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LETTER TO THE EDITOR

Phases of the 2D Hubbard model at low doping

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Abstract. We study the equilibrium spin configuration of the 2D Hubbard model for a low degree of doping, x, when a long-range magnetic order is still present. We show that the conventional planar spiral phase has negative bosonic modes and is therefore unstable. The novel equilibrium state that we find at low doping is incommensurate and *non-coplanar* with the inverse pitch of the spiral varying as $\sqrt{x}$; nevertheless this state has a dominant peak in the susceptibility at (π, π).

Magnetic properties of the CuO_2 layers in the high-temperature superconductors have recently been attracting intense interest, as magnetism is possibly a major contributor to the mechanism of superconductivity [1]. There are numerous reasons for believing that the low-energy properties of cuprates are quantitatively captured by the 2D Hubbard model

$$\mathcal{H} = -\sum_{i,j} t_{i,j} a^\dagger_{i,\alpha} a_{j,\alpha} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}. \qquad (1)$$

Here α is a spin index, $n = a^\dagger a$, and $t_{i,j}$ is a hopping integral, which we assume to act only between nearest neighbours. According to numerical calculations, making this last assumption is more justified for $La_{2-x}Sr_xCuO_4$ than for $YBa_2Cu_3O_{6+x}$.

At half-filling, the ground state of the 2D Hubbard model exhibits a long-range commensurate Néel order. Shraiman and Siggia first pointed out [2] that holes introduced into a commensurate antiferromagnet give rise to a long-range dipolar distortion of the staggered magnetization. In their mean-field scenario, this leads to a spiral spin configuration with the momentum (π, Q). The incommensurate (π, Q) phase was also obtained in the early perturbative studies of the Hubbard model with small U [3] and in several other mean-field [4, 5] and self-consistent [6] calculations.

In this communication we use the spin-density-wave (SDW) approach and study the structure of magnetic correlations in the Hubbard model at small but finite doping when long-range magnetic order is still present. We will show that the (π, Q) spiral state is actually *unstable*, and find an equilibrium state which will be not only incommensurate but also non-coplanar in the spin space. This in turn leads to a novel scenario of spin reorientation upon doping.

As an input for our analysis, we will need an expression for the energy spectrum, E_k, of a single hole in a quantum antiferromagnet. The mean-field theory gives [7] $E_k = -\sqrt{\epsilon_k^2 + \Delta^2}$, where $\epsilon_k = -2t(\cos k_x + \cos k_y)$, t is the nearest-neighbour hopping, and Δ is a gap which separates valence and conduction bands [4, 8, 7, 9]. This energy is obviously degenerate along the whole edge of the magnetic Brillouin zone. However, both perturbative [10] and variational [11] studies have shown that this degeneracy does

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not survive the effects of quantum fluctuations, and the actual dispersion has a maximum at four points $(\pm\pi/2, \pm\pi/2)$. In the neighbourhood of these points E_k can be presented as $E_k = -\Delta + p_\parallel^2/2m_\parallel + p_\perp^2/2m_\perp$ (near $(\pi/2, \pi/2)$, we have $p_\parallel = (k_x - k_y)/2$, $p_\perp = (k_x + k_y)/2$). Self-consistent calculations predict that at large U, both masses scale as the inverse bandwidth $J = 4t^2/U$ but numerically, $m_\parallel$ is several times larger than $m_\perp$. Notice, however, that the mass anisotropy is present only in the nearest-neighbour model: a negative second-neighbour hopping t' yields pockets at $(\pi/2, \pi/2)$ even in the mean-field approximation, and the two masses become equal for $t' \sim J/2 \ll t$.

We now turn to the description of our calculations. Consider first a Néel-ordered state for a small but finite degree of doping. Near $Q_0 = (\pi, \pi)$, the static transverse susceptibility should have a hydrodynamic form [12] $\chi_{\mathrm{st}}^{xx}(q \approx Q_0) = N_0^2/(\rho_s(q - Q_0)^2)$, where N_0 is the on-site magnetization, and ρ_s is the spin stiffness. This form of transverse susceptibility is reproduced in the SDW formalism by summing the ladder series of bubble diagrams. At half-filling, only bubbles containing valence and conduction fermions are allowed, while for a finite degree of doping one also has contributions to χ from bubbles with only valence fermions as chemical potential moves inside the valence band. These last contributions are proportional to the Pauli susceptibility, which in two dimensions does not depend on carrier concentration. As a result, we obtain a finite correction to the spin stiffness even for a very small degree of doping [8]: $\rho_s = \rho_s^0(1 - z)$, where ρ_s^0 is the spin stiffness for half filling, and $z = 4T\chi_{2\mathrm{D}}^{\mathrm{Pauli}} = 2T\sqrt{m_\perp m_\parallel}/\pi$ where T is the effective interaction between two holes. In a systematic perturbative expansion around the mean-field state (which holds for the inverse number of orbitals $n = 2S$, and yields antiferromagnet with spin S), this interaction is of the order of U and therefore $z \gg 1$. However, for physical $S = 1/2$, the perturbative approach is irrelevant because of the strong self-energy and vertex corrections which contribute powers of U/tS. Self-consistent calculations for $S = 1/2$ have shown that these corrections reduce T to the order of the bandwidth J [2, 8, 13], which in turn implies that z is simply a number, independent of U/t. For these reasons, for the rest of this work, we will consider z as a phenomenological input parameter [14].

It follows from stiffness considerations that the Néel state remains stable for a finite degree of doping if $z < 1$, but becomes unstable if $z > 1$ in which case we have to consider incommensurate spin configurations as possible candidates for the ground states. Let us first focus on the two simplest candidates [2, 6, 15]: the spiral states with the ordering vectors (π, Q) and (Q, Q). For definiteness, we choose the ordering to be in the XY-plane such that $S_R^X = S_{\bar{Q}} \cos(\bar{Q}R)$, and $S_R^Y = S_{\bar{Q}} \sin(\bar{Q}R)$, where $\bar{Q}$ is the ordering momentum.

The mean-field analysis for the incommensurate states proceeds in the same way as for the Néel state: one has to introduce a single-particle condensate, decouple a Hubbard term and diagonalize the quadratic form. Performing the calculations, we find that only two pockets, at $(\pm\pi/2, \pi/2)$, are actually occupied in the (π, Q) state, and that $Q = \pi - (U/t)x$ and $E^{(\pi,Q)} - E^{(\pi,\pi)} = \pi x^2(1 - z)/(4\sqrt{m_\perp m_\parallel})$. Clearly, the (π, Q) phase has lower energy than the (π, π) phase for $z > 1$, exactly where the stiffness of the (π, π) state becomes negative.

For the (Q, Q) phase, the inverse pitch Q is the same, but only one hole pocket, at $(\pi/2, \pi/2)$, is occupied, and the energy difference is $E^{(Q,Q)} - E^{(\pi,\pi)} = \pi x^2(3 - 2z)/(4\sqrt{m_\perp m_\parallel})$. Comparing the two expressions for energy, we observe that the spiral (π, Q) phase has the lowest energy at $1 < z < 2$. This is consistent with the results from other mean-field approaches [2, 5]. For $z > 2$, the (Q, Q) state has the lowest energy. However, we found that $\partial E^{(Q,Q)}/\partial x^2 \sim (1 - z/2)$ is negative for $z > 2$. This suggests that a phase-separated solution will have lower energy than the homogeneous state [16]. In contrast, for $1 < z < 2$, where mean-field considerations favour a (π, Q)

spiral, $\partial E^{(Q,Q)}/\partial x^2 > 0$, i.e. the system is stable towards phase separation. In view of this, we will only consider the case $1 < z < 2$.

We now turn to the central topic of our work, which is the stability analysis of the spiral phases. Stability requires that the static bosonic susceptibility is positive everywhere except for at three points in momentum space where χ^{-1} is zero due to the breakdown of SO(3) symmetry. The calculation of the susceptibilities in the SDW approach is straightforward but lengthy because we have to solve a set of four coupled equations (three for spin–spin correlators and one for the density–density correlator). A similar analysis for the Hubbard model on a triangular lattice is presented in [17]. For in-plane (longitudinal) spin fluctuations, a simple symmetry analysis predicts that the zero modes are located at $q = \mp\bar{Q} \equiv (\pi, Q)$ for χ_q^{+-} and χ_q^{-+} correspondingly. We have performed calculations and indeed found that near the pole, static χ_q^{+-} behaves as $\chi_q^{+-} = 2[J(q+\bar{Q})^2(2-z)]^{-1}$, i.e., it is *positive* for $z < 2$ which means that the (π, Q) phase is stable with respect to phase separation [18]. Note in passing that for the dynamical susceptibility, we found a pole at $\omega = c|q+\bar{Q}|$ with the same c (up to O(x) terms) as at half filling. This is in agreement with other results [19, 15].

We now consider magnetic susceptibility χ_q^{zz} associated with the fluctuations of the plane of spin ordering. These fluctuations are coupled to the charge and in-plane spin fluctuations only dynamically, so for the full static susceptibility one has the simple RPA-like formula $\chi_q^{zz}(\omega=0) = \overline{\chi}_q^{zz}(\omega=0)/(1 - U\overline{\chi}_q^{zz}(\omega=0))$ where $\overline{\chi}_q^{zz}$ is the bare bubble. From general symmetry considerations, we would expect the Goldstone modes in χ_q^{zz} to be at $q = \pm\bar{Q}$. Performing calculations to the lowest non-trivial order in the density (i.e. to O(x^2)), we have, indeed, found that $(\chi_q^{zz})^{-1}$ at $q = \pm\bar{Q}$ is equal to zero. However, with the same accuracy, we also find that the stiffness for excitations near these momenta is equal to zero! Moreover, to O(x^2), all fluctuation modes between $\bar{Q}$ and $-\bar{Q}$, including the mode at (π, π), turn out to be gapless. A similar degeneracy was found in the macroscopic consideration by Shraiman and Siggia [19]. This degeneracy is not related to any kind of broken symmetry and is only an artifact of the lowest order in the expansion in hole density. At the same time, the divergence of the static susceptibility in a finite range of momenta implies that there are an infinite number of spin configurations which to the lowest order in the hole density are degenerate with the (π, Q) state.

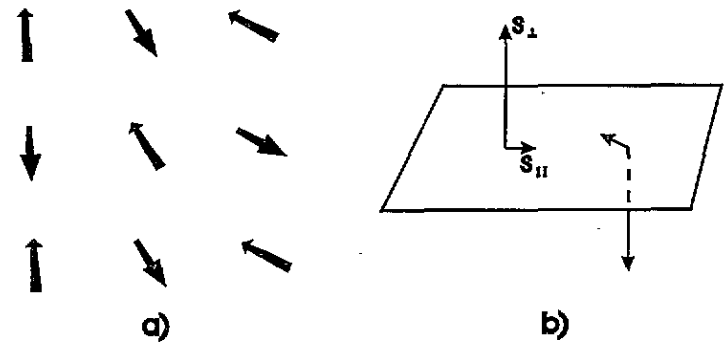

Figure 1. (a) The spin configuration of a non-coplanar state. Arrows with thick heads point out of the plane, while those with thick tails point into the plane. This configuration is different from the double spiral considered by Chakraborty *et al* [5]. (b) Two adjacent spins in the equilibrium configuration. The in-plane component, $S_\perp \sim x^{1/2}$, is small compared with the off-plane component, $S_\|$.

To specify this set of states, we observe that zero modes in χ^{zz} are centred around

(π, π). The zero mode in the transverse susceptibility at (π, π) means that the system is indifferent to generation of a spontaneous commensurate antiferromagnetic order along the Z-direction in addition to the incommensurate spin ordering in the XY-plane. Accordingly, we introduce two different SDW order parameters, $\Delta_\perp = U\langle S_\perp \rangle$ and $\Delta_\parallel = U\langle S_\parallel \rangle$, where $\langle S_\perp \rangle$ and $\langle S_\parallel \rangle$ are the magnitudes of the off-plane and in-plane components of the on-site magnetization, respectively. Notice that the states with both $\Delta_\parallel$ and $\Delta_\perp$ finite are non-coplanar (see figure 1). The inverse pitch of the spiral in the XY-plane is related to $\Delta_\perp$ by the requirement that the two SDW self-consistency conditions for two order parameters be compatible with each other. Solving the self-consistency equations, we obtain ($q_Q = \pi - Q$) $q_Q = (U/t)(\Delta/\Delta_\parallel)x = O(x^2)$ where $\Delta^2 = \Delta_\perp^2 + \Delta_\parallel^2$ is the total order parameter constrained by the self-consistency conditions to be $\Delta \approx U/2$. We then evaluate the ground-state energy of non-coplanar states and find that to order x^2, it *does not depend* on $\Delta_\perp$. In other words, all non-coplanar states with finite $\Delta_\perp$ are degenerate in energy with the (π, Q) spiral and therefore belong to a set of degenerate ground states.

As we have already discussed, the degeneracy found so far is not related to any kind of broken symmetry and must be lifted due to higher-order terms in the hole density. However, it seems impossible to predict in advance which configuration (planar spiral or some other) will be the true ground state. We therefore perform calculations of the ground-state energy to next-to-leading order in x, and find after some tedious algebra that when $\Delta_\perp$ and $\Delta_\parallel$ are both of the order of U,

$$\Delta E = -Ux^3 \left(\frac{\Delta_\perp}{\Delta_\parallel}\right)^2 \left(\frac{2}{z} - 1\right) \tag{2}$$

where $\Delta E = E_{\Delta_\perp} - E_{\Delta_\perp \to 0}$, and $E_{\Delta_\perp \to 0}$ is the ground-state energy in the limit when the Z-component of the order parameter tends to zero [20]. It is apparent from (2) that the energy *decreases* as the ratio $\Delta_\perp/\Delta_\parallel$ increases—that is, the (π, Q) spiral phase corresponds to a maximum rather than minimum of energy.

As an independent check that the planar (π, Q) phase is unstable, we also calculate the static susceptibility $\chi^{zz}(q)$ in this state beyond the leading order in the hole density and after some algebra obtain along $q_x = \pi$

$$(\chi^{zz})_q^{-1} = \frac{4x^3}{U}\left(1 - \frac{\tilde{q}^2}{q_Q{}^2}\right)\left(1 - \frac{2}{z} - \frac{\tilde{q}^2}{q_Q{}^2}\right) \tag{3}$$

where $\tilde{q} = \pi - q_y$, and $q_Q = \pi - Q$. We see that while the Goldstone mode at $\tilde{q} = \pm q_Q$ survives to $O(x^3)$ (as it should), the static susceptibility for out-of-plane fluctuations at and near (π, π) is *negative* for $z < 2$. This implies that the spiral (π, Q) state is unstable at low doping which is entirely consistent with energy considerations. Notice that the RHS of (2) contains the same positive factor $x^3((2/z) - 1)$ as the expression for χ^{zz} at (π, π). Also note that all $O(x^3)$ terms in (2) and (3) come from the integration within the hole pockets (the bubbles with conduction and valence fermions yield regular corrections in powers of x^2). Near the minima, the hole spectrum has a quadratic dispersion for an arbitrary form of the hopping integral, and we therefore expect our result for the instability of the (π, Q) phase to be valid also for the models with more complex hole dispersion, the only necessary condition being the existence of hole pockets around $(\pm\pi/2, \pm\pi/2)$.

We now turn to the issue of what is the actual equilibrium state at finite doping. We see from equation (2) that the ground-state energy decreases as $\Delta E \sim -x^3/\Delta_\parallel$ when one moves away from planar spiral. However, as we have already mentioned, this equation holds as long as $\Delta_\parallel$ remains of the order of U. For smaller $\Delta_\parallel$, particularly when $\Delta_\parallel$ and

$q_Q \sim x\Delta_\parallel$ both become of the order of $\sqrt{x}$, equation (2) and the self-consistency condition on $\bar{q}$ have more complex forms. In this region, we find

$$\Delta E = \frac{Ux^2}{2}\left[1 + (\alpha^2+2)\beta^2 - \frac{\beta z}{6}\left(\left(\alpha^2 + \frac{8}{z}\right)^{3/2} - \alpha^3\right)\right] \tag{4}$$

where we introduced $\Delta_\parallel = \alpha\Delta x^{1/2}, q_Q = \beta(U/t)x^{1/2}$. The self-consistency condition on $\bar{q}$ relates α and β as follows: $\beta = z(\sqrt{\alpha^2 + 4/z} - \alpha)/2$. Substituting this relation into (4) and minimizing ΔE with respect to α, we obtain the equilibrium values of α, β and ΔE. To the lowest order in $2 - z$ they are: $\alpha \approx \sqrt{7z/(12(2-z))}$, $\beta \approx 1/\alpha$ and

$$\Delta E = -\frac{Ux^2}{2}\left[\frac{12}{7}\left(1 - \frac{2}{z}\right)^2\right]. \tag{5}$$

As expected, ΔE is negative which implies that equilibrium state has smaller energy than the (π, Q) spiral. Also observe that because in equilibrium $\Delta_\parallel \sim \sqrt{x}$, ΔE in fact scales as x^2, instead of x^3, which in turn implies that this state in principle could be selected even without considering a degenerate set of states. However, the discovery of the instability of the planar spiral state has given us a hint of where to search for the equilibrium state.

Consider next the magnetic susceptibility in the equilibrium state. By virtue of being an energy minimum, it is indeed positive, diverging only at the Goldstone points. The peculiar thing is that the order parameter now has two components, an XY-component with momentum $\bar{Q} \equiv (\pi, Q)$ and the Z-component with momentum $\boldsymbol{\pi} \equiv (\pi, \pi)$. As a result, the in-plane (XY) spin susceptibility will have *two* static zero modes at these points. We can therefore approximate $\chi_q^{\pm}$ via

$$\chi^{+-}(q) \approx \frac{\chi_\pi}{(q-\pi)^2} + \frac{\chi_{\bar{Q}}}{(q+\bar{Q})^2} \tag{6}$$

where the residues χ_π and $\chi_{\bar{Q}}$ are proportional to $\Delta_\perp^2$ and $\Delta_\parallel^2$ respectively. Now observe that because $\Delta_\parallel \sim \sqrt{x}$, the residue of the pole at the incommensurate wave vector $q = -\bar{Q}$ is proportional to the hole concentration, and is suppressed with respect to the pole at the commensurate wave vector (π, π). This implies that as long as long-range order is present, the in-plane spin susceptibility remains peaked at (π, π) even when the commensurate phase is unstable. For χ_q^{zz}, however, simple symmetry considerations show that zero modes are located at $q = \pm\bar{Q}$.

The above results lead to a novel scenario of spin reorientation with doping. In the Shraiman–Siggia picture, spins remain in the same plane as at half-filling, but for $z > 1$, they are twisted into a spiral with incommensurate momentum (π, Q). In our scenario, the commensurate antiferromagnetic ordering (the same as at half-filling) does not vanish when $z > 1$, and doping only introduces a transverse component of the order parameter which forms a spiral in the plane perpendicular to the direction of commensurate order. This transverse component is small for small x, and the low-T behaviour at finite doping remains nearly the same as in the commensurate antiferromagnet [21, 22]. Notice, however, that our our analysis has been performed only for frequencies smaller than the energy scale ΔE associated with the lifting of the degeneracy. At larger frequencies, the static selection is irrelevant, and one has to solve the full dynamical problem which at the moment seems rather difficult to do.

The analysis above is valid for the magnetically ordered phase. We therefore cannot pretend to resolve the well-known discrepancy between neutron scattering and NMR experiments for $La_{2-x}Sr_xCuO_4$ [23, 24], which have both been performed well inside the metallic phase. Notice in this regard that, as neutron data indicate, incommensurability at (π, Q) observed at 7.5% and 14% doping *is not* correlated with the magnetic behaviour in the ordered phase. This implies that our results are not in conflict with neutron data. At the same time, no incommensurability has been found in neutron experiments in the magnetically ordered phases of Y123 and electron-doped compounds.

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