A mean field calculation of the Hubbard model finds a rich phase diagram. The antiferromagnetic phase is generally unstable away from half filling, and there are several regions of phase separation. One solution in particular closely resembles the stripe phase of White and Scalapino. By comparison to unrestricted Hartree-Fock calculations (for which this phase is metastable), it is demonstrated that this phase arises from phase separation. The interface surface tension is found to change sign below a particular stripe width, at which point the stripes begin to meander, gradually crossing over to diagonal.

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 [8] 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 [9], and how these features are related to ‘stripes’ in cuprates and other oxides. Similarly, in the doped tJ model, various calculations find that the ground state is striped [10], or uniform [11], or phase separated [12]. Inclusion of realistic values of t’ into the model further reduces stripe stability [13]. Reference to earlier calculations may be found in these articles and in the reviews [1].

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 [6,7] 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) [1] 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, \( q_x, q_y \approx 0 \) or \( Q_z = \pi/a \). The resulting mean-field phase diagrams involve phase separation between the AFM phase and a metallic phase, either ferromagnetic (FM), or 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 [13]: 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 = \( U \sum_i (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2) \)] with bare dispersion \( \epsilon_k = -2t(c_x + c_y) - 4t'c_xc_y, \) with \( c_i = \cos k_ia \). In the presence of a mean-field magnetization \( m_q \) at wave vector \( \vec{q} \), the quasiparticle dispersion becomes

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

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

\[
m_q = \sum_k (f(E_-) - f(E_+))\frac{Um_q}{E_0}, \tag{2}
\]

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

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

where \( S \) is the entropy.

The phase with \( \vec{q} = Q \equiv (\pi, \pi) \) 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]. A fit to the dispersion of the magnetic insulator SrCuO2Cl2 finds \[ t = 325meV, \ U = 6.03t, \ \text{and} \ t' = -0.276t, \] which will be assumed below unless stated otherwise. We use the same model, with different choices of \( \vec{q} \neq Q \), 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 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) \( \vec{q} = Q \), a ferromagnet (FM) with \( \vec{q} = (0, 0) \), and a linear antiferromagnet (LAF) with \( \vec{q} = (\pi, 0) \) (see Fig. 3g, 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 doping the
magnetic phases terminate when $m_q \to 0$. The inset to Fig. 3 shows the dispersions for the stable phases, AFM at $x = 0$ (solid lines) and LAF at $x = 0.353$ (dashed lines).

![Fig. 1](image1.png)

**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 $\Gamma = (0, 0)$, $X = (\pi, 0)$, $S = (\pi, \pi)$.

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 true UHF ground state, which has filled $(x = 1)$ 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 $U > U_c$. When $t' \neq 0$, the phase diagram is completely different, with phase separation between the AFM and a FM phase. For large $U$, the Hubbard model should reduce to the tJ model; agreement with recent calculations for the phase separation boundary in the Hubbard [2] and tJ [3] models is satisfactory (triangles and $+$'s in Fig. 2). 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 tJ model is usually taken as paramagnetic, the WS results may hint that it is an LAF phase near $U = 11t$.

![Fig. 2](image2.png)

**FIG. 2.** Phase diagram, $x(U)$ for the Hubbard model, with $t' = 0$. Triangles = Hubbard model results, estimated from Fig. 1 of Ref. 3; dot-dashed line with $+$'s = tJ model results, Ref. 3b, assuming $J/t = 4t/U$.

Figure 2 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 midgap, as found in ordered stripe arrays [2] and for randomly distributed magnetic polarons (Fig. 2a,b). [For the left-hand panels of Fig. 3, the UHF calculations were iterated to self-consistency on 24×24 (a), 32×6 (b), 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. 2b) was on a 24×24 lattice).]

The LAF stripes resemble the WS stripes of the tJ model: the minimum LAF stripe is two cells wide, and acts as an antiphase boundary between AFM domains, Fig. 3: In both calculations, the doped ground state is found to involve mixtures of LAF and AFM stripes, with no sign of insulating, empty stripes. The doping is comparable: the star in Fig. 2a represents the WS stripe, assuming an effective $U/t = 4t/J$, with $J = 0.35t$. Both kinds of stripe have similar fractional transfer of holes onto adjacent AFM rows (see caption of Fig. 3), and both are destabilized by non-zero $t'$. We find that the charged stripes have a fixed, minimal width for $x \leq 1/6$, 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 [1]. An LAF-like state has also been found in recent Monte Carlo calculations in the manganites [2]: interestingly, a spin flux phase can form from a coherent superposition of two LAF phases.
Excess holes pushed onto the magnetic bounding layers, wall atom). The magnetic contribution, associated with tension but different stripe widths and (b) the resulting surface with large lattices, up to 128 \times 128 per domain wall atom for an \( \sigma \) LAF stripe array, of the same average doping (\( x = 1/8 \)).

For the widest stripes, the surface tension \( \sigma \) starts to level off to a value of \( \sim 0.1t \) per domain wall atom for an isolated domain wall. As the stripes move closer \( \sigma \) decreases, ultimately changing sign (negative surface tension). When the LAF stripe has a width of 8 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 generally high (dotted lines...
in Fig. 3(a)). On larger lattices, the UHF spontaneously evolves to a meandering stripe pattern, Fig. 3(b), with free energy lower than the tieline (Fig. 3(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. 3(a) (although the difference is very small, and 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. 4c) from vertical 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 4c 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 $96 \times 6$ (for $x = 1/9$ and $2/9$), $128 \times 6$ (for all $x = 1/12$, and for the largest period at $x = 1/6$), or $64 \times 6$ (for the remaining $x = 1/6$), with periodic boundary conditions assumed. The meandering stripes were all on $48 \times 12$ lattices, and the diagonal on $24 \times 24$ ($48 \times 16$ 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: $12 \times 24$ 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 UHF: $E_{AFM}/t = 2.46577$ (mean field) vs 2.46588 (UHF) (UHF’s on $24 \times 24$ 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 tJ 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 tJ model are really magnetic polarons. A recent Quantum Monte Carlo study of the Hubbard model [13] also finds that holes add new dispersionsless bands, and do not uniformly dope the AFM phase. (See also Ref. 12.) Hence, the three-sided debate about ‘uniform’ (or magnetic polaron) vs stripe vs (macroscopically) phase-separated tJ ground state is in all probability really a debate about three kinds of phase separated ground state. 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.

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