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(Article begins on next page)

Local moments and magnetic order in the two-dimensional Anderson-Mott transition

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We study the role of electronic correlation in a disordered two-dimensional model by using a variational wave function that can interpolate between Anderson and Mott insulators. Within this approach, the Anderson-Mott transition can be described both in the paramagnetic and in the magnetic sectors. In the latter case, we find evidence for the formation of local magnetic moments that order before the Mott transition. The charge gap opening in the Mott insulator is accompanied by the vanishing of the $\lim_{q \rightarrow 0} \langle n_q \rangle \langle n_{-q} \rangle$ (the bar denoting the impurity average), which is related to the compressibility fluctuations. The role of a frustrating (second-neighbor) hopping is also discussed, with a particular emphasis to the formation of metastable spin-glass states.

PACS numbers:

The combined action of electron-electron interaction and disorder is known to heavily influence the physical behavior of electron systems. [1] Recently, the observation of metallic behavior in high-mobility two-dimensional electron-gas devices [2] has opened new perspectives in this subject, suggesting the possibility that a metallic behavior could be stabilized by a strong electron-electron interaction in two dimensions, in spite of the standard scaling theory of Anderson localization. [3, 4] Such a proposal was first put forward theoretically by means of a weak-coupling renormalization group approach within a Fermi-liquid description, [5] and later developed along similar directions. [6, 7] A common feature of the above renormalization-group calculations is the crucial role played by the spin fluctuations that grow large as the renormalization group procedure is iterated. This tendency, which has been interpreted as signaling the emergence of local moments, suggests that electron-electron correlations become effectively very strong that, in turn, makes doubtful the validity of a Fermi liquid description. [8, 9]

Apart from the debated issue of a metal-insulator transition in two-dimensional high-mobility devices, [10, 11, 12, 13] there are less controversial systems where the role of strong correlations concomitantly with disorder is well testified. Particularly emblematic is the case of Si:P and Si:B, [14, 15] which are three-dimensional materials that show a *bona fide* metal-insulator transition. Here, the randomly distributed impurities form a very narrow band within the semiconducting gap. Since the local Coulomb repulsion is sizable compared to the width of the impurity band, this system is particularly suitable to investigate the interplay between disorder and interaction. Indeed, clear signatures of local magnetic moments are found in several thermodynamic quantities. [16, 17, 18, 19] Theoretically, the interplay of disorder and interaction is a very difficult question. Any approach based on a single-particle description, like unrestricted Hartree-Fock, [20, 21] can uncover the emer-

gence of local moments only if spin-rotational symmetry is explicitly broken, introducing spurious effects due to magnetism that can be dealt with using further approximate schemes. [23, 24] More sophisticated approaches, like those based on dynamical mean-field theory, [25] can in principle manage without magnetism, [26, 27, 28] but they usually miss important spatial correlations.

In this Letter, we will generalize the variational approach that has been successfully used to describe the Mott transition in finite-dimensional clean systems [29, 30, 31]. We will show that, for a half-filled disordered Hubbard model on a square lattice and when the variational wave function is forced to be paramagnetic, the Anderson to Mott insulator transition exists and it is continuous. When magnetism is allowed, we find two successive second order phase transitions: from a compressible paramagnetic Anderson insulator with local moments to a compressible magnetic Anderson insulator and then to an incompressible magnetic Mott insulator. Unlike previous unrestricted Hartree-Fock [21] or Monte Carlo calculations, [22] we do not find any evidence of an intermediate truly metallic behavior.

We consider a half-filled Hubbard model on a square lattice with on-site disorder:

$$\mathcal{H} = \sum_{i,j,\sigma} t_{i,j} c_{i,\sigma}^\dagger c_{j,\sigma} + H.c. + \sum_i (\epsilon_i n_i + U n_{i,\uparrow} n_{i,\downarrow}), \quad (1)$$

where $c_{i,\sigma}^\dagger$ ($c_{i,\sigma}$) creates (destroys) one electron at site i with spin σ , $n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}$, and $n_i = \sum_\sigma n_{i,\sigma}$. ϵ_i are random on-site energies chosen independently at each site and uniformly distributed in $[-D, D]$. $t_{i,j}$ are the hopping parameters that we will consider limited either to nearest-, $t_{ij} = -t$, or to next-nearest-neighbor, $t_{ij} = -t'$, sites. In the calculations we will consider 45 degree rotated clusters with $N = 2n^2$ sites, n being an odd integer, and periodic boundary conditions, so that the non-interacting ground state is always non-degenerate at half filling.

Following the approach developed for clean systems, [29] we define a variational wave function containing a Gutzwiller and a long-range Jastrow factor that apply to an uncorrelated state:

$$|\Psi\rangle = \mathcal{P}_G \mathcal{J} |\Phi_0\rangle, \quad (2)$$

where $|\Phi_0\rangle$ is the ground state of a non-interacting Hamiltonian with the same hopping parameters as in Eq. (1) but with variational spin-dependent on-site energies $\tilde{\epsilon}_{i\sigma}$ to be determined by minimizing the total energy. A paramagnetic wave function is obtained by forcing $\tilde{\epsilon}_{i,\uparrow} = \tilde{\epsilon}_{i,\downarrow}$, while, to discuss magnetism, we allow the wave function to break spin-rotational symmetry with $\tilde{\epsilon}_{i,\uparrow} \neq \tilde{\epsilon}_{i,\downarrow}$. $\mathcal{P}_G = \exp[\sum_i g_i n_i^2]$ is a Gutzwiller correlator that depends upon the *site-dependent* parameters g_i 's, while $\mathcal{J} = \exp[1/2 \sum_{i \neq j} v_{i,j} (n_i - 1)(n_j - 1)]$ is a Jastrow factor. The latter one spatially correlates valence fluctuations, $\delta n_i = \langle n_i - 1 \rangle \neq 0$, on different sites, binding those with $\delta n_i \delta n_j < 0$ and unbinding those with $\delta n_i \delta n_j > 0$. This fact has been shown to be crucial to describe a Mott transition in clean systems. [29, 30] We shall assume that v_{ij} is translationally invariant, which makes the numerical calculations feasible but neglects any clustering effects. All the parameters contained in the variational wave function $|\Psi\rangle$, i.e., $\tilde{\epsilon}_{i,\sigma}$, g_i , and $v_{i,j}$, [32] are optimized to minimize the variational energy by using the Monte Carlo technique of Ref. [33].

As discussed in Refs. [29, 30] for clean systems, it is possible to discriminate variationally metals from Mott insulators by looking to the equal-time density-density structure factor $N_q = \langle \Psi | n_q n_{-q} | \Psi \rangle / \langle \Psi | \Psi \rangle$, where n_q is the Fourier transform of the electron density n_i . Indeed, $N_q \sim |q|$ implies the existence of gapless modes, while $N_q \sim |q|^2$ indicates that charge excitations are gapped. Moreover, there is a tight connection between the long-wave-length behavior of N_q and the Fourier transform of the Jastrow factor v_q , namely $v_q \sim 1/|q|$ for a metal and $v_q \sim 1/|q|^2$ for an insulator. [29, 30] This distinction should equally work in (1) after disorder average. However, particular care must be taken to interpret N_q in a disordered system, where the structure factor includes a *disconnected* term, $N_q^{\text{disc}} = \overline{\langle n_q \rangle \langle n_{-q} \rangle}$ (where the quantum average is taken at fixed disorder configuration and the overbar indicates the disorder average) as well as a connected one, i.e., $N_q^{\text{conn}} = N_q - N_q^{\text{disc}}$. For a clean system, the disconnected term gives rise to the elastic scattering peaks at q equal to the reciprocal lattice vectors, the Bragg reflections. On the contrary, in the presence of disorder N_q^{disc} is finite for any finite momentum q . [34] The diagrammatic representation of N_q^{disc} is shown in Fig. 1 and one can realize that, for $q \rightarrow 0$, it reduces to the electron compressibility fluctuations. For non-interacting electrons, N_q^{disc} is finite for $q \rightarrow 0$, whereas $N_q^{\text{conn}} \sim |q|$, indicating the absence of a gap in the spectrum of charge-density fluctuations. [34]

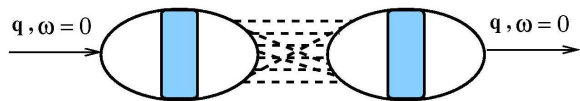


FIG. 1: (Color online) Density-density fluctuations $N_q^{\text{disc}} = \overline{\langle n_q \rangle \langle n_{-q} \rangle}$. Dotted lines denote impurity averages, and the squares indicate vertex corrections that include both interaction and impurity insertions. Continuous lines are fully corrected Green's functions.

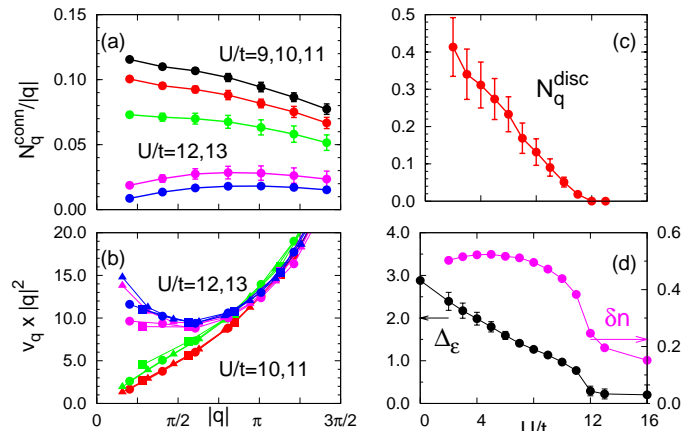


FIG. 2: (Color online) (a) Connected term of the density-density correlation function N_q^{conn} divided by $|q|$. (b) Jastrow parameters v_q multiplied by $|q|^2$. (c) Disconnected term of the density-density correlation function N_q^{disc} as a function of U . (d) Fluctuations of the on-site variational energies Δ_ϵ and of the local densities. All calculations have been done for $D/t = 5$.

We start our analysis with the case of nearest-neighbor hopping only by using a paramagnetic wave function, namely imposing $\tilde{\epsilon}_{i,\uparrow} = \tilde{\epsilon}_{i,\downarrow}$. In Fig. 2, we show the variational N_q^{conn} and the Fourier transform of the optimized Jastrow potential v_q for different values of the interaction U and $D/t = 5$ (we take such a large value of D in order to have a localization length that, at $U = 0$, is smaller than the numerically accessible system sizes). A clear change in the behavior of these quantities is observed at $U_c^{\text{Mott}}/t = 11.5 \pm 0.5$. For small values of the electron interaction, $N_q^{\text{conn}} \sim |q|$ and $v_q \sim 1/|q|$, whereas $N_q^{\text{conn}} \sim |q|^2$ and $v_q \sim 1/|q|^2$ in the strong-coupling regime. The latter behavior is symptomatic of the presence of a charge gap hence of a Mott insulating behavior. [29] We notice that, for the clean case $D = 0$ and within the same approach, a metal-insulator transition at $U_c^{\text{Mott}} = 8.5 \pm 0.5$ was found, [35] indicating that disorder competes with U and pushes the Mott transition to higher values of U/t . It should be emphasized that, with respect to the clean system, for $U < U_c^{\text{Mott}}$, $N_q^{\text{conn}} \sim |q|$ is not associated to a metallic behavior but only to a gapless spectrum, also characteristic of an An-

derson insulator. Remarkably, we find that the Mott and Anderson insulators can also be discriminated through the behavior of the $\lim_{q \rightarrow 0} N_q^{\text{disc}}$. In Fig. 2 we plot this quantity for different values of U , demonstrating that it is finite in the Anderson insulator, whereas it vanishes in the Mott phase. This identifies a simple and variationally accessible order parameter for the Anderson-Mott transition.

Even though within this approach we cannot access dynamical quantities like DC conductivity, hence we can not address the question of a possible stabilization of a conducting phase with moderate Coulomb repulsion, [22] we note that the linear slope of N_q^{conn} has a non-monotonic behavior as a function of U , showing a peak for $U/t \sim 7$ that indicates an accumulation of low energy states around the Fermi energy. The same qualitative behavior is also present in the fluctuations of the local densities, $\delta n^2 = 1/N \sum_i (\langle n_i^2 \rangle - \langle n_i \rangle^2)$. Though the single-particle eigenstates of the variational Hamiltonian may have a very long localization length, because of the suppression of the effective on site disorder $\tilde{\epsilon}_i$, yet this length is still finite in two dimensions hence the many-body wave function $|\Psi\rangle$ always describes an Anderson insulator below the Mott transition. Indeed, as shown in Fig. 2, the fluctuations of the on-site variational disorder $\Delta_\epsilon^2 = 1/N \sum_i \tilde{\epsilon}_i^2 - (1/N \sum_i \tilde{\epsilon}_i)^2$ are always finite, though sizably renormalized by the electron interaction U .

Let us now move to the more interesting case in which we allow magnetism in the variational wave function, which amounts to permit $\tilde{\epsilon}_{i,\uparrow} \neq \tilde{\epsilon}_{i,\downarrow}$. In this case the ground state may acquire a finite *local* magnetization on each site $m_i = n_{i,\uparrow} - n_{i,\downarrow}$. A magnetically ordered phase will have a finite value of the total magnetization $M = 1/N \sum_j e^{iR_j Q} m_j$ for a suitable momentum Q , like for instance $Q = (\pi, \pi)$ for the Néel state. In the presence of disorder, a finite value U_c^{AF} is needed to have long-range antiferromagnetic order. We find that, also in presence of a small t' , $U_c^{\text{AF}} < U_c^{\text{Mott}}$, giving rise to an extended region with antiferromagnetic order and finite compressibility (i.e., a vanishing charge gap). These results are in agreement with previous mean-field calculations. [21, 36, 37] In Fig. 3, we show the results for $t' = 0$ either by fixing $D/t = 5$ and varying U (for which $U_c^{\text{AF}}/t = 6.5 \pm 0.5$ and $U_c^{\text{Mott}}/t = 10.5 \pm 0.5$) or by fixing $U/t = 4$ and changing D (for which $D_c^{\text{AF}}/t = 1 \pm 0.5$ and $D_c^{\text{Mott}}/t = 2.5 \pm 0.5$). We note that the onset of antiferromagnetism is preceded by a magnetically disordered phase (i.e., $M = 0$) in which local moments appear. In Fig. 4, the pattern of the local density $\langle n_i \rangle$ and local magnetization $\langle m_i \rangle$ are shown for a typical realization of disorder. For $U/t = 4$, the ground state is an Anderson insulator with a large number of empty and doubly occupied sites with $m_i \sim 0$. However, some sites have finite magnetization, but they are not spatially correlated hence long-range magnetism is absent. We interpret these magnetic sites as local moments. When the electron

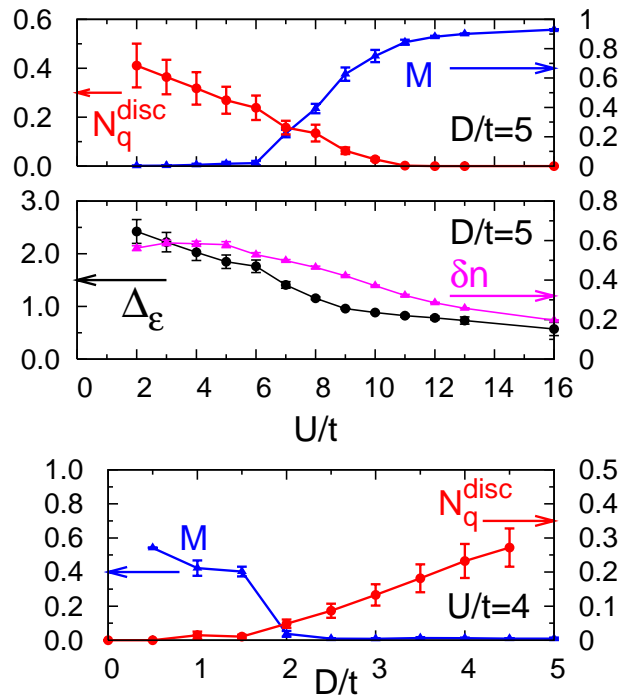


FIG. 3: (Color online) Staggered magnetization M for $Q = (\pi, \pi)$ and compressibility fluctuations N_q^{disc} as a function of U for disorder $D/t = 5$ (upper panel) and as a function of D for $U/t = 4$ (bottom panel). Fluctuations of the on-site variational energies Δ_ϵ and of the local densities (middle panel). Calculations have been done for $N = 98$ and error-bars indicate the average over different realizations of disorder.

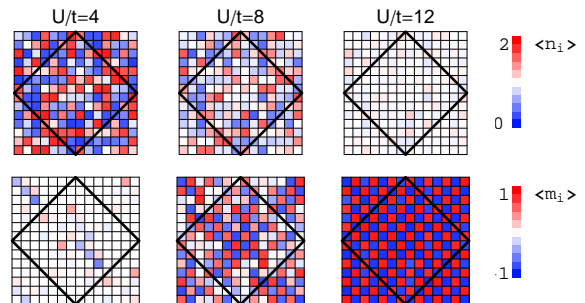


FIG. 4: (Color online) Local density $\langle n_i \rangle$ (upper panels) and local magnetization $\langle m_i \rangle$ (lower panels) for a given disorder realization with $D/t = 5$ and different values of U/t . The black contour shows the elementary cell of the lattice which is repeated to mimic the infinite lattice with periodic boundary conditions.

interaction U increases, the number of magnetic sites increases rapidly and the local moments eventually display the typical staggered pattern of Néel order. Nevertheless, charge excitations are still gapless, with $N_q^{\text{conn}} \sim |q|$. For $U/t = 12$ the system is a gapped insulator with antiferromagnetic order and a vanishing compressibility. Variationally, the charge gap opens by the combined effect

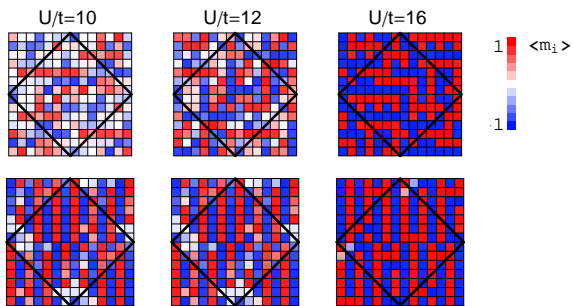


FIG. 5: (Color online) Local magnetization $\langle m_i \rangle$ for the best variational state (lower panels) and for a metastable solution (upper panels) for a given disorder configuration with $D/t = 5$ and $t'/t = 1$.

of the Jastrow correlations, i.e., $v_q \sim 1/|q|^2$, and the finite antiferromagnetic gap in the mean-field Hamiltonian (due to staggered $\tilde{\epsilon}_{i,\sigma}$'s).

In the presence of a large frustrating hopping $t'/t \gtrsim 0.9$ we find evidences of a spin glass behavior. In the large U regime, the optimal wave function displays magnetic long-range order with $Q = (\pi, 0)$ or $(0, \pi)$. However, the energy landscape contains other local minima very close in energy in which most of the sites of the lattice have a net magnetization but an overall vanishing magnetic order, a “glassy” spin patterns, see Fig. 5. These solutions are incompressible, i.e., $N_q^{\text{disc}} \sim 0$ and, therefore, may be viewed as disordered Mott insulators. By decreasing the interaction strength U , these metastable states turn compressible, still having a large number of local moments. However, the actual variational minimum shows, as before, a Mott transition from a Mott to an Anderson insulator, both magnetically ordered, followed, at lower U , by a further transition into a paramagnetic Anderson insulator. The only role of t' is to shrink the region in which a magnetic Anderson insulator is stable.

In conclusion, we have shown that a relatively simple variational wave function is able to describe the Anderson-insulator to Mott-insulator transition in two dimensions. In the paramagnetic sector, this phase transition is continuous, in agreement with dynamical mean field theory. [25, 27] When spontaneous spin symmetry breaking is allowed, we find two successive phase transition, the first from a paramagnetic Anderson insulator to a magnetic one, followed by a transition from a magnetic Anderson insulator to a magnetic Mott insulator. Upon increasing frustration, the stability region of the magnetic Anderson insulator decreases. In general, the paramagnetic Anderson insulator develops local magnetic moments, but we do not find any evidence of a truly metallic behavior induced by interaction.

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