Indications of a metallic antiferromagnetic phase in the two-dimensional U-t-t' model

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We present mean-field and quantum Monte Carlo results that suggest the existence of an itinerant antiferromagnetic ground state in the half-filled U-t-t' model in two dimensions. In particular, working at $t'/t=-0.2$ we found that antiferromagnetic long-range order develops at $U_{c_1}/t\approx 2.5\pm 0.5$, while a study of the density of states $N(\omega)$ and the response to an external magnetic field indicates that the system becomes insulating at a larger coupling $4<U_{c_2}/t<6$. [S0163-1829(97)50406-1]

The interest in metal-insulator transitions started several decades ago with the observation that nickel oxide (NiO), a transparent nonmetal, should be metallic according to its electronic band structure.[1] Afterwards, several models were proposed to study metal-insulator transitions, including the well-known Hubbard model. Brinkman and Rice found that when the on-site Coulomb repulsion U reaches $U_c=1.15W$, where W is the electronic bandwidth,[2] the ground state should change from metallic to insulating. However, a variety of numerical and analytical studies have convincingly shown that the half-filled Hubbard model with electronic hopping between nearest-neighbor sites has an insulating antiferromagnetic ground state for any finite value of the coupling U. The addition of a hopping along the plaquette diagonals to the Hubbard Hamiltonian destroys the nesting, and the possibility of a finite critical coupling (U_c) at half filling is recovered. U_c depends on the diagonal hopping t', and in previous work it has been obtained by monitoring the value of U at which antiferromagnetic long-range order (AFLRO) develops.[3] Mean-field and quantum Monte Carlo methods have been the techniques most used for this purpose. It is generally accepted that the half-filled U-t-t' model has a metallic ground state for $U<U_c$ and an antiferromagnetic insulating (AFI) state for $U>U_c$.

The aim of our work is the study of the metal-insulator transition (MIT) in the U-t-t' model using updated numerical techniques. We will monitor the development of AFLRO from the behavior of the spin correlations, and we will search for the onset of an insulating phase by studying the density of states and the response of the system to magnetic fields. The main result is that we have found indications of the existence of an intermediate phase between the paramagnetic metal and the AF insulator. The phase can be characterized as an AF metal (AFM). The existence of two-dimensional systems with nonordered metallic, AFI, and AFM phases has recently been discussed.[4]

The U-t-t' Hamiltonian is given by

$$H=-t\sum_{\langle \mathbf{ij}\rangle,\sigma}(c^{\dagger}_{\mathbf{i},\sigma}c_{\mathbf{j},\sigma}+\text{H.c.})-t'\sum_{\langle \mathbf{in}\rangle,\sigma}(c^{\dagger}_{\mathbf{i},\sigma}c_{\mathbf{n},\sigma}+\text{H.c.})+U\sum_{\mathbf{i}}(n_{\mathbf{i}\uparrow}-1/2)(n_{\mathbf{i}\downarrow}-1/2)+\mu\sum_{\mathbf{i},\sigma}n_{\mathbf{i}\sigma}, \tag{1}$$

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, the sum $\langle \mathbf{ij}\rangle$ runs over pairs of nearest-neighbor lattice sites, and the sum $\langle \mathbf{in}\rangle$ runs over pairs of lattice sites along the plaquette diagonals. U is the on-site Coulombic repulsion, t the nearest-neighbor hopping amplitude, t' the hopping amplitude along the plaquette diagonals, and μ is the chemical potential. In the following $t=1$ will be used.

As a first step, the Hamiltonian will be studied using the spin density wave (SDW) mean-field (MF) approximation.[5] Proposing as an ansatz an AF ground state and following the standard Bogoliubov procedure to diagonalize exactly the resulting MF Hamiltonian, we found two energy bands given by

$$E^{\pm}_{\mathbf{k}}=E^{d}_{\mathbf{k}}-\mu\pm E^{0}_{\mathbf{k}}, \tag{2}$$

where

$$E^{d}_{\mathbf{k}}=-4t'\cos k_x\cos k_y, \tag{3}$$

$$E^{0}_{\mathbf{k}}=\sqrt{\epsilon^2_{\mathbf{k}}+\Delta^2}, \tag{4}$$

and

$$\epsilon_{\mathbf{k}}=-2t(\cos k_x+\cos k_y). \tag{5}$$

Δ is the MF parameter that, when finite, indicates that the ground state has AFLRO. Both Δ and μ are obtained by solving the self-consistent equations

$$\frac{1}{U}=\frac{1}{N}\sum_{\mathbf{k}}\frac{[f(E^{-}_{\mathbf{k}})-f(E^{+}_{\mathbf{k}})]}{E^{0}_{\mathbf{k}}}, \tag{6}$$

and

$$\langle n\rangle=\sum_{\mathbf{k}}n(\mathbf{k}), \tag{7}$$

where $f(x)$ is the Fermi function given by $1/(e^{\beta x}+1)$, N is the number of sites in the lattice, and

$$n(\mathbf{k})=\frac{1}{2}\left(1-\frac{\epsilon_{\mathbf{k}}}{E^{0}_{\mathbf{k}}}\right)f(E^{-}_{\mathbf{k}})+\frac{1}{2}\left(1+\frac{\epsilon_{\mathbf{k}}}{E^{0}_{\mathbf{k}}}\right)f(E^{+}_{\mathbf{k}}). \tag{8}$$

Equations (6)–(8) can be solved at any temperature T but since we are trying to study ground state properties we will

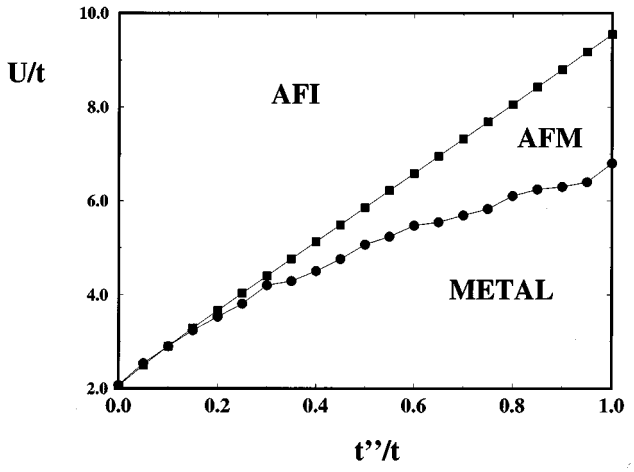

FIG. 1. SDW mean-field phase diagram of the U-t-t'-t'' model at half filling and $T=0$, for $t=1$ and $t'=-0.2$.

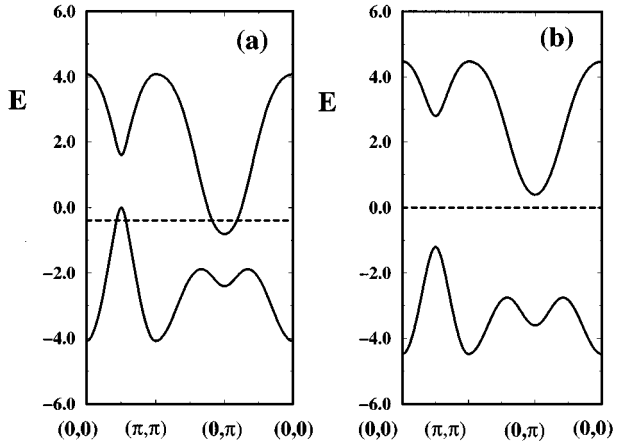

FIG. 2. SDW mean-field band structure of the half-filled U-t-t'-t'' model for $t=1$, $t'=-0.2$, and $t''=0.2$ (a) in the AFM phase with $U=3.57$ and $\Delta=0.8$ and (b) in the AFI phase with $U=5.1$ and $\Delta=2.0$. The dashed line indicates the position of the chemical potential.

work at $T=0$. To study the MIT discussed above $\langle n\rangle=1$ is fixed in our calculations. When $t'=0$ it is found that as soon as Δ becomes different from zero, indicating the existence of an AF ground state, a gap of size 2Δ opens between the two bands given by Eq. (2), and the chemical potential lies inside the gap. However, when $t'\neq 0$, the shape of the bands is distorted, and even when AF has developed, the two bands overlap if $\Delta\leqslant 2|t'|$. This occurs because the actual gap is defined by the separation between the highest state in the lower band and the lowest state in the upper band. For $t'<0$ these states have $\mathbf{k}=(\pi/2,\pi/2)$ and $\mathbf{k}=(\pi,0)$, respectively (for $t'>0$ the momenta are reversed). For example, for $t'<0$, the lowest state in the upper band has energy $\Delta-4|t'|$ while the highest state in the lower band has energy $-\Delta$. An analogous condition is obtained for $t'>0$. Then, an effective finite gap exists if $\Delta>2|t'|$. Therefore, in the region where the bands overlap the ground state is antiferromagnetic, but it has metallic properties because the chemical potential cuts both the lower and upper bands. Unfortunately, solving the MF equations we found that the AFM is not stable in this case since Δ changes *discontinuously* from zero to $2|t'|$ at a particular value of U which depends on t'. This is due to the fact that the energy as a function of Δ, in this case, has a two minima structure. Then, the AFM phase exists only at one point in parameter space. However, it is reasonable to expect that the AFM phase might be stabilized by including the effect of fluctuations beyond the MF approximation. Rather than adding these fluctuations, we intuitively believe that their effect could be mimicked by introducing longer-range hopping terms in the kinetic energy. Thus, we have added to the MF calculation an additional hopping term between second nearest neighbors in the x and y directions with strength regulated by the parameter t''. The MF equations are modified simply by replacing $E^d_{\mathbf{k}}$ in Eq. (3) by

$$E^d_{\mathbf{k}}=-4t'\cos k_x\cos k_y-2t''(\cos 2k_x+\cos 2k_y). \qquad (9)$$

In this case we found that the overlap of the bands occurs if $0\leqslant\Delta\leqslant 2|t'|+4t''$. The introduction of t'' stabilizes the AFM phase in the MF approximation as can be seen in the phase diagram presented in Fig. 1 for $t'=-0.2$. The circles indicate the values of U_{c_1} where the ground state changes from paramagnetic metal to AF metal, i.e., where Δ becomes nonzero but the bands still overlap. The squares represent a second critical coupling, U_{c_2}, at which the ground state becomes an AF insulator. This occurs when Δ becomes larger than $2|t'|+4t''$ and the bands no longer overlap. In Fig. 2(a) the energy bands along certain directions in momentum space in the AFM phase are shown. As was discussed above, it is clear that the two bands overlap and the position of the chemical potential, denoted with a dashed line, indicates that the top of the lower band is empty while the bottom of the upper band is filled. The energy bands in the AFI phase are presented in Fig. 2(b). In this case, μ lies in the middle of the gap and the system is clearly an insulator. Then, at the MF level, the addition of longer-range hopping terms stabilizes the AFM ground state.[6]

To find further support for the existence of the AFM ground state, quantum Monte Carlo (QMC) techniques have been here applied to the study of the U-t-t' model, working at $t'=-0.2$ on 8×8 lattices and temperatures $T=1/8$ and $1/6$. For these values of the parameters the MF approximation (with $t''=0$) predicts $U_c=2.1$. Previous quantum Monte Carlo results suggested that AFLRO develops for $U_{c_1}\approx 2.5$.[3] We have independently analyzed the spin-spin correlation function $C(r)$ as a function of distance for several values of U/t on an 8×8 cluster. The results are shown in Fig. 3. Note that a finite tail is already developed for $U/t=3$ but it is not present for $U/t=2$. Thus, a critical coupling $U_c\approx 2.5\pm 0.5$ is here estimated.[7] Now let us focus our attention to the coupling $U=4$ where AFLRO is clearly developed (Fig. 3). The next issue is whether the system is metallic or insulating for $U=4$. To investigate this important point, the density of states $N(\omega)$ was calculated using the maximum entropy technique.[8] The stability of the results was checked by making four independent long runs for each set of parameters. In Fig. 4(a) the results for $U=4$, $t'=-0.2$, and $\beta=6$ are presented. Three main peaks are observed in the results: those to the left and to the right of μ can be identified with the lower and upper Hubbard bands, while the

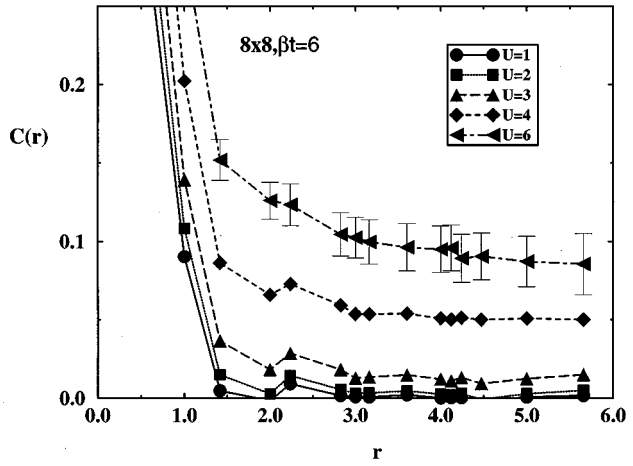

FIG. 3. QMC spin-spin correlation $C(\mathbf{r})=\langle S^z_{\mathbf{i}}S^z_{\mathbf{i}+\mathbf{r}}\rangle(-1)^{|\mathbf{r}|}$ for several values of U/t, $T=t/6$ on an 8×8 lattice at half filling for $t'/t=-0.2$. Points without error bars have errors smaller than the size of the dots.

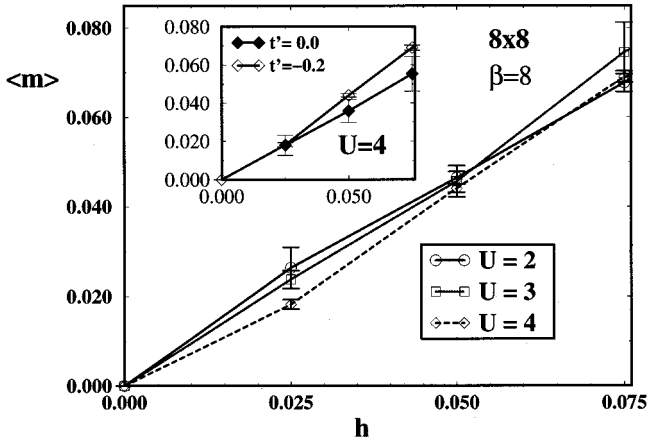

FIG. 5. Magnetization m versus magnetic field h for the half-filled U-t-t' model. $t'=-0.2$ and $U=2$, 3, and 4 at $T=t/8$. In the inset m versus h is shown for $U=4$ and $t'=0$ (filled diamonds) and -0.2 (open diamonds).

peak at μ corresponds to the quasiparticle weight, indicating that the system is metallic. This metallic behavior disappears as U increases and an effective gap develops. In Fig. 4(b) $N(\omega)$ for $U=6$, $t'=-0.2$ and $\beta=4$ is shown. Here the finite temperature precursor of an insulating gap in the density of states has developed and the chemical potential lies inside the gap. Notice that these results are in agreement with those we obtained in Ref. 9, where the gap was studied by monitoring the behavior of the density $\langle n\rangle$ versus μ, as well as the spectral functions $A(\mathbf{k},\omega)$. In Fig. 4(c) the mean-field result for $N(\omega)$ in the AFM region is presented. It is remarkable that the three main peak structure is qualitatively similar to that found numerically for $U=4$. The MF density of states in the AFI phase is presented in Fig. 4(d), where there is also good qualitative agreement with the QMC numerical results for $U=6$.

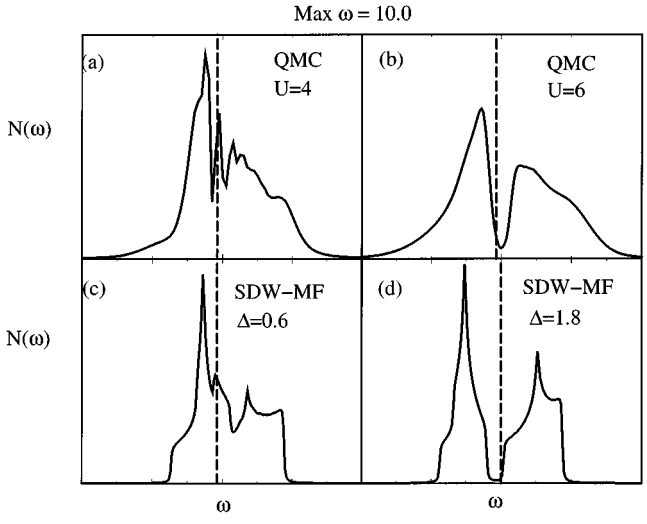

FIG. 4. QMC density of states $N(\omega)$ for the U-t-t' model at half filling for $t'=-0.2$ and (a) $U=4$, $\beta=6$, on an 8×8 lattice; (b) same as (a) for $U=6$ and $\beta=4$; (c) mean-field results on a 200×200 lattice at $T=0$ using $t''=0.2$, $\Delta=0.6$, and $\mu=-0.382$; (d) same as (c) with $\Delta=1.8$ and $\mu=0$. The MF transition between AFM and AFI occurs for $\Delta=1.2$.

In spite of the good agreement between the SDW-MF and QMC numerical data suggesting the existence of an AFM phase and a metal-insulator transition somewhere in the interval $4<U_{c_2}<6$, we decided to study the lower limit for U_{c_2} using an alternative technique. It is well known that when a metallic system is close to its critical coupling towards an insulator, a magnetic field can induce a metal-insulator transition.[10,11] The signature of the transition at low temperature is a discontinuity (''metamagnetic transition'') in the magnetization m as a function of the magnetic field h for U slightly smaller than U_{c_2}. For a coupling close to but smaller than U_{c_2}, the system is still metallic at zero magnetic field. The magnetization curve follows a metallic behavior until the field reaches a critical value h_c that drives the system to become an insulator and, thus, produces the metamagnetic transition. Since we are working at small but finite temperature, we do not expect to find a perfect discontinuity but instead a very rapid crossover. In fact, in Ref. 11, where the Hubbard model in infinite dimension was studied, it was shown that only for $T<0.01$ a proper first-order phase transition is observed. However, defining $\chi=dm/dh$ as the magnetic susceptibility, at low but finite temperatures and at low magnetic fields we expect $d\chi/dh>0$ to be the signature of the metamagnetic transition that should occur at lower temperature. On the other hand, $d\chi/dh\leqslant 0$ would indicate normal behavior.[11] For a standard Fermi liquid, m vs h should be linear for small magnetic fields (i.e., $d\chi/dh=0$). With increasing h, the slope will decrease as m saturates to 1. The numerical calculation of m as a function of h is very difficult because the behavior that we want to study occurs at very small magnetic field, i.e., $h<0.1$. We found that the anomalous behavior is not observed for temperatures higher than $T=0.125$. To obtain numerical values with small enough error bars we needed to perform about 100 000 measuring QMC sweeps per point. In Fig. 5, m vs h for $t'=-0.2$ is shown at different values of U for $\beta=8$ on an 8×8 lattice. $d\chi/dh\leqslant 0$ is observed for $U=2$ and 3. However, for $U=4$, $d\chi/dh>0$ is found. This suggests that at $t'=-0.2$, $U=4$ is a lower bound for U_{c_2}. It could be argued that a

quantum antiferromagnet will have $d\chi/dh>0$ because its magnetization is given by $m=\chi h+$ sgn h $h^2/4\pi c^2$.[12] However, for the small values of h used here the linear term prevails as can be seen in the inset of Fig. 5, where the magnetization as a function of the magnetic field is shown for $U=4$ and $t'=0$. Since antiferromagnetism is reduced by the addition of a finite t' the upturn observed for $t'=-0.2$ cannot be caused by staggered spin correlations. Then, by comparing the two curves in the inset of Fig. 5, it is clear that $d\chi/dh$ becomes larger than zero due to the effect of the diagonal hopping. It appears that in the half-filled U-t-t' model when $t'=-0.2$, AFLRO develops at $U_{c_1}=2.5\pm0.5$, but the system becomes an insulator for U_{c_2} larger than 4. These numerical results again suggest that the AFM region exists, and it is actually broader than what was predicted at the mean-field level. Notice that the existence of AFM phases is not just an academic curiosity. Magnetically ordered metallic phases have been observed experimentally.[13] In particular, an AFM phase was found in organic κ-(BEDT-TTF)$_2X$.[14]

Summarizing, in this paper we have provided numerical and analytical results that suggest the existence of an antiferromagnetic metallic ground state in the two-dimensional U-t-t' model.[15]

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[6] It is important to remark that the cluster sizes that can be studied with quantum Monte Carlo impose limitations in our detection abilities of potential incommensurate order before the insulator phase is reached as U grows at fixed t'. Previous Hartree-Fock studies on triangular lattices have suggested such incommensurate intermediate phases [H. R. Krishnamurthy *et al.*, Phys. Rev. Lett. **64**, 950 (1990)]. In doped U-t Hubbard clusters short range incommensurability has been detected using clusters similar to those used here [A. Moreo *et al.*, Phys. Rev. B **41**, 2313 (1990)].

[7] The critical coupling U_{c_1} found here is in good agreement with the U_c reported in Ref. 3 though the bulk extrapolation used there was incorrect [see, for example, S. White *et al.*, Phys. Rev. B **40**, 506 (1989)].

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[15] An additional procedure to show numerically that the intermediate phase is indeed metallic would be to study the behavior of the Drude weight that acts as order parameter [see E. Dagotto, Rev. Mod. Phys. **63**, 763 (1994) and references therein]. However, the standard sum rule as well as the definition of the current are modified by the introduction of the diagonal hopping. Work along this line is in progress.