Dimensional and temperature dependence of metal-insulator transition in correlated and disordered systems

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Abstract – We study the dimensional dependence of the interplay between correlation and disorder in two dimensions at half-filling using the 2D \(t-t'\) disordered Hubbard model with deterministic disorder both at zero and finite temperatures. Inclusion of \(t'\) without disorder leads to a metallic phase at half-filling below a certain critical value of \(U\). Above this critical value \(U_c\) correlation favours an antiferromagnetic phase. Since disorder leads to double occupancy over the lower-energy site, the competition between Hubbard \(U\) and disorder leads to the emergence of a metallic phase, which can be quantified by the calculation of Kubo conductivity, gap at half-filling, density of states, spin order parameter, inverse participation ratio (IPR) and bandwidth. We have studied the effect of disorder on the system in a very novel way through a deterministic disorder which follows a Fibonacci sequence. The behaviour of different quantities shows interesting features on going from a two- to quasi–one-dimensional system.

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Introduction. – Kravchenko et al. [1] in a series of experiments on very weakly disordered 2D semiconductors (Si MOSFETS) at very low filling, in the absence of magnetic field showed that it is possible for a 2D system to undergo a metal-insulator transition. Recently, Punnoose and Finkelstein have shown that it is possible to identify a quantum critical point separating a metallic phase stabilized by electronic interactions from the insulating phase where disorder prevails over electronic interactions in certain systems [2].

Recently, the Mott insulator has been realised for fermionic atoms in an optical lattice in 3 dimensions [3], whereas most of the previous results were for bosonic atoms. Further, the experimental realisation of Anderson insulators for Bose gas has been realised [4] by disordering the optical lattice site potentials. It is possible to disorder the lattice in a rather controlled manner on optical lattices. This has facilitated the controlled experimental study of the phase diagram arising due to the competition of strong correlations and disorder in these systems, causing us to revisit this topic.

The present work emphasises on the dimensional dependence of the interplay between electronic correlation and deterministic disorder (and the consequential reflection in metal-insulator transition (MIT)) as one goes from a two-dimensional system to a quasi–one-dimensional system. Also the important aspect of the role of temperature in this whole scenario has been duly addressed.

A Hartree-Fock mean-field treatment of the non-disordered \(t-t'\) Hubbard Hamiltonian [5] shows a paramagnetic-to-antiferromagnetic transition at \(U_c = 2.1\). The disordered Hubbard Hamiltonian was shown to have persistent currents [6], Milovanović et al. [7] investigated it numerically and Bhatt et al. [8] studied local moment formation. Dobrosavljević and co-workers [9] use the generalized DMFT method to report the interesting fact that increasing disorder from a clean Mott insulator results in the closing of the Mott gap and the stabilization of a metallic phase.

The possibility that a metallic phase may exist in 2D due to the interplay of strong correlations and random disorder for the half-filled disordered Hubbard model has been suggested [10].

We solve the problem numerically using the unrestricted Hartree-Fock (UHF) technique. The UHF method works remarkably well even in 1D at half-filling and is in excellent agreement with results obtained from the real-space renormalization method [11]. In 2D at half-filling the UHF method gives a result in close proximity with that of the
quantum Monte Carlo method [5]. However, one should mention here that the correlated Kondo-like processes that lead to large effective-mass renormalization in the vicinity of the Mott transition can only be captured by a method like DMFT and not by the present method [12]. The importance of inelastic scattering processes for calculating the conductivity was shown by a DMFT calculation by Aguiar et al. [13]. We choose a deterministic binary disorder (that follows a Fibonacci sequence), motivated largely by optical lattice realisations. Deterministic disorder has been one of the forefront areas of research in condensed-matter physics for the past two and a half decades both in experiments [14] and theory [15]. Theoretical studies of the quasi-periodic systems have shown that in the non-interacting limit the wave function shows a power law localization both in one [16] and two [17] dimensions. A very recent experiment in a 1D quasi-periodic optical lattice [18], where the system was described by an Aubry-Andre Hamiltonian, has shown exponentially localized states (Anderson localization) in the large disorder limit. A theoretical explanation has been published recently [19] using a Fibonacci sequence in 1D. We benchmark our results and trends against old results obtained with random disorder. Zero- and finite-temperature calculations have been carried out for different values of the disorder strength. The impurity concentration remained almost constant as we reduced the dimension, which is an artifact of the Fibonacci sequence. We have taken a 40 × 40 lattice which is fairly large to rule out finite-size effects.

The system, though insulating in the $U > U_c$ regime, undergoes a depletion of the charge gap at half-filling as the disorder is increased, till it reaches a stage where the lower-energy sites would be doubly occupied in spite of the large value of $U$. A narrow metallic regime emerges while going from the Neel state to the state with a distribution of doubly occupied and unoccupied sites. The low-temperature metallic phase gives way to an insulating phase upon heating. It has residual spin order (very low value) and is thus not a perfect paramagnet. One of our objectives in the present work is to investigate the evolution of the interplay between disorder and interactions and relatively whose effect gets more dominant as one reduces the dimension. The effect of next-nearest-neighbour hopping makes the delocalized phase more robust.

**Disordered Hubbard Hamiltonian.** – The disordered 2D $t - t'$ Hubbard Hamiltonian considered by us is as follows:

$$H_0 = \sum_i \epsilon_i n_{i\sigma} - t \sum_i (c_{i\sigma}^\dagger c_{i+\delta_{i\sigma}} + h.c.)$$

$$+ t' \sum_i (c_{i\sigma}^\dagger c_{i+\delta_{i\sigma}} + h.c.),$$

$$H_{int} = U \sum_i n_{i\uparrow} n_{i\downarrow},$$

$$H = H_0 + H_{int}. \tag{1}$$

Here $t$ and $t'$ are nearest and next-nearest-neighbour hopping terms, $U$ is the on-site Hubbard interaction, $\epsilon_i$ is the site potential at the $i$-th site, while $c_{i\sigma}^\dagger$, $c_{i\sigma}$, $n_{i\sigma}$ are creation, annihilation operators for the electron of spin $\sigma$, and the number operators for up- and down-spins, respectively, at site $i$.

**Deterministic disorder.** – Deterministic disorder is neither periodic nor fully random and have long-range correlations (correlated disorder). The site potential $\epsilon_i$ is deterministically disordered. It follows a Fibonacci sequence which is generated as $A \rightarrow AB$ and $B \rightarrow A$, where $A$ and $B$ are the two different sites. In our case site $B$ has a higher site potential than site $A$ ($\epsilon_B > \epsilon_A$, $W = \epsilon_B - \epsilon_A$, being the disorder strength). A typical Fibonacci chain in a particular generation looks like: ABAABABAABABAABABAABABAABABA . . . We have used the Fibonacci sequence and generalised the idea of quasi-periodicity in one dimension to two dimensions by essentially wrapping up the one-dimensional Fibonacci sequence over the two-dimensional square lattice. Moreover, the number of lattice sites need not be a Fibonacci number. In our case the $N$ lattice sites picks up the first $N$ entries of the sequence from the left, thus allocating the site potentials. This sort of disorder can also be referred to as correlated disorder.

**Discussion of the numerical method.** – We solve the Hartree-Fock decoupled Hamiltonian with an initial guess (seed) of $n_{i\uparrow}$ and $n_{i\downarrow}$, and solve it self-consistently till the solutions of $n_{i\uparrow}$ and $n_{i\downarrow}$ converge to a difference of less than $10^{-7}$ for every site. We settled up with that initial seed which minimises the ground-state energy. This strict convergence criterion has been employed to ensure that we stay away from local minima while exploring the energy landscape. This is extremely important as we approach the disorder-induced localized phase using a variational approach like Hartree-Fock to treat interactions as our only guiding principle in choosing the ground-state configuration is energetics. In the low and medium disorder regime if we start from the Neel order state as the starting seed, we get the desired convergence very quickly, while in the high disorder regime near the MIT, we have found the desired results starting with a near paramagnetic configuration as the initial seed (PM seed).

*Unrestricted Hartree-Fock.* In UHF theory the Hubbard interaction term is decoupled keeping in the site dependence and thus one obtains modified site potentials for up- and down-spins which read as

$$\epsilon_i^\uparrow = \epsilon_i + U \langle n_{i\uparrow} \rangle; \quad \epsilon_i^\downarrow = \epsilon_i + U \langle n_{i\downarrow} \rangle. \tag{4}$$

This gives us the following Hamiltonian which is decoupled into up- and down-spin parts:

$$H_\sigma = \sum_i \epsilon_i^\sigma n_{i\sigma} - t \sum_i (c_{i\sigma}^\dagger c_{i+\delta_{i\sigma}} + h.c.)$$

$$+ t' \sum_i (c_{i\sigma}^\dagger c_{i+\delta_{i\sigma}} + h.c.), \tag{5}$$

where $\epsilon_i^\sigma$ are now defined by eq. (4).
Calculated quantities. – Once the energy spectrum is obtained the energy gap at half-filling is calculated by the difference between the energy level at half-filling and the one just above it. The expression reads as

\[ E_{\text{gap}} = E_{N/2+1} - E_{N/2}, \]  

(6)

where \( N \) is the number of sites in the 2D lattice. The ground-state energy \( E_g \) is calculated by summing up the single-particle energy states for both spin species up to the Fermi level corresponding to the desired filling. The Fermi level at half-filling is calculated as the mean of the highest filled state and the lowest unoccupied one. For finite-temperature calculations are performed with respect to the Fermi level at half-filling. The single-particle energy states for both spin species up to highest filled state and the lowest unoccupied one are converged values of the occupation numbers of up- and down-spins, respectively, at the \( i \)-th site, then the spin order is defined as

\[ S = \frac{1}{N} \left( \sum_{i, \text{even row}} (-1)^i (n_{i\uparrow} - n_{i\downarrow}) + \sum_{i, \text{odd row}} (-1)^{(i+1)} (n_{i\uparrow} - n_{i\downarrow}) \right). \]  

(7)

For disordered non-interacting systems, the Kubo formula, at any temperature is given by

\[ \sigma(\omega) = \frac{A}{N} \sum_{\alpha, \beta} (n_\alpha - n_\beta) \left| f_{\alpha\beta} \right|^2 \delta(\omega - (\epsilon_\beta - \epsilon_\alpha)) \]  

(8)

with \( A = \pi e^2/\hbar a_0 \), \( a_0 \) being the lattice spacing, and \( n_\alpha = \) Fermi function with energy \( \epsilon_\alpha - \mu \). The \( f_{\alpha\beta} \) are matrix elements of the current operator \( j_{x}\delta = \sum_{s, \sigma} \langle c_{s+1, \sigma} c_{s, \sigma} - c_{s, \sigma} c_{s+1, \sigma} \rangle \), between exact single-particle eigenstates \( |\psi_\alpha\rangle \), \( |\psi_\beta\rangle \), etc., and \( \epsilon_\alpha \), \( \epsilon_\beta \) are the corresponding eigenvalues. In this paper, conductivity/ conductance is expressed in units of \( A = \pi e^2/\hbar a_0 \).

We calculate the “average” conductivity over 3–4 small frequency intervals \( \Delta \omega(\Delta \omega = n\omega_r, n = 1, 2, 3, 4) \), and then differentiate the integrated conductivity to get \( \sigma(\omega) \) at \( \omega = n\omega_r, n = 1, 2, 3. \) These three values are then extrapolated to \( \omega = 0 \) to get \( \sigma_{dc} \). For the sake of simplicity, and keeping all other consistency checks in mind [20], we have taken the value of \( \sigma(\omega_r) \) as the actual value of \( \sigma_{dc} \).

The average of \( \sigma(\omega) \) over the interval \( [0, \omega_r] \) is

\[ \sigma_{int}(\omega_r, \mu, N) = \frac{1}{\omega_r} \int_0^{\omega_r} \sigma(\omega, \mu, N) \, d\omega, \]  

(9)

\( \omega_r \) is set to be sufficiently larger than the average spacing between energy levels, given by \( D/N \), where \( D \) is the full bandwidth for the interacting 2D disordered Hubbard model that we are considering and is simply calculated as \( D = E_N - E_1 \), where \( E_N \) and \( E_1 \) refer to the topmost and lowermost eigenvalues. For \( N = 1600, \omega_r = 0.05 \).

| Size     | \( A \) | \( B \) | \( A/B \) |
|----------|--------|--------|---------|
| 40 \( \times \) 40 | 989     | 611    | 1.608   |
| 40 \( \times \) 14 | 346     | 214    | 1.616   |
| 40 \( \times \) 10 | 247     | 153    | 1.614   |
| 40 \( \times \) 6  | 148     | 92     | 1.608   |

Table 1: Number of \( A \) and \( B \) sites for different system sizes.

![Fig. 1: (Colour on-line) (a) Effect of reducing \( n_y \) on the gap at half-filling. For \( t' = 0.2 \), the gap is zero till \( U \leq 2.1 \). \( U \) is unchanged all the way down to 40 \( \times \) 14 below which \( U \) starts decreasing slowly at first, and below 40 \( \times \) 8, it shows a steep fall, as the quasi-1D effect sets in and electronic motion gets constrained. (b) Fall in the gap at half-filling with increasing \( t' \). The plot is for \( W = 0, \ U = 3 \) and \( N = 40 \times 40 \).](image)

In the discussion below, all length scales are normalized by the lattice parameter \( a \), and we use dimensionless energy parameters \( U, W \) and \( t' \), scaled by the hopping amplitude \( t \)

Fig. 1: Disorder-induced metal in 2D correlated system

Numerical results. – We have calculated the gap at half-filling, charge and spin order, bandwidth, IPR and the \( \sigma_{dc}^x \) of the 2D \( t-t' \) disordered Hubbard model at half-filling as we vary the \( t' \), disorder potential \( W \) and also reduce the dimensionality along the \( y \)-direction. We study the problem for the intermediate disorder strength \( (W < U) \) where the underlying Neel magnetic ordering (due to \( U \)) is not killed and is predominantly present, for a \( 40 \times 40 \) lattice. We have shown here our calculations for system sizes \( 40 \times 40, 40 \times 14, 40 \times 10 \) and \( 40 \times 6 \). We have tabulated the number of \( A \) and \( B \) sites and the ratio \( A/B \) for the different sizes which are given in table 1.

In fig. 1(a) we study the effect of size reduction along the \( y \)-axis. We show that for \( t' = 0.2 \), \( E_{\text{gap}} \) is zero till a critical
of there, allowing some double occupancies on the lower spin species will try to avoid the sitewith higher energy, thereby allowing some double occupancies on the lower-spin energy. The gap decreases rather slowly for low values of $\Delta$ and finally falls sharply at a certain $W = W_c$, for fixed system size. We find that for a fixed disorder, though $E_g$ increases as we reduce $n_y$, the rate of fall in $E_g$ increases with increase in disorder as we reduce $n_y$, highlighting that effect of disorder is more pronounced than the effect of Hubbard $U$ as one reduces $n_y$. We will see the effect of this in our Kubo conductivity results.

The corresponding spin order plot also follows a similar trend (fig. 2(b)). However, the reduction in this case is more gradual than the gap at half-filling. This is because the system prefers to retain the antiferromagnetic configuration to gain maximum kinetic energy due to hopping, till a critical value of $W$ up to which $U$ is effective, and beyond which the spin order reduces very rapidly. We find this critical $W \approx 1.75$, at which point the Hubbard gap roughly diminishes from first to second place of decimal. The reduction in magnetic ordering is much slower than the gap at half-filling, and there is significant residual magnetic ordering ($S \approx 0.25$) when $\Delta$ has already gone to zero.

Figure 3(a) shows the plot of the dc conductivity ($\sigma_0$) against the disorder strength $W$ at $T = 0$ for $U = 3$, 3.2 and 3.4, which is well in the antiferromagnetic regime even for $t' = 0.2$. Due to interplay between correlation and disorder, $\sigma_0$ increases from zero at a critical value of $W = W_c$, whose value increases with $U$. Thus it takes higher values of disorder to form doubly occupied sites as one increases $U$ at half-filling. This plot cannot be extrapolated indefinitely on the lower side as $U$ has to be greater than $U_c$.

Figure 3(b) shows the plot of Kubo conductivity at zero temperature as we change $t'$ for the disordered problem. It is found that as we increase $t'$ from zero it takes a lower value of disorder to first generate a non-zero value of the Kubo conductivity and then render the system metallic.

Figure 3(c) shows the plot of the $T = 0$ $\sigma_0$ against $W$ as we reduce the system size along the $y$-direction, thus going over to a quasi-1D system. We need a lower disorder value to annul the effect of $U$, as we lower the dimensionality again highlighting the fact that the effect of disorder, for a fixed value of $U$ becomes more robust as we decrease the dimensionality from 2D to quasi-1D. The faster rate of depletion of the Hubbard gap $\Delta$ as we reduce the dimensionality, as seen in fig. 2(a), is thus connected to the $\sigma_0-W$ curves for different $n_y$ in this way.

Figure 3(d) show the plots of $\sigma_0$ against temperature for $U = 3.2$ and shows an insulator-to-metal transition with increasing $W$ at low temperatures. Our calculation shows a finite conductivity at zero temperature, which is
consistent with experimental results. The region $kT < 0.02$ corresponds to the diffusive sector while for $kT > 0.05$ we are in the ballistic regime. $W_c$ corresponds to the value of $W$ for which $\sigma_0$ at $T = 0$ becomes non-zero and slowly starts to increase, while at $W = W_m$ the system becomes a metal as the Hubbard gap is completely killed by the disorder. In between there is a narrow range of $W$ within which $\sigma_0$ starts increasing from zero, but the system is still however not a metal. Further increasing $W$, we enter a metallic regime where the rate of fall in conductivity with temperature decreases. This indicates that it is a highly disordered metallic phase (dirty metal). The ground state of the highly disordered insulator is extremely difficult to obtain within Hartree-Fock, which takes a very long time to converge to the required precision. Even when it does, there is a possibility of the system getting stuck in one of the many local minima and not being able to access the true ground state. We therefore venture up to the point where there are no convergence problems (the system is metallic).

Though the effect of $U$ becomes stronger, with the Hubbard gap becoming larger as we decrease the dimensionality of the system, it is clear that the disorder effect surpasses the effect of $U$ as one lowers the dimension, as is evident from figs. 3(d)–(f). Figures 3(d)–(f) show the finite-temperature plots of $\sigma_0$ for different parametric values of $W$ for $n_y = 40, 14$ and 6, respectively. We again observe the general behaviour that the dc conductivity of an insulator/metal rises/falls with increasing temperature in the low-temperature regime. However, the onset of the metallic phase occurs for lower values of $W$ as we reduce the dimensionality.

We see that as we heat the system, the system goes from a low-temperature metallic phase to a high-temperature insulator phase. This effect is further seen to go away as we reduce the dimensionality.

Figures 4(a), (b) show the plot of the density of states (DOS) for a fixed value of $U = 3$ for $n_y = 40$ and 6, respectively, highlighting how disorder closes the gap when we reach $W_m$. However, the gap closes for a lower value of $W$ as we decrease $n_y$ again emphasising the increased effectiveness of disorder as we reduce the dimensionality. We compare our result with the work done in the first reference of [9]. We observe from their LDOS plot that the MIT for the random disordered 2D Hubbard model occurs roughly at $W = 2.7$ for $U = 1.25$. In our work for the 2D $t - t'$ (for $t' = 0.2$) deterministically disordered Hubbard model the MIT occurs at $W = 1.85$ for $U = 3$ (fig. 4(a)). Figures 4(c), (d) show the IPR and the bandwidth of the system for a fixed value of $U > U_c$, as we increase the disorder strength. Figure 4(d) clearly shows that for the interacting case the effect of disorder on the bandwidth is quite non-monotonic and non-trivial. The bandwidth increases for very weak (low) disorder, then it stops growing and surprisingly starts decreasing with increasing disorder. This is the regime where the states at the Fermi energy have already become delocalized, as can be seen from fig. 4(c) (the IPR curve also behaves non-monotonically). In this regime more and more states are introduced in the gap region. Since the total number of levels are fixed, the bandwidth decreases.

The localization in the Hartree-Fock single-particle excitations for $t' = 0$, as reflected in the IPR peak below $W = W_m$ is rapidly eroded as we increase $t'$. This is seen in the rapidly falling peak structure in the IPR curve as we increase $t'$. Thus with increasing $t'$, there is a subtle transition in the nature of the wave functions itself (localized to delocalized) as the metallic phase sets in.

Figure 5(a) represents the plot of the gap at half-filling against disorder, for three different realizations of the Fibonacci sequence. One can see from these plots that the results remain almost invariant as we change the realization. The results shown here are for $U = 3$ and $t' = 0.2$ for a $40 \times 40$ system.

Figure 5(b) shows our results of the dc conductivity at zero temperature as a function of disorder, in the range where the dc conductivity just starts to pick up from zero. We have shown the results for 2 system sizes, namely $32 \times 32$ and $40 \times 40$. It is clearly observed that the critical value of disorder $W_c$, where the dc conductivity picks...
up from zero, is almost the same. This shows that the finite-size effects are already quite small by the time we reach the $32 \times 32$ system size.

We believe that our simulation results provides useful and direct insight into the competition between correlations and disorder, which has been introduced in a simplified (deterministic) manner and is capable of capturing all the subtleties involved. It gives a good estimate of the Kubo conductivity as one goes from 2D to quasi-1D systems in the presence of disorder and correlation and indicates the emergence of a metallic phase. As we tune the disorder to a very high value, the system becomes a metallic glass (highly disordered metal).

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