Can Disorder Drive a Mott Insulator into a Metal in 2D?

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We find that isoelectronic disorder generates novel phases in a Mott insulator at half filling. For both binary disorder potentials and for random site disorder models, the Mott gap is destroyed locally generating puddles of gapless excitations. With increasing disorder, these puddles grow and rather surprisingly, form an inhomogenous metal in 2D. Antiferromagnetic long range order is more robust than the Mott gap and persists into the metal, getting destroyed close to a critical disorder where doubly occupied and empty sites percolate.

§1. Introduction

The simplest disorder driven quantum phase transition is the Anderson localization problem that describes the properties of non-interacting electrons in a random potential. It was shown by the scaling theory$^{1,2}$ that in dimensions $d > 2$ the disordered system shows a transition from a conducting to an insulating phase. In a conductor, the wave functions are extended across the system and respond to perturbations at the boundaries. On the other hand in an insulating phase the wave functions are localized around deep potentials and are therefore insensitive to boundary conditions. The scaling theory further showed that for non-interacting electrons, the destructive quantum interference from time reversed paths localizes all the states in 2d and therefore no metallic behavior is possible in a 2d system.

However, in a condensed matter system, interactions cannot be ignored. In fact, the effect of localizing the particles by disorder only enhances the effective interactions.$^3$ The perturbative renormalization group work of Finkelstein$^4$ showed that the effective interaction parameter scaled to large values outside the regime of validity of the calculations. It is non-trivial to include the effects of interactions numerically. Given the many body nature of basis states, the Hilbert space grows exponentially with system size, and exact diagonalization is limited to about 16–20 sites. Quantum Monte Carlo techniques are powerful as they can incorporate disorder and interaction effects exactly for about 100 fermions.$^5$ However, in many cases the simulations are restricted to temperatures greater than $T \simeq 0.2t$ because of the “sign problem”.$^6$ Another method that has been applied to interacting disordered systems is the dynamical mean field theory.$^7$–$^9$ While it has been successful in describing quantum fluctuations at an effective single site, this method has not been applied to treat the spatially varying disorder in 2D.

Experimentally, our motivation is derived from the behavior of the resistivity in 2d MOSFETs and quantum wells$^{10,11}$ which give a clear indication of a transition from an insulating behavior (with $dp/dT < 0$) to metallic behavior (with $dp/dT > 0$)
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as the density of carriers $n$ is increased. The data can further be scaled by plotting the resistivity vs a scaled variable $|n - n_c| / T^{1/\nu z}$ where $n_c$ is the critical density that marks the metal-insulator transition and $\nu$ and $z$ are critical exponents.

In this paper we discuss the still open question of the combined effect of repulsive interactions and disorder in a fermionic system. In particular, we would like to understand whether the scaling result of the absence of metallic behavior in 2d remains robust when interactions are included or whether we get something new. We have previously studied the interplay of attractive interactions and disorder in superconductors\textsuperscript{12} as well as the interplay of repulsive interactions and disorder in superfluids.\textsuperscript{13}

Given the limitations of exact diagonalization, quantum Monte Carlo and dynamical mean field theory techniques, we are motivated to explore an alternative approach, the inhomogeneous Hartree Fock method.\textsuperscript{14} Though it treats interactions within mean field, this method includes disorder effects exactly and has the virtue of being able to deal with $\sim 5000$ fermions at $T = 0$ as well as finite $T$. Our results of the inhomogeneous mean field theory have provided a very intriguing picture of the phases that emerge with increasing disorder. Amongst our most striking results is a novel metallic phase in 2D which is sandwiched between a Mott insulator for small disorder and an Anderson insulator at large disorder.\textsuperscript{14} Here we explore the effects of a different model of disorder, the binary disorder model, which is conceptually simpler and we hope will elucidate the underlying physics of the phenomenon better.

§2. Disordered Hubbard model

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

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

The first term is the kinetic energy of electrons for hopping from site $i$ to site $j$ on a 2D square lattice. For 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 $\sigma$. $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the occupation number and $\mu$ 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 $\mu$ 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 disorder $V_i$. We choose two different models of disorder: In Model A the site energies $V_i$ are chosen randomly from a uniform distribution between $-V$ and $V$. In Model B (binary disorder model) a certain fraction of sites $n_{\text{dis}}$ chosen at random have a site potential $\pm V$, half of these sites have $V_i = V$ and for the other half $V_i = -V$. The rest of the sites, a fraction $(1-n_{\text{dis}})$ have zero potential $V_i = 0$. In the binary disorder model the disorder is described by two parameters $V$ and $n_{\text{dis}}$. Tuning each of them leads to different results. The electron density is fixed at $\langle n \rangle = 1$, and the temperature is zero. We have previously studied the behavior for Model A type disorder.\textsuperscript{14} Here we report our results for Model B type binary disorder for a fixed value of interaction $U = 4t$. 
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 the Appendix). The effective Hamiltonian is

$$H_{\text{eff}} = -t \sum_{\langle ij \rangle, \sigma} (c^\dagger_{i \sigma} c_{j \sigma} + c^\dagger_{j \sigma} c_{i \sigma}) + \sum_i \left( V_i + \frac{U}{2} \langle n_i \rangle - \mu \right) n_i - \sum_i h_i \cdot S_i \quad (2)$$

in which

$$h_i = 2U\langle S_i \rangle,$$

$$S_i = \frac{1}{2} c^\dagger_{i \sigma} \tilde{\tau}_{\sigma \sigma'} c_{i \sigma'}.$$

$h_i$ and $\langle n_i \rangle$ represent local fields and density and are variational parameters which have to be determined self-consistently, and $\tilde{\tau}$ are the Pauli spin matrices. We tune $\mu$ such that the half filling condition is satisfied. For an $N$ site system starting with an initial guess for the variational parameters, we have to solve the problem self-consistently for $3N + 1$ variables. An efficient algorithm requires special mixing schemes e.g. the Broyden method (see the Appendix) to achieve self-consistency in a reasonable amount of computer time. We have studied system sizes up to $50 \times 50$ at zero and finite temperatures.

§3. Results: Interplay of disorder and interaction

We now present results in the presence of both disorder and interaction obtained within a self consistent Hartree Fock approximation.

3.1. Magnetization, density and gap

For the pure system with no disorder, the system is a Mott insulator with a finite gap in the excitation spectrum and antiferromagnetic AF long range order. Disorder is introduced in the form of a certain fraction of sites $n_{\text{dis}}$ having a potential $V_i = \pm U/2$. The presence of valley sites with $V_i = -U/2$ favors double occupancy whereas the hill sites with $V_i = U/2$ favors empty sites. As a result of the tendency to form doubly occupied and empty sites, the local staggered magnetization $m^\dagger_i = (-1)^i x + i y 2\langle S^\dagger_i \rangle$ gets reduced. Figure 1 shows $m^\dagger_i$ for three values of $n_{\text{dis}} = 0.23, 0.43$ and 0.72 at fixed values of interaction ($U = 4t$) and disorder strength ($V_i = \pm 2t$). The left panels give the disorder profile; black circles correspond to $V_i = V$ and empty circles to $V_i = -V$. The right panels show the corresponding behavior of $m^\dagger_i$. The uniform black background indicates AF long range order (AFLRO) (since the obvious alternating Neel order has been factored out), while white regions in the right panels indicate paramagnetic sites. The AFLRO persists even to $n_{\text{dis}} = 0.72$. In addition to the reduction of AFLRO with increasing disorder, panel (c) also shows that there are clusters with staggered magnetization opposite to the majority of sites (shown as black circles).

Three panels in Fig. 2 exhibit the probability distribution of the local staggered magnetization, local density and effective potential for three values of the binary
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Disorder Profile

\( n_{\text{dis}} = 0.23 \)

(a)

\( n_{\text{dis}} = 0.43 \)

(b)

\( n_{\text{dis}} = 0.72 \)

(c)

Stagg. Mag.

Fig. 1. Left panels give disorder profile for a binary disorder model: black circles indicate sites with \( V_i = V \) and white circles indicate sites with \( V_i = -V \) for \( U = 4t \) and \( V = U/2 = 2t \) on a system of size \( N = 28 \times 28 \). The rest of the sites (not marked) are non-disordered. The right panels show the corresponding local staggered magnetization \( m^\uparrow \). The uniform black background in the right panels identifies sites with finite staggered magnetization forming a Neel ordering pattern, though with reduced moment. The white regions interrupt the AFRO with paramagnetic sites and grow with increasing \( n_{\text{dis}} \). The black circles indicate local AF regions but with sublattice magnetization opposite to that of the original system.

disorder \( n_{\text{dis}} \). For \( n_{\text{dis}} = 0.23 \), \( P(S_i/n_i/V_{\text{eff}}) \) has a sharp peak dominated largely by the sites with weak disorder. With increasing \( n_{\text{dis}} \), in panel (a) most of the weight of the distribution shifts to the smaller values of staggered magnetization dominated by sites which have close to double occupancy or are empty. In panel (b), the local density which is peaked at one per site at low disorder gets redistributed near occupancies of two and zero. Panel (c) shows the effective disorder potential screened by the Hartree shift \( V_{\text{eff}}(i) = V_i + (U/2)\langle n_i \rangle \); note that the disordered sites with \( V_i = \pm 2t \) are screened most prominently.

These data show that the properties of a disordered system can be effectively modeled as a two-component system with distinct contributions from sites that have zero disorder showing characteristics close to the pure system, whereas sites which are disordered show paramagnetic behavior. In the classical system for \( t = 0 \), the hills are empty and valleys are doubly occupied; upon including the quantum effects,
Fig. 2. (a), (b) and (c) show the probability distribution of the local AF magnetization, local density and local effective potential respectively on \( N = 28 \times 28 \) and averaged over 3 realizations of disorder. The interaction and disorder strength are fixed at \( U = 4t \) and \( V = 2t \).

The corresponding occupancies fluctuate near zero and two.

Figure 3(a) shows the staggered magnetization as a function of \( n_{\text{dis}} \) for different disorder strengths. For \( V < U/2 \) the system continues to display AFLRO even when all the sites are disordered. On the other hand, for \( V \geq U/2 \) AFLRO is lost beyond a critical \( n_{\text{dis}} \) and the fraction of disordered sites that are required to kill AFLRO
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Fig. 3. (a) Staggered magnetization as a function of number of disordered sites \( \langle n_{\text{dis}} \rangle \) for four different values of \( V \) on \( N = 28 \times 28 \). Neel ordered initial inputs are chosen for the parameters of the HF Hamiltonian. It becomes difficult to achieve self consistency at higher values of \( n_{\text{dis}} \). (b) Staggered magnetization vs. disorder strength \( V \) for three different values of \( n_{\text{dis}} \), the interaction is \( U = 4t \). The data are averaged over three realizations of disorder.

decreases with increasing \( V \) i.e. for higher values of \( V \) the magnetization falls faster. Panel (b) shows that the staggered magnetization for small \( V \) is almost independent of \( n_{\text{dis}} \).

Figure 4 shows the spectral gap in the DOS as a function of disorder strength \( V \) for three values of \( n_{\text{dis}} \). Our results show that the gap strongly depends on the strength of disorder \( V \) rather than \( n_{\text{dis}} \). This is largely because we are defining the gap as the lowest energy excitation above the ground state. In the case of binary disorder it measures the local destruction of the gap once the disorder at a site becomes on the order of \( U/2 \). At this point, the disorder is successful in overcoming the repulsion \( U \) and generates charge fluctuations from having just singly occupied sites to having paramagnetic sites with zero and double occupancy. As a result of these charge fluctuations the gap closes locally. So obviously, the gap is more sensitive to the local potential rather than to how many such disorder sites exist in the system.

3.2. Nature of eigenstates

The presence of extended states at the Fermi surface is an indication of a metallic phase. Figure 5 shows a real space image of the eigenstate \( |\psi^2(i)|^2 + |\psi^1(i)|^2 \) at the Fermi energy for three values of \( n_{\text{dis}} \). For \( n_{\text{dis}} = 0.23 \) and \( n_{\text{dis}} = 0.43 \) these states are localized, while for \( n_{\text{dis}} = 0.72 \) they become extended. This implies a metal insulator transition with \( n_{\text{dis}} \) as the tuning parameter.

To quantify the extent of the wave function, we calculate the inverse participation
Fig. 4. Lowest energy excitation gap in the single particle density of states as a function of disorder strength for different values of $n_{\text{dis}}$. The interaction is $U = 4t$.

Fig. 5. Eigenstates at the Fermi energy for three different values of $n_{\text{dis}}$ and fixed $U = 4t$ and $V = 2t$. Surprisingly, with increasing $n_{\text{dis}}$ these states become extended. The system size is $N = 28 \times 28$.

ratio $\text{IPR}^{15}$ defined by

$$\text{IPR}(\Psi_n) = \sum_{i,\sigma} |\psi^n_\sigma(i)|^4. \quad (4)$$

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

$$|\Psi(r)|^2 = A \exp(-\alpha r/\xi), \quad (5)$$
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Fig. 6. The inverse participation ratio (IPR) (a measure of the inverse localization length) for all states vs energy. The disorder strength is $V = U/2$ and $N = 28 \times 28$. $n_{\text{dis}}$ is the fraction of disordered sites with potential $V_i = \pm V$.

Fig. 7. (a) The inverse participation ratio (IPR) as a function of $n_{\text{dis}}$ for different $V/t$. For larger values of $V$'s, IPR falls faster. (b) IPR as a function $V$ for different values of $n_{\text{dis}}$. With increasing $n_{\text{dis}}$, the metallic phase gets expanded to a wider range of $V$. 
where $\alpha$ is a positive constant, $\xi$ is the localization length. In 2D, the normalization factor is $A = \alpha^2/\xi^2$. Therefore IPR is

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

(6)

Thus $\text{IPR}(|\Psi|)$ is a measure of the localization of a state $\Psi$. The more a state is localized the higher its IPR. For an extended state $\text{IPR} \sim O(1/N)$, where $N$ is the number of sites.

To get a better idea about the nature of eigenstates as a function of energy, we show in the different panels of Fig. 6 the 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 which are near the Fermi energy indicated by 0, are localized, while in (c) with increasing number of disordered sites these states become extended.

Figure 7(b) shows the IPR as a function $n_{\text{dis}}$ for different $V$'s. IPR has sharper fall for larger $V$'s. Panel (b) shows the highly non-monotonic behavior of the IPR vs $V$ for three different $n_{\text{dis}}$. At higher values of $n_{\text{dis}}$ the system has metallic behavior for larger range $V$; as $n_{\text{dis}} \to 1$, IPR has the lowest value for $V = U/2$.

### 3.3. Percolation of kinetic bonds

In order to get a picture of the metallic phase and understand why it arises upon introducing disorder, we have looked at the expectation value of the hopping amplitude or the kinetic energy on all the bonds. In the absence of disorder all the bonds have equal kinetic energy $|K_{ij}| = 0.34t$. By adding disorder, the kinetic energy of the bonds surrounding the disordered site get lower (their absolute values increase), in other words, bonds linking the specific disordered site to nearest neighbor sites get active because of enhanced hopping. In Fig. 8 we show the kinetic energy of the active bonds for 3 different disorder profiles. In these figures, the open circles are sites with $V_i = 0$, the black circles and those with $+$ inside are sites with disorder potential $U/2$ and $-U/2$ respectively. The fraction of disordered sites varies in the three figures. The gray scale squares measure the expectation values of the corresponding bonds, only “active bonds” bonds with kinetic energy more than a threshold (say 0.34$t$) are shown. Notice that the kinetic energy is highest for the bonds with opposite signs of disorder $V_i = V$ and $V_j = -V$ for adjacent sites $i$ and $j$. Recently we have addressed the magnetic properties of such defects and found that they show definitive signatures in the specific heat and spin susceptibility as a function of temperature. The kinetic energy is the lowest for the weakly disordered sites ($V_{i,j} = 0$), however if such non-disordered bonds are surrounded by active bonds their kinetic energy increases because of quantum tunneling. Figure 9 shows the probability distribution of the kinetic energy of all the bonds for three values of $n_{\text{dis}}$. For higher values of $n_{\text{dis}}$ the distribution gets broader accessing higher values that are conducive to metallic behavior. The presence of a percolating cluster of such active bonds gives rise to the metallic phase as seen from Fig. 8(c).
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\[ n_{\text{dis}} = 0.23 \quad (a) \]
\[ n_{\text{dis}} = 0.43 \quad (b) \]
\[ n_{\text{dis}} = 0.72 \quad (c) \]

Fig. 8. Open circles are sites with \( V_i = 0 \), the filled black circles have an on-site potential \( V_i = U/2 \), whereas the white circles with a + inside have \( V_i = -U/2 \). The number of sites with repulsive and attractive on-site potentials are equal. The total density of disordered sites is (a) \( n_{\text{dis}} = 0.21 \); (b) \( n_{\text{dis}} = 0.43 \); and (c) \( n_{\text{dis}} = 0.72 \). The gray squares are the expectation value of the corresponding bond in units of \( t \). Bonds with energy equal to 0.34 in the pure system are not shown in order to distinguish those that are affected by the disorder.

§4. The role of inhomogeneous magnetic field

A crucial question arises from our discovery of a metallic phase in the disordered Mott insulator in 2D. The calculations are performed using the HF approximation which ultimately results in an effective single particle Hamiltonian. We know from the scaling theory on the non-interacting model that in 2D the system is always an
insulator. So the question that arises is how can the HF approximation produce a metallic phase? It is useful to examine the conditions of the scaling theory. The theoretical result of all states being localized in 2D is obtained for (i) potential or hopping disorder that is completely uncorrelated, and (ii) absence of any magnetic fields. Within the Hartree Fock approximation, the interactions screen the bare disorder potential and produce an effective potential $\tilde{V}_{\text{eff}}(i) = V_i + (U/2)\langle n_i \rangle$. The interactions also result in an inhomogeneous magnetic field $h_i$. Thus there are two possibilities for the breakdown of the scaling argument: (i) Even though the bare potential is completely uncorrelated, there are non-trivial spatial correlations of the effective potential. (ii) The inhomogeneous magnetic field $h_i$ is correlated with the disorder.

To investigate these possibilities further, we have used the distribution of the effective potential shown in Fig. 2 as the disorder input for a “non-interacting” problem. Figure 10 shows the IPR for the eigenstates at the Fermi energy as a function of $n_{\text{dis}}$ for the HF solution of the interacting problem. In comparison, we also show the IPR for the non-interacting problem with a screened disorder potential $V_{\text{eff}}$. In the metallic regime (for $n_{\text{dis}} > 0.6$) where the states are extended as seen from Fig. 5, we find that the IPR obtained for the interacting HF problem is lower indicating that the states are more extended that what one would deduce from a pure screening picture. This implies that the inhomogeneous magnetic fields also have an important role to play in delocalizing the electrons. Thus the metallic phase arises from a combination of both effects: screening of strong disorder sites and the presence of an inhomogeneous magnetic field. It is important to note that the lowest
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Fig. 10. IPR of the states at the Fermi energy as a function of the fraction of disordered sites \( n_{\text{dis}} \). 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 the IPR for non-interacting electrons but with the disorder chosen from effective screened potential obtained in the interacting problem.

The value of the IPR of 0.003 is limited by the saturation of the correlation length at the system size.

§5. Physical picture: Two component model

The physical picture that emerges from the data given above is intimately related to percolation. For this it is useful to consider the extreme classical limit \( t = 0 \). Figure 11 shows the effect of adding B type sites to a system composed of A type sites. In our model the A type sites correspond to the AF sites which have occupancy 1 and based on Fig. 2 arise from the sites with zero or less disorder. Type B sites correspond to doubly occupied sites that arise from potentials wells of depth \( V_i \leq -U/2 \) or empty sites at sites with potential hills of height \( V_i \geq U/2 \). In the classical limit at a density of 41% B sites, the single occupied sites stops percolating\(^{16}\) and the system loses AFLRO. Figure 3 shows that upon including quantum effects the critical point can change and depends on the strength of the local disorder potential. We also find that the self consistency condition is more difficult to achieve near the critical point and the system develops sensitivity to the initial conditions. As a result we are unable to pursue the calculations to smaller values of the staggered magnetization. Finite size effects are also important near the critical point.

The bond kinetic energy plots in Fig. 8 are extremely pertinent in understanding the emerging metallic behavior. Disorder generates charge fluctuations along the bonds that connect the disorder sites to the neighbors. Pairs of nearest neighbor sites with opposite signs of potentials \( V_i = \pm U/2 \) and \( V_j = 0 \) or \( V_i = U/2 \) and
Fig. 11. For a 2D lattice made up of two types of sites A and B that are randomly distributed, if $N_B/(N_A + N_B) > x_c$, 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 0.59.16

$V_j = -U/2$ have the most contribution to the conductivity.17 The metallic state arises from a percolating cluster of these active bonds.

Appendix A

We give the details of the Hartree Fock (HF) approximation and the numerical method that we have used.

A.1. Details of Hartree-Fock approximation

Starting with the repulsive Hubbard model with site disorder in Eq. (1), we use the following mean field approximation (MFA):

\[
\begin{align*}
n_{i\uparrow}n_{i\downarrow} &= c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} \\
&= \langle n_{i\uparrow} \rangle n_{i\uparrow} + \langle n_{i\downarrow} \rangle n_{i\downarrow} - \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle \\
&\quad - c_{i\uparrow}^\dagger c_{i\downarrow} (c_{i\downarrow}^\dagger c_{i\uparrow}) - c_{i\downarrow}^\dagger c_{i\uparrow} (c_{i\uparrow}^\dagger c_{i\downarrow}) + \langle c_{i\uparrow}^\dagger c_{i\downarrow} \rangle (c_{i\downarrow}^\dagger c_{i\uparrow}). \tag{A.1}
\end{align*}
\]

This unrestricted mean field approximation results in the effective Hamiltonian:

\[
H_{eff} = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + \sum_i \tilde{V}_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} + \sum_i (h_i^- c_{i\uparrow}^\dagger c_{i\downarrow} + h_i^+ c_{i\downarrow}^\dagger c_{i\uparrow}), \tag{A.2}
\]

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

We are now faced with the mammoth task of obtaining the $3N + 1$ variational parameters: $\langle n_{i\sigma} \rangle$, $h_i = h_i^+ = h_i^-$ at the N sites and the chemical potential $\mu$ self-consistently. $h_i^\pm$ is the expectation value of $S_i^\pm$ and is given by

\[
\begin{align*}
h_i^+ &= -U \langle c_{i\uparrow}^\dagger c_{i\downarrow} \rangle, \\
h_i^- &= -U \langle c_{i\downarrow}^\dagger c_{i\uparrow} \rangle.
\end{align*}
\]
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The chemical potential $\mu$ has to be tuned such that the half filled condition $1/N \sum_{i,\sigma} \langle n_{i\sigma} \rangle = 1$ is satisfied.

$H_{\text{eff}}$ is written as

$$
H_{\text{eff}} = C^\dagger \begin{pmatrix}
\tilde{V}_1^{\uparrow} & -t & 0 & \ldots & h_1^- & 0 & 0 & \ldots \\
-t & \tilde{V}_2^{\uparrow} & -t & \ldots & 0 & h_2^- & 0 & \ldots \\
0 & -t & \tilde{V}_3^{\uparrow} & \ldots & 0 & 0 & h_i^- & \ldots \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots \\
h_1^+ & 0 & 0 & \ldots & \tilde{V}_1^{\downarrow} & -t & 0 & \ldots \\
0 & h_2^+ & 0 & \ldots & -t & \tilde{V}_2^{\downarrow} & -t & \ldots \\
0 & 0 & h_3^+ & \ldots & 0 & -t & \tilde{V}_3^{\downarrow} & \ldots \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots \\
\end{pmatrix} C \quad (A.3)
$$

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

$$
C = \begin{pmatrix} c_1^{\uparrow} \\ c_2^{\uparrow} \\ c_3^{\uparrow} \\ \vdots \\ c_N^{\uparrow} \\ c_1^{\downarrow} \\ c_2^{\downarrow} \\ c_3^{\downarrow} \\ \vdots \\ c_N^{\downarrow} \end{pmatrix} \quad (A.5)
$$

We perform a unitary transformation on $c_{i\sigma}$ which diagonalizes $H_{\text{eff}}$.

$$
H_{\text{eff}} = \epsilon_n c_{n\uparrow} c_{n\downarrow} \quad (A.6)
$$

and

$$
c_{i\sigma} = \sum_n \psi_{i\sigma}^n c_{n\sigma},
$$

$$
\sum_{i,\sigma} |\psi_{i\sigma}^n|^2 = 1, \quad (A.7)
$$

where $\psi_{i\sigma}^n$ are the components of the eigenvectors of $\hat{A}$ in the site basis and $\epsilon_n$ are the corresponding eigenvalues. Since eigenvectors of $\hat{A}$ are real $\psi_{i\sigma}^n \ast = \psi_{i\sigma}^n$.

A.2. Observables

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

- Local density:

$$
\langle n_{i\sigma} \rangle = \sum_n \left( |\psi_{i\sigma}^n|^2 \right) f(\epsilon_n). \quad (A.8)
$$
Local magnetic fields:

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

\[
h_i = -U \langle c_i^\dagger c_i \rangle = -U \sum_n \psi_{i\uparrow}^n \psi_{i\downarrow}^n f(\epsilon_n),
\]  

(A.9)

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

Spin-spin correlation function:

\[
\langle S_i^+ S_j^- \rangle = \langle c_{i\uparrow}^\dagger c_{j\downarrow} c_{j\uparrow}^\dagger c_{i\downarrow} \rangle
= \sum_{n,m,k,l} \psi_{i\uparrow}^n \psi_{i\downarrow}^m \psi_{j\uparrow}^k \psi_{j\downarrow}^l (\tilde{c}_{i\uparrow} \tilde{c}_{i\downarrow} \tilde{c}_{j\uparrow} \tilde{c}_{j\downarrow})
= \sum_{n,m,n\neq m} (\psi_{i\uparrow}^n \psi_{i\downarrow}^m \psi_{j\uparrow}^m \psi_{j\downarrow}^n (\tilde{c}_{i\uparrow} \tilde{c}_{i\downarrow} \tilde{c}_{j\uparrow} \tilde{c}_{j\downarrow}) + \psi_{i\uparrow}^n \psi_{i\downarrow}^m \psi_{j\uparrow}^n \psi_{j\downarrow}^m (\tilde{c}_{i\uparrow} \tilde{c}_{i\downarrow} \tilde{c}_{j\uparrow} \tilde{c}_{j\downarrow}))
+ \sum_n \psi_{i\uparrow}^n \psi_{i\downarrow}^n \psi_{j\uparrow}^n \psi_{j\downarrow}^n (\tilde{c}_{i\uparrow} \tilde{c}_{i\downarrow} \tilde{c}_{j\uparrow} \tilde{c}_{j\downarrow})
= \sum_{n,m,n\neq m} (\psi_{i\uparrow}^n \psi_{i\downarrow}^m \psi_{j\uparrow}^m \psi_{j\downarrow}^n f(\epsilon_n)f(\epsilon_m) + \psi_{i\uparrow}^n \psi_{i\downarrow}^m \psi_{j\uparrow}^n \psi_{j\downarrow}^m f(\epsilon_n)(1 - f(\epsilon_m)))
+ \sum_n \psi_{i\uparrow}^n \psi_{i\downarrow}^n \psi_{j\uparrow}^n \psi_{j\downarrow}^n f(\epsilon_n).
\]

(A.10)

A.3. Self consistency procedure

The input parameters of the matrix \( \hat{A} \) are unknown quantities \( \langle n_{i\sigma} \rangle, h_i \) and \( \mu \). We start with guess inputs for these quantities. For small disorder the ground state has AF long range order therefore it is efficient to start with an AF initial input. Similarly for high disorder, a good guess is to start with a random initial input for the local fields. Using these inputs in Eq. (A.4) we then calculate the eigenfunctions. The output local density and fields are obtained from Eqs. (A.8) and (A.9) in terms of these eigenfunctions. If these output fields are different from the input, the problem is reiterated with these new output fields as the new parameters in Eq. (A.4). The most obvious method is to take as the new input to be the resultant output of the previous iteration; however convergence to the self-consistent solution is improved by adding some mixing. These mixing methods are discussed in the next subsection.

We have found that the final self-consistent solution is independent of the initial starting inputs (e.g. random or Neel) in the low disorder regime. In the strongly disordered regime, on the other hand, we found that different initial inputs can result in different final states, and from these we choose the one with the lowest energy as the ground state.

At half filling \( \mu = U/2 \), 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.3.1. Newton method

Given an input and the resulting output parameters after a single iteration, we next discuss two different important mixing schemes\(^{18} \) that determine the input parameters for the subsequent iteration.
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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 $h_i$ 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 $\mathbf{F} = \mathbf{x}_{\text{output}} - \mathbf{x}_{\text{input}}$. Our aim is to find the values of $\mathbf{x}$ for which this difference becomes smaller than a threshold (e.g. $10^{-4}$). We can write $\mathbf{F}$ as:\(^{18}\)

$$F_i(\mathbf{x} + \delta \mathbf{x}) = F_i(\mathbf{x}) + \sum_j \frac{\partial F_i}{\partial x_j} \delta x_j + \cdots,$$

$$\mathbf{F}(\mathbf{x} + \delta \mathbf{x}) = \mathbf{F}(\mathbf{x}) + \mathbf{J} \cdot \delta \mathbf{x},$$

(A-11)

where the Jacobian

$$J_{ij} = \frac{\partial F_i}{\partial x_j}. \quad (A-12)$$

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

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

(A-13)

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

A.3.2. Broyden mixing scheme

A more efficient mixing scheme, The Broyden method allows $\mathbf{J}$ to change in each iteration. Equation (A-12) can be written as

$$\mathbf{J}^{(n+1)}(\mathbf{x}) = \frac{\delta \mathbf{F}^{(n)}}{\delta \mathbf{x}^{(n)}}, \quad (A-14)$$

The upper index $n$ is the iteration number.

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

(A-15)

$$\mathbf{v} = \delta \mathbf{x}^{(n)} \dagger, \quad u = \frac{\delta \mathbf{F}^{(n)} - \mathbf{J}^{(n)} \delta \mathbf{x}^{(n)}}{\delta \mathbf{x}^{(n)} \dagger \delta \mathbf{x}^{(n)}}, \quad (A-16)$$

$$\mathbf{J}^{(n+1)-1} = \left(\mathbf{J}^{(n)} + uu^\dagger\right)^{-1}. \quad (A-17)$$
Now we have to use this expansion for the matrices \( A = J^{(n)} \) and \( B = uv^\dagger \),
\[
(A + B)^{-1} = (A(I + A^{-1}B))^{-1} = (I + A^{-1}B)^{-1}A^{-1}
= (I - A^{-1}B + A^{-1}BA^{-1}B - (A^{-1}B)^2 + \cdots)A^{-1}
= A^{-1} - A^{-1}BA^{-1} + A^{-1}BA^{-1}BA^{-1} - A^{-1}BA^{-1}BA^{-1}BA^{-1} + \cdots,
\]
(A·18)
\[
A^{-1}BA^{-1}BA^{-1} = J^{(n)-1}v^\dagger J^{(n)-1}u^\dagger J^{(n)-1}u
\]
(A·19)
in this relation \( \lambda \) is a scalar and has been defined as
\[
\lambda = v^\dagger J^{(n)-1}u
= \delta x^\dagger J^{(n)-1} \left( \frac{\delta F^{(n)} - J^{(n)} \delta x^{(n)}}{\delta x^{(n)} \delta x^{(n)}} \right) = \delta x^\dagger J^{(n)-1} \frac{\delta F^{(n)}}{\delta x^{(n)}} - 1,
\]
(A·20)
and therefore
\[
\frac{1}{1 + \lambda} = \frac{\delta x^\dagger \delta x^{(n)}}{J^{(n)-1} \delta F^{(n)}}
\]
(A·21)
from Eqs. (A·18) and (A·19)
\[
J^{(n+1)-1} = J^{(n)-1} - J^{(n)-1}uv^\dagger J^{(n)-1} \left( 1 - \lambda + \lambda^2 - \cdots \right)
= J^{(n)-1} - J^{(n)-1}uv^\dagger J^{(n)-1} \frac{1}{1 + \lambda}
= J^{(n)-1} - \left( \frac{J^{(n)-1} \delta F^{(n)} - \delta x^{(n)}}{\delta x^{(n)} \delta x^{(n)}} \right) \delta x^\dagger J^{(n)-1} \frac{1}{1 + \lambda}
\]
(A·22)
by using Eq. (A·21) in the above equation
\[
J^{(n+1)-1} = J^{(n)-1} + \left( \frac{\delta x^{(n)} - J^{(n)-1} \delta F^{(n)}}{\delta x^{(n)} \delta x^{(n)}} \right) \delta x^\dagger J^{(n)-1}
\]
(A·23)
having found \( J^{-1} \), from Eq. (A·13) \( \delta x \) can be found for the next iteration. In our problem there are \( 3N \) variational parameters \( (h_i \text{ and } n_i) \) therefore \( x \) is a vector in \( 3N \) dimensional space, and \( F = x^{out} - x^{in} \) in which \( x^{in} = x^{(n)} \).

A.4. 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 a mixing scheme is used to generate the next set of input fields.

Typical lattice sizes that we have used are \( 28 \times 28, 32 \times 32, 40 \times 40 \) and \( 50 \times 50 \). For a lattice of size \( 28 \times 28 \), the CPU time (in a pentium 4 machine) required for
one iteration in the self-consistent loop is about one minute. In the Mott regime, it takes approximately 250 iterations for a fixed value of $V_d$, $U$ and temperature in order to get the self consistent result with an accuracy $10^{-4}$ on a $28 \times 28$ system. In the strongly disordered regime this number can be of the order of several thousand iterations. The number of iterations increases with the system size. For larger sizes (above $L = 32$), the computation were performed on the dec-alpha machines.

References

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