A correlated Anderson insulator on the honeycomb lattice

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We study the effect of disorder on the semimetal – Mott insulator transition in the half-filled repulsive Hubbard model on a honeycomb lattice, a system that features vanishing density of states at the Fermi level. Using the determinant quantum Monte Carlo method, we characterize various phases in terms of the bulk-limit antiferromagnetic (AF) order parameter, compressibility, and temperature-dependent DC conductivity. In the clean limit, our data are consistent with previous results showing a single quantum critical point separating the semi-metallic and AF Mott insulating phases. With the presence of randomness, a non-magnetic disordered insulating phase emerges. Inside this disordered insulator phase, there is a crossover from a gapless Anderson-like insulator to a gapped Mott-like insulator.

Introduction — The study of the metal-insulator transition (MIT) has a long history. A classification of metals and insulators based on band theory was established in the early years of quantum mechanics.1 After the discovery of transition-metal oxides2 (e.g., NiO) where the d-orbitals are partially filled, it was realized that the band theory is insufficient and interactions between electrons should be taken into account.3 The resulting Mott insulator has become a paradigm for the physics of MIT in strongly correlated systems.4 While non-interacting systems typically show metallic properties, Anderson, in a seminal work, showed that, in the presence of strong disorder, electron eigenstates can be localized and fall off exponentially with distance due to coherent backscattering.5 This phenomenon has been verified by experiments,6, 7 and the Anderson localization mechanism provides a third route to the metal-insulator transition.

In real materials, since disorder and interactions are both present, understanding the interplay of the two sources of localization and their combined impact on the MIT has become a focus of research8–11. On the theory side, progress has been made by treating correlations at the Hartree-Fock level12, 13 and via diagrammatic12 and perturbative renormalization group calculations13–15. However, questions remain when both disorder and interactions are strong,4 in which case they should be treated on the same non-perturbative footing. New theoretical concepts challenging existing paradigms have also emerged.16 For experiments, recent progress in controlling disorder and interaction parameters precisely is allowing detailed comparison with theoretical predictions.17

In order to shed light on the physics of disordered interacting fermions, we study the half-filled repulsive Hubbard model on the honeycomb lattice with off-diagonal disorder using the numerically exact determinant quantum Monte Carlo (DQMC) method.18 While most previous DQMC and other numerical studies have examined the interplay of disorder and correlations in ‘conventional’ geometries with a finite density of states at the Fermi level EF, our study addresses the interesting issue of how this interplay manifests within a Dirac-like dispersion near EF.

We focus on electronic, transport, as well as magnetic properties of the system, and highlight the phases that emerge from the competition of disorder and interaction. The key results are summarized in the phase diagram Fig. 1: Whereas in the absence of disorder the metal-insulator and AF phase transitions coincide at a common critical coupling,19 the addition of disorder reduces the threshold coupling strength for insulating behavior, while increasing that for AF order, thereby opening up an intervening insulating phase with no long range magnetic order.

Model and numerical method — We consider the bond disordered Hubbard Hamiltonian

\[
\hat{H} = - \sum_{\langle i,j \rangle \sigma} t_{ij} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma}) - \mu \sum_{i \sigma} \hat{n}_{i\sigma} + U \sum_{i} \left( \hat{n}_{i\uparrow} - \frac{1}{2} \right) \left( \hat{n}_{i\downarrow} - \frac{1}{2} \right).
\]

\(\hat{c}_{i\sigma}^\dagger (\hat{c}_{i\sigma})\) are the spin-σ electron creation (annihilation) operator at site \(i\). \(U > 0\) is the on-site Coulomb repulsion. \(t_{ij}\) is the hopping integral between two near-neighbor sites \(i\) and \(j\). The chemical potential \(\mu\) determines the average density of the system. \(\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}\) is the number operator. Disorder is introduced through the hopping matrix elements \(t_{ij}\) chosen uniformly \(P(t_{ij}) = 1/\Delta\) for \(t_{ij} \in [t-\Delta/2,t+\Delta/2]\), and zero otherwise. Here \(\Delta\) represents a measure of disorder strength, and \(t = 1\) sets the scale of energy. In this work, we focus on the case \(\mu = 0\) where the system is half-filled and the Hamiltonian remains particle-hole symmetric20 even in the presence of disorder.

The model is solved numerically using the finite-temperature DQMC method.18 In this approach,
FIG. 1. Phase diagram of the disordered Hubbard model on the honeycomb lattice at half-filling. ∆ labels the disorder strength and U represents the local Coulomb repulsion. The metallic phase boundary is determined by the temperature dependence of the conductivity σ_{dc} and the region of long range AF order by finite size scaling of the AF structure factor. Although these transitions coincide in the clean limit, for non-zero ∆ an intermediate, magnetically disordered, insulator phase intervenes. This phase itself contains a crossover from Anderson-like to Mott-like behavior based on the behavior of the compressibility κ. The inset shows the geometry of the L = 6 honeycomb lattice.

the interacting Hamiltonian is mapped onto free fermions coupled to space and imaginary-time dependent Ising fields. The integration over all possible field configurations is carried out by Monte Carlo sampling. This approach allows us to compute static and dynamic (in imaginary time) observables at a given temperature T. Because of the particle-hole symmetry, the system is sign-problem free and the simulation can be performed at large enough β = 1/T to converge to the ground state. Data reported are obtained on 2 × L^2 (L = 3, 6, 9, 12, and 15) honeycomb lattices with periodic boundary conditions. The inset of Fig. 1 shows the L = 6 geometry. In the presence of disorder, results are averaged over 20 disorder realizations; the error bars reflect both statistical and disorder sampling fluctuations.

We use the temperature-dependent DC conductivity σ_{dc}(T) to characterize the metal-insulator transition. According to the fluctuation-dissipation theorem, σ_{dc}(T) is related to the zero frequency limit of the current-current correlation function. While real-frequency quantities can be obtained through analytic continuation of imaginary-time QMC data, we implement an approximation[21] that has been extensively benchmarked in previous work,[20–22]

\[ \sigma_{dc}(T) = \frac{\beta^2}{\pi} \Lambda_{xx}(q = 0, \tau = \beta/2). \]  

Here \( \Lambda_{xx}(q, \tau) = \langle \hat{j}_x(q, \tau) \hat{j}_x(-q, 0) \rangle \), where \( \hat{j}_x(q, \tau) \) is the Fourier transform of the time-dependent current operator \( \hat{j}_x(r, \tau) \) in the x-direction. Eq. (2) provides a good approximation if the temperature is lower than the energy scale at which there is significant structure in the density of states.[21] Checks of the applicability to the present problem will be discussed below.

In addition to transport properties, we also examine the charge excitation gap and the antiferromagnetic (AF) structure factor at wave vector Q = Γ,

\[ S_{AF} = \frac{1}{N_c} \sum_r \left( \langle \hat{S}_{r,A} \rangle - \langle \hat{S}_{r,B} \rangle \right)^2. \]  

FIG. 2. (a) DC conductivity σ_{dc} versus temperature T in the clean limit ∆ = 0 computed at various coupling strengths for the L = 12 honeycomb lattice. (b) Scaling behavior of the normalized AF spin structure factor S_{AF}/N_c at corresponding U values. Solid and dashed lines represent third-order polynomial fits to the data.

Here N_c is the number of unit cells. \( \hat{S}_{r,A} \) and \( \hat{S}_{r,B} \) are total spin operators for sublattices A and B of the bipartite honeycomb lattice.

Results and discussion — We first demonstrate results for the disorder-free system. Fig. 2(a) shows σ_{dc}(T) measured on the L = 12 lattice across several U values. As shown by the figure, the conductivity increases with decreasing temperature for T \( \lesssim 0.25 \), regardless of U. Upon further lowering T, the data indicate that dσ_{dc}/dT < 0 and σ_{dc} diverges as T → 0 for U \( \lesssim 3.8 \). This low temperature behavior is an indication that the system is metallic.[20] For U \( \gtrsim 4.0 \), the low-T behavior of σ_{dc} points to an insulating state: dσ_{dc}/dT > 0 and the conductivity vanishes as T → 0. Fig. 2(b) shows finite-size scaling of the normalized AF spin structure factor S_{AF}/N_c. By extrapolating the data to the thermodynamic limit, it appears that the onset of AF order is 3.8 \( \lesssim U \lesssim 4.0 \). These findings suggest that there is a transition from paramagnetic semimetal to an AF insulator at 3.8 \( \lesssim U \lesssim 4.0 \), a result that is consistent with previous finding of a quantum critical point U_c \( \sim 3.85 \) which separates the semimetallic and Mott insulating phases.[23]

Next we move to the disordered case. In disordered graphene and without interactions, electronic transport has been extensively investigated.[24–32] In order to
establish the phase diagram for interacting electrons, we first examine transport properties. Fig. 3 shows \( \sigma_{dc}(T) \) computed in a range of disorder strengths at four representative coupling strengths across the \( \Delta = 0 \) quantum critical point \( U_c \).

Fig. 3(a) \( \sim \) (c) examine the semi-metallic region \( U \lesssim U_c \). The low temperature behavior of \( \sigma_{dc} \) indicates that there is a change from metallic to insulating behavior with increasing disorder \( \Delta \): For \( U = 1, T \lesssim 0.14, \) and \( \Delta = 0.5 \), the conductivity is metallic. \( \sigma_{dc}(T) \) grows with decreasing temperature: \( d\sigma_{dc}/dT < 0 \). At \( \Delta = 2.5 \), on the other hand, \( \sigma_{dc}(T) \) decreases as the temperature is lowered, and approaches zero as \( T \to 0 \), suggesting insulating behavior. The crossover from a metallic to an insulating state takes place at \( \Delta_c \sim 1.7 \) for \( U = 1 \). By raising the interaction strength, the crossover sets in at a reduced disorder strength: \( \Delta_c \sim 1.5 \) and \( 1.0 \) for \( U = 2 \) and \( 3 \) respectively. The critical disorder strength reduces to \( \Delta = 0 \) at roughly \( U \sim 3.9 \) where the system enters the correlation-induced Mott-Slater insulator regime. The conductivity data exhibit an insulating response \( d\sigma_{dc}/dT > 0 \) and vanish as \( T \to 0 \) for any \( \Delta \). See Fig. 3(d).

The “metallic” region of the phase diagram Fig. 1 summarizes these transport results. As previously found for the quarter-filled square lattice Hubbard model [20] with bond disorder, our DQMC calculations suggest that the onsite Hubbard repulsion can introduce metallic behavior in the 2D honeycomb lattice even at the Dirac point where the density of states \( N(E_F) = 0 \) for \( U = 0 \).

Another electronic property of interest is the single-particle gap. Without disorder, the half-filled Hubbard model on the honeycomb lattice exhibits a charge (Mott) excitation gap for \( U > U_c \).[19, 23] The non-interacting Anderson insulator, on the other hand, is gapless at the Fermi level (in the thermodynamic limit).[5, 33] Although the gap is not an order parameter associated with symmetry breaking, it nevertheless can be used to establish the existence of the Mott insulator. In general the single-particle gap can be extracted from the density of states \( N(\omega) \). Here we extract information of the gap by examining the behavior of charge compressibility \( \kappa = -d\langle \hat{n}(\mu) \rangle / d\mu \) at the Fermi level \( \mu = 0 \), where \( \langle \hat{n}(\mu) \rangle \) is the average density at the chemical potential \( \mu \). Using this formula, the compressibility can be deduced from local densities which are easy to compute within DQMC. A finite \( \kappa \) indicates that the system is compressible, i.e., gapless.

In Fig. 4, the compressibility \( \kappa \) is plotted as a function of \( \mu \) for various disorder strength \( \Delta \) and local repulsion \( U \). Each data point is obtained by averaging results from 20 disorder realizations on the \( L = 12 \) lattice. Tuning the chemical potential away from \( \mu = 0 \) breaks particle-hole symmetry and leads to a sign problem. However, the problem is less severe in the presence of disorder[20, 34], and we are still able to extract accurate local density results. In the weak disorder region \( \Delta \ll U \), Fig. 4

![FIG. 3. Temperature dependence of the DC conductivity \( \sigma_{dc} \) measured on the \( L = 12 \) lattice with disorder. Panels correspond to different couplings: (a) \( U = 1.0 \), (b) \( U = 2.0 \), (c) \( U = 3.0 \), and (d) \( U = 4.0 \). In each figure, lines are guides to the eyes. Metallic and insulating behaviors are indicated by solid and dashed lines respectively.](image)

![FIG. 4. Charge compressibility \( \kappa \) versus chemical potential \( \mu \) at four representative disorder strengths. A finite \( \kappa \) means the system is compressible, i.e., gapless; while \( \kappa = 0 \) implies an gapped incompressible state. The criterion \( \kappa \lesssim 0.04 \) is adopted to distinguish the gapped and gapless states.](image)
properties of the disordered Hubbard model on the honeycomb lattice using DQMC simulations. In the absence of disorder, we verified this geometry has a quantum critical point at $3.8 \lesssim U \lesssim 4.0$ separating the semimetallic and Mott insulating phases, a result that is consistent with previous (higher resolution) findings.[19] In the $U = 0$ limit, the semimetallic phase is driven into an gapless Anderson insulating state. By switching on the local Coulomb repulsion $U$, the critical disorder strength for the metal-insulator transition decreases, indicating that the presence of both disorder and interactions becomes more effective in localizing electrons. At $U \gtrsim 4.0$, electrons are localized by strong Coulomb correlations in the absence of disorder: the AF transition and metal-insulator transitions coincide in the clean limit. Our key finding is that adding random bond disorder reduces the threshold $U$ required for insulating behavior, but increases the $U$ required for AF. Thus the magnetic and metal-insulator transitions no longer coincide, and a disordered insulating phase intervenes. Furthermore, within this disordered insulator, there is a crossover from an Anderson-like region where the compressibility $\kappa \neq 0$ to a Mott-like region where $\kappa = 0$.

Already, certain unique features of the interplay of disorder and interactions in models with a Dirac dispersion have been noted, including the possibility that disorder might enhance superconductivity for attractive interactions.[36] Our work expands this understanding to repulsive interactions, where similar anomalous effects such as an enhancement of Néel temperature by randomness are known[37] for conventional geometries. Moreover, the reduced critical coupling strength for the metal-insulating transition in the presence of disorder might be relevant for practical applications of honeycomb structural materials such as a low power Mott transistor.

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Summary — We have studied electronic and magnetic

indicates that $\kappa$ vanishes near $\mu = 0$ for $4.0 \lesssim U \lesssim 5.0$, i.e., the system becomes incompressible and acquires an energy gap for charge excitations. For strong disorder $\Delta \gtrsim U$, it is clear that the compressibility tends to become zero at a weaker coupling strength $3.0 \lesssim U \lesssim 4.0$. We are not able to pin-point the exact location where the gap opens at each disorder strength due to the sparse data. Nonetheless, an estimated cross-over separating the gapless and gapped regions, using the criterion $\kappa \lesssim 0.04$, is presented in Fig. 1.

We now consider magnetic properties and the effect of bond disorder on long-range AF, generalizing the discussion of Fig. 2(b). Fig. 5 summarizes finite-size scaling studies of the AF structure factor on lattices up to $L = 15$ (450 sites). For $\Delta = 0$, it is known that the ground state of the system is an antiferromagnet for $U > U_c \sim 3.85$. For $U = 1, 2$, where there is no AF order even in the clean limit, bond disorder has almost no effect on $S_{AF}$ for sufficiently large lattices (Figs. 5(a) and (b)). On the other hand, above the clean limit $U_c$, $\Delta > 0$ suppresses $S_{AF}$ and increases the interaction strength needed for long range AF order to appear. The mechanism for the suppression of AF is the tendency towards singlet formation on pairs of sites with large $t_{ij}$[35]. Based on the extrapolated behavior of $S_{AF}/N_c$ in the thermodynamic limit, a magnetic phase boundary for the paramagnetic-antiferromagnetic transition can be established for nonzero $\Delta$, and is shown in Fig. 1.

FIG. 5. Finite-size scaling studies of the AF spin structure factor. In (c) and (d), antiferromagnetic spin structure factor, $S_{AF}$, is plotted as a function of $1/L$ for various values of disorder strength at $U = 4.5t$ (c) $U = 5.0t$ (d); Lines are cubic polynomial (in $1/L$) fits to the data.
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