Antiferromagnetism in the Two-Dimensional Hubbard Model

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Magnetic properties of the two-dimensional Hubbard-model are inferred from results of Monte Carlo simulations. Lattice sizes up to 8×8 and temperatures down to $T=t/20$ (t =hopping) were studied. The half-filled system is found to exhibit antiferromagnetic long-range order for all values of the Coulomb repulsion U. The low-temperature magnetic properties are found to be well described by spin-wave theory with renormalized local moment and spin-wave velocity. Numerical evidence presented suggests that when doped the system loses the long-range order immediately away from half filling.

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The magnetic properties of the two-dimensional Hubbard model are of great current interest, as the model is likely to describe at least approximately some of the properties of the recently discovered oxide superconducting materials.[1] More generally, since it is the simplest quantum model of magnetism involving itinerant electrons, a detailed understanding of its properties is desirable. We discuss here results of extensive Monte Carlo simulations of the model. In the half-filled band case, we determine the long-range order as a function of U and discuss to what extent spin-wave theory correctly describes the magnetic properties. For the non-half-filled band, we present numerical evidence that suggests that the system loses its long-range order immediately under doping.

Earlier Monte Carlo results[2] on magnetic properties only reached temperatures down to $\beta=4.5$ (in units where the hopping $t=1$). A recent algorithmic advance[3] now allows us to reach much lower temperatures. Here we discuss results down to temperatures $\beta=20$ on lattice sizes up to 8×8. It is necessary to reach such low temperatures to be able to infer the ground-state properties of the system.

The model is defined by the Hamiltonian

$$H=-t\sum_{(ij)}(c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c.})+U\sum_{i}n_{i\uparrow}n_{i\downarrow}-\mu\sum_{i\sigma}n_{i\sigma}. \quad (1)$$

We have studied lattices of sizes 4×4, 6×6, and 8×8, for values of $U=2$, 4, and 8 (in units where $t=1$). A detailed discussion of the model and early Monte Carlo results can be found in Ref. 2. Comparison with exact results in a 2×2 lattice demonstrates that the program is running properly. For most simulations we chose our time-slice size $\Delta\tau$ such that $\Delta\tau^2tU\sim0.125$.

In the half-filled band case, the magnetic structure factor

$$S(\mathbf{q})=\frac{1}{N}\sum_{i,j}e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\langle(n_{i\uparrow}-n_{i\downarrow})(n_{j\uparrow}-n_{j\downarrow})\rangle \quad (2)$$

exhibits a sharp peak at wave vector $\mathbf{q}_m=(\pi,\pi)\equiv\pi$. We will discuss in detail the q dependence elsewhere.[4] Results for $S(\pi)$ are shown in Fig. 1 for values of $U=4$, 2, and 8. Note the different horizontal and vertical scales in the three cases. We have reached in each case temperatures low enough that $S(\pi)$ has essentially saturated at its ground-state values. Results for the spin-spin correlation between the two farthest points on the $L\times L$ lattice

$$C_{L/2,L/2}=\langle\sigma_0^z\sigma_{x=L/2,y=L/2}^z\rangle \quad (3)$$

exhibit similar behavior,[4] except that they go to zero more rapidly as T is increased. Both quantities are useful to extrapolate the long-range magnetic order.

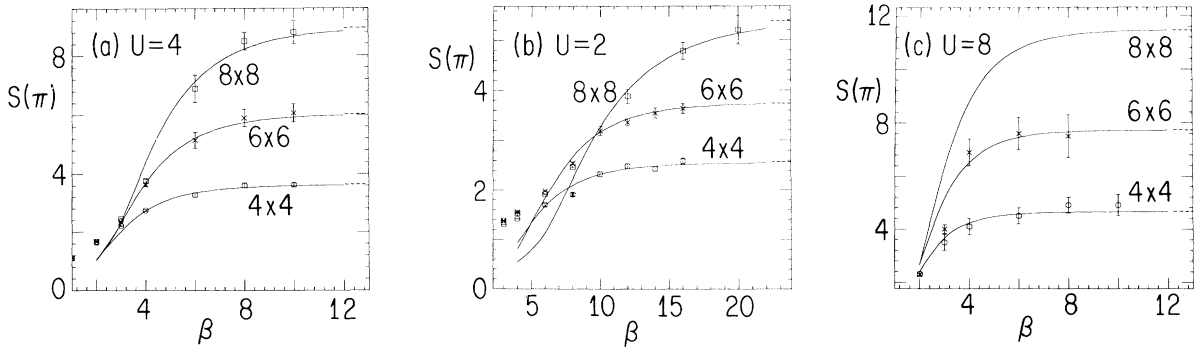

FIG. 1. Magnetic structure factor $S[\mathbf{q}=(\pi,\pi)]$ vs temperature for lattices of size 4×4, 6×6, and 8×8. The solid lines are results of spin-wave theory (see text). The dashed lines at the right side indicate the $T=0$ limits of the spin-wave results.

In addition to statistical error, the results in Fig. 1 have some systematic error due to the finite time-slice size $\Delta\tau$. Figure 2 shows the extrapolation to $\Delta\tau=0$ for $U=4$ and lattice sizes 4×4 and 2×2, for temperatures $\beta=2$, 4, and 8. We note that the $\Delta\tau$ error is not strongly dependent either on temperature or on lattice size. It is very expensive in computer time to perform accurate $\Delta\tau^2$ extrapolations on larger lattices, and the systematic error will be buried in the statistical error unless very long runs are performed. Based on the results in Fig. 2 and similar results for $C_{L/2,L/2}$ we estimate that finite $\Delta\tau$ ($=0.167$ in this case) increases our measured magnetic properties by about 5% for the case $U=4$, and thus we will use this to correct our final estimates for the long-range order. Our statistical error should be much larger than any residual systematic error. Similar estimates yield a correction of 8% for $U=2$, $\Delta\tau=0.25$, and 2% for $U=8$, $\Delta\tau=0.125$.

To further convince ourselves that the results of Fig. 1 are close to ground-state values at the lowest temperatures it is desirable to have a theoretical model that fits the data and can carry us to much lower temperatures. As there is spin rotational invariance for any U and a gap for charge excitations, we would expect spin waves to be the dominant low-lying excitations (except perhaps for very small U) that determine the low-temperature properties of the system. Recently, Arovas and Auerbach[5] (AA) have shown how to obtain magnetic correlations for the two-dimensional Heisenberg model at finite temperatures within spin-wave theory. The spin-wave dispersion relation within their mean-field theory is given by

$$\epsilon_k=\sqrt{2}c(1-\eta^2\gamma_k^2)^{1/2}, \tag{4a}$$

with

$$\gamma_k=\tfrac{1}{2}(\cos k_x+\cos k_y). \tag{4b}$$

$\eta\to1$ as $T\to0$, and at finite-temperatures it generates a gap for the low-lying excitations that destroys the magnetic long-range order. The value of η is determined by the mean-field constraint equation[5]

$$2=\frac{1}{N}\sum_k\frac{\coth\frac{1}{2}\beta\epsilon_k}{(1-\eta^2\gamma_k^2)^{1/2}}, \tag{5}$$

and the spin structure factor at wave vector (π,π) is given by

$$S_{\mathrm{AA}}(\pi)=\frac{1}{3N}\sum_k\frac{1+(\eta\gamma_k)^2}{1-(\eta\gamma_k)^2}\coth^2\left(\frac{\beta\epsilon_k}{2}\right)-\frac{1}{3}. \tag{6}$$

Equation (6) is obtained from the expressions for the spin-spin correlations given by AA normalized so that the "local moment" $\langle\sigma_z^2(R)\rangle=1$. In the Hubbard model, it is reasonable to scale the spin correlation functions by a factor that takes into account the reduction in the local spin by charge fluctuations, and we write

$$S(\pi)=m_L^2S_{\mathrm{AA}}(\pi). \tag{7}$$

It would seem natural to take m_L^2 to equal the squared local moment $\langle(n_{i\uparrow}-n_{i\downarrow})^2\rangle$. However, we find that such a choice in general does not fit the Monte Carlo data. Thus, we take both m_L^2 and the spin-wave velocity c as adjustable parameters.

The solid lines in Fig. 1 show the spin-wave fit to our data. For the case $U=4$, the best fit is obtained with a spin-wave velocity $c\cong0.49$ and squared effective local moment $m_L^2=0.62$. The on-site local moment is $\langle(n_{i\uparrow}-n_{i\downarrow})^2\rangle=0.78$ for this case. The reason the effective local moment is smaller is that charge fluctuations suppress more effectively long-range spin correlations than on-site spin correlations. As $U\to\infty$, both the effective local moment and the on-site local moment approach unity.

For $U=2$, there is no unique choice of c and m_L that gives reasonable fits for the three lattices studied: c has to be taken smaller in the 8×8 lattice, and m_L larger in the 4×4 lattice. Presumably, large charge fluctuations make the simple spin-wave fit not very good in this case. Still, the fit is useful in allowing us to estimate the error introduced by finite temperatures.

A consistency check as well as another estimate of the spin-wave velocity can be obtained from studying the

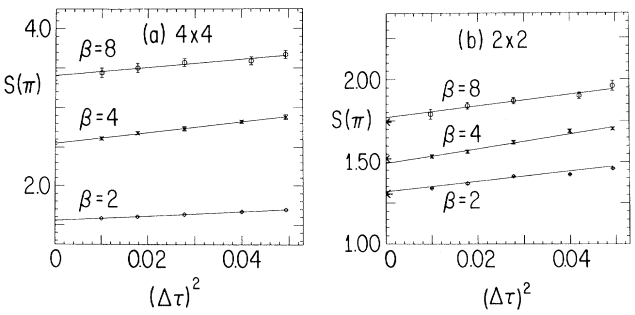

FIG. 2. $\Delta\tau$ dependence of the $\mathbf{q}=(\pi,\pi)$ magnetic structure factor for $U=4$ and temperatures $\beta=2$, 4, and 8 on (a) 4×4 and (b) 2×2 lattices. The points for $\Delta\tau=0$ on (b) are results of exact diagonalization, the straight lines are least-squares fits to the data.

TABLE I. Estimates of the squared effective local moment m_L^2 [Eq. (7)] and spin-wave velocity c that give the best fit to the Monte Carlo data. The squared local moment obtained from Monte Carlo simulations is $m_L^2\sim0.67$, 0.78, and 0.90 for $U=2$, 4, and 8, respectively.

	m_L^2	c [From $S(\pi)$]	c (From energy)
$U=2$	0.43(2) (4×4)	0.28(4) (4×4)	0.32(4) (4×4)
	0.38(2) (6×6)	0.28(4) (6×6)	0.35(4) (6×6)
	0.36(2) (8×8)	0.23(3) (8×8)	0.32(4) (8×8)
$U=4$	0.62(2)	0.49(4)	0.57(5)
$U=8$	0.79(10)	0.71(14)	0.64(7)

temperature dependence of the energy at low temperatures. The Monte Carlo results are found[4] to be well fitted by the form

$$E=\epsilon_0+\frac{1}{N}\sum_k \frac{\epsilon_k}{e^{\beta\epsilon_k}-1}, \quad (8)$$

with ϵ_0 a (lattice dependent) adjustable parameter, ϵ_k given by Eq. (4a), and c adjusted to give the best agreement. Again for $U=2$ a slightly better fit can be obtained by taking different c's on different size lattices. The values of c obtained this way are slightly larger than the ones that give the best fit for the magnetic structure factor but have the same qualitative trend (i.e., increasing with U). Table I summarizes our results for m_L and c, with the error bars a rough estimate of the range of parameters that give a reasonable fit to the Monte Carlo data.

In Fig. 3 we show the extrapolation for the magnetic long-range order. We plot the low-temperature limit of $S(\pi)/N$ and $C_{L/2,L/2}$ vs $1/\sqrt{N}$. For $U=8$, the results for $C_{L/2,L/2}$ have too large a statistical error to be useful and are not shown. According to spin-wave theory, the points plotted should lie approximately on a straight line.[6] We find this to be the case (within error) for $U=4$ and 8 but not for $U=2$. We attribute this deviation to the fact that short-distance charge fluctuations are masking the spin-wave behavior in the smallest lattice for $U=2$. Thus, we used only the 6×6 and 8×8 lattices for extrapolation in that case. Note that the upward curvature for both $S(\pi)/N$ and $C_{L/2,L/2}$ for $U=2$ leaves no doubt that they extrapolate to a *finite* value of m_z^2. Both quantities give approximately the same estimate for the long-range order for $U=2$ as well as for $U=4$.[7]

The inset in Fig. 3 shows the antiferromagnetic long-range order $m=(3m_z^2)^{1/2}$, with m_z^2 the extrapolated ordinates, versus U. The values obtained are $m=0.25(5)$, 0.39(5), and 0.44(10) for $U=2$, 4, and 8, respectively. The short-dashed line labeled SW is the spin-wave estimate $m=0.606$[8] in the limit $U\to\infty$, which is believed to be close to the true value.[9] We also show the Hartree-Fock prediction (dashed line), and the product of the Hartree-Fock values with the spin-wave estimate (solid line). It can be seen that the Hartree-Fock results, which account for charge fluctuations, corrected for zero-point fluctuations by the spin-wave result, give reasonable agreement with our numerical estimates.

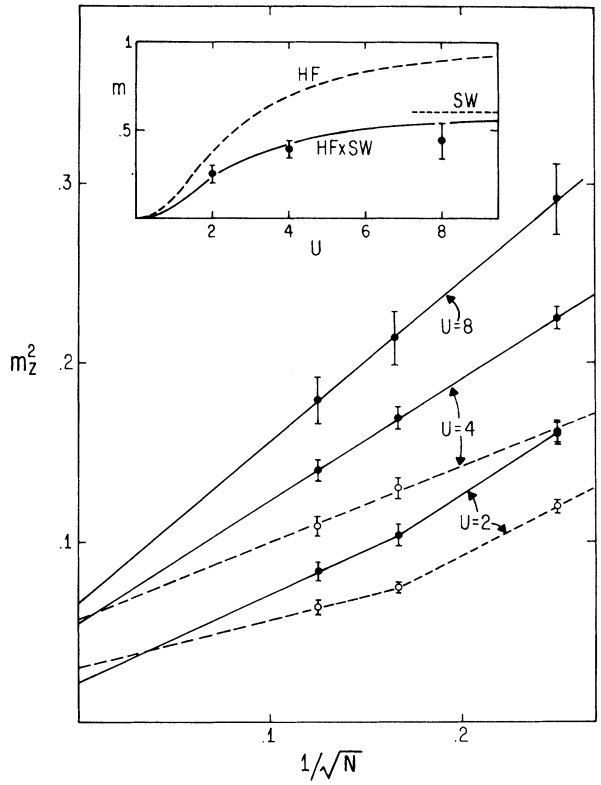

FIG. 3. Extrapolation of magnetic long-range order m_z^2. $S(\pi)/N$ (filled circles, solid lines) and $C_{L/2,L/2}$ (open circles, dashed lines) are plotted vs $1/\sqrt{N}$, N is the number of lattice points. Inset: The extrapolated long-range order $m=\sqrt{3}m_z$, the Hartree-Fock prediction (dashed line), the $T=0$ spin-wave prediction for the Heisenberg model (short-dashed line), and the product of Hartree-Fock and spin-wave results (solid line).

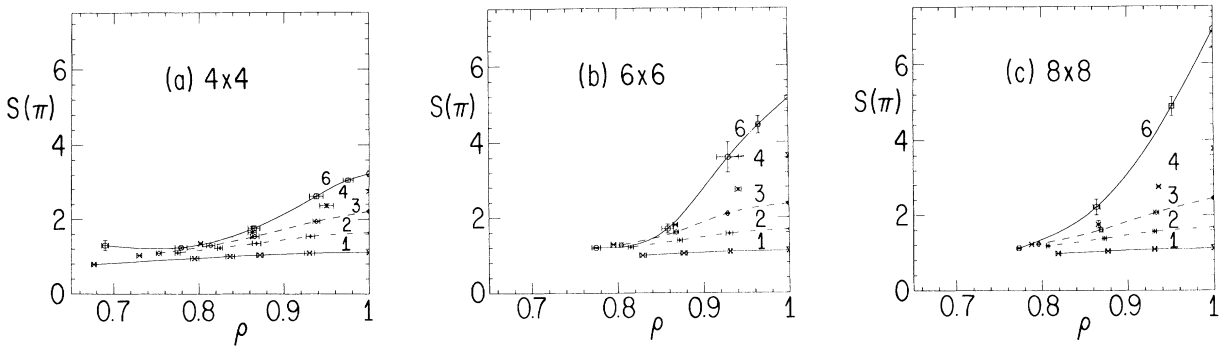

FIG. 4. Magnetic structure factor at wave vector $\mathbf{q}=(\pi,\pi)$ vs band filling for $U=4$, with 4×4, 6×6, and 8×8 lattices at various temperatures. The numbers next to the curves indicate β, the curves are drawn through the points to guide the eye.

We now discuss briefly the magnetic behavior of the system under doping. It was observed in Ref. 2 that antiferromagnetic correlations are suppressed extremely rapidly with doping, and conjectured that the antiferromagnetic order disappears immediately away from half filling. We present here some further evidence in support of this conjecture. Figure 4 shows the magnetic structure factor versus band filling for $U=4$, lattices of size 4×4, 6×6, and 8×8 and various temperatures. Unfortunately, away from half-filling negative signs in the fermion determinants prevent us from carrying out simulations beyond $\beta=6$ (except for the 4×4 lattice where $\beta=8$ can be reached) in a range of band filling close to $\frac{1}{2}$. Nevertheless, Fig. 4 shows that the suppression of $S(\pi)$ as ρ deviates from 1 becomes sharper as $T\rightarrow 0$ and $N\rightarrow\infty$, suggesting that no long-range order exists except for $\rho=1$. As a further argument, we remark that to have finite long-range order, the quantity $S(\pi)/\sqrt{N}$ should be an *increasing* function of N; in the range of parameters shown in Fig. 4, this is not the case except for $\rho>0.98$. Of course, in a real material other effects not included here, like anisotropy or a three-dimensional coupling, could easily stabilize long-range antiferromagnetic order in a finite range around the half-filled band case.

In summary, we have presented results of Monte Carlo simulations of the two-dimensional Hubbard model that demonstrate that long-range antiferromagnetic order exists down to the smallest U studied ($U=2$), and suggest that it exists for arbitrary nonzero U. We also obtained estimates for the long-range order and spin-wave velocity as functions of U. Our results for the long-range order are consistent with the Hartree-Fock results corrected by zero-point spin fluctuations as described by spin-wave theory. We found the spin-wave velocity to decrease as U decreases in the parameter range studied, evidently because charge fluctuations are weakening the effective exchange (for sufficiently large U, c should of course increase with decreasing U).[10] A more detailed discussion of our results, particularly away from half filling, and implications of our results for theoretical models such as resonating-valence-bond theory[11] and spin bags[12] will be presented in a separate publication.

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Note added.— For the Heisenberg model we have recently found that the Arovas-Auerbach mean-field theory or a closely related sublattice-symmetric spin-wave theory yield the exact spin-spin correlations to better than 1% for the lattices studied here (J.E. Hirsch and S. Tang, University of California at San Diego preprint).

[1]See, for example, *Proceedings of the International Conference on High-Temperature Superconductors and Materials and Mechanisms of Superconductivity, Interlaken, Switzerland, 1988,* edited by J. Müller and J. L. Olsen (North-Holland, Amsterdam, 1988).

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[6]D. A. Huse, Phys. Rev. B **37**, 2380 (1988); previous numerical work [J. Oitmaa and D. Betts, Can. J. Phys. **56**, 897 (1978) and Ref. 2] erroneously used a $1/N$ extrapolation.

[7]A recent Monte Carlo estimate of $C_{L/2,L/2}=(0.37)^2$ for $U=4$ on a 16×16 lattice (S. Sorella *et al.*, to be published) is inconsistent with our results in Fig. 3. We do not know the origin of the discrepancy.

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[10]The spin-wave theory prediction for the spin-wave velocity in the Heisenberg model is $c=6.55$ in units where the exchange constant J multiplying the Pauli matrices is unity, in good agreement with finite-lattice calculations (H. Neuberger and T. Ziman, to be published). For the Hubbard model at large U, $J=t^2/U$ yielding $c(U=8)=0.82$, not too far from our estimate for this case.

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