statistical error given by the standard deviation of the different samples is also estimated for each quantity. In case of Approximation A, B, C it is calculated from the spectral function using Eq. 6.12 given by

$$n_{i\sigma} = \int_{-\infty}^{+\infty} A_{i\sigma}(\omega) f(\omega) d\omega. \quad (6.12)$$

where \(\omega \rightarrow \omega + i\eta\), \(\eta\) being the broadening parameter. The integration is performed numerically using Trapezoid rule. We need to carefully choose the frequency cut-offs such that the significant part of spectra is covered. The grid of the integration should be greater than the broadening parameter.

3. Neighbourhood screening charge or N-screening charge

In order to quantitatively study the effect of screening on the electrons due to the single impurity, in the neighbourhood of the impurity we calculate the N-screening charge defined by,

$$Z_{sc} = \sum_{i \neq i_{imp}} (n_i - \bar{n}), \quad (6.13)$$

where the summation runs over all the lattice sites excluding the impurity site. \(n_i\) is the local occupation per lattice site corresponding to the inhomogeneous system \((V \neq 0)\) used from our previous calculations. \(\bar{n}\) gives the average occupation of the system.

6.3 Numerical results on local electronic occupation

We now present our results from the local electronic occupation. We judge if the behaviour of FO in finite interacting lattice system follow the same trend of non-interacting continuous system in the asymptotic limit as given by Eq. 2.1.

6.3.1 Approximation A (\(\Sigma\text{model}\))

We start with presenting the results from the simplest method, i.e. Approximation A for 1D and 2D systems. The parameters chosen for our simulation are \(a = 2, b = 3\), in Eq. 6.8 and the broadening parameter \(\eta = 0.008\). We choose the frequency cut-off between ±20 and the frequency grid as 0.004.

1D interacting system at half-filling with repulsive impurity potential

In Fig. 6.3 we present the local occupation \(n_i\) in a one-dimensional lattice with \(N_L = 100\) sites where the impurity is located at the 20\(^{th}\) site. The repulsive potential is \(V_0 = 2\). The particles are repelled from the impurity site and the screening cloud is built around it. There is a dip at the impurity site due to the repulsive potential which gets shallower with the increasing interactions. This feature is discussed in more details in the Sec. 6.4 where we discuss about the N-screening charge. We can clearly see the characteristic FO. The screening cloud is seen for all \(g\) parameters, however, the amplitudes of the density oscillations are suppressed. Since
for $d = 1$, the Fermi vector $k_F$ is unchanged for the model self-energy, the period of oscillations must be the same for different $g$ at half-filling. In addition the phase $\delta$ is unchanged as well since we impose the PBC.

![Figure 6.3: Variation of the local occupation and FO in presence of the single impurity potential $V_0 = 2.0$ placed at 20th site in a 1D lattice chain. Different colours correspond to different electronic interactions accounted for using Approximation A. The inset shows behaviour of FO in the neighbourhood of the impurity site.](image)

In order to have a quantitative idea about the decay of FO with the interactions we extract the local maxima in Fig. 6.3 on the right side of the impurity (site 21 to 50) and plot it against the inverse of the relative distance from the impurity in Fig. 6.4(a). It is seen that even for the interacting system the oscillations follow a linear asymptotic decay described by the $1/r$ law as predicted by Eq. 2.1 for the 1D case. Thus due to the interaction only the pre-factor $A$ in Eq. 2.1 behaves as a decreasing function of $g$ as shown in Fig. 6.5. We obtained similar results for other values of $V_0$ and positions of the impurity.

In Fig. 6.6 we show FO in non-interacting systems using different boundary conditions. We have also repeated similar studies in case of interacting systems. It is observed that the behaviour of FO with the interactions is independent of the boundary conditions. In the rest of the thesis we restrict ourselves to periodic boundary conditions.

**1D interacting system away from half-filling with a repulsive impurity potential**

In case of half-filled one-dimensional systems we saw that the periodicity and the phase of FO remain unchanged with the interactions. However, if we shift slightly away from the half-filling interactions appreciably influence the periodicity of FO. In Fig. 6.7 we present cases where the average density of the system is equal to $\bar{n} = 0.9$. We show FO is damped faster away from half-filling with increasing interactions. The period and phases are noticeably changed with the interactions. In Eq. 2.1, the term $\cos(2k_Fr + \delta)$ decides the period of the FO. Now in case of 1D systems the Brillouin zone extends from $-\pi/a$ to $\pi/a$, and thus at half-filling the Fermi vector is given by $k_F = \pi/2a$. Now substituting $k_F$ at half-filling in the cosine term and replacing $r$ of the continuous system with $r = na$ for the finite lattice system where $a$ is the lattice constant and $n$ is any integer we get $\cos(2k_Fr + \delta) = \pi n$. Thus the periodicity remains unchanged. However, away from half-filling $k_F \neq \pi/2a$ and hence the above argument does not hold and the period changes.
1D interacting system at half-filling with an attractive impurity potential

Fig. 6.8 shows FO in presence of an attractive impurity potential $V_0 = -2$. The only difference observed from the repulsive case is a peak instead of a dip at the impurity site. The height of the peak decreases with the increasing interactions. The behaviour of FO with interactions remains the same as the repulsive case. This is because of the particle-hole symmetry which appears at the half-filling.

2D interacting system with a repulsive potential

The FO on a surface with non-interacting particles is shown in Fig. 6.9(a) where the system has 31 by 31 lattice sites and the impurity $V_0 = -10$ is located at the center. The symmetry of the square lattice is visible. In Fig. 6.9(b) we show the FO in the interacting case with $g = 3$. The FO are more localised due to the interactions and the oscillation pattern is richer. This sub-section is concluded with a small remark. In case of Approximation A we did not increase the interaction beyond $g = 4$ as the model self-energy is designed to give physically correct result only for low $g$-values in the metallic regime. Thus, it is not possible to study FO
Figure 6.5: Logarithmic variation of the slope of the linear fits with the interactions accounted for using Approximation A in 1D systems. The amplitude of oscillations varies as a decreasing function of interaction.

Figure 6.6: FO for Periodic Boundary Condition (PBC), Open Boundary Condition (OBC), and Natural Boundary Condition (NBC) in 1D interacting system with $N_L = 50$. An impurity potential $V_0 = 2$ is placed at the center. Electronic correlations are accounted for using Approximation A and we present results for $g = 1$.

around the Mott transition and in the insulating system using the model self-energy. Moreover, the results obtained from the model even in the metallic regime needs further validation using the more numerically accurate and reliable DMFT method. Nevertheless, still this simple model offers nice initial insights in the metallic regime and confirms that it is a promising problem to study the effect of interactions on FO.

### 6.3.2 Approximation B ($\Sigma^{Hubl}$)

We now present the results from Approximation B for 1D and 2D systems. We consider a 1D lattice chain with $N_L = 50$ and place a repulsive impurity $V_0 = 2$ at the 25th lattice site. In Fig. 6.10 we see there is no FO for any finite $U$. Some numerical artifact are seen around the impurity for $U = 0.1, 0.5$ due to discretization in our system. It apparently contradicts the results for the low $U$ values as predicted by Approximation A where FO was damped with the interactions but did not completely disappear. The anomalous behaviour happens as the Hubbard I approximation is valid only in the atomic limit for any finite $U$ at which the system is an insulator. Thus Approximation B can only describe FO in insulators.
Figure 6.7: Variation of the local occupation and FO in presence of a single impurity potential \( V_0 = 2.0 \) placed at 20\textsuperscript{th} site in a 1D lattice chain, slightly away from half-filling, where the average occupation of the system is equal to \( \bar{n} = 0.9 \). Different colours correspond to different electronic interactions accounted for using Approximation A.

Figure 6.8: Variation of the local occupation and FO in presence of an attractive single impurity potential \( V_0 = -2.0 \) placed at 25\textsuperscript{th} site in a 1D lattice chain with \( N_L = 50 \). Different colours correspond to different electronic interactions accounted for using Approximation A. The inset shows behaviour of FO in the neighbourhood of the impurity for the different interactions.

Absence of FO for any finite \( U \) has also been observed in case of a 2D (31 by 31 lattice) with an impurity potential \( V_0 = +4 \) at the center using Approximation B. (See Fig. 6.11)

At this point we see that Approximation A cannot describe the system for high interactions in the insulating regime. The behaviour predicted by Approximation A in the metallic regime do not agree with the results from Approximation B. Moreover, using either of these methods it is not possible to judge the behaviour of FO in the intermediate regime around the Mott transition.
6.3.3 Approximation C \((\Sigma^{NRG})\)

Next we attempt to see the behaviour of the system in the metallic, insulating regime and around the Mott transition using Approximation C in 1D, 2D, and 3D systems.

We further test if the critical value \(U_c\) for the homogeneous system at which the Mott transition happens is in accordance to

\[
U_c = 6\sqrt{zt},
\]

as derived by Bulla et.al using linearized Dynamical Mean-Field Theory [124]. The coordination number \(z = 2, 4, 6\) for 1D, 2D, and 3D systems respectively.
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Figure 6.10: Variation of local electronic occupation and absence of FO in 1D system with an impurity $V_0 = 2$, placed at the 25th site. Different colours correspond to different interactions accounted for using Approximation B. Absence of oscillation is already observed for $U = 1$ since in this approximation the Hubbard gap opens for any finite $U$ and the system behaves as an insulator. We only observe numerical noise.

Figure 6.11: Absence of FO in 2D interacting lattice system in presence of single impurity potential using Approximation B for $U = 2$. Contour plot of the local occupation $n_i$ for electrons on a $31 \times 31$ square lattice with impurity potential $V_0 = -24$ located at the center is shown. We observe only numerical noise.

1D systems

Again we start our discussion with the 1D lattice chain. We place a repulsive single impurity potential $V_0 = 2$ at the 25th site of a 1D lattice chain with $N_L = 50$.

In Fig. 6.12 we present the variation of the local electronic occupation for the different interaction parameters $U$. We observe that in the metallic phase for $U < 8$ the amplitude of oscillations decreases with interactions while the period and phase-shift remain unchanged. However, oscillations are hardly visible around $U = 8$ and completely disappears beyond it in the insulating phase. Thus apparently a Mott transition happens around $U \approx 8$ as predicted by Eq. 6.14. Thus it shows that FO is absent at the Mott transition and beyond it at the insulating phase. In order to have a more quantitative understanding on the decay of
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Figure 6.12: Variation of electronic density per lattice site and FO. An impurity potential $V_0 = 2$ is applied at the 25th site in a 1D lattice with $N_L = 50$. Different colours correspond to different electronic interactions accounted for using Approximation C. The Mott transition occurs between $U = 8$ and $U = 9$ around which FO just disappears. The inset shows behaviour of FO with interactions in the neighbourhood of the impurity site.

The amplitudes with the interaction we plot $|n_i|$ from Fig. 6.12 vs the inverse of the relative distance from the impurity site, i.e. $1/|r_i - r_{imp}|$.

In Fig. 6.13(a) we see that Eq. 2.1 is obeyed and even for the interacting systems the oscillations follow an asymptotic linear decay. We perform a linear regression fit and compute the slopes of the straight lines which decrease with the interactions as shown in Fig. 6.14. The logarithm of the slopes versus the interaction is shown in Fig. 6.14. We observe that in the metallic phase it decreases as $\exp(-U^2)$ up to the Mott transition. Then in the insulating phase it decreases as $\exp(-U)$. A sharp change of behaviour is seen around the Mott transition at $U \approx 8$.

Thus in the metallic phase the results are in agreement as predicted by Approximation A. A qualitative comparison of the local occupation calculated by using the Approximation A and Approximation C is presented in Fig. 6.15. We find that FO is damped faster in case of Approximation A. However, the reader should note that the parameter $g = 1$ and $U = 1$ are not equivalent though both corresponds to the electronic interactions in the system.

The absence of oscillations in the insulating phase as described by the Approximation B is also confirmed. Thus Approximation C gives us a complete picture of both metallic and insulating phases and the behaviour at the Mott transition at zero temperature. This further proves the uniqueness of DMFT in studying FO at Mott transitions.

2D systems

We next attempted to study higher dimensional (2D and 3D) systems where Landau quasi-particles exist and for which the DMFT approximation is more physically suitable. 2D and 3D systems are also interesting from an experimental point of view for real materials. In case of 2D we consider a 31 by 31 square lattice system and place an impurity potential $V_0 = 4$ at the center. In order to facilitate computation we map the 2D lattice into a 1D system such that nearest neighbour hopping and periodic boundary conditions are still preserved. The mapping procedure is discussed in details in the Appendix B. Once the densities are computed we perform an inverse mapping to recover results for the two-dimensional systems. We plot the surface density profile Fig. 6.16, contour plot Fig. 6.17 to visualize FO in the square lattice for different interactions. We observe that the range of oscillations are suppressed and FO is more localized around the impurity with the increasing interaction on the metallic side.
Figure 6.13: Variation of the maxima of the local occupation with the inverse of the relative distance from the impurity site for different interactions accounted for using Approximation C. An impurity potential $V_0 = 2$ is applied at the 25th site of a 1D lattice with $N_L = 50$. The $1/r$ relation is in principle obeyed as in the non-interacting case. Slopes decrease with the increasing interactions tending to zero on the insulating side. Points show the data while the dotted lines show linear fits. (a) We present the variation for all lattice sites, (b) We zoom in the variation in the asymptotic regime of Fig. 6.13(a).

Damping of FO in 2D with the increase in the interactions have been also observed by Andrade et.al using slave boson theory [18]. According to Eq. 6.14, $U_c = 12$ for 2D system. In Fig. 6.17 we see FO is heavily suppressed for $U = 8$ and no FO is observed for $U = 12$ apart from some numerical noise.
Figure 6.14: Logarithmic variation of the slopes in Fig. 6.13(a) with the interaction (U) where the interactions are accounted for using Approximation C. The left region of the plot with $U < 8$ corresponds to the metallic regime where FO decays as a decreasing function of U. The right region with $U > 9$ corresponds to the insulating regime where the decay exponentially decreases with U. A distinct change in behaviour is observed in the cross-over region (Mott transition) between $U = 8$ and $U = 9$ which is indicated with a dotted box.

Figure 6.15: A qualitative comparison of FO in the metallic phase $g = 2$ and $U = 2$ where electronic interactions are accounted for using Approximation A and Approximation C respectively. An impurity potential $V_0 = 2$ is applied at the $25^{th}$ site of a 1D lattice with $N_L = 50$.

In order to have a similar quantitative analysis of the decay of FO like in case of 1D, we map the lattice surface such that the density variation in each row of the square lattice is plotted with a small lateral shift in Fig. 6.18. We want to study if the decay follow Eq. 2.1 for $d=2$. No oscillations are observed along the diagonal of the square lattice due to the symmetry in the geometry of the system. In Fig. 6.19(a), we study $|n_i|$ versus the square of the relative distance from the impurity along a sectional cut slightly away from the diagonal.

We see FO decays as $1/r^2$ and thus obeys Eq. 2.1. We perform a linear regression fit and calculate the slopes of the straight lines in Fig. 6.19(a).

Again we present the logarithm of slopes vs interaction in Fig. 6.20. The behaviour is exactly similar to 1D as depicted in Fig. 6.14 and a sharp change around $U_c = 12$ is observed this
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Figure 6.16: Variation of the local electronic occupation on a $31\times31$ square lattice with impurity potential $V_0 = 24$ located at the center. A surface density profile is shown for $U = 0, U = 2, U = 8, U = 12$ where the electronic correlations are accounted for using Approximation C. The white area in the plots implies that the data is out of the range of plot. It corresponds to the impurity site which has a very low density.

Even for the 2D systems the results obtained from Approximation C matches with those from Approximation A in the metallic regime and the Approximation B in the insulating regime. Note that in Fig. 6.17 the contour plots may apparently indicate absence of the symmetry of square lattice. However, the same data represented in Fig. 6.18 plotted using another method exhibits the symmetry. Thus it is confirmed there is no debate over the data. Rather, the lack of symmetry in the contour plot is understood a numerical artifact of contour plots.

3D systems

The study of FO in 3D systems is the most interesting case in the context of real materials. However, as already mentioned conducting the studies for higher dimensions using our method is computationally demanding. In order to study a commensurately large system (e.g. $31 \times 31 \times 31$) lattice like in the case of 2D, one faces problems with the huge computer memory requirement. In our techniques we map higher dimensional lattices to 1D for facilitating computation. In case of a cubic lattice the number of lattice sites is $N_v^3$ after such a mapping where $N_v$ is the number of lattice sites in each row. Thus in case of a $(31 \times 31 \times 31)$ lattice one
Figure 6.17: Variation of the local electronic occupation on a $31 \times 31$ square lattice with impurity potential $V_0 = 24$ located at the center. A contour density profile is shown for $U = 0, U = 2, U = 8, U = 12$ where the electronic correlations are accounted for using Approximation C. The white area in the plots implies that the data is out of the range of plot. It corresponds to the impurity site which has a very low density.

needs to invert a matrix of dimension $(29791 \times 29791)$ where each element of the matrix is a complex number with 64-bits. This was not achievable with our present scheme of calculation and available computation power. However, using our present techniques it was possible to generate a $11 \times 11 \times 11$ lattice.

We studied FO placing an impurity $V_0 = 6$ at the body center of the cubic lattice. We divide the lattice into horizontal planes which are enumerated from zero to ten. The crystallographic direction can be interpreted from the Miller indices of each plane given by $(0 \ 0 \ n)$, where $n$ is the number of the plane [125]. Fig. 6.21 shows the surface density plot of different cross-sections of the cubic lattice for $U = 0$.

In Fig. 6.22, we present the local electronic occupation in the planes (005) (containing the impurity), plane (007), (two planes away from the impurity), plane (009) (four planes away from the impurity). In plane (005) we observe the presence of impurity in the center, FO is observed and it is damped with the interactions. No oscillations are observed for $U = 6$ and beyond it.

In case of the planes away from the impurity we see surface patterns which change for the different interactions and FO is absent for $U = 6$ and beyond in each case. This confirms that the oscillations propagate inside the cube and also affect the planes neighbouring to the
Figure 6.18: Surface map to show variation of the local electronic occupation on a $31 \times 31$ square lattice with impurity potential $V_0 = 24$ located at the center for $U = 2, \ U = 5, \ U = 8, \ U = 10$ where the electronic correlations are accounted for using Approximation C. The density variation in each lattice chain is plotted with a lateral shift of 0.001. The site containing the impurity is removed.

impurity plane. We have further studied the local occupation in equidistant planes on either sides of the impurity planes (e.g. (003) and (007) in Fig. 6.23 and found the behaviour of oscillations for the different interactions very similar. This further confirms that the screening cloud is compressed on whole by volume due to the interactions but the shape of it is not changed. In other words the compression is isotropic and the symmetry of the screening cloud is preserved.

Owing to the small lattice size the number of data points are not adequate for a comprehensive study of the behaviour of the decay.

6.3.4 R-DMFT+CTQMC

Finally we present the results from the RDMFT+CTQMC method. We first comment on the choice of different parameters used in our simulations.

Convergence criterion

This method is numerically exact provided we perform a sufficient number of Monte Carlo steps to reach the convergent solution. We start with an initial number of Monte Carlo steps ($\approx 10^5$) which is increased by a factor of 1.1 after each DMFT iteration. Several Monte Carlo steps need to be performed till a convergent solution is achieved, e.g. a convergence of the order of $\text{conv} = 0.005$ where the variable $\text{conv}$ denotes the convergence criteria, is achieved after $8 \times 10^5$ Monte Carlo steps for 1D systems with $U = 1$ and $\beta = 20$. Next we explain what do we mean by a convergent solution and how we measure it. A solution is accepted to be convergent if the difference between the maximal values of the Green’s function in $\tau$ space for the last two iteration is less than the value of a given critical convergence criteria set by us for all lattice sites, i.e. $\max_{\tau,i}|G_i(\tau)^{\text{iter}} - G_i(\tau)^{\text{iter}-1}| < \text{conv}_{\text{crit}}$. $G_i(\tau)^{\text{iter}}$ stands for the Green’s function in the $\tau$ space for a particular iteration (iter), $\text{conv}_{\text{crit}}$ denotes the critical convergence criteria, $\max$ denotes the maximal values. Lower value of the convergence criteria corresponds to a better accuracy but larger time for calculations. We optimize the degree of accuracy in order to achieve our desired physical results. Moreover, we also verify if local occupation calculated using Eq. 5.19 for the last three consistently convergent iterations differ within the statistical error limit to confirm if solutions are convergent. In Fig. 6.25 we present the density profile of 1D systems for $\beta = 20$ in the last three iterations with a convergence
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Figure 6.19: A chain is cut along slightly away from the diagonal of a 31 × 31 square lattice with impurity $V_0 = 24$ at the center. Variation of the maxima of the local occupation $|n_i|$ with the square of the relative distance from the impurity site is studied for different interactions accounted for using Approximation C. Points show the data while dashed lines show linear fits.

criteria ($\text{conv} = 0.005$). We see the variation in the density is within the statistical error limit.

It was more difficult and time consuming in case of 2D systems to reach lower convergence criteria and hence we have performed our calculations for $\text{conv} = 0.01$ which was tested to have a fair accuracy to be close to the true solution.
Figure 6.20: The logarithmic variation of the slope of the straight lines in Fig. 6.19(a) for different interactions. Distinct change of behaviour of the slope at the Mott transition is visible like in case of 1D. Electronic correlations are accounted for using Approximation C.

Figure 6.21: Variation of the local electronic occupation on a \((11 \times 11 \times 11)\) 3D cubic lattice, for a non-interacting system \((U=0)\), with impurity potential \(V_0 = 6\) located at the body center of the cube \((5, 5, 5)\). A 3D surface density profile of the plane \((005)\) containing the impurity (left figure); \((007)\) which is two planes away from the impurity (middle figure); and \((009)\) which is four planes away from the impurity (right figure) is shown for \(U = 0\). The bar legend at the bottom shows the density gradient.

**Choice of temperature**

As already mentioned, FO can only be studied at finite temperatures using this method. This brings us to two important points - i) what is the maximum temperature at which FO are visible and the effects of interactions can be still significantly observed in them? ii) what would be the value of \(U_c\) for Mott transition in case of 1D, 2D, and 3D lattices in finite temperature. The second information is required to make a judgment if FO disappears at the Mott transition even at finite temperature. It is further interesting to see if the general behaviour of FO is consistent for \(T = 0\) and finite temperature.
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Figure 6.22: Variation of the local electronic occupation on a $11 \times 11 \times 11$ 3D cubic lattice, for different interactions, with impurity potential $V_0 = 6$ located at the body center of the cube $(5, 5, 5)$. A 3D surface density profile of the plane (005) containing the impurity (upper panel); (007) which is two planes away from the impurity (middle panel); and (009) which is four planes away from the impurity (lower panel) is shown each for $U = 1$, $U = 3$, $U = 6$ where the electron correlations are accounted for Approximation C. The bar legend at the bottom shows the density gradient.

At finite temperature two factors contribute in quenching of FO:

- Effect of temperatures
- Effect of electronic correlations

At low-temperature a sharp-edge at the Fermi surface exists in the k-space. However, as the temperature increases the edge softens and thus FO in the real-space also decays. Again, as the electronic correlations $U$ is increased, the Fermi edge disappears due to the appearance of the Hubbard gap and consequently FO slowly disappears.

It is of potential interest to further estimate the temperature for which the Fermi-edge is sharp enough to observe FO in non-interacting systems. For such an optimised temperature, the effect of correlations on FO and hence the behaviour of FO across the metal to insulator transition can be well-understood. In Fig. 6.26 we show how the Fermi edge behaves with $\beta$. 

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Figure 6.23: Variation of the local electronic occupation on a $11 \times 11 \times 11$ 3D cubic lattice with impurity potential $V_0 = 6$ located at the body center of the cube (5 5 5) at equidistant plane on either direction of the impurity potential. A 3D surface density profile of the plane (003) (upper panel) and (007) (lower panel) which are equi-distant from either sides of the plane (005) containing the impurity is shown each for $U = 1$ and $U = 3$ where the electron correlations are accounted for Approximation C. The bar legend at the bottom shows the density gradient.

It is observed that for $\beta = 1$ the Fermi edge does not exist. It slowly appears from $\beta = 5$ where still the edge is very soft. At $\beta = 20$ one clearly sees the Fermi edge. The sharpness of the edge at $\beta = 50$ is very close to $\beta = 10000$ and negligible changes occur on further increasing $\beta$ or in other words lowering the temperature. It is computationally expensive and time consuming to perform our simulations using CTQMC for higher values of $\beta$, $\beta = 20$ is chosen to be an acceptable limit of low temperature to study the behaviour of FO in Mott insulators. We have performed our studies for low values (e.g. $\beta = 5$), high values (e.g. $\beta = 20$) and have made a comparative analysis. A rough estimation of $U_c$ for Mott transition at finite temperature for finite lattice systems has been made from the $U$-$T$ phase diagram for a cubic lattice as presented in the Appendix A.
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Figure 6.24: Comparison of the calculation of the electronic density per lattice site calculated using $\langle \hat{n} \rangle = 1 + G(\tau) = 1 + G(0^+) + G(0^+)$ where $G(0^+)$ is the Green’s function for $\tau = 0$ and directly from the Monte Carlo average using Eq. 5.80 and Eq. 5.19. $G(\tau)$ in turn was calculated from the Green’s function in Matsubara space which is again calculated directly using Monte Carlo. We consider a 1D lattice chain with $N_L = 50$, $U = 1$, $\beta = 20$ and $\text{conv} = 0.005$. We choose the i) number of Matsubara frequency = 200, ii) number of Monte Carlo steps = $10^5$, iii) a convergence criteria $\text{conv} = 0.005$.

Figure 6.25: Density profile in 1D lattice system with $N_L = 50$ and $V_0 = 2$ at the 5$th$ lattice site for $U = 1$, $\beta = 20$, convergence criteria $\text{conv} = 0.005$ is shown. We choose the i) number of Matsubara frequency = 200, ii) number of Monte Carlo steps = $10^5$. The densities computed using $\langle \hat{n} \rangle = 1 + G(\tau)$ as explained in Fig. 6.24 in the last three consistently convergent iteration is presented. The differences are seen to be within the statistical error limit showing that the required convergence is achieved.

1D system

Our analysis follows exactly a similar trend like the previous methods. We consider a one-dimensional lattice chain with $N_L = 50$ and place a repulsive impurity potential $V_0 = 2$ at the 5$th$ lattice site. We present our results for $\beta = 5$ in Fig. 6.27(a) which corresponds to a higher temperature and $\beta = 20$ in Fig. 6.27(b) which is an acceptable low temperature to replicate...
the results close to $T = 0$. In Fig. 6.27(a) we see that the oscillations appear only around the impurity and thus the range is small. However, still one sees the damping of amplitudes with the interactions even if one takes into account the error due to statistical fluctuations. The period and phase-shift of oscillations remain unchanged. In Fig. 6.27(b) we see that the oscillations get sharper with the decrease in the temperature as expected. Moreover, the effect of damping of the amplitudes due to the interactions is more prominently visible in case of low temperatures. The constancy in the period and phase of oscillation remain unaffected by the decrease in the temperature.

Again in order to have a quantitative idea about the decay of FO we plot $|n_i|$ with its statistical error versus the relative distance from the impurity in Fig. 6.28(a) ($\beta = 5$) and Fig. 6.28(b) ($\beta = 20$). The asymptotic linear decay is visible in agreement with Eq. 2.1 even in the presence of interactions for both the temperatures. In case of $\beta = 5$ we see more noise in the asymptotic regime as compared to $\beta = 20$. This is due to the small range of FO only around the impurity for higher temperature or low $\beta$. We make a cut in order to reject the noise and perform a linear regression fit on the linear part of the data. (See Fig. 6.29(a) and Fig. 6.29(b)). Then we measure the slope of straight line in Fig. 6.29(a) and see the logarithm of slope decreases with $U$ in Fig. 6.30. Thus all behaviour is consistent with our previous methods, particularly Approximation C. It is further seen that the Mott transition occurs earlier ($U = 6$) for $\beta = 5$ due to finite temperature effect as compared to the $T = 0$ case where $U_c = 8$.

**2D system**

We extend our studies also for the 2D systems using this method. We placed a repulsive impurity potential $V_0 = 6$ at the center of a $31 \times 31$ square lattice. It was indeed a difficult system to solve which needed a long time on a single processor with 1.2 GHz. However, since the impurity was placed at the center we could use the four-fold symmetry of the square lattice and solve the SIAM only at the non-equivalent sites and copied the results for the equivalent sites. In this way we reduced our computational time by a factor of four. Still it was difficult to perform calculations beyond a convergence criteria of $\text{conv} = 0.01$ owing to the time factor. It needed about 3-4 weeks of calculation to achieve results for e.g. $\beta = 20$, $U = 6$ even for the above mentioned convergence criteria. It has been hard to visualize the effects of interactions on FO in 2D using this method. However, in Fig. 6.31(a); Fig. 6.31(b) ($U = 1$) and Fig. 6.32(a); Fig. 6.32(b) we present similar surface maps like in the case of Approximation C for $U = 1$ and $U = 5$ respectively. The density of the lattice sites corresponding to each row is shifted by a small factor and the site containing the impurity potential is excluded. Weak effects of the damping on the oscillations with the increase in the interactions are visible. It was...
Figure 6.27: Variation of the local occupation and FO in presence of the single impurity potential $V_0 = 2.0$ placed at 5$^{th}$ site in a 1D lattice chain with $N_L = 50$ for finite temperatures. Different colours correspond to different electronic interactions which is accounted for using R-DMFT+CTQMC. Since it is a Monte Carlo calculation the corresponding stochastic error bars are also shown. The inset shows the behaviour of FO in the neighbourhood of the impurity. We choose the i) number of Matsubara frequencies $= 200$, ii) number of Monte Carlo steps $= 10^5$, iii) a convergence criteria $\text{conv} = 0.005$. (a) Shows the behaviour for a high temperature corresponding to $\beta = 5$. (b) Shows the behaviour for a low temperature corresponding to $\beta = 20$.

difficult to perform further quantitative analysis concerning the decay of FO with the existing data. However, we would see in the next section that screening effects were visible even for the 2D systems using RDMFT+CTQMC which gave indirect evidence of the significant effect of interactions on the oscillations.

6.4 Numerical results for N-screening charge

We see in Fig. 6.12 that there is a dip in the local occupation at the lattice site containing the repulsive impurity potential. The dip gets shallower with the increasing interactions. In order to preserve the charge neutrality of the system it is required that the change in the local
Figure 6.28: Variation of the maxima of the local occupation with the inverse of the relative distance from the impurity site using R-DMFT+CTQMC. A single impurity potential $V_0 = 2.0$ is placed at the 5th site in a 1D lattice chain with $N_L = 50$. The corresponding Monte Carlo error bars in the density is shown. The electronic densities are the same as in Fig. 6.27(a) and Fig. 6.27(b). The $1/r$ relation is in principle obeyed as in the non-interacting case. Slopes decrease with the increasing interactions tending to zero on the insulating side. (a) Shows the behaviour for a high temperature corresponding to $\beta = 5$. (b) Shows the behaviour for a low temperature corresponding to $\beta = 20$.

occupation at the impurity site should be compensated by an appropriate change in the local occupation at other sites. In order to quantitatively study the phenomenon we calculate the $N$-screening charge of the system defined by Eq. 6.13 for different interactions. We calculate the $N$-screening charge corresponding to the electronic densities obtained from Approximation C and R-DMFT+CTQMC respectively.

6.4.1 Approximation C ($\Sigma^{NRG}$)

The variation of the $N$-screening charge with a) the impurity potential and b) the electronic interactions is studied for the 1D, 2D, and 3D lattice systems.
N-screening charge in 1D systems

In Fig. 6.34 we observe that the variation of the N-screening charge with the impurity charge for different interactions is a family of sigmoid curves. Systems in the metallic, insulating and Mott insulating phases have been studied. The steepness of the curves decreases with the increasing interaction showing that electronic interactions weaken the screening effects. In Fig. 6.33 a comparative study using Approximation A shows a similar behaviour.
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We further study the variation of the N-screening charge with interaction for a small impurity $V_0 = 2$ and a large impurity $V_0 = 7$ in Fig. 6.35. We see the decrease of N-screening charge with increasing $U$ in the metallic phase. In the insulating phase the decrease is exponential. The rate of change is faster in case of a small impurity potential. However, in both cases a sharp change of behaviour near the Mott transition is observed. $U_c$ for the Mott transition is again in agreement with Eq. 6.14. The behaviour for the corresponding negative impurity potentials obeys a point symmetry. We attempted to find an effective potential for which the N-screening charge is invariant. However, such an invariance in the N-screening charge could not be observed.

N-screening charge in higher dimensional systems

We further compute the N-screening charge for the 2D and 3D systems from Eq. 6.13. In Fig. 6.37 the variation of $Z_{sc}$ with $U$ is studied for different impurities. We show the variation of $Z_{sc}$ with the impurity potential for different interactions in Fig. 6.13. In Fig. 6.39 and Fig. 6.38 the variation of $Z_{sc}$ with $U$ and $V$ is shown for 3D system respectively. Fig. 6.37 and Fig. 6.39 show that the Mott transition happens at $U_c = 12$ and $U_c = 15$ for 2D and 3D respectively which is again in agreement with Eq. 6.14.

In all the above cases the behaviour of the N-screening charge is similar to the 1D case. It is difficult to visualize the effect of interactions on FO in 3D owing to the small system size. However, the trend in behaviour of the N-screening charge is universal for the 1D, 2D and 3D case. It also establishes that the initial results from the 1D studies give us a reliable idea about the higher dimensional cases. The behaviour of the N-screening charge with $U$ in case of 3D shows that the screening cloud is compressed on whole with increasing the interactions.

Comparison of the N-screening charge with Fermi Renormalization factor

In order to get a better understanding of the mathematical form of the N-screening charge, we try to numerically find its relation with the Fermi-renormalization factor as calculated by R. Bulla using linearized DMFT [126]. It is defined by

$$Z_F = \left( \frac{1}{1 - \frac{d\text{Re} (\Sigma(\omega))}{d\omega}} \right)_{\omega=0}.$$

(6.15)
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Figure 6.31: Surface map to show variation of the local electronic occupation on a (31 × 31) square lattice with impurity potential $V_0 = 6$ located at the center for $U = 1$ where correlations are accounted for R-DMFT+CTQMC. The density variation in each lattice chain is plotted with a lateral shift. The site containing the impurity is removed. We choose the i) number of Matsubara frequencies $= 200$, ii) number of Monte Carlo steps $= 10^5$, iii) a convergence criteria $conv = 0.01$. (a) Shows the behaviour for a high temperature corresponding to $\beta = 5$. (b) Shows the behaviour for a low temperature corresponding to $\beta = 15$.

We use the real part of the self-energy calculated using Approximation C for the homogeneous system to compute the derivative around $\omega = 0$. A log-log plot in Fig. 6.40(a), Fig. 6.40(b), Fig. 6.40(c), shows a power-law dependence between the two quantities for a 1D, 2D and 3D lattice respectively. Based on our studies in the 1D, 2D and 3D case, we universally observe

$$Z_{sc} = AZ^B,$$

where $A$ is an increasing function of the impurity potential $V$ while $B$ is a decreasing function of $V$. We could not determine any universal constant value for the exponent with our existing data.
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Figure 6.32: Surface map to show variation of the local electronic occupation on a $31 \times 31$ square lattice with impurity potential $V_0 = 6$ located at the center for $U = 5$ where correlations are accounted for R-DMFT+CTQMC. The density variation in each lattice chain is plotted with a lateral shift. The site containing the impurity is removed. We choose the i) number of Matsubara frequency $= 200$, ii) number of Monte Carlo steps $= 10^5$, iii) a convergence criteria $\text{conv} = 0.01$. (a) Shows the behaviour for a high temperature corresponding to $\beta = 5$. (b) Shows the behaviour for a low temperature corresponding to $\beta = 15$.

Explicit dependence of electronic density at the impurity site on $V$ and $U/g$

As mentioned in the previous section, we observed a power law dependence between $Z$ and $Z_{sc}$ given by Eq. 6.16. Analysing the fitted values of $A$ and $B$ for the different dimensions we arrived at an approximate empirical relation of $A$ and $B$ with the impurity potential $V$ given by $A = k_1 V$ and $B = k_2 V$ where $k_1$ and $k_2$ are constants having a magnitude around one. Assuming this approximate relation holds we tried to find the explicit dependence of the electronic density at the impurity site with $V$ and $U$. Plugging in $A$ and $B$ in Eq. 6.16 and using Eq. 6.15 we get

$$Z_{sc} = k_1 V \left( \frac{1}{1 - \left. \frac{d \text{Re} \Sigma(\omega)}{d\omega} \right|_{\omega=0}} \right)^{\frac{k_2}{k_1}}. \quad (6.17)$$
Figure 6.33: Variation of the N-screening charge ($Z_{sc}$) defined by Eq. 6.13 with the impurity potential for different interactions in a 1D lattice chain with $N_L = 50$. In each case the impurity is placed at the 25th site. Electronic correlations are accounted using Approximation A.

Figure 6.34: Variation of the N-screening charge ($Z_{sc}$) defined by Eq. 6.13 with the impurity potential for different interactions in a 1D lattice chain with $N_L = 50$. In each case the impurity is placed at the 25th site. Electronic correlations are accounted using Approximation C.

Let \( \left( \frac{d\rho_{\Sigma}}{d\omega} \right) \mid_{\omega=0} \) be a function of interaction only, given by $F(U)$. Combining the original definition of the N-screening charge Eq. 6.13, and Eq. 6.17 we get

\[
\sum_{i \neq i_{\text{imp}}} (n_i - \bar{n}) = k_1 V \left( \frac{1}{1 - F(U)} \right)^{k_2}. \tag{6.18}
\]

If $N_L$ is the total number of lattice sites, and $\bar{n}$ be the average occupation, we obtain the total occupation in all lattice sites excluding the impurity site as,

\[
\sum_{i \neq i_{\text{imp}}} n_i = (N_L - 1)\bar{n} + k_1 V \left( \frac{1}{1 - F(U)} \right)^{k_2}. \tag{6.19}
\]
Figure 6.35: Variation of the N-screening charge with interaction (U) for different impurities in a 1D lattice chain with $N_L = 50$. In each case the impurity is placed at the 25th site. Electronic correlations are accounted using Approximation C. Change of behaviour at the Mott transition (between $U = 8$ and $U = 9$) as predicted by Eq. 6.14 is observed.

Figure 6.36: Variation of the N-screening charge defined by Eq. 6.13 with the impurity potential for different interactions in 2D systems. An impurity potential $V_0 = 4$ is applied at the center of the $31 \times 31$ square lattice. Electronic correlations are accounted for using Approximation C.

In the above summation we used the fact $\sum_{i \neq i_{imp}} \bar{n} = (N_L - 1)\bar{n}$, since $\bar{n}$ is a constant. Now knowing the total occupation including the impurity site is $N_L\bar{n}$, and using Eq. 6.19, the occupation at the impurity site is given as

$$n_{imp} = \bar{n} - k_1 V \left(\frac{1}{1 - F(U)}\right)^{\frac{k_2}{k_1}}. \tag{6.20}$$

Thus we see that the occupation at the impurity site differs from the average occupation by a reduction factor $\lambda = k_1 V \left(\frac{1}{1 - F(U)}\right)^{\frac{k_2}{k_1}}$. $k_1, k_2$ are positive, and $F(U) < 1, \lambda > 0$, for a
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Figure 6.37: Variation of the N-screening charge with the interaction (U) in 2D systems. Change of behaviour at the Mott transition, $U = 12$ is seen. Electronic correlations are accounted using Approximation C.

Figure 6.38: Variation of the N-screening charge with $V$ for the 3D, $11 \times 11 \times 11$ lattice with impurity $V_0 = 6$ placed at the center. Electronic correlations are accounted using Approximation C. We present the cases for $U = 1$, $U = 6$, and $U = 15$.

repulsive impurity potential $V > 0$. Hence the occupation at the impurity site is less than the average occupation and we see a dip. In case of attractive potential $V < 0$, $\lambda < 0$, and thus the local occupation at the impurity site is higher than the average occupation. We have also seen similar behaviour in our numerical results.

Next we attempt to estimate the functional dependence of the density at the impurity site with the interaction parameter for a constant impurity potential. Using the model self-energy in Eq. 6.8, we can analytically calculate $F(U) = -g$, as $g$ is the interaction parameter. Substituting $F(U)$ in Eq. 6.21 we get

$$n_{imp} = \bar{n} - k_1 V \left( \frac{1}{1 + g} \right)^{k_2}.$$

(6.21)

Again for a constant impurity potential, we take $k_1 V = k'_1$, $k_2 V = k''_2$ as constants. Rear-
ranging the terms and taking logarithm on both sides we get

\[ \log \left( \frac{\bar{n} - n_{\text{imp}}}{k''_1} \right) = -k''_2 \log(1 + g). \]  

(6.22)

Using the Taylor expansion, \( \log(1 + g) = (g - \frac{g^2}{2} + \frac{g^3}{3} - \ldots) \) and keeping the first order term only, we obtain from Eq. 6.22 as

\[ n_{\text{imp}} = \bar{n} - k''_1 e^{-k''_2 g}. \]  

(6.23)

Thus we attempted to have some analytical understanding of the dependence of local occupation at the impurity site with the interaction. According to this analysis an exponential dependence is preliminarily observed.

### 6.4.2 RDMFT+CTQMC

We study the variation of the N-screening charge with \( a) \) interactions and \( b) \) temperature using densities obtained from RDMFT+CTQMC. The inverse temperature \( \beta = 1/k_B T \) is has the energy scale in the units of hopping such that \( t\beta = 1 \). The variation of \( Z_{\text{sc}} \) with the temperature also gives us an idea of the \( \beta \) value which can be considered as a low temperature in the context of screening and FQ. Considering the computational complications of this method we have calculated the densities only for two impurity potentials \( V_0 = 2 \) and \( V_0 = 4 \).

Thus we lacked sufficient data for studying the variation of the N-screening charge with the impurity potential in this case. Since this method is based on stochastic sampling like in the case of local occupation we have also calculated the statistical error of the N-screening charge defined by

\[ \Delta Z = \sqrt{\sum_{i \neq \text{imp}} (\Delta n_i)^2}, \]  

(6.24)

where \( \Delta n_i \) is the statistical error of individual densities given by the corresponding standard deviation of the variable.
Figure 6.40: We plot the logarithm of N-screening charge defined by Eq. 6.13 against the logarithm of the Fermi renormalization factor defined by Eq. 6.15. Fig. 6.40(a), Fig. 6.40(b), and Fig. 6.40(c) represents the 1D ($N_L = 50$), 2D ($31 \times 31$), and 3D ($11 \times 11 \times 11$) lattice systems respectively. The power law dependence is observed described by Eq. 6.16 is observed for the 1D, 2D and 3D case. $A$ is an increasing function of $V$ while $B$ is a decreasing function of $V$. Electronic correlations are accounted for using Approximation C. (a) 1D, (b) 2D, (c) 3D lattices.
1D systems

In case of 1D systems we observe in Fig. 6.41 the N-screening charge decreases with the interaction and a sharp change occurs at the Mott transition. The dependence of $Z_{sc}$ with $U$ differs appreciably with $\beta$ till $\beta = 10$, beyond which it becomes independent of $\beta$. Moreover, in case of $\beta = 5$ the Mott transition occurs at $U = 7$ while from $\beta = 10$ onwards, $U_c = 8$ which also agrees with Eq. 6.14 for $T = 0$. This confirms that $\beta = 10$ can already replicate the behaviour of the system in $T = 0$ regime. This fact is further established in Fig. 6.44 where we see that the N-screening charge becomes constant with $\beta$ beyond $\beta = 10$ for all the interactions. Thus we further argue that our choice of $\beta = 20$ as a low temperature where the oscillations are significant, is well-justified. It can thus also be predicted that for real systems even at finite temperature as high as $\beta = 20$ the effects of interactions on FO can be similar as for $\beta = \infty$. It should be promising from an experimentalist's point of view to observe FO in high $T_c$ cuprates or other strongly correlated systems.

![Figure 6.41: Variation of the N-screening charge with the interaction (U) for different temperatures. We consider a 1D lattice chain with $N_L = 50$ and impurity potential $V_0 = 2$ placed at the 5th lattice site. Electronic correlations are accounted for using RDMFT+CTQMC. Since it is a Monte Carlo calculation the statistical error bars are also shown.](image)

2D systems

The trend of behaviour of $Z_{sc}$ with $U$ and $\beta$ in the 2D system shows universality with the 1D case (see Fig. 6.43, Fig. 6.44, Fig. 6.44). However, due to technical issues we could not reach high $U$ values upto $U_c$ where the Mott transition is expected for 2D. Still the decrease in $Z_{sc}$ with increasing $U$ is observed in Fig. 6.44.

6.5 Numerical results for spectral functions

We present the result of the spectral function at different lattice sites (near and far away from the impurity) accounting for the interaction using different methods. It is of particular interest to observe the effects of the additional external impurity on the spectral function at the impurity site.

6.5.1 Approximation A ($\Sigma^{\text{model}}$)

The model self-energy also has both real and imaginary part and thus can capture the effect of interactions in the spectral function. Moreover, it has a generic definition independent of
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Figure 6.42: Variation of the N-screening charge with the inverse temperature ($\beta$) for different interactions. We consider a 1D lattice chain with $N_L = 50$ and impurity potential $V_0 = 2$ placed at the 5th lattice site. Electronic correlations are accounted for using RDMFT+CTQMC. Since it is a Monte Carlo calculation the statistical error bars are also shown.

Figure 6.43: Variation of the N-screening charge with the interaction ($U$) for different temperatures. We consider a 2D square lattice with $(31 \times 31)$ sites and impurity potential $V_0 = 6$ placed at the center. Electronic correlations are accounted for using RDMFT+CTQMC. Since it is a Monte Carlo calculation the statistical error bars are also shown.

...the filling of the system. Thus it is also justified to study the behaviour at the impurity in presence of electronic interactions using this self-energy.

In Fig. 6.47 we present the Local Density of States (LDOS) at the impurity site ($25^{th}$) site for a 1D system having $N_L = 50$. In case of a non-interacting system where $g = 0$ we see the continuous band together with a peak due to an anti-bound state at the energy of the order of $V_0$ at the impurity site. As we go further away from the impurity the height of the anti-bound state decreases, there is a redistribution of the spectral weight and the spectrum slowly resembles like that of a homogeneous system as shown in Fig. 6.46. Moreover, even for small values of the impurity the peak always lies outside the continuous band as seen in Fig. 6.45.
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Figure 6.44: Variation of the N-screening charge with the inverse temperature ($\beta$) for different interactions. We consider a 2D lattice chain with $31 \times 31$ sites and an impurity potential $V_0 = 6$ placed at the center. Electronic correlations are accounted for using RDMFT+CTQMC. Since it is a Monte Carlo calculation the statistical error bars are also shown.

Figure 6.45: Local Density of States at the impurity site for a non-interacting system ($g = 0$) in the presence of different external impurity potential $V_0$. We consider a 1D chain with $N_L = 50$. The additional anti-bound state due to the impurity always lies outside the continuous band.

The peak disappears with increasing $g$ and in addition a pseudo-gap opens at the Fermi energy and resonances appear. The width of the resonances increases with the interaction.

We further study the variation of the spectral function at different lattice sites along the lattice chain for different interactions in Fig. 6.48(a), and Fig. 6.48(b).

In Fig. 6.49(a) and Fig. 6.49(b) we show the behaviour of the spectral function far away from the impurity site (e.g. $40^{th}$ site). We see that the spectral function resembles a homogeneous system and the additional effect of the impurity is not observed.

An universality in the behaviour of the spectral function at the different lattice sites has been observed for 2D systems. In Fig. 6.50(a) and Fig. 6.50(b) we present the spectral function at
Figure 6.46: Local Density of States at different lattice sites for a non-interacting system with \( g = 0 \). The upper panel shows the impurity site (20\textsuperscript{th}) where an anti-bound state corresponding to the impurity potential \( V_0 = 2 \) appears. The peak for has finite width due to the numerical broadening parameter \( \eta = 0.008 \). The middle panel shows the 23\textsuperscript{rd} which is near to the impurity site where we see the height of the peak is reduced and spectral re-distribution occurs. The lower panel shows 40\textsuperscript{th} site far away from the impurity where effect of impurity is not observed and the spectral function resembles that of a homogeneous system.

Figure 6.47: Spectral function at the impurity site for different interactions for a 1D lattice chain with \( N_L = 50 \). Redistribution of spectral weights occur with increasing interaction \( (g) \). The anti-bound state \( V_0 = 2 \) peak for \( g = 0 \) has finite width due to the numerical broadening parameter \( \eta = 0.008 \). Electronic correlations are accounted for using Approximation A.

the impurity site of a 31 by 31 lattice with an impurity potential \( V_0 = -10 \) at the center.

We have also performed semi-analytical calculations on the spectral functions using the model Bethe DOS and the model self-energy in presence of a single impurity which has been presented in Chp 9. The results from those calculations agree with our numerical results presented above.

6.5.2 Approximation B (\( \Sigma^{Hubb} \))

The Hubbard I self-energy used in this approximation only has a real term and is valid for the system at half-filling. In absence of any imaginary term we see discreet bound state as a manifestation of the single impurity. Moreover, at the impurity site the system is far away from half-filling. Thus, the case when the bound state interacts with the continuous lattice is not reproduced in the spectral function in this case. In Fig. 6.51 and Fig. 6.52 we observe a
splitting of the bound-state with the Hubbard sub-bands as we increase the interactions. However, in this approximation it is difficult to comment about the splitting of the peaks as any physical effect of interaction or simple numerical artifact. Far away from the impurity site the spectral function resembles that of a homogeneous system. The universality in the behaviour of the spectral function for different dimensions has also been observed. Some analytical calculations showing the behaviour of the peak with $U$ and $V$ have been presented in Chap 9.

### 6.5.3 Approximation C ($\Sigma^{NRG}$)

The self energy, $\Sigma^{hom}_{NRG}$ obtained from Approximation C has both real and imaginary parts. As already mentioned Approximation C is justified in the asymptotic limit where the system is at half-filling. The system is very far away from half-filling at the impurity site. Though we present our results using this method further verification is required to confirm the features observed in the spectral function at the impurity site.

Fig. 6.53 shows the spectral function at the impurity site i.e. the 25$^{th}$ site for different interactions. At $U = 2$ in the metallic regime a sharp resonance peak is observed at a frequency corresponding to the impurity potential $V_0 = 2$. The quasi-particle peak is seen while the Hubbard sub-bands are still not distinctly visible. Near the Mott transition at $U = 7$ the height of the resonance peak and quasi-particle peak decreases and the Hubbard sub-bands are clearly visible. Resonance humps are observed in the sub-band as an effect of the external impurity. $U = 10$ corresponds to the insulating case where the two sub-bands split completely. The resonance peak and the quasi-particle peak disappears, and the effect of the impurity is only visible in the resonance humps of the sub-bands.
Figure 6.49: A comparative study of spectral function far away from the impurity and a homogeneous system for a 1D lattice chain with $N_L = 50$. Electronic correlations are accounted for using Approximation A. (a) Shows the spectral function at the 40th site which is far away from the impurity site for different interactions. An impurity potential $V_0 = 2$ is placed at the 25th site. (b) Shows spectral function at any lattice site of a homogeneous (without any external impurity) 1D lattice chain with $N_L = 50$ for different interactions. The spectral function far away from the impurity site resembles that of a homogeneous system.

We have also studied the spectral functions at different lattice sites and also for the homogeneous system near the Mott transition in Fig. 6.54. We observe a resonance peak at $V_0 = 2$ and resonance humps in the sub-bands in the spectral function of the impurity site i.e. 25th site. However, far away from the impurity site i.e. at the 40th site no significant effects of the impurity are visible. Rather, the spectral function looks very similar to the one for a homogeneous system. The similarity in the spectral function far away from the impurity site with the homogeneous system reconfirms our assumption of neglecting the inhomogeneous part of the self-energy is well justified at least in the asymptotic limit.

In Fig. 6.55 we observe that the behaviour of the spectral functions in the higher dimensions (2D, 3D) is the same as in 1D.
6.5.4 R-DMFT+CTQMC

Approximation B and Approximation C are suitable only for a half-filled system and cannot describe the spectral function correctly at the impurity site where the system is far away from...
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Figure 6.52: Spectral function at the impurity site for $U = 5.0$ and $U = 10.0$ using Approximation B. An impurity potential $V_0 = 2$ is applied at the 25th site of a 1D chain with $N_L = 50$. The bound state splits more uniformly and the gap between the two subbands increases with the increasing interactions.

Figure 6.53: The spectral function at the impurity site (25th) for different interactions using (Approximation C). An impurity potential $V_0 = 2$ is applied at the 25th site in a 1D lattice chain with $N_L = 50$. The left panel $U = 2$ correspond to the metallic case; middle panel $U = 7$ is close to the Mott transition; right panel $U = 11$ is a Mott insulator. Behaviour of the bound state and resonances due to the impurity are compared for the different interactions.

half-filling. The model self-energy used in Approximation A, which has a generic definition independent of the filling of the system can predict the behaviour of the spectral functions in the presence of the impurity and interactions in the metallic phase only. Still, it needs further validation. Thus we study the spectral function in presence of impurity and interactions using RDMFT+CTQMC in which all inhomogeneities in the self-energy are taken into account. The MaxEnt method discussed in Sec. 6.2 is used for this purpose. We use a classic type of Maxent analysis in order to obtain the Green’s function in real space from the Matsubara space via analytical continuation as described in [123].

Here we present the technical computational details used for computing the Green’s function as input to Maxent. We start our calculations with a convergent solution of self-energy for a criteria of $\text{conv} = 0.005$ in case of 1D systems with a certain value of the impurity potential obtained from our previous analysis using RDMFT+CTQMC. We then make thousand copies of Green’s function with a high number of Monte Carlo steps $2 \times 10^5$. We ensure that the
Figure 6.54: Spectral function at different lattice sites for $U = 7$, i.e., near the Mott transition where correlations are accounted for using Approximation C. An impurity potential $V_0 = 2$ is applied at the 25th site in a 1D lattice chain with $N_L = 50$. The left panel corresponds to the impurity site (25th); middle panel the (40th) site which is far away from the impurity site; right panel shows the spectral function corresponding to $U = 7$ for a homogeneous, continuous, infinite system.

Figure 6.55: Behaviour of the spectral function at the impurity site near Mott transition is presented for 1D, 2D, and 3D. The upper panel shows a 1D system with an impurity potential $V_0 = 2$. The middle panel shows a 2D system with an impurity potential $V_0 = 24$. The middle panel shows a 3D system with an impurity potential $V_0 = 6$. In each an additional anti-bound state is observed at an energy of the order of $V_0$. Resonance effects in the Hubbard sub-bands are observed. Electronic correlations are accounted for using Approximation C.

input data is normally distributed around the mean and uncorrelated in order to have a proper estimate of the statistical error required for the analytical continuation using Maxent.

Fig. 6.56 shows the spectral functions in 1D systems calculated for different interactions corresponding to metallic, insulating and Mott insulating phases in presence of a single impurity potential $V_0 = 4$ at $\beta = 1$. Fig. 6.57 presents the corresponding homogeneous spectral function in absence of any external impurity potential, all other parameters remaining the same as in Fig. 6.56. Some asymmetry is observed in the spectral function corresponding to $U = 1$ in Fig. 6.57 which is unphysical. It is a numerical artifact which arises from the statistical error of the input data and the error from the Maxent. Nevertheless, the additional resonance effects in the presence of the impurity is clearly observed if we make a comparative study between Fig. 6.56 and Fig. 6.57. In Fig. 6.58 we show the spectral functions at different lattice sites for $U = 1$, and it is observed that as we go further away from the impurity site the spectral function resembles more that of a homogeneous system. The behaviour of the spectral function is in agreement with the predictions from Approximation A and semi-analytical calculations.
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Figure 6.56: Spectral functions at the impurity site for 1D lattice with $N_L = 50$ and an impurity potential $V_0 = 4$ at the 5th site. We consider the case of $\beta = 1$ for different interactions using R-DMFT+CT-QMC. The spectral functions are calculated using an analytic continuation of the Green’s function from the Matsubara to the real space using the Maximal Entropy method (Maxent).

using the Bethe DOS presented in Chp. 9. However, the spectral features at the impurity site as seen by Approximation B and Approximation C are not reproduced confirming that these methods cannot explain the interaction of the bound state with the continuous band. Studies of the spectral functions of 2D systems using Maxent are left as future work.

Figure 6.57: Spectral functions for a homogeneous 1D interacting lattice with $N_L = 50$. We consider the case of $\beta = 1$ for different interactions using R-DMFT+CT-QMC. The spectral functions are calculated using an analytic continuation of the Green’s function from the Matsubara to the real space using the Maximal Entropy method (Maxent). All other parameters are the same as in Fig. 6.56.
Figure 6.58: Spectral functions at 5th site containing the impurity, 6th (neighbouring site to impurity), and 2th site (far away from the impurity) are presented. We consider a 1D lattice with $N_L = 50$ and impurity potential $V_0 = 4$. We consider $\beta = 1$ and the interaction is $U = 1$, accounted for using R-DMFT+CT-QMC. The spectral functions are calculated using an analytic continuation of the Green’s function from the Matsubara to the real space using the Maximal Entropy method (Maxent).

6.6 Friedel Sum Rule in interacting systems in presence of single impurity

We numerically verify the conservation of FSR in presence of a single impurity following the formulation presented in subsection 5.5.2. According to Eq. 5.124 there exists a linear relation between the scattering phase-shift and screening charge with a pre-factor of $\frac{\pi}{2}$ in case of a non-interacting system. Our derivation and other literature sources show that FSR is obeyed when all effects of many-body correlations are accounted for [100, 103, 104, 105]. We are interested to see if the linearity is also obeyed, i.e. the screening charge is equal to the scattering phase-shift, if interactions are taken into account using our methods.

We first study the FSR at the finite temperatures $\beta = 5$ and $\beta = 20$. The screening charge is defined by $Z = \sum_i (n_i - n_{hom})$, where $n_i$ is the local occupation per lattice site corresponding to inhomogeneous system ($V \neq 0$). $n_{hom}$ corresponds to the local occupation per lattice site of a homogeneous system ($V = 0$). $Z$ is computed using $n_i$ obtained from R-DMFT+CT-QMC in a 1D system with $N_L = 50$, and an impurity potential $V_0 = 4$ placed at the 5th site for the respective $\beta$ values. We again note that in R-DMFT+CT-QMC the effect of all inhomogeneities in the self-energy are included. However, it is non-trivial to calculate the scattering phase-shift from R-DMFT+CT-QMC since the Green's functions are computed in the Matsubara space and we need to perform an analytic continuation. Hence we compute the phase-shift for the continuous homogeneous systems using Approximation C for $T = 0$. We assume that the Green’s function around the Fermi energy and hence the phase-shift is independent of temperature. The FSR predicts ideally the screening charge should be equal to the phase-shift. Due to our numerical inaccuracies (e.g. choosing a criteria of convergence $conv = 0.005$ for solving DMFT equations), we do not obtain the exact agreement but the sum rule is in principle obeyed with some error. We define the relative percentage error for the deviation of the phase-shift at the Fermi level and screening charge by,

$$D_{FSR} = \left| \frac{\delta(\epsilon_f) - Z}{\delta(\epsilon_f)} \right| \times 100\%$$

(6.25)
Figure 6.59: Verification of Friedel Sum Rule in 1D interacting lattice system with $N_L = 50$. Variation of the percentage error of deviation between the screening charge and scattering phase-shift, defined by Eq. 6.25 with the interaction is shown. An impurity $V_0 = 4$ is placed at the 5th lattice site. Electronic interactions are accounted for using R-DMFT+CTQMC for calculating the screening charge and Approximation C for calculating the scattering phase-shift.

We plot $D_{FSR}$ vs. the interaction $U$ in Fig. 6.59 for $\beta = 5$ and $\beta = 20$. We see that the maximum error is 14 percent while the average value of error is less than 10 percent. We further see the error increases with the increase in interaction and temperature. Thus, even for finite temperatures we obtain a moderate agreement with FSR when the interactions are accounted for using R-DMFT+CT-QMC for calculating the screening charge. We are working to minimize the error in deviation by increasing the accuracy of our calculations. However, if $Z$ is calculated using Approximation A and Approximation C where the inhomogeneities in the self-energy are neglected we could not obtain a good agreement of the numerical results with FSR. Currently we are conducting further investigations to clarify and understand this behaviour.
6.7 Conclusions

Thus, in this chapter we have discussed our numerical results on the effect of electronic interactions on FO in the presence of a single impurity potential using different approximate methods and finally the numerically exact RDMFT+CTQMC method. The results obtained from the different methods have been consistent. The effect of interactions on the oscillation is found to be similar both for finite temperature and in the limit of $T = 0$. In the 1D, 2D and 3D case FO decays as $1/r^d$ both for interacting and non-interacting systems where $d$ is the dimension of the system, and $r$ is the relative distance from the impurity. At half-filling, the amplitude of FO decreases with the interactions while the period and phase remain unchanged. FO disappears at the Mott transition and no oscillations are observed beyond it in the insulating phase. A bound state is observed in the spectral function at the impurity site for the non-interacting system which is replaced by resonances when interaction is switched on. The N-screening charge defined as the sum of deviation in the local occupation in each lattice site from the average occupation, increases with the impurity charge and the behavior is symmetric for positive and negative impurities. The N-screening charge decreases with interactions and an abrupt change in the behavior is observed at the Mott transition. This shows that interactions weaken screening effects. An universality in the variation of the N-screening charge with the impurities and interactions is observed for the 1D, 2D and 3D case. The FSR for interacting system is not obeyed apparently when inhomogeneities in the self-energy of the system are neglected.

The problem of single impurity is revisited in Chp. 9 where we also discuss about the effect of interactions on the scattering phase-shift, calculate the spectral function with a model Bethe DOS and model self-energy using a semi-analytical approach.
Chapter 7

Two/Multiple single-site impurities

In the previous chapter we studied the behaviour of FO in interacting fermionic systems, in the presence of a single-site impurity potential. Now, what happens if we place a second impurity potential in another lattice site and also change its position? The current chapter addresses this issue. Such a two impurity potential is modeled by

$$V_i = V_1 \delta_{i_1} + V_2 \delta_{i_2}$$

where $V_1$ and $V_2$ are the magnitudes of the first and second impurity located at sites $i_1$ and $i_2$ respectively. We also perform some qualitative studies of FO in the presence of more than two impurities, or multiple impurities scattered at different sites of an interacting lattice system. These cases are discussed in Sec. 7.1, and Sec. 7.2 respectively.

7.1 Two impurities

I. Grosu et al. studied the problem of FO in one-dimensional non-interacting electron gas in the presence of two impurities using the linear response theory [15]. The potential in the continuous system was modeled by two delta functions separated by a finite distance given by $V(r) = V_1 \delta(r) + V_2 \delta(r + a)$. They observed that the presence of the second $\delta$ impurity significantly changes the density oscillations (changing the positions of the maxima, minima) depending on the distance between the impurities. They pointed out that this behaviour is due to the interference effect induced by the impurities. Motivated by our results on effects of electronic correlations on FO in the presence of a single impurity, we expect significant effects of electronic repulsion on the interference pattern of FO due to the electronic repulsion. In case of a single impurity we further observed resonances in the spectral function at the impurity site in the presence of correlations due to the external impurity. In this case it is also interesting to see if additional resonance effects are also visible in the spectral functions at the intermediate sites around the neighbourhood of the two impurities. This issue was not addressed in Grosu's work. Moreover, Grosu studied the problem only for 1D continuous systems while we study it in discreet finite lattice systems both in one and two-dimensions.

Like in the case of single impurity we study the i) local occupation, ii) screening charge and iii) spectral function at different lattice sites, particularly the intermediate sites in between the two impurities. In order to save computational time we have performed detailed studies mostly on 1D systems. We have seen the universality in the behaviour of FO with respect to dimensions in our previous studies for the single impurity. Thus, the results obtained from 1D systems are expected to replicate the results of the higher dimensional systems also in this case. This can be verified as a future work performing the studies for higher dimensional systems. However, some preliminary results on the local occupation of 2D systems have also been presented.

The electronic correlations are accounted for using Approximation A and Approximation C only for all the cases of this problem. We study the problem at low temperatures $T = 0$ for a half-filled system using periodic boundary conditions. The local occupation and spectral function have been respectively calculated using Eq. 6.12 and Eq. 5.9 like in Chp. 6. The
definition of the screening charge has been slightly modified and two types of screening charge are calculated which is discussed in details in subsection 7.1.2. However, we could not use the R-DMFT+CTQMC method for this problem due to paucity of time but its scientific merits have been outlined as a future work in Chp. 11.

Figure 7.1: Variation of FO in 1D interacting system in presence of two impurities of equal magnitude for large relative distances between the impurities using Approximation A. We consider a 1D system with \( N_L = 50 \). \( V_1 = 2 \) is kept fixed at the 3\(^{rd}\) lattice site while the position of \( V_2 = 2 \) is varied along the lattice chain. The relative distances between the impurities is given by \( r \). Electronic repulsion in the system is accounted for using Approximation A. Different values of the parameter \( g \) correspond to different interactions.

7.1.1 Local occupation

In the following subsections we present the behaviour of FO for different magnitudes and signs of the second impurity, and varying its position w.r.t. the first impurity. The magnitude and position of the first impurity is always kept constant for the sake of simplicity.

Two repulsive impurity potential of equal magnitude

We place two impurities of equal magnitude, \( V_{01} = 2 \) and \( V_{02} = 2 \), in a 1D lattice chain with \( N_L = 50 \). The position of the first impurity is fixed at the 3\(^{rd}\) lattice site while the position of the second impurity is varied along the 1D lattice chain. We present the variation of the local electronic occupation per lattice site in the presence of electronic interactions as the relative distance between the impurities is changed using Approximation A (see Fig. 7.1 and Fig. 7.2) and Approximation C (see Fig. 7.4 and Fig. 7.5). The behaviour of FO is consistent for both the methods. Interference effects are observed in FO up to a certain cross-over distance \( r = 10 \). For \( r = 1 \) there is an interference minima, while for \( r = 2 \) there is a maxima between the two impurities. FO is observed only in the neighbourhood of the second impurity unlike the single impurity case where the range of FO spreads over the whole lattice chain. This can be interpreted as a consequence of destructive interference between the two impurities. Some oscillations appear at the boundary owing to PBC. Electronic correlations reduce the height/depth of the maxima/minima, or in other words correlations minimize the effects of the
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Figure 7.2: Variation of FO in 1D interacting system in presence of two impurities of equal magnitude for medium relative distances between the impurities using Approximation A. We consider a 1D system with $N_L = 50$. $V_1 = 2$ is kept fixed at the 3rd lattice site while the position of $V_2 = 2$ is varied along the lattice chain. The relative distances between the impurities is given by $r$. Electronic repulsion in the system is accounted for using Approximation A. Different values of the parameter $g$ correspond to different interactions. 

interference. However, correlations do not cause any shift in the positions of maxima/minima. Also in the presence of the second impurity, the amplitudes of FO are damped while the period and phase remain unaffected due to the correlations. Further we see in Fig. 7.4 and Fig. 7.5 at $U = 11$ corresponding to an insulating system beyond the Mott transition no oscillations or interference effects are observed even in the presence of the second impurity. This shows the absence of FO in Mott insulators like the single impurity case even in the presence of the second impurity. A closer investigation on the behaviour of oscillations with the distance between the two impurities in the metallic regime shows complex yet systematic interference patterns till $r = 6$. FO appears in between the impurities from $r = 8$. As we go on increasing the distance between the impurities, beyond a certain cut-off distance (in this case $r = 10$) the oscillations localize with the interactions around the impurities, and they behave more as two independent single-site impurities.

The second impurity has a different sign and magnitude

In Fig. 7.6, Fig. 7.7 we consider the case where the second repulsive impurity potential has different magnitude than the first, $V_{01} = 2$, $V_{02} = 10$. We see the shape of the maxima and minima are different as compared to the previous case where both the potentials have equal magnitude. The other behaviour with the distance is similar, and in this case already beyond $r = 6$ the impurities behave independently. Correlations only suppresses the height of the maxima but do not affect their positions.

In Fig. 7.8 and Fig. 7.9 we study the case where the first impurity potential is repulsive $V_{01} = 2$, while the second is attractive but of equal magnitude $V_{02} = -2$. In this case the behaviour of the oscillations in between the two impurities is complicated. However, again beyond a certain cut-off distance the two impurities behave independently.
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Figure 7.3: Variation of FO in 1D interacting system in presence of two impurities of equal magnitude for large relative distances between the impurities using Approximation A. We consider a 1D system with $N_L = 50$. $V_1 = 2$ is kept fixed at the 3rd lattice site while the position of $V_2 = 2$ is varied along the lattice chain. The relative distances between the impurities is given by $r$. Electronic repulsion in the system is accounted for using Approximation A. Different values of the parameter $g$ correspond to different interactions.

Comparison with the single-site impurity case

In Fig. 7.10 we present a comparative study for a single repulsive impurity ($V_0 = 2$) and two repulsive impurities of equal magnitude ($V_{01} = 2, V_{02} = 2$) in presence of electronic correlations. It is evident that the presence of a second impurity influences the oscillation which is again modified by different electronic correlations. We observed FO in the presence of two impurities have higher amplitude compared to the single-site impurity case.

Local occupation in 2D lattice systems

We further studied the local occupation in a 2D, $31 \times 31$ interacting lattice system at half-filling with PBC in the presence of two impurities. Two impurities of equal magnitude (compare Fig. 7.11) and different magnitude (compare Fig. 7.12) were placed in two lattice sites having coordinates (10,10) and (16,16) along the diagonal of the square lattice. FO were studied for different interactions in metallic and Mott insulating phases. We observe FO around the impurity sites and also interference effects in the metallic phase. FO are absent beyond the Mott insulating phase and only the signature of impurities is observed. However, the results present only a glimpse of the qualitative picture while detailed studies like how the position of the maxima varies with the distance between the impurities as in the case of 1D system were not performed due to lack of time. Interactions localize FO and complex interference pattern in FO are seen in the metallic phase. This problem can be studied for larger lattice systems to estimate a cut-off distance as in case of 1D, beyond which the impurities behave independently.

7.1.2 N- Screening charge

We define two types of screening charge in this case:
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Figure 7.4: Variation of FO in 1D interacting system in presence of two impurities of equal magnitude for small relative distances between the impurities using Approximation C. We consider a 1D system with \( N_L = 50 \). \( V_1 = 2 \) is kept fixed at the 3\(^{rd}\) lattice site while the position of \( V_2 = 2 \) is varied along the lattice chain. The relative distances between the impurities is given by \( r \). Electronic repulsion in the system is accounted for using Approximation C. Different values of the parameter \( U \) correspond to different interactions. \( U = 11 \) corresponds to a Mott insulating phase where no oscillations are observed.

- Total N- screening charge
- Partial screening charge

Total N- screening charge

The total N- screening charge gives the deviation of the electronic density of all lattice sites apart from the impurity sites, from the average density. It is similarly defined as in Chp. 6 by

\[
Z_{sc} = \sum_{i \neq i_{imp1}, i_{imp2}} (n_i - \bar{n})
\]  

(7.1)

where \( i_{imp1} \) and \( i_{imp2} \) corresponds to the first and second impurity site.

The total N- screening charge remains nearly constant as the distance between the impurities is changed with mild oscillations for small distances up to \( r = 10 \). However, the constant magnitude is suppressed with the interactions. We have also studied the cases where the second impurity potential has different magnitude and signs. The behaviour of the total N-screening charge remains similar in case of other repulsive impurity potential with different magnitude. However, if the second impurity potential is attractive, while the first impurity potential is repulsive, and both have equal magnitude the total N-screening charge becomes zero for all the interactions.

Partial screening charge

In case of the partial screening charge we compute the deviation only for the lattice sites lying in between the two impurities. This quantity aims to measure the overall screening effect in
We consider a 1D system with $N_L = 50$. $V_1 = 2$ is kept fixed at the 3rd lattice site while the position of $V_2 = 2$ is varied along the lattice chain. The relative distances between the impurities is given by $r$. Electronic repulsion in the system is accounted for using Approximation C. Different values of the parameter $U$ correspond to different interactions. $U = 11$ corresponds to a Mott insulating phase where no oscillations are observed.

The lattice sites lying in between the two impurities. It is defined by

$$Z_{\text{par}} = \sum_{i=1_{\text{imp1}}+1}^{i_{\text{imp2}}-1} (n_i - \bar{n})$$

We present the variation of partial screening charge with the relative distance between the impurities using Approximation A in Fig. 7.15 and Approximation C in Fig. 7.16. The partial screening charge varies more significantly as the relative distance between the impurities is changed. It oscillates with the distance and the period of oscillation increases for larger distances. The amplitude of oscillations in the partial screening charge is also suppressed by the interactions. The oscillatory behaviour of the partial screening charge should not be confused with the standard FO which are the central topic of this thesis. In Fig. 7.16 we see at $U = 11$, the partial screening charge has no oscillations but increases monotonically with the distance between the impurities. Thus, a sharp change of behaviour in case of this quantity is observed at the Mott transition. It confirms the absence of FO in Mott insulators, even in the presence of the second impurity.

Next we present the variation of the partial screening charge with the distance between the impurities in the presence of interactions. The first impurity potential is repulsive, $V_1 = 2$ while three different cases of second impurity potential are considered: i) $V_2 = +2$ (repulsive potential with same magnitude as the first impurity, see Fig. 7.16) ii) $V_2 = 10$ (repulsive potential with different magnitude than the first impurity), iii) $V_2 = -2$ (attractive potential with equal magnitude as the first impurity).

### 7.1.3 Spectral functions

We further studied the spectral function numerically at different lattice sites with the first impurity potential kept fixed at the 3rd lattice site and different positions of the second impurity.
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Figure 7.6: Variation of FO in 1D interacting system in presence of two impurities of unequal magnitude for small relative distances between the impurities using Approximation C. We consider a 1D system with $N_L = 50$. $V_1 = 2$ is kept fixed at the 3rd lattice site while the position of $V_2 = 10$ is varied along the lattice chain. The relative distances between the impurities is given by $r$. Electronic repulsion in the system is accounted for using Approximation C. Different values of the parameter $U$ correspond to different interactions. $U = 11$ corresponds to a Mott insulating phase where no oscillations are observed.

Potential. We present the case where the second impurity is placed at the 5th lattice site in the following.

Non-interacting case

We first discuss the features of the spectral functions for the non-interacting case. At the 4th site lying exactly between the two impurities one bound state is observed in the energy range of the impurity potential. Moreover, due to interference effects, the continuous band is distorted from that of a homogeneous non-interacting system. However, at other sites in the neighbourhood of the impurity sites, including the impurity sites two bound states with different heights are observed. As we move further away from the second impurity site (i.e. the 5th site), the height of the two bound states decreases till it disappears from the 11th site onwards. The distortion in the continuous band also reduces and it resembles more the homogeneous system as we move away from the second impurity site. This behaviour for the non-interacting lattice system is illustrated in Fig. 7.17

Thus we see that the behaviour of the spectral function, already for the non-interacting case is quite different in the presence of the second impurity as compared to the single impurity case.

Interacting case

When interaction is turned on, the bound state disappears as in the case of the single impurity. Instead, resonance humps appear which shows a certain complex behaviour pattern at different sites along the lattice chain up to a certain distance. Further investigation and experimental studies using STM can offer more insights about this phenomenon. Far away from the second
Figure 7.7: Variation of $F_O$ in 1D interacting system in presence of two impurities of unequal magnitude for large relative distances between the impurities using Approximation C. We consider a 1D system with $N_L = 50$. $V_1 = 2$ is kept fixed at the 3rd lattice site while the position of $V_2 = 10$ is varied along the lattice chain. The relative distances between the impurities is given by $r$. Electronic repulsion in the system is accounted for using Approximation C. Different values of the parameter $U$ correspond to different interactions. $U = 11$ corresponds to a Mott insulating phase where no oscillations are observed.

impurity the spectral function again resembles that of an interacting homogeneous system, as shown in Fig. 7.19.

As we increase the interactions, the general pattern of behaviour of the resonances still remains the same. However, the height of the resonance peak is suppressed and the resonances become wider. Fig. 7.18 shows the behaviour of the spectral function at different lattice sites when the interaction is switched on. We have also performed our studies placing the second impurity at $(r = 11)$. Similar behaviour due to interference at the intermediate lattice sites has been observed.

Finally, we may comment that we could not explain every detailed feature of the spectral functions with our numerical method which involves different approximations. However, it is evident that the interference between the two impurities significantly affects the spectral functions at the neighbouring impurity sites. The inclusion of electronic correlations systematically adds to the complexity in the interference pattern.

### 7.2 Multiple impurities

Kolesnichenko et al. studied the surface electronic structure of transition metal Cr(001) using low temperature scanning tunneling microscopy and spectroscopy [127]. They observed Friedel oscillations around the impurity atoms and the oscillations were anisotropic, i.e. not circular like in the non-interacting case but had distinct asymmetry. Cr(001) produced by the cleavage of a single crystal are automatically clean except surface areas where impurity concentrations slightly exceed the bulk concentration due to the existence of a high dopant zone in the crystal. In order to explain their experimental results they performed first principle calculations using
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Figure 7.8: Variation of FO in 1D interacting system in presence of two impurities of equal magnitude but opposite sign (i.e. attractive and repulsive) for small relative distances between the impurities using Approximation C. We consider a 1D system with $N_L = 50$. $V_1 = 2$ is kept fixed at the 3rd lattice site while the position of the $V_2 = -2$ is varied along the lattice chain. The relative distances between the impurities is given by $r$. Electronic repulsion in the system is accounted for using Approximation C. Different values of the parameter $U$ corresponds to different interactions. $U = 11$ corresponds to a Mott insulating phase where no oscillations are observed.

ab-initio methods mostly based on density functional theory which is essentially a static mean-field approximation approach. Cr(001) belongs to the class of strongly correlated compounds. Motivated by this experiment we wanted to study FO in presence of multiple impurities in interacting lattice systems using DMFT to account for all local electronic correlations. The contaminated surface in their system was modeled by placing multiple single site impurities scattered over our 2D interacting lattice.

We consider five impurities each of magnitude $V_0 = 10$, randomly scattered over a $31 \times 31$ square lattice at sites: $(3,3)$, $(20,5)$, $(5,20)$, $(25,22)$, $(17,28)$. Electronic correlations have been accounted for using Approximation C. Again, we consider a half-filled system with PBC. All other formalism to compute the local occupation follow the description of Chp. 6. In Fig. 7.20, we present results for a weakly correlated ($U = 2$), strongly correlated ($U = 5$), and also the Mott insulating phase ($U = 12$). We see oscillations around the impurities for $U = 2$, and $U = 5$ together with a complex interference pattern in between the impurities which also changes with the interactions. However, no FO is observed at the Mott transition.

7.3 Conclusions

In presence of two/multiple impurities, correlation minimizes the interference effects between the impurities but does not change positions of the maxima and minima of the oscillations at half-filling. Beyond a certain cross-over distance interference effects are negligible and the two impurities behave more as independent single impurities. This distance reduces with the interactions. No oscillation is observed at the Mott transition and beyond it in the Mott insulating phase.

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Figure 7.9: Variation of FO in 1D interacting system in presence of two impurities of equal magnitude but opposite sign (i.e. attractive and repulsive) for large relative distances between the impurities using Approximation C. We consider a 1D system with $N_L = 50$. $V_1 = 2$ is kept fixed at the 3rd lattice site while the position of $V_2 = -2$ is varied along the lattice chain. The relative distances between the impurities is given by $r$. Electronic repulsion in the system is accounted for using Approximation C. Different values of the parameter $U$ correspond to different interactions. $U = 11$ corresponds to a Mott insulating phase where no oscillations are observed.

Figure 7.10: Comparative study of FO in 1D interacting system in the presence of a single impurity potential and two impurities. We consider a 1D system with $N_L = 50$. Electronic correlations are accounted for using Approximation A for $g = 1$. We compare the cases where (i) An impurity $V_0 = 2$ is placed at the 10th site (ii) Two impurities of equal magnitude $V_1 = V_2$ is placed at the 10th and 12th site respectively.
Figure 7.11: Contour plot showing FO in 2D interacting system in presence of two impurities of equal magnitude using Approximation C. $V_1 = V_2 = 24$ is placed at lattice sites (10,10), (16,16) respectively along the diagonal of a $(31 \times 31)$ square lattice. The left panel ($U = 2$) corresponds to a weakly correlated phase, middle panel ($U = 5$) is a strongly correlated phase, the right panel $U = 12$ is the Mott insulating phase where the oscillations are absent.

Figure 7.12: Contour plot showing FO in 2D interacting system in presence of two impurities of different magnitude using Approximation C. $V_1 = 6$ is placed at lattice site (10,10) and $V_2 = 24$ is placed at site (16,16) along the diagonal of a $(31 \times 31)$ square lattice. The left panel ($U = 2$) corresponds to weakly correlated phase, middle panel ($U = 5$) is a strongly correlated phase, the right panel $U = 12$ is the Mott insulating phase where the oscillations are absent.

Phase even in the presence of the second impurity. The total N-screening charge remains nearly constant when the distance between the impurities is varied while the partial screening charge shows oscillations with the variation in distance for the metallic case. However, at the Mott transition the partial charge increases monotonically with the distance thus showing a sharp change in behaviour. In case of multiple impurities we see that the oscillations localize around the impurities with the increasing interactions. The preliminary results in case of multiple impurities offer initial insights on how point defects would manifest FO in real heavy fermionic systems.
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Figure 7.13: Variation of the total N-screening charge with the relative distance between the two impurities, $V_1 = V_2 = 2$. Electronic repulsion in the system is accounted for using Approximation A. Different values of the parameter $g$ correspond to different interactions.

Figure 7.14: Variation of the total N-screening charge with relative distance between the impurities, $V_1 = V_2 = 2$. Electronic repulsion in the system is accounted for using Approximation C. Different values of the parameter $U$ correspond to different interactions. Some mild oscillations are observed for small distances in the metallic phase only.
Figure 7.15: Variation of the partial screening charge with relative distance between the two impurities, $V_1 = V_2 = 2$. Electronic repulsion in the system is accounted for using Approximation A. Different values of the parameter $g$ correspond to different interactions.

Figure 7.16: Variation of the partial screening charge with relative distance between the two impurities, $V_{01} = 2$, $V_{02} = 2$. Electronic repulsion in the system is accounted for using Approximation C. Different values of the parameter $U$ corresponds to different interactions. It oscillates with $r$ in the metallic phase. A sharp change in the behaviour is observed at the Mott transition, where it monotonically increases with $r$. 

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Figure 7.17: Spectral function at different lattice sites for a 1D non-interacting (g=0) lattice system with $N_L = 50$. Two impurities each of magnitude $V_1 = V_2 = 2$ is placed at the $3^{rd}$ and $5^{th}$ site respectively. The upper panel shows the behaviour of the spectral function at the $3^{rd}$ site (impurity site). The behaviour of the spectral function at the other impurity site $5^{th}$ site is also similar. The middle panel shows the behaviour at the $4^{th}$ site which lies in between the two impurities. The lower panel shows the behaviour at the $6^{th}$ site, which is neighbouring to the impurity site.

Figure 7.18: Spectral function at different lattice sites for a 1D interacting lattice system with $N_L = 50$ is shown for $g = 1$ and $g = 4$ where interactions are accounted for using Approximation A. Two impurities each of magnitude $V_1 = V_2 = 2$ is placed at the $3^{rd}$ and $5^{th}$ site respectively. The upper panel shows the behaviour of the spectral function in the $3^{rd}$ site (impurity site). The behaviour of the spectral function at the other impurity site $5^{th}$ site is also similar. The middle panel shows the behaviour at the $4^{th}$ site which lies in between the two impurities. The lower panel shows the behaviour at the $6^{th}$ site which is neighbouring to the impurity site.
Figure 7.19: Spectral function at the 30th site, far away from both the impurity sites for a 1D lattice system with $N_L = 50$ and different interactions using Approximation A. Two impurities each of magnitude $V_1 = V_2 = 2$ is placed at the 3rd and 5th site respectively. It resembles that of a homogeneous system. Different values of the parameter g correspond to different interactions.

Figure 7.20: A contour density plot of a $(31 \times 31)$ square lattice with five impurities each of magnitude $V_1 = V_2 = V_3 = V_4 = V_5 = 10$, randomly scattered over the lattice sites: (3,3), (20,5), (5,20), (25,22), (17,28) for different interactions using Approximation C is shown. The left panel ($U = 2$) corresponds to weakly correlated phase, middle panel ($U = 5$) is a strongly correlated phase, the right panel $U = 12$ is the Mott insulating phase where the oscillations are absent.
Chapter 8

Extended inhomogeneity

In this chapter we present our studies for an extended inhomogeneous potential for one and two dimensional lattices. Models of both spin independent and spin dependent potentials are studied. In case of a spin independent potential the electronic correlations are accounted for by self-energy calculated using Approximation A and Approximation C. In case of spin dependent potential correlations are accounted by the spin dependent Hubbard I self-energy (Approximation B). The system is subjected to periodic boundary conditions in all cases. In case of spin independent systems we choose the chemical potential such that the system is at half-filling. In case of spin-dependent systems we conduct our studies for arbitrary chemical potentials.

8.1 Numerical results for spin independent systems

In this case, the extended inhomogeneity is modeled by a step potential given by \( V_{\sigma} = h\Theta(R - R_i) \), where \( \Theta \) is the step function.

8.1.1 Approximation A

1D

We again start our discussion with a 1D lattice chain with \( N_L = 50 \). We apply a step potential with \( h = 2 \) upto the 25\textsuperscript{th} site and then cut if off. In Fig. 8.1(b) we observe FO upto a certain value of impurity beyond which oscillations disappear for non-interacting systems. The band is completely filled inside the region of step potential while nearly empty outside. In case of an optimized value of impurity (e. g. \( V_0 = +2 \)) for which FO are still observed for the non-interacting case we see that oscillations are damped on increasing interactions. Moreover, the difference in average occupation of electrons inside and outside the potential range minimizes and the system becomes more homogeneous with increasing interactions as shown in Fig. 8.1(a).

2D

In this case we put an impurity +3 at all sites in the first half-plane of a 32 × 32 square lattice while the second half-plane contains no impurities. We again make a contour density plot to study the effects of interactions. As we see in Fig. 8.2(a) and 8.2(b) a higher redistribution of the electronic density takes place at the interface which shows that the system becomes more homogeneous with the increasing interactions.

8.1.2 Approximation C

In Fig. 8.3 the 1D lattice with \( N_L = 50 \) is subjected to a step potential \( V_0 = 2 \). Electronic interactions are accounted for using Approximation C and the cases of metallic, Mott insulating and insulating phases are presented. We see that the behaviour of FO with the interactions
Figure 8.1: FO in the presence of extended inhomogeneity in 1D systems using Approximation A. We consider a finite system with $N_L = 50$ subjected to a step potential given by $V_{i\sigma} = h\Theta(R - R_i)$, where $h$ is non-zero for the sites (0-25) and $h$ is zero for the sites (25-50). We consider periodic boundary conditions. (a) Shows the variation of local occupation for different values of $g$ accounting for the interaction when $h = 2$. (b) Shows the variation of local occupation for different values of $h$ for a non-interacting system ($g = 0$).
is similar to the case when we account for the interactions using Approximation A. Moreover, in this case it is observed that no oscillations are present even at the interface beyond Mott transition when $U = 11$. 

In Fig. 8.4(a), Fig. 8.4(b) and Fig. 8.4(c) we present the contour density plot of FO for a 32 x 32 square lattice subjected to an external inhomogeneous potential $V_0 = 3$ in the first half-plane i.e. upto the coordinates (16,0) and (16,32) for $U = 1$, $U = 5$ and $U = 10$ respectively. Oscillatory effects at the interface decrease with the interactions and the system becomes more homogeneous. The observations are in agreement with those from Approximation A.

### 8.2 Spin-dependent systems with Approximation B

The study of FO has been extended for spin-dependent external magnetic potential in the presence of electronic correlations accounted for using the spin dependent Hubbard I self-energy (Approximation B). We consider a) a smoothly varying potential b) a step potential. The results from the two cases are presented in the following subsections.

#### 8.2.1 Smoothly varying potential

We consider a smoothly varying potential given by

$$V_{\text{ext}} = \sigma V_{\text{ext}} \tanh \left( \frac{R_i - R}{\xi} \right)$$

where $V_{\text{ext}}$ is the maximum height of the potential, $\xi$ gives the characteristic length over which the potential varies. $R$ is any particular lattice site at which we cut off the external magnetic field. $R_i$ is the lattice site in which we calculate the local occupation. We choose $V_{\text{ext}} = 5$ and $\xi = 1$ for our simulations.

In Fig. 8.5(a) we show the absence of FO in the presence of such a smoothly varying potential. Fig. 8.5(b) further shows that even the presence of an additional impurity $V_0 = 2$ at the 40th site does not produce any oscillations. One just sees a dip or a peak at the impurity site based on the nature of the impurity charge.
Figure 8.3: FO in the presence of extended inhomogeneity in 1D systems using Approximation C. We consider a finite system with \( N_L = 50 \) subjected to a step potential given by \( V_{i\sigma} = h\Theta(R - R_i) \), where \( h = 2 \) for the sites (0-25) and \( h = 0 \) for the sites (25-50). We consider periodic boundary conditions. The variation of local occupation for different values of \( U \) accounting for the interaction is shown.

Figure 8.4: FO in the presence of extended inhomogeneity in 2D systems using Approximation C. We consider a 32 × 32 lattice subjected to a step potential given by \( V_{i\sigma} = h\Theta(R - R_i) \), where \( h = 3 \) placed in the first half of lattice plane (upto (16,0),(16,32)). The variation of local occupation is shown for (a) \( U = 1 \), (b) \( U = 5 \), (c) \( U = 10 \).
Figure 8.5: Variation of the local occupation with the lattice site in the presence of a smoothly varying potential. We consider the potential given by Eq. 8.1 is applied $\xi = 1$, $V_0 = 5$, polarization $m=2$. Periodic boundary conditions applied. (a) An additional impurity potential $V_0 = 2$ is placed at the interface ($25^{th}$ site), (b) An additional impurity potential $V_0 = 2$ is placed at the $40^{th}$ site outside the field.
8.2.2 Step potential

Next we consider the case of a step potential given by

\[ V_{i\sigma} = \sigma m(R - R_i) \quad (8.2) \]

where \( \sigma \) gives the spin index and \( m \) is the magnetic field which can be interpreted as a polarization parameter of the system. The maximum polarization is equal to the bandwidth of the system which is twice the hopping amplitude \( t \). In our bandwidth is 2 and maximum value of \( m \) is also 2. We study the system for full polarization and also for partial polarization like \( m = 1, 0.5, 0.2 \) etc. The problem is extended by putting a single impurity at different positions of the lattice and study the interference between the effect of impurity and the magnetic field. Studies are conducted for both non-interacting and interacting systems using both PBC and OBC. Electronic correlations or interactions are accounted for by considering the spin-dependent self-energy under Hubbard I approximation.

In Fig. 8.6(a) we consider a 1D interacting lattice chain with \( N_L = 50 \) for \( U = 1 \). We apply a magnetic field with the full polarization \( m = 2 \) for the first 25 sites and sharply cut-off the field from the 25th site. The system is subjected to PBC. It is observed that for the region under the influence of the magnetic field the band is fully occupied with spin-down electrons and no spin up electrons are present indicating a complete polarization. Oscillations are observed at the interface (25th) site onwards where the field is suddenly cut-off in contrast to the case of a smoothly varying potential as shown in Fig. 8.5(a) and Fig. 8.5(b). Also we see that beyond the region of the magnetic field the average number of spin up and spin down electrons become nearly equal. The small finite difference between the average occupation of spin-up and spin-down electrons outside the field in the absence of any additional impurity is defined by,

\[ L = |\bar{n}_{i\uparrow} - \bar{n}_{i\downarrow}| \quad (8.3) \]

where \( \bar{n}_{i\uparrow} \) and \( \bar{n}_{i\downarrow} \) correspond to the average occupation of the spin-up and spin down electrons respectively. The finite difference can be due to the boundary effects and induced magnetization. Boundary effects include the overall system boundary and our imposed boundary conditions, i.e. PBC or OBC. In Fig. 8.6(b) we show the behaviour of the system in the presence of an additional impurity \( V_0 = 2 \) placed at the 40th site outside the field. We observe interference effects in the oscillations due to residual magnetism and the presence of the impurity.

In Fig. 8.7(a) and Fig. 8.7(b) we present a comparative study of the behaviour of 1D interacting system in the presence of full polarization \( (m = 2) \) and partial polarization \( (m = 1) \). We see that in contrast to full polarization, oscillations are observed both for spin up and spin down electrons within the field for \( m = 1 \).

In Fig. 8.8(a) and Fig. 8.8(b) we study how the finite difference in the average occupation of the spin up and spin down electrons, outside the field as defined by Eq. 8.3 change with the polarization parameter for different boundary conditions.

In Fig. 8.8(a) we see that the finite difference increases with the polarization beyond \( m = 0.5 \) for a non-interacting system subjected to OBC. The rate of this increase decreases and shows a linear behaviour for an interacting system with \( U = 1 \). In Fig. 8.8(b) we present the behaviour of the finite difference with the polarization of an interacting system with \( U = 1 \) for different boundary conditions. We observe that the rate of increase is higher in case of PBC as compared to OBC due to feedback effects by virtue of periodicity.

If we put a large impurity \( V_0 = +2 \) at the interface of the magnetic field, we see that the difference between spin-up and spin-down electrons tends to zero or in other words the impurity at the interface divides the system into two halves; the region where the magnetic field is absent feels no induced magnetism as the impurity being appreciably large completely shields the effect of magnetic field as shown in Fig. 8.9(a). However, if the value of the impurity is small, e.g. \( V_0 = 0.2 \) Fig. 8.9(b) the shielding effect is not so significant and still some effects of induced magnetism can be observed.

In Fig. 8.10(a) and Fig. 8.10(b) we have made a comparative study of the non-interacting case and for \( U = 1 \) in presence of an external magnetic field with an additional impurity placed
Figure 8.6: Effect of a step polarization on local occupation in a spin dependent 1D interacting system using Approximation B for $U = 1$. We consider $N_L = 50$ subjected to a step potential as in Eq. 8.2 with $m = 2$ corresponding to the maximum polarization. Periodic boundary conditions are applied. We show the cases where (a) No additional impurity is kept, (b) $V_0 = 2$ is placed at the 40th site outside the field.
Figure 8.7: Local occupation in a spin dependent 1D interacting system using Approximation B for $U = 1$ and different polarization. (a) Oscillations are observed for partial polarization $m = 1$, in absence of impurity and oscillation parameters are spin dependent. (b) No oscillation is observed for $m = 2$, full polarization. Periodic boundary conditions are applied.
Figure 8.8: The variation of the difference in average occupation for spin up and spin down electrons given by $L$ outside the region of magnetic field in the presence of a step polarization. The relative difference in occupation for the two spins increases with the polarization. (a) We show the case for different interactions when the system is subjected to OBC in absence of any impurity. (b) We show the case for different boundary conditions with $U = 1$ in absence of any impurity. Electronic correlations are accounted for using Approximation B.
Figure 8.9: FO in non-interacting 1D systems with \( N_L = 50 \), in the presence of step-polarization and an additional impurity potential at the interface. The impurity potential \( V_0 \) is placed exactly at the interface, i.e. at the 25\textsuperscript{th} site and the polarization is \( m=1 \). (a) In case of a large impurity \( V_0 = 2 \) there is no difference in local occupation of spin up and spin down electrons at different lattice sites outside the field, (b) In case of a small impurity, \( V_0 = 0.2 \) the difference in occupation between the spin up and spin down electrons at different lattice sites outside the field is visible. It is numerically calculated as \( 3.8559E - 002 \).
inside the field. We observe that inside the magnetic field the oscillations are damped for the interacting case both for spin up and spin down electrons. Outside the field we see that the difference in occupation for the two spins due to residual magnetism is suppressed when interaction is switched on.

One sees a relative shift in the local density of states of spin up and spin down electrons which is proportional to the polarization parameter $m$.

In Fig. 8.11(a) and Fig. 8.11(b) we show the spectral functions for the spin-up and spin-down electrons at the 10th site located inside the field and 40th located outside the field respectively. No additional impurity is present in the system.

### 8.3 Conclusion

We conclude that in the presence of extended inhomogeneities the system becomes more homogeneous with the increasing interactions for spin independent systems. Oscillations are observed only for a step potential and no oscillations appear for a smoothly varying potential. A systematic relative shift is observed for the spectral function of spin up and spin down electrons at the 10th site, inside the field due to polarization, $m = 1$. The relative shift in the spectral functions of the spin up and spin down electrons at the 40th site outside the field is absent. However, one sees the spectral function of the two spins do not exactly overlap. This may be due effects of residual magnetism, random fluctuations and numerical errors.
Figure 8.10: FO in the presence of a step polarization and additional impurity for interacting and non-interacting system. We consider a 1D system with $N_L = 50$ subjected to a step polarization with $m = 1$. An additional impurity potential $V_0 = 2$ is placed on the $10^{th}$ site inside the field. (a) Shows the non-interacting case with $U = 0$, (b) shows the interacting case with $U = 1$ where correlations are accounted for using Approximation B.
Figure 8.11: Spectral functions for spin-up and spin-down electrons in non-interacting system subjected to step polarization without any additional impurity. (a) A systematic relative shift is observed for the spectral function of spin up and spin down electrons at the 10th site, inside the field due to polarization, $m = 1$. (b) The relative shift in the spectral functions of the spin up and spin down electrons at the 40th site outside the field is absent. However, one sees the spectral function of the two spins do not exactly overlap. This may be due effects of residual magnetism, random fluctuations and numerical errors.
Chapter 9

Semi-analytical studies on many-body scattering in interacting systems

In this chapter we study the spectral function and scattering phase-shift for interacting systems using a semi-analytical approach. We use a model Bethe density of states and the phenomenological model self-energy given by Eq. 6.8 to account for the electronic interactions. The results obtained are compared with the numerical results of Chp. 6. We also present some analytical calculations to explain the behaviour of the spectral functions obtained in Chp. 6 using Approximation B (Hubbard I self-energy).

9.1 Semi-analytical calculations using the model Bethe DOS and model self-energy for a single impurity

9.1.1 Spectral function for interacting Bethe DOS in presence of a single impurity

In Chp. 6 we numerically observed the appearance of the additional peak in the spectral function of the impurity site for the non-interacting case due to the formation of a single bound-state in presence of the single impurity. The sharp bound state disappeared with the interactions, and resonances appeared instead. The width of the resonances increased with the increasing interactions. We now try to study the spectral function using a semi-analytical method and compare it with our numerical results.

Evaluating the homogeneous interacting Green’s function

We consider a model Bethe lattice. It is a standard text-book problem to compute the Green’s function for a homogeneous, non-interacting Bethe lattice which is given by

\[ G_{\text{nonint}}^0 = \frac{2}{\omega - \varepsilon_0 + i\eta + \sqrt{(\omega - \varepsilon_0)^2 - W^2}}. \] (9.1)

[128]. In our system the ground state energy \( \varepsilon_0 = 0 \), the half band-width \( W = 2t^* \) where \( t^* = t/\sqrt{z} \). \( t \) is the hopping amplitude, \( z \) is the co-ordination number and in case of Bethe lattice \( z \rightarrow \infty \). Further, we replace \( \omega \) by \( (\omega - \Sigma(\omega)) \) in Eq. 9.1 in order to include the effects of electronic interactions. Thus the Green’s function for a homogeneous Bethe lattice in presence of electronic interactions is given by

\[ G_{\text{int}}^0 = \frac{2}{\omega - \Sigma(\omega) + \sqrt{(\omega - \Sigma(\omega))^2 - W^2}}. \] (9.2)
\[ G^0_{\text{int}} = \frac{2}{\omega - \text{Re} \Sigma(\omega) - i\text{Im} \Sigma(\omega) + \sqrt{(\omega - \text{Re} \Sigma(\omega) - i\text{Im} \Sigma(\omega))^2 - W^2}}. \] (9.5)

Let \( A = \omega - \text{Re} \Sigma(\omega) \), \( D = \text{Im} \Sigma(\omega) \), making the following substitutions in Eq. 9.5 we get

\[ G^0_{\text{int}} = \frac{2}{(a - iD) + \sqrt{(A - iD)^2 - W^2}}. \] (9.6)

After rationalization of Eq. 9.6 we get

\[ G^0_{\text{int}} = \frac{2((A - iD) - \sqrt{(A - iD)^2 - W^2})}{W^2}. \] (9.7)

We make use of the De Moivre’s theorem to extract the complex square-root. It states that \( \sqrt{M + iN} = \sqrt{r}(\cos(\theta) + i\sin(\theta)) \) where \( r = \sqrt{M^2 + N^2}, \cos(\theta) = \frac{M}{r}, \sin(\theta) = \frac{N}{r} \). In the square root appearing in Eq. 9.7 we have \( M = A^2 - D^2 - W^2, \ N = -2AD \). Finally, evaluating the square-root the real and imaginary part of the non-interacting Green’s function have the following expressions:

\[ G^0_{\text{int}} = \frac{2(A - \sqrt{(M + r)^2})}{W^2} \] (9.8)

\[ G^0_{\text{int}} = -(D + \frac{N}{\sqrt{2\sqrt{M + r}}}) \] (9.9)

where \( G^0_{\text{int}} \) and \( G^0_{\text{int}} \) are the real and imaginary parts of the interacting homogeneous Green’s function. It was not possible to solve the problem analytically beyond this point. Hence we numerically calculated \( G^0_{\text{int}} \) and \( G^0_{\text{int}} \) using Eq. 9.8, Eq. 9.9. It follows from their definition that \( A, B, M, N \) and \( r \) can be evaluated from the real and imaginary parts of the model self-energy.

**Green’s function for model Bethe lattice in presence of a single impurity**

The Green’s function for the interacting Bethe lattice \( G^V_{\text{int}} \), in presence of a single impurity can be obtained from \( G^0_{\text{int}} \), following the Dyson equation [128]:

\[ G^V_{\text{int}} = \frac{G^0_{\text{int}}}{1 - VG^0_{\text{int}}}. \] (9.10)

Since \( G^0_{\text{int}} = G^0_{\text{int}} + iG^0_{\text{int}} \), the impurity Green’s function in Eq. 9.10, can be further resolved into the real and imaginary parts as follows:

\[ G^{VR}_{\text{int}} = \frac{G^0_{\text{int}} - V((G^0_{\text{int}})^2 - (G^0_{\text{int}})^2)}{(1 - VG^0_{\text{int}})^2 + V^2(G^0_{\text{int}})^2}, \] (9.11)

\[ G^{VI}_{\text{int}} = \frac{G^0_{\text{int}}}{(1 - VG^0_{\text{int}})^2 + V^2(G^0_{\text{int}})^2}. \] (9.12)
CHAPTER 9. SEMI-ANALYTICAL STUDIES ON MANY-BODY SCATTERING IN INTERACTING SYSTEMS

We can use $G^0_{int}$ and $G^{0R}_{int}$, from our previous calculations to again calculate $G^{VI}_{int}$ and $G^{VR}_{int}$. Once we know $G^{VI}_{int}$ we can calculate the spectral function using Eq. 5.9. In Fig. 9.1(a) and Fig. 9.1(b), we present the spectral functions calculated using the above method for external impurity potentials $V = 0.1$ and $V = 2$. The behaviour of the spectral functions is consistent with the spectral functions obtained from numerical methods in Fig. 6.47.

![Spectral function obtained semi-analytically for a model Bethe DOS in presence of a single impurity potential ($V_0$) for different interactions. We consider (a) $V_0=0.1$, (b) $V_0=2$. Electronic interactions have been accounted for using the phenomenological model self-energy in Eq. 6.8 where we choose $a = 0.2$, $b = 0.3$. The parameter $g$ is tuned to vary the interactions.](image)

**Disappearance of the peak for interacting system**

We see that the bound state corresponding to the impurity potential disappears as we switch on the interaction and resonances appear instead. Here, we try to provide an analytical explanation for the above phenomena. It follows from Eq. 9.10, that a singularity in the Green’s Function exists for $1 - V G^0_{int} = 0$. Since $V$ is real, the condition for the singularity in the non-interacting system is given by

$$\text{Re } G^0_{\text{non-int}} = 1/V.$$  \hfill (9.13)
Thus we see the discreet bound state for the non-interacting case. However, in case of interacting system, even $G_{0R}^{\text{int}}$ has contributions from the imaginary parts of the self-energy and is not purely real. Hence, Eq. 9.13 does not hold and the bound state disappears with the interactions.

9.1.2 Effects of interaction on the scattering phase-shift for a model Bethe DOS in presence of a single impurity potential

In Fig. 9.2(a) we study the variation of scattering phase-shift in presence of a single impurity for a Bethe DOS calculated using Eq. 5.122 with the frequency for different interactions. Electronic interactions have been accounted for using the model self-energy in Eq. 6.8. We see the behaviour of scattering phase-shift significantly changes with the interactions.

![Figure 9.2: Scattering phase-shift in a model Bethe DOS in presence of a single impurity potential for different interactions. We consider (a) $V_0=0.1$, (b) $V_0=2$. Electronic interactions have been accounted for using the phenomenological model self-energy in Eq. 6.8 where we choose $a=0.2$, $b=0.3$. The parameter $g$ is tuned to vary the interactions.](image-url)
9.2 Analytical approach to explain the behaviour of the spectral function using Hubbard I self-energy in presence of single impurity

We attempt to explain the behaviour of the spectral function from our numerical studies, presented in Fig. 6.52 using Approximation B. The one-particle Green’s function can be analytically obtained for the Hubbard I self-energy (used in Approximation B) as,

\[
G(i,i,z) = \frac{1 - \bar{n}}{z} + \frac{\bar{n}}{z - U} \quad (9.14)
\]

where the frequency \(z = \omega + i\eta\), \(U\) is the Hubbard interaction and \(\bar{n}\) is the average occupation of electrons in the lattice. Again Eq. 9.14 can be resolved into real and imaginary parts as

\[
G(i,i,z) = \frac{(1 - \bar{n})\omega}{\omega^2 + \eta^2} + \frac{\bar{n}(\omega - U)}{(\omega - U)^2 + \eta^2} - i \left( \frac{(1 - \bar{n})\eta}{\omega^2 + \eta^2} + \frac{\bar{n}\eta}{(\omega - U)^2 + \eta^2} \right) \quad (9.15)
\]

Here, we see the real part of the Green’s function is purely real and thus the condition of the singularity is given by \(\text{Re}G(i,i,z) = \frac{1}{V}\). We get from Eq. 9.15, the condition of singularity for \(\eta \rightarrow 0\) as

\[
\frac{1 - \bar{n}}{\omega} + \frac{\bar{n}}{\omega - U} = \frac{1}{V} \quad (9.16)
\]

[128]. Solving the above quadratic Eq. 9.16, we get two roots of \(\omega\), which corresponds to the two singular peaks given by

\[
\omega_{1,2} = \frac{U + V}{2} \pm \frac{1}{2} \sqrt{(U - V)^2 + 4UV\bar{n}}. \quad (9.17)
\]

Eq. 9.17 can be expanded using series expansion and simplified as

\[
\omega_{1,2} = \frac{U + V}{2} \pm \frac{U - V}{2} \left( 1 + \frac{4UV\bar{n}}{2(U - V)} + .... \right). \quad (9.18)
\]

Thus, keeping the leading order terms we see the positions of the two peaks are given by

\[
\omega_1 = U + \frac{UV\bar{n}}{U - V}, \quad (9.19)
\]

\[
\omega_2 = V - \frac{UV\bar{n}}{U - V}. \quad (9.20)
\]

For \(U \gg V\) we can neglect \(V\) and \(\omega_2 = V(1 - \bar{n})\), i.e. proportional to the impurity potential. This provides an understanding of the spectral function in Fig. 6.52.

It is also worthy to attempt further analytical studies in order to support our numerical calculations. Particularly a similar analytical formula like Eq. 2.1 to describe the modulation of densities in the interacting systems including the interaction parameter would be particularly useful to validate our numerical results.
Chapter 10

Summary of Thesis

In this thesis we have presented our studies on screening of charged impurities and the associated phenomenon of Friedel oscillations in correlated fermionic systems. Friedel oscillations appear in metals at low temperature due to the spatial density oscillations of the conduction electrons in the neighbourhood of a charged impurity. Several studies have been conducted both theoretically and experimentally on these oscillations for non-interacting and weakly interacting systems. We have investigated the behaviour of oscillations in strongly correlated electronic systems for metals, insulators and particularly the Mott insulating phases. We further studied the effect of correlations on the screening charge and spectral function at different lattice sites.

The strongly correlated electronic system has been modeled by the Hubbard Hamiltonian. We have conducted our studies in the presence of a single impurity, two impurities and extended inhomogeneous potentials in one-, two-, and three dimensional finite lattice systems with periodic boundary conditions. The Hubbard model has been solved using the Real space Dynamical Mean-Field Theory which is the best known unique method to solve it in the regime of Mott transition. Electronic correlations in the system have been accounted for by solving the self-consistent DMFT equations using Continuous Time Monte Carlo (CTQMC) method which accounts for all the inhomogeneities in the self-energy. However, it is computationally time-consuming and works for finite temperatures only. Hence we also use other approximate methods to study these oscillations in the limit of low temperature and also to obtain quick initial insights regarding the effect of interactions on the oscillation parameters. We assume that in the asymptotic limit the effect of impurity on the self-energy is weak enough and it is justified to neglect the inhomogeneities in the self-energy at different lattice sites due to the impurity. The homogeneous part of the self-energy is then obtained by solving the DMFT equations using NRG (Approximation C), using a model self-energy (Approximation A), using the self-energy under Hubbard I approximation (Approximation B). In each of the approximate methods the homogeneous self-energy is transferred to the real-space Dyson equation containing the impurity potential to obtain the single-particle Green’s function from which other local properties of the system like a) local electronic occupation per lattice site, b) screening charge and c) spectral function are calculated. Approximation A can explain FO in metallic systems, Approximation B in insulating systems but DMFT methods (Approximation C and R-DMFT+CTQMC) uniquely present a complete picture both for metallic and insulating regime. The results from Approximation C and R-DMFT+CTQMC have been consistently showing that the effect of interactions on FO both at finite and zero temperature is similar.

We have studied the problem in case of an extended inhomogeneous potential. We have also studied the oscillations for spin dependent potentials in the presence of a magnetic field and observed the effect of magnetic polarization on the oscillations of electrons of different spins. Our studies confirm that electronic interactions significantly influence the screening and FO. In all the three dimensions FO decay as \( \frac{1}{r^d} \) both for interacting and non-interacting systems where \( d \) is the dimension of the system, and \( r \) is the relative distance from the impurity. The amplitude of FO decreases with the interactions while the period and phase remain unchanged.
for the system at half-filling. FO disappear at the Mott transition and no oscillations are observed beyond it in the insulating phase. In case of a single impurity a bound state is observed in the spectral function at the impurity site for the non-interacting system. It is replaced by resonances when interaction is switched on. This feature in the spectral function has been observed using Approximation A, and R-DMFT+CTQMC where we have used Max-Ent to perform an analytic continuation of the Green’s function in the Matsubara space to obtain the spectral functions.

The screening effect decreases with the interactions and an abrupt change in the behavior is observed at the Mott transition in all three dimensions. The screening charge around the neighbourhood of the impurity defined by “N-screening charge” increases with the impurity for a given interaction and a symmetry in the behavior about the zero impurity is observed for positive and negative impurities. Beyond a certain temperature the screening charge remains constant with the variation in temperature. We have verified the Friedel sum rule which states that the screening charge should be equal to the scattering phase-shift at the Fermi energy for interacting systems and observed an approximate agreement within some error limits using our methods.

In the presence of two impurities it is seen that the interaction weakens the interference effects between the impurities. No interference effects are observed beyond a certain cut-off distance and the impurities behave independently. We have studied the variation of the total N-screening charge and partial screening charge as the distance between the impurities is varied. It is observed that while the total screening charge remains almost constant with the distance, the partial screening charge shows appreciable variation. We have also extended the problem for multiple impurities randomly scattered over a 2D surface. We see that the oscillations localize around the impurities with the increase of interactions. In the presence of extended inhomogeneities it is observed that the system becomes more homogeneous with the increasing interactions. FO weaken with increase in temperature, however effects of interaction on FO have also been observed of finite temperatures far away from $T = 0$. We see the effect of interactions on FO is universal for all the three dimensions.

The thesis presents numerical results on the significant effects of electronic interactions on FO. It can serve as a nice motivation for similar experimental studies on real strongly correlated electronic systems, eg. heavy fermionic compounds, high-$T_c$ cuprates in the future.
Chapter 11

Outlook and open questions

This thesis can serve as nice background to provide initial insights and ideas for various future problems related to this topic. In this chapter some initial ideas for few of such potential problems are proposed. Firstly we would discuss about the studies which can be done as a direct extension to this work. We would then also highlight a few novel and related questions which may be probed.

11.1 More studies on 3D systems

We have used the technique of dense matrix inversion for our program to compute the Green’s function inverting the Dyson equation. The matrix corresponding to the Dyson equation is actually a sparse matrix, i.e. most of its elements are zero. Thus instead of using dense matrix inversion one can implement sparse matrix inversion to our existing program. This would minimize the computational time and also resolve the computer memory problems for larger lattice systems in higher dimensions. One can simulate larger lattice systems in three-dimensions using such an implementation and study FO in it. This can eliminate the problem of boundary effects due to the small system size as faced by us and provide better information on the decay of FO with distance in 3D.

11.2 Further studies using R-DMFT+CTQMC+MaxEnt

Single impurity

We have conducted preliminary studies of the spectral function only for 1D systems at high temperatures $\beta = 1$. It is worth to probe the behaviour of the spectral functions in the lower-temperature limit (higher $\beta$) for higher dimensional systems (e.g. 2D and 3D). This would reflect on the temperature dependence of the spectral functions. One can also test if the universal behaviour at different dimensions is observed like in the case of Approximation A, Approximation B and Approximation C.

We commented that the Friedel Sum Rule is apparently not obeyed for the interacting systems using Approximation A and Approximation C as we neglect the contribution from the inhomogeneous part of the self-energy. This can actually be verified by studying the FSR using the site dependent self-energies from CTQMC where all the inhomogeneities are accounted for. In this case we need to again perform an analytical continuation of the real and imaginary parts of the Green’s function using Max-Ent and calculate the phase shifts at corresponding lattice sites using Eq. 5.122.

Two impurity

The interference effects on the spectral functions at intermediate sites in the presence of two impurities can be performed using RDMFT+CTQMC+MaxEnt, where all the inhomogeneities in the self-energy are taken into account. The results in turn can be used to verify
CHAPTER 11. OUTLOOK AND OPEN QUESTIONS

the features of the spectral functions as predicted by the model self-energy. Moreover, the
temperature dependence on the interference effect induced by the second impurity can also be
studied.

FSR can be verified in case of two and multiple impurities as in the case of single impurity
using Approximation C, RDMFT + CTQMC + Max-ENT.

As discussed in Chap. 7, a further quantitative study of two and three dimensional systems
in the presence of two and multiple impurities using Approximation C, RDMFT + CTQMC is
promising from an experimentalist's point of view.

11.3 Friedel oscillation in materials with strongly correlated electrons

All our studies have been conducted on model correlated systems. Studying FO in realistic
crystal structures e.g. metallic perovskites, $V_2O_3$, heavy fermionic systems which belong to
the class of strongly correlated compounds would be interesting. Dopant and crystal defects
would play the role of inhomogeneity in such real crystals. Here we sketch a very preliminary
idea of studying such problems. A combination of Dynamical Mean-Field Theory and b-initio
Density Functional Theory (DMFT + DFT) approach can be used to numerically study the
problem. A full implementation of DMFT + DFT approach used to calculate the total-energy
and reproduce the metal-insulator and structural phase-diagram of rare-earth nickelate per-
ovskite is presented in [129]. In our case one has to calculate the hopping and interaction
parameters for the Hubbard Hamiltonian corresponding to the real atoms using DFT. These
parameters can then be used as inputs to calculate the electronic densities with the DMFT
self-consistency loop. The results obtained from such studies can validate the predictions from
our theoretical model. It would further stimulate future experiments to study the effect of
interaction and temperature on FO in real SCES compounds.

11.4 Friedel Oscillations in Attractive Hubbard Model

We conclude presenting a short proposal of studying FO in an attractive Hubbard model using
R-DMFT.

At very low temperatures electrons can form Cooper pairs or fermionic condensates according
to the BCS theory of superconductivity. They can conduct current with zero resistance and
thus behave as superconductors. Friedel oscillations have been observed in superconducting
systems at low temperature. A. Fetter et al. examines the modification in a superconducting
medium due to a single, spherically symmetric, non-magnetic impurity using the BCS theory
of superconductivity [130]. It is observed that FO diminish in the Meissner state. However, M.
Machida et al. calculated microscopically the charge distribution around the vortex of a Tyre
II superconductor using Bogoliubov-de Gennes equation and Poisson equation simultaneously.
M. Machida concluded that Friedel Oscillations play an important role in the formation of
vortex core states in high-$T_c$ superconductors [131]. In M. Zhitomirskiy et al. work it has been
pointed out that the density variations near the impurity sites are significant for short-
coherence length superconductors and can increase the transition temperature in the case of
s-wave superconductors [132]. A. Koga et al. studied the dynamical properties of ultra-cold
fermions with attractive interactions solving the attractive Hubbard model using DMFT-
CTQMC for homogeneous systems [42]. They studied the low energy properties of the system
in one dimension, two dimensions and higher dimensions. They have found that weakly coupled
Cooper pairs are formed in case of small $U$ and the BCS type of phase is realized while in
case of large $U$ strong attraction tightly couples the fermions and the BEC type of super-fluid
state is realized. Koga’s work would be helpful in studies of FO in inhomogeneous systems
for the attractive Hubbard model using DMFT-CTQMC. Evidences of studies of FO in the
superconductors using the attractive Hubbard model within the framework of R-DMFT are
still not available in the literature to the best of our knowledge. Thus the study of behaviour
of FO in the superconducting phase, superconducting to normal phase transition under the framework of DMFT solving the attractive Hubbard model is a novel problem. It is expected that the theoretical results hence obtained can motivate and explain future experiments. It can also predict the role of FO in future nano devices, optical lattices, real cold atoms and thus make original contributions in the field of low temperature physics.
Appendices
Appendix A

Estimation of critical interaction and temperature for Mott transition in finite lattice systems

In general the inverse temperature of the system given by $\beta$ has the inverse dimension of energy while the interaction of the system ($U$) has the dimension of energy. We rescale $\beta$ and $U$ such that they are dimensionless. Such a rescaling can be done in the units of band-width ($W$) or hopping amplitude ($t$). The relation between the band-width and the hopping amplitude is given by:

$$W = 2zt,$$  \hspace{1cm} (A.1)

where $z$ is the coordination number of the system. It is given by the number of nearest neighbours corresponding to a lattice site and hence dependent on the dimension of the lattice. $t$ is the hopping amplitude and $t = 1$ in our system. Let $\beta_t$, $\beta_W$, $U_t$, $U_W$, be the rescaled dimensionless quantity with the units indicated by the suffix as follows

$$\beta_t = \frac{t}{k_BT},$$  \hspace{1cm} (A.2)

$$\beta_W = \frac{W}{k_B},$$  \hspace{1cm} (A.3)

$$U_t = \frac{U}{t},$$  \hspace{1cm} (A.4)

$$U_W = \frac{U}{W}.$$  \hspace{1cm} (A.5)

Using Eq. (22), (23), (24) we can find the relation between $\beta_t$ and $\beta_W$ as

$$\beta_t = \frac{\beta_W}{2z}.$$  \hspace{1cm} (A.6)

Similarly using Eq. (22), (25) and (26) we obtain the relation between $U_t$ and $U_W$ as

$$U_t = 2zU_W.$$  \hspace{1cm} (A.7)

The numerical values for the different dimensions

As mentioned earlier the coordination number $z$ is dependent on the dimension of the lattice. Consequently the scaling factor changes with the dimensions. We present some numerical values to illustrate the dimensional dependence in Tab. A.1, Tab. A.2 and Tab. A.3. Moreover, in our program $t$ scales the energy units and thus we measure $\beta_t$ and $U_t$. In the following
Table A.1: 1D

<table>
<thead>
<tr>
<th>$\beta_t$</th>
<th>$\beta_W$</th>
<th>$k_B T/W$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4</td>
<td>0.25</td>
</tr>
<tr>
<td>5</td>
<td>20</td>
<td>0.05</td>
</tr>
<tr>
<td>10</td>
<td>40</td>
<td>0.025</td>
</tr>
<tr>
<td>15</td>
<td>60</td>
<td>0.0167</td>
</tr>
<tr>
<td>20</td>
<td>80</td>
<td>0.0125</td>
</tr>
</tbody>
</table>

Figure A.1: Variation of $k_B T/W$ with $\beta_t$ for the different dimensions. $k_B T/W$ and $\beta_t$ are the inverse temperatures measured in the units of band-width and hopping respectively.

In Fig. A.1 the variation of $K_B T/W$ with $\beta_t$ is shown. In Fig. A.2 the phase-diagram for the Mott transition in a cubic lattice is shown.

Table A.2: 2D

<table>
<thead>
<tr>
<th>$\beta_t$</th>
<th>$\beta_W$</th>
<th>$k_B T/W$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>8</td>
<td>0.125</td>
</tr>
<tr>
<td>5</td>
<td>40</td>
<td>0.025</td>
</tr>
<tr>
<td>10</td>
<td>80</td>
<td>0.0125</td>
</tr>
<tr>
<td>15</td>
<td>120</td>
<td>0.0083</td>
</tr>
<tr>
<td>20</td>
<td>160</td>
<td>0.0063</td>
</tr>
</tbody>
</table>

In Fig. A.2 the critical values of interactions and temperature at which Mott transition occurs is given by $U_{cW} = 1$ and $\beta_{cW} = 100$ ($k_B T/W = 0.01$). Comparing Fig. A.1 and Fig. A.2 we can have an estimate of $\beta_t$ for which the critical region is reached. It is observed that with the increase in dimension the critical regime is achieved for a lower value of $\beta_t$ as the rescaling factor $z$ increases with the dimension. According to Tab. A.1, Tab. A.2 and Tab. A.3 the Mott
transformation is already achieved for $\beta_t = 15$, $\beta_t = 10$, $\beta_t = 5$ in case of 1D, 2D, 3D lattice respectively. While comparing our values with Fig. A.2 we assume $U_{cW}$, $\beta_{cW}$ in 1D and 2D are the same order of magnitude as 3D.

Table A.3: 3D

<table>
<thead>
<tr>
<th>$\beta_t$</th>
<th>$\beta_{#W}$</th>
<th>$\frac{K_B T}{W}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>12</td>
<td>0.0833</td>
</tr>
<tr>
<td>5</td>
<td>60</td>
<td>0.0167</td>
</tr>
<tr>
<td>10</td>
<td>120</td>
<td>0.0083</td>
</tr>
<tr>
<td>15</td>
<td>180</td>
<td>0.0056</td>
</tr>
<tr>
<td>20</td>
<td>240</td>
<td>0.0042</td>
</tr>
</tbody>
</table>
Appendix B

Mapping the Hamiltonian of higher dimensional lattices into equivalent one-dimensional systems.

Two dimensional lattice

The position vector of any point on a lattice in d dimensions is given by \( \mathbf{R}_i = (n_1, n_2, \ldots, n_d) \) where \( n_1, n_2, \ldots, n_d \) are the indices along respective directions.

In case of a 2D lattice, if we directly work with the position vector we need to deal with two indices to denote the position of the lattice which adds to the computational complications. Hence we attempt to reduce the problem to an equivalent one-dimensional case. The position vector \( \mathbf{R}_{n_1, n_2} \) can be mapped into an integer number \( i \) as follows:

\[
i = n_1 + N_1 \cdot (n_2 - 1),
\]

where \( N_1 \) is the total number of lattice sites in each row. Since it is a square lattice the number of lattice sites in each column is also \( N_1 \). Hopping from \( \mathbf{R}_{n_1, n_2} \) to \( \mathbf{R}_{n_1, n_2+1} \) is represented by

\[
i' = n_1 + N_1 \cdot n_2.
\]

Then the total number of lattice sites in 1D will be equal to \( N_1^2 \). However, while mapping we need to preserve the nearest neighbour hopping and periodic boundary conditions both in horizontal and vertical directions. This is achieved by the following procedure to define the hopping matrix elements. These rules were determined using an inductive approach.

- **Hopping in the horizontal direction**
  \[ \langle i | H | i + 1 \rangle = \langle i + 1 | H | i \rangle = t \]
  where \( t \) is the hopping amplitude.

  However, if \( i \) is a multiple of \( N_1 \) which is the maximum number of lattice sites in a particular row then we reach the end of a particular row. The above rule is not valid in that case as the \( (N+1) \)th or \( (i+1) \)th position is not available for the electron to hop on.

- **Hopping in vertical direction**
  \[ \langle i | H | i + N_1 \rangle = \langle i + N_1 | H | i \rangle = t \]
  In general the procedure repeats for \( (N_1^2 - N_1) \) times.

- **Horizontal Boundary Condition**
  \[ \langle i | H | i + (N_1 - 1) \rangle = \langle i + (N_1 - 1) | H | i \rangle = t \]
  We need to choose \( i \) from 1 to \( N_1^2 \) in steps of 3.

- **Vertical Boundary Condition**
  \[ \langle (i + N_1(N_1 - 1)) | H | i \rangle = \langle i | H | (i + N_1(N_1 - 1)) \rangle = t \]
APPENDIX B  MAPPING THE HAMILTONIAN OF HIGHER DIMENSIONAL LATTICES INTO EQUIVALENT ONE-DIMENSIONAL SYSTEMS.

All other hopping matrix elements are equal to zero apart from the site containing the impurity. The equivalent lattice index for the impurity site is calculated using Eq. B.2, once we know the position of the impurity. In the above enumeration technique every \((i + (N_1 - 1))^{th}\) element is a diagonal element while every \((i + N_1 + 1)^{th}\) element is an anti-diagonal element.

Figure B.1: 2D DOS for non-interacting \((31 \times 31)\) finite square lattice in absence of impurity using our equivalent mapping technique.

In order to test if the mapping is correct we compute the total density of states and compare the results of 2D DOS from the literature. The shape of 2D DOS with the logarithmic divergence at the center and a corresponding bandwidth of -4 to +4 is reproduced (since \(t = 1\) and \(d = 2\) in this case) in Fig. B.1 using our method confirming that our enumeration technique and mapping is correct.

Three dimensional lattice

In case of 3D if we directly work with the position vector we even need to deal with three indices. Thus we perform a similar equivalent one-dimensional mapping such that the equivalent index \(i\) is given by,

\[
i = n_1 + N_1 \cdot (n_2 - 1) + N_1 \cdot N_2 \cdot (n_3 - 1),
\]

where \(N_1, N_2, N_3\) are the number of lattice sites in three directions. Since it is a cubic lattice \(N_1 = N_2 = N_3\) hopping from \(\mathbf{R}_{n_1,n_2}\) to \(\mathbf{R}'_{n_1,n_2+1}\) is represented by

\[
i' = n_1 + N_1 \cdot n_2 + N_1 \cdot N_2 \cdot (n_3 - 1)
\]

Then the total number of lattice sites in 1D will be equal to \(N_1^3\). We again need to take care that the nearest neighbour hopping and periodic boundary conditions is preserved in all possible directions in our equivalent mapping. Like in the case of 2D we explicitly illustrate the procedure as follows:

- **Hopping in the horizontal direction**

  \[\langle i | H | i + 1 \rangle = \langle i + 1 | H | i \rangle = t\]

  where \(t\) is the hopping amplitude.

  However if \(i\) is a multiple of \(N_1\) which is the maximum number of lattice sites in a particular row then we reach the end of a particular row. The above rule is not valid in that case as the \((N+1)\)th or \((i+1)\)th position is not available for the electron to hop.
on. Thus this rule is the same as in case of 2D.

- Hopping in vertical direction
\[ \langle i | H | i + N_1 \rangle = \langle i + N_1 | H | i \rangle = t \]
Unlike in case of 2D lattice we have a collection of 2D slices in this case. Thus we need to impose an additional restriction that the end of a column in a particular slice is identified and the above rule will not work beyond it as there is no nearest neighbour for vertical hopping.

- Interlayer hopping
In this case we need to also consider nearest neighbour hopping in between the slices which is given by,
\[ \langle i | H | i + N_2 \rangle = \langle i + N_2 | H | i \rangle = t \]
We choose to repeat the procedure for \( i \) running from 1 to \( (N_1^3 - N_2^3) \).

- Horizontal Boundary Condition
\[ \langle i | H | i + (N_1 - 1) \rangle = \langle i + (N_1 - 1) | H | i \rangle = t \]
We need to choose \( i \) from 1 to \( N_1^3 \) in steps of \( N_1 \).

- Vertical Boundary Condition
\[ \langle (i + N_1(N_1 - 1)) | H | i \rangle = \langle i | H | (i + N_1(N_1 - 1)) \rangle = t \]

- Boundary condition for the third direction.
\[ \langle (i + N_2^2(N_1 - 1)) | H | i \rangle = \langle i | H | (i + N_2^2(N_1 - 1)) \rangle = t \]
In this case \( i \) runs from 1 to \( N_2^3 \) and no additional restriction is imposed.

All other hopping matrix elements are equal to zero apart from the site containing the impurity. The equivalent lattice index for the impurity site is calculated using Eq. B.3, once we know the position of the impurity.

![3D DOS for a non-interacting finite cubic lattice](image)

**Figure B.2:** 3D DOS for a non-interacting finite cubic lattice \((11 \times 11 \times 11)\) in absence of impurity using our equivalent mapping technique.

In order to test if the mapping is correct we compute the total density of states and compare the results of 3D DOS for continuous homogeneous non-interacting systems. We see in Fig. B.2 that 3D DOS with a corresponding bandwidth of -6 to +6 is reproduced (since \( t = 1 \) and \( d = 3 \) in this case) in using our method confirming that our enumeration technique and
mapping is correct. However, the shape is not completely reproduced owing to numerical discretization effects in our small $11 \times 11 \times 11$ finite cubic lattice.
Appendix C

Technical numerical details of RDMFT+CTQMC calculations

We discuss about the various computational details and numerical tricks used in our computational program implementing RDMFT+CTQMC.

Initial choice of self-energy

In RDMFT+CTQMC loop in Fig. 5.2, we need to start from an initial value of self-energy. A smart choice of the initial value of self-energy which is expected to be close to the true solution optimizes computational time and power. Moreover, the code is structured such that if the initial value of self-energy is too far away from the true solution then after a few iterations calculations are stopped. We start our calculations with a high-value of convergence criteria $\text{conv} = 0.02$ and low value of $\beta$ and $U$, i.e. $\beta = 1$ and $U = 1$. In this case we choose the initial self-energy equal to zero for all lattice sites. While calculating the higher values of $\beta$ or $U$ we use the self-energies calculated for the low-values of the corresponding parameter as an initial input. In order to calculate with a better accuracy i.e. lower convergence criteria we use the self-energies calculated for the corresponding $\beta$ and $U$ in higher convergence limits as initial input.

Fourier transform of different quantities

In the DMFT self-consistency loop the hybridization function is calculated in the Matsubara frequency space from the local Dyson equation Eq. 5.79. In the CTQMC method we need to perform a Fourier transform of the hybridization function from Matsubara frequency space to $\tau$ space (see Eq. 6.4). We use the method of moments to calculate the Fourier transform of the hybridization function in the asymptotic limit, i.e. for large values of $i\omega_n$. In order to calculate the moments of the hybridization function we also need to calculate the moments of self-energy and Green’s function.

The moments of self-energy at the lattice site $i$ are given by

$$\Sigma_{ii}(z) = \sum_{m=0}^{\infty} \frac{\Sigma^{(m)}_{ii}}{(i\omega_n)^m}. \tag{C.1}$$

$\Sigma^{(0)}, \Sigma^{(1)}$ denote the first, second and third order moments respectively.

We show the basic idea of evaluating the moments of the Green's function obtained from the Dyson equation.
Let $M$ be the matrix with the elements, $M_{ii} = \mu/(i \omega_n) = \Sigma_{ii}/(i \omega_n) - t_{ii}/(i \omega_n)$. $M_{ii}$ is small for large $i \omega_n$ and we can write the Green's function in the moment expansion form as

$$G(i \omega_n) = \frac{1}{i \omega_n} [1 + M + \mathbb{M}^2] + O \left( \frac{1}{(i \omega_n)^n} \right). \quad (C.3)$$

The moments $M_i^m$ of local Green's function on the lattice site $i$ would then be given by

$$G_{ii}(i \omega_n) = \sum_{m=0}^{\infty} \frac{M_i^m}{(i \omega_n)^{m+1}}. \quad (C.4)$$

The moments hence calculated are:

$$M_i^{(0)} = 1, \quad (C.5)$$

$$M_i^{(1)} = \mu_i + \Sigma_i^{(0)} + t_{ii}, \quad (C.6)$$

$$M_i^{(2)} = \Sigma_i^{(1)} + (\mu_i - \Sigma_i^{(0)})^2 + 2t_{ii}(\mu_i - \Sigma_i^{(0)}) + [t^2]_{ii}. \quad (C.7)$$

Note that $t_{ii}^2$ means element by element multiplication, i.e. $t_{ii} \ast t_{ii}$, while $[t^2]$ refers to matrix multiplication $t \times t$. The program is designed to optimally choose the cut-off Matsubara frequency for asymptotic limit. Note that below the asymptotic limit we perform real Monte Carlo simulations.

The relation between the Green's function and hybridization function is given by Eq. 5.69 and Eq. 5.79.

The moments of hybridization function are given by

$$\Delta_{ii}(i \omega_n) = \sum_{m=0}^{\infty} \frac{\Delta_{ii}^{(m)}}{(i \omega_n)^{m+1}}. \quad (C.8)$$

The moments hence calculated are as follows:

$$\Delta_i^{(0)} = -t_{ii}^2 + [t_{ii}^2], \quad (C.9)$$

$$\Delta_i^{(1)} = t_{ii}^2 + \mu(t_{ii}^2 - [t_{ii}^2]) - 2t_{ii}t_{ii}^2. \quad (C.10)$$

$$\Delta_i^{(2)} = -\Sigma_i^{(1)}t_{ii}^2 - r_{ii}^2 + \Sigma_i^{(1)}[t^2]_{ii} + 3t_{ii}^2[t^2]_{ii} - [t^2]_{ii}^2$$

$$+ \mu^2(-t_{ii}^2 + [t^2]_{ii}) + (\Sigma_i^{(0)})^2(-t_{ii}^2 + [t^2]_{ii}) - 2t_{ii}[t^3]_{ii}$$

$$+ 2\Sigma_i^{(0)}([t^3]_{ii} - 2t_{ii}[t^2]_{ii} + [t^3]_{ii}) - 2\mu([t^3]_{ii} - 2t_{ii}[t^2]_{ii})$$

$$+ \Sigma_i^{(0)}(-t_{ii}^2 + [t^2]_{ii} + [t^3]_{ii}) + [t^4]_{ii}. \quad (C.11)$$

The moments of the new Green's function obtained after solving SIAM using CTQMC are given by

$$G(-i \omega_n) = \frac{M_i^{(0)}}{(i \omega_n)} + \frac{M_i^{(1)}}{(i \omega_n)^2} + \frac{M_i^{(2)}}{(i \omega_n)^3}. \quad (C.12)$$

$$M_i^{(0)} = 1, \quad (C.13)$$

$$M_i^{(1)} = -\mu + t_{ii} + U + \langle n_i \rangle. \quad (C.14)$$
APPENDIX C. TECHNICAL NUMERICAL DETAILS OF RDMFT+CTQMC CALCULATIONS

\[ M_i^{(2)} = \delta_i^{(0)} + (-\mu + t_{ii})^2 + 2(\mu + t_{ii})U\langle n_i \rangle + U^2\langle n_i \rangle \quad (C.15) \]

The new moments of self-energy can also be calculated using moments of Green’s function and hybridization functions are

\[ \Sigma_i^{(0)} = \mu - t_{ii} + M_i^{(1)}, \quad (C.16) \]
\[ \Sigma_i^{(1)} = -(M_i^{(1)})^2 + M_i^{(2)} - \delta_i^{(0)}. \quad (C.17) \]

In order to reduce the computation time we do not compute the Green’s function for all the frequencies using Eq. 5.73. The property of Fourier transform of the Green’s function given by

\[ G(-i\omega_n) = G(i\omega_n)^*, \quad (C.18) \]

is used. Thus it is enough to compute the Green’s function for half of the Matsubara frequencies.

Computational time and memory in R-DMFT+CTQMC

R-DMFT+CTQMC were performed using the cluster facility "KRUK" of the University of Warsaw having a total of 1020 cores. The cores used for these calculations typically have CPUs with 1.2 GHz and 16 GB RAM. We have performed serial computation for any one set of parameters \((\beta, U)\). However, we have parallely performed our calculations for different parameter values of \(iU\) and \(\beta\) in different nodes. In such a computational setup the time scaled upto 3-4 weeks to perform calculations on 2D lattices at high \(\beta\) values. The systematic increase in the CPU time (in hrs) with the increase in \(U\) and \(\beta\) in case of a 1D lattice is shown in Fig. C.1.

The estimated memory needed to perform our serial computation for any-one set of parameter was 16 MB for a 1D lattice with \(N_L = 50\) and 5.6 GB for a \(31 \times 31\), 2D lattice.

![CPU Time vs Beta](image)

Figure C.1: Variation of computational time with \(\beta\) in 1D system for different interactions using R-DMFT+CTQMC (CT-HYB). Calculations have been performed in a CPU with 1.2 GHz, 16 GB RAM and we show the cpu-time in hrs.
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Author’s scientific contribution and training

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ORAL PRESENTATIONS at conferences/seminars:

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3. “Seminar at Institute for Theoretical Physics C, RWTH Aachen University, Germany.” (2016)


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