Metal-Insulator Transitions in Two Dimensions

A Thesis submitted to the Tata Institute of Fundamental Research, Mumbai For the degree of Doctor of Philosophy in Physics

by

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This thesis is a presentation of my original research work. Wherever contributions of others are involved, every effort is made to indicate this clearly, with due reference to the literature, and acknowledgment of collaborative research and discussions.

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Dariush Heidarian

In my capacity as supervisor of the candidate's thesis, I certify that the above statements are true to the best of my knowledge.

Nandini Trivedi

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Introduction

1.1 Is there a metallic phase in two dimensions?

The interplay of disorder and interaction in low dimensional systems has given rise to many interesting phenomena such as metal-insulator transition (MIT), quantum Hall effect, superconducting-insulator transition, superfluid-Bose glass transition and magnetic to non-magnetic transitions.

Analysis within the scaling theory predicted absence of any metallic state in 2D and 1D while it predicted a MIT in a 3D system of non-interacting disordered electron gas[1, 2]. Based on this theory in 2D, in the weak disorder limit, the resistivity increases logarithmically with lowering temperature while in the strong disorder regime it increases exponentially.

Including a weak electron-electron interaction within the perturbation theory found that the localization effects get even stronger[3]. In the opposite limit of strong coupling and no disorder, the 2D electronic system forms a Wigner crystal and any disorder pins the electrons so the conductivity tends to zero[4]. Attempts to use renormalization group methods were inconclusive due to runaway flows to the strong coupling limit[5]. Experiments done in this period on thin metallic films were consistent with the predictions of weak localization theory.

In 1990's, experiments on the 2D electron gas in high mobility quantum wells in Si-MOSFET's and GaAs/AlGaAs for the first time questioned the results obtained by the scaling theory[6, 7, 8, 9]. In these experiments, at low carrier density the conductance shows insulating behavior (ρ_{dc} increases by lowering temperature) and at high carrier density it is metallic (ρ_{dc} decreases upon lowering T). All curves for different densities n can be scaled to two curves (one for metal and one for insulator) when ρ_{dc} plotted against appropriately scaled temperature. This is an indication of a quantum phase transition with density as tuning parameter.

It is evident that the failure of scaling theory in predicting a 2D MIT seen in the experiments is related to ignoring the interaction among electrons. Since this transition is happening in the regime where both interaction and disorder are comparable, perturbation theories which are based on weak interaction or weak disorder limits cannot address it.

The question that we are trying to answer is: What is the combined effect of electron-electron interaction and disorder on a system of 2D electrons? We address this question within the context of the disordered Hubbard model which is the simplest model that includes both interaction and disorder effects. Furthermore we study the magnetic transitions which accompany the MIT. We have chosen two models of disorder. (1) In the first model we have modeled disorder as a random potential at all the sites of a square lattice taken from a uniform distribution; the width of the distribution is then a measure of the strength of disorder. (2) In the second model the strength of site disorder is fixed at V or -V, but only a fraction of sites are disordered and their locations are chosen randomly. The Hubbard model at half filling is a Mott-Insulator and in the large disorder limit the system is an Anderson-Insulator. How does the system evolve from a Mott-Insulator to an Anderson-Insulator? This is the question we focus on in this thesis.

1.2 Anderson localization

In the traditional view of disorder, electrons scatter from impurities and this leads to a finite width of the momentum eigenstates, though the wave functions remain extended. Anderson[10] pointed out that while the above is true for weak disorder, sufficiently strong disorder localizes the wave functions such that they decay exponentially in space with a localization length ξ , about a point r_0 where the potential is relatively deep given by

$$|\psi(r)| \propto \exp(-|r - r_0|/\xi).$$
 (1.1)

In one dimension all states get localized in the presence of even a small amount of disorder. In higher dimensions, for the first time, Banyai[11] and Mott[12] pointed out that the disorder may not be strong enough to localize all the states. For a mixture of localized wave functions, if their eigenvalues are close they are far apart in space, and if



Fig 1.1: The states in the hatched region are localized and the states at the un-hatched region are extended. The mobility edge, E_c , separates the localized and extended states.

they are nearby in space their energies mismatch, hence their overlap is exponentially small.

In a disordered system, localized states sit in the tails of the spectrum and for moderate regime of disorder the states at the middle of the band can be extended. If the Fermi energy lies deep in the localized side of the band (the hatched region in Fig. 1.1), the system is an Anderson insulator, and if it is in middle of the band, the system is a metal with finite conductivity at T = 0. Increasing the disorder strength localizes more states and for a fixed chemical potential it can lead to a metal insulator transition (MIT). Another route leading to MIT is to tune the Fermi energy at fixed disorder strength. MIT occurs at a critical energy $E_F = E_c$ — known as mobility edge. E_c separates the metallic extended states from the localized insulating states (see Fig. 1.1).

In 1972, Mott[13] pointed out that conductivity for a metal should have a discontinuous transition, which implies a minimal conductivity σ_{min} for a metal at the critical point (see Fig. 1.2), identified as the point where the mean free path l in the metal becomes on the order of the lattice spacing a or the inverse of the Fermi wave vector (k_F^{-1}) which are the smallest length scales in the system. From the Boltzmann equation for conductivity

$$\sigma = \frac{e^2 n\tau}{m} = \left(\frac{e^2}{\hbar}\right) \left(\frac{nl}{k_F}\right) \ge \left(\frac{e^2}{\hbar}\right) \left(\frac{n}{k_F^2}\right) \equiv \sigma_{min}^{3D} \tag{1.2}$$

where $l = v_F \tau$ and τ is the scattering time between collisions. In 3D with N electrons on a lattice we have

$$N = 2 \times \frac{4\pi k_F^3/3}{(2\pi/L)^3} \tag{1.3}$$



Fig 1.2: The conductivity as a function of scaled electron density (n_s/n_c) The solid line is continuous transition of conductivity observed experimentally for uncompensated samples of Si:P and Ge:Sb, which can be fitted to Eq. 1.7 with $\nu = 0.5$. The dashed line shows conductivity for compensated samples with exponent parameter to be $\nu = 1$ (From Ref. [15]). The dotted line is discontinuous transition in conductivity.

or

$$n = \frac{k_F^3}{3\pi^2}.$$
 (1.4)

therefore the minimum conductivity is

$$\sigma_{\min}^{3D} = \left(\frac{e^2}{3\pi^2\hbar^2}\right) \left(\frac{1}{a}\right) \tag{1.5}$$

Early experiments seem to support the existence of σ_{min}^{3D} (for a review see Ref. [14]). The consequence of Mott's argument in 2D is even more drastic; it predicts the minimum conductivity to be independent of any microscopic length scale and universal for all materials, given by

$$\sigma_{\min}^{2D} = \frac{e^2}{2\pi\hbar} \tag{1.6}$$

Mott's expectation was questioned by the experiments on doped semiconductors (for a review see [15]) in 3D which showed a continuous metal insulator transition.

Within the framework of the scaling theory in 3D the conductivity has a continuous transition, is given by (see also Ref. [16])

$$\sigma_{dc} = \sigma_{min}^{3D} (1 - n_s/n_c)^{\nu} \tag{1.7}$$

where n_s is the electron density and n_c is the critical electron density. For doped uncompensated semiconductors such as Si:P[15] the exponent ν is ≈ 0.5 ; upon compensating¹

¹Compensating refers to the cases where the number of dopants are more than the number of carriers, in other words, some of the carriers are trapped by defects, impurities or another type of dopants.

these materials [15] ν was found to be one (see Fig. 1.2) which agrees with prediction of the scaling theory. It is believed that this difference from unity for the exponent ν in the uncompensated Si:P arises from electron-electron interactions; however the precise value of ν is a matter of debate among experimentalists and theorists.

In the next section we review some of the theoretical works mainly focused on 2D MIT with an emphasis on including electron-electron interaction beyond the Anderson model.

1.3 Previous studies

There have been over 500 papers over the last ten years on the 2D MIT. Here we review the most relevant ones to the subject and to our work. For reviews on the subject, see Refs. [2, 9, 17, 18, 19].

Efros-Shklovskii conductivity: In 1975, Efros and Shoklovskii [20] argued that the Coulomb interaction between localized states reduces the density of states at the Fermi surface. Based on their argument if there is a localized state at position r_i with energy E_i just below the Fermi energy, there cannot be another localized state at position r_j with energy E_j above the Fermi energy such that $(E_j - E_i) < e^2/|r_i - r_j|$, otherwise the electron at state i can hop to the state j, leaving behind a hole at r_i . This is because, the energy reduction from Coulomb interaction between a hole at r_i and an extra electron at r_j is larger in magnitude than the energy increase $E_j - E_i$. This effect is at the root of reduction of density of states close to the Fermi energy, leading to dc-conductivity $\sigma \propto \exp[-(T_0/T)^{1/2}]$, where $T_0 = e^2/\epsilon\xi$, ξ is the localization length and ϵ is the dielectric constant. This results were obtained for three dimensions but the same argument in 2D leads to the similar conclusions; However as Mott [21, 22] and Pollak and Knotek^[23] pointed out, this argument is based on single particle density of states and cannot be applied to a many body interacting system. For a detailed discussion of the subject see reference [24]. At the end, these arguments could only address the insulating phase. Below we summarize some of the analytical attempts for describing the metallic phase.

Renormalization group (RG) method : In 1984 Finkelstein [5], for the first time, within a perturbative RG method, suggested existence of a metallic state in 2D. In this theory, before reaching zero temperature, the interaction parameter scales to infinity, outside the range of validity of perturbation. However it predicts a metallic state at all densities at very low temperature. Further it point out that application of magnetic field suppresses metallicity, leading to an insulating state. Due to the runaway flows of the RG, that were hard to interpret, it did not receive general acceptance.

Most recently, Punnoose and Finkelstein [25] re-summed over the most divergent terms. In their theory they gave N flavors to electrons, corresponding to degenerate regions in the conduction band of semiconductors, known as valleys, they assumed the intervally scattering to be absent, including those from disorder. The theory remains under control in all temperatures only if $N \to \infty$, in Si-MOSFET, the electron band in [001] plane has two valleys ($n_v = 2$), leading to N = 4, the extra factor of two is due to the two possible spin states of an electron. They argued for the existence of a metallic and an insulating phase separated by a quantum critical point. As the transition point is approached, various thermodynamic quantities are expected to show critical singularities. However, such perturbative approaches are valid only in the weak *e-e* coupling regime and cannot be applied to the regime where disorder and interaction are comparable.

Renormalizing of compressibility and scaling analysis: In the RG approach, the compressibility remains unrenormalized. This holds at high carrier density where the screening length is much less than mean free path ($s \ll l$) — in the general view when compressibility is reduced, the screening get weaker[26] or vice versa, in other words compressibility is proportional to the inverse of screening length $\kappa \sim 1/s$. In 1998 Si and Varma[27] within an scaling analysis approached the transition point from the metallic side. They argued that at low carrier density, where $s \gg l$, the compressibility vanishes, leading to strong suppression of conductivity, therefore a 2D MIT is expected with s as the tuning parameter. However this theory assumes existence of a metallic phase at high carrier densities (based on RG results) and therefore fails to address the features of the metallic state.

In 1997, Dobrosavljevic *et al.*[28], made the assumpsion of enhancement of conductivity by interaction, as noted in the previous RG studies, and *assumed* that the beta function in leading order of 1/g (at large g) has a positive coefficient (g is the conductance and $\beta(g) = d \ln(g)/d \ln(L)$). Applying scaling arguments used in the *non-interacting* electrons along with the above assumption give a metallic state in a 2D system. They pointed out that quantum critical behavior of the 2D MIT leads to the symmetries, observed experimentally, in conductivity and resistivity. They argued that a 2D disordered metal most likely to be non-Fermi liquid. In partial conformation of this, Chakravarty *et al.*[29] showed that at the sufficiently strong interaction limit, the non-Fermi liquid in the presence of disorder in 2D is a perfect conductor. At the carrier density $n_s < n_c$ the system forms a Wigner crystal and at the critical density n_c the Wigner glass melts to a non-Fermi liquid with short range magnetic correlations.

Percolation of screened charged impurity centers: Recently a number of papers[30, 31, 32] has argued that 2D MIT at zero temperature is not a quantum phase transition but it is a classical/or semi-classical phase transition. They argue that this can be realized in the semiconductor structures where the impurity is quenched disorder of random charged impurity centers. At high carrier density screening is strong, with decreasing the carrier density the distribution of disorder sites does not change. At low carrier density the screening is non-linear, leading to formation of hills and puddles of electron liquid density associated with the distribution of disorder. At the critical carrier density n_c there is a percolating cluster of strong screened centers. Below n_c the screened islands are isolated leading to an insulating phase.

The analyses mentioned above were in 2D, in 3D, within the scaling theory MIT has been already expected, and it has been discussed extensively in the literature, for a review see Ref. [18]. In the framework of HF approximation, in 1995, Tusch *et al.*[33] showed that the localization effects has non-monotonic behavior with disorder and at intermediate regime of disorder and interaction, the disorder enhances metallic behavior — this has a resemblance to what we have obtained in our HF approximation in 2D.

1.4 Numerical approaches

1.4.1 Quantum Monte Carlo

This method allows us to work with the full many-body wavefunction at the cost of statistical uncertainity, which can be reduced by increasing number of measurements. One finds the expectation value of operators by stochiastically sampling a probability distribution. For reveiws in the method see references [34, 35, 36]. Although Quantum Monte Carlo (QMC) is exact, it suffers from fermionic sign problem and it is not applicable to very low temperature, it is also limited to very small system sizes.

Numerical simulation using QMC [37, 38] in a 2D disordered Hubbard model have suggested a MIT by analyzing the dc-conductivity. They predicted possibility of a metallic phase at an intermediate regime of disorder and interaction. They pointed out if the particle hole (p - h) symmetry is broken, increasing disorder enhances the conductivity. On the other hand if the p-h symmetry is preserved, increasing disorder suppresses conductivity. Site disorder in the latter case is like random Zeeman magnetic field at all the sites. They showed that application of a uniform magnetic field, restores localization further. This is consistent with the experimental observations. Contrary to these findings, there have been also a number of papers (see [39, 40, 41]), within QMC approach, which did not report metallicity in the 2D disordered Hubbard model. Therefore, theoretically, existance of a metallic state in 2D is still an open question.

1.4.2 Dynamical mean field theory

Byczuk *et al.*[42], in a very recent work using dynamical mean field theory (DMFT) proposed a phase diagram for a correlated disordered system. In this method, the disordered Hubbard model is mapped[19] to an ensemble of effective single impurity Anderson Hamiltonian with a random site potential V_i uniformly distributed in the all the sites. By analyzing the averaged local density of states they concluded presence of a metallic phase sandwiched between Mott and Anderson insulators. The metallic state is characterized with a finite averaged local DOS. In this approach, or similar DMFT approaches, the disorder is not treated exactly and the geometry of the lattice is coming to the picture through a non-interacting DOS for calculating local Green's functions, in this work non-interacting DOS was chosen to be a semi elliptic function of energy. In a separate work, Tanaskovic *et al.*[43] showed strong enhancement of screening in the strong coupling regime despite reduction of compressibility. In $d = \infty$, MIT in disordered Hubbard model has been already discussed within this approach (see [44, 45]).

It would be interesting to know if the metallic phase survives by solving the DMFT equations simultaneously in all the sites in a 2D lattice. This way, the disorder is treated exactly, however the number of self-consistent DMFT equations increases substantially.

1.4.3 Inhomogeneous Hartree-Fock approximation

Hartree-Fock (HF) approximation maps the disordered Hubbard model to an effective Hamiltonian with quadratic terms in annihilation and creation operators. The variational local fields and densities of the effective Hamiltonian have to be determined self-consistently (for details see appendix A). In this thesis, mainly within this approach, we have studied the effects arising from interplay of disorder and interaction in a 2D electron gas. While this method treats the disorder exactly it ignores the effects of quantum fluctuations and its finite temperature results are not reliable.

1.5 Summary of the results

Here are our main results for the disordered Hubbard model within inhomogeneous HF approximation:

- At low disorder limit, the system is a Mott insulator and it has antiferromagnetic long range order. With increasing disorder the Mott gap closes around V ≈ U/2 U is the interaction and the random disorder in all sites V_i is chosen from a uniform distribution of random numbers between -V and V, therefore V measures the strength of disorder.
- At an intermediate regime of disorder, the system becomes a metal with extended states at the Fermi energy. Scaling analysis to the larger system sizes confirms that metallic behavior is not a finite size effect.
- In the metallic phase there is a percolating cluster of bonds with high kinetic energy.
- At large disorder limit, the excitations are gapless but the states at the Fermi energy are localized. The system is made of clusters of AF sites with no long order, with increasing disorder the size of cluster shrinks further. At limit of small interaction the system is a paramagnetic Anderson insulator.
- AF long range order vanishes at the percolation threshold of weakly disordered sites.
- At the limit of large interaction limit U/t, we found a new type of magnetic state arising from a binary disorder potential (U/2 and −U/2) at two neighboring sites. This state, which we call it resonant pair exchange (RPE), is a mixture of a singlet state of two singly occupied sites and another state with zero and double electron occupancies (|0,2⟩). Such pairs have lower magnetic moment than a purely singlet state, however their energy difference with the triplet excited state is of the order of hopping parameter t which is higher than J = 4t²/U.

In the next chapter we briefly present the scaling theory and its consequences in low dimensions. The third chapter is some of the key experiments which for the first time questioned the scaling theory predictions. Our results in the framework of the HF approximation come in the fourth chapter, in this chapter we present the detailed results which conclude existence of a metallic state in an intermediate regime of interaction and disorder. In the fifth chapter we study the disordered Hubbard model within a perturbation approach and propose a new of type of magnetic state with reduced antiferromagnetic (AF) moment and enhanced AF coupling.

Scaling theory of localization

2.1 Introduction

In this chapter we review briefly the scaling theory and its consequences for a disordered electronic system. In 1979, Abrahams *et al.*[1] within a perturbative approach showed that for a weakly disordered system the β function — defined as $d \ln g/d \ln L$ where g is the conductance and L is the length scale — deviates from its Ohmic value (d-2) by -a/g, where a is a positive constant. For two dimensions, analysis of the β function has important consequences, it predicts the absence of a metallic state. However it should be noted that this theory ignores the effects of electron-electron interaction which plays an important role in real experimental systems showing metal-insulator transitions. In the next section we review the scaling theory analysis and its predictions in different dimensions.

2.2 Localization within scaling theory

In 1970's Thouless showed that for a system of non-interacting disordered electron gas the localization problem can be formulated as a scaling analysis of one parameter, the conductance [46, 47].

The basis of the scaling theory is to relate the conductance of a system size L to perturbation in the boundry conditions. States with a localization length smaller than the length scale of the system, are essentially insensitive to the boundary conditions, whereas extended states or localized states with a localization length larger than Lshould be affected to changes in the boundry conditions. For a system of length scale L, much larger than the mean free path, it takes time T to travel L/2 with diffusion constant D. Based on uncertainty principle between time and energy

$$\Delta E = \frac{\hbar}{T} = \frac{\hbar D}{L^2} \tag{2.1}$$

 ΔE is the sensitivity to the boundary conditions. From Einstein relation for conductivity [48]

$$\sigma = \frac{e^2}{2} D \frac{dn}{dE} \tag{2.2}$$

where $dn/dE = dN/L^d dE$ is the density of states. From Eq. 2.1 we have

$$\Delta E = \frac{2\hbar^2}{e^2} L^{d-2} \sigma \frac{dE}{dN} \tag{2.3}$$

For simplicity we choose a square lattice of size $L \times L$. In the tight bonding model,

$$H = -t \sum_{\langle ij \rangle} c_i^{\dagger} c_j + \sum_i V_i n_i \tag{2.4}$$

where t is the hopping amplitude from a site to the nearest neighboring sites. c_i^{\dagger} and c_i are the creation and anihilation operators at site i. V_i is a site dependent potential randomly distributed between -V and V in all the sites. If we increase the length scale from L to L^2 then in the new lattice there are L^2 squares each with length L. We denote the hopping amplitude for a square to the nearest neighboring squares by t' and this is proportional to the sensitivity of the boundary conditions ΔE . The energy mismatch between two close by energy levels of two neighboring squares is V' and is proportional to the inverse density of states dE/dN. In other words, if we pick one energy level, say the closest to E = 0, from each square then all these energy levels have random distribution between -V' and V'. At the end we have the original problem with the rescaled parameters t' and V'; for this system

$$\frac{t'}{V'} = \frac{\Delta E}{dE/dN} = \frac{2\hbar}{e^2} L^{d-2} \sigma = \frac{2\hbar}{e^2} g$$
(2.5)

One can repeat this procedure and find rescaled parameters t'' and V''. For a localized state, with rescaling the length scale the hopping amplitude get weaker and weaker and tends to zero, leading to divergence in resistivity. Therefore the localization problem of non-interacting electrons can be solved in the framework of scaling analysis of the resistivity.

2.3 Scaling theory of β function

In this section we start with the asymptotic behavior of the conductance g in two limits of weak and strong scattering (for details see Ref. [1]). Then we analyze the leading order correction of the β function in the weak disorder regime. Finally we discuss the conductance behavior in different dimensions with emphasis on two dimensions.

In the limit of weak scattering in an electronic system, the wave functions are extended and the mean free path l is large in comparison to the inverse Fermi wave vector k_F^{-1} . The conductivity σ to leading order in $(k_F l)^{-1}$ is $\sigma = ne^2 \tau/m = ne^2 l/\hbar k_F$, where n is the electron density, $\tau = l/v_F$ is the relaxation time and m is the effective electron mass. σ is an intensive quantity provided $L \gg l$, L is the length scale. Based on Ohm's law for a d-dimensional system, the conductance is

$$g(L) = \sigma L^{d-2}.$$
(2.6)

In the limit of strong scattering the wave-functions at the Fermi energy are localized with the localization length ξ_{loc} , since in the real space these states are far apart – despite their close energies – the hopping amplitude from one state to another is exponentially small, in this regime for length scales $L \gg \xi_{loc}$, the conductance is:

$$g(L) \propto \exp(-L/\xi_{loc}) \tag{2.7}$$

For a particular choice of disorder, as the length scale increases from l, g(L) smoothly changes, starting from g_0 (conductance at the length scale of the mean free path) and it finally reaches one of the limiting cases of Eq. 2.6 or Eq. 2.7. The final state depends on the microscopic disorder, g_0 and dimensionality. In 1D where the localization length ξ_{loc} is of the order of l, all the states are localized and the system does not obey Ohm's law on any length scales.

 $\beta(g) \equiv d \ln g/d \ln L$ is a function of conductance g. Next we discuss the scaling behavior of $\beta(g)$ for various dimensions. From Eqs. 2.6 and 2.7

$$\beta(g) = d - 2 \qquad g \gg g_0$$

= $\ln(g/g_0) \qquad g \ll g_0$ (2.8)

In the localized regime $\beta(g)$ is negative corresponding to decrease in conductance as L increases. In the limit of weak scattering $((k_F l)^{-1} \ll 1)$ the next higher order contribution to σ is summation of all maximally crossed diagrams[49]. With this correction σ is

$$\sigma_{3D} = \sigma_0 - \frac{e^2}{\hbar \pi^3} \left(\frac{1}{l} - \frac{1}{L} \right)$$



Fig 2.1: β function versus conductance g. From Ref. [1]

$$\sigma_{2D} = \sigma_0 - \frac{e^2}{\hbar\pi^2} \ln\left(\frac{l}{L}\right)$$

$$\sigma_{1D} = \sigma_0 - \frac{e^2}{\hbar\pi} (L - l)$$
(2.9)

this gives a β function of the form:

$$\beta(g) = d - 2 - \frac{a}{g} \tag{2.10}$$

for an electron gas $a = g_0 = \pi^{-2}$. Therefore for a disordered system $\beta(g)$ is always less than its Ohmic value.

Three dimensions: At very large g, β is one and at small g, β is negative, it passes zero at g_3 (see Fig. 2.1). If the state of the microscopic disorder is such that the conductance g_0 at length scale l is greater than g_3 , one starts somewhere in the positive side of the β curve, and with increasing length scale, β increases further i.e. the system approaches the Ohmic regime. Finally at macroscopic length scales, β reaches one. If g_0 is less than g_3 , β is negative and with increasing L, β tends to the logarithmic form in the localized regime.

Two dimensions: In 2D $\beta \leq 0$, therefore at large length scales the system tends to localized behavior. Consider very weak disorder, with conductance g_0 on the length scale l. Upon increasing the length scale L, g decreases and consequently one moves downward in the scaling curve until it reaches $\beta \approx \ln(g/g_0)$. Thus in 2D states are localized in the thermodynamic limit. One can estimate the localization length from the perturbative value of β . Conductance at the length scale L is $g(L) = g_0 - (e^2/\hbar\pi^2) \ln(l/L)$ where g_0 is given by $(e^2/2\pi\hbar)(k_F l)$. Conductance at the length scale of localization length is zero, therefore $g_0 = (e^2/\hbar\pi^2) \ln(\xi_{loc}^{2D}/l)$ and $\xi_{loc}^{2D} \approx l \exp(\pi k_F l/2)$. Since the localization length depends on l exponentially, it can be difficult to observe localization in 2D. In the presence of an arbitrary small disorder a 2D electronic system has non-Ohmic behavior on the entire range of the length scales. The β function shown in Fig. 2.1 is obtained in the absence of spin-orbit coupling. In the presence spin-orbit coupling the β function can be positive, leading to a metallic phase in 2D[50].

One dimension: In 1D, β always remains negative and it decreases further with increasing the length scale. All states are localized due to repeated backscattering, the localization length is of the order of backscattering mean free path.

Experimental Findings

3.1 Introduction

In this chapter we present experiments on two dimensional electron systems which for the first time questioned the conventional scaling theory.

In 1980, experiments on thin metallic films and MOSFET's showed the expected logarithmic increase in the resistivity with lowering temperature [51, 52] and at low electron densities, an exponential increase of the resistivity versus inverse temperature was observed [52].

Recent development on high quality 2D MOSFET's and GaAs/AlGaAs heterostructure[53, 6, 7, 8] made it possible for electrons (or holes) to move exactly in 2D by confinement and low temperature. In these samples with low disorder and low carrier densities MIT were observed with electron density (or holes) as tuning parameter. At electron density n_s (or p_s for holes) above some critical density n_c (or p_c) the system has metallic behavior and below this critical density the system is an insulator. In the next section we present some of the key experimental findings which confirmed MIT in 2D and at the end of the section we study the effects of electric and magnetic fields in MIT.

3.2 Experimental results

The first experiments that reported MIT in 2D were performed on ultrahigh mobility $(7.1 \times 10^4 cm^2/Vs)$ and very low disordered Si MOSFET's [6, 7] at zero magnetic field. The electron densities were below $10^{11} cm^{-2}$. The electron-electron interaction can be estimated by

$$E_{e-e} \sim \frac{e^2}{\epsilon r_0} = \frac{e^2}{\epsilon} \sqrt{\pi n_s} \tag{3.1}$$

where ϵ is the dielectric constant, and r_0 is the distance between two electrons. We have used the relation $N/L^2 = n_s = 1/\pi r_0^2$ for N electrons in an area L^2 . The Fermi energy, which measures the kinetic energy of electrons, is given by

$$E_F = \frac{\hbar^2 k_F^2}{2m^*} = \frac{\hbar^2 \pi}{2m^*} n_s \tag{3.2}$$

 m^* is the effective mass of electron in Si MOSFET. We have used the relation $N = 4 \times (\pi k_F^2)/(2\pi/L)^2$ (the extra factor of two is due to the degeneracy in [100] surface of MOSFET's). The ratio of these two energies is a dimensionless parameter r_s and quantifies the strength of interaction relative to the Fermi energy

$$r_s \equiv \frac{E_{e-e}}{E_F} = \left(\frac{2e^2m^*}{\hbar^2\epsilon\sqrt{\pi}}\right)\frac{1}{\sqrt{n_s}}$$
(3.3)

At the low electron densities (around $10^{11}cm^{-2}$) the repulsive electron-electron interaction is around $E_{e-e} \approx 9meV$ (by taking the electric constant to be around 9), while the Fermi energy is¹ $E_F \approx 0.6meV$, hence the dimensionless parameter r_s is 15. In the very dilute regime of the electron density and low disorder, 2D electrons are expected to form Wigner crystal. For a 2D disordered system numerical works[54] have suggested the critical r_s beyond which a crystal is formed is 37 ± 5 . Therefore it is natural to assume at $r_s \approx 10$ 2D electrons form strongly correlated liquid.

Summary of the experimental findings are given in the following figures. Fig. 3.1 is the temperature dependence of the resistivity for Si MOSFET at low disorder and low electron densities $7.12 \times 10^{10} - 13.7 \times 10^{10} cm^{-2}$ with corresponding r_s between 18 to 13. In this figure there are two sets of curves, for the upper curves with $n_s < n_c$ the resistivity increases with lowering the temperature $(d\rho/dT < 0)$ at temperatures $T > T^* \approx 2K$, while for the lower curves $n_s > n_c$ the resistivity decreases. Therefore $n_c = 9.02 \times 10^{10} cm^{-2}$ is the critical density which separates the metallic from the insulating phase; the corresponding r_s is around 15.7.

Fig. 3.2.a shows the resistivity versus scaled temperature T/T_0 for Si MOSFET corresponding to Fig. 3.1. All data for different electron densities collapse to two scaling curves, corresponding to the metallic and the insulating phases. The data set in the insulating regime of the Fig. 3.1 for the range of $(T/T_0)^{-1/2} \ge 2$ can be fitted well with the function $\rho = \rho_0 \exp[(T_0/T)^{1/2}]$ while in the metallic side for temperatures

¹Rydberg constant is $\hbar^2/2m_e a_0^2 = 13.61 eV$ and the Bohr radius is $a_0 = 0.52 \times 10^{-8} cm$, in MOS-FET's the effective electron mass is $m^* \simeq 0.21 m_e$ therefore $\hbar^2 \pi/2m^* = 0.6 \times 10^{-14} eV cm^2$. For the electron-electron energy we have used this relation: $e^2 = (e^2/\hbar c)\hbar c \approx 1.44 \times 10^{-7} eV cm$.



Fig 3.1: The temperature dependence of the resistivity for Si MOSFET for different electron densities ranging from $7.12 \times 10^{10} cm^{-2}$ to $13.7 \times 10^{10} cm^{-2}$ at zero magnetic field. (From Ref. [7]).

 $[T_0/T]^{1/2} \ge 6$ it decreases monotonically as $[T_0/T]^{1/2}$ with lowering temperature. As it is shown in Fig. 3.2.b, T_0 depends on electron density n_s .

Fig. 3.3 is the resistivity of 2D electron gas formed in a different system: p-GaAs/AlGaAs[8]. In this figure the hole densities range from $8.9 \times 10^9 cm^{-2}$ to $6.4 \times 10^{10} cm^{-2}$, corresponding to r_s from 24 to 9. At low hole densities $p_s < p_c$ (upper curves) the sample is insulator while for $p_s \ge p_c$ (lower curves) it is metal. The dashed lines correspond to the intermediate regime with metallic like behavior. Range of carrier densities in this figure is much higher than Fig. 3.1, all these curves can be scaled to $\rho = \rho_0 + \rho_1 \exp(-T_0/T)$ [8].

Effect of magnetic field: Application of a magnetic field suppresses the metallic behavior. Extensive studies in Si MOSFET's [55] have reported a rise of resistivity by four orders of magnitude in the presence of a magnetic field parallel to the 2D plane; experiments on 2D hole gas p-GaAs/AlGaAs [56] reached similar conclusions. Fig. 3.4 shows the effect of magnetic field on the resistivity for Si MOSFET at a fixed electron density. The zero field curve is the typical behavior in the metallic regime, however in the presence of a parallel magnetic field the 2D electron gas becomes an insulator (curves for the fields above 0.9 Tesla). At temperatures above $T > T^* \approx 2K$ the effect of magnetic field is negligible. This is the temperature above which the sample has insulating behavior $(d\rho/dT < 0)$ even in the absence of the magnetic field.

Nonlinear regime: All the results mentioned so far were obtained in the linear regime where the electric field tends to zero, in situations that electric field exceeds the thermal energy kT, the V-I curves become nonlinear [57]. In the vicinity of a critical point the dominant nonlinearities are coming from critical fluctuations, an scaling argument [57] in this regime shows that if the resistivity scales with the temperature it should also scale with the electric field. Fig. 3.5.a shows the resistivity versus electric field at various electron densities for Si MOSFET. Plotting resistivity versus the scaled electric field ($\delta_n E^{1/a}$) in Fig. 3.5.b shows that all data can be collapsed to two distinct curves corresponding to insulating and metallic regimes.

3.2.1 Enhancement of Effective mass

Shashkin *et al.*[59] in a recent experiment on 2D MOSFETs showed that for T > 0.2 - 0.5 conductivity linearly decreases with increasing temperature, this can be realized within a Fermi liquid approach[60] where it predicts, in the intermediate of regime of



Fig 3.2: (a) Resistivity vs scaled temperature T/T_0 for different electron densities corresponding to Fig. 3.1. (b) Scaling parameter T_0 vs electron density n_s . In both panels the open symbols correspond to the insulating side of the transition and the filled symbols to the metallic side. (From Ref.[7]).



Fig 3.3: Resistivity per square vs temperature in 2D hole gas of p-GaAs/AlGaAs at zero magnetic field. Different curves exhibits various hole densities. There are three distinct regimes, the upper and lower solid curves correspond to the insulating and the metallic phases respectively, and the dashed lines are metallic like regime at high densities. The inset is the schematic picture of the p-type 2D hole gas used in the experiment (From Ref. [8]).



Fig 3.4: Resistivity vs temperature in heterostructure Si MOSFET at various magnetic fields parallel to the 2D plane. The electron density is $8.83 \times 10^{10} \text{cm}^{-2}$ (From Ref. [8]).



Fig 3.5: (a) Resistivity vs temperature in heterostructure Si MOSFET at zero magnetic field vs electric field for electron densities ranging form $7.81 \times 10^{10} \text{cm}^{-2}$ to $10.78 \times 10^{10} \text{cm}^{-2}$ at T = 0.22K. (b) This panel shows resistivity vs scaled electric field. In the \hat{x} axis the parameter δ_n is $|n_c - n_s|/n_s$ (From Ref. [58]).



Fig 3.6: Normalized conductivity versus temperature for different electron densities (in units of 10^{11} cm⁻²) above the critical density. The dashed lines are the linear fits. (From Ref. [59]).

temperature $(T > \hbar/k_B \tau, \tau \text{ is the elastic relaxation time})$, conductivity has a linear dependence on T:

$$\frac{\sigma(T)}{\sigma_0} = 1 - Ak_B T,\tag{3.4}$$

where A is determined by the Fermi liquid parameters and is

$$A = -\frac{(1+8F_0^a)gm}{\pi\hbar^2 n_s},$$
(3.5)

in this relation m is the effective mass and F_0^a is a Fermi liquid constant related to the normalized g factor:

$$\frac{g}{g_0} = \frac{1}{(1+F_0^a)},\tag{3.6}$$

Fig. 3.6 shows the temperature dependency of normalized conductivity $(\sigma(T)/\sigma_0)$ for various n_s in the metallic phase, in this sample the critical density is $n_c = 8 \times 10^{10} \text{ cm}^{-2}$. As seen in this picture for a wide range of temperature, conductivity is linear in T, the dashed lines show the extrapolations of the linear fits.

For the region $n_s > n_c$ the experimental data indicated a linear dependence of 1/A on n_s , while product of g and m remains almost constant, therefore F_0^a is n_s



Fig 3.7: Normalized effective mass (filled squares) and g factor (filled circles) as a function of electron density n_s . m_b is the band mass and is equal to $0.19m_e$ where m_e is the free electron mass. The inset shows the Fermi liquid parameter dependency on n_s , the solid line in the theoretical value (obtained in Ref. [60]) and circles are experimental data points evaluted from Eq. 3.6 (From Ref. [59]).

independent (≈ -0.2); However as $n_s \rightarrow n_c$ a sharp increase of m was observed while g remains constant (see Fig. 3.7). This indicates that growing effective mass is reponsible for the anomalous behavior of the 2D electron system near metal insulator transition. Traditionally it was belived that the effective mass remains constant $m \approx m_b$ (m_b is mass band), and therefore the elastic relaxation time τ was obtained from mobility and it was decreasing with decreasing n_s in the critical regime. But, now, by taking into account the anomalous behaviour of m, the elastic relaxation time increases with lowering n_s (for more details see Fig.4 of reference [59]). Hence, the drop in mobility at low n_s is originated from the enhancement of m rather than decrease of τ , although τ tends to zero in the insulating phase.

Separate measurements in dilute, high mobility GaAs, 2D electron systems reached to similar conclusions, for details see reference [61].

3.3 Conclusion

The experiments which carried out on 2D samples of electron gas with high mobility and low carrier densities lead us to the following conclusions:

(i) In the clean and dilute 2D samples of Si MOSTFET and p-GaAs/AlGaAs, the metallic state $(d\rho/dT > 0)$ have been obtained at carrier densities n_s (or p_s for holes) above some critical value n_c (or p_c). For $n_s < n_c$ (or $p_s < p_c$) these systems show insulating behavior $(d\rho/dT < 0)$. The metallic behavior persist to exist upto the lowest accessible temperature, which is in contrast with the theory of Anderson localization for noninteracting electrons.

(*ii*) The application of a magnetic field at any angle with respect to the 2D plane suppresses the metallic behavior and restores the localization behavior.

(*iii*) All data for resistivity vs temperature/or electric field at different carrier densities collapse to two distinct curves for the metallic and insulating phases indicating a quantum phase transitions[62] driven by magnetic field or carrier density. There is no consensus among community about the nature of either of these effects.

(iv) The anomalous behavior obsevered near metal insulator transition of low density 2D MOSFETs, originates from the effective mass enhancement, this effect also lead to a sharp increase in elastic scattering time as $n_s \rightarrow n_c$.

Disordered Hubbard Model

4.1 Introduction

In the scaling theory mentioned earlier the effects of electron-electron interaction were ignored. In this chapter we study the interplay of disorder and interaction in 2D systems within the context of the disordered Hubbard model which is the simplest model that includes both disorder and interaction. However this model is difficult to solve exactly, even in the absence of disorder. We use an inhomogeneous Hartree-Fock (HF) approximation in which we treat the disorder exactly while using a mean field approximation for the interaction (see appendix A).

Amongst our most striking results is a novel metallic phase which is sandwiched between a Mott insulator for small disorder and an Anderson insulator at large disorder. In the next section we present the model and subsequent sections contain results obtained within the HF approximation. We conclude with a phase diagram based on our numerical results.

4.2 Model

We study the repulsive Hubbard model with site disorder. The Hamiltonian is:

$$H = -\sum_{ij,\sigma} t_{ij} (c_{i\sigma}^{\dagger} c_{j\sigma} + h.c.) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \sum_{i,\sigma} (V_i - \mu) n_{i\sigma}$$
(4.1)

The first term is the kinetic energy of electrons for hopping from site *i* to site *j* on a 2D square lattice. We assume for the nearest neighbors $t_{ij} = t$ and for the rest $t_{ij} = 0$. $c_{i\sigma}^{\dagger}(c_{i\sigma})$ is the creation (annihilation) operator at site *i* with spin σ . $n_{i\sigma} = c_{i\sigma}^{\dagger}c_{i\sigma}$ is the occupation number and μ is the chemical potential that fixes the total density of electrons. In this work, we fix the density at half filling $\langle n \rangle = 1$ for which μ is close to U/2. The second term is the repulsive interaction energy when two electrons of opposite spin are on the same site *i*. The last term is the site energy, V_i , chosen randomly from a uniform distribution between -V and V.

We use an inhomogeneous Hartree-Fock approximation to change the interaction term which is quartic in $c_{i\sigma}$ to quadratic terms in $c_{i\sigma}$. The eigenstates of the effective Hamiltonian can be found by diagonalizing a $2N \times 2N$ matrix (for details see appendix A). The effective Hamiltonian is

$$H_{eff} = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma}) + \sum_{i} \left(V_{i} + \frac{U}{2} \langle n_{i} \rangle - \mu \right) n_{i} - \sum_{i} \mathbf{h}_{i} \cdot \mathbf{S}_{i}$$
(4.2)

in which

$$\mathbf{h}_{i} = 2U\langle \mathbf{S}_{i} \rangle$$

$$\mathbf{S}_{i} = \frac{1}{2} c_{i\sigma}^{\dagger} \vec{\tau}_{\sigma\sigma'} c_{i\sigma'}$$

$$(4.3)$$

 \mathbf{h}_i and $\langle n_i \rangle$ represent local fields and density and are variational parameters which have to be determined self-consistently, and $\vec{\tau}$ is the Pauli spin matrices. We tune μ such that the half filling condition is satisfied. We have studied system sizes up to 50 × 50 at zero and finite temperatures. For an N site system starting with an initial guess for the variational parameters, we have to solve the problem self-consistently for 3N variables. An efficient algorithm requires special mixing schemes e.g. the Broyden method (see the appendix B) to achieve self-consistency in a reasonable amount of computer time.

4.3 Results in three different limits

4.3.1 Non-Interacting electrons

In the non-interacting case and without disorder (V = 0 and U = 0) the system is a metal. The energy spectrum for nearest neighbor hopping is

$$\epsilon_k = -2t(\cos k_x + \cos k_y) \tag{4.4}$$

The density of states (DOS) has a logarithmic divergence at half filling and is given by Eq. C.18:

$$g(\epsilon) = \frac{\theta(\epsilon - 4t)}{4\pi^2 t} K(\sqrt{1 - (\epsilon/4t)^2})$$
(4.5)



Fig 4.1: Pauli Susceptibility $\chi(\vec{\mathbf{q}} = 0, \omega = 0) = \chi^0$ as a function of chemical potential μ scaled by the band width at T = 0 for free electrons on a 2D square lattice (1500×1500).

where K is the elliptic integral of the first kind. For this system the spin susceptibility at wave vector \mathbf{q} and frequency ω is (see appendix D)

$$\chi_{zz}(q, i\omega) = \frac{1}{2} \sum_{k} \frac{f(\epsilon_{k+q}) - f(\epsilon_k)}{\epsilon_k - \epsilon_{k+q} - i\omega},$$
(4.6)

where $f(\epsilon_k)$ is the Fermi function at energy ϵ_k . At q = 0, $\omega = 0$ and T = 0

$$\chi^{0} \equiv \chi_{zz}(0,0) = -\frac{1}{2} \sum_{k} \frac{\partial f(\epsilon_{k})}{\partial \epsilon_{k}} = \frac{1}{2} \sum_{k} \delta(\epsilon_{k} - \epsilon_{F})$$
$$= \frac{1}{2} \int g(\epsilon) d\epsilon \delta(\epsilon - \epsilon_{F}) = \frac{1}{2} g(\epsilon_{F})$$
(4.7)

is the Pauli susceptibility. In Eq. 4.7 $g(\epsilon_F)$ is the DOS at the Fermi energy.

Fig. 4.1 shows the filling dependence of the Pauli susceptibility (Eq. 4.7) for a 2D lattice $N = 1500 \times 1500$ at T = 0. There is a logarithmic divergence in χ^0 (at half filling) which is in agreement with Eq. 4.5. Fig. 4.2 shows T dependent of χ^0 at two different filling factors n = 1 and n = 1/2. Since $\chi^0 \propto g(\epsilon_F)$ as $T \to 0$ we see a divergence in χ^0 at half filling but it approaches a constant value away from half filling. For T > t the system becomes non-degenerate¹ and $\chi^0 \propto 1/T$.

In Fig. 4.3 we show the wave-vector dependent susceptibility $\chi(\mathbf{q}, \omega = 0)$ for $\mathbf{q} = (\pi, \pi)$ as a function of filling. By comparison between Fig. 4.2 and Fig. 4.3 we see

¹In general for any **q** the spin susceptibility has Curie behavior at $T \gg t$.


Fig 4.2: The susceptibility χ^0 as a function of temperature T shown for two different filling factors. At half filling (n = 1) and at low T, χ^0 has a divergence which tracks the divergence of the density of states. At quarter filling $(n = 1/2) \chi^0$ shows a bump at $T \simeq 0.5t$ because at this temperature the electrons can access the high density of zero energy states. For T > t, $\chi^0 \propto 1/T$, indicating Curie behavior from independent local moments.

stronger divergence for $\chi(\pi,\pi)$ at T = 0 and n = 1 than for χ^0 primarily because of the effect of nesting at half filling. **Nesting** refers to the existence of parallel sections on the Fermi surface which are separated by the wave vector \mathbf{q}_{nest} (see Fig. 4.4).

Fig. 4.4 shows the Fermi surface for different filling factors. It is evident that at half filling, there are parallel sections at $\mathbf{q} = (\pi, \pi)$ which gives rise to nesting.

From Fig. 4.5 it is quite clear that $\chi(\vec{\pi})$ is a constant near T = 0 except at the half filling and $\chi(\vec{\pi}) \propto 1/T$ for $T \gg t$ for all filling.

The Pauli susceptibility χ^0 (Eq. 4.7) is dependent on the DOS at the Fermi energy but $\chi(\mathbf{q})$ at finite \mathbf{q} depends on the Fermi surface geometry, in particular its nesting property. The nesting effects are more dramatic in 1D at any filling and in 2D at half filling. It provides a large number of small energy denominators $|\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}_{nest}}| \ll \delta$ in Eq. 4.6 which enhances $\chi(\mathbf{q}_{nest})$. This divergence can produce a magnetic ground state. In 2D at half filling nesting happens for $\mathbf{q} = (\pi, \pi)$ and produces an antiferromagnet ground state (Fig. 4.3 and Fig. 4.4).

In the classical limit the susceptibility has a different behavior. In that case instead



Fig 4.3: The wave-vector dependent susceptibility $\chi(\mathbf{q}, \omega)$ at $\mathbf{q} = (\pi, \pi)$ and $\omega = 0$ as a function of filling at T = 0. The singularity at $\mu = 0$ is because of nesting at half filling.

of considering electrons in the lattice, we assign each site an spin label. Magnetization for this system is $\langle S \rangle = \partial \ln Z / \beta \partial h$, h is the external magnetic field and Z is the partition function, therefore susceptibility is $\chi = \partial \langle S \rangle / \partial h = (\partial^2 Z \ln Z / \partial h^2) / \beta$. This limit gives rise to 1/T behavior of the susceptibility known as the Curie susceptibility.

4.3.2 Effect of interaction: Mott insulator

In the weak coupling limit, the ground state is unstable against spin density wave fluctuations. At half filling, there is ordering of the electronic spin density in the wave vector $Q = (\pi, \pi)$ mode. By assuming the ordering to be in the z direction, analysis within a mean field approximation shows that (see Ref. [63]) in addition to the AF order for small coupling U, the system also has a gap in the single particle spectrum $\Delta \propto -t \exp(-2\pi\sqrt{t/U})$ [63] (see appendix E).

In the strong coupling limit, the system has a Mott gap $\propto U$ (see Fig. 4.6). At half filling, a second order perturbation expansion in t/U maps the repulsive Hubbard model to the spin-1/2 Heisenberg model with a coupling between nearest neighbor spins given by $J = 4t^2/U$ (see appendix F). The ground state for this model has AFLRO (for a review on spin-1/2 Heisenberg model see Ref. [64]). The AF ground state is highly



Fig 4.4: The Fermi surface for $\epsilon_{\mathbf{q}} = -2t(\cos q_x + \cos q_y)$ at different filling factors. At half filling for $\mathbf{q} = (\pi, \pi)$ there are parallel sections in the Fermi surface which give rise to an instability towards an antiferromagnetic ground state.



Fig 4.5: The wave-vector dependent susceptibility $\chi(\vec{\pi}, 0)$ as a function of temperature T shown for two different filling factors. $\chi(\vec{\pi}, 0)$ has a divergence at half filling (n = 1) at low T because of nesting. For T > t, $\chi(\vec{\pi}, 0) \propto 1/T$.



Fig 4.6: (a) DOS for an interacting fermionic model in a square lattice $N = 24 \times 24$. This is obtained by using HF approximation at zero temperature at U = 4t. (b) Spin-Spin correlation in the z direction at U = 4t, V = 0 and T = 0. At distance l = L/2, $\langle S_i^z S_{i+l}^z \rangle$ approaches $|m_{op}^z|^2 = 0.24$.

unstable against filling. For a single hole, Nagaoka showed that the ground state is a ferromagnet[65]. For higher number of holes, AFLRO is destroyed and the system describes a superconducting ground state[66], which is basically the high T_c problem.

At finite temperatures, HF equations overestimate magnetic ordering and underestimates disorder effects arising from an insufficient inclusion of spin fluctuations, leading to a magnetic ground state with long range order. This violates Mermin-Wagner theorem[67] which predicts no long range in a 2D or 1D Heisenberg model with short range interaction.

4.3.3 Effect of disorder: Anderson-Insulator

In a non-interacting disordered system there is no gap in the DOS (Fig. 4.7) and with increasing disorder, the van Hove singularity at $\omega = 0$ is washed out. Although the excitations are gapless, for any amount of disorder all the states are localized and spatially far apart so that their contribution to the conductance is zero. Fig. 4.8.a shows the spatial extent of the wave function at the Fermi energy. As the disorder is increased, the wave-function gets more and more localized.



Fig 4.7: DOS for noninteracting disordered fermionic model at different disorder width.

4.4 Results: Interplay of Disorder and interaction

Having discussed the various limits, we now present results in the presence of both disorder and interaction obtained within a self consistent Hartree Fock approximation.

4.4.1 Magnetization and spectral gap

In the weak disorder limit, the system is a Mott insulator with a gap in the DOS and AF long range order. Fig. 4.9 shows that the local magnetization $m^{\dagger}(i) = (-1)^{i_x+i_y} 2\langle S_z(i) \rangle$ has AF order for V = 2t. Defect sites in this panel are those with site disorder close to U/2. With increasing disorder the defective regions with reduced AF order grow in size. This also can be seen in Fig. 4.10.a and Fig. 4.10.b where the distribution of $m^{\dagger}(i)$ shows a growth of paramagnetic (PM) sites with $m^{\dagger} \approx 0$ as disorder increases and correspondingly an increase in sites with the local density away from $\langle n_i \rangle = 1$. Appearance of red sites in the right panels of Fig. 4.9 at V = 3t, 5t — these sites have staggered magnetization opposite to the rest of the surrounding AF cluster — is the signature of higher order couplings; crudely speaking, whenever a site with weak disorder has nearest neighbors (nn) with strong disorder it get coupled to the next



Fig 4.8: Plot of $\sum_{\sigma} |\psi_{n\sigma}(i)|^2$ of the eigenstates at the Fermi surface for the noninteracting and interacting (U = 4t) disordered Hubbard model at T = 0. For non-interacting model by increasing V the states (at the Fermi surface) get more localized while for the interacting case for V = 2t and V = 5t these states are localized and for V = 3tthey are extended.



Fig 4.9: Magnetization for different disorder widths and system size $N = 28 \times 28$. Left panels show $\langle S_z(i) \rangle$ but right panels show the staggered magnetization $m^{\dagger}(i) = (-1)^{i_x+i_y} 2 \langle S_z(i) \rangle$. For V = 2t there are a few PM sites. The uniform blue color is indication of AF long range order for V = 2t and V = 3t; for V = 5t the system looses AF order. The red sites in the right panels are evidence of next nearest neighbor coupling among spins.



Fig 4.10: (a) Probability distribution $P(m^{\dagger})$ for different values of V. With increasing V, $P(m^{\dagger})$ gets broader and develops weights near 0 indicating the growth of paramagnetic regions. (b) Probability distribution P(n) of the site occupancy $\langle n_i \rangle$ showing a peak near $\langle n_i \rangle \approx 1$ for V = 1 which gets broader with increasing V and develops weight for doubly occupied and unoccupied sites.

nn's, leading to a mismatch in the AF pattern of that particular cluster. Details of obtaining the next nn coupling from a perturbation expansion up to fourth order is in the appendix C.

In Fig. 4.11 we show the correlation between the local disorder potential V_i , the local AF order $m^{\dagger}(i)$, and the local density $\langle n_i \rangle$. For a fixed disorder at V = 3t for a given realization, the sites with AF moment greater than 0.3 are marked as the AF sites and those with AF moment less than 0.1 are the PM sites. Then we find the probability distributions of site potential V_i and the local densities $\langle n_i \rangle$ of the AF, PM and all the sites. Finally we average over realizations of disorder. It clearly shows that regions with AF order [defined crudely as those with $m^{\dagger}(i) \geq 0.3$] originate from the weakly disordered (WD) regions of the disorder potential. These regions also have a local density close to unity. On the other hand, the PM sites (with m^{\dagger}) are correlated with strongly disordered (SD) regions that also have a bimodal density clustering near zero and double occupancy.

The spectral gap and AF order are the two defining characteristics of a Mott insulator. There is a gap in the single particle density of states for $V < V_{c1} = 2t$ (see Fig. 4.12) and it closes at U/2; however AF order persist to exist upto disorder strength $V = V_{c2} \approx 3.4$ (Fig. 4.13), which is the classical percolation threshold of WD sites, further details of the percolation picture is given in the next chapter. AF order parameter is obtained from the spin-spin correlation function. Surprisingly, even though the energy scale for charge fluctuation is $U \gg J \sim t^2/U$, the scale for AF coupling, the spectral gap vanishes at a lower value of disorder than the AF long range order. Our results are consistent with the results obtained within DMFT[68] in prediction of closing gap. However HF overestimates the AF moment. For a comparison between HF estimate of staggered magnetization and exact results in a non-disordered system see Ref. [63], the discrepancy increases with increasing U. Surprisingly, in the presence of disorder, HF approximation gives better estimate of the ground state (for detailed comparison see Ref. [69]). Fig. 4.14 compares the local density of states (LDOS) for paramagnetic and AF sites at V = 3t. In both types of sites there is no gap in the LDOS; however for the paramagnetic sites, one side of the spectrum gets higher weight than the other side depends on the sign of the disorder at that site.



Fig 4.11: Correlation between the local disorder potential V_i , the local staggered magnetization $m^{\dagger}(i)$ and the local density $\langle n_i \rangle$ for V = 3t. The distribution $P(m^{\dagger})$ of $m^{\dagger}(i)$ is shown in (b). We define those sites with $m^{\dagger}(i) \geq 0.3$ to be AF sites (region shown filled); and sites with $m^{\dagger}(i) \leq 0.1$ to be PM (shown hatched). The AF sites correlate with the weakly disordered (WD) (filled) region in the disorder distribution in (a) and the density distribution P(n) centered around unity (filled) in (c), whereas the PM sites correlate with the strongly disordered (SD) (hatched) regions in (a) and a bimodal P(n) with weight near zero and double occupancy (hatched).



Fig 4.12: DOS averaged over 10 different realizations of disorder for U = 4t, T = 0 and $N = 28 \times 28$. At V = t there is a gap in DOS, at V = 2t the gap closes and at V = 3t not only the gap vanishes but also DOS at $\epsilon_F = 0$ has a higher value than other V's.



Fig 4.13: (a) Spin-Spin correlation in the z direction. for V < 4t there is a long range order. U = 4t, T = 0 and $N = 24 \times 24$. (b) AF order parameter vs the disorder width, the system sieze is $N = 28 \times 28$. AF long range order disappears at $V_{cr} = 3.4t$. For $V > V_{cr}$ the final state of the self-consistency loops highly depends on the initial inputs for the variational local fields, and it consists of clusters of AF sites with no long range order. Since all these clusters are not oriented in the same direction the total staggered magnetization is zero while locally there is AF order. This leads to a jump in the magnetization at V_{cr} .



Fig 4.14: Local density of states (LDOS) for paramagnetic and AF sites, averaged over 15 disorder realizations. The disorder strength is fixed at V = 3t and the interaction is U = 4t. LDOS of the PM sites with $V_i < 0$ has more weight in the negative side of the spectrum (dotted curve) while for the repulsive PM sites $(V_i > 0)$ it is opposite (dashed curve). For the AF sites the LDOS is symmetric.

4.4.2 Nature of eigenstates and inverse participation ratio

We argue below that for an intermediate regime of disorder the system is an inhomogeneous metal. We establish our claim by an extensive study of the inverse participation ratio (IPR) and its scaling behavior with system size. Fig. 4.8.b shows the eigenstates at the Fermi energy for the interacting system with U = 4t. For small V = 2t and large disorder V = 5t, the states at the Fermi surface are localized while at an intermediate disorder V = 3t these states are extended. This is very different from the behavior for the non-interacting case.

To quantify the extent of the wave function, we calculate the inverse participation ratio IPR defined by

$$IPR(\Psi_n) = \sum |\psi_n(i)|^4.$$
(4.8)

In the continuum limit, in general a localized wave function $\psi(r)$ at r = 0 is of the form

$$|\Psi(r)|^2 = A \exp(-\alpha r/\xi), \qquad (4.9)$$



Fig 4.15: Inverse participation ratio for all the states at three different disorder strength.

where α is a positive constant, ξ is the localization length. In 2D, the normalization factor is $A = \alpha^2 / \xi^2$. Therefore IPR is

IPR =
$$\int_0^\infty |\Psi(r)|^4 r dr = (\alpha/\xi)^4 \int_0^\infty \exp(-2\alpha r/\xi) r dr \propto 1/\xi^2.$$
 (4.10)

Thus IPR(Ψ) is a measure of the localization of a state Ψ . The more a state is localized the higher its IPR. For an extended state IPR ~ O(1/N), where N is the number of sites.

Fig. 4.15 is IPR for all the single particle eigenstates at U = 4t. For disorder strength V = 2t and V = 5t the localized states are at the middle and edges of the spectrum while for V = 3t the states at the Fermi energy (E = 0) are extended.

In Fig. 4.16.a we compare IPR of the states at the Fermi energy for the noninteracting and interacting cases. For the non-interacting case IPR increases monotonically whereas for the interacting case IPR increases and then, surprisingly, has a sudden drop around $V \approx 2t$, further increasing V restores localization. A careful finite size scaling of IPR in the phase marked by **II** shows that IPR tends to zero at infinite length scales whereas in the insulating phase (as well as the non-interacting case) it extrapolates to a finite value as $L \to \infty$ (see Fig. 4.16.b). This is a clear indication of a metallic phase in a 2D disordered system.



Fig 4.16: (a) Inverse participation ratio IPR $\propto \xi_{loc}^{-2}$, where ξ_{loc}^{-2} is the localization length, as a function of disorder strength V for states at the Fermi surface at U = 4tand T = 0 averaged over 15 realizations of disorder. For non-interacting case IPR is monotonically increasing with V (Red curve) but in interacting case IPR is increasing upto V = 2t and then there is sudden drop upto V = 3t. In region I and III the localized states are at the Fermi surface but in the intermediate regime II IPR is small which is indication of large localization length (or extended states). (b) Scaling behavior of the IPR vs 1/L for $L \times L$ systems. In the non-interacting case (open squares) the IPR extrapolates to a finite value for V = 3t, whereas for the interacting case the IPR extrapolates to zero for V = 3t (filled triangles) and V = 3.4t (filled circles) indicating a divergence of the localization length in the metallic regime. Further increase to V = 4t (open hexagons) once again gives a finite localization length.



Fig 4.17: IPR and gap for an $N = 16 \times 16$ system. V and U are in units of hopping parameter t. At strong disorder limit and strong coupling limit IPR approaches one which implies states are localized and the system is an insulator. Only at an intermediate regime of disorder and interaction the IPR has small value and this is the metallic region. In the right panel gap closes at V = U/2. The region with non-zero gap is the Mott insulator.

In Fig. 4.17 at an intermediate regime of disorder and interaction, the metallic region, IPR and the spectral gap have their lowest values. The gap vanished at $V_{c1} = U/2$ (Figs. 4.12, 4.17.b). Thereafter the density of states at the Fermi energy increases with V and has its maximum in the metallic phase.

4.4.3 Screening of the strongly disordered sites

The effective potential at each site defined as

$$\hat{V}_i = V_i + U \frac{\langle n_i \rangle}{2} - \mu \tag{4.11}$$

is a measure of the screening of the bare random potential by repulsive interaction. An analytical work by Herbut [70] within HF approximation in the weak disorder regime has shown that the screened potential is correlated and it enhances dc conductivity. Even recent investigation using DMFT [43] has reported in the strong disorder regime screening to be more significant, if the interaction is treated beyond HF level. Fig. 4.18 is a comparison between probability distributions of site potential V_i and effective potential \hat{V}_i for the PM sites (dotted and dashed-dotted curves), defined as sites with AF moment less than 0.1, as well as all the sites (solid and dashed lines). It indicates screening of the strongly disordered sites, which are the PM sites; screening of the AF sites (defined as sites with AF moment more than 0.3) is minute. The bimodal form



Fig 4.18: The solid and dashed lines are probability distributions of the uniform disorder V_i and the effective potential respectively. The hashed and filled regions are the probability distributions of disorder and effective potential for the PM sites. The data is averaged over 15 realizations of disorder at system size $N = 28 \times 28$ for U = 4t and V = 3t.

of $P(V_{eff})$ is due to the bimodal form of the $P(n_i)$ seen in Fig. 4.10.b.

4.4.4 Compressibility

In the insulating phase most of the sites are frozen with no charge fluctuations while in the metallic phase electrons/holes are more mobile, leading to higher charge fluctuations. Compressibility — defined as deviation of the occupation number of a site to a slight shift in the chemical potential — is a measure of charge stiffness and is given by

$$\kappa(i) = \frac{\delta n_i}{\delta \mu}.\tag{4.12}$$

In Fig. 4.19 we compare the probability distribution of κ in the metallic and the insulating phases. In the insulating phase $P(\kappa)$ has a sharp peak close to zero while in the metallic phase it is very broad. In the Mott region ($V \leq U/2$) compressibility is zero. Fig. 4.20 shows that probability distribution of the compressibility for AF sites is close to zero while $P(\kappa)$ for the PM sites is broader.



Fig 4.19: Probability distribution of compressibility (κ_i) for all the sites in two insulating and metallic phases. For V = 2.4t, in the insulating phase, $P(\kappa)$ has a sharp peak close to zero while for V = 3t, in the metallic phase, $P(\kappa)$ is very broad (note the difference in x and y scales in these plots).



Fig 4.20: Probability distribution of compressibility at V = 2.4, U = 4 for a lattice of size $N = 28 \times 28$ (a) $P(\kappa_i)$ for AF (blue) and PM (red) sites. (b) $P(\kappa_i)$ for all the sites.



Fig 4.21: (a) Probability distribution of kinetic energy in all the bonds for three values of V. (b) Averaged kinetic energy as a function disorder strength. The interaction is fixed at U = 4t. The data is averaged for 15 realizations of disorder. The system size is $N = 28 \times 28$.

4.4.5 Kinetic energy

In the low disorder limit, the probability distribution of the kinetic energy of all the bonds P(K) is peaked at a specific value determined by V, with increasing disorder strength P(K) gets broader such that kinetic energy of some of the bonds even increases. In the large disorder limit most of the weight of P(|K|) shift to smaller values of |K|. Interestingly, the average of kinetic energy does not change monotonically with disorder (see Fig. 4.21), it initially decreases to its lowest value at V = 2.5t then it increases with further increasing of disorder.

4.4.6 Frequency-dependent conductivity

The nature of the frequency dependent conductivity $\text{Re}\sigma(\omega) = \text{Im}\Lambda(\omega)/\omega$ gives insight into the conducting properties of the phases. $\Lambda(\omega)$ is the Fourier transform of $\Lambda(\tau) = \langle j(\tau)j(0) \rangle$ the disorder averaged current-current correlation function (for details see



Fig 4.22: Frequency dependence of the conductivity for V = t in region I showing a gap ω_0 in the joint density of states; for V = 3t in region II showing a linear dependence indicative of metallic behavior; and for V = 5t in region III showing ω^3 dependence indicative of Anderson localization. The inset shows the decrease of the gap ω_0 with increasing disorder V and its vanishing around $V_{c1} \approx 2t$.



Fig 4.23: Temperature dependent of the conductivity for the three disorder strengths. For V = 2t and V = 5t the conductivity is zero at zero temperature while for V = 3t it has a finite value; however it increases with temperature for all three disorder strengths. The system size 32×32 and the data is averaged over four disorder realizations.

appendix A). As shown in Fig. 4.22 the low frequency behavior of $\text{Im}\Lambda(\omega)$ has a finite gap in the Mott region I for V = t; shows a linear ω dependence in the metallic region II for V = 3t which implies that there is a finite dc conductivity $\sigma(\omega \to 0)$; and shows a ω^3 dependence in the Anderson insulating regime III for V = 5t, which implies that there are gapless excitations but nevertheless $\sigma \to 0$.

Fig 4.23 shows that dc-conductivity for V = 3t has a finite value at zero temperature which is a metallic behavior but it increases with temperature — an insulating character. For other values of disorder V = 2t and V = 5t dc-conductivity is zero at zero temperature.

4.4.7 Glassy behavior

After passing the metallic phase with increasing V the system has glassy behavior and locks into different metastable states with close by energies. In this regime of disorder we find that the self-consistent procedure is highly dependent on the initial conditions that we have started with (see Fig. 4.24). Normally in this regime of disorder the number of self-consistent loops highly increases due to large number of metastable states with close energies to the groundstate. The glassy behavior is observed in both metallic and insulating phases. We believe the reason for this glasslike behavior is the local frustration, resulting from competition of nearest neighbor (n.n) coupling with higher orders of coupling in disordered sites, for instance the next n.n. coupling is also AF and in certain situations it may overcome the n.n. coupling. The details of higher order couplings are in the appendix C.

In a recent experiment, Popovic *et al.*[71] studied the transport and low frequency resistance noise measurements in 2D MOSFET's. They reported a glassy phase shared in the metallic and the insulating phases, the width of the glassy phase depends on disorder and becomes small in the low disorder samples. The glassy phase is manifested by a sudden slowing down of electron dynamics and by an abrupt change to the sort of statistics characteristic of complicated multistate systems.

Within DMFT approach, a recent work [72] reported existence of a glassy phase in the metallic and the insulating states in the disordered extended Hubbard model with spinless fermions, Anderson localization stabilizes the glassy phase while the Mott localization weakens it. In the context of Mott-Anderson transition also the glassy behavior has been discussed using scaling analysis (see reference [73]).



Fig 4.24: Staggered magnetization pattern $(-1)^{i_x+i_y} \langle S_i^z \rangle$ for one realization of disorder using HF approximation at U = 4t and V = 3.6t. Two different initial inputs for the variational parameters have given different final states. In panel (a) the initial inputs for variational local fields are AF while in (b) they are randomly chosen from a uniform distribution.

4.4.8 Phase diagram

Based on our results we propose an schematic phase diagram for the disordered Hubbard model on a square lattice in Fig. 4.25.

- Mott insulator: At V = 0 and $U \neq 0$ system is a Mott insulator with a gap in the DOS and AF long range order. The spectral gap closes at V = U/2.
- Insulator A: This phase is characterized with the gapless excitations, AF long range order and localized eigenstates at the Fermi energy. In this phase paramagnetic sites start appearing for sites with $|V_i| > U/2$.
- Insulator B: In this phase, the states at the Fermi energy are localized; excitations are gapless and the system is made of clusters of AF sites with no long range order. With further increasing of disorder the size of these clusters shrinks and at the limit of $V \gg U$ the system becomes an Anderson insulator with no magnetic order. In the limit of strong disorder and strong coupling the electrons are essentially pinned at the lattice sites and since $t \ll U$ and $t \ll V$ they cannot hop from site to site and the system is insulator.
- *Metallic phase*: Our new finding is that in an intermediate coupling regime once the disorder destroys the gap we have a metallic regime. This phase, characterized



Fig 4.25: Calculated phase diagram for the disordered Hubbard model at half filling and zero temperature. The x axis is the interaction U and the y axis is the disorder width V. There are four phases: (i) $0 \le V < U/2$, Mott Insulator (brown region): The system is a Mott insulator with AF long range order (AFLRO) and finite charge gap in the single particle density of states. (ii) $U/2 \le V < 5U/6$, Insulator A (pink region): New insulating phase that we predict with AFLRO but gapless charge excitations. The states at the Fermi energy are localized. (iii) $V \ge 5U/6$, Insulator B (light blue region): This phase is also an insulator, with gapless excitation and localized states at the Fermi energy and clusters of AF spins. At the limit of small interaction the system becomes a paramagnetic Anderson insulator. As we get closer to the line $V \approx 5U/6$ the size of clusters increases. (iv) Novel metallic phase (gray region) is sandwiched between the insulating phases.

by gapless excitations and extended states at the Fermi energy, is sandwiched among three other insulating phases. In the metallic phase the charge fluctuation induced by disorder screens out the random potential. For $2V \leq U/0.59$ there is AF long range order.

4.5 Binary Disorder Model

4.5.1 Model

Another interesting model which gives insights to the 2D MIT is the binary disorder model. Since often the disorder is from one or two types of atoms (with a fixed V_i)

this model is more realistic in describing the disorder. A fraction of sites (n_{dis}) have site potentials $\pm V$, half of these sites have $V_i = V$ and for the other half $V_i = -V$, for the rest of the sites $(1-n_{dis}) V_i = 0$. In this model the disorder is described by two parameters V and n_{dis} . Tuning either of them lead to different results. Further it can help us in understanding which types of bonds contribute most to the conduction. The electron density is fixed at $\langle n \rangle = 1$, and the temperature is zero. Here we report results for a fixed value of interaction U = 4t. These results are obtained within the framework of HF approximation.

4.5.2 Magnetization, density and gap

Figure 4.26 shows the staggered magnetization for three values of $n_{dis} = 0.23$, 0.43 and 0.72 at fixed values of interaction (U = 4t) and disorder strength (V = 2t). The left panels indicate disorder profile; red and blue correspond to two values of the disorder strength $V_i = \pm V$. The right panels are local staggered magnetization $m^{\dagger} = (-1)^{i_x+i_y} 2\langle S_i^+ \rangle$, and the uniform blue color in the background indicates AF long range order while white color in these panels (right panels) show the paramagnetic sites. The AF long range order persist even to $n_{dis} = 0.72$; however there are clusters with staggered magnetization opposite to the majority of sites (the red patches in the blue background in panel (c)). Fig. 4.27 shows the staggered magnetization as a function of n_{dis} for different disorder strengths. For higher values of V the magnetization falls faster. In Fig. 4.28, the staggered magnetization for small V is almost independent of n_{dis} . Fig. 4.29 shows the spectral gap in the DOS as a function of disorder strength V for three values of n_{dis} . The gap strongly depends on the strength of disorder V rather than n_{dis} .

Three panels in Fig. 4.30 exhibits the probability distribution of the local staggered magnetization, local density and effective potential for three values of n_{dis} in the binary disorder model. For $n_{dis} = 0.23$, $P(S_i/n_i/V_{eff})$ has a sharp peak corresponding to the non-disordered sites. With increasing n_{dis} , in panel (a) most of the weight of the distribution shifts to the smaller values of staggered magnetization. In panels (b) and (c), despite broadening the peaks, with increasing n_{dis} , the distributions of non-disordered sites do not overlap. Panel (c) shows a significant amount of screening for the disordered sites with $V_i = \pm 2t$.



Fig 4.26: Left panels are disorder profile and right panels show staggered magnetization m^{\dagger} for U = 4t and V = 2t in the binary disorder model. Uniform blue color in the right panels indicate AF long range order, which survives even at $n_{dis} = 0.72$. The red color in the left panels indicates sites with $V_i = V$, the blue color sites have potential disorder $V_i = -V$ and uncolored sites correspond to non-disordered sites. The system size is $N = 28 \times 28$.



Fig 4.27: Staggered magnetization as a function of number of disordered sites (n_{dis}) for four different values of V. The data is averaged over three realizations of disorder. Antiferromagnetic initial inputs were chosen for the variational parameters of the HF Hamiltonian.



Fig 4.28: Staggered magnetization versus disorder strength V for three different values of n_{dis} , the interaction is U = 4t. Data is averaged over three realizations of disorder.



Fig 4.29: Gap in the single particle density of states as a function of disorder strength for different values of n_{dis} . The interaction is U = 4t.



Fig 4.30: (a), (b) and (c) show the probability distribution of the local AF magnetization, local density and local effective potential respectively. The interaction and disorder strength are fixed at U = 4t and V = 2t.



Fig 4.31: Eigenstates at the Fermi energy for three different values of n_{dis} and fixed U = 4t and V = 2t. With increasing n_{dis} these states become extended. The system size is $N = 28 \times 28$.

4.5.3 Nature of eigenstates

Like the previous section, the presence of extended states at the Fermi surface is the indication of a metallic phase. Fig. 4.31 shows the extent of an eigenstate $|\psi_{\sigma}^{n}(i)|^{2}$ at the Fermi energy for three values of n_{dis} . For $n_{dis} = 0.23$ and $n_{dis} = 0.43$ these states are localized, while for $n_{dis} = 0.72$ they become extended. This implies a metal insulator transition with n_{dis} as the tuning parameter. Each panel of Fig. 4.32 shows IPR of all the single particle eigenstates for one realization of disorder; the disorder strength is fixed at V = U/2. In (a) and (b) the states at the center of the band are localized, while in (c) with increasing number of disordered sites these states become extended.

Figure 4.33 shows IPR as a function n_{dis} for different V's. IPR has sharper fall for larger V's. Fig. 4.34 is IPR vs V for three different n_{dis} ; at higher values of n_{dis} the system has metallic behavior for larger range V; As $n_{dis} \rightarrow 1$, IPR has the lowest value for V = U/2.

4.5.4 Percolation of kinetic bonds

In order to get a better picture of the metallic phase and how is it arising from disorder, we have looked at the expectation value of kinetic energy of all the bonds. In the



Fig 4.32: IPR for all states vs energy, the disorder strength is V = U/2 and $N = 28 \times 28$. n_{dis} is the fraction of disordered sites with potential $V_i = \pm V$.



Fig 4.33: For larger values of V's, IPR falls faster.



Fig 4.34: IPR as a function V for different values of n_{dis} . With increasing n_{dis} the metallic phase get expanded to wider range of V.

absence of disorder all bonds have equal kinetic energy. By adding disorder, the kinetic energy of the bonds surrounding the disordered site get lower (their absolute values increase), in other words, nearest bonds linked to the disorder get active since disorder induces hopping. The presence of a percolating cluster of such active bonds gives rise to the metallic phase. In order to locate the active bonds in the lattice we have plotted the expectation values of the bonds and their disorder profile in one figure, shown in Fig.'s 4.35, 4.36 and 4.37. In these figures, the open circles are sites with $V_i = 0$, the blue and red circles are sites with disorder potential U/2 and -U/2 respectively. The gray scale squares measure the expectation values of the corresponding bonds, only bonds with kinetic energy more than a threshold (say 0.34t) are shown. Generally kinetic energy is the highest for the bond) — we study the magnetic properties of such bonds in the next chapter — and it is the lowest for the weakly disordered sites $(V_{i,j} = 0)$, however if such non-disordered bonds are surrounded with active bonds their kinetic energy increases which is indication of quantum tunneling.

Figures 4.35, 4.36 and 4.37 are a comparison of number of active bonds at three different disorder densities (n_{dis}) , conductivity enhances with increasing the number of disorder sites but it gets suppressed at disorder strengths away from U/2. These information can be summarized in Fig. 4.38, where the probability distribution of the



Fig 4.35: Open circles are sites with $V_i = 0$, the blue and red circles are sites with potential $V_i = U/2$ and $V_i = -U/2$ respectively; number of sites with repulsive potential (blue) is equal to the sites with attractive potential (red), total number of disordered sites is $n_{dis} = 0.21$. The gray squares are the expectation value of the corresponding bond in units of t. Bonds with energy less than 0.34 are not shown, this is in order to distinguish the active bonds (with higher kinetic energy) easily.



Fig 4.36: In this figure: $n_{dis} = 0.43$.



Fig 4.37: $n_{dis} = 0.72$.



Fig 4.38: Probability distribution of the kinetic energy for all the bonds for three values n_{dis} , corresponding to the previous gray scale figures.

kinetic energy in all the bonds is plotted for three values of n_{dis} . For higher values of n_{dis} the distribution gets broader.

4.6 The role of inhomogeneous magnetic field

By doing HF approximation we get an effective Hamiltonian which is combined of kinetic energy, effective potential (\hat{V}_i) and an inhomogeneous magnetic field (\mathbf{h}_i) in all the sites, practically this is a non-interacting model; within the scaling theory analysis, mentioned in the second chapter, a 2D non-interacting system is an insulator, then the question arises how can HF approximation produces a metallic phase. For that there two possibilities: *(i)* There is correlation in the effective potential. *(ii)* Inhomogeneous magnetic field is correlated with the disorder and it can lead a metallic phase. We have studied the role of either of cases and we found that, there is no correlation in the effective potential but the inhomogeneous field plays an important role in the metallic


Fig 4.39: IPR of the states at the Fermi energy as a function of the fraction of disordered sites n_{dis} . The curve with triangle symbol is the IPR for the binary disorder model at U = 4t and V = U/2, averaged over two realizations of disorder, the curve with square symbols shows IPR for non-interacting electrons with the disorder chosen from effective potential obtained in the interacting problem.

phase.

We have used the effective potential obtained in Eq. 4.11 as the disorder input for the non-interacting case. Based on our results in the binary disorder model, the inhomogeneous field enhances the metallic behavior and in their absence states would be less extended; however in the model with uniform disorder these local fields do not enhance the metallic behavior. Fig. 4.39 shows IPR for the eigenstates at the Fermi energy as a function of n_{dis} , in the metallic regime where IPR is small (for $n_{dis} > 0.6$) the case with non-zero \mathbf{h}_i has smaller IPR. Therefore the metallic phase is arising from two distinct effects, screening of strong disorder sites and presence of an inhomogeneous magnetic field.

4.7 Conclusion

Uniform disorder at all the sites:

• The spectral gap vanishes at the disorder strength $V_{c1} = U/2$. The states at the Fermi surface are localized on the paramagnetic sites.

- AF long range order persists upto the classical percolation threshold of almost singly occupied sites which is $V_{c2} \simeq 5U/6$.
- Once the spectral gap is closed by increasing V, the states at the Fermi surface get extended and the system shows metallic behavior which is very surprising. Our finite size scaling of the states at the Fermi energy shows that the localization length of these states tend to infinity as the system size tends to infinity which is a strong evidence for metallic states.
- Further increasing V restores localization and the system becomes an Anderson insulator with gapless excitations.
- At disorder limit V > 5U/6 the system has glassy behavior.
- Strongly disordered sites get screened by interaction. However screening alone is not sufficient for the appearance of a metallic phase but presence of an inhomogeneous effective field (h_i) which is correlated with the effective potential (V
 _{iσ}) gives rise to a metallic phase in the absence of inhomogeneous field, the effective Hamiltonian reduces to the problem of 2D non-interacting electrons where the disorder is given by the effective potential and this system is an Anderson insulator based on scaling theory.

Binary disorder model:

• Pairs of nearest neighbor sites with opposite signs of potentials have the most contribution to the conductivity. The metallic state arises from a percolating cluster of active bonds, these bonds are siting on pairs with $V_i = \pm U/2$ and $V_j = 0$ or $V_i = U/2$ and $V_j = -U/2$; the latter have magnetic moment which is more stable towards thermal fluctuations as we describe it in details in the next chapter.

The large U limit

5.1 Introduction

In the repulsive Hubbard model for large interaction strength, one can use perturbation expansion in t/U, where t is the hopping parameter and U is the interaction. The first order perturbation moves eigenstates out of the ground state subspace and does not reconnect back to the ground state making the matrix element zero. A second order perturbation couples two nearest neighbor sites leading to an effective Hamiltonian known as t - J model[74]; at half filling this model simplifies to spin-1/2 Heisenberg model with an antiferromagnetic (AF) coupling given by $J = 4t^2/U$.

Electron/Hole doping: At large U and half filling each site has exactly one electron, and therefore the system is a Mott insulator. Doping suppresses AF order. Based on Nagaoka theory[65] at infinite U limit in the presence of even one hole at half filling $(N_e = N - 1, \text{ where } N_e \text{ is the number of electrons and } N \text{ is the number of sites})$ the ground state is a ferromagnet. Addition of electrons/holes (doping) in the quantum Heisenberg model gives rise to interesting effects such as high T_c superconductors which is a subject of great interest to the condensed matter community.

Percolation of magnetic sites: Another direction would be to investigate the effects of quenched disorder in the large U limit at half filling which we are discussing in this chapter. This is like diluting a quantum antiferromagnet (for a review in diluted Heisenberg model see Ref. [75]). Experimental realization of this would be to substitute Copper ions, which are magnetic, with non-magnetic ions such as Zinc or Magnesium in La_2CuO_4 the parent compound of High T_c superconductors. This diluted quantum Heisenberg model has been studied since past ten years, some concluded the destruction of AFLRO before reaching the percolation threshold of doping. Theoretical studies using quantum Monte Carlo [76, 77, 78], spin wave theory and T-matrix approximation [79]



Fig 5.1: Normalized magnetization as a function of dilution for spin-1/2 Quantum Heisenberg model. Different curves show results obtained within different approaches, the symbols are the experimental data points (for details see the Ref. [78]).

concluded that the critical value of dilution for disappearance of AFLRO is the same as percolation threshold. Recent experiments by Vajk *et al.*[78] verified the theoretical predictions (see Fig. 5.1). In the context of the Hubbard model, strong disorder generates two types of sites: non-magnetic unoccupied or doubly occupied sites, and magnetic sites with a single spin[80]. We find that a percolation-based description then becomes possible, as electron hopping results in coupling between neighboring magnetic sites; upon increasing disorder, the number of magnetic sites decreases and eventually leads to a transition marking the loss of long range AF order. At the end of the chapter we compare our HF results (presented in the previous chapter) with the percolation picture and the studies of diluted Heisenberg model using different approaches.

In addition to the destruction of the AF order, disorder may induce new type of magnetic coupling, absent in the non-disordered case. We study the effects of such coupling on different properties of the system. We show that, presence of potential disorder $V_i = U/2$ and $V_j = -U/2$ at two nearest neighbor (nn) sites leads to new type of magnetic coupling that we call resonant pair exchange (RPE). This interaction is the outcome of the resonance to order t between two configurations of spins on

adjacent sites: (a) a spin singlet formed by single spins on adjacent sites and (b) a nonmagnetic doublon formed by a doubly occupied and empty pair. This sort of 'defect pair' occurs with a finite probability in a disordered system, and has several important characteristics: (i) Similar to two-level systems in glasses, these defects bring about a characteristic maximum in the specific heat. (ii) The staggered spin susceptibility is suppressed because of the mixing of the singlet configurations with a non-magnetic configuration. However, interestingly, the non-Curie behavior persists to temperatures $T \sim t$, which is much higher than the kinetic exchange scale $J \sim t^2/U < t$. (iii) The resonant tunneling produces high kinetic energy on the bond connecting the two sites. This provides a source of noise in RPE defects that should be trackable in conductance noise experiments[71].

5.2 Magnetic Properties

We show that close to the atomic limit $(t/U \rightarrow 0)$, the magnetic properties of the strongly disordered half-filled Hubbard model can be understood in terms of a percolationbased model with a concentration of magnetic sites which depends on the ratio V/U. Electron hopping induces two types of magnetic coupling — kinetic exchange between neighboring magnetic sites, and resonant pair exchange between particular pairs of neighboring magnetic and nonmagnetic sites. These couplings and their effects are discussed subsequently.

Consider first the limit t = 0. The competition between repulsive interactions and disorder produces site-dependent occupancies n_i in the ground state (see Fig. 5.2). Sites with $V_i > U/2$ are unoccupied; and those with $V_i < -U/2$ are doubly occupied; neither of these two types of sites has a free spin. On the other hand, sites with $|V_i| < U/2$ have $n_i = 1$ with a free spin residing on each such site. Thus the fraction of singly-occupied (magnetic) sites is x = U/2V, while the remaining sites are nonmagnetic. The spin degeneracy of the ground state is 2^{N_x} , where $N_x = xN$ (In Fig. 5.2, N_x is the number of gray sites.) is the number of singly occupied sites and N is the total number of sites.

The effect of turning on a small value of the hopping amplitude t is to lift the ground state degeneracy. To second order in t, an AF coupling of magnitude J_{ij} is induced between the spins on nearest-neighbor singly-occupied sites i and j, by the well-known mechanism of kinetic exchange. The coupling $J_0 = 4t^2/U$ in the pure system is modified

1	0	0	2	0
2	0	1	1	2
2	1	2	1	1
0	1	0	0	2
2	0	1	2	1

Fig 5.2: A typical ground ground state of the disordered Hubbard model at the atomic limit (t = 0). The number shown at each site indicates the occupancy of the corresponding site. gray sites are the singly occupied sites.

by the site potentials V_i and V_j (for details see appendix F, equation F.12):

$$J_{ij} = \frac{2t^2}{U + V_i - V_j} + \frac{2t^2}{U - V_i + V_j} = \frac{J_0}{1 - (\delta V/U)^2}$$
(5.1)

where $\delta V = |V_i - V_j|$. The effective leading-order Hamiltonian is $\mathcal{H} = \sum_{\langle ij \rangle} J_{ij}S_i \cdot S_j$ where the summation is only over sites with $|V_{i/j}| < U/2$ which are singly occupied and magnetic. In other words, $J_{ij} = 0$ if either of the sites is nonmagnetic.

5.3 Resonant Pair Exchange (RPE)

It is evident from the above analysis that there will be some rare regions where the disorder at a pair of neighboring magnetic sites V_i and V_j is such that the conditions $|V_i - V_j - U| < t \ll U$ and $|V_{i/j}| \simeq U/2$ hold. In that case, the denominator in Eq. 5.1 becomes very large, and the perturbative expression is no longer valid. In fact, in this regime the electron hopping couples these pairs of sites to *first* order in *t*, and we show that it induces a new type of coupling, which we call resonant pair exchange (RPE). The RPE process differs qualitatively from normal kinetic exchange, and has important consequences for the thermodynamic and transport properties of the system.

Consider states with only two electrons on a pair of sites characterized by disorder parameters V_1 , V_2 , when the hopping t = 0. Of the total of 6 states (without half filling condition there are totally 16 possible states for two sites), there are 3 singlet (S = 0)



Fig 5.3: Eigenstates for two sites. (a) Resonant pair exchange: With $V_1 = -V_2 = U/2$; the difference in energy between the RPE singlet ground state and triplet excited state is $\Delta \sim t$. (b) Kinetic exchange: With $V_1 = V_2 = 0$; the energy difference between the magnetic singlet ground state and the triplet excited state is $\Delta = J \sim t^2/U$.

states $|1,1\rangle_S$, $|2,0\rangle$, $|0,2\rangle$ and 3 triplet (S = 1) states $|\uparrow,\uparrow\rangle$, $|\downarrow,\downarrow\rangle$, $|1,1\rangle_t$. Since the Hamiltonian conserves total spin S, we examine each subspace separately. Of the three singlet states, two states $|2,0\rangle$ and $|0,2\rangle$ involve unequal charges at each of the two sites, whereas one state $|1,1\rangle_S = 1/\sqrt{2}(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle)$ involves one electron on each site. The Hamiltonian in the singlet subspace with eigenstates $|1,1\rangle_S$, $|2,0\rangle$ and $|0,2\rangle$ is (see appendix H for details)

$$H = \begin{pmatrix} V_1 + V_2 - 2\mu & -\sqrt{2}t & -\sqrt{2}t \\ -\sqrt{2}t & 2V_1 + U - 2\mu & 0 \\ -\sqrt{2}t & 0 & 2V_2 + U - 2\mu \end{pmatrix}.$$
 (5.2)

We are interested in the case when one of the two unequal-charge states is nearly degenerate with $|1,1\rangle_S$. For specificity, let us take $V_1 = -V_2 = U/2$. Then 5 of the six states (the 3 triplet states and 2 singlet states $|1,1\rangle_S$ and $|0,2\rangle$) are degenerate with energy -U, while $|2,0\rangle$ has energy U. The primary effect of nonzero but small hopping is to mix the two degenerate singlets. In the large U limit, the $|0,2\rangle$ (with energy U) has a large splitting with respect to the ground state. Since we are interested in the ground state and the low level excitations, we estimate the Hamiltonian in (5.2) by

$$H = \begin{pmatrix} -U & -\sqrt{2}t \\ -\sqrt{2}t & -U \end{pmatrix}$$
(5.3)



Fig 5.4: $\chi(\pi)t$ and $\chi(0)t$ versus T/t for different U/t for two sites at half filling and with $V_1 = U/2$ and $V_2 = -U/2$. The square symbol is for U = 8t and the circle symbol for U = 16t. When scaled by t, the curves for different T and U collapse to one curve. The inset depicts $T\chi$ versus $\ln(T/t)$, showing that χ has Curie behavior at large T.

The eigenstates for this effective Hamiltonian are

$$\begin{aligned} |\psi_s^+\rangle &= \frac{1}{\sqrt{2}} \Big(|1,1\rangle_S + |0,2\rangle \Big) \\ |\psi_s^-\rangle &= \frac{1}{\sqrt{2}} \Big(|1,1\rangle_S - |0,2\rangle \Big) \end{aligned}$$
(5.4)

with eigenvalues $-U - \sqrt{2}t$ and $-U + \sqrt{2}t$ respectively. The resulting pattern of energy levels is as shown in Fig. 5.3.a.

It is interesting to contrast the effect of the resonant condition $V_1 = -V_2 = U/2$ on the magnetic properties of the dimer with the magnetic properties arising from the familiar case $V_1 = V_2 = 0$. In the latter case, the states $|2,0\rangle$ and $|0,2\rangle$ have a high energy U, while the hopping lowers the energy of $|1,1\rangle_S$ with respect to the triplet state by an energy of order t^2/U (Fig. 5.3.b). This is the familiar mechanism of kinetic exchange, which produces AF correlations in the dimer ground state; in that case, correlations persist up to temperatures of order t^2/U . With resonant pair exchange, by contrast, the AF correlations in the ground state are reduced (as the state $|0,2\rangle$ is mixed in); but these correlations persist to much higher temperature T (of order t) than in the case of kinetic exchange. This is well brought out by the behavior of the magnetic susceptibility (both the uniform susceptibility $\chi(q = 0)$ and the ordering susceptibility $\chi(q = \pi)$) shown in Fig. 5.4. Deviations from Curie (free moment) behavior are evident at temperatures T below t, signaling the onset of AF correlations due to resonant pair exchange. The static susceptibility for wave vectors q = 0 and $q = \pi$ is

$$\chi^{zz}(q=0) = \beta \langle S^z S^z \rangle$$

$$\chi^{zz}(q=\pi) = \int_0^\beta d\tau \langle e^{\tau H} S^z(\pi) e^{-\tau H} S^z(\pi) \rangle, \qquad (5.5)$$

H is the Hamiltonian, for two site $S^z = S_1^z + S_2^z$ and $S^z(\pi) = S_1^z - S_2^z$. We have also studied the behavior of a four site cluster with sites labeled 1,2,3,4, with $V_i = (-1)^{i+1}U/2$ (see appendix H). We find that the ground state resonates between two types of singlets — one type involving unequal charges at different sites, and the other involving one electron per site. The first excited state is also a singlet, and involves states with one electron per site (as opposed to a triplet for the dimer). Hence thermal occupation of this state increases AF correlations, leading to an increase of $T\chi(\pi)$ (see Fig. 5.5) up till temperatures of the order of the gap. The lowest energy levels are given at the bottom of Fig. 5.5 for U = 8t.

It should be noted that similar magnetic effects are expected whenever the conditions $|U + V_i - V_j| \leq t$ and $|V_{i/j}| \simeq U/2$ are satisfied for neighboring pairs of sites $\langle ij \rangle$. The fraction of such pairs in the disordered Hubbard model is of the order of $(t/2V)^2$. As the contribution to energy lowering from each pair is t, the overall contribution to the ground state energy is of order t^3/V^2 , which is of higher order in t than from the majority of pairs, which are coupled by normal kinetic exchange.

5.4 Specific Heat and Spin Susceptibility:

Since sites coupled by resonant pair exchange are relatively rare and have a very different level structure (see Fig. 5.3) from the majority of pairs, they act as localized



Fig 5.5: $t\chi(\pi)$ and $t\chi(0)$ versus T/t for different U and t for four sites [1-2-3-4] at half filling with periodic boundary conditions, $V_i = (-1)^{i+1}U/2$. By scaling the temperature with t spin susceptibility for different values of U and t collapses to one curve. This is due to the energy splitting of order t between the ground state and the triplet excited state. $\chi(\pi)$ has a rise at $T/t \sim 0.5$, this is because the first excited state is singlet magnetic and rise in temperature makes this state accessible and magnetization increases. At large U the ground state is a mixture of a singlet non-magnetic state $|0, 2, 0, 2\rangle$ and a set of magnetic singlet states (Details are in appendix H). The lower right inset is the energy spectrum at U = 8t upto the third excited state. The lower center inset is $T\chi$ versus temperature in logarithmic scale. At high temperature $T\chi$ approaches a constant.

centers and give rise to a distinctive signature in the specific heat C_v and χ_{avg} , much as two level centers do in glasses.

For an arbitrary pair, by shifting the energies of the singlet subspace (given in Eq. 5.2) with $V_i + V_j$ and taking $\mu = U/2$, the new energies are -U, $\pm |V_i - V_j|$ corresponding to states $|1, 1\rangle_S$, $|2, 0\rangle$ and $|0, 2\rangle$. We assume that the state with energy $|V_i - V_j|$ decouple from rest of Hamiltonian, within this approximation the energy splitting Δ between the singlet ground state and the triplet states is (for details see appendix G)

$$\Delta = \sqrt{2t^2 + \left(\frac{U - \delta V}{2}\right)^2} - \frac{U - \delta V}{2} \tag{5.6}$$

where $\delta V = |V_1 - V_2|$. Here we have assumed the state with energy $U + \delta V$ decouples from other two levels. If V_1 and V_2 are chosen from a uniform distribution between -V to V and we regard each pair as isolated from the others, then the probability distribution for the splitting Δ can be found

$$P(\Delta) = \frac{1}{2V} \left[\frac{\Delta}{V} \left(\frac{4t^4}{\Delta^4} - 1 \right) + \frac{2V - U}{V} \left(\frac{2t^2}{\Delta^2} + 1 \right) \right].$$
(5.7)

The total specific heat from such pairs is then $C_v = \int_{\Delta_{min}}^{\Delta_{max}} d\Delta P(\Delta)c_v(\Delta)$ where Δ_{min} and Δ_{max} can be obtained by substituting 0 and U for δv in Eq. 5.6, since the integration is only over singly occupied sites. $P(\Delta)$ is zero for $\Delta < \Delta_{min}$ and it has a sharp peak at Δ_{min} (see the inset of Fig. 5.6). Noting that the average energy for this two level system is $E(\Delta) = -\Delta \exp(\Delta/T)/[\exp(\Delta/T) + 3]$, the corresponding specific heat $c_v(\Delta) = \partial E/\partial T$ can be obtained (see Fig. 5.6).

We see that at $T \ge t$ most of the contribution to the total specific heat is from RPE sites, due to their large splitting. In this regime C_v varies as $1/T^2$. On lowering T, C_v has a peak at $T = 2t^2/\lambda U$ with $\lambda \simeq 2.85$. Most of the peak weight comes from pairs with small splitting ($\Delta \propto t^2/U$). In the low-T regime, C_v decays exponentially as $T \to 0$; this form of the decay found within the pair approximation would change if the system supports extended (spin wave like) states.

The above arguments hold also for the averaged susceptibility. For the two level system mentioned above spin susceptibility is $\chi^{+-}(\Delta, T) = 2/T[\exp(\Delta/T) + 3]$. The susceptibility averaged over pairs has Curie behavior ($\propto 1/T$) at high T and a peak at $T \approx 2t^2/U$ (see Fig. 5.6); below this temperature triplet states make very small contribution to the susceptibility. As T tends to zero χ^{+-}_{aver} falls as $\exp(-\Delta/T)$. Therefore the



Fig 5.6: The averaged susceptibility χ_{avg}^{+-} and specific heat versus the temperature. Both quantities show a peak at $T \sim J$ where $J \sim t^2/U$ is the exchange coupling. The resonating pair exchange defects contribute at higher temperatures $T \sim t$. The distribution of the energy level splittings is shown in the inset and shows that it is dominated by small splittings $\sim J$.

high temperature $(T \ge t)$ behavior of the specific heat and susceptibility is determined by the RPE sites while the low temperature behavior is governed by pairs of sites with small energy splittings.

5.5 Percolation of Magnetic Sites

Equation 5.1 defines the coupling in the antiferromagnetic Heisenberg model, with random site dilution. It is well known that a necessary condition to have long-range order is that there be an infinite number of connected sites with free spin — i.e. that x exceed the percolation threshold x_c for the lattice in question. This defines a classical percolation picture for the disordered Hubbard model. For the square lattice (the case of primary interest here), $x_c \simeq 0.59[81]$ (see Fig. 5.7), so that to second order in t, antiferromagnetic long range order would be lost for $U/2V < x_c$.

It should be noted that the reduction of the disordered Hubbard model to the site-



Fig 5.7: For a 2D lattice, made of two type of sites A and B randomly distributed, if $N_B/(N_A + N_B) > x_c$ then with probability P_B there is a percolating cluster of B sites (region B), and if $N_B/(N_A + N_B) < 1 - x_c$ with probability P_A there is percolating cluster of A sites (region A). N_A and N_B are the number of sites of type A and B respectively. The x axis is $N_B/(N_A + N_B)$, x_c is the percolation threshold which is close to 0.59[81].

dilute antiferromagnet is valid on any lattice, in any dimension, and is easily generalized to arbitrary distributions P(V) of the disorder variable V. The corresponding threshold value is given by $x_c = \int_{-U/2}^{U/2} P(V) dV$.

Also, the assumed symmetry of the disorder-distribution guarantees that the expected number of sites with $n_i = 0$ is the same as the number with $n_i = 2$. However, in any particular configuration of disorder, we may expect an imbalance of order $\sqrt{N_s}$ in this number, which in turn would imply a corresponding number of holes or extra particles on the $n_i = 1$ sites. These carriers may have interesting consequences, which we have not addressed.

We thus arrive at the following description in the limit of strong disorder $(V \ge U/2)$ and small hopping $(t \ll U)$. First, the ratio x = U/2V determines the fraction of randomly placed singly occupied (magnetic) sites. Second, neighboring magnetic sites are coupled through AF Heisenberg interactions (Eq. (1)), so that we have a random site-dilute Heisenberg antiferromagnet. Third, for V > U/2, a small fraction $\sim t^2/V^2$ of pairs of sites satisfies the condition $|V_i - V_j - U| < t$ and $|V_{i/j}| \simeq U/2$, resulting in resonant-pair coupling between the sites in such pairs.

For x below the percolation concentration x_c , the system consists of isolated clusters of magnetically coupled sites, and there is no possibility of long range order. For x exceeding x_c , an infinite connected cluster of magnetically coupled sites forms, and AF



Fig 5.8: Solid line is AF order parameter m^{\dagger} vs 1 - x = 1 - U/2V using HF approximation for a 2D square lattice of the model mentioned in Eq. 4.1 the system size is 28×28 , U = 4 and T = 0. The dashed and dotted lines are staggered magnetization vs dilution in the 2D quantum Heisenberg model with spin-1/2 using quantum Monte Carlo[78, 77] and spin wave theory[79]. The square symbols are experimental data points using neutron scattering[78]. The percolation threshold is $1 - x_c \simeq 0.41$.

long range order sets in at T = 0. The occurrence of resonant pairs, one site of which is attached to the infinite cluster, would result in a slight loss of AF order in the ground state. On the other hand, as the temperature is raised to values much larger than t^2/U but still of the order of t, only the resonant pairs make a non-Curie contribution to magnetic properties.

5.6 Comparison with HF results

From previous chapter recall that upon adding site disorder in the repulsive Hubbard model, we found the Mott gap in the density of states (DOS) closed at V = U/2, while AFLRO persist upto the percolation threshold of magnetic sites, $2V_{cr} \simeq U/0.59$ (Fig. 5.8). Within the classical picture that we described earlier (at the atomic limit), sites with $|V_i| > U/2$ are non-magnetic and sites with $|V_i| \le U/2$ are magnetic, within HF approximation, the paramagnetic sites start appearing only when $|V_i| > U/2$. Further we found that for disorder strength $V > V_{cr}$ the system breaks into clusters of AF sites with no long range order, and displays a glassy behavior; the final state of self-consistent iterations depends on the initial inputs of the variational parameters of the trial HF Hamiltonian. With increasing disorder the size of AF clusters shrinks further, and at the limit of very large disorder the system is a paramagnetic Anderson insulator. This results are consistent with the percolation picture for appearing of paramagnetic sites and the critical threshold for AFLRO.

Figure 5.8 shows a good consistency of the staggered magnetization obtained within the HF approximation with results of other theoretical and experimental studies of the diluted Heisenberg model. The HF approximation captures rather subtle effects as well. In particular the next nn coupling, coming from a fourth order expansion in t can compete with the nn coupling to produce occasional mismatches in the alignments of particular spins/clusters — and these are reproduced by HF treatment (for details of higher order coupling see appendix F). Further for a honeycomb lattice at half filling the AFLRO vanishes at a disorder strength, predicted by the percolation picture.

5.7 Higher order coupling

Figure 5.9 is a comparison between probability distribution of the nn coupling J and the next nn coupling J' (given by equations F.14, F.15 and F.16) in the disordered



Fig 5.9: Probability distribution of nearest neighbor coupling and the next nearest neighbor coupling at half filling for 2D square lattice.

Hubbard model. For $V < V_{cr}$, P(J) has a sharp peak at $J = 4t^2/U$, while P(J') is small with a peak at J' close to zero. With increasing disorder strength, probability distribution of the nn coupling drops whereas probability distribution of the next nn coupling does not change much. There are fraction of sites for which the inequality $J' \ge J$ holds, this implies competition of J and J' for such sites, leading to frustration or occasional spin mismatch in a cluster of AF sites.

5.8 Discussion and future direction

Recently a number of papers have studied ionic Hubbard model (each site has an extra local potential V and its sign changes alternatively) in a 1D system at half filling[82, 83, 84]. They found that, by increasing U, at a fixed V, there would be a phase transition from band insulator (BI) to a broken-symmetry bond ordered (BO) insulator. References [83, 84] reported another phase transition from BO to Mott insulator (MI), with *no* long range order, as U increases further. Contrary to this, reference [82], using QMC approach, did not find MI phase at any finite V, however, it predicted at the transition point between BI and BO the system is a *metal*, characterized with no charge gap and divergent localization length. In the BO phase a chain of length L forms L/2 bonds similar to RPE bonds in our notation. Another study [85], using

DMFT approach, in a Bethe lattice with $z = \infty$, has reported a metallic phase (not a point) sandwiched between BI and MI.

If a chain of RPE bonds can give rise to a metallic state then it is plausible to assume a percolating cluster of such bonds can also give a metal in a 2D system. Further, even in the absence of classical bond percolation, the quantum tunnelling in 2D can enhance conductivity by connecting disjointed clusters, leading to metallic state. This gives a motivation to study the disordered binary model where $\pm V$'s are randomly distributed on all the sites. The next step could be: *(i)* To write an effective Hamiltonian (simpler to handle), where it has terms corresponding to RPE bonds (with opposite signs of disorder on both sites) and other types of bonds, where disorder in two sites have the same sign. *(ii)* Another direction would be to check for the presence of a percolating cluster of RPE bonds in the disordered model and its role in conductivity. *(iii)* The RPE picture may also give an insight to the kind of wavefunction in a variational QMC approach. The magnetic properties of this model are uncertain.

5.9 Conclusion

We found that disorder induced defects involving pairs of binary potentials leads to a new type of magnetic state in which the staggered magnetization is reduced though the coupling is enhanced. The disordered Hubbard model at large U can be mapped to a disordered diluted AF spin-1/2 quantum Heisenberg model. Based on the percolation picture developed, only sites with $|V_i| < U/2$ can contribute to AF order. Existence of a percolating infinite cluster of such magnetic sites is necessary for AFLRO. We find a remarkable consistency between the percolation picture and HF approximation results even in an intermediate range of interaction U.

Details of Hartree-Fock approximation

In this appendix we give the details of the HF approximation and the numerical method that we have used.

A.1 HF approximation

The repulsive Hubbard model with site disorder model is

$$H = -\sum_{i \neq j,\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i} (V_i - \mu) c_{i\sigma}^{\dagger} c_{i\sigma} + \sum_{i} U n_{i\uparrow} n_{i\downarrow}$$
(A.1)

Within a mean-field approximation for $n_{i\uparrow}n_{i\downarrow}$ we have:

$$n_{i\uparrow}n_{i\downarrow} = c^{\dagger}_{i\uparrow}c_{i\uparrow}c^{\dagger}_{i\downarrow}c_{i\downarrow}$$
$$= \langle n_{i\downarrow}\rangle n_{i\uparrow} + \langle n_{i\uparrow}\rangle n_{i\downarrow} - \langle n_{i\downarrow}\rangle \langle n_{i\uparrow}\rangle$$
$$- c^{\dagger}_{i\uparrow}c_{i\downarrow}\langle c^{\dagger}_{i\downarrow}c_{i\uparrow}\rangle - c^{\dagger}_{i\downarrow}c_{i\uparrow}\langle c^{\dagger}_{i\uparrow}c_{i\downarrow}\rangle + \langle c^{\dagger}_{i\uparrow}c_{i\downarrow}\rangle \langle c^{\dagger}_{i\downarrow}c_{i\uparrow}\rangle.$$
(A.2)

Therefore the effective Hamiltonian is

$$H_{eff} = -t \sum_{\langle ij \rangle, \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i} \tilde{V}_{i\sigma} c^{\dagger}_{i\sigma} c_{i\sigma} + \sum_{i} (h^{-}_{i} c^{\dagger}_{i\uparrow} c_{i\downarrow} + h^{+}_{i} c^{\dagger}_{i\downarrow} c_{i\uparrow})$$
(A.3)

where $\tilde{V}_{i\sigma} = V_i - \mu + U \langle n_{i\bar{\sigma}}^{\dagger} \rangle$

There are 3N + 1 variational parameters. $\langle n_{i\sigma} \rangle$, $h_i = h_i^+ = h_i^-$ at the N sites and the chemical potential μ which have to be found self-consistently. h_i^{\pm} is the expectation value of S_i^{\pm} and is given by

$$h_i^+ = -U\langle c_{i\uparrow}^\dagger c_{i\downarrow}\rangle$$
$$h_i^- = -U\langle c_{i\downarrow}^\dagger c_{i\uparrow}\rangle.$$

The chemical potential μ has to be tuned such that the half filled condition $1/N \sum_{i,\sigma} \langle n_{i\sigma} \rangle = 1$ is satisfied.

 H_{eff} is written as

$$H_{eff} = \mathbf{C}^{\dagger} \begin{pmatrix} V_{1\uparrow} & -t & 0 & \dots & h_{1}^{-} & 0 & 0 & \dots \\ -t & \tilde{V}_{2\uparrow} & -t & \dots & 0 & h_{2}^{-} & 0 & \dots \\ 0 & -t & \tilde{V}_{3\uparrow} & \dots & 0 & 0 & h_{3}^{-} & \dots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots \\ h_{1}^{+} & 0 & 0 & \dots & \tilde{V}_{1\downarrow} & -t & 0 & \dots \\ 0 & h_{2}^{+} & 0 & \dots & -t & \tilde{V}_{2\downarrow} & -t & \dots \\ 0 & 0 & h_{3}^{+} & \dots & 0 & -t & \tilde{V}_{3\downarrow} & \dots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}_{2N \times 2N} \mathbf{C} \quad (A.4)$$
$$= \mathbf{C}^{\dagger} \mathbf{\hat{A}} \mathbf{C} \qquad (A.5)$$

where $N = L_x \times L_y$ is the number of lattice sites and

$$\mathbf{C} = \begin{pmatrix} c_{1\uparrow} \\ c_{2\uparrow} \\ c_{3\uparrow} \\ \vdots \\ c_{N\downarrow} \\ c_{1\downarrow} \\ c_{2\downarrow} \\ c_{3\downarrow} \\ \vdots \\ c_{N\downarrow} \end{pmatrix}$$
(A.6)

by doing a transformation on $c_{i\sigma}$:

$$H_{eff} = \epsilon_n \tilde{c}_n^{\dagger} \tilde{c}_n \tag{A.7}$$

and

$$c_{i\sigma} = \sum_{n} \psi_{i\sigma}^{n} \tilde{c}_{n},$$

$$\sum_{i,\sigma} |\psi_{i,\sigma}|^{2} = 1.$$
 (A.8)

Since eigenvectors of $\hat{\mathbf{A}}$ are real $\psi_{i\sigma}^{n\,*} = \psi_{i\sigma}^{n}$.

A.2 Self consistency procedure

The input parameters of the matrix $\hat{\mathbf{A}}$ are $\langle n_{i\sigma} \rangle$, h_i and μ . For small disorder the ground state has AF long range order therefore it is efficient to start with a AF initial

input which allows one to reache the self-consistent solution faster. However we have found that the final self-consistent solution is independent of the startup initial inputs (e.g. random) in this regime. Similarly for the paramagnetic regime we start with a random initial input for the local fields. In the strongly disordered regime we found that different initial inputs result in different final states, and from them we choose the one with the lowest energy as the ground state. At half filling μ is U/2, but in the presence of disorder this value must be modified by a self-consistent loop in order to satisfy the half filling condition precisely.

A.3 Computational details

At the end of each iteration we compare the input fields with the output fields. If the difference is smaller than 10^{-4} then the self-consistency loop is exited. otherwise we use the Broyden mixing scheme (see appendix B) to generate the next set of input fields.

Typical lattice sizes that we have used are 28×28 , 32×32 , 40×40 and 50×50 . For a lattice of size 28×28 , the amount of CPU time (in a pentium 4 machine) which takes for running one iteration in the self-consistent loop is one minute and in the Mott regime for fixed values of V_d , U and temperature in order to get final answer with accuracy 10^{-4} 250 iteration is needed. In the strongly disordered regime this number can be of the order of couple of thousands. Number of iteraction increases with the system size. For larger sizes (above L = 32) we did the computation in the dec-alpha machines.

A.4 Observables

Here are the expectation values of some of the operators of our interest.

• Local magnetic fields:

$$\langle S_i^z \rangle = \frac{1}{2} \langle n_{i\uparrow} - n_{i\downarrow} \rangle = \frac{1}{2} \sum_n \left(|\psi_{i\uparrow}^n|^2 - |\psi_{i\downarrow}^n|^2 \right) f(\epsilon_n)$$

$$h_i = -U \langle S_i^+ \rangle = -U \langle c_{i\uparrow}^\dagger c_{i\downarrow} \rangle = -U \sum_n \psi_{i\uparrow}^{*n} \psi_{i\downarrow}^n f(\epsilon_n)$$
(A.9)

where $f(\epsilon)$ is the Fermi function.

• Spin-spin correlation function:

$$\langle S_{i}^{+}S_{j}^{-}\rangle = \langle c_{i\uparrow}^{\dagger}c_{i\downarrow}c_{j\downarrow}^{\dagger}c_{j\uparrow}\rangle = \sum_{n,m,k,l} \psi_{i\uparrow}^{n}\psi_{i\downarrow}^{m}\psi_{j\downarrow}^{k}\psi_{j\uparrow}^{l}\langle\tilde{c}_{n}^{\dagger}\tilde{c}_{m}\tilde{c}_{k}^{\dagger}\tilde{c}_{l}\rangle$$

$$= \sum_{n,m,n\neq m} \left(\psi_{i\uparrow}^{n}\psi_{i\downarrow}^{n}\psi_{j\uparrow}^{m}\psi_{j\uparrow}^{m}\langle\tilde{c}_{n}^{\dagger}\tilde{c}_{n}\tilde{c}_{m}^{\dagger}\tilde{c}_{m}\rangle + \psi_{i\uparrow}^{n}\psi_{i\downarrow}^{m}\psi_{j\downarrow}^{n}\psi_{j\uparrow}^{n}\langle\tilde{c}_{n}^{\dagger}\tilde{c}_{m}\tilde{c}_{n}\rangle \right)$$

$$+ \sum_{n} \psi_{i\uparrow}^{n}\psi_{i\downarrow}^{n}\psi_{j\downarrow}^{n}\psi_{j\uparrow}^{n}\langle\tilde{c}_{n}^{\dagger}\tilde{c}_{n}\tilde{c}_{n}\tilde{c}_{n}^{\dagger}\tilde{c}_{n}\rangle$$

$$= \sum_{n,m,n\neq m} \left(\psi_{i\uparrow}^{n}\psi_{i\downarrow}^{n}\psi_{j\uparrow}^{m}\psi_{j\uparrow}^{m}f(\epsilon_{n})f(\epsilon_{m}) + \psi_{i\uparrow}^{n}\psi_{i\downarrow}^{m}\psi_{j\uparrow}^{n}f(\epsilon_{n})(1-f(\epsilon_{m})) \right)$$

$$+ \sum_{n} \psi_{i\uparrow}^{n}\psi_{i\downarrow}^{n}\psi_{j\downarrow}^{n}\psi_{j\uparrow}^{n}f(\epsilon_{n})$$

$$(A.10)$$

• Current-current correlation function:

$$\Lambda_{xx}(\mathbf{q}, i\omega_M) = \int_0^\beta d\tau e^{i\omega_M \tau} \langle j_x(\mathbf{q}, \tau) j_x(-\mathbf{q}, 0) \rangle \tag{A.11}$$

 e_{j_x} is the x component of the paramagnetic current density and $\omega_M = 2M\pi/\beta$ is the Matsubara frequency for $j(\mathbf{q})$ which is a bosonic operator (M is an integer).

$$j_{x}(\mathbf{i}) = it \sum_{\sigma} \left(c_{\mathbf{i}+\hat{x}\sigma}^{\dagger} c_{\mathbf{i}\sigma} - c_{\mathbf{i}\sigma}^{\dagger} c_{\mathbf{i}+\hat{x}\sigma} \right)$$
$$j_{x}(\mathbf{q}) = \frac{it}{N^{1/2}} \sum_{\mathbf{i}\sigma} e^{-i\mathbf{q}\cdot\mathbf{i}} \left(c_{\mathbf{i}+\hat{x}\sigma}^{\dagger} c_{\mathbf{i}\sigma} - c_{\mathbf{i}\sigma}^{\dagger} c_{\mathbf{i}+\hat{x}\sigma} \right)$$
(A.12)

therefore

$$\langle j_{x}(\mathbf{q},\tau)j_{x}(-\mathbf{q},0)\rangle = -\frac{t^{2}}{N}\sum_{\mathbf{i},\mathbf{j},\sigma,\sigma'}e^{i(\mathbf{j}-\mathbf{i})\cdot\mathbf{q}}\Big\langle \Big(c^{\dagger}_{\mathbf{i}+\hat{x}\sigma}(\tau)c_{\mathbf{i}\sigma}(\tau) - c^{\dagger}_{\mathbf{i}\sigma}(\tau)c_{\mathbf{i}+\hat{x}\sigma}(\tau)\Big) \\ \times \Big(c^{\dagger}_{\mathbf{j}+\hat{x}\sigma'}c_{\mathbf{j}\sigma'} - c^{\dagger}_{\mathbf{j}\sigma'}c_{\mathbf{j}+\hat{x}\sigma'}\Big)\Big\rangle.$$
(A.13)

As an example we find one of these terms:

$$\begin{aligned} \langle c_{\mathbf{i}\sigma}^{\dagger}(\tau)c_{\mathbf{i}+\hat{x}\sigma}(\tau)c_{\mathbf{j}\sigma'}^{\dagger}c_{\mathbf{j}+\hat{x}\sigma'}\rangle &= \sum_{n,m,k,l} \psi_{\mathbf{i}\sigma}^{n}\psi_{\mathbf{j}+\hat{x}\sigma}^{m}\psi_{\mathbf{j}\sigma'}^{k}\psi_{\mathbf{j}+\hat{x}\sigma'}^{l}\langle \tilde{c}_{n}^{\dagger}(\tau)\tilde{c}_{m}(\tau)\tilde{c}_{k}^{\dagger}\tilde{c}_{l}\rangle \\ &= \sum_{n} \psi_{\mathbf{i}\sigma}^{n}\psi_{\mathbf{i}+\hat{x}\sigma}^{n}\psi_{\mathbf{j}\sigma'}^{n}\psi_{\mathbf{j}+\hat{x}\sigma'}^{n}\langle \tilde{c}_{n}^{\dagger}(\tau)\tilde{c}_{n}(\tau)\tilde{c}_{n}^{\dagger}\tilde{c}_{n}\rangle \\ &+ \sum_{n,m,n\neq m} \psi_{\mathbf{i}\sigma}^{n}\psi_{\mathbf{i}+\hat{x}\sigma}^{m}\psi_{\mathbf{j}\sigma'}^{m}\psi_{\mathbf{j}+\hat{x}\sigma'}^{n}\langle \tilde{c}_{n}^{\dagger}(\tau)\tilde{c}_{n}(\tau)\tilde{c}_{m}^{\dagger}\tilde{c}_{n}\rangle \\ &+ \sum_{n,m,n\neq m} \psi_{\mathbf{i}\sigma}^{n}\psi_{\mathbf{i}+\hat{x}\sigma}^{n}\psi_{\mathbf{j}\sigma'}^{m}\psi_{\mathbf{j}+\hat{x}\sigma'}^{m}\langle \tilde{c}_{n}^{\dagger}(\tau)\tilde{c}_{n}(\tau)\tilde{c}_{m}^{\dagger}\tilde{c}_{m}\rangle \\ &= \sum_{n} \psi_{\mathbf{i}\sigma}^{n}\psi_{\mathbf{i}+\hat{x}\sigma}^{n}\psi_{\mathbf{j}\sigma'}^{n}\psi_{\mathbf{j}+\hat{x}\sigma'}^{n}f(\epsilon_{n}) \end{aligned}$$

+
$$\sum_{\substack{n,m,n\neq m}} \psi_{\mathbf{i}\sigma}^{n} \psi_{\mathbf{j}\sigma'}^{m} \psi_{\mathbf{j}\sigma'}^{n} \psi_{\mathbf{j}+\hat{x}\sigma'}^{n} e^{(\epsilon_{n}-\epsilon_{m})\tau} f(\epsilon_{n})(1-f(\epsilon_{m}))$$

+
$$\sum_{\substack{n,m,n\neq m}} \psi_{\mathbf{i}\sigma}^{n} \psi_{\mathbf{i}+\hat{x}\sigma}^{n} \psi_{\mathbf{j}\sigma'}^{m} \psi_{\mathbf{j}+\hat{x}\sigma'}^{m} f(\epsilon_{n}) f(\epsilon_{m})$$
(A.14)

From equation A.11 and $e^{i\omega_M\beta} = 1$:

$$\operatorname{Im}\Lambda_{xx}(\mathbf{q}=0,i\omega_{M}) = \operatorname{Im}\left[\frac{-t^{2}}{N}\sum_{n,m,n\neq m}\Psi^{n,m}f(\epsilon_{n})(1-f(\epsilon_{m}))\left(\frac{e^{\beta(\epsilon_{n}-\epsilon_{m})}-1}{i\omega_{M}+\epsilon_{n}-\epsilon_{m}}\right)\right]$$
$$= \operatorname{Im}\left[\frac{-t^{2}}{N}\sum_{n,m,n\neq m}\Psi^{n,m}\left(\frac{f(\epsilon_{m})-f(\epsilon_{n})}{i\omega_{M}+\epsilon_{n}-\epsilon_{m}}\right)\right]$$
(A.15)

in which

$$\Psi^{n,m} = \sum_{\mathbf{i},\mathbf{j},\sigma,\sigma'} \left(\psi^n_{\mathbf{i}\sigma} \psi^m_{\mathbf{i}+\hat{x}\sigma} \psi^m_{\mathbf{j}\sigma'} \psi^n_{\mathbf{j}+\hat{x}\sigma'} + \psi^n_{\mathbf{i}+\hat{x}\sigma} \psi^m_{\mathbf{i}\sigma} \psi^m_{\mathbf{j}+\hat{x}\sigma'} \psi^n_{\mathbf{j}\sigma'} - \psi^n_{\mathbf{i}+\hat{x}\sigma} \psi^m_{\mathbf{j}\sigma'} \psi^n_{\mathbf{j}+\hat{x}\sigma'} - \psi^n_{\mathbf{i}\sigma} \psi^m_{\mathbf{i}+\hat{x}\sigma} \psi^m_{\mathbf{j}+\hat{x}\sigma'} \psi^n_{\mathbf{j}\sigma'} \right)$$
(A.16)

by replacing $i\omega_M = \omega + i\eta$ in which $\eta \to 0$ and

$$\frac{1}{\omega + \epsilon_n - \epsilon_m + i\eta} = P \frac{1}{\omega + \epsilon_n - \epsilon_m} - i\pi\delta(\omega + \epsilon_n - \epsilon_m).$$
(A.17)

Therefore

$$\operatorname{Im}\Lambda_{xx}(\mathbf{q}=0,\omega) = \frac{t^2}{N} \sum_{n,m,n\neq m} \Psi^{n,m} \left(f(\epsilon_m) - f(\epsilon_n)\right) \delta(\omega + \epsilon_n - \epsilon_m) (A.18)$$

$$\sigma(\omega) = \frac{\mathrm{Im}\Lambda(\mathbf{q}=0,\omega)}{\omega} \tag{A.19}$$

• Spin susceptibility:

$$\chi(\mathbf{q},\tau)^{+-} = \langle S_{\mathbf{q}}^{+}(\tau)S_{-\mathbf{q}}^{-}(0)\rangle = \frac{1}{N}\sum_{i,j}e^{i\mathbf{q}\cdot(\mathbf{i}-\mathbf{j})}\langle S_{i}^{+}(\tau)S_{j}^{-}(0)\rangle$$

$$= \frac{1}{N}\sum_{i,j}e^{i\mathbf{q}\cdot(\mathbf{i}-\mathbf{j})}\langle c_{i\uparrow}^{\dagger}(\tau)c_{i\downarrow}(\tau)c_{j\downarrow}^{\dagger}c_{j\uparrow}\rangle$$

$$= \frac{1}{N}\sum_{i,j}e^{i\mathbf{q}\cdot(\mathbf{i}-\mathbf{j})}\psi_{i\uparrow}^{n}\psi_{i\downarrow}^{m}\psi_{j\downarrow}^{k}\psi_{j\uparrow}^{l}\langle \tilde{c}_{n}^{\dagger}(\tau)\tilde{c}_{m}(\tau)\tilde{c}_{k}^{\dagger}\tilde{c}_{l}\rangle$$

$$= \frac{1}{N}\sum_{i,j,n,m,k,l}e^{i\mathbf{q}\cdot(\mathbf{i}-\mathbf{j})}\psi_{i\uparrow}^{n}\psi_{i\downarrow}^{m}\psi_{j\downarrow}^{k}\psi_{j\uparrow}^{l}e^{\tau(\epsilon_{n}-\epsilon_{m})}\langle \tilde{c}_{n}^{\dagger}\tilde{c}_{n}\tilde{c}_{k}^{\dagger}\tilde{c}_{l}\rangle$$

$$= \frac{1}{N}\sum_{i,j,n\neq m}e^{i\mathbf{q}\cdot(\mathbf{i}-\mathbf{j})}\psi_{i\uparrow}^{n}\psi_{i\downarrow}^{n}\psi_{j\downarrow}^{m}\psi_{j\uparrow}^{m}f(\epsilon_{n})f(\epsilon_{m})$$

$$+ \frac{1}{N} \sum_{i,j,n\neq m} e^{i\mathbf{q}\cdot(\mathbf{i}-\mathbf{j})} \psi_{i\uparrow}^{n} \psi_{i\downarrow}^{m} \psi_{j\downarrow}^{m} \psi_{j\uparrow}^{n} e^{\tau(\epsilon_{n}-\epsilon_{m})} f(\epsilon_{n}) \left[1-f(\epsilon_{m})\right] \\ + \frac{1}{N} \sum_{i,j,n} e^{i\mathbf{q}\cdot(\mathbf{i}-\mathbf{j})} \psi_{i\uparrow}^{n} \psi_{i\downarrow}^{n} \psi_{j\downarrow}^{n} \psi_{j\uparrow}^{n} f(\epsilon_{n})$$
(A.20)

for $\mathbf{q} = (\pi, \pi)$ and $\omega = 0$

$$\chi(\vec{\pi}, \omega = 0) = \int_{0}^{\beta} \chi(\vec{\pi}, \tau) d\tau$$

$$= \sum_{i,j} (-1)^{|\mathbf{i}-\mathbf{j}|} \left\{ \frac{\beta \langle c_{i\uparrow}^{\dagger} c_{i\downarrow} \rangle \langle c_{j\downarrow}^{\dagger} c_{j\downarrow} \rangle}{N} + \frac{\beta}{N} \sum_{n} \psi_{i\uparrow}^{n} \psi_{i\downarrow}^{n} \psi_{j\downarrow}^{n} \psi_{j\uparrow}^{n} [1 - f(\epsilon_{n})] f(\epsilon_{n}) + \frac{1}{N} \sum_{n \neq m} \psi_{i\uparrow}^{n} \psi_{i\downarrow}^{m} \psi_{j\downarrow}^{m} \psi_{j\uparrow}^{n} \frac{f(\epsilon_{n}) - f(\epsilon_{m})}{\epsilon_{m} - \epsilon_{n}} \right\}$$
(A.21)

Mixing methods

B.1 Newton method

We want to find values of \mathbf{x} for which $\mathbf{F}(\mathbf{x}) = 0$, in this notation \mathbf{x} is a vector of all 3N variational input parameters, including \mathbf{h}_i and $\langle n_i \rangle$ in all the sites, and \mathbf{F} is the difference between variational parameters in the last two iterations, in other words $\mathbf{F} = \mathbf{x}|_{output} - \mathbf{x}|_{input}$; we want to find the values of \mathbf{x} for which this difference become zero or smaller than a threshold (e.g. 10^{-4}). We can write \mathbf{F} as[86]

$$F_{i}(\mathbf{x} + \delta \mathbf{x}) = F_{i}(\mathbf{x}) + \sum_{j} \frac{\partial F_{i}}{\partial x_{j}} \delta x_{j} + \dots$$

$$\mathbf{F}(\mathbf{x} + \delta \mathbf{x}) = \mathbf{F}(\mathbf{x}) + \mathbf{J} \cdot \delta \mathbf{x}$$
(B.1)

$$J_{ij} = \frac{\partial F_i}{\partial x_j} \tag{B.2}$$

since $\mathbf{F}(\mathbf{x} + \delta \mathbf{x}) = 0$ therefore

$$\delta \mathbf{x} = -\mathbf{J}^{-1} \cdot \mathbf{F} \tag{B.3}$$

in this method \mathbf{J} is fixed for all the iterations.

B.2 Broyden mixing scheme

In this method \mathbf{J} is changing in each iteration. Equation (B.2) can be written as

$$\mathbf{J}^{(n+1)} = \frac{\delta \mathbf{F}^{(n)}}{\delta \mathbf{x}^{(n)}}
\mathbf{J}^{(n+1)} \delta \mathbf{x}^{(n)} = \delta \mathbf{F}^{(n)}
= \delta \mathbf{F}^{(n)} + \mathbf{J}^{(n+1)} \delta \mathbf{x}^{(n)} - \mathbf{J}^{(n+1)} \delta \mathbf{x}^{(n)}
= \mathbf{J}^{(n)} \delta \mathbf{x}^{(n)} + \frac{(\delta \mathbf{F}^{(n)} - \mathbf{J}^{(n)} \delta \mathbf{x}^{(n)})(\delta \mathbf{x}^{(n)^{\dagger}} \delta \mathbf{x}^{(n)})}{(\delta \mathbf{x}^{(n)^{\dagger}} \delta \mathbf{x}^{(n)})}$$
(B.4)

The upper index n is the iteration number.

$$\mathbf{J}^{(n+1)} = \mathbf{J}^{(n)} + \frac{(\delta \mathbf{F}^{(n)} - \mathbf{J}^{(n)} \delta \mathbf{x}^{(n)}) \delta \mathbf{x}^{(n)^{\dagger}}}{(\delta \mathbf{x}^{(n)^{\dagger}} \delta \mathbf{x}^{(n)})}$$
$$= \mathbf{J}^{(n)} + uv^{\dagger}$$
(B.5)

$$v^{\dagger} = \delta \mathbf{x}^{(n)^{\dagger}}, \qquad u = \frac{\delta \mathbf{F}^{(n)} - \mathbf{J}^{(n)} \delta \mathbf{x}^{(n)}}{\delta \mathbf{x}^{(n)^{\dagger}} \delta \mathbf{x}^{(n)}}$$
(B.6)

$$\mathbf{J}^{(n+1)^{-1}} = \left(\mathbf{J}^{(n)} + uv^{\dagger}\right)^{-1}$$
(B.7)

Now we have to use this expansion for the matrices $\mathbf{A} = \mathbf{J}^{(n)}$ and $\mathbf{B} = uv^{\dagger}$,

$$(\mathbf{A} + \mathbf{B})^{-1} = (\mathbf{A}(I + \mathbf{A}^{-1}\mathbf{B}))^{-1} = (I + \mathbf{A}^{-1}\mathbf{B})^{-1}\mathbf{A}^{-1}$$

= $(I - \mathbf{A}^{-1}\mathbf{B} + \mathbf{A}^{-1}\mathbf{B}\mathbf{A}^{-1}\mathbf{B} - (\mathbf{A}^{-1}\mathbf{B})^3 + \dots)\mathbf{A}^{-1}$
= $\mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{B}\mathbf{A}^{-1} + \mathbf{A}^{-1}\mathbf{B}\mathbf{A}^{-1}\mathbf{B}\mathbf{A}^{-1}$
- $\mathbf{A}^{-1}\mathbf{B}\mathbf{A}^{-1}\mathbf{B}\mathbf{A}^{-1} + \dots$ (B.8)

$$\mathbf{A}^{-1}\mathbf{B}\mathbf{A}^{-1}\mathbf{B}\mathbf{A}^{-1} = \mathbf{J}^{(n)^{-1}}u\underbrace{v^{\dagger}\mathbf{J}^{(n)^{-1}}u}_{\lambda}v^{\dagger}\mathbf{J}^{(n)^{-1}}$$
(B.9)

in this relation λ is a scalar and has been defined as

$$\lambda = v^{\dagger} \mathbf{J}^{(n)^{-1}} u$$

= $\delta \mathbf{x}^{\dagger} \mathbf{J}^{(n)^{-1}} \left(\frac{\delta \mathbf{F}^{(n)} - \mathbf{J}^{(n)} \delta \mathbf{x}^{(n)}}{\delta \mathbf{x}^{(n)^{\dagger}} \delta \mathbf{x}^{(n)}} \right) = \frac{\delta \mathbf{x}^{(n)^{\dagger}} \mathbf{J}^{(n)^{-1}} \delta \mathbf{F}^{(n)}}{\delta \mathbf{x}^{(n)^{\dagger}} \delta \mathbf{x}^{(n)}} - 1 \qquad (B.10)$

therefore

$$\frac{1}{1+\lambda} = \frac{\delta \mathbf{x}^{(n)\dagger} \delta \mathbf{x}^{(n)}}{\delta \mathbf{x}^{(n)\dagger} \mathbf{J}^{(n)^{-1}} \delta \mathbf{F}^{(n)}}$$
(B.11)

from (B.8) and (B.9)

$$\mathbf{J}^{(n+1)^{-1}} = \mathbf{J}^{(n)^{-1}} - \mathbf{J}^{(n)^{-1}} u v^{\dagger} \mathbf{J}^{(n)^{-1}} (1 - \lambda + \lambda^{2} - \dots)
= \mathbf{J}^{(n)^{-1}} - \mathbf{J}^{(n)^{-1}} u v^{\dagger} \mathbf{J}^{(n)^{-1}} \frac{1}{1 + \lambda}
= \mathbf{J}^{(n)^{-1}} - \frac{\left(\mathbf{J}^{(n)^{-1}} \delta \mathbf{F}^{(n)} - \delta \mathbf{x}^{(n)}\right)}{\delta \mathbf{x}^{(n)^{\dagger}} \delta \mathbf{x}^{(n)}} \delta \mathbf{x}^{(n)^{\dagger}} \mathbf{J}^{(n)^{-1}} \frac{1}{1 + \lambda} \quad (B.12)$$

by using (B.11) in the above equation

$$\mathbf{J}^{(n+1)^{-1}} = \mathbf{J}^{(n)^{-1}} + \frac{\left(\delta \mathbf{x}^{(n)} - \mathbf{J}^{(n)^{-1}} \delta \mathbf{F}^{(n)}\right) \delta \mathbf{x}^{(n)^{\dagger}} \mathbf{J}^{(n)^{-1}}}{\delta \mathbf{x}^{(n)^{\dagger}} \mathbf{J}^{(n)^{-1}} \delta \mathbf{F}^{(n)}}$$
(B.13)

having found \mathbf{J}^{-1} , from (B.3) $\delta \mathbf{x}$ can be found for the next iteration. In our problem there are 3N variational parameters (\mathbf{h}_i and n_i) therefore \mathbf{x} is a vector in 3N dimensional space, and $\mathbf{F} = \mathbf{x}^{out} - \mathbf{x}^{in}$ in which $\mathbf{x}^{in} = \mathbf{x}^{(n)}$.

Density of States in 2D

We derive the exact expression for the density of states in 2D for electrons described by the tight binding Hamiltonian $\epsilon_k = -2t(\cos k_x + \cos k_y)$. The Green's function is[87]

$$G(z) = \sum_{\mathbf{k}} \frac{|\mathbf{k}\rangle \langle \mathbf{k}|}{z - \epsilon_k} \tag{C.1}$$

in which

$$|\mathbf{k}\rangle = \frac{1}{\sqrt{N}} \sum_{i} e^{i\mathbf{k}\cdot\mathbf{x}_{i}} |i\rangle$$
$$\langle i|\mathbf{k}\rangle = e^{i\mathbf{k}\cdot\mathbf{x}_{i}}$$
(C.2)

therefore

$$G_{ii}(z) = \sum_{k} \frac{1}{z - \epsilon_k} = \int_{1BZ} \frac{d\mathbf{k}}{z - \epsilon_k}$$
(C.3)

where the integration in (C.3) is over the first Brillioun zone. Now

$$\lim_{\varepsilon \to 0} \frac{1}{z - \epsilon_k} = P\left(\frac{1}{E - \epsilon_k}\right) - i\pi\delta(E - \epsilon_k) \tag{C.4}$$

where

$$z = \lim_{\varepsilon \to 0} E + i\varepsilon$$

and

$$\int_{1BZ} \delta(E - \epsilon_k) d\mathbf{k} = \int_{1BZ} d\epsilon g(\epsilon) \delta(E - \epsilon_k) = g(E)$$
(C.5)

hence

$$G_{ii}(z) = \int P\left(\frac{1}{E - \epsilon_k}\right) - i\pi g(E) \tag{C.6}$$

and the density of states can be written in terms of the imaginary part of the Green's function as

$$g(E) = -\frac{1}{\pi} \lim_{\varepsilon \to 0} \operatorname{Im} G_{ii}(z)$$
(C.7)

Now we perform the integration in (C.3)

$$G_{ii}(z) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dk_x \int_{-\pi}^{\pi} dk_y \frac{1}{z + 2t(\cos k_x + \cos k_y)}$$
(C.8)

we know that

$$\cos k_x + \cos k_y = 2\cos\left(\frac{k_x + k_y}{2}\right)\cos\left(\frac{k_x - k_y}{2}\right) \tag{C.9}$$

by defining new variables $\alpha = (k_x + k_y)/2$ and $\beta = (k_x - k_y)/2$ and Eq. C.8 we have[89]

$$G_{ii}(z) = \frac{2}{(2\pi)^2} \int_{-\pi}^{\pi} d\alpha \int_{0}^{\pi} d\beta \frac{1}{z + 4t(\cos\alpha\cos\beta)}$$
(C.10)

also we know that (from Eq. 2.553 in Ref. [90])

$$\int \frac{dx}{a+b\cos x} = \frac{2\pi}{\sqrt{a^2 - b^2}} \tan^{-1}\left(\frac{\sqrt{a^2 - b^2}\tan(x/2)}{a+b}\right) \qquad a^2 > b^2 \qquad (C.11)$$

$$\int \frac{dx}{a+b\cos x} = \frac{1}{\sqrt{b^2 - a^2}} \ln\left[\frac{\sqrt{b^2 - a^2}\tan(x/2) + (a+b)}{\sqrt{b^2 - a^2}\tan(x/2) - (a+b)}\right] \qquad a^2 < b^2 \quad (C.12)$$

so that for $a^2 > b^2$ (see :

$$G_{ii}(z) = \frac{2\pi}{(2\pi)^2} \int_{-\pi}^{\pi} d\alpha \frac{1}{\sqrt{z^2 - 16t^2 \cos^2 \alpha}} \\ = \frac{1}{\pi z} \int_{0}^{\pi} \frac{d\alpha}{\sqrt{1 - (4t/z)^2 \cos^2 \alpha}} \\ = \frac{2}{\pi z} K(4t/z)$$
(C.13)

where K is the elliptic integral of the first kind. For $a^2 < b^2$:

$$\int_0^{\pi} \frac{dx}{a+b\cos x} = \frac{1}{\sqrt{b^2 - a^2}} \left[\ln(1) - \ln(-1) \right] = \frac{-i\pi}{\sqrt{b^2 - a^2}}$$
(C.14)

therefore

$$G_{ii}(z) = \frac{-i}{\pi} \int_0^{\pi} \frac{d\alpha}{\sqrt{(4t\cos\alpha)^2 - z^2}} \\ = \frac{-i}{\pi 4t \sqrt{1 - (z/4t)^2}} K\left(\frac{1}{\sqrt{1 - (z/4t)^2}}\right)$$
(C.15)

We use the relation[90]:

$$\frac{1}{q}K\left(\frac{1}{q}\right) = K(q) + iK(\sqrt{1-q^2}) \tag{C.16}$$

in which q is a complex number, therefore when |z| < 4t:

$$G_{ii}(E) = -\frac{i}{4t\pi}K(\sqrt{1 - (E/4t)^2}) + \frac{1}{4t\pi}K(E/4t)$$
(C.17)

by using Eq. C.7 the density of states can be written as:

$$g(E) = \frac{\theta(E-4t)}{4\pi^2 t} K(\sqrt{1-(E/4t)^2})$$
(C.18)

Spin Susceptibility

In this appendix we derive an expression for the spin susceptibility as a spin-spin correlation function. Consider a system described by a Hamiltonian H_0 (with ground state $|\phi_0\rangle$) which is perturbed by a time-dependent magnetic field $\mathbf{h}(\mathbf{x}, t)$. The perturbation is $H'(t) = \int d^d x \mathbf{S}(\mathbf{x}, t) \cdot \mathbf{h}(\mathbf{x}, t)$. Our aim is to calculate the expectation $\langle \psi_S(t) | \hat{O} | \psi_S(t) \rangle$ of an operator \hat{O} (e.g. spin operator) in the modified states $|\psi_S(t)\rangle = e^{-iHt} |\phi_0\rangle$ in which $H = H_0 + H'(t)$. The subscript S denotes the Schrodinger picture (symbol S should not be confused with spin operator). It is useful to use the interaction picture (I)where the evolution of operators is governed by the unperturbed Hamiltonian H_0 .

$$\hat{O}_I = e^{iH_0 t} \hat{O} e^{-iH_0} \tag{D.1}$$

$$\begin{aligned} |\psi_I(t)\rangle &= e^{iH_0t} |\psi_S(t)\rangle = e^{iH_0t} e^{-iHt} |\psi_S(0)\rangle \\ &= U(t) |\psi_S(0)\rangle \end{aligned}$$
(D.2)

where U is defined as

$$U = e^{iH_0 t} e^{-iHt} \tag{D.3}$$

We show that the average of any operator in two pictures are equal.

$$\begin{aligned} \langle \psi_I(t) | \hat{O}_I(t) | \psi_I(t) \rangle &= \langle \psi_S(0) | e^{iHt} e^{-iH_0} e^{iH_0t} \hat{O} e^{-iH_0t} e^{iH_0t} e^{-iHt} | \psi_S(0) \rangle \\ &= \langle \psi_S(0) | e^{iHt} \hat{O} e^{-iHt} | \psi_S(0) \rangle \\ &= \langle \psi_S(t) | \hat{O} | \psi_S(t) \rangle \end{aligned}$$
(D.4)

From Eq. D.3 we have

$$\frac{\partial U(t)}{\partial t} = ie^{iHt} (H_0 - H) e^{-iHt}$$
$$= -ie^{iH_0 t} H' e^{-iHt}$$
(D.5)

By integrating this equation we have

$$U(t) = 1 - i \int_{0}^{t} dt_{1} H'(t_{1}) U(t_{1})$$

= $1 - i \int_{0}^{t} dt_{1} H'(t_{1}) + (-i)^{2} \int_{0}^{t} dt_{1} \int_{0}^{t_{1}} dt_{2} H'(t_{1}) H'(t_{2}) \dots H'(t_{n})$
= $T \exp\left[-i \int_{0}^{t} dt_{1} H'(t_{1})\right]$ (D.6)

The factor T is a time ordering operator with earliest t to the right.

S-matrix (not to be confused with spin operator) is a propagator in the interaction picture such that it changes $|\psi_I(t')\rangle$ into the $|\psi_I(t)\rangle$ [91].

$$|\psi_I(t)\rangle = U(t)|\psi_S(0)\rangle = S(t,t')|\psi_I(t')\rangle$$

$$S(t,t') = U(t)U^{\dagger}(t')$$
(D.7)

and

$$S(t,t') = T\left[\exp\left(-i\int_{t'}^{t} dt_1 H'(t_1)\right)\right]$$
(D.8)

We assume that the system is in the ground state of H_0 and at $t = -\infty$, H' is adiabatically turned on.

$$|\psi_I(t)\rangle = S(t, -\infty)|\phi_0\rangle \tag{D.9}$$

where we have used Eq. D.7 and the fact that at $t = -\infty$: $|\psi_I(-\infty)\rangle = |\phi_0\rangle$.

The magnetization $\mathbf{M}(\mathbf{x}, t)$ in the presence of the perturbation is

$$\mathbf{M}(\mathbf{x},t) = \langle \psi_I(t) | \mathbf{S}(\mathbf{x},t) | \psi_I(t) \rangle$$

= $\langle \phi_0 | S^{\dagger}(t,-\infty) \mathbf{S}(\mathbf{x},t) S(t,-\infty) | \phi_0 \rangle$ (D.10)

By expansion of $S(-\infty, t)$ in powers of H' we have

$$S(t, -\infty) |\phi_0\rangle = \left[1 - i \int_{-\infty}^t dt' H'(t') \right] |\phi_0\rangle + O(H')^2 |\phi_0\rangle$$
 (D.11)

Therefore

$$M_{\alpha}(\mathbf{x},t) = \langle \phi_0 | \{ S_{\alpha}(\mathbf{x},t) - i \int_{-\infty}^t dt' [S_{\alpha}(\mathbf{x},t), H'(t')] \} | \phi_0 \rangle$$
(D.12)

Since $\langle \phi_0 | S_\alpha(\mathbf{x},t) | \phi_0 \rangle = 0$ and $H'(t') = -\int d^d x \mathbf{S}(\mathbf{x},t') \cdot \mathbf{h}(\mathbf{x},t')$ therefore

$$M_{\alpha}(\mathbf{x},t) = -i \int_{-\infty}^{t} dt' \langle \phi_{0} | [S_{\alpha}(\mathbf{x},t), H'(t')] | \phi_{0} \rangle$$

$$= i \int_{-\infty}^{t} dt' \int d^{d}x' \langle \phi_{0} | [S_{\alpha}(\mathbf{x},t), \sum_{\alpha'} S_{\alpha'}(\mathbf{x}',t')h_{\alpha'}(\mathbf{x}',t')] | \phi_{0} \rangle$$

$$= \sum_{\alpha'} i \int_{-\infty}^{t} dt' \int d^{d}x' \langle \phi_{0} | [S_{\alpha}(\mathbf{x},t), S_{\alpha'}(\mathbf{x}',t')] | \phi_{0} \rangle h_{\alpha'}(\mathbf{x}',t') \quad (D.13)$$

from the definition of susceptibility within linear response [93]

$$\delta M_{\alpha}(\mathbf{x},t) = \int_{-\infty}^{t} dt' \int d^{d}x' \chi_{\alpha\alpha'}(\mathbf{x},\mathbf{x}';t,t') \delta h_{\alpha'}(\mathbf{x}',t')$$
(D.14)

then we have

$$\chi_{\alpha\alpha'}(\mathbf{x}, \mathbf{x}'; t, t') = i\theta(t - t') \langle [S_{\alpha}(\mathbf{x}, t), S_{\alpha'}(\mathbf{x}', t')] \rangle$$
(D.15)

 $\theta(t-t')$ is an step function and the average is taken with respect to the ground state of H_0 . Since H_0 is independent of time therefore χ depends only on the difference t-t'. Upon Fourier transforming,

$$\chi_{\alpha\alpha'}(\mathbf{x}, \mathbf{x}'; \omega) = \int_{-\infty}^{\infty} d(t - t') e^{i\omega(t - t')} \chi_{\alpha\alpha'}(\mathbf{x}, \mathbf{x}'; t, t')$$
$$= i \int_{-\infty}^{0} dt e^{i\omega t} \langle [S_{\alpha}(\mathbf{x}, t), S_{\alpha'}(\mathbf{x}', 0)] \rangle$$
(D.16)

Susceptibility has been defined in Matsubara formalism as

$$\chi_{\alpha\alpha'}(\mathbf{x}, \mathbf{x}'; i\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} \langle \mathbf{T}_\tau S_\alpha(\mathbf{x}, \tau) S_{\alpha'}(\mathbf{x}', 0) \rangle \tag{D.17}$$

In which τ is imaginary time $\tau = it$ and $\beta = 1/T$. We can repeat all this calculation in the q space and like real space the result is

$$\chi_{\alpha\alpha'}(\mathbf{q},\mathbf{q}';i\omega_n) = \int_0^\beta d\tau e^{i\omega_n\tau} \langle T_\tau S_\alpha(\mathbf{q},\tau) S_{\alpha'}(\mathbf{q}',0) \rangle \tag{D.18}$$

For a translationally invariant system

$$\chi_{\alpha\alpha'}(q,i\omega) = \int_0^\beta d\tau e^{i\omega\tau} \langle S_\alpha(q,\tau) S_{\alpha'}(-q,0) \rangle \tag{D.19}$$

For the case that $\mathbf{S}(\mathbf{x}, \tau)$ is given in terms of creation and annihilation operators then

$$S_z(q,0) = \frac{1}{2} \sum_{k,\sigma} \sigma c^{\dagger}_{k\sigma} c_{k+q\sigma}$$

$$S_{x}(q,0) = \frac{1}{2} \sum_{k} \left(c_{k\uparrow}^{\dagger} c_{k+q\downarrow} + c_{k\downarrow}^{\dagger} c_{k+q\uparrow} \right)$$

$$S_{y}(q,0) = \frac{i}{2} \sum_{k} \left(c_{k\uparrow}^{\dagger} c_{k+q\downarrow} - c_{k\downarrow}^{\dagger} c_{k+q\uparrow} \right)$$
(D.20)

From (D.19)

$$\chi_{zz}(q,0) = \frac{1}{4} \sum_{k,k,\sigma,\sigma'} \sigma\sigma' \int_0^\beta d\tau \langle \mathcal{T}_\tau c_{k\sigma}^\dagger(\tau) c_{k+q\sigma}(\tau) c_{k'\sigma'}^\dagger(0) c_{k'-q\sigma'}(0) \rangle \tag{D.21}$$

This a general formula for susceptibility. For the special case of a system of noninteracting electron (or quasi-particles) with the Hamiltonian $H = \sum_{k,\sigma} \epsilon_k c_{k\sigma}^{\dagger} c_{k\sigma}$ the susceptibility is

$$\chi_{zz}(q,0) = \frac{1}{4} \sum_{k,k,\sigma,\sigma'} \sigma \sigma' \int_0^\beta d\tau e^{(\epsilon_{k+q}-\epsilon_k)\tau} \langle c_{k\sigma}^{\dagger} c_{k+q\sigma} c_{k'\sigma'}^{\dagger} c_{k'-q\sigma'} \rangle$$

$$= \frac{1}{4} \sum_{k,\sigma} \sigma^2 \frac{e^{(\epsilon_{k+q}-\epsilon_k)\beta} - 1}{\epsilon_k - \epsilon_{k+q}} f(\epsilon_k) (1 - f(\epsilon_{k+q}))$$

$$= \frac{1}{2} \sum_k \frac{e^{\beta\epsilon_k} - e^{\beta\epsilon_{k+q}}}{(1 + e^{\beta\epsilon_k})(1 + e^{\beta\epsilon_{k+q}})} \frac{1}{\epsilon_k - \epsilon_{k+q}}$$

$$\chi_{zz}(q,0) = \sum_k \frac{1}{2} \frac{f(\epsilon_{k+q}) - f(\epsilon_k)}{\epsilon_k - \epsilon_{k+q}}$$
(D.22)

Hartree-Fock approximation for a non-disordered system

In this appendix we use Hartree-Fock approximation to obtain staggered magnetization of the repulsive Hubbard model (we follow Ref.[63]). Within this approximation the interaction term which is quartic in annihilation and creation operators ($c_{i\sigma}$ and $c_{i\sigma}^{\dagger}$) changes to quadratic terms in $c_{i\sigma}$ and $c_{i\sigma}^{\dagger}$. Therefore

$$n_{i\uparrow}n_{i\downarrow} = c^{\dagger}_{i\uparrow}c_{i\uparrow}c^{\dagger}_{i\downarrow}c_{i\downarrow}$$

$$= \langle n_{i\downarrow} \rangle n_{i\uparrow} + \langle n_{i\uparrow} \rangle n_{i\downarrow} - \langle n_{i\downarrow} \rangle \langle n_{i\uparrow} \rangle$$

$$- c^{\dagger}_{i\uparrow}c_{i\downarrow} \langle c^{\dagger}_{i\downarrow}c_{i\uparrow} \rangle - c^{\dagger}_{i\downarrow}c_{i\uparrow} \langle c^{\dagger}_{i\uparrow}c_{i\downarrow} \rangle + \langle c^{\dagger}_{i\uparrow}c_{i\downarrow} \rangle \langle c^{\dagger}_{i\downarrow}c_{i\uparrow} \rangle.$$
(E.1)

By using the relation

$$[n_{i\uparrow} \langle n_{i\downarrow} \rangle + n_{i\downarrow} \langle n_{i\uparrow} \rangle] = \frac{1}{2} [(n_{i\uparrow} + n_{i\downarrow})(\langle n_{i\uparrow} \rangle + \langle n_{i\downarrow} \rangle) - (n_{i\uparrow} - n_{i\downarrow})(\langle n_{i\uparrow} \rangle - \langle n_{i\uparrow} \rangle)]$$

= $\frac{1}{2} [(n_i \langle n_i \rangle - 4S_i^z \langle S_i^z \rangle],$ (E.2)

where

$$S_i^{\alpha} = \frac{1}{2} c_{is_1}^{\dagger} \sigma_{s_1 s_2}^{\alpha} c_{is_2} \tag{E.3}$$

and $\sigma^{\alpha}_{s_1s_2}$ are Pauli matrices, s_1 and s_2 are spin indices, the effective Hamiltonian can be written as

$$H_{\text{eff}} = -\sum_{\langle ij \rangle, \sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i,\sigma} \left(\frac{U \langle n_i \rangle}{2} - \mu \right) c_{i\sigma}^{\dagger} c_{i\sigma} - 2U \sum_i \langle \mathbf{S}_i \rangle \cdot \mathbf{S}_i.$$
(E.4)

At half filling $(\langle n_i \rangle = 1)$ the chemical potential is $\mu = U/2$. With a Fourier transformation of $c_{i\sigma}$ and $c_{i\sigma}^{\dagger}$ in Eq. E.4 the effective Hamiltonian is

$$H_{\text{eff}} = \sum_{q,\sigma} \epsilon_q n_{q\sigma} - 2NU \sum_{\mathbf{q}} \langle \mathbf{S}(-\mathbf{q}) \rangle \cdot \mathbf{S}(\mathbf{q})$$
(E.5)



Fig E.1: First Brillion zone for the non-interacting electrons in a tight binding model on a square lattice. The hatched region is filled at half filling.

where N is the number of sites and

$$S^{\alpha}(\mathbf{q}) = \frac{1}{2N} \sum_{k+\mathbf{q}} c^{\dagger}_{ks_1} \sigma^{\alpha}_{s_1, s_2} c_{ks_2}$$
(E.6)

At half filling and for a small interaction the ground state has non-zero expectation value of $\mathbf{S}(q)$ for wave vector $Q = (\pi, \pi)$. The ground state is invariant under the rotation of the order parameter $\mathbf{S}(Q)$, for generality we assume the order is in the z direction. Therefore

$$\langle \Omega | S_Q^z | \Omega \rangle = m^{\dagger} \tag{E.7}$$

 m^{\dagger} is the staggered moment and is a variational parameter and $|\Omega\rangle$ is true ground state of the system. The effective Hamiltonian is

$$H_{\text{eff}} = \sum \epsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} - U m^{\dagger} \sum_k \left(c^{\dagger}_{k+Q\uparrow} c_{k\uparrow} - c^{\dagger}_{k+Q\downarrow} c_{k\downarrow} \right)$$
(E.8)

The above summation on the wave vector k which is in the first Brillion zone can be written as two separate summations, one for k_{\leq} inside the hatched region in Fig. E.1 and the other k_{\geq} for outside this region which can be written as $k_{\geq} = k_{\leq} + Q$. For simplicity we denote all k_{\leq} with k. Therefore Eq. E.8 changes to

$$H_{\text{eff}} = \sum_{k,\sigma} \epsilon_k \left(c_{k\sigma}^{\dagger} c_{k\sigma} - c_{k+Q\sigma}^{\dagger} c_{k+Q\sigma} \right) - Um^{\dagger} \sum_k' \left(c_{k+Q\uparrow}^{\dagger} c_{k\uparrow} + c_{k\uparrow}^{\dagger} c_{k+Q\uparrow} - c_{k+Q\downarrow}^{\dagger} c_{k\downarrow} - c_{k\downarrow}^{\dagger} c_{k+Q\downarrow} \right)$$
(E.9)

where the prime in the sum denotes only k vectors inside the hatched region of the Fig. E.1. We have used the relation $\epsilon_k = -\epsilon_{k+Q}$. Now we use another transformation to γ basis chosen so as to diagonalize H_{eff}

$$\begin{cases} \gamma_{k\uparrow}^c = u_k c_{k\uparrow} + v_k c_{k+Q\uparrow} \\ \gamma_{k\uparrow}^v = v_k c_{k\uparrow} - u_k c_{k+Q\uparrow} \end{cases} \begin{cases} \gamma_{k\downarrow}^c = u_k c_{k\downarrow} - v_k c_{k+Q\downarrow} \\ \gamma_{k\downarrow}^v = v_k c_{k\downarrow} + u_k c_{k+Q\downarrow} \end{cases}$$
(E.10)

The inverse transformation is

$$\begin{cases}
c_{k\uparrow} = u_k \gamma_{k\uparrow}^c - v_k \gamma_{k\uparrow}^v \\
c_{k+Q\uparrow} = v_k \gamma_{k\uparrow}^c + u_k \gamma_{k\uparrow}^v
\end{cases}
\begin{cases}
c_{k\downarrow} = u_k \gamma_{k\downarrow}^c + v_k \gamma_{k\downarrow}^v \\
c_{k+Q\downarrow} = -v_k \gamma_{k\downarrow}^c + u_k \gamma_{k\downarrow}^v
\end{cases}$$
(E.11)

We now find the first summation in Eq. E.9

$$n_{k\uparrow} - n_{k+Q\uparrow} = \left(u_k^2 \gamma_{k\uparrow}^{c\dagger} \gamma_{k\uparrow}^c + v_k^2 \gamma_{k\uparrow}^{v\dagger} \gamma_{k\uparrow}^v - u_k v_k (\gamma_{k\uparrow}^{c\dagger} \gamma_{k\uparrow}^v + \gamma_{k\uparrow}^{v\dagger} \gamma_{k\uparrow}^c) \right) - \left(v_k^2 \gamma_{k\uparrow}^{c\dagger} \gamma_{k\uparrow}^c + u_k^2 \gamma_{k\uparrow}^{v\dagger} \gamma_{k\uparrow}^v + u_k v_k (\gamma_{k\uparrow}^{c\dagger} \gamma_{k\uparrow}^v + \gamma_{k\uparrow}^{v\dagger} \gamma_{k\uparrow}^c) \right)$$
(E.12)

$$n_{k\downarrow} - n_{k+Q\downarrow} = \left(u_k^2 \gamma_{k\downarrow}^{c\dagger} \gamma_{k\downarrow}^c + v_k^2 \gamma_{k\downarrow}^{v\dagger} \gamma_{k\downarrow}^v + u_k v_k (\gamma_{k\downarrow}^{c\dagger} \gamma_{k\downarrow}^v + \gamma_{k\downarrow}^{v\dagger} \gamma_{k\downarrow}^c) \right) - \left(v_k^2 \gamma_{k\downarrow}^{c\dagger} \gamma_{k\downarrow}^c + u_k^2 \gamma_{k\downarrow}^{v\dagger} \gamma_{k\downarrow}^v - u_k v_k (\gamma_{k\downarrow}^{c\dagger} \gamma_{k\downarrow}^v + \gamma_{k\downarrow}^{v\dagger} \gamma_{k\downarrow}^c) \right)$$
(E.13)

therefore

$$n_{k\uparrow} - n_{k+Q\uparrow} = (u_k^2 - v_k^2)(\gamma_{k\uparrow}^{c\dagger}\gamma_{k\uparrow}^c - \gamma_{k\uparrow}^{v\dagger}\gamma_{k\uparrow}^v) - 2u_k v_k(\gamma_{k\uparrow}^{c\dagger}\gamma_{k\uparrow}^v + \gamma_{k\uparrow}^{v\dagger}\gamma_{k\uparrow}^c)$$

$$n_{k\downarrow} - n_{k+Q\downarrow} = (u_k^2 - v_k^2)(\gamma_{k\downarrow}^{c\dagger}\gamma_{k\downarrow}^c - \gamma_{k\downarrow}^{v\dagger}\gamma_{k\downarrow}^v) + 2u_k v_k(\gamma_{k\downarrow}^{c\dagger}\gamma_{k\downarrow}^v + \gamma_{k\downarrow}^{v\dagger}\gamma_{k\downarrow}^c) \quad (E.14)$$

We now find the second summation in (E.9).

$$c_{k+Q\uparrow}^{\dagger}c_{k\uparrow} + c_{k\uparrow}^{\dagger}c_{k+Q\uparrow} = 2u_{k}v_{k}(\gamma_{k\uparrow}^{c\dagger}\gamma_{k\uparrow}^{c} - \gamma_{k\uparrow}^{v\dagger}\gamma_{k\uparrow}^{v}) + (u_{k}^{2} - v_{k}^{2})(\gamma_{k\uparrow}^{c\dagger}\gamma_{k\uparrow}^{v} + \gamma_{k\uparrow}^{v\dagger}\gamma_{k\uparrow}^{c})$$

$$c_{k+Q\downarrow}^{\dagger}c_{k\downarrow} + c_{k\downarrow}^{\dagger}c_{k+Q\downarrow} = -2u_{k}v_{k}(\gamma_{k\downarrow}^{c\dagger}\gamma_{k\downarrow}^{c} - \gamma_{k\downarrow}^{v\dagger}\gamma_{k\downarrow}^{v}) + (u_{k}^{2} - v_{k}^{2})(\gamma_{k\downarrow}^{c\dagger}\gamma_{k\downarrow}^{v} + \gamma_{k\downarrow}^{v\dagger}\gamma_{k\downarrow}^{c}) \quad (E.15)$$

The effective Hamiltonian in the γ basis is

$$H_{\text{eff}} = \sum_{k,\sigma} \left\{ \left(\epsilon_k (u_k^2 - v_k^2) - 2USu_k v_k \right) (\gamma_{k\sigma}^{c\dagger} \gamma_{k\sigma}^c - \gamma_{k\sigma}^{v\dagger} \gamma_{k\sigma}^v) \right. \\ \left. + \sigma \left(US(u_k^2 - v_k^2) - 2\epsilon_k u_k v_k \right) (\gamma_{k\sigma}^{c\dagger} \gamma_{k\sigma}^v + \gamma_{k\sigma}^{v\dagger} \gamma_{k\sigma}^c) \right\}$$
(E.16)

By putting the coefficient of the off-diagonal term zero and $\Delta=-US$ we get

$$\Delta(u_k^2 - v_k^2) + 2\epsilon_k u_k v_k = 0 \tag{E.17}$$
and since $u_k^2 + v_k^2 = 1$, we have

$$u_{k} = \left[\frac{1}{2}\left(1 + \frac{\epsilon_{k}}{E_{k}}\right)\right]^{1/2}$$
$$v_{k} = \left[\frac{1}{2}\left(1 - \frac{\epsilon_{k}}{E_{k}}\right)\right]^{1/2}$$
(E.18)

where $E_k = (\epsilon_k^2 + \Delta^2)^{1/2}$. For the diagonal terms in (E.16) we have

$$\epsilon_k (u_k^2 - v_k^2) - 2USu_k v_k = \epsilon_k \left(\frac{\epsilon_k}{E_k}\right) + \Delta \left(1 - \frac{\epsilon_k}{E_k}\right)^{1/2} = E_k$$
(E.19)

Finally the effective Hamiltonian is

$$H_{\text{eff}} = \sum_{k,\sigma}' E_k (\gamma_{k\sigma}^{c\dagger} \gamma_{k\sigma}^c - \gamma_{k\sigma}^{v\dagger} \gamma_{k\sigma}^v)$$
(E.20)

The spin density wave ground state $|\Omega\rangle$ for a half filled band is defined by

$$\gamma_{k\sigma}^{v\dagger}|\Omega\rangle = \gamma_{k\sigma}^{v}|\Omega\rangle = 0 \tag{E.21}$$

The variational parameter is

$$\langle \Omega | S_Q^z | \Omega \rangle = S = -\frac{1}{2N} 2 \sum_k' u_k v_k$$
$$= \frac{1}{4N} \sum_k' \frac{\Delta}{E_k} = -\frac{\Delta}{U}$$
(E.22)

$$\frac{1}{4N}\sum'\frac{1}{(\epsilon_k^2 + \Delta^2)^{1/2}} = \frac{1}{U}$$

We change the above summation to integration on ϵ and for that we use the density of states of a 2D non-interacting system that we obtained in appendix C (see Eq. C.18). The DOS has a log singularity at $\epsilon = 0$; we approximate the elliptic integral with \sinh^{-1} function, therefore the self consistent solution is

$$\frac{1}{U} \approx \int_{0}^{t/\Delta} \frac{1}{4\pi^{2}t} \frac{\sinh^{-1}(\epsilon')}{\sqrt{\epsilon'^{2}+1}} d\epsilon' = \frac{1}{4\pi^{2}t} \int_{0}^{t/\Delta} \sinh^{-1}(\epsilon') d(\sinh^{-1}(\epsilon'))$$
$$= \frac{1}{4\pi^{2}t} \left(\sinh^{-1}(t/\Delta)\right)^{2}$$
(E.23)

where $\epsilon' = \epsilon / \Delta$.

$$\frac{t}{\Delta} = \sinh\left(2\pi\sqrt{\frac{t}{U}}\right)$$
$$\Delta = \frac{2t}{e^{2\pi\sqrt{t/U}} - e^{-2\pi\sqrt{t/U}}}$$
(E.24)

at the large U limit

$$\Delta \sim t e^{-2\pi \sqrt{t/U}} \tag{E.25}$$

Finding Higher Order Coupling

In the limit of large interaction U in Eq. 4.1 we treat the kinetic energy t/U as a perturbation on the Hamiltonian H_0 . In the ground state of the unperturbed Hamiltonian each site can accommodate 0, 1 or 2 electrons. The perturbation t/U can couple two singly occupied sites that are separated by a number of zero and doubly occupied sites (for instance in Fig. F.1 singly occupied sites A and B are separated at least by five sites with zero and doubly occupancies). In this appendix our aim is to give a general relation for this coupling in terms of parameters of the Hamiltonian on a square lattice (see also Ref. [92] for higher order coupling in 1D).

The unperturbed ground state has four fold degeneracy for different spin configurations at sites A and B. These states are given below (we have used the notation $|S_A^z, S_B^z\rangle$)

$$\begin{aligned} |1\rangle &= |\uparrow,\downarrow\rangle, \quad |2\rangle = |\downarrow,\uparrow\rangle \\ |3\rangle &= |\uparrow,\uparrow\rangle, \quad |4\rangle = |\downarrow,\downarrow\rangle \end{aligned}$$
 (F.1)

Generally in Hamiltonian $H = H_0 + \lambda H'$, the perturbation breaks the degeneracy of the unperturbed ground state. In this case the perturbation can only mix the states $|1\rangle$ and $|2\rangle$, therefore we do not consider states $|3\rangle$ and $|4\rangle$ in the perturbation expansion. If the distance between sites A and B is n (in Fig. F.1: n = 5) a perturbation expansion of the order of 2n + 2 is needed in order to couple states $|1\rangle$ and $|2\rangle$ in Eq. F.1.

 $E_D^{(0)}$ and E are the ground state energies for H_0 and H and $|l^0\rangle$ and $|l\rangle$ are the corresponding eigenstates. $|l\rangle$ approaches $|l^0\rangle$ as λ tends to zero. P_0 is the projection operator to the subspace of degenerate states $|l^0\rangle$ and P_1 is the complementary projection. Therefore

$$(E - E_D^{(0)} - \lambda H')P_0|l\rangle + (E - H_0 - \lambda H')P_1|l\rangle = 0$$

в

Fig F.1: Two singly occupied sites A and B are separated by at least five zero and doubly occupied sites. There would be an AF coupling between these two sites.

by applying P_0 and P_1 from the left to the above equation

$$(E - E_D^{(0)} - \lambda P_0 H') P_0 |l\rangle - \lambda P_0 H' P_1 |l\rangle = 0$$
(F.2)

$$-\lambda P_1 H' P_0 |l\rangle + (E - H_0 - \lambda P_1 H') P_1 |l\rangle = 0$$
(F.3)

using these two equations we get

$$\left(E - E_D^{(0)} - \lambda P_0 H' P_0 - \lambda P_0 H' P_1 \frac{\lambda}{\left(E - H_0 - \lambda P_1 H' P_1\right)} P_1 H'\right) P_0 |l\rangle = 0 \qquad (F.4)$$

Expansion of the denominator in the third term gives

$$\left(E - E_D^{(0)} - \lambda P_0 H' P_0 - \lambda P_0 H' P_1 \frac{\lambda}{(E - H_0)} \sum_{m=0}^{\infty} \left[\frac{\lambda P_1 H' P_1}{E - H_0}\right]^m P_1 H'\right) P_0 |l\rangle = 0 \quad (F.5)$$

All the odd powers of H' give rise to states out of the degenerate subspace, therefore they can be canceled. Lower orders of m (with m < 2n) also cannot couple sites A and B. The lowest order contribution from the summation in Eq. F.5 would be m = 2n, therefore

$$\left(E - E_D^{(0)} - \lambda^{2n+2} P_0 H' P_1 \frac{1}{(E_D^{(0)} - H_0)} \left[\frac{P_1 H' P_1}{E_D^{(0)} - H_0}\right]^{2n} P_1 H'\right) P_0 |l\rangle = 0 \qquad (F.6)$$

in order to find the energy shift of the ground state $\Delta^{(2n+2)} = E - E_D^{(0)}$ we have to solve the secular equation

$$\det\left(\Delta^{(2n+2)} - \hat{\mathbf{J}}^{(2n+2)}\right) = 0 \tag{F.7}$$

in which

$$\hat{\mathbf{J}}^{(2n+2)} = \lambda^{2n+2} P_0 H' P_1 \frac{1}{(E_D^{(0)} - H_0)} \left[\frac{P_1 H' P_1}{E_D^{(0)} - H_0} \right]^{2n} P_1 H' P_0$$
(F.8)



Fig F.2: Possible spin configurations for the next nearest neighbor coupling for n = 1. by defining $J_{lk}^{(2n+2)}$ as $\langle l | \hat{\mathbf{J}}^{(2n+2)} | k \rangle$ and from the symmetry of the problem

$$J_{11}^{(2n+2)} = J_{22}^{(2n+2)} = -J_{12}^{(2n+2)} = -J_{21}^{(2n+2)} = -J^{(2n+2)}$$
(F.9)

The indices 1 and 2 are referred to the states defined in Eq. F.1. The negative sign for $J_{12}^{(2n+2)}$ and $J_{21}^{(2n+2)}$ is coming from the fact that when H' acting on $|1\rangle$ even number of times gives $-|2\rangle$.

In Eq. F.8 each $1/(E_D^{(0)} - H_0)$ gives a negative factor and there are odd number of such factors, hence $J^{(2n+2)}$ becomes a positive number, therefore for Eq. F.7 we have

$$\begin{aligned} \Delta_s^{(2n+2)} &= -2J^{(2n+2)}, \\ \Delta_t^{(2n+2)} &= 0, \\ |1,1\rangle_s &= \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle), \\ |1,1\rangle_t &= \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle) \end{aligned}$$
(F.10)

for the case of two nearest neighbor sites n = 0 and (F.8) changes to

$$\det\left(\Delta^{(2)} - \lambda^2 P_0 H' P_1 \frac{1}{(E_D^{(0)} - H_0)} P_1 H' P_0\right) = 0$$

$$J_{11}^{(2)} = \langle 1 | \lambda^2 P_0 H' P_1 \frac{1}{(E_D^{(0)} - H_0)} P_1 H' P_0 | 1 \rangle$$

$$= \lambda^2 \sum_{k \notin D} \frac{1}{E_D^{(0)} - E_k^{(0)}} |\langle 1 | H' | k^{(0)} \rangle|^2$$
(F.11)

for two nearest neighbor i and j we have

$$\Delta_s^{(2)} = -2J^{(2)}$$

= $-2\left(\frac{t^2}{V_i - V_j + U} + \frac{t^2}{V_j - V_i + U}\right)$ (F.12)

since for sites *i* and *j* with the separation of *n* sites there are three triplet state with zero energy and one singlet state with energy $-2J^{(2n+2)}$ we can write an effective Hamiltonian for these two sites in terms of spin operators as

$$H_{eff}^{ij} = 2J^{(2n+2)}\mathbf{S}_i \cdot \mathbf{S}_j + const \tag{F.13}$$

Now we find coupling between a site and its next nearest neighbor. There are six different spin configurations for this system which are shown in Fig. F.2 and for each configuration only specific moves which can couple these two spins are allowed.

$$J_{a} = -J_{11}^{(2n+2)}$$

$$J_{a} = \left\{ \frac{t^{4}}{(V_{2} - V_{1})^{2}(U - V_{3} + V_{1})} + \frac{t^{4}}{(V_{2} - V_{3})^{2}(U - V_{1} + V_{3})} + \frac{t^{4}}{U - 2V_{2} + V_{1} + V_{3}} \left[\frac{1}{V_{2} - V_{1}} + \frac{1}{V_{2} - V_{3}} \right]^{2} \right\}$$
(F.14)

$$J_{b} = \left\{ \frac{t^{4}}{(V_{1} - V_{2})^{2}(U + V_{3} - V_{1})} + \frac{t^{4}}{(V_{3} - V_{2})^{2}(U + V_{1} - V_{3})} + \frac{t^{4}}{U + 2V_{2} - V_{1} - V_{3}} \left[\frac{1}{V_{1} - V_{2}} + \frac{1}{V_{3} - V_{2}} \right]^{2} \right\}$$
(F.15)

for the other cases (c), (d), (e) and (f) we get

$$J_{c} = J_{a} + J_{b}(2 \rightarrow 4) + \frac{2t^{4}}{(V_{2} - V_{1})(U + V_{1} - V_{3})(V_{3} - V_{4})} + \frac{2t^{4}}{(V_{1} - V_{4})(U + V_{3} - V_{1})(V_{2} - V_{3})} J_{d} = J_{b} + J_{b}(2 \rightarrow 4) + \frac{2t^{4}}{(V_{1} - V_{2})(U + V_{3} - V_{1})(V_{1} - V_{4})} + \frac{2t^{4}}{(V_{3} - V_{4})(U + V_{1} - V_{3})(V_{3} - V_{2})} J_{f} = J_{a} + J_{a}(2 \rightarrow 4) + \frac{2t^{4}}{(V_{2} - V_{1})(U + V_{1} - V_{3})(V_{4} - V_{1})} + \frac{2t^{4}}{(V_{4} - V_{3})(U + V_{3} - V_{1})(V_{2} - V_{3})} J_{e} = J_{c}(2 \rightleftharpoons 4).$$
(F.16)

Specific Heat Calculation

In this appendix we give a general relation for the specific heat of disordered Hubbard model (Eq. 4.1). First we break up the lattice to sum of pairs, for a pair of sites we find the ground state and the next excited state. For simplicity we assume the state with the highest energy in the singlet subscape decouples from other two states (this state is $|2,0\rangle$ or $|0,2\rangle$). Knowing probability distribution of V_1 and V_2 of a pair, one can find the probability distribution of the splitting between the singlet ground state and the triplet excited state. Therefore we can think of the original model as sum of two level systems with energies $-\Delta$ and zero, probability distribution of Δ is $P(\Delta)$. The total specific heat or spin susceptibility is sum of contributions of all two level system with splitting Δ weighted by $P(\Delta)$.

G.1 Probability distribution of splittings

For a pair of sites there are six states: three triplet states:

$$|\uparrow,\uparrow\rangle, |\downarrow,\downarrow\rangle, |1,1\rangle_t = \frac{1}{\sqrt{2}} (|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle)$$

and three singlet states:

$$|2,0\rangle, |0,2\rangle, |1,1\rangle_s = \frac{1}{\sqrt{2}} \left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right),$$
 (G.1)

the kinetic term does not couple these two subspaces; however there would be energy splitting for the singlet states. The Hamiltonian in the subspace of singlet states is (see Eq. 4.1):

$$H = \begin{pmatrix} V_1 + V_2 - 2\mu & -\sqrt{2}t & -\sqrt{2}t \\ -\sqrt{2}t & 2V_1 + U - 2\mu & 0 \\ -\sqrt{2}t & 0 & 2V_2 + U - 2\mu \end{pmatrix}$$
(G.2)

for the simplicity we define new variables $\gamma = V_1 + V_2$ and $v = |V_1 - V_2|$. The energy of triplet states is γ . Since we are interested in the energy splitting, we shift all energies by $\gamma - 2\mu$. Therefore Eq. G.2 becomes

$$H = \begin{pmatrix} 0 & -\sqrt{2}t & -\sqrt{2}t \\ -\sqrt{2}t & U - v & 0 \\ -\sqrt{2}t & 0 & U + v \end{pmatrix}.$$
 (G.3)

In the limit of $v = |V_1 - V_2| = 0$ the eigenvalues are

$$\begin{aligned}
\epsilon_1 &= \frac{1}{2} \left(U - \sqrt{16t^2 + U^2} \right), \\
\epsilon_2 &= U, \\
\epsilon_3 &= \frac{1}{2} \left(U + \sqrt{16t^2 + U^2} \right).
\end{aligned}$$
(G.4)

For large U limit and $v \gg t$ one of the states $|0,2\rangle$ or $|2,0\rangle$ (with energy U + v) can be decoupled from the rest of H in Eq. G.3. Therefore the effective Hamiltonian in the low energy sector is

$$H = \begin{pmatrix} 0 & -\sqrt{2}t \\ -\sqrt{2}t & U - v \end{pmatrix}$$
(G.5)

with eigenvalues

$$\epsilon_1 = \frac{U - v}{2} - \sqrt{2t^2 + \left(\frac{U - v}{2}\right)^2}, \quad \epsilon_2 = \frac{U - v}{2} + \sqrt{2t^2 + \left(\frac{U - v}{2}\right)^2}.$$
 (G.6)

The energy splitting between the ground state and the triplet states Δ is given by

$$\Delta = 0 - \epsilon_1 = \sqrt{2t^2 + \left(\frac{U - v}{2}\right)^2} - \frac{U - v}{2}.$$
 (G.7)

Comparing this splitting at the limit v = 0 with Eq. G.4 which is exact, the approximation G.7 for the splitting is not so good at small v.

The corresponding eigenvectors of G.6 are (with assumption $V_1 < V_2$)

$$|\psi_1\rangle = \frac{1}{\sqrt{1+{\Delta'}^2}} \Big(|1,1\rangle_s - \Delta'|2,0\rangle\Big)$$

$$|\psi_2\rangle = \frac{1}{\sqrt{1+{\Delta'}^2}} \Big(\Delta'|1,1\rangle_s + |2,0\rangle\Big)$$
(G.8)

where $\Delta' = \Delta/\sqrt{2t}$.



Fig G.1: (a) The hatched area of integration on V_1 and V_2 which is transformed to the hatched area in (b) with v and γ as new variables.

Within this approximation the probability distribution of the splitting Δ is

$$P(\Delta) = \int_{-V}^{V} dV_1 \int_{-V}^{V} dV_2 P(V_1) P(V_2) \delta(\Delta - \Delta(V_1, V_2))$$
(G.9)

 V_1 and V_2 are chosen from a uniform distribution: $P(V_1) = P(V_2) = 1/2V$; hence

$$P(\Delta) = \frac{1}{2V^2} \int_{-V}^{V} dV_1 \int_{V_1}^{V} dV_2 \delta(\Delta - \Delta(V_1, V2))$$

= $\frac{1}{2V^2} \int_{0}^{2V} dv \int_{0}^{2V-v} d\gamma \delta(\Delta - \Delta(v, \gamma))$ (G.10)

The hatched area in Fig. G.1.a shows the region of integration in V_1 and V_2 which is transformed to the hatched area in Fig. G.1.b with variables $v = |V_1 - V_2|$ and $\gamma = V_1 + V_2$ in Eq. G.10.

In order to carry out the integration in Eq. G.10 we need to use the relation given below for the delta function:

$$\delta(f(x)) = \frac{\delta(x - x_0)}{|f'(x)|_{x_0}}, \qquad f(x_0) = 0$$
(G.11)

therefore

$$f(v) = \Delta + \frac{U - v}{2} - \sqrt{\left(\frac{U - v}{2}\right)^2 + 2t^2}$$

$$f'(v) = \frac{1}{2} \left(1 - \frac{(U - v)/2}{\sqrt{((U - v)/2)^2 + 2t^2}}\right).$$
 (G.12)

Now we find the roots of f(v)

$$f(v_0) = 0$$

$$\Delta + \frac{U - v_0}{2} = \sqrt{\left(\frac{U - v_0}{2}\right)^2 + 2t^2}$$
(G.13)

therefore

$$U - v_0 = \frac{2t^2}{\Delta} - \Delta \tag{G.14}$$

and the delta function transform to

$$\delta(f(v)) = \delta(v - v_0) \left(\frac{2t^2}{\Delta^2} + 1\right). \tag{G.15}$$

From Eq. G.10 and Eq. G.14 we have

$$P(\Delta) = \frac{2V - v_0}{2V^2} \left(\frac{2t^2}{\Delta^2} + 1\right)$$
$$= \frac{\Delta}{2V^2} \left(\frac{2t^2}{\Delta^2} + 1\right) \left(\frac{2t^2}{\Delta^2} - 1 + \frac{2V - U}{\Delta}\right)$$
(G.16)

$$P(\Delta) = \frac{1}{2V} \left[\frac{\Delta}{V} \left(\frac{4t^4}{\Delta^4} - 1 \right) + \frac{2V - U}{V} \left(\frac{2t^2}{\Delta^2} + 1 \right) \right]$$
(G.17)

 $P(\Delta)$ has a sharp peak at Δ_{min} (see the inset in Fig. 5.6), and is non-zero only for $\Delta_{min} < \Delta < \Delta_{max}$, where Δ_{min} and Δ_{max} are obtained by substituting 0, and U in Eq. G.7.

G.2 Specific Heat for two level systems

Now we find the specific heat for a two level system. For two sites the ground state has energy $-\Delta$ and the excited state with three fold degeneracy has zero energy, hence the average energy is

$$E = \frac{-\Delta e^{\beta \Delta}}{e^{\beta \Delta} + 3} \tag{G.18}$$

and the specific heat is

$$c_{v} = \frac{\partial E}{\partial T} = -\beta^{2} \frac{\partial E}{\partial \beta}$$

$$c_{v} = \beta^{2} \Delta^{2} \frac{3e^{\beta \Delta}}{(e^{\beta \Delta} + 3)^{2}}$$
(G.19)

the total specific heat would be

$$C_{v} = \int_{\Delta_{min}}^{\Delta_{max}} d\Delta P(\Delta) c_{v}(\Delta)$$

= $\frac{3}{2V^{2}} \left[4t^{4}\beta^{2} \int \frac{dx}{x} \frac{e^{x}}{(e^{x}+3)^{2}} - \frac{1}{\beta^{2}} \int x^{3} \frac{e^{x}}{(e^{x}+3)^{2}} \right]$
+ $\frac{3(2V-U)}{2V^{2}} \left[2t^{2}\beta \int \frac{e^{x}}{(e^{x}+3)^{2}} dx + \frac{1}{\beta} \int \frac{x^{2}e^{x}}{(e^{x}+3)^{2}} \right]$ (G.20)

in the above integral the minimum splitting is $\Delta_{min} = \sqrt{U^2/4 + 2t^2} - U/2$ (from Eq. G.4) and from Eq. G.7 for the maximum splitting $(v_0 = 2V)$

$$\Delta_{max} = \frac{2V - U}{2} + \sqrt{\left(\frac{2V - U}{2}\right)^2 + 2t^2}.$$
 (G.21)

By putting parameters U and V we find total specific heat numerically. Fig. G.2 is the specific heat versus temperature for U = 8, t = 1 and V = 5 in three different range of temperatures. The red curve is the total specific heat. The other curves are different terms in the Eq. G.20 which are given below:

$$F_{1}(T) = \frac{6t^{4}}{V^{2}} \left[\beta^{2} \int_{x_{min}}^{x_{max}} \frac{dx}{x} \frac{e^{x}}{(e^{x}+3)^{2}} \right]$$

$$F_{2}(T) = \frac{3}{2V^{2}} \left[\frac{1}{\beta^{2}} \int_{x_{min}}^{x_{max}} x^{3} \frac{e^{x}}{(e^{x}+3)^{2}} dx \right]$$

$$F_{3}(T) = \frac{3(2V-U)t^{2}}{V^{2}} \left[\beta \int_{x_{min}}^{x_{max}} \frac{e^{x}}{(e^{x}+3)^{2}} dx \right]$$

$$F_{4}(T) = \frac{3(2V-U)}{2V^{2}} \left[\frac{1}{\beta} \int_{x_{min}}^{x_{max}} \frac{x^{2}e^{x}}{(e^{x}+3)^{2}} dx \right]$$

$$C_{v}(T) = F_{1}(T) - F_{2}(T) + F_{3}(T) + F_{4}(T)$$
(G.22)

in these integrations $x_{min} = \beta \Delta_{min}$ and $x_{max} = \beta \Delta_{max}$. As we see in figure G.2 contributions from $F_2(T)$ and $F_4(T)$ are equal and they cancel each other in the relation G.22, therefore the main contribution to the specific heat are from $F_1(T)$ and $F_3(T)$. Further analysis of specific heat is in the fourth chapter.

Upon a high temperature expansion in Eq. G.22:

$$\frac{e^x}{(e^x+3)^2} \approx \frac{1+x}{16}\left(1+\frac{x}{2}\right)$$
(G.23)

all terms $F_i(T)$ become proportional to β^2 . Therefore specific heat at large temperatures decays as $1/T^2$.



Fig G.2: Specific heat (the red curve) for three different temperature regimes. Four other curves are different contributions to the specific heat in Eq. G.20. These functions are given in Eq. G.22.

G.3 Spin susceptibility for two level systems

Spin susceptibility for two level systems can be obtained similar to what we have done for the specific heat. In general spin susceptibility for the wave vectors \mathbf{q} and \mathbf{q}' is written as:

$$\chi^{\alpha\alpha'}(\mathbf{q},\mathbf{q}';i\omega_n) = \int_0^\beta d\tau e^{i\omega_n\tau} \langle T_\tau S^\alpha(\mathbf{q},\tau) S^{\alpha'}(\mathbf{q}',0) \rangle \tag{G.24}$$

in the above relation $S^{\alpha}(\mathbf{q},\tau) = e^{-\tau H} S^{\alpha}(\mathbf{q}) e^{\tau H}$. For $i\omega_n = 0$ and $\mathbf{q} = 0$ spin susceptibility is

$$\chi^{\alpha\alpha'} = \int_0^\beta d\tau \langle T_\tau S^\alpha(\mathbf{q}=0,\tau) S^{\alpha'}(\mathbf{q}'=0,0) \rangle \tag{G.25}$$

Since the uniform magnetization S^α operator commutes with the Hamiltonian therefore $S^\alpha(\tau)=S^\alpha$ and

$$\frac{1}{\beta}\chi_{tot}^{+-} = \langle S^+S^- \rangle$$

$$T\chi_{tot}^{+-} = \sum_{\langle ij \rangle} \langle S_i^+S_j^- \rangle \qquad (G.26)$$

for two sites the uniform spin susceptibility is

$$T\chi^{+-} = \langle S_1^+ S_1^- + S_1^+ S_2^- + S_2^+ S_1^- + S_2^+ S_2^- \rangle$$
 (G.27)

knowing the eigenstates G.8, we find these expectation values

$${}_{s}\langle 1,1|S_{1}^{+}S_{1}^{-} + S_{2}^{+}S_{2}^{-}|1,1\rangle_{s} = 1$$

$${}_{s}\langle 1,1|S_{1}^{+}S_{2}^{-} + S_{2}^{+}S_{1}^{-}|1,1\rangle_{s} = -1$$

$${}_{t}\langle 1,1|S_{1}^{+}S_{1}^{-} + S_{2}^{+}S_{2}^{-}|1,1\rangle_{t} = 1$$

$${}_{t}\langle 1,1|S_{1}^{+}S_{2}^{-} + S_{2}^{+}S_{1}^{-}|1,1\rangle_{t} = 1$$

$$\langle \uparrow,\uparrow |S_{1}^{+}S_{1}^{-} + S_{2}^{+}S_{2}^{-}|\uparrow,\uparrow\rangle = 2$$

$$\langle \uparrow,\uparrow |S_{1}^{+}S_{2}^{-} + S_{2}^{+}S_{1}^{-}|\uparrow,\uparrow\rangle = 0$$

$$\langle \downarrow,\downarrow |S_{1}^{+}S_{1}^{-} + S_{2}^{+}S_{2}^{-}|\downarrow,\downarrow\rangle = 0$$

$$\langle \downarrow,\downarrow |S_{1}^{+}S_{2}^{-} + S_{2}^{+}S_{1}^{-}|\downarrow,\downarrow\rangle = 0$$
(G.28)

Therefore the spin susceptibility of two sites with two levels $-\Delta$ and zero is

$$T\chi^{+-} = \frac{2}{e^{\beta\Delta} + 3},\tag{G.29}$$

and for the total spin susceptibility

$$T\chi_{tot}^{+-} = \left[\frac{2t^4}{V^2}\right]\beta^2 \int \frac{dx}{x^3} \frac{2}{e^x + 3} \\ + \left[\frac{-1}{2V^2}\right] \frac{1}{\beta^2} \int x dx \frac{2}{e^x + 3} \\ + \left[\frac{t^2(2V - U)}{V^2}\right] \beta \int \frac{dx}{x^2} \frac{2}{e^x + 3} \\ + \left[\frac{2V - U}{2V^2}\right] \frac{1}{\beta} \int dx \frac{2}{e^x + 3}.$$
 (G.30)

The limits of the integrals are $\beta \Delta_{min}$ and $\beta \Delta_{max}$. High temperature expansion of χ gives

$$T\chi^{+-} = \frac{2}{e^x + 3} \approx \frac{2}{4+x} = \frac{1}{2} \left(1 + \frac{x}{4} \right)^{-1} = \frac{1}{2} \left(1 - \frac{x}{4} \right).$$
(G.31)

Within this approximation $T\chi_{tot}$ converges to a constant at small β .

Exact solution of 2 and 4 sites problem

H.1 Two sites solution

In the context of disordered Hubbard model given in Eq.4.1 for two sites at half filling there are six states:

- Three singlet states
 - 1. two non-magnetic $|2,0\rangle$ and $|0,2\rangle$,
 - 2. one magnetic $(S = 0, S_z = 0)$ $|1, 1\rangle_s = \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle |\downarrow, \uparrow\rangle).$
- Three triplet states
 - 1. $S = 1, S_z = \pm 1$: $|\uparrow,\uparrow\rangle$, $|\downarrow,\downarrow\rangle$, 2. $S = 1, S_z = 0$: $|1,1\rangle_t = \frac{1}{\sqrt{2}} (|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle)$.

For $|V_{1,2}| \leq U/2$ and at the limit t = 0 the ground state has 4 fold degeneracy $(|1,1\rangle_s, |1,1\rangle_t, |\uparrow,\uparrow\rangle, |\downarrow,\downarrow\rangle)$. Perturbation expansion of the kinetic term breaks the degeneracy, and the ground state will be combination of the singlet magnetic state and singlet non-magnetic states. At $U \gg t$ the main contribution to the ground state is from the magnetic one.

In the limit $V_1 \simeq -U/2$ and $V_2 \simeq U/2$ we use different perturbation expansion. The Hamiltonian H in the basis $|1,1\rangle_s$, $|2,0\rangle$ and $|0,2\rangle$ is

$$H = \begin{pmatrix} V_1 + V_2 - 2\mu & -\sqrt{2}t & -\sqrt{2}t \\ -\sqrt{2}t & 2V_1 + U - 2\mu & 0 \\ -\sqrt{2}t & 0 & 2V_2 + U - 2\mu \end{pmatrix}$$

$$= \begin{pmatrix} -U & -\sqrt{2}t & -\sqrt{2}t \\ -\sqrt{2}t & -U & 0 \\ -\sqrt{2}t & 0 & U \end{pmatrix}.$$
 (H.1)

At the limit $U \gg t$ the state $|0,2\rangle$ will decouple from the rest of Hamiltonian and the effective Hamiltonian is

$$H = \begin{pmatrix} -U & -\sqrt{2}t \\ -\sqrt{2}t & -U \end{pmatrix}$$
(H.2)

with eigenvalues $\epsilon_s^{\pm} = \pm \sqrt{2t} - U$, corresponding eigenstates are $|\psi_s^{\pm}\rangle = 1/\sqrt{2}(|2,0\rangle \pm |1,1\rangle_s)$ (see Fig. 5.3). The rest of the spectrum is $E_t = -U$ and $E_U = U$. Indices s and t correspond to singlet and triplet. The energy difference between the singlet ground state and the triplet excited state is $\sqrt{2t}$. For the case $|V_{1,2}| < U/2$ this energy difference is J_{12} , given in Eq. 5.1.

H.2 Four sites solution

For four sites [1-2-3-4] with periodic boundary conditions there are 70 states,

• Singlet states: sector with S = 0

6 non-magnetic states (e.g. $|2, 0, 2, 0\rangle$), 12 partially magnetic (e.g. $|2, 1, 1, 0\rangle_s$),

3 singlet states such as $\frac{1}{\sqrt{2}} \Big(|\uparrow,\downarrow,\uparrow,\downarrow\rangle + |\downarrow,\uparrow,\downarrow,\uparrow\rangle \Big),$

• Triplet states, sector with $S_z = 0$:

12 states with
$$S = 1$$
 (e.g. $|2, 1, 1, 0\rangle_t$),
3 states with $S = 2$ such as $\frac{1}{\sqrt{2}} \left(|\uparrow, \downarrow, \uparrow, \downarrow\rangle - |\downarrow, \uparrow, \downarrow, \uparrow\rangle \right)$,

• Triplet states, sector with $S_z = 1$:

12 states with S = 1 (e.g. $|2, \uparrow, \uparrow, 0\rangle$),

4 states with
$$S = 2$$
 (e.g. $|\downarrow,\uparrow,\uparrow,\uparrow\rangle$),

• Triplet states, sector with $S_z = -1$:

12 states with S = 1 (e.g. $|2, \downarrow, \downarrow, 0\rangle$),

4 states with S = 2 (e.g. $|\uparrow, \downarrow, \downarrow, \downarrow\rangle$),

• Triplet states, sectors with $S_z = \pm 2$:

two states: $|\uparrow,\uparrow,\uparrow,\uparrow\rangle$ with $S_z = 2$ and $|\downarrow,\downarrow,\downarrow,\downarrow\rangle$ with $S_z = 2$.

When $V_{1,2,3,4} = 0$ and t < U the ground state is singlet and the energy difference from the first triplet excited state upto second order perturbation in t is of the order t^2/U . For $V_i = (-1)^{i+1}U/2$ the ground state $|\psi_0^s\rangle$ is from the singlet sector and it is resonating between a set of magnetic and one non-magnetic states. At large U limit it is

$$\begin{aligned} |\psi_{0}^{s}\rangle &\approx \frac{1}{\sqrt{2}} \left(\frac{1}{2} \Big[|0,2,1,1\rangle_{s} + |1,2,0,1\rangle_{s} + |0,1,1,2\rangle_{s} + |1,1,0,2\rangle_{s} \Big] \right) \\ &+ \frac{1}{\sqrt{2}} \Big(\frac{2}{\sqrt{5}} |0,2,0,2\rangle \\ &+ \frac{1}{\sqrt{10}} \Big[|\uparrow,\uparrow,\downarrow,\downarrow\rangle + |\downarrow,\downarrow,\uparrow,\uparrow\rangle - |\downarrow,\uparrow,\uparrow,\downarrow\rangle - |\uparrow,\downarrow,\downarrow,\uparrow\rangle \Big] \Big). \end{aligned}$$
(H.3)

The first excited state is also from the singlet sector and is given by

$$\begin{aligned} |\psi_{1}^{s}\rangle &\approx \frac{1}{\sqrt{2}} \left(\frac{1}{2} \Big[|0, 2, 1, 1\rangle_{s} - |1, 2, 0, 1\rangle_{s} - |0, 1, 1, 2\rangle_{s} + |1, 1, 0, 2\rangle_{s} \Big] \right) \\ &+ \frac{1}{\sqrt{2}} \Big(-\frac{2}{\sqrt{6}} \Big[|\uparrow, \downarrow, \uparrow, \downarrow\rangle + |\downarrow, \uparrow, \downarrow, \uparrow\rangle \Big] \\ &+ \frac{1}{\sqrt{6}} \Big[|\uparrow, \uparrow, \downarrow, \downarrow\rangle + |\downarrow, \downarrow, \uparrow, \uparrow\rangle + |\downarrow, \uparrow, \uparrow, \downarrow\rangle + |\uparrow, \downarrow, \downarrow, \uparrow\rangle \Big] \Big). \end{aligned}$$
(H.4)

The next excited state is from the triplet subspaces and it has three fold degenerate and triplet. One of these states is

$$\begin{aligned} |\psi_{2}^{t}\rangle &\approx \frac{1}{\sqrt{2}} \left(\frac{1}{2} \Big[|0,2,1,1\rangle_{t} - |1,2,0,1\rangle_{t} + |0,1,1,2\rangle_{t} - |1,1,0,2\rangle_{t} \Big] \right) \\ &+ \frac{1}{\sqrt{2}} \Big[|\uparrow,\downarrow,\uparrow,\downarrow\rangle - |\downarrow,\uparrow,\downarrow\rangle \Big] \end{aligned} \tag{H.5}$$

The energy difference between the ground state and the first triplet excited state is of order of t. The first few energy spectrum are given in the inset of Fig.(5.5).

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