PHYSICAL REVIEW B, VOLUME 65, 041102(R)

White-Scalapino-like stripes in a mean-field Hubbard model

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(Received 17 October 2001; published 28 December 2001)

In stripe phases, a ''hidden order'' can exist as an order parameter *on* the charged stripes. A simple example arises in an unrestricted Hartree-Fock calculation of the Hubbard model, where a (metastable) solution is found which closely resembles the stripe phase of White and Scalapino. By comparison with uniform mean-field solutions, it is demonstrated that this phase develops from phase separation, and the order on the charged stripes is identified. The interface surface tension becomes negative for sufficiently narrow stripes, at which point the stripes begin to meander, gradually crossing from vertical to diagonal with decreasing doping.

DOI: 10.1103/PhysRevB.65.041102 PACS number(s): 71.10.Fd, 74.25.Dw

When the Hubbard model is doped away from the antiferromagnetic insulator at half filling, a number of calculations find evidence for spatially inhomogeneous solutions. There is considerable debate[1,2] as to whether these solutions are generic features of the Hubbard model, or arise only in a restricted parameter domain. Related issues are whether the inhomogeneity is driven by phase separation or antiferromagnetic (AFM) domain wall formation,[3] and how these features are related to ''stripes'' in cuprates and other oxides. It is well known[4] that stripes can develop from a frustrated phase separation, and a phase on the charged stripes is a good candidate for ''hidden order'' in the cuprates. Similar issues arise in the doped t-J model, where the ground state is variously found to be striped,[5] or uniform,[6] or phase separated.[7,8] Reference to earlier calculations may be found in these articles and in the reviews.[9]

Unrestricted Hartree-Fock (UHF) calculations[10–12] find that the holes form filled (one additional hole per row) stripes which act as antiphase boundaries between AFM domains. Such filled domain wall stripes are not found in more advanced calculations[5,7] of the Hubbard model, and are not consistent with experiment on the cuprates.[13] We here analyze a *metastable* state of the UHF calculations, which closely resembles the White-Scalapino (WS) (Ref. 5) stripes, and agrees better with experiment. These stripes can be understood from a phase separation approach, comparing the free energies of low-order commensurate magnetic phases, $q_x, q_y \sim 0$ or $Q_i = \pi/a$. The resulting mean-field phase diagrams involve phase separation between the AFM phase and a metallic phase, either ferromagnetic (FM), as in early ferron phase approaches to the Hubbard model,[14] or a phase resembling WS stripes, depending on the value of second neighbor hopping parameter t'. These stripes are stable local free-energy minima in UHF calculations, but globally there are alternative states of lower free energy.[12] However, these solutions can be stabilized by *additional interactions* beyond the pure Hubbard model (e.g., charge-density wave or superconducting), and hence may be relevant to experiment. These additional interactions will be discussed in a companion publication;[15] here we introduce the mean-field model and utilize UHF calculations to calculate the surface tension in the resulting stripe phases. We find that WS-like stripes are stable against macroscopic phase separation.

We study a one-band electron-hole symmetric Hubbard model [interaction $= U\Sigma_i (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2)$] with bare dispersion $\epsilon_k = -2t(c_x + c_y) - 4t' c_x c_y$, with $c_i = \cos k_i a$. In the presence of a mean-field magnetization m_q at wave vector $\vec{q}$, the quasiparticle dispersion becomes

$$E_\pm = \frac{1}{2}(\epsilon_k + \epsilon_{k+q} \pm E_0), \tag{1}$$

where $E_0 = \sqrt{(\epsilon_k - \epsilon_{k+q})^2 + 4U^2 m_q^2}$. The site magnetization is found self-consistently from

$$m_q = \sum_k (f(E_-) - f(E_+)) \frac{U m_q}{E_0}, \tag{2}$$

with Fermi function $f(E) = 1/(1 + e^{(E - E_F)/k_B T})$. The free energy is

$$F = \sum_{k, i=\pm} E_i f(E_i) - TS + U\left(m_q^2 + \frac{x^2}{4}\right), \tag{3}$$

where S is the entropy.

The phase with $\vec{q} = \vec{Q} \equiv (\pi, \pi)$ provides a good model for the AFM phase at half filling with Mott gap, successfully describing the spin-wave dispersion[16] and Monte Carlo results,[17,18] and serving as the basis for a number of treatments of strong correlation effects.[19] While a fit to the dispersion of the magnetic insulator $SrCuO_2Cl_2$ finds[20] $t = 325$ meV, $U = 6.03t$, and $t' = -0.276t$, here we study $t' = 0$. We use the same model, with different choices of $\vec{q} \neq \vec{Q}$, to describe a number of competing magnetically-ordered states. While at half filling the AFM state has lowest free energy, this is not true for finite-average doping x, leading to a rich phase diagram, with regimes of phase separation. Figure 1 shows the low-temperature free energy as a function of doping for the case $t' = 0$ for three magnetic phases, the standard antiferromagnet (AFM) $\vec{q} = \vec{Q}$, a ferromagnet (FM) with $\vec{q} = (0,0)$, and a linear antiferromagnet (LAF) with $\vec{q} = (\pi, 0)$ [see Fig. 3(g), below]. The curves are symmetric about half filling ($x = 0$). For $|x| \leq 0.25$ the AFM lies lowest in energy; between $0.25 \leq |x| \leq 0.65$ the LAF lies lowest, and beyond that, the ground state is nonmagnetic ($m_q = 0$). For all dopings, the FM state is metastable. At high

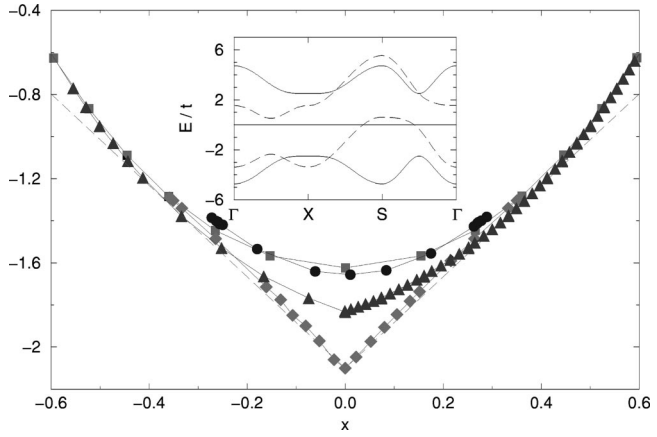

FIG. 1. Free energy vs doping for several magnetic phases of the Hubbard model ($U=6.03t$, $t'=0$). Diamonds=AFM, triangles =LAF, circles=FM, and squares=PM phase. Dashed lines =tangent construction. Inset: Dispersion of magnetic phases: solid lines=AFM at $x=0$, dashed lines=LAF at $x=0.353$; Brillouin zone points $\Gamma=(0,0)$, $X=(\pi,0)$, $S=(\pi,\pi)$.

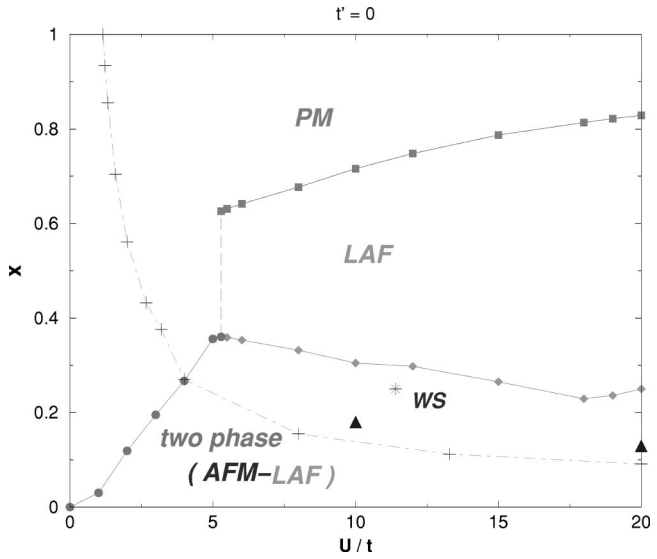

FIG. 2. Phase diagram, $x(U)$ for the Hubbard model, with $t'=0$. Triangles=Hubbard model results, estimated from Fig. 1 of Ref. 2; dot-dashed line with $+$'s=t-J model results, Ref. 7(b), assuming $J/t=4t/U$. The WS point is defined by x_0, the doping on the charged stripes, which is also approximately the doping where the two-phase regime terminates.

doping the magnetic phases terminate when $m_q \to 0$. The inset to Fig. 1 shows the dispersions for the stable phases, AFM at $x=0$ (solid lines) and LAF at $x=0.353$ (dashed lines).

The antiferromagnetic state has a cusp at half filling, with the slope discontinuity being the Mott-Hubbard gap. Away from half-filling, this state is always *thermodynamically unstable*–the compressibility $\sim \partial^2 f/\partial x^2$ is negative. The tangent construction (dashed lines) shows that the equilibrium state between zero doping and $|x|=x_c=0.353$ consists of a *phase separation* between the AFM and LAF phases. Note that the mean-field model misses the UHF ground state,[12] which has ''filled'' (one hole per row) stripes in an AFM background. It can be shown that, if the last term in Eq. (3) is omitted, this ground state would be recovered for large U, with the LAF phase stable only for a small parameter range near $U/t=6-8$ $(t'=0)$.

The resulting phase diagram x vs U is shown in Fig. 2. Phase separation persists for all finite U, but while the insulating state is always AFM, there is a crossover in the metallic stripe component from paramagnetic phase for $U<U_c=5.3t$ to LAF for $U>U_c$). The termination of the two-phase regime occurs approximately when $x=x_0$, the doping on the charged stripes. When $t'\neq 0$, the phase diagram is completely different, with phase separation between the AFM and a FM phase.[15] For large U, the Hubbard model should reduce to the t-J model; agreement with recent calculations for the phase separation boundary in the Hubbard[2] and t-J (Ref. 7) models is satisfactory [triangles and $+$'s in Fig. 2(a)]. The deviation at small U (large J) is expected, since the models are equivalent only in the large-U limit. While the metallic phase in the t-J model is usually taken as paramagnetic, the WS results may hint that it is an LAF phase near $U=11t$.

Figure 3 illustrates some of the low-energy textures found in UHF calculations, and shows that in the LAF stripe phase dispersions the added states form additional bands near mid-gap, as found in ordered stripe arrays[20] and for randomly-distributed magnetic polarons [Figs. 3(a) and 3(b)]. [For the left-hand panels of Fig. 3, the UHF calculations were iterated to self-consistency on 24×24 (a), 32×6 (c), or 12×12 (e,g) lattices with periodic boundary conditions. For the dispersions of the right-hand panels of Fig. 3, these solutions were extended to a 32×32 (d,h) or 36×36 (f) lattice, with one additional iteration (Fig. 3(b) was on a 24×24 lattice)].

The LAF stripes resemble the WS stripes of the t-J model: the minimum LAF stripe is two cells wide, and acts as an antiphase boundary between AFM domains, Fig. 3(c). In both calculations, the doped ground state is found to involve mixtures of LAF and AFM stripes, with no sign of insulating, ''filled'' stripes. The doping is comparable: the star in Fig. 2(a) represents the WS stripe phase, assuming an effective $U/t=4t/J$, with $J=0.35t$. Both kinds of stripes have similar fractional transfer of holes onto adjacent AFM rows (see caption of Fig. 3), and both are destabilized by nonzero t' (cf. Ref. 21). We find that the charged stripes have a fixed, minimal width for $x\leqslant 1/6$, with the charge per row of a stripe doubling at higher doping, and the stripe phase terminating near $x=1/3$; WS find similar doping dependences, systematically shifted due to the difference in hole density (1/3 vs 1/4) on a stripe. Similar LAF stripes were found previously as metastable UHF solutions.[11] An LAF-like state has also been found in recent Monte Carlo calculations in the manganites;[22] interestingly, a spin flux phase can form from a coherent superposition of two LAF phases.

It is clear from Fig. 3 that the LAF-AFM stripes arise from phase separation, with the stripe spacing evolving as expected with doping. The question remains as to whether the stripes are stable against macroscopic phase separation, i.e., is the free energy of the stripe phase F_{str} higher or lower than that of the separated bulk phases (tie-line) F_{sep}? We

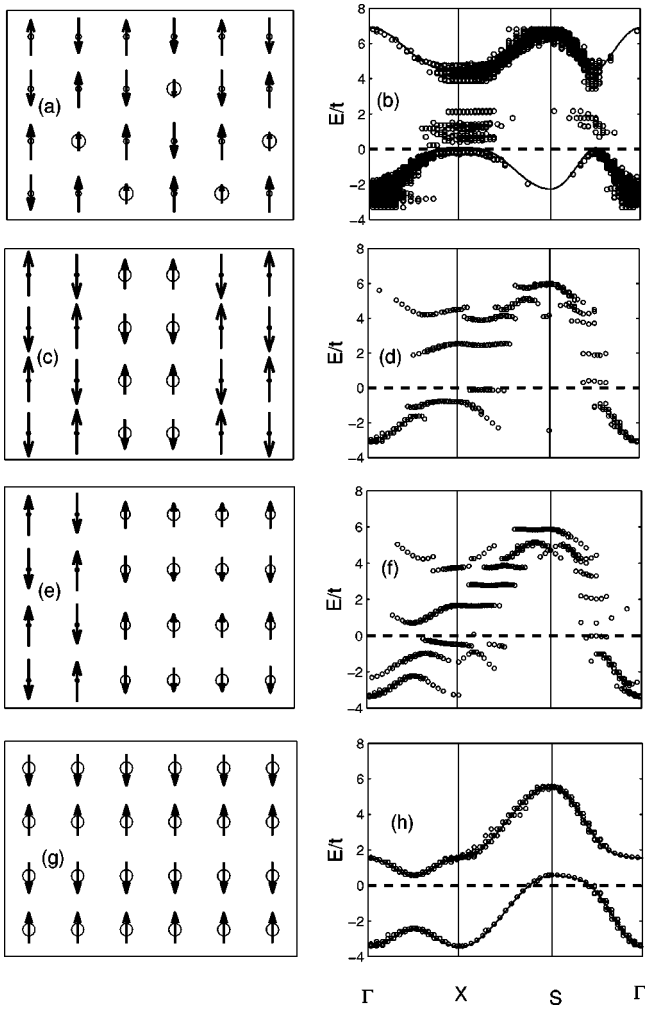

FIG. 3. Unrestricted Hartree-Fock calculations of the Hubbard model. Left panels: the hole configurations for $x=1/8$, 1/6, 2/9, and 1/3 average dopings minimizing the free energy. Right panels: the corresponding dispersions (open circles); solid lines=mean-field bands for undoped AFM (b) and LAF (h); dashed lines=chemical potential. (a,b): Random distribution of holes in an antiferromagnetic background forming magnetic polarons at $x=1/8$ doping. (c,d): LAF stripes at $x=1/6$ doping–on the charge stripes the hole density is 0.27 and the magnetization is 0.46; on the antiferromagnetic stripes the hole density is 0.06 and the magnetization is 0.77. (e,f): AFM stripes in LAF background at $x=2/9$; there is a weak modulation of the hole density on the LAF stripe: 0.245 (0.365) holes on the outer (inner) rows. (g,h): LAF configuration at 1/3 doping.

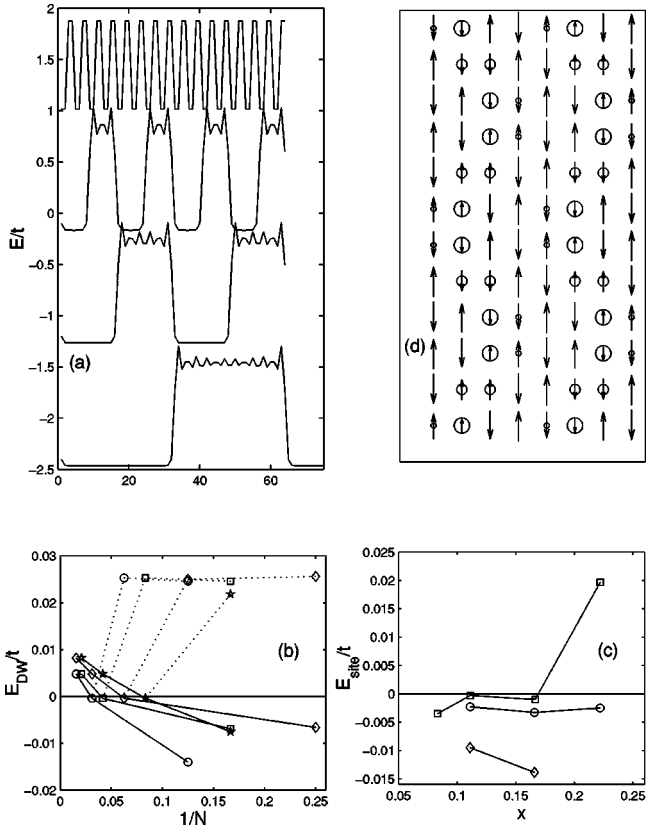

FIG. 4. (a) Free energy $f(x)$ per row for a LAF stripe array in the Hubbard model, with $t'=0$, $U=8t$ and $x=1/6$, comparing several different lattice periodicities: $(N,M)=(32,32)$ on a 128×6 lattice, and, for 64×6 lattices, (16,16), (8,8), and (2,2). Energies of narrower arrays are offset for clarity. (b) Excess free energy *per domain wall atom* E_{DW} plotted vs $1/N$, where N is the charge stripe periodicity, for $x=1/12$ (circles), 1/9 (squares), 1/6 (diamonds), and 2/9 (stars). Dotted lines connect unstable vertical stripes. (c) Comparison of energy per site E_{site} of meandering (circles) and diagonal (squares) stripes compared to the filled diagonal stripes (diamonds) 12. (d) Pattern of spin and charge order on meandering $x=1/6$ stripe.

answer this via UHF calculations, taking care to minimize finite-size effects. This is done by (a) adjusting U so that the charged-stripe doping x_0 is a simple rational fraction (at $U/t=8$, $x_0\simeq1/3$), and (b) working with large lattices, up to 128×6. Figure 4 shows (a) the average free energy on each row of a series of AFM-LAF stripe arrays, of the same average doping ($x=1/6$) but different stripe widths and (b) the resulting surface tension σ (free energy difference $F_{str}-F_{sep}$ per domain wall atom). We label the stripe array with $N+M$ copper (charge) periodicity by (N,M), where N (M) is the width in coppers of a charge (magnetic) stripe. The magnetic contribution to σ, associated with excess holes pushed onto the magnetic bounding layers, is positive and saturates for wider stripes, while the LAF energy is negative, and oscillates on the stripes, in parallel with hole density oscillations. These oscillations are due to quantum confinement, similar to the Friedel oscillations seen in electrons confined on a step on a Cu surface.[23] The confinement oscillations lead to a long-range interaction between domain walls (across a charged stripe), which explains why the net surface tension saturates so slowly as a function of stripe width, and why it depends mainly on the width of the LAF stripes.

For the widest stripes, the surface tension σ starts to level off to a value of $\sim0.01t$ per domain wall atom for an isolated domain wall. As the stripes move closer σ decreases, ultimately changing sign (*negative surface tension*). When the LAF stripe has a width of eight cells, the surface tension is essentially zero. For narrower LAF stripes straight vertical stripes are unstable, but can be pinned by commensurability effects on specially chosen lattices; the free energy is gener-

ally high [dotted lines in Fig. 4(b)]. On larger lattices, the UHF spontaneously evolves to a meandering stripe pattern, Fig. 4(d), with free energy lower than the tie-line [Fig. 4(b), lowest points of solid lines]. The meandering LAF stripes are composed of straight diagonal segments, separated by kinks. On the straight segments, holes on successive rows are shifted diagonally by one Cu site, leading to ferromagnetic alignment between kinks. Remarkably, the free energy of the meandering stripes is lower than that of the corresponding straight diagonal stripes, Fig. 4(c) (although the small difference could be a finite-size effect). The crossover appears to be kinetic energy driven: the holes in the LAF phase are delocalized along the (FM) rows, but when the LAF stripes get too narrow, adjacent rows shift to provide a FM coupling. Due to commensurability pinning effects, it will be hard to repeat this calculation for arbitrary values of U, although $x_0 \sim 1/4$ at $U=16t$.

There is a gradual crossover [Fig. 4(c)] from vertical (at $x=2/9$) to meandering (1/6, 1/9) to diagonal stripes (1/12). At $x=1/12$, the diagonal stripes have a low free energy, and meandering configurations are unstable. Figure 4(c) also includes the free energy of the diagonal, one hole per row stripes which are the UHF ground state.[12] The free energy differences are small, and the order of states may be reversed by including some additional (perhaps phononic or Coulomb) interactions.

Some mention must be made about the size of the lattice used. Most of the results correspond to lattices 96×6 (for $x=1/9$ and 2/9), 128×6 (for all $x=1/12$, and for the largest period at $x=1/6$), or 64×6 (for the remaining $x=1/6$), with periodic boundary conditions assumed. The meandering stripes were all on 48×12 lattices, and the diagonal on 24×24 (48×16 for 1/12). Straight stripes are metastable when the LAF stripe width is 4, and we had to use special lattices to stabilize this configuration: 12×24 for $x=2/9$, and $N'\times 12$, with $N'=48(1/6)$, 24 (1/9), and 32 (1/12) (there was no similar problem for the LAF width=2 stripes, which are also metastable). The surface tension also depends sensitively on the free energies of the reference end phases. These can be calculated either exactly, from the mean-field theory, or numerically from the UHF. For the LAF the agreement is quite good: energy per site $E_{LAF}/t=1.46579$ (mean field) vs 1.46578 (UHF); $E_{AFM}/t=2.46577$ (mean field) vs 2.46588 (UHF) (UHF's on 24×24 matrices). It was necessary to use the UHF value for E_{AFM} to calculate surface tensions.

The present calculations shed some light on the controversy in the t-J model. The doped AFM phase is so unstable in the Hubbard model, that it is likely that the elementary excitations in the ''uniform'' lightly-doped t-J model are really magnetic polarons. A recent quantum Monte Carlo study of the Hubbard model[18] also finds that holes add dispersionless bands, and do not uniformly dope the AFM phase. (See also Ref. 24.) Hence, the three-sided debate about ''uniform'' (or magnetic polaron)[7] vs stripe[5] vs (macroscopically) phase-separated[8] t-J ground state is in all probability really a debate about three kinds of phase-separated ground states. Our results favor (meandering) stripes.

In conclusion, we find WS-like stripes at the HF level in the Hubbard model (albeit as metastable states), and we demonstrate that they arise from a tendency to phase separation, providing the first estimate of their surface tension.

C.K.'s research was supported in part by NSF Grant No. NSF-9711910. These computations were carried out using the facilities of the Advanced Scientific Computation Center at Northeastern University (NU-ASCC). Their support is gratefully acknowledged. Publication 783 of the Barnett Institute.

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