Magnetic correlations in the two-dimensional Anderson-Hubbard model

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The two-dimensional Hubbard model in the presence of diagonal and off-diagonal disorder is studied at half-filling with a finite-temperature quantum Monte Carlo method. Magnetic correlations as well as the electronic compressibility are calculated to determine the behavior of local magnetic moments, the stability of antiferromagnetic long-range order (AFLRO), and properties of the disordered phase. The existence of random potentials (diagonal or ''site'' disorder) leads to a suppression of local magnetic moments which eventually destroys AFLRO. Randomness in the hopping elements (off-diagonal disorder), on the other hand, does not significantly reduce the density of local magnetic moments. For this type of disorder, at half-filling, there is no ''sign problem'' in the simulations as long as the hopping is restricted between neighbor sites on a bipartite lattice. This allows the study of sufficiently large lattices and low temperatures to perform a finite-size scaling analysis. For off-diagonal disorder, AFLRO is eventually destroyed when the fluctuations of antiferromagnetic exchange couplings exceed a critical value. The disordered phase close to the transition appears to be incompressible, and shows an increase of the uniform susceptibility at low temperatures. [S0163-1829(97)10007-8]

I. INTRODUCTION

Electrons in crystals are scattered both by their mutual interaction and by static disorder potentials. These processes typically lead to quite different or even competing effects. For example, on a bipartite lattice close to half-filling the strongly screened Coulomb interaction between electrons can generate antiferromagnetic long-range order (AFLRO), while disorder tends to destroy such correlations. The simultaneous presence of interaction and disorder cannot in general be considered as a simple superposition of both contributions, but interesting many-body phenomena may emerge. This has been found for instance in the study of the metal-insulator transitions in doped semiconductors[1] or in the stability of AFLRO against disorder within a dynamical mean-field theory.[2] In spite of the great progress that has been achieved in understanding interacting as well as disordered systems in recent years, there is still no controlled and at the same time tractable theoretical method to describe their combined effects, in particular when the interactions and/or disorder cannot be considered as small.

It is the purpose of the present paper to provide approximation-free results for a very simple microscopic model that incorporates electron interactions as well as disorder, namely, the disordered Hubbard model, or ''Anderson-Hubbard model'' in two dimensions, $D=2$. The Hamiltonian of the model in the usual notation reads:

$$\hat{H} = \sum_{\langle \mathbf{i},\mathbf{j} \rangle, \sigma} t_{\mathbf{i},\mathbf{j}} \hat{c}^{\dagger}_{\mathbf{i}\sigma} \hat{c}_{\mathbf{j}\sigma} + \sum_{\mathbf{i}\sigma} (\epsilon_{\mathbf{i}} - \mu) \hat{n}_{\mathbf{i}\sigma}$$
$$+ U \sum_{\mathbf{i}} (\hat{n}_{\mathbf{i}\uparrow} - \tfrac{1}{2})(\hat{n}_{\mathbf{i}\downarrow} - \tfrac{1}{2}). \qquad (1)$$

$\mathbf{i}$ and $\mathbf{j}$ are lattice vectors. The distributions of the random hopping elements $t_{\mathbf{i},\mathbf{j}}$ and random local potentials $\epsilon_{\mathbf{i}}$ will be specified later on. Note that hopping processes are restricted between nearest neighbors on a square lattice; hence there is no magnetic frustration.

Model (1) has been investigated within various approaches: the formation of localized magnetic moments has been studied in $D=3$ for a very broad distribution of $t_{\mathbf{i},\mathbf{j}}$ within an unrestricted Hartree-Fock approximation.[3] The case of random potentials has been treated by a real-space renormalization-group method in $D=1$ and 3 (Ref. 4) and $D=2$.[5] In $D=2$ this treatment provides a transition from a Mott to an Anderson insulator with no metallic phase. However, in these investigations the formation of AFLRO which will set in, at least in the unfrustrated case close to half-filling, is not taken into account. The (in)stability of AFLRO with respect to diagonal disorder and two types of metal-insulator transition were examined[2] in a dynamical mean-field theory which becomes exact in the limit of $D \to \infty$.[6] Diagonal disorder has also been studied in $D=3$ by Hartree-Fock approximations.[7] The strong-coupling limit of model (1) with diagonal disorder was studied[8] using a slave-boson formulation of the corresponding t-J model. In the case of off-diagonal disorder at half-filling the model maps in this limit onto the spin-$\tfrac{1}{2}$ Heisenberg model with random (not frustrated) exchange couplings. This model has also been investigated numerically in $D=2$.[9] Finally, the one-dimensional Hubbard model with either type of disorder was studied using quantum Monte Carlo (QMC) simulations.[10]

Here we will concentrate on the effect of disorder on the magnetic correlations. We will address the following questions:

(i) How are short- and long-range magnetic correlations affected by the two different kinds of disorder?

(ii) Is there a critical disorder strength where AFLRO ceases to exist?

(iii) How do the magnetic susceptibility and charge compressibility behave in the disordered state?

II. COMPUTATIONAL METHOD

We will study the Anderson-Hubbard model in $D=2$ using a finite-temperature, grand-canonical QMC method[11] which is stabilized at low temperatures by the use of orthogonalization techniques.[12,13] The algorithm is based on a functional-integral representation of the partition function by discretizing the ''imaginary-time'' interval $[0,\beta]$, where β is the inverse temperature. The interaction is decoupled by a two-valued Hubbard-Stratonovich transformation[14] yielding a bilinear time-dependent fermionic action. For the positive-U model, the $D+1$-dimensional auxiliary field ($s_{\mathbf{i}l}=\pm1$, where $\mathbf{i}$ is the lattice and l the ''time'' index) couples to the local magnetization ($n_{i\uparrow}-n_{i\downarrow}$). The fermionic degrees of freedom can be integrated out analytically, and the partition function (as well as observables) can be written as a sum over the configurations of the auxiliary field with a weight proportional to the product of two determinants, one for each spin species. The two determinants are not equal, since $s_{\mathbf{i}l}$ couples with different sign to the two fermion species, and, in general, their product is not positive definite and thus cannot serve as a weight function in an importance sampling procedure. The formally exact treatment of this ''minus-sign problem'' can lead in some regimes of the model parameters to very small signal-to-noise ratios in physical quantities, that become in fact exponentially small with inverse temperatures and system size.

In the case of a bipartite lattice, under the particle-hole transformation of one spin species,

$$\hat{c}_{\mathbf{i}\downarrow}\rightarrow(-1)^{\mathbf{i}}\hat{c}_{\mathbf{i}\downarrow}^{\dagger}. \tag{2}$$

Hamiltonion (1) is mapped onto the *negative-U* Hubbard model:

$$\hat{H}(U)\rightarrow\hat{H}(-U)+\sum_{\mathbf{i}}(\epsilon_{\mathbf{i}}-\mu)(1-2\hat{n}_{\mathbf{i}\downarrow}). \tag{3}$$

If the Hamiltonion is now spin symmetric, i.e., $\epsilon_{\mathbf{i}}=\mu$ for all $\mathbf{i}$, the two determinants for spin-up and -down are identical, since in the case of the negative-U model the Hubbard-Stratonovich field couples to the charge ($n_{i\uparrow}+n_{i\downarrow}$), that is, with the same sign for the two fermion species. Hence the determinant product is positive (semi) definite and there is no ''minus-sign problem.'' For this reason the local random potentials $\epsilon_{\mathbf{i}}$ lead to a minus-sign problem even at half-filling, whereas the sign is always positive at half-filling for off-diagonal disorder as long as the hopping remains restricted between nearest neighbors.

We will consider the case of static, uncorrelated disorder in either the hopping elements $t_{\mathbf{i},\mathbf{j}}$ or the on-site potentials $\epsilon_{\mathbf{i}}$. Therefore we have to average all quantities over a sufficient number of disorder realizations, and calculate the averaged expectation values

$$\langle\langle\hat{A}\rangle\rangle_h=\prod_{\langle\mathbf{i},\mathbf{j}\rangle}\left[\int dt_{\mathbf{i},\mathbf{j}}P_h(t_{\mathbf{i},\mathbf{j}})\right]\langle\hat{A}\rangle(\{t_{\mathbf{i},\mathbf{j}}\}), \tag{4}$$

$$\langle\langle\hat{A}\rangle\rangle_s=\prod_{i}\left[\int d\epsilon_{\mathbf{i}}P_s(\epsilon_{\mathbf{i}})\right]\langle\hat{A}\rangle(\{\epsilon_{\mathbf{i}}\}). \tag{5}$$

$\langle\hat{A}\rangle$ denotes the thermal expectation value of the operator $\hat{A}$ for a given disorder configuration; $\langle\ \rangle_{h(s)}$ stands for the average over hopping (site) disorder. We will assume uniform distributions of either the hopping elements $t_{\mathbf{i},\mathbf{j}}$ with an average value of $t\equiv-1$ or the on-site potentials $\epsilon_{\mathbf{i}}$ with an average of zero. The width of the distributions $P_{h(s)}$ is denoted by Δ,

$$P_h(t_{\mathbf{i},\mathbf{j}})=\frac{1}{\Delta}\Theta\left(\frac{\Delta}{2}-|t_{\mathbf{i},\mathbf{j}}-t|\right), \tag{6}$$

$$P_s(\epsilon_{\mathbf{i}})=\frac{1}{\Delta}\Theta\left(\frac{\Delta}{2}-|\epsilon_{\mathbf{i}}|\right). \tag{7}$$

(We use the same symbol for the width Δ, since each type of disorder is considered separately.) Restricting to the half-filled band case ($\mu=0$) the remaining three parameters are interaction U, disorder strength Δ, and temperature $T\equiv1/\beta$.

In the present study we will concentrate on the following observables: (i) magnetic correlation functions

$$C(\mathbf{l})=\frac{1}{N}\sum_{\mathbf{j}}\langle\langle\hat{m}_{\mathbf{j}}\hat{m}_{\mathbf{j}+\mathbf{l}}\rangle\rangle. \tag{8}$$

Here $\hat{m}_{\mathbf{j}}=\Sigma_{\sigma}\sigma\hat{n}_{\mathbf{j}\sigma}$ is the local spin operator, and N is the total number of lattice sites. $\sqrt{C(0,0)}$ measures the density of local magnetic moments and is equal to $n-2d$ with the electronic density $n=\Sigma_{\mathbf{j}\sigma}\langle\langle\hat{n}_{\mathbf{j}\sigma}\rangle\rangle$ and the density of doubly occupied sites $d=\Sigma_{\mathbf{j}}\langle\langle\hat{n}_{\mathbf{j}\uparrow}\hat{n}_{\mathbf{j}\downarrow}\rangle\rangle$. (The indices h and s of the disorder averages are suppressed for convenience.) (ii) Magnetic structure factors and the Fourier transformation of $C(\mathbf{l})$,

$$S(\mathbf{q})=\sum_{\mathbf{l}}C(\mathbf{l})e^{i\mathbf{q}\cdot\mathbf{l}}, \tag{9}$$

[note that $\beta S(0,0)$ is equal to the uniform spin susceptibility]. (iii) Charge compressibility

$$\kappa\equiv\frac{\partial n}{\partial\mu}=\frac{\beta}{N}\left[\sum_{\mathbf{i},\mathbf{j}}\langle\langle\hat{n}_{\mathbf{i}}\hat{n}_{\mathbf{j}}\rangle\rangle-Nn^2\right], \tag{10}$$

with local charge operator $\hat{n}_{\mathbf{j}}=\Sigma_{\sigma}\hat{n}_{\mathbf{j}\sigma}$.

We found $S(\mathbf{q})$ to be largest at the commensurate vector $\mathbf{q}=(\pi,\pi)$. At sufficiently low temperatures the magnetic correlation length exceeds the system size, and $S(\pi,\pi)$ saturates with β for a given system size. Using the saturated values we can extrapolate the behavior in the thermodynamic limit by a finite-size scaling according to spin-wave theory,[15] which in the case of AFLRO in the ground state with sublattice magnetization M predicts

$$C(N_x/2,N_x/2)=\frac{M^2}{3}+O(N_x^{-1})$$

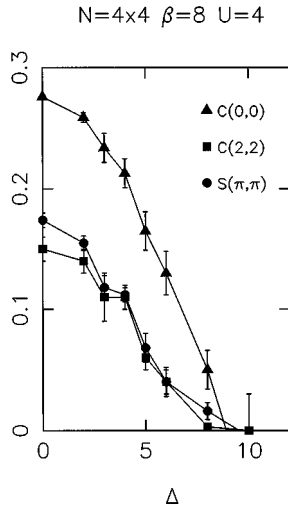$$\frac{S(\pi,\pi)}{N}=\frac{M^2}{3}+O(N_x^{-1}), \tag{11}$$

FIG. 1. Local moment $C(0,0)$ (triangles), longest-range spin correlation $C(2,2)$ (squares) and antiferromagnetic structure factor $S(\pi,\pi)/N$ (circles) on 4x4 lattices at $U=4$ and $T=\frac{1}{8}$, as a function of site disorder Δ. The noninteracting values of each quantity have been subtracted.

where $(N_x/2,N_x/2)$ is the maximal separation on a square lattice of linear size $N_x=\sqrt{N}$ with periodic boundary conditions. Thus we have two independent quantities to extrapolate the value of the ground-state order parameter. The finite-size extrapolation is technically only possible in the case of off-diagonal disorder, where there is no ''minus-sign problem'' and hence sufficiently large lattices at low temperatures can be simulated.

III. DIAGONAL DISORDER

Diagonal disorder describes the idealized situation of a random alloy with negligible lattice distortions but varying values of the chemical potentials of the constituents. While the repulsive interaction U tends to induce singly occupied sites, i.e., local magnetic moments, a wide spectrum of random potentials has the opposite effect because electrons tend to doubly occupy the lower potentials. Intuitively one would expect that a disorder strength Δ of the order of U may be sufficient to destroy AFLRO. This has actually been observed in the limit $D\to\infty$,[2] where the disorder effects are exactly treated by the coherent potential approximation.[16] Since the magnetic moment formation is a local effect, we expect qualitatively the same behavior in $D=2$. Figure 1 shows the local spin-spin correlation fuction $C(0,0)$ on a 4×4 lattice at $U=4$ as a function of Δ. $C(0,0)$ decreases monotonically with Δ, and reaches the noninteracting value 0.5 about $\Delta=2U$. This local effect is indeed independent of dimensionality and has been observed in $D=1$ (Ref. 10) and $D=\infty$.[2] A similar behavior is seen in the spin-spin correlation function at the largest separation $C(2,2)$, and the AF structure factor $S(\pi,\pi)/N$. They are slightly more stable than $C(0,0)$ for small disorder, and decrease more rapidly for $\Delta>4$, also reaching their noninteracting values of 0 and 0.0508, respectively, about $\Delta=2U$.

More interesting is the behavior of the compressibility κ (Fig. 2). In a Fermi liquid in the limit $T\to0$, κ is equal to the one-particle density of states (DOS) at the Fermi energy. For

the pure tight-binding model without interaction and disorder, κ diverges logarithmically with T at half-filling due to perfect nesting.[17] Turning on the disorder removes the van Hove singularity, leading to a finite DOS at the Fermi level and to a broadening of the DOS. For large Δ the DOS is dominated by the disorder spectrum, giving a bandwidth proportional to Δ, and due to normalization a value at the Fermi energy proportional to $1/\Delta$. This relation is also observed for the compressibility at $U=0$ at a finite temperature (Fig. 2).

On the other hand, when the interaction strength U is nonzero, for small values of Δ the compressibility vanishes due to the charge gap induced by antiferromagnetic ordering. AFLRO is strictly present only in the ground state, but for a finite lattice the AF correlation length at a finite temperature
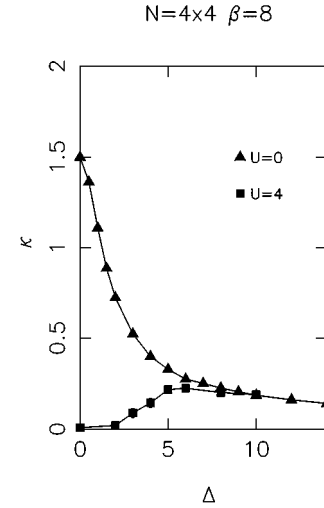

FIG. 2. Compressibility κ at $U=0$ (triangles) and $U=4$ (squares) on 4x4 lattices and $T=\frac{1}{8}$, as a function of site disorder Δ. The very different behavior at $\Delta=0$ reflects the suppression of the divergent density of states in the noninteracting limit and the opening of a charge gap.
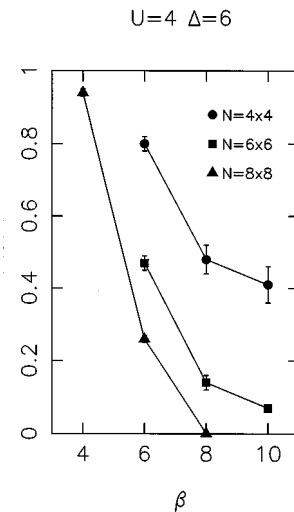

FIG. 3. Average sign $\langle\langle\sigma\rangle\rangle$ for the site-disordered problem at $U=4$ and $\Delta=3$ as a function of inverse temperature β. Circles are 4x4 lattices, while squares and triangles are 6x6 and 8x8 lattices, respectively. This sign problem is absent in the case of hopping disorder at half-filling.
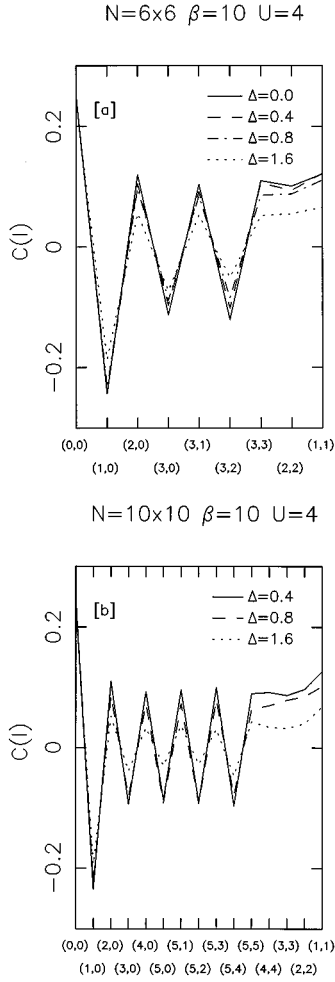
FIG. 4. Spin-spin correlations as a function of separation on (a) 6×6 and (b) 10×10 lattices at $T=\frac{1}{10}$ and $U=4$. The value shown at (0,0) is $C(0,0)-\frac{1}{2}$.
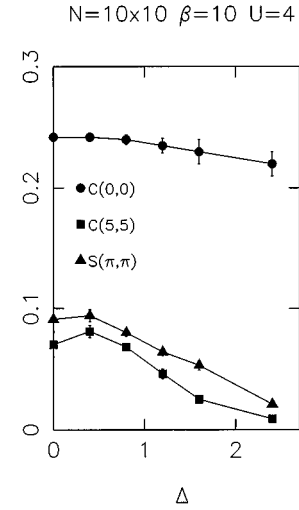

FIG. 5. Local moment $C(0,0)$ (circles), longest range spin correlation $C(5,5)$ (squares) and antiferromagnetic structure factor $S(\pi,\pi)/N$ (triangles) on 10x10 lattices at $U=4$ and $T=\frac{1}{10}$, as a function of site disorder Δ. The noninteracting values of each quantity have been subtracted.

IV. OFF-DIAGONAL DISORDER

In the case of random hopping elements $t_{\mathbf{i,j}}$ restricted to near-neighbor sites on a bipartite lattice, there is no ''minus sign problem'' at half-filling. Therefore we can do a much more detailed analysis of the phase diagram. We study square lattices with periodic boundary conditions up to the size $N=100$ ($N_x=10$). For a given disorder configuration, 500–700 Monte Carlo sweeps were performed for equilibration, followed by 1000–1500 measurement sweeps. Then all measured quantities were averaged over 10–20 different disorder configurations. The disorder average is the main source of the statistical errors.

As in Sec. III, we first study the spin-spin correlations as a function of disorder strength Δ for a given lattice size. Figure 4(a) shows $C(\mathbf{l})$ over a path in real space for different values of Δ on a 6×6 lattice. AF correlations are present for all values of Δ. They are only slightly reduced for $\Delta\lesssim0.8$ and much more significantly reduced when $\Delta\sim1.6$. Larger lattices show a quite similar picture [Fig. 4(b)]. The local moments $\sqrt{C(0,0)}$ are apparently stable for off-diagonal disorder, as is shown in Fig. 5, where the behavior of $C(\mathbf{l})$ for $\mathbf{l}=(0,0)$ and $(N_x/2,N_x/2)$ and the AF structure factor $S(\pi,\pi)/N$ are plotted as a function of Δ. Unlike the case of random site energies (Fig. 1), $C(0,0)$ is almost unchanged by Δ. However, measures of the long-range order are strongly affected. While the longer-range correlations break down for strong disorder ($\Delta\sim2$), they slightly *increase* for small Δ. This slight increase between $\Delta=0.0$ and 0.2 might be due to an enhanced averaged Heisenberg exchange coupling

$$\langle J_{\mathbf{i\cdot j}}\rangle = \frac{4\langle t_{\mathbf{i,j}}^2\rangle}{U} = J_0 + \frac{\Delta^2}{3U}, \tag{12}$$

with $J_0=4t^2/U$ for the undisordered case. However, this is essentially a strong-coupling argument ($J_0\ll t$), while the present value is only $J_0=t$.

can exceed the lattice size.[13] Even with a fully established charge gap, κ is always finite at finite temperature, however exponentially suppressed (Fig. 2). κ starts to increase significantly for $\Delta>2$, and reaches a maximum at about $\Delta=6$. Since the κ vs Δ curve for $U=4$ approaches the noninteracting curve for large Δ, the finite compressibility is quite likely not thermally activated, but due to the closing of the charge gap. Further, κ becomes finite for relatively small values of $\Delta<4$, where the AF correlations are still strong. Although the lattice size is much too small for a definite conclusion, this indicates that the charge gap may close within the AF phase. Evidence of a disorder-induced AF metal at half-filling has previously been found in $D=\infty$,[2] and also in a Hartree-Fock treatment in $D=3$.[7] Note, however, that in the presence of disorder a finite compressibility does not necessarily imply metallicity because of localization effects.

Fig. 3 shows why we cannot study large lattices and low temperatures in the case of diagonal disorder. The averaged values of the sign of the product of determinants, $\langle\langle\sigma\rangle\rangle$, vanishes rapidly with spatial lattice size N and inverse temperature β. A value $\langle\langle\sigma\rangle\rangle$ smaller than about 0.2 precludes reliable simulations due to a vanishing signal-to-noise ratio in the data.

$\beta=10$ $U=4$ $\Delta=0.4$

[a]
▲ $C(N_x/2,N_x/2)$
● $S(\pi,\pi)$

$1/N_x$

$\beta=10$ $U=4$ $\Delta=1.2$

[c]
▲ $C(N_x/2,N_x/2)$
● $S(\pi,\pi)$

$1/N_x$

$\beta=10$ $U=4$ $\Delta=0.8$

[b]
▲ $C(N_x/2,N_x/2)$
● $S(\pi,\pi)$

$1/N_x$

$\beta=10$ $U=4$ $\Delta=1.6$

[d]
▲ $C(N_x/2,N_x/2)$
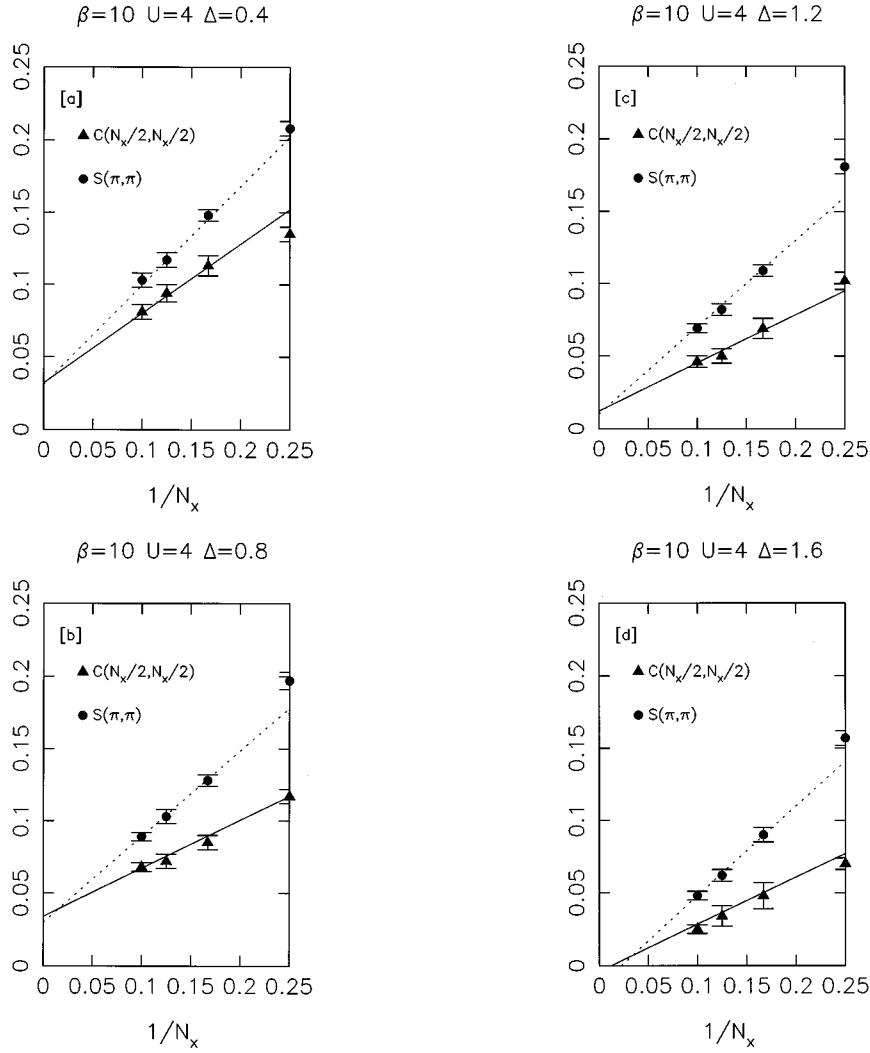● $S(\pi,\pi)$

$1/N_x$

FIG. 6. Finite size scaling analysis of the AF structure factor and long-range spin correlations. These quantities, appropriately scaled, are plotted as a function of the linear lattice size $1/N_x$. A nonzero extrapolation to $1/N_x=0$ indicates AFLRO. The extrapolated values should be identical.

In order to answer the question if there is AFLRO in the ground state, we calculate $C(N_x/2,N_x/2)$ and $S(\pi,\pi)$ for different lattice sizes, and extrapolate the results assuming a finite-size scaling according to Eq. (11). For the present lattice sizes (up to 10×10 sites) the magnetic correlations are saturated at a temperature of about $T=\frac{1}{10}$, where the finite system is essentially in its ground state. For disorder strength $\Delta \leq 1.2$ both $C(N_x/2,N_x/2)$ and $S(\pi,\pi)$ extrapolate to a nonzero order parameter M at $N_x\rightarrow\infty$ (Fig. 6). The values for M are obtained by a least-square fit of the data with $N_x\geq6$. For $N_x=4$ there are apparently deviations from scaling (11). Within the statistical error the independent extrapolations lead to the same value of M. For $\Delta=1.6$, however, there is no long-range order.

The values of M as a function of Δ are shown in Fig. 7 where the value for $\Delta=0$ is taken from the literature.[13] M is apparently stable for small disorder strength $\Delta\leq0.8$, and then decreases and eventually vanishes about $\Delta\approx1.4$. The slight increase of magnetic correlation for small disorder at a given system size (Fig. 5) is not observed in the values of the order parameter.

The physical reason for the destruction of AFLRO is not obvious for this type of disorder. There is no magnetic frustration and also no destruction of local moments. One possible approach to understanding the transition is a weak-coupling analysis. Within the random-phase approximation (RPA) the magnetic susceptibility of the interacting system χ_{RPA} is expressed in terms of the noninteracting value χ_0,

$$\chi_{RPA}(\pi,\pi)=\frac{\chi_0(\pi,\pi)}{1-U\chi_0(\pi,\pi)}. \qquad (13)$$

The perfect nesting relation of the pure tight-binding model without interactions and disorder $\varepsilon(\mathbf{q}+(\pi,\pi))=-\varepsilon(\mathbf{q})$ at half-filling leads to a divergent susceptibility

$$\chi_0(\pi,\pi)\propto(\ln T)^{\gamma}. \qquad (14)$$

For the square lattice at half-filling we have $\gamma=2$ due to the logarithmic van Hove singularity in the DOS at the Fermi energy. In general, for bipartite lattices without this DOS singularity, like the simple cubic lattice the exponent becomes $\gamma=1$. Since χ_0 diverges at $T=0$ the RPA predicts that the system will order at any finite U.
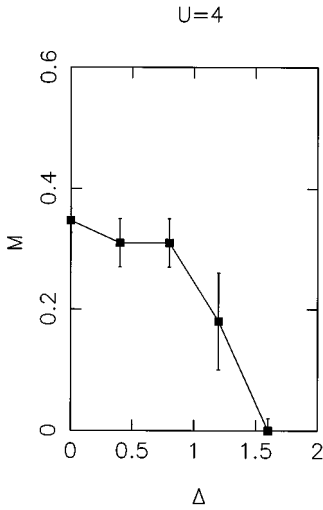
U=4

FIG. 7. The order parameter M inferred from Fig. 6 as a function of Δ. For $\Delta < \Delta_c \approx 1.4$ there is AFLRO. For $\Delta > \Delta_c \approx 1.4$ there is a transition into a disordered phase.

One effect of the disorder is removing the perfect nesting relation of the pure tight-binding model, reducing χ_0 and leading to the destruction of AFLRO within this RPA analysis. However, off-diagonal disorder does not the remove the bipartite structure of the lattice, so we expect Eq. (14) still to hold with $\gamma = 1$ although $\mathbf{q}$ is no longer a good quantum number. Since there exists no analytic solution for $\langle \chi(\mathbf{q}) \rangle$ for the disordered lattice even without interaction, we calculate it numerically for finite lattices. $\chi_0(\pi,\pi)$ is indeed well described by a logarithmic fit (Fig. 8). In fact, we further observe that in the disorder-averaged RPA susceptibility $\chi_{\mathrm{RPA}}(\pi,\pi)$ for finite U, one can to a very good approximation replace $\chi(\pi,\pi)$ for a given disorder configuration by its average value $\langle \chi(\pi,\pi) \rangle$,

$\Delta = 1.6$

FIG. 8. The behavior of the noninteracting susceptibility χ_0 (circles) with temperature T in the presence of disorder. χ_0 still diverges logarithmically as $T \to 0$. The full line is a fit with $\chi_0 = 0.054 - 0.245 \ln T$. Also shown are the inverse RPA susceptibility $\chi_{\mathrm{RPA}}^{-1}(\pi,\pi)$ (triangles) and the approximation $\chi_{\mathrm{approx.}}^{-1}(\pi,\pi)$ (squares). They are indistinguishable within the statistical errors and vanish at the same critical temperature. The dotted line is only a guide to the eye.

$$\chi_{\mathrm{RPA}}(\pi,\pi) = \left\langle \frac{\chi(\pi,\pi)}{1 - U\chi(\pi,\pi)} \right\rangle \approx \chi_{\mathrm{approx.}}(\pi,\pi)$$

$$= \frac{\langle \chi(\pi,\pi) \rangle}{1 - U\langle \chi(\pi,\pi) \rangle}. \quad (15)$$

In particular the estimated Néel temperatures for a given U obtained from the divergence of $\chi_{\mathrm{RPA}}(\pi,\pi)$ and $\chi_{\mathrm{approx.}}(\pi,\pi)$ are identical within the errors due to disorder averaging (Fig. 8). We observe that $\chi_{\mathrm{RPA}}(\mathbf{q})$ for different momenta $\mathbf{q} \neq (\pi,\pi)$ is always more strongly suppressed by disorder than $\chi_{\mathrm{RPA}}(\pi,\pi)$. We conclude that off-diagonal disorder does not remove the low-temperature divergence of the AF susceptibility. Thus an explanation of the transition based, for example, on the inducement of a finite $U_{\mathrm{crit}} > 4$ as the disorder is increased is not viable.

While the above considerations might be suited in the case of weak interaction, we will now consider the opposite case of $U \gg t$. Here the half-filled Hubbard model with random $t_{\mathbf{i,j}}$ at half-filling becomes equivalent to the disordered, but *unfrustrated*, AF spin-$\frac{1}{2}$ Heisenberg model with random couplings $J_{\mathbf{i,j}}$, see Eq. (12). This model has been studied in $D = 2$ by a quantum Monte Carlo technique in the case of a binary distribution of $J_{\mathbf{i,j}} \in \{J_1, J_2\}$.[9] This numerical work incorporated disorder in two ways—both through the difference of the exchange energies $\tilde{\Delta} = |J_1 - J_2|$ and also through different concentrations of strong and weak bonds. Depending on the concentration p of, say the J_1 bonds, and the difference $\tilde{\Delta}$, AF ordered and disordered phases were identified. The basic physics is that spin singlets form on the strong bonds, driving the formation of a paramagnetic phase, as has been discussed by Bhatt and Lee[19] and Kirkpatrick and Belitz.[20] We have made a quantitative comparison of our data for the Hubbard model at $U = 4$ with this strong-coupling theory, which incorporates spin degrees of freedom only. We first note that the result of Ref. 9, for the phase boundary in the $p - \tilde{\Delta}$ plane, is reasonably well described by setting the variance of $J_{\mathbf{i,j}}$,

$$v \equiv \frac{\langle J_{\mathbf{i,j}}^2 \rangle - \langle J_{\mathbf{i,j}} \rangle^2}{\langle J_{\mathbf{i,j}}^2 \rangle} = \frac{p(1-p)\tilde{\Delta}^2}{pJ_1^2 + (1-p)J_2^2}, \quad (16)$$

to a critical value $v = v_c$.[21] That is, the fact that there are two distinct types of randomness appears irrelevant—they can be modeled together in a simple way by their effect on the variance of $J_{\mathbf{i,j}}$. The fit to the calculated phase boundary is best for $v_c \approx 0.40$–0.42. The variance of J in the Hubbard model with disorder distribution (6) is independent of U, and reads

$$v = \frac{\langle t_{\mathbf{i,j}}^4 \rangle - \langle t_{\mathbf{i,j}}^2 \rangle^2}{\langle t_{\mathbf{i,j}}^4 \rangle} = \frac{4}{9} \left(\frac{\Delta^4 + 60t^2\Delta^2}{\Delta^4 + 40t^2\Delta^2 + 80} \right). \quad (17)$$

v has its maximum of $\frac{5}{9}$ at $\Delta = 4\sqrt{5}t$. If we now apply the same criterion $v = v_c$ as in the Heisenberg model, we obtain a critical disorder strength of $\Delta_c = 1.7t$–$1.8t$. This estimation is surprisingly close to the critical Δ obtained by finite-size scaling at $U = 4$ (Fig. 7) in spite of the fact that $U = 4$, corresponding to $J_0 = 1$ is not in the strong-coupling limit of the Hubbard model.[18] The agreement might be due to the fact that for $U = 4$ the double occupancies are already strongly suppressed, and the density of local moments has reached
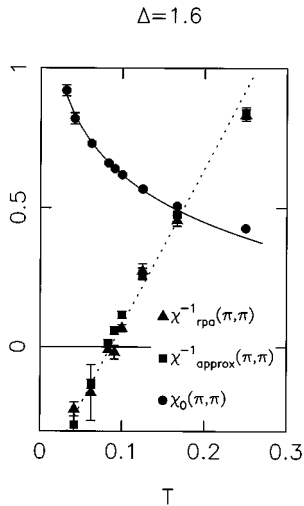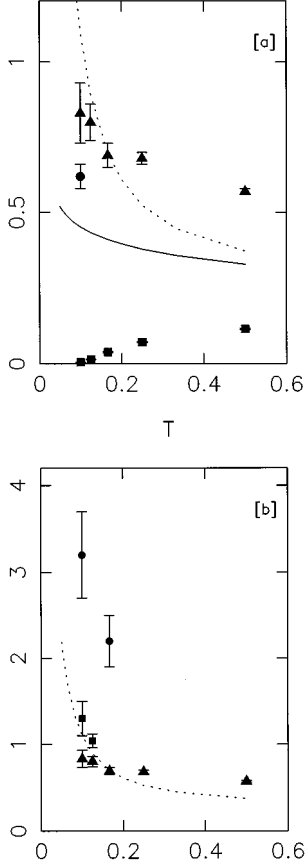
FIG. 9. Uniform susceptibility $\chi(0,0)$ vs T on a 8×8 lattice. (a) $\chi(0,0)$ for $U = 4$ and $\Delta = 1.6$ (triangles); $\chi(0,0)$ for $U = 4$, $T = t/10$, and $\Delta = 0.0$, 0.4, and 0.8 (circle) are indistinguishable within the error-bars. Also shown is the noninteracting $\kappa = \chi(0,0)$ for $\Delta = 0.0$ (dotted line) and $\Delta = 1.6$ (full line). The compressibility κ for $U = 4$ and $\Delta = 1.6$ (squares) vanishes exponentially at low temeratures. The key point of this data is that while randomness suppresses the susceptibility at $U = 0$, it enhances it for nonzero U. (b) $\kappa = \chi(0,0)$ for $U = \Delta = 0$ (dashed line) and $\chi(0,0)$ for $U = 4$ and $\Delta = 1.6$ (triangles) are again shown as in (a). However, here they are now compared with $\chi(0,0)$ for $\Delta = 2.4$ (squares) and for the case of correlated hopping randomness with $\Delta' = 1.6$ (circles) (see text).

about 75% of the maximal value 1.0 independent of disorder strength (see Fig. 5). Further, Δ_c is small compared to $3U$, so that the averaged $\langle J_{\mathbf{i},\mathbf{j}} \rangle$ is only slightly enhanced (by a factor of ~ 1.25) according to Eq. (12), which is a consistency check of the arguments above.

To characterize the properties of the disordered phase ($\Delta > 1.4$), we study the temperature dependence of the uniform spin susceptibility $\chi(0,0) = \beta S(0,0)$ [Eq. (9)] and the charge compressibility κ [Eq. (10)]. In the noninteracting case both quantities are identical, and diverge logarithmically in $D = 2$ for $\Delta = 0$, as mentioned before.[17] This singularity is removed by interactions, and $\chi(0,0)$ reaches a maximum at a finite temperature, approaching a finite value at $T = 0$.[13] Disorder suppresses the noninteracting susceptibility too, but for a different reason because it removes the van Hove singularity in the density of states [Fig. 9(a)]. In the interacting case, however, disorder has the opposite effect of enhancing $\chi(0,0)$ if the disorder is strong enough

($\Delta = 1.6$). For $\Delta \lesssim 0.8$ there is no significant effect on $\chi(0,0)$ due to disorder at the lowest temperature under consideration ($T = t/10$). In the present temperature regime at $\Delta = 1.6$, $\chi(0,0)$ decreases monotonically with T, a behavior also found in the disordered phase of the random bond Heisenberg model.[9] Stronger disorder [$\Delta = 2.4$; see Fig. 9(b)], where some of the hopping elements become negative, leads to a further enhancement of $\chi(0,0)$. In systems with longer-range interactions a low-temperature divergence of $\chi(0,0)$ has been predicted.[19] This divergence is explained by the presence of localized moments, i.e., spins on lattice sites which are effectively decoupled from the rest of the system. Such isolated sites are particulary likely in the case of a special type of *correlated* hopping randomness with $t_{\mathbf{i},\mathbf{j}} = x_{\mathbf{i}} x_{\mathbf{j}}$, where the site variables $\{x_{\mathbf{i}}\}$ are randomly distributed.[22] In contrast to the uncorrelated distribution (6), here a site $\mathbf{i}$ with a small variable $x_{\mathbf{i}}$ is weakly connected to *all* its neighbors. We consider a bimodal, symmetric distribution of site variables,

$$ P(x_{\mathbf{i}}) = \frac{1}{2}\left[\delta\left(x_{\mathbf{i}} - \left(t - \frac{\Delta'}{2} \right)^{1/2} \right) + \delta\left(x_{\mathbf{i}} - \left(t + \frac{\Delta'}{2} \right) \right)^{1/2} \right], \tag{18} $$

with $\Delta' \leq 2t$. This distribution corresponds to a binary alloy where the hopping amplitudes $t_{\mathbf{i},\mathbf{j}}$ depend only on the (three possible) combinations of atoms on neighboring sites. $t_{\mathbf{i},\mathbf{j}}$ are always positive, and can take the values $t - \Delta'/2$, $\sqrt{t^2 - (\Delta'/2)^2}$, and $t + \Delta'/2$. The average Heisenberg coupling remains $\langle J_{\mathbf{i},\mathbf{j}} \rangle = J_0 = 4t^2/U$ independent of Δ'. We find that, for $\Delta' = 1.6$, $\chi(0,0)$ increases for lower temperatures, and is enhanced by almost one order of magnitude at $T = t/10$ compared to the case without disorder. Although the statistical errors and limited temperatures do not allow us to extract the functional dependence on T, this dramatic increase supports the existence of a finite density of localized moments.

As in the interacting case without disorder, the compressibility κ for $\Delta = 1.6$ shows activated behavior with temperature [Fig. 9(a)], with an estimated charge gap of 0.5.[23] A quite similar behavior is found even for stronger disorder $\Delta = 2.4$, and also for the correlated hopping randomness with $\Delta = 1.6'$ (not shown): κ is very small [$\sim O(10^{-3})$], and decreases strongly for lower T consistent with an activated behavior. Hence the systems remains uncompressible even in the absence of long-range magnetic order.

V. SUMMARY AND CONCLUSIONS

In this paper we have presented quantum Monte Carlo calculations for the magnetic phase diagram of the disordered repulsive Hubbard model at half-filling. When the randomness is in the site energy, the sign problem precludes the study of large systems at low temperatures necessary for a proper finite-size scaling analysis. However, on 4x4 lattices we are able to see the destruction of local moments and longer-range spin-spin correlations. We also studied the compressibility κ as a function of disorder strength. The incompressible state with $\kappa = 0$ at nonzero U in the absence of disorder is replaced by a finite κ at $\Delta \approx 2$, indicating a disorder-induced closing of the charge gap.

When the randomness is in the hoppings $t_{\mathbf{i,j}}$, a particle-hole transformation proves that the product of determinants which gives the Boltzmann weight is positive at half-filling. That is, there is no sign problem at arbitrarily low temperatures and large lattices. In this case we were able to do a finite-size scaling analysis of our results, and determined $\Delta_c \approx 1.4$ for the destruction of antiferromagnetism. This value was in reasonable agreement with that obtained for the disordered Heisenberg model[9]. The paramagnetic phase is driven by singlet formation. Unlike the random-site energy case, the local moments remain well formed through the transition. The strong enhancement of the uniform susceptibility at low temperatures, in particular for the correlated hopping randomness, indicates the formation of effectively localized magnetic moments. The compressibility is appar-ently activated even for strong disorder where there are no long-range magnetic correlations. We are currently studying the dependence of the density of states in this model, as it has recently been suggested that this may provide an alternate way to describe transitions in the Anderson-Hubbard model and its experimental realizations.[24]

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