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 sector and in the magnetic sector. 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 $\lim_{q\to 0}\overline{\langle n_q\rangle\langle n_{-q}\rangle}$ (the bar denoting the impurity average). The role of a frustrating (second-neighbor) hopping is also discussed, with a particular emphasis to the formation of metastable spin-glass states.

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The combined action of Coulomb repulsion and disorder is known to heavily influence the physics 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] Such a proposal has been put forward theoretically by several weak-coupling renormalization-group approaches.[4] A common feature of the above calculations is the crucial role played by the spin fluctuations that grow large as the renormalization-group procedure is iterated. This tendency has been interpreted as signaling the emergence either of local moments or, in the continuum, of a ferromagnetic instability.[5] In a lattice, the latter one is likely substituted by a magnetic instability at some wave vector determined by the topology of the lattice and the form of the hopping elements.

Apart from the debated issue of a metal-insulator transition in two-dimensional high-mobility devices,[6–8] there are less controversial systems where the role of strong correlations concomitantly with disorder is well testified. Emblematic is the case of Si:P and Si:B,[9] three-dimensional materials that undergo a bona fide metal-insulator transition. Here, the randomly distributed impurities form a 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 for studying the interplay between disorder and interaction. Indeed, clear signatures of local magnetic moments are found in several thermodynamic quantities.[10–13] Theoretically, the interplay of disorder and interaction is a difficult question. Any approach based on single-particle descriptions, such as unrestricted Hartree-Fock,[14,15] can uncover the emergence of local moments only if spin-rotational symmetry is explicitly broken, introducing spurious effects that can be dealt with using further approximate schemes.[16] More sophisticated approaches, such as those based on dynamical mean-field theory,[17] can in principle manage without magnetism,[18–20] but they usually miss important spatial correlations.

Here, we extend the variational approach that has been successfully used to describe the Mott transition in finite-dimensional clean systems.[21] We 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 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[15] or Monte Carlo calculations,[22] we do not find any clear evidence of an intermediate metallic behavior.

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

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

where $c^{\dagger}_{i,\sigma}$ ($c_{i,\sigma}$) creates (destroys) one electron at site i with spin σ, $n_{i,\sigma}=c^{\dagger}_{i,\sigma}c_{i,\sigma}$, and $n_i=\Sigma_\sigma n_{i,\sigma}$. 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° rotated clusters with $N=2n^2$ sites, n being an odd integer, and periodic boundary conditions, so that the noninteracting ground state is always nondegenerate at half filling.

Following the approach developed for clean systems,[21] we define a variational wave function containing Gutzwiller and long-range Jastrow factors that apply to an uncorrelated state:

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

$|\Phi_0\rangle$ is the ground state of a noninteracting 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 assess magnetism, we allow for $\tilde{\epsilon}_{i,\uparrow} \neq \tilde{\epsilon}_{i,\downarrow}$. $\mathcal{P}_G=\exp[\Sigma_i g_i n_i^2]$ is a Gutzwiller correlator that depends on the *site-dependent* parameters g_i's,

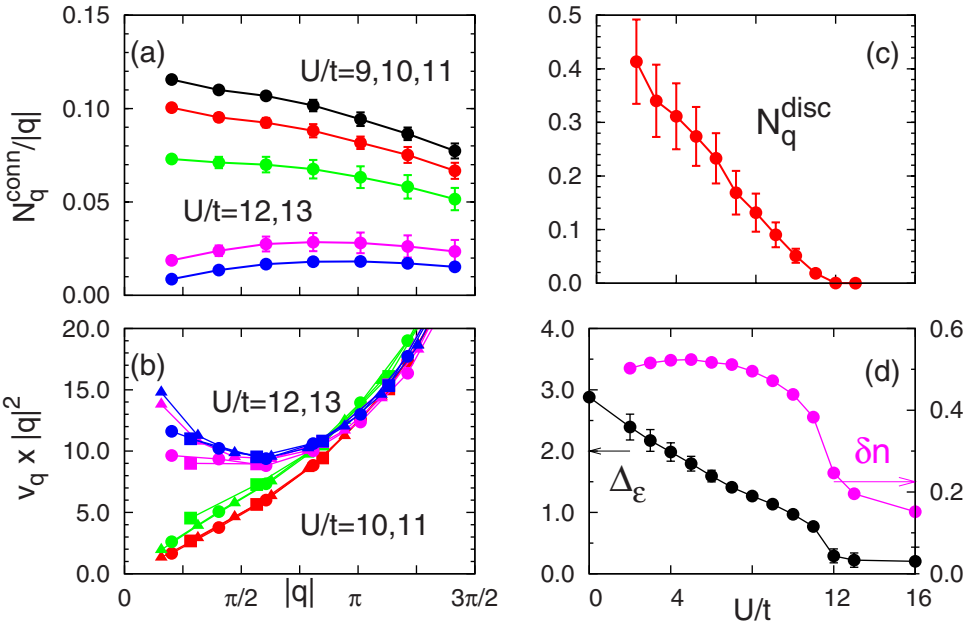

FIG. 1. (Color online) (a) Connected term of the density-density correlation function N_q^{conn} divided by $|q|$. (b) Jastrow parameters v_q multiplied by $|q|^2$. (c) Disconnected term of the density-density correlation function N_q^{disc} as a function of U. (d) Fluctuations of the on-site variational energies Δ_ϵ and of the local densities. All calculations have been done for $D/t=5$.

while $\mathcal{J}=\exp[1/2\Sigma_{i\neq j}v_{i,j}(n_i-1)(n_j-1)]$ is a Jastrow factor. The latter one spatially correlates valence fluctuations, $\delta n_i=n_i-1$, 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.[21] We shall assume that v_{ij} is translationally invariant, which makes the numerical calculations feasible but neglects any clustering effects. All variational parameters, i.e., $\tilde{\epsilon}_{i,\sigma}$, g_i, and $v_{i,j}$, are optimized to minimize the variational energy by the Monte Carlo technique of Ref. 23.

As discussed in Ref. 21, it is possible to discriminate variationally metals from Mott insulators by looking to the equal-time density-density structure factor $N_q=\langle\Psi|n_qn_{-q}|\Psi\rangle/\langle\Psi|\Psi\rangle$, 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 small q 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.[21] This distinction should equally work in Eq. (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, $N_q^{\mathrm{disc}}=\overline{\langle n_q\rangle\langle n_{-q}\rangle}$ (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., $N_q^{\mathrm{conn}}=N_q-N_q^{\mathrm{disc}}$. For a clean system, the disconnected term gives rise to the elastic Bragg peaks. On the contrary, in the presence of weak disorder N_q^{disc} is finite for any finite momentum q, whereas $N_q^{\mathrm{conn}}\sim|q|$, indicating the absence of a gap in the spectrum of charge-density fluctuations.[24]

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. 1, 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 for two reasons. First of all, a reliable calculation requires a localization length that, at least at $U=0$, is within the numerically accessible system sizes. Furthermore, we expect that, should a metallic phase exist, it would intrude between the Anderson insulator and the Mott insulator, hence in the region of parameters where the competition between Anderson and Mott localization phenomena is maximum. Since in the clean case the paramagnetic Mott transition occurs at $U_c^{\mathrm{Mott}}=8.5\pm0.5$,[25] we expect that a sizable D is needed to uncover the aforementioned competition. It could well happen that a metallic phase is instead confined at weak U and D within the Anderson insulating phase, while, the large U transition is always between an Anderson insulator and a Mott one. However, this possibility is outside a reliable finite-size numerical approach.

Going back to our variational calculation, we note that a clear change in the behavior of the wave function occurs at $U_c^{\mathrm{Mott}}/t=11.5\pm0.5$. For small values of U, $N_q^{\mathrm{conn}}\sim|q|$ and $v_q\sim 1/|q|$, whereas $N_q^{\mathrm{conn}}\sim|q|^2$ and $v_q\sim 1/|q|^2$ for large U. The latter behavior is symptomatic of the presence of a charge gap, hence of a Mott insulating behavior.[21] We note that the increase in U_c with respect to the clean case[25] indicates that disorder does compete with U. It should be emphasized that, with respect to the clean model, for $U<U_c^{\mathrm{Mott}}$, $N_q^{\mathrm{conn}}\sim|q|$ is not associated to a metallic behavior but only to a gapless spectrum, also characteristic of an Anderson insulator. Remarkably, we find that the Mott and Anderson insulators can also be discriminated through the behavior of the $\lim_{q\to0}N_q^{\mathrm{disc}}$. In Fig. 1 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.

We note that the linear slope of N_q^{conn} has a nonmonotonic behavior as a function of U, showing a peak for $U/t\sim7$ 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, $\delta n^2=1/N\Sigma_i(\langle n_i^2\rangle-\langle n_i\rangle^2)$ (see Fig. 1) which might indicate an increase in *me-*

tallicity. However, as shown in Fig. 1, although the fluctuations of the on-site variational disorder $\Delta_\epsilon^2 = 1/N\Sigma_i \tilde{\epsilon}_i^2 - (1/N\Sigma_i \tilde{\epsilon}_i)^2$ decrease upon increasing U, they stay finite no matter how strong U is. Therefore, the single-particle eigenstates of the variational Hamiltonian keep a finite localization length. Hence the uncorrelated wave function $|\Phi_0\rangle$ always describes an Anderson insulator below the Mott transition. A key question is whether the action of the Gutzwiller correlator and the Jastrow factor could turn a localized $|\Phi_0\rangle$ into a delocalized $|\Psi\rangle$. Since the variational method does not give access to dynamical quantities such as dc conductivity, we have no definite answer to this intriguing question. Nevertheless, we tend to believe that such a transmutation of a localized $|\Phi_0\rangle$ into a delocalized $|\Psi\rangle$ is unlikely.

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 $M = 1/N\Sigma_j e^{iR_jQ} m_j$ for a suitable momentum Q, such as, 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', $U_c^{\mathrm{AF}} < U_c^{\mathrm{Mott}}$, 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,[15,26,27] although the latter ones overestimate the extension of the magnetic phase. In Fig. 2, we show the results for $t'=0$ either by fixing $D/t=5$ and varying U (for which $U_c^{\mathrm{AF}}/t = 6.5 \pm 0.5$ and $U_c^{\mathrm{Mott}}/t = 10.5 \pm 0.5$) or by fixing $U/t=4$ and changing D (for which $D_c^{\mathrm{Mott}}/t = 1 \pm 0.5$ and $D_c^{\mathrm{AF}}/t = 2.5 \pm 0.5$). We remark that our wave function is more robust against long-range magnetism and slightly more compressible than the Hartree-Fock one (see Fig. 2). One could take these facts as another signal of a tendency toward delocalization, induced unexpectedly by the action of the Jastrow and Gutzwiller correlators. Once again we are led to face the question of whether an uncorrelated and localized $|\Phi_0\rangle$ could give rise, after projection, to a delocalized $|\Psi\rangle$.

The onset of antiferromagnetism is preceded by a magnetically disordered phase (i.e., $M=0$) in which local moments appear. In Fig. 3, the patterns 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 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 $N_q^{\mathrm{conn}} \sim |q|$. 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 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).

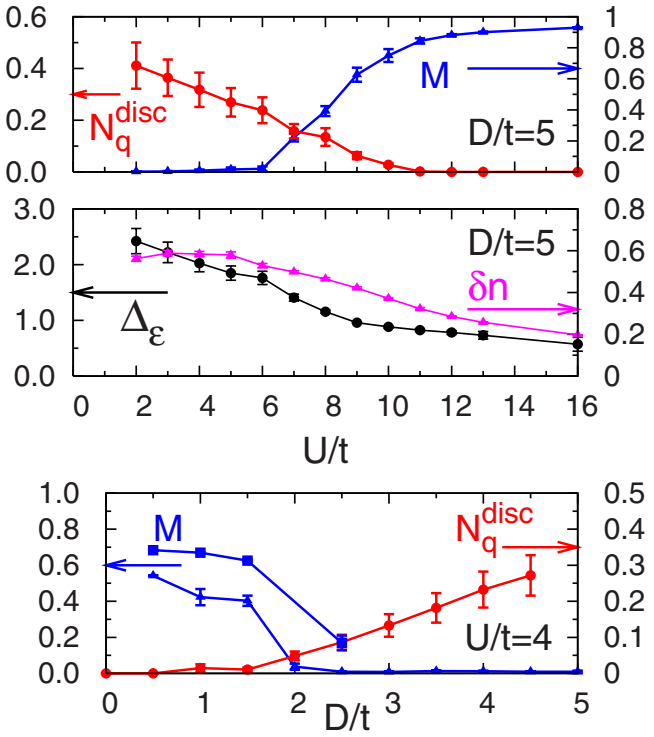

FIG. 2. (Color online) Staggered magnetization M for $Q=(\pi,\pi)$ and compressibility fluctuations N_q^{disc} as a function of U for disorder $D/t=5$ (upper panel) and as a function of D for $U/t=4$ (bottom panel). In the bottom panel, we also report the results of M for the unprojected wave function $|\Phi_0\rangle$ (upper curve). 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.

In the presence of a large frustrating hopping $t'/t \gtrsim 0.9$ we find evidence 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 pattern (see Fig. 4). These solutions are incompressible, i.e., N_q^{disc}

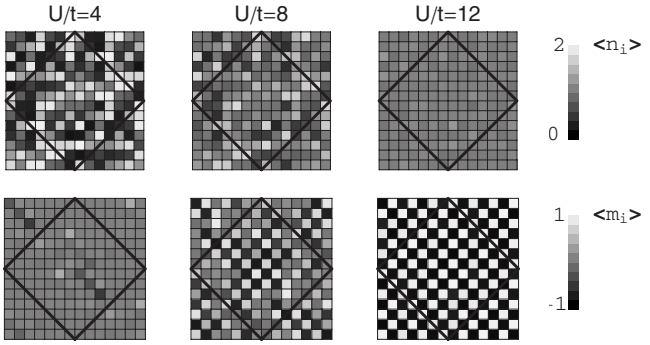

FIG. 3. Local density $\langle n_i \rangle$ (upper panels) and local magnetization $\langle m_i \rangle$ (lower panels) for a given disorder realization with $D/t=5$ and different values of U/t. The black contour shows the elementary cell of the lattice which is repeated to mimic the infinite lattice with periodic boundary conditions.

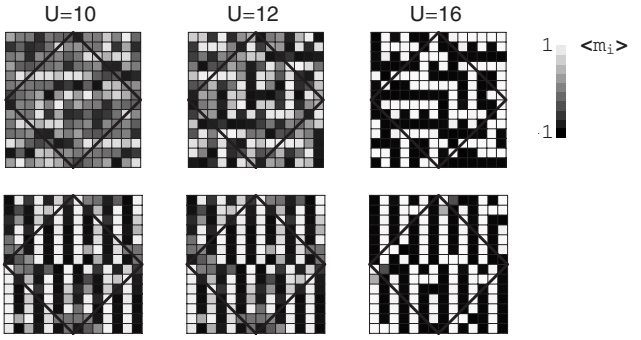

FIG. 4. Local magnetization $\langle m_i \rangle$ for the best variational state (lower panels) and for a metastable solution (upper panels) for a given disorder configuration with $D/t=5$ and $t'/t=1$.

~ 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 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.[17,19] When spontaneous spin symmetry breaking is allowed, we find two successive transitions: 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 clear-cut evidence, at least within the limits of our variational approach, of a truly metallic behavior induced by interaction.

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