Magnetic susceptibility of the two-dimensional Hubbard model

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Using quantum Monte Carlo techniques we study the magnetic susceptibility of the Hubbard model on a two-dimensional square lattice for values of the coupling U/t ranging from 4 to 20, and as a function of temperature and doping. For $U/t=4$ the magnetic susceptibility has a maximum at half filling and decreases with doping, in qualitative agreement with recent random-phase-approximation calculations. However, for $U/t=10$ the susceptibility increases with hole doping near half filling resembling the experimental results obtained for $La_{2-x}Sr_xCuO_4$. At low electronic density the temperature dependence of the susceptibility is compatible with that of a Fermi liquid.

Superconductivity in the high-temperature copper-oxides[1] appears in the vicinity of antiferromagnetic order. This may have important implications for the pairing mechanism. Studies of the uniform magnetic susceptibility, χ, in $La_{2-x}Sr_xCuO_4$ (Refs. 2 and 3) have shown that as the doping x increases from zero at a fixed temperature so does χ. Fixing the electronic density at half filling and changing the temperature, the susceptibility reaches a maximum value at a finite temperature T_m that eventually goes to zero as the material is doped with holes. This behavior, in turn, leads to an anomalous temperature dependence of the Knight shift and the nuclear-spin-relaxation rates $1/TT_1$.[4]

It is widely believed that the interesting low-temperature magnetic behavior in the cuprate high-T_c superconductors comes predominantly from the copper-oxide planes. Some of the experimental properties of these planes, like antiferromagnetism, spin incommensurability at finite doping, and the optical conductivity, have been successfully qualitatively reproduced using two-dimensional purely electronic models, like the *t-J* and the one-band Hubbard models.[5,6] Since the qualitative behavior of some of these magnitudes does not depend strongly on U/t, weak-coupling techniques have successfully described them, but more quantitative comparisons with experimental results suggest that $U/t\approx 10$ is more realistic to phenomenologically describe the cuprate materials.[7] For the *t-J* model, on the other hand, qualitative changes in the ground state, such as phase separation and *d*-wave superconductivity,[8] are observed as J/t increases. Other properties of the copper-oxide compounds are not theoretically understood. Among them is the behavior of the uniform magnetic susceptibility as a function of temperature and doping. Its study will be the subject of this paper.

The magnetic susceptibility has been analyzed in the context of the Hubbard model using weak-coupling methods like random-phase approximation (RPA).[9] Under this approximation T_m is always zero, and in addition the susceptibility decreases with doping in disagreement with experiments on $La_{2-x}Sr_xCuO_4$. However, recent high-temperature expansions (HTE's) up to ninth order in $1/T$, and extrapolated to low temperatures by Padé approximants were carried out for the *t-J* model.[10] The observed behavior is in qualitative agreement with experiments for $J/t\approx 0.5$. The discrepancy between RPA and HTE is difficult to explain.[11] One possibility is that the behavior of the susceptibility is different in the weak-coupling and strong-coupling limits and that RPA is capturing only the weak-coupling behavior. Another possibility is that the behavior that resembles experiments is characteristic of the *t-J* rather than the Hubbard model and appears at some finite value of J/t. One of the goals of this paper is to solve this paradox. Analytical approaches such as mean-field, RPA, and high-temperature expansions have proved to be very useful in describing bulk properties of Hamiltonians, but are somewhat uncontrolled. RPA sums an arbitrary set of Feynman diagrams, while HTE relies on analytic continuation to extract low-temperature properties. On the other hand, there are numerical methods, like exact diagonalization and quantum Monte Carlo, that provide exact results on finite lattices. Hence, in order to obtain bulk results with these techniques finite-size effects have to be considered. Thus, numerical and analytical techniques are complementary to each other.

The goal of this paper is to study the uniform magnetic susceptibility of the Hubbard model for U/t ranging from weak to strong coupling, using an unbiased method such as quantum Monte Carlo.[12] Finite-size effects will be analyzed and comparisons with experiments and previous analytical results will be made. The Hubbard model is defined by the standard Hamiltonian

$$H=-t\sum_{\langle \mathbf{ij}\rangle,\sigma}(c^\dagger_{\mathbf{i},\sigma}c_{\mathbf{j},\sigma}+\mathrm{H.c.})+U\sum_{\mathbf{i}}n_{\mathbf{i}\uparrow}n_{\mathbf{i},\downarrow}\ , \qquad (1)$$

where $c^\dagger_{\mathbf{i},\sigma}$ creates an electron at site $\mathbf{i}$ with spin projection σ, $n_{\mathbf{i},\sigma}$ is the number operator, and the sum $\langle \mathbf{ij}\rangle$ runs over pairs of nearest-neighbor lattice sites. U is the on site Coulombic repulsion, and t the hopping parameter. The *t-J* model is defined by

$$H=-t\sum_{\langle \mathbf{ij}\rangle,\sigma}(\bar{c}^\dagger_{\mathbf{i},\sigma}\bar{c}_{\mathbf{j},\sigma}+\mathrm{H.c.})+J\sum_{\langle \mathbf{ij}\rangle}\mathbf{S_i}\cdot\mathbf{S_j}\ , \qquad (2)$$

where $\bar{c}^\dagger_{\mathbf{i},\sigma}$ creates a hole at site $\mathbf{i}$ with spin projection σ, and $\mathbf{S_i}$ are spin operators. As the Hubbard coupling increases, double occupancy of a lattice site becomes less likely and the Hubbard Hamiltonian approximately maps on the t-J model with $J=4t^2/U$. The two are strictly equivalent in the limit $J/t=4t/U=0$. Then the t-J model can be regarded as the strong-coupling limit of the Hubbard model although Zhang and Rice derived it directly from the copper oxide planes.[13] It is important to notice that as J/t increases the mapping is no longer accurate. Actually, exact diagonalizations on 4×4 lattices show that the one band Hubbard and the t-J models are no longer equivalent for $J/t\geq0.4$.[14]

The magnetic susceptibility is given by

$$\chi=\lim_{\mathbf{q}\to0}\frac{1}{N}\sum_{l}e^{i\mathbf{q}\cdot l}\int_0^\beta d\tau\langle[n_{\mathbf{i}+l,\uparrow}(\tau)-n_{\mathbf{i}+l,\downarrow}(\tau)]\times[n_{\mathbf{i},\uparrow}(0)-n_{\mathbf{i},\downarrow}(0)]\rangle\ , \quad (3)$$

where $\beta=1/T$ and T is the temperature, $\mathbf{q}$ denotes momentum and N is the number of lattice sites. Before presenting our results, let us discuss the expected behavior of χ in several limits. For a Fermi liquid χ is finite at low temperature (proportional to the density of states) and as T increases it decreases to zero following the Curie-Weiss law. We should expect to observe this behavior at very low fillings, where double occupancy is unlikely, and certainly also at $U/t=0$. When U/t is large and the system is half filled, Eq. (1) maps onto the Heisenberg model. In this case χ reaches a maximum at $T\approx J$ and then drops by about a factor of 2 at $T=0$.[15] As the system is doped away from half filling the maximum value of χ is expected to increase. This occurs because $\chi\propto1/J$, and we can mimic the effect of doping by replacing J by an effective coupling J_{eff} with $J_{\text{eff}}<J$. Neither the increase of χ with doping starting at half filling nor the increase with temperature starting at $T=0$, have been reproduced by RPA calculations.

In Fig. 1 we show χ vs T for $U/t=4$ at different fillings obtained with quantum Monte Carlo. We present results on 4×4 and 8×8 lattices in order to discuss finite-size effects. It can be seen that they are small at low hole doping including half filling. As the doping increases they become important at low temperature. Let us try to understand why this occurs and what we should expect at larger values of the coupling. At $U=0$, finite-size effects are significant, since we expect that $\chi\propto\beta e^{-\beta\Delta_{SW}}$, where Δ_{SW} is the gap between the ground state and the first excited state with total spin 1. For $U=0$ there are degeneracies that in small lattices will cause χ to diverge as β at low temperature for some dopings. In small systems there are finite gaps between states then for certain fillings χ will go to 0 below temperatures of the order of these gaps. As U/t increases we expect less degeneracies and smaller gaps, and thus finite size effects should be less important.

At half filling [Fig. 1(a)] Heisenberg-like behavior is observed showing the existence of long-range antiferromagnetic order. Of course, the position of the peak in χ is not well predicted by the relation valid in the Heisenberg model, $T_m\approx J=4/U$, since U/t is small. As the filling decreases to 0.75 [Fig. 1(b)] the susceptibility *decreases* and becomes flatter. This behavior is in agreement with RPA calculations but not with that observed experimentally in the cuprate superconductors. At quarter filling finite-size effects are strong [Fig. 1(c)], since even on an 8×8 lattice an spurious divergence in the susceptibility is observed at low temperature. At low density, $\langle n\rangle=0.25$ [Fig. 1(d)], Monte Carlo results for $U/t=4$ are compared

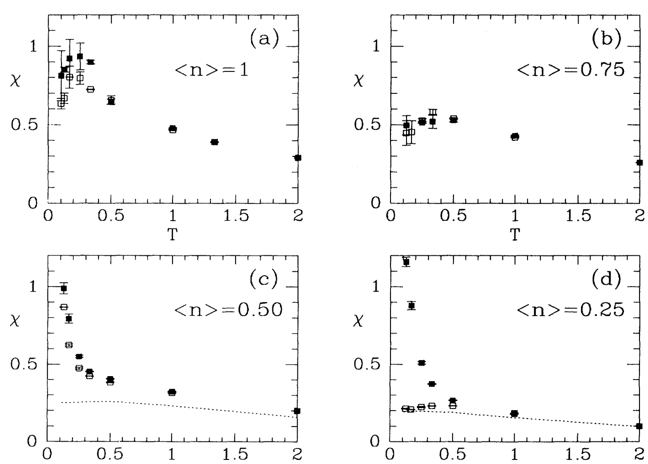

FIG. 1. Uniform magnetic susceptibility χ as a function of temperature for $U/t=4$ on a 4×4 (full squares) and on an 8×8 lattice (open squares) for $\langle n\rangle=1.0$ (a), 0.75 (b), 0.50 (c); and 0.25 (d). The dotted line denotes the $U=0$ susceptibility.

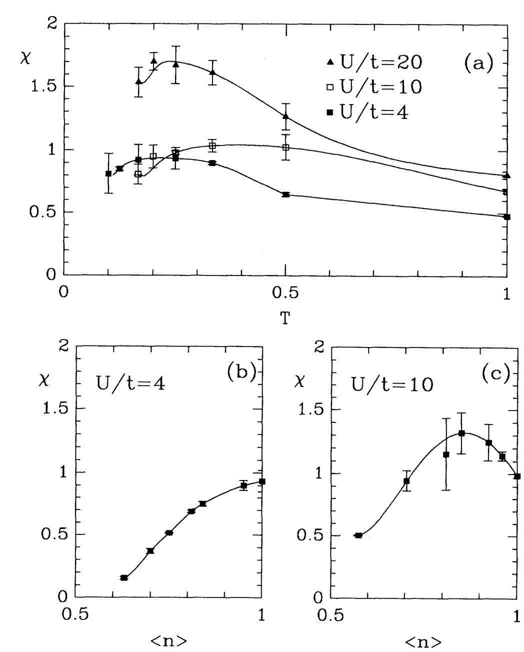

FIG. 2. (a) Uniform magnetic susceptibility as a function of temperature at half-filling on a 4×4 lattice for different values of U/t. (b) Uniform magnetic susceptibility as a function of density at temperature 0.25 on a 4×4 lattice for $U/t=4$. (c) Uniform magnetic susceptibility as a function of density at temperature 0.25 on a 4×4 lattice for $U/t=10$.

with $U=0$ results. We had to use a 32×32 lattice to obtain a behavior without finite-size effects for $U=0$ at T as low as 0.1. Similar behavior, though, was obtained for $U/t=4$ on an 8×8 lattice in agreement with our earlier remark stating that finite-size effects are expected to diminish as the value of the coupling increases. Clearly at this low-filling Fermi-liquid-like behavior is observed.

Our results for $U/t=4$ indicate that RPA successfully reproduces the physics of the Hubbard model in this limit. What happens when the coupling increases? In Fig. 2(a) we present the behavior of χ as a function of temperature for different values of U/t at half filling on 4×4 clusters. For $U/t=4$ finite-size effects are not strong for $\langle n\rangle>0.5$ and, as shown before, we expect them to become smaller as U/t increases. χ increases with the coupling because the magnetic correlations become stronger. At large U, when the Heisenberg model is a good approximation to Eq. (1) the susceptibility is expected to peak at $T\approx4/U$, as it occurs for $U/t=10$ and 20. In Figs. 2(b) and 2(c) we show the behavior of χ at $T=0.25$ for $U/t=4$ and 10, respectively, as a function of doping. In Fig. 2(b) we see that χ clearly decreases with doping for $U/t=4$. The behavior of χ changes qualitatively for $U/t=10$ as it is shown in Fig. 2(c). As the system is doped away from half filling, the susceptibility increases reaching a maximum at $\langle n\rangle\approx0.83$. Figure 2(c) is in qualitative agreement with experiments. These results suggest that the RPA approach successfully describes the behavior of the one band Hubbard model for $U/t\approx4$ but fails for stronger couplings. On the other hand, comparisons with the *t-J* model imply that for $U/t=4t/J\geq10$ Hubbard and *t-J* models are very similar. It is important to notice that the behavior of χ for the Hubbard model in two dimensions appears to be different than one dimension,[16] where a maximum at finite T is present for all values of U/t and χ increases slightly with doping at very small U.

In this paper we have shown that the qualitative behavior of the magnetic susceptibility of the one-band Hubbard model strongly depends on the coupling U/t. We found that RPA calculations failed to reproduce the experimental results for χ in the superconducting cuprates because the method only captures weak-coupling behavior, while experimental results are well reproduced using couplings equal or larger than $U/t=10$ in the one-band Hubbard model.

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[1]J. G. Bednorz and K. A. Müller, Z. Phys. B **64**, 188 (1986); C. W. Chu *et al.*, Phys. Rev. Lett. **58**, 405 (1987).
[2]J. B. Torrance *et al.*, Phys. Rev. B **40**, 8872 (1989).
[3]D. Johnston, Phys. Rev. Lett. **62**, 957 (1989).
[4]W. W. Warren *et al.*, Phys. Rev. Lett. **62**, 1193 (1989); R. E. Waldstedt *et al.*, Phys. Rev. B **41**, 9574 (1990); **44**, 7760 (1991); M. Takigawa *et al.*, *ibid.* **43**, 247 (1991); H. Alloul *et al.*, Phys. Rev. Lett. **63**, 1700 (1989).
[5]E. Dagotto, A. Moreo, F. Ortolani, D. Poilblanc, and J. Riera, Phys. Rev. B **45**, 10 741 (1992).
[6]A. Moreo, E. Dagotto, J. Riera, F. Ortolani, and D. J. Scalapino, Phys. Rev. B **45**, 10 107 (1992).
[7]Hybertsen *et al.*, Phys. Rev. B **41**, 11 068 (1990).
[8]E. Dagotto and J. Riera, Phys. Rev. Lett. **70**, 682 (1993).
[9]N. Bulut, D. W. Hone, D. J. Scalapino, and N. E. Bickers, Phys. Rev. B **41**, 1797 (1990); J. Lu, Q. Si, J. H. Kim, and K. Levin, Phys. Rev. Lett. **65**, 2466 (1990).
[10]R. Singh and R. Glenister, Phys. Rev. B **46**, 11 871 (1992).
[11]Studies of χ for the *t-J* model based on a slave-boson mean-field approximation do not agree with the HTE results. See T. Tanamoto, K. Kuboki, and H. Fukuyama, J. Phys. Soc. Jpn. **60**, 3072 (1991).
[12]S. R. White *et al.*, Phys. Rev. B **40**, 506 (1989).
[13]F. C. Zhang and T. M. Rice, Phys. Rev. B **37**, 3759 (1988).
[14]A. Moreo, Phys. Rev. B **45**, 4907 (1992).
[15]G. Gómez-Santos, J. D. Joannopoulos, and J. W. Negele, Phys. Rev. B **39**, 4435 (1989); S. Bacci, E. Gagliano, and E. Dagotto, *ibid.* **44**, 285 (1991).
[16]T. Usuki, N. Kawakami, and A. Okiji, J. Phys. Soc. Jpn. **59**, 1357 (1990).