Incommensurate Antiferromagnetism in the Two-Dimensional Hubbard Model

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The magnetic states occurring in the two-dimensional Hubbard model in the vicinity of half filling of the conduction band are studied in the case of weak correlations, using Hartree-Fock theory. It is shown that at zero temperature the commensurate antiferromagnetic state is unstable against domain-wall formation for arbitrarily small deviations from half filling. The resulting incommensurate antiferromagnet remains initially insulating. The predictions of the model for the polarization and modulation wave vector of the incommensurate antiferromagnet are discussed.

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One of the most interesting properties of the copper-oxide-based high-T_c superconductors[1,2] is the close proximity of insulating antiferromagnetic[3,4] and superconducting phases: Fairly small compositional changes transform an insulating antiferromagnet into a superconductor. The insulating and magnetic properties can be explained by the effects of Coulomb repulsion in a half-filled band (e.g., one electron per site), whereas superconductivity typically occurs slightly away from half filling. A model containing the basic ingredients for the transition from an insulating antiferromagnet to a metal (and possibly a superconductor) is the two-dimensional Hubbard model.[5] For exactly one electron per site, i.e., a half-filled band, it is by now rather clear that this model has a two-sublattice (commensurate) antiferromagnetic ground state. Considerable effort has been devoted to the understanding of the effect of small deviations from half filling.[6-10] In most of these investigations it is assumed that the extra holes move in an essentially unchanged *commensurate* antiferromagnetic background and form a band of mobile carriers. Here I will show that, at least for relatively weak Coulomb repulsion, any finite concentration of holes changes the magnetic structure drastically, leading to an *incommensurate* antiferromagnet which remains insulating up to a critical concentration of holes. The recent observation of short-range incommensurate antiferromagnetic order[11] seems to lend some support to this picture.

In real compounds, correlation energies are probably (at least) comparable to the bandwidth. Here I will consider the limit of weak correlation, where the Hartree-Fock approximation is a valid starting point. It is hoped that the present results will shed some light on the physics in more strongly correlated cases. I consider the standard Hubbard Hamiltonian

$$H=-t\sum_{\langle i,j\rangle,s}(a_{is}^{\dagger}a_{js}+a_{js}^{\dagger}a_{is})+U\sum_{i}n_{i\uparrow}n_{i\downarrow}\,, \tag{1}$$

where a_{is} destroys an electron at site i with spin projection s, and $\langle i,j\rangle$ indicates summation over all nearest-neighbor pairs on a square lattice. For exactly one electron per site the model has a two-sublattice (commensurate) antiferromagnet ground state. To understand the physics away from half filling (i.e., for nonzero chemical potential μ), I use the Stoner criterion for the stability of the paramagnetic metallic state: A magnetically ordered state becomes stable as soon as $1-(U/2)\chi_0(\mathbf{k},T)<0$, where χ_0 is the magnetic susceptibility of the noninteracting system at wave vector $\mathbf{k}$ and temperature T. In the present case an expansion for $|\mu|,T\ll t,|\mathbf{q}|\ll\pi$ gives

$$\chi_0(\mathbf{Q}_0+\mathbf{q},T)=\chi_0(\mathbf{Q}_0,T)-\frac{1}{4\pi^2 t}[f(\tilde{\mu},\tilde{q}_+)+f(\tilde{\mu},\tilde{q}_-)]\,, \tag{2}$$

where $\mathbf{Q}_0=(\pi,\pi)$, $\tilde{q}_{\pm}=t(q_x\pm q_y)/2\pi T$, $\tilde{\mu}=\mu/2\pi T$, and

$$f(x,y)=\mathrm{Re}\int_{-\pi}^{\pi}\frac{du}{|\sin u|}[\psi(\tfrac{1}{2}+ix+iy\sin u)-\psi(\tfrac{1}{2}+ix)]\,. \tag{3}$$

At zero temperature the limiting form

$$\lim_{x,y\to\infty}f(x,y)=-2\,\mathrm{Re}[\arcsin^2(y/x+i0^-)]$$

is more useful. One can easily show that $f(x,y)$ has a minimum at $y\neq 0$ if $x>x_0=0.30409\ldots$, and therefore $\chi_0(\mathbf{k})$ has degenerate maxima at $\mathbf{Q}_1=(\pi\pm\delta,\pi)$ and $\mathbf{Q}_2=(\pi,\pi\pm\delta)$, with δ nonzero. At $T=0$ one has $\delta=\mu/t$. Consequently, the antiferromagnetically ordered phase appears with the *incommensurate* wave vectors $\mathbf{Q}_1$ and/or $\mathbf{Q}_2$ if $|\mu|>2x_0\pi T$.[12] Naively, one might have expected a modulation wave vector along the diagonal of the Brillouin zone: $\mathbf{Q}_3=(\pi\pm\delta,\pi\pm\delta)$. That the vectors $\mathbf{Q}_{1,2}$ lead to the stable state can be seen from the following argument: The antiferromagnetic state is stabilized with respect to the metallic state due to the opening of a gap on parts of the Fermi surface. For a given modulation wave vector $\mathbf{Q}$ a gap is opened along lines in the Brillouin zone given by $\epsilon_{\mathbf{k}}=\epsilon_{\mathbf{k}\pm\mathbf{Q}}$, where $\epsilon_{\mathbf{k}}=-2t(\cos k_x+\cos k_y)$ is the single-electron dispersion. The corresponding lines for $\mathbf{Q}_1$ and $\mathbf{Q}_3$ are shown in Fig. 1. One immediately sees that a $\mathbf{Q}_1$ modulation, with $\delta=2\times\sin^{-1}(|\mu|/2t)$, opens gaps on *all* the flat parts of the

Fermi surface, and thus leads to a lower energy than the $\mathbf{Q}_3$ modulation, which only opens a gap on half the flat parts of the Fermi surface.

Given the instability at wave vectors $\mathbf{Q}_{1,2}$, two questions remain: (i) Will there be a modulation with a single wave vector, $\mathbf{Q}_1$ or $\mathbf{Q}_2$, or a "double-Q" phase? (ii) Will this be a linearly polarized, spiral, or more complicated magnetic structure? To answer these questions, I write the moment at site $\mathbf{R}$ as

$$\langle \mathbf{m}(\mathbf{R}) \rangle = (4\mu_B/U)\mathrm{Re}(\Delta_1 e^{i\mathbf{Q}_1\cdot\mathbf{R}} + \Delta_2 e^{i\mathbf{Q}_2\cdot\mathbf{R}}) , \tag{4}$$

where $\Delta_{1,2}$ are *complex vector* order parameters. The Landau expansion of the free energy per site is then

$$\begin{aligned} F(\Delta_1,\Delta_2) = {} & a(\mathbf{Q}_1)[|\Delta_1|^2 + |\Delta_2|^2] + b_1[|\Delta_1|^2 + |\Delta_2|^2]^2 + b_2|\Delta_1|^2|\Delta_2|^2 \\ & + b_3[(\Delta_1\cdot\Delta_1)(\Delta_1^*\cdot\Delta_1^*) + (\Delta_2\cdot\Delta_2)(\Delta_2^*\cdot\Delta_2^*)] + b_4[(\Delta_1\cdot\Delta_2)(\Delta_1^*\cdot\Delta_2^*) + (\Delta_1\cdot\Delta_2^*)(\Delta_1^*\cdot\Delta_2)] , \end{aligned} \tag{5}$$

where $a(\mathbf{Q}) = 1/U - \chi_0(\mathbf{Q},T)/2$, and the analytical expressions for the b_i are rather involved and will be given in a subsequent paper. The Landau expansion (5) contains all symmetry-allowed quartic terms, and therefore allows discussion of all possible magnetic structures, independent of the underlying mechanism: For example, $b_2 > 0$ ($b_2 < 0$) leads to a single-$\mathbf{Q}$ (double-$\mathbf{Q}$) structure, $b_3 < 0$ ($b_3 > 0$) leads to a linearly polarized (spiral) antiferromagnet. In the present weak-coupling calculation $b_2 > 0$, $b_3 < 0$, and consequently I find a *linearly polarized single-*$\mathbf{Q}$ incommensurate antiferromagnet. The linear polarization is in agreement with general arguments for spin-density waves.[13] The phase diagram obtained from (5) for $U = 2t$ is shown in Fig. 2.[14] For the C-IC line, only the vicinity of the triple point and the $T \to 0$ limit (see below) are given by the present calculations. For different values of U, the general shape of the diagram remains unchanged; only the temperature and density scales have to be rescaled by a factor $\exp[-2\pi(t/U)^{1/2}]$. It should be emphasized here that this figure is obtained in the small-U approximation. It is quite possible that for stronger U the coefficients in (5) change, giving rise to a different (e.g., spiral[10]) structure.

A complete investigation of the phase diagram requires considerable calculational effort. In the following I will concentrate on ground-state properties. Close to the critical number of holes ($n_c = 0.857$ in Fig. 2), the amplitude of the spin modulation is small, and the Hartree-Fock wave functions are linear combinations of plane waves with wave vectors $\mathbf{k}$ and $\mathbf{k}+\mathbf{Q}$ only, with eigenenergies

$$E_{\mathbf{k}} = \tfrac{1}{2}\{\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{k}+\mathbf{Q}} \pm [(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{Q}})^2 + 4\Delta^2]^{1/2}\} . \tag{6}$$

The modulation wave vector $\mathbf{Q} = (\pi \pm \delta, \pi)$ and the gap Δ are determined variationally, with results shown in Fig. 3. The initially linear increase of Δ below n_c is due to the presence of nonanalytic terms in the ground-state energy. In that region a gap is only opened on parts of the Fermi surface, leaving pockets of holes in the vicinity of the points $(\pm\pi, 0)$ and $(0, \pm\pi)$ in Fig. 1; i.e., close to n_c the system remains metallic. With increasing electron concentration Δ increases and $\mathbf{Q}$ changes, leading to a progressive shrinking of these pockets. For a critical value of Δ [$\Delta = 2\sin^2(\delta/2) - \mu$ in the present approximation] the pockets disappear completely, leading to an *insulating incommensurate antiferromagnet for less than*

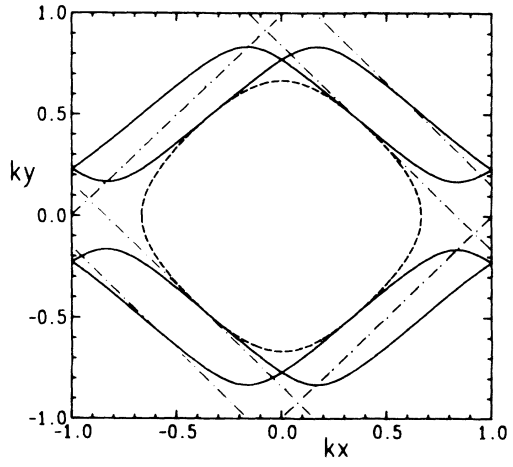

FIG. 1. Lines in the Brillouin zone along which a gap is opened for modulation vectors $\mathbf{Q}_1$ (solid lines) and $\mathbf{Q}_3$ (dash-dotted lines). The dashed line is the Fermi surface for $\mu = -t$. Momenta are in units of π.

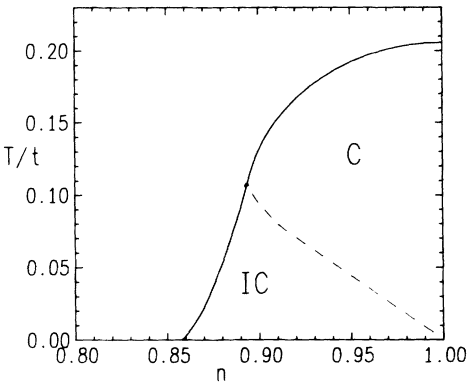

FIG. 2. Phase diagram (Ref. 14) in the temperature-density (n) plane for $U = 2t$, with commensurate (C) and incommensurate (IC) antiferromagnetic phases, and the paramagnetic state. Most of the C-IC line is only schematic (see text). For $n < n_c = 0.857$ the IC phase is metallic; for $n > n_c$ it is insulating.

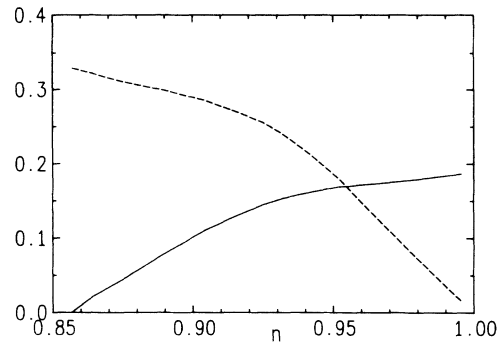

FIG. 3. Particle-density dependence of the gap parameter Δ/t (solid line) and the modulation wave vector δ (dashed line) at $T=0$ for $U=2t$. In this case, the hole pockets vanish for $n>0.942$.

one electron per site.

Well away from n_c, and in particular close to half filling, Δ can no longer be treated as small, and higher harmonics of the spin structure need to be considered. Then the full Hartree-Fock equations have to be used. Unless there is another phase transition in the incommensurate phase, the magnetic structure will be the same as that found from the systematic expansion in Eq. (5), e.g., linearly polarized and single **Q**. Assuming the modulation to be along the x direction, the Hartree-Fock single-particle eigenstates can be written as $\psi(x,y)=e^{ipy}[u_+(x)+(-1)^{x+y}u_-(x)]$, with $u_\pm$ depending *only* on x. These functions then obey the equations

$$-jt[u_j(x+1)+2\cos(p)u_j(x)+u_j(x-1)] -\Delta(x)u_{-j}(x)=Eu_j(x), \quad (7)$$

where $j=\pm$, $|p|\le\pi/2$, and $\Delta(x)$ has to be determined self-consistently: $\Delta(x)=U\langle n_\uparrow(x)-n_\downarrow(x)\rangle/2$, with the average taken over the occupied eigenstates of (7). In a commensurate antiferromagnet Δ is spatially constant, and Eq. (7) leads to two bands of extended states, separated by a gap 2Δ. By analogy with one-dimensional charge-density-wave systems, close to half filling (i.e., $n\ll n_c$) the spin structure is expected to be an equally spaced array of domain walls. I therefore have studied domain-wall-type solutions to Eq. (7) [a *variational Ansatz* would be $\Delta(x)=\Delta_0\tanh(x/x_0)$]. The following general statements can be made: (i) Provided $\Delta(-x)=-\Delta(x)$, $u_+(x),u_-(x)$ and $u_-(-x),u_+(-x)$ are solutions with energies E and $-E$, respectively, and consequently the spectrum of (7) is symmetric; (ii) for any domain-wall solution [$\Delta(\pm\infty)=\pm\Delta_0$] there are at least *two bound states* in the gap. The existence of bound states opens the possibility of the formation of a domain-wall structure as soon as there is less (or more) than one electron per site: The extra holes (electrons) gain energy by occupying the bound states, rather than the extended states of the commensurate structure. In order to decide whether the domain wall or the commensurate structure is more stable, the energies of the two states have to be compared. I have therefore solved Eq. (7) self-consistently for various values of U and system sizes up to 96×24. In all cases the domain wall has a lower energy than the commensurate structure, with a binding energy (e.g., difference between commensurate and domain-wall state) of about 0.34Δ per hole.[15] I therefore conclude that the commensurate state is *unstable against domain-wall formation as soon as there is less or more than one electron per site.* The extra holes or electrons are localized on the domain walls, and thus this state remains insulating.[16] A single domain wall of length N_y can accommodate N_y holes, and therefore at $1+\epsilon$ electrons per site the distance between walls is $1/|\epsilon|$, leading to a modulation wave vector $\delta=\pi|\epsilon|$. This agrees with the numerical results in Fig. 3, for $n\to1$. With increasing ϵ, domain walls start to overlap considerably, and then a rather complicated electronic structure is expected, which only in the limit of small Δ reduces to the rather simple form (6).

The formation of domain walls parallel to the y axis agrees with the fact that the instability of the paramagnetic phase appears at wave vector $\mathbf{Q}_1$, and not at $\mathbf{Q}_3$. For a $\mathbf{Q}_3$ instability one would expect diagonal walls, e.g., along $x=-y$. In that case the single-particle wave functions can be written as $\psi(x,y)=e^{ipr_-}u(r_+)$, with $r_\pm=x\pm y$ and u depending on r_+ only. The analog of Eq. (7) is then

$$-2\cos(p)t[u(r_++1)+u(r_+-1)] -(-1)^{r_+}\Delta(r_+)u(r_+)=Eu(r_+), \quad (8)$$

where $|p|\le\pi/2$. These are exactly the Su-Schrieffer-Heeger equations, with Fermi velocity proportional to $\cos(p)$.[17,18] Comparing numerical results for (8) to the solution of (7), I find that the binding energy per hole is always larger than (7) as long as U is smaller or comparable to the bandwidth $8t$, and therefore *the domain wall parallel to the y axis is stable.* For very large U Poilblanc and Rice find the diagonal wall energetically favorable.[19] One may also wonder whether a long-wavelength spiral state might be energetically favorable, due to the fact that the order parameter remains nonzero everywhere. However, one then does not form bound states in the gap, so that the holes have to go into the band of extended states, at energy $\cos t\approx0.34\Delta$ compared to the domain-wall state.

I have shown here that the introduction of holes (or extra electrons) into a half-filled Hubbard model leads to immediate changes in the magnetic structure: First, a widely spaced array of domain walls is formed, with the extra carriers bound to the domain walls. This is similar to "soliton doping" in one-dimensional systems.[17] With increasing doping the magnetic structure gradually transforms into a sine wave, and pockets of free carriers appear; i.e., the metal-insulator transition occurs *within the incommensurate antiferromagnetic phase.* Only

with further increase of carrier concentration does the antiferromagnetic order vanish completely. The finite interval of insulating behavior around half filling is in contrast to assumptions made in previous work, in both the weak-U and large-U limits, that carriers become immediately mobile in extended states. To what extent a finite insulating interval exists even for large U remains to be seen.[20] Beyond the sequence of different phases with increasing number of holes, the present model makes specific predictions about the polarization of the incommensurate antiferromagnet (longitudinal, not spiral) and about the direction of the wave vector (along x or y, not along the diagonal). These predictions could be tested on $La_{2-x}Sr_xCuO_4$, where incommensurate short-range order has been found.[11]

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[15]More detailed calculations show that this binding energy is considerably bigger than that found for spin bags by W. P. Su and X. Y. Chen, Phys. Rev. B **38**, 8879 (1988); e.g., for $U=2t$ I find a binding energy of $0.095t$, whereas the spin-bag result of Su and Chen is only $0.046t$. Thus the incommensurate domain-wall state is stable with respect to the commensurate state even if spin-bag effects are included.

[16]Motion of domain walls as a whole, in principle, gives rise to electrical current. However, the walls are extended objects, and therefore (i) are easily pinned by small inhomogeneities, and (ii) their tunneling probability through the Peierls barrier (due to the underlying lattice) is vanishingly small in the thermodynamic limit.

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