

Magnetic phases of the two-dimensional Hubbard model at low doping

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We study the equilibrium spin configuration of the two-dimensional (2D) Hubbard model at low doping, when a long-range magnetic order is still present. We use the spin-density-wave formalism and identify three different low-doping regimes depending on the value of $z = 4U\chi_{2D}$ where χ_{2D} is the Pauli susceptibility of holes. When $z < 1$, the collinear antiferromagnetic state remains stable upon low doping. As candidates for the ground state for $z > 1$ we first examine the planar spiral phases with the pitch Q either in one or in both spatial directions. Mean-field calculations favor the spiral (π, Q) phase for $1 < z < 2$, and (Q, Q) phase for $z > 2$. Analysis of the bosonic modes of the spiral state shows that the (Q, Q) state has a negative longitudinal stiffness and is unstable towards domain-wall formation. For the (π, Q) state, the longitudinal stiffness is positive, but to the lowest order in the hole concentration, there is a degeneracy between this state and a whole set of noncoplanar states. These noncoplanar states are characterized by two order parameters, one associated with a spiral, and the other with a commensurate antiferromagnetic ordering in the direction perpendicular to the plane of a spiral. We show that in the next order in the hole concentration this degeneracy is lifted, favoring noncoplanar states over the spiral. The equilibrium, noncoplanar configuration is found to be close to the Néel state with a small spiral component whose amplitude is proportional to the square root of the hole concentration. These findings lead to a new scenario of spin reorientation upon doping in Hubbard antiferromagnets.

I. INTRODUCTION

Magnetic properties of the CuO_2 layers in high-temperature superconductors have been recently attracting intense interest as magnetism is possibly a major contributor to the mechanism of superconductivity.¹ There are numerous reasons to believe that the magnetic properties of weakly doped cuprates are quantitatively captured by the effective two-dimensional (2D) theory for one degree of freedom per CuO_2 unit which is provided by a one-band Hubbard model

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

Here α is a spin index, $n = a^\dagger a$, and $t_{i,j}$ is a hopping integral which acts mainly between nearest (t) and next-nearest (t') neighbors. We will assume that t' is negative.²

At half-filling, the ground state of the 2D Hubbard model exhibits a long-range commensurate Néel order provided t' is not very large. It has been known for many years^{3,4} that holes introduced into a commensurate antiferromagnet give rise to a long-range dipolar distortion of the staggered magnetization. In 2D this effect was studied in detail by Shraiman and Siggia.⁵ They found that in the simplest scenario, the dipolar distortion leads to a spiral spin configuration with the momentum (π, Q) at any nonzero doping. The incommensurate (π, Q) phase was also obtained in the early perturbative studies of the Hubbard model with small U ,⁶ and in several other mean-field⁷⁻⁹ and self-consistent¹⁰ calculations.

In this paper, 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, depending on the strength of the interaction between the holes, three different solutions of the Hubbard model at low doping are possible: (i) a commensurate Néel phase at small interaction (precise criteria will be derived below), (ii) phase separation at sufficiently strong interaction, and (iii) an intermediate homogeneous incommensurate phase which, however, differs from the planar spiral suggested by the mean-field analysis. This incommensurate phase is noncoplanar in spin space, and its properties are much closer to the properties of a commensurate (π, π) spin configuration than those of a planar spiral.

The analysis presented here is related to other works on incommensurate magnetic phases at finite doping. Previous mean-field studies of the Hubbard and t - J models^{5,7-9,11} have focused on the three configurations with ordering momenta (π, π) , (π, Q) , and (Q, Q) , and have shown that in a certain range of parameters, any of these configurations can have energy lower than that of the other two states. Our energy analysis is consistent with their results. These mean-field studies also found that for short-range repulsion, the (Q, Q) phase is likely to be unstable towards domain-wall formation,^{5,9} while the (π, Q) phase is stable. Shraiman and Siggia¹² developed a macroscopic theory of the bosonic excitations in the (π, Q) spiral phase. Surprisingly, to the lowest order in density they found a peculiar degeneracy in the ground-state energy for the planar spiral state and for a whole set of noncoplanar magnetic configurations with the plane

of the spiral varying in space. This degeneracy is also present in our microscopic calculations reported below. However, the further assumption of Shraiman and Siggia, that the next-order terms in doping concentration stabilize the planar spiral state, is inconsistent with our microscopic calculations which favor a noncoplanar spin configuration for the same range of parameters as in Ref. 12.

The paper is organized as follows. In Sec. II we consider the mean-field theory of the spiral phases in the Hubbard model and compare the ground-state energies of different phases. In Sec. III we compute the dispersion of the bosonic excitations in the (π, Q) and (Q, Q) spiral phases to the lowest order in hole density and find that the (Q, Q) spiral has negative longitudinal susceptibility, while the (π, Q) spiral has an infinite number of zero modes. We will identify the set of magnetic states which are degenerate in energy with the planar (π, Q) spiral. In the next section, we show that the degeneracy is lifted by the next-to-leading order terms in hole density. We compute the ground-state energy and find the equilibrium spin configuration at a finite doping. We then discuss the properties of this equilibrium state, in particular, the behavior of the dynamical spin susceptibility. Finally, Sec. VI states our conclusions.

II. SPIRAL PHASES

In this section, we describe spin-density-wave (SDW) calculations for the Hubbard model at and near half-filling. Let us start with the commensurate Néel state. The SDW approach for this state has been discussed several times in the literature^{7,13–16} and we will use the results of these studies. At half-filling, the fermionic spectrum consists of conduction and valence bands separated by the energy gap $\Delta = U\langle S_z \rangle$. The dispersion relation for the valence fermions is $E_k^d = -E^- + \epsilon^+$ where $E_- = \sqrt{\Delta^2 + (\epsilon^-)^2}$ and $\epsilon^- = -2t(\cos k_x + \cos k_y)$, $\epsilon^+ = 4|t' \cos k_x \cos k_y|$. This dispersion has a maximum at four points $(\pm\pi/2, \pm\pi/2)$ in the center of each of the edges of the magnetic Brillouin zone, provided that t' is not too large. In the neighborhood of these points, E_k^d can be presented as $E_k^d = -\Delta + p_{\parallel}^2/2m_{\parallel} + p_{\perp}^2/2m_{\perp}$. Thus, near $(\pi/2, \pi/2)$, we have $p_{\parallel} = (k_x - k_y)/2$, $p_{\perp} = (k_x + k_y)/2$, $m_{\parallel} = (4t')^{-1}$, $m_{\perp} = (4J - 4|t'|)^{-1}$ where $J = 4t^2/U$ is the inverse bandwidth. For both La- and Y-based materials, $t' \sim J$ and therefore both masses scale as $1/J$. Note that the minimum at $(\pi/2, \pi/2)$ is rather robust, even if $t' = 0$, and the mean-field spectrum is degenerate along the whole edge of the magnetic Brillouin zone; the actual dispersion still has four minima at $(\pm\pi/2, \pm\pi/2)$ due to quantum fluctuations (not included in our present SDW treatment).^{17,18}

At finite doping, the chemical potential moves into a valence band, and the states near the maximum of E_k^d become empty. These states are often referred to as hole pockets. For a commensurate spin ordering, all four pockets become equally occupied. Performing then simple calculations, we obtain that in the presence of holes, the ground-state energy of the (π, π) phase changes to

$$E^{(\pi, \pi)} = \frac{\pi x^2}{4\sqrt{m_{\perp} m_{\parallel}}} . \quad (2)$$

We will also need the expression for the static magnetic susceptibility of the (π, π) state. In the SDW formalism, the susceptibility is obtained by summing up the series of bubble diagrams, and the result is

$$\bar{\chi}^{+-}(q) = \frac{\chi(q)}{1 - U\chi(q)} , \quad (3)$$

where for $\Delta > t, t'$

$$\begin{aligned} \chi^{+-}(q) = & \frac{1}{N} \sum'_{E_k^d < \mu} \left[1 - \frac{\epsilon_k^- \epsilon_{k+q}^- - \Delta^2}{E_k^- E_{k+q}^-} \right] \frac{1}{E_k^c - E_{k+q}^d} \\ & + \frac{1}{N} \sum'_{\substack{E_{k+q}^d < \mu \\ E_k^d > \mu}} \left[1 + \frac{\epsilon_k^- \epsilon_{k+q}^- - \Delta^2}{E_k^- E_{k+q}^-} \right] \frac{1}{E_k^d - E_{k+q}^d} . \end{aligned} \quad (4)$$

The prime at the summation signs indicates that the summation is over the magnetic Brillouin zone. Near $\bar{Q} = (\pi, \pi)$, the static transverse susceptibility should obey the hydrodynamic relation¹⁹ $\chi_{st}^{+-}(q) = 2N_0^2/\rho_s(q - \bar{Q})^2$, where N_0 is the on-site magnetization, and ρ_s is the spin stiffness. At half-filling only bubbles containing valence and conduction fermions are allowed, and performing simple calculations, we obtain $\rho_s = \rho_s^0 = J[1 - 2(t'/t)^2]/4$, where $J = 4t^2/U$. At finite doping, there is also a contribution to the stiffness from the last term in (4) which contains only valence fermions. This last contribution is proportional to the Pauli susceptibility, which in two dimensions does not depend on carrier concentration. As a result, in the SDW approximation, the spin stiffness acquires a finite correction at an arbitrarily small deviation from half-filling,^{5,9,16}

$$\rho_s = \rho_s^0(1 - z), \quad (5)$$

where

$$z = 4U\chi_{2D}^{\text{Pauli}} = 2U \frac{\sqrt{m_{\perp} m_{\parallel}}}{\pi} . \quad (6)$$

We see that if $z < 1$, the Néel state remains stable at finite doping, while if $z > 1$, it becomes unstable, and we have to consider incommensurate states as possible candidates to the ground state. In the naive mean-field calculations discussed so far, we have $z \sim U/J \gg 1$, which implies that the commensurate state becomes unstable immediately upon doping. However, we have explicitly verified that all our conclusions are valid for arbitrary ratios of t/U and t'/t provided that magnetic order at half-filling is commensurate, and the hole pockets are located at $(\pm\pi/2, \pm\pi/2)$. We therefore will consider z as an input parameter which can, in principle, have any value. Some rigorous results about the dispersion of bosonic excitations at arbitrary t, t', U will be presented in Appendix B.

It is worth emphasizing that even in the large U limit,

the value of z can in fact be of the order of unity. The point is that the mean-field results at large U must be taken with caution in view of a strong self-energy and vertex corrections which both contribute powers of U/tS . Self-consistent consideration of these corrections indicates that they do not change the momentum dependence of the vertices at small $q - \bar{Q}$, but reduce the overall scale of the effective interaction between holes from U to U_{eff} which is of the order of the bandwidth J .^{5,16,20} This in turn implies that z is in fact simply a number, independent of U/t . Furthermore, strictly speaking, instead of U_{eff} we have to consider the total scattering amplitude of two holes, T . In two dimensions,

$$T = \frac{U_{\text{eff}}}{1 + \frac{mU_{\text{eff}}}{4\pi} \log \frac{mU_{\text{eff}}p_F}{4\pi}}. \quad (7)$$

Hence T and, consequently, z vanish logarithmically as the hole concentration $\delta \propto \sqrt{p_F}$ tends to zero. This always makes the collinear antiferromagnetic state stable at *very* low doping.¹⁶ However, the range of doping where logarithmic corrections are important is likely to be very small, and in this paper we simply set $T = U_{\text{eff}}$ and consider $z = O(1)$ as a doping-independent parameter. For simplicity, throughout the paper, we will focus on large U and present the results for the quantities not related to Pauli susceptibility, only to the leading order in t/U .

We now consider incommensurate spin configurations at finite doping. Let us first focus on the two simplest candidates: the spiral states with the ordering vectors (π, Q) and (Q, Q) .^{5,9-11} As before, we will label the ordering momentum as \bar{Q} [\bar{Q} can be either (π, Q) or (Q, Q)]. The spin order parameter now has two components, and in terms of the fermionic operators is expressed as

$$S_{\bar{Q}}^+ = \frac{1}{N} \sum_k \langle a_{k,\uparrow}^\dagger a_{k+\bar{Q},\downarrow} \rangle \equiv S_{\bar{Q}}, \quad (8)$$

$$S_{-\bar{Q}}^- = \frac{1}{N} \sum_k \langle a_{k,\downarrow}^\dagger a_{k-\bar{Q},\uparrow} \rangle = (S_{\bar{Q}})^*.$$

For definiteness, we choose the order parameter to be in the XY plane. Without a loss of generality one can also choose $S_{\bar{Q}}$ to be real. The real space spin configuration described by (8) is then $S_R^X = S_{\bar{Q}} \cos(\bar{\mathbf{Q}} \cdot \mathbf{R})$, and $S_R^Y = S_{\bar{Q}} \sin(\bar{\mathbf{Q}} \cdot \mathbf{R})$, where \mathbf{R} denotes the lattice site.

The SDW calculations proceed in the same way as before: One has to decouple the interaction term in (1) using (8) and diagonalize the quadratic form. Performing the computations, we obtain

$$E_k^{c,d} = \epsilon_+ \pm E_-, \quad (9)$$

where as before $E_- = \sqrt{\Delta^2 + (\epsilon_-)^2}$, but now

$$\epsilon_+ = \frac{\epsilon_{k+\bar{Q}/2} + \epsilon_{k-\bar{Q}/2}}{2}, \quad \epsilon_- = \frac{\epsilon_{k+\bar{Q}/2} - \epsilon_{k-\bar{Q}/2}}{2}. \quad (10)$$

Note that for XY ordering, these new electron states appear as hybridization of the original electrons with op-

posite spins and thus contain no spin labels. In this situation, there is no doubling of the unit cell, and the summation over momenta in (8) is extended to the whole first Brillouin zone ($-\pi/a < k_{x,y} < \pi/a$).

The gap Δ is related to the parameters of the Hubbard model via the self-consistency condition

$$\frac{1}{U} = \frac{1}{N} \sum_k \frac{1}{2\sqrt{\Delta^2 + E_-^2}}, \quad (11)$$

where the summation goes over the momenta of occupied states.

Consider now specifically the spiral (π, Q) state. The mean-field fermionic spectrum for this state is not symmetric with respect to the reflection $k_y \rightarrow -k_y$, although it is still symmetric with respect to $k_x \rightarrow -k_x$. Consequently, the minima at $(\pm\pi/2, \pi/2)$ have lower hole energy than those at $(\pm\pi/2, -\pi/2)$.

Suppose that the concentration of holes filling the lower-energy pocket is x_1 and filling the higher-energy pocket is x_2 ($x_1 + x_2 = x$). Simple calculations then show that the ground-state energy of the (π, Q) phase is given by

$$E^{(\pi, Q)} = -t\bar{q}(x_1 - x_2) + \frac{t^2\bar{q}^2}{4\Delta} + \frac{\pi(x_1^2 + x_2^2)}{2\sqrt{m_\perp m_\parallel}}, \quad (12)$$

where $\bar{q} \equiv \bar{q}_y = \pi - Q$. The first term reflects the decrease in total energy due to the ϵ_+ term in the spectrum, the second term results from the redistribution of the energy levels below the Fermi level, and the last term corresponds to the increase of the total energy due to unequal occupation of pockets. Minimizing the total energy of the (π, Q) state with respect to \bar{q} we obtain to the lowest order in hole concentration

$$\bar{q} = \frac{U}{t}(x_1 - x_2). \quad (13)$$

For the energy of the (π, Q) state, we then have

$$E^{(\pi, Q)} = \frac{\pi(x_1 - x_2)^2}{4\sqrt{m_\perp m_\parallel}}(1 - z) + \frac{\pi x^2}{4\sqrt{m_\perp m_\parallel}}. \quad (14)$$

We see that the ground-state energy of the (π, Q) phase becomes smaller than that of the (π, π) phase at $z > 1$, exactly when the stiffness for the (π, π) phase becomes negative. In the latter case, we also have $x_1 = x$ and $x_2 = 0$, which implies that only two out of four pockets are occupied, and $\bar{q} = (U/t)x$. A similar analysis was performed in Ref. 9.

Finally, consider the (Q, Q) phase. Now the fermionic spectrum is not symmetric with respect to either the $k_x \rightarrow -k_x$ or $k_y \rightarrow -k_y$ reflections. The point $(\pi/2, \pi/2)$ becomes the only absolute minimum of the hole spectrum. Suppose that the concentration of holes filling the lowest-energy pocket is x_1 , filling the two intermediate-energy pockets is x_2 , and filling the highest-energy pocket is x_3 ($x_1 + 2x_2 + x_3 = x$). Then the ground-state energy of the (Q, Q) phase is given by

$$E^{(Q,Q)} = -2t\bar{q}(x_1 - x_3) + \frac{t^2\bar{q}^2}{2\Delta} + \frac{\pi(x_1^2 + 2x_2^2 + x_3^2)}{\sqrt{m_\perp m_\parallel}}. \quad (15)$$

The inverse pitch of the spiral $\bar{q} = \pi - Q$ is found by minimizing the energy:

$$\bar{q} = \frac{U}{t}(x_1 - x_3). \quad (16)$$

The total energy then assumes the following form:

$$E^{(Q,Q)} = \frac{\pi}{2\sqrt{m_\perp m_\parallel}} [(x_1 - x_3)^2(1 - z) + (x_1 - 2x_2)^2 + 4x_2^2]. \quad (17)$$

It is immediately obvious that if $z < 1$, then the lowest possible energy is achieved when $x_1 = x_2 = x_3$, and $\bar{q} = 0$, i.e., in the (π, π) phase. If $z > 1$, then $x_3 = 0$. Minimizing the energy with respect to x_1 , we find

$$x_1 = \frac{4}{6 - z}x \quad (18)$$

when $z < 2$ and

$$x_1 = x \quad (19)$$

when $z > 2$. In the former case only the highest-energy pocket has no holes, and the total energy is equal to

$$E^{(Q,Q)} = \frac{2\pi x^2}{\sqrt{m_\perp m_\parallel}} \frac{2 - z}{6 - z}. \quad (20)$$

It is straightforward to see that it is always higher than the energy of the (π, Q) phase, given by Eq. (14). In case of $z > 2$, only the pocket with the lowest hole energy is occupied, and the total energy is

$$E^{(Q,Q)} = \frac{\pi x^2}{2\sqrt{m_\perp m_\parallel}}(2 - z). \quad (21)$$

Comparing (2), (14), and (21), we observe that the Néel state is the minimum for $z < 1$ and the (π, Q) spiral phase has the lowest energy at $1 < z < 2$, while the

(Q, Q) state has the lowest energy at $z > 2$.

Observe, however, that in the latter case, $\partial^2 E^{(Q,Q)}/\partial x^2 \sim (2 - z)$ is negative. On general grounds, this result suggests that the homogeneous solution is unstable. We will see in the next section that the longitudinal stiffness for the (Q, Q) state is in fact negative — this will be another argument in favor of an inhomogeneous ground state. On the other hand, for the (π, Q) phase in its region of stability ($1 < z < 2$) we have $\partial E^{(\pi,Q)}/\partial x^2 > 0$; i.e., the homogeneous solution is stable.

III. COLLECTIVE EXCITATIONS

Now we proceed to examining the stability of the spiral states by considering collective bosonic excitations. It follows from general considerations that in a spiral phase one should have a Goldstone mode with one velocity related to the spin rotation in the plane of the spiral, and two Goldstone modes with another velocity related to the rotations of the plane of the spiral around the X and Y axes.²¹ The former Goldstone mode results in the divergence of the total static susceptibility $\chi^{+-}(q)$ at the wave vector $q = -\bar{Q}$, while the latter leads to divergences of the total $\chi^{zz}(q)$ at the wave vectors $\pm\bar{Q}$.

The spectrum of collective excitations is determined by the poles of dynamic susceptibility

$$\chi_q^{ij} = i \int dt e^{i\omega t} \langle T S_q^i(t) S_{-q}^j(0) \rangle. \quad (22)$$

Here S^i represents either one of the three spin densities S^+, S^-, S^z or the charge density ρ . For the (π, π) state, fluctuations in transverse spin channels are completely decoupled from fluctuations in the density and longitudinal spin channels. Dynamical susceptibility is then a 2×2 problem. For planar spiral states, however, all four channels are coupled, and the dynamical susceptibility has to be found by solving a set of four coupled Dyson equations. Doing the standard SDW manipulations, we obtain that the poles of dynamical susceptibility are given by solving $D(q, \omega) = 0$ where $D(q, \omega)$ is the determinant of a 4×4 matrix given by

$$\begin{pmatrix} 1 - U\chi_{q,-q}^{+-} & -U\chi_{q+2\bar{Q},-q}^{--} & -U\sqrt{2}\chi_{q+\bar{Q},-q}^{z-} & U\sqrt{2}\chi_{q+\bar{Q},-q}^{\rho-} \\ -U\chi_{q,-(q+2\bar{Q})}^{++} & 1 - U\chi_{q+2\bar{Q},-(q+2\bar{Q})}^{+-} & -U\sqrt{2}\chi_{q+\bar{Q},-(q+2\bar{Q})}^{z+} & U\sqrt{2}\chi_{q+\bar{Q},-(q+2\bar{Q})}^{\rho+} \\ -U\sqrt{2}\chi_{q,-(q+\bar{Q})}^{+z} & -U\sqrt{2}\chi_{q+2\bar{Q},-(q+\bar{Q})}^{-z} & 1 - 2U\chi_{q+\bar{Q},-(q+\bar{Q})}^{zz} & 2U\chi_{q+\bar{Q},-(q+\bar{Q})}^{\rho z} \\ -U\sqrt{2}\chi_{q,-(q+\bar{Q})}^{+\rho} & -U\sqrt{2}\chi_{q+2\bar{Q},-(q+\bar{Q})}^{-\rho} & -2U\chi_{q+\bar{Q},-(q+\bar{Q})}^{z\rho} & 1 + 2U\chi_{q+\bar{Q},-(q+\bar{Q})}^{\rho\rho} \end{pmatrix}.$$

The expressions for the irreducible susceptibilities are presented in Appendix A. A similar expression for $D(q, \omega)$ was recently obtained by Cote and Tremblay²² in their SDW analysis of collective excitations in a 2D Hubbard model on a triangular lattice at half-filling. For our present consideration, it is essential that at zero fre-

quency, $\chi_{q,-(q+\bar{Q})}^{+z} = \chi_{q+2\bar{Q},-(q+\bar{Q})}^{-z} = \chi_{q+\bar{Q},-(q+\bar{Q})}^{z\rho} = 0$ at any q , and therefore static transverse spin fluctuations *decouple* from the longitudinal spin fluctuations and density fluctuations (we remind the reader that spin ordering is in the XY plane). We now consider the transverse and longitudinal fluctuations separately.

A. Longitudinal spin fluctuations

Consider first the solution for the density and longitudinal spin fluctuations. At $q = -\bar{Q}$, the evaluation of the expressions in Appendix A yields at zero frequency $\chi_{-\bar{Q},0}^{\rho} = \chi_{\bar{Q},0}^{\rho} = \chi_{-\bar{Q},\bar{Q}}^{\rho,\rho} = z/8U$, $\chi_{-\bar{Q},-\bar{Q}}^{++} = \chi_{\bar{Q},\bar{Q}}^{--} = (z-4)/8U$, and $\chi_{-\bar{Q},\bar{Q}}^{+-} - \chi_{\bar{Q},\bar{Q}}^{-+} = \sum_k 1/(2E_k^-) \equiv 1/U$. Elementary manipulations then show that there is indeed a Goldstone mode at $q = -\bar{Q}$. Expanding around this point, we obtain after straightforward but lengthy calculations, that to quadratic order in $q + \bar{Q}$

$$D(q, \omega) = \frac{2t^2}{U^2} (q + \bar{Q})^2 \left(1 - \frac{z_\omega}{2}\right) - \frac{\omega^2}{U^2}. \quad (23)$$

The $q + \bar{Q}$ term comes from the expansion of $1 - U\chi_{q,-q}^{+-} + U\chi_{q,-(q+2\bar{Q})}^{++}$, and the ω^2 term comes from χ^{+z} and χ^{-z} . We also introduced $z_\omega = 4U\chi_{2D}(\omega)$ where $\chi_{2D}(\omega)$ is the susceptibility of a 2D Fermi gas at finite frequency,

$$\chi_{2D}(\omega) = \frac{\sqrt{m_{\parallel}m_{\perp}}}{2\pi} \left[1 - \left(\frac{\delta^2}{\delta^2 - 1}\right)^{1/2}\right], \quad (24)$$

where to the leading order in the hole density,

$$\delta^2 = \frac{\omega^2 m_{\parallel} m_{\perp}}{(q + \bar{Q})^2 p_F^2} \quad (25)$$

and $p_F \sim \sqrt{x}$ is the Fermi momentum of holes. At zero frequency we indeed have $z_\omega = z$.

The explicit expression for the total longitudinal susceptibility $\bar{\chi}$ is

$$\bar{\chi}^{+-}(q, \omega) = \frac{A(q, \omega)}{D(q, \omega)}. \quad (26)$$

The numerator can be evaluated right at $q = -\bar{Q}$, $\omega = 0$ where it reduces to

$$A(-\bar{Q}, 0) = (\chi_{-\bar{Q},\bar{Q}}^{+-} - \chi_{-\bar{Q},-\bar{Q}}^{++}) \left[(1 - U\chi_{-\bar{Q},\bar{Q}}^{+-})(1 + 2U\chi_{-\bar{Q},\bar{Q}}^{\rho,\rho}) + 2U^2\chi_{-\bar{Q},0}^{\rho,\rho}\chi_{\bar{Q},0}^{\rho,\rho} \right]. \quad (27)$$

Substituting the values for irreducible susceptibilities, we obtain that $A = 1/2U$ and does not depend on z . For the total longitudinal susceptibility we then have

$$(\bar{\chi}_{q,-q}^{+-})^{-1} = J(q + \bar{Q})^2 \left(1 - \frac{z_\omega}{2}\right) - \frac{\omega^2}{2J}. \quad (28)$$

This expression is valid for the (π, Q) phase and for the (Q, Q) phase at $q_x = q_y$. We see that the stiffness for longitudinal fluctuations is $\rho_L \propto (1 - z/2)$. For the (π, Q) phase ($1 < z < 2$), the stiffness is positive, while for the (Q, Q) phase ($z > 2$) it is *negative*. This last result implies that the homogeneous (Q, Q) phase is in fact unstable. This agrees with our observation in the previous section that $\partial E^{(Q,Q)}/\partial x^2$ is negative.

The negative longitudinal stiffness of the (Q, Q) phase was earlier obtained by Dombre⁹ in the macroscopic calculations in the framework of the Shraiman-Siggia model. He argued that this instability leads to a formation of domain walls, but can be prevented by a long-range Coulomb interaction. Phase separation at large z is also a possibility.²³ We, however, have not studied inhomogeneous spin configurations.

It is also essential to observe that z_ω behaves as a constant ($= z$) only at frequencies comparable to $(q + \bar{Q})p_F$; at larger frequencies, the dynamical susceptibility $\chi_{2D}(\omega)$ rapidly decreases, and near a spin-wave pole $\omega^2 \sim 2J^2(q + \bar{Q})^2$, we have $\chi_{2D}(\omega) \sim p_F|q + \bar{Q}|/\omega \ll 1$. Then, near the pole, to the lowest order in the hole density we have

$$\bar{\chi}^{+-} \sim [c^2(q + \bar{Q})^2 - \omega^2]^{-1}, \quad (29)$$

where the spin-wave velocity $c = \sqrt{2}J$ is the same as in the (π, π) . This result agrees with the macroscopic consideration by Shraiman and Siggia¹² and with the Schwinger-boson analysis by Gan, Andrei, and Coleman.¹¹

B. Transverse spin fluctuations

We now consider the magnetic susceptibility $\chi_{q,q}^{zz}$ associated with the out-of-plane fluctuations. We found above that this channel is coupled to density and longitudinal spin fluctuations only dynamically. For the full static susceptibility we then have a simple random-phase-approximation (RPA) formula

$$\bar{\chi}_{q,-q}^{zz} = \frac{\chi_{q,-q}^{zz}}{1 - 2U\chi_{q,-q}^{zz}}. \quad (30)$$

From the above considerations, we expect the Goldstone modes in $\bar{\chi}_{q,-q}^{zz}$ to be at $q = \pm\bar{Q}$. Consider first the (π, Q) spiral. Using Eq. (A1) from Appendix A, and expanding near $q = \pm\bar{Q}$, to the lowest order in the hole density we obtain

$$\chi_{q,-q}^{zz} = \frac{1}{2U} + \frac{x^2}{U} \left(\frac{t\bar{q}}{Ux}\right)^2 \left(1 - \frac{\bar{q}^2}{\bar{q}^2}\right) - \frac{x^2}{U} \left(\frac{t\bar{q}}{Ux}\right) \left(1 - \frac{\bar{q}^2}{\bar{q}^2}\right), \quad (31)$$

where $\tilde{q} = \pi - q$ and $\bar{q} = \pi - Q$. The second term comes from the integration over the regions away from

pockets, while the last term comes from the integration inside the hole pockets. We see that at $\tilde{q} = \pm\bar{q}$; i.e., at $q = \pm Q$, χ^{zz} precisely equals $1/2U$, and $\bar{\chi}^{zz}$ diverges as it indeed should. At the same time, neither of the last two terms in (31) has a form of a quadratic expansion around $q = \pm Q$. To the lowest order in hole density, $\bar{q} = Ux/t$, and the last two terms in (31) cancel each other at any $q \sim Q$. This means that $\bar{\chi}^{zz}$ is infinite in a whole range of momenta which in turn implies that there exists an infinite number of other states which are degenerate in energy with the spiral states to the leading order in hole density. In Appendix B we show that this degeneracy is in fact a quite general phenomenon and it exists for an arbitrary ratio of t , t' , and U . Furthermore, we found that at least to the leading order in t/U , $\chi_{q,-q}^{zz} \equiv 1/2U$ for $q = (\pi, \tilde{q}_y)$ and arbitrary \tilde{q}_y . This last result means that there exists a whole line of zero modes in $\bar{\chi}^{zz}$. At $q = (\tilde{q}_x, \tilde{q}_y)$, we found that $\chi_{q,-q}^{zz} = 1/2U + O((\tilde{q}_x)^4)$. For typical $\tilde{q}_x \sim \bar{q} \sim x$, the last term is $O(x^4)$; i.e., it contains two extra powers of x compared to the terms we consider.

We will discuss the set of degenerate states in the next section, and here merely notice that the degeneracy is not related to any kind of broken symmetry and, therefore, should be lifted by higher-order terms in the expansion in the hole density which we are proceeding to discuss.

It is not difficult to make sure that the contributions to χ^{zz} from the regions far from the hole pockets form regular series in powers of \tilde{q}^2 ; odd powers of \tilde{q} disappear due to momentum integration. As typical $\tilde{q} \sim \bar{q}$, the next-to-leading order terms have an extra factor of $\tilde{q}^2 \propto x^2$. On the other hand, the expansion near pockets involve only fermions with momenta near $k = (\pi/2, \pi/2)$ and $k = (-\pi/2, \pi/2)$; i.e., there is no summation over momenta. As a result, the next subleading term in χ^{zz} from hole pockets has an extra power of x rather than x^2 . We computed this term explicitly by expanding in (A1) and in the ground-state energy (from which we extract \bar{q}) beyond the leading order in hole density, and obtained

$$\bar{q} = \frac{Ux}{t} \left(1 - \frac{\pi}{8} x \frac{m_{\parallel} + m_{\perp}}{\sqrt{m_{\parallel}m_{\perp}}} \right) \quad (32)$$

and

$$\chi_{q,-q}^{zz} = \frac{1}{2U} - \frac{2x^3}{U} \left(1 - \frac{\tilde{q}^2}{\bar{q}^2} \right) \left[\left(1 - \frac{2}{z} \right) - \frac{\tilde{q}^2}{\bar{q}^2} \right]. \quad (33)$$

Notice that the correction term in \bar{q} which explicitly depends on the mass ratio does not show up in the expression for χ^{zz} .

We see that the Goldstone mode in $\bar{\chi}^{zz} \sim (1 - 2U\chi^{zz})^{-1}$ at $\tilde{q} = \pm\bar{q}$ survives as it should, but $(\bar{\chi}^{zz})^{-1}$ still *does not* have a form of a quadratic expansion around the Goldstone points (Fig. 1). For $1 < z < 2$, when the (π, Q) phase is a candidate for the ground state, $1 - 2U\chi^{zz}$, and hence $\bar{\chi}^{zz}$ is negative in the region $\tilde{q}^2 < \bar{q}^2$. This implies that the (π, Q) planar spiral phase is also unstable, and one should look for other candidates for the ground state.

For completeness, consider also the transverse suscep-

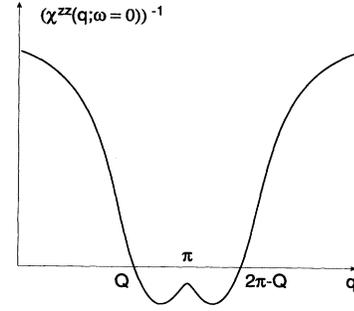


FIG. 1. The out-of-plane static susceptibility for the planar (π, Q) spiral. The susceptibility is negative around (π, π) , indicating instability towards spontaneous magnetization in the out-of-plane direction.

tibility in the (Q, Q) phase. At $\tilde{q}_x \neq \tilde{q}_y$, the total transverse susceptibility is positive already at the quadratic order in \tilde{q} :

$$1 - 2U\chi^{zz} = \frac{t^2}{U^2} (\tilde{q}_x - \tilde{q}_y)^2. \quad (34)$$

However, along the Brillouin zone diagonal, at $\tilde{q}_x = \tilde{q}_y = \tilde{q}$, $(\bar{\chi})^{-1}$ is again zero, to order $O(x^2)$, at arbitrary \tilde{q} . We performed calculations to order $O(x^3)$ and obtained

$$1 - 2U\chi^{zz} = 16x^3 \left(1 - \frac{\tilde{q}^2}{\bar{q}^2} \right) \left[1 - \frac{2}{z} - \frac{\tilde{q}^2}{\bar{q}^2} \right]. \quad (35)$$

The total transverse susceptibility $\bar{\chi}^{zz} = \chi^{zz}/(1 - 2U\chi^{zz})$ then has one zero associated with the Goldstone mode at $\tilde{q} = \bar{q}$, and another “accidental” zero at

$$\tilde{q} = \bar{q} \sqrt{1 - \frac{2}{z}}. \quad (36)$$

Between these two zeros the total static transverse susceptibility is negative, indicating an instability. Contrary to the previously found instability of the (Q, Q) state towards domain-wall formation, the latter instability is unlikely to be removed by including the long-range component of Coulomb interaction. We, however, have not performed any further calculations for the (Q, Q) phase.

The result that the planar spiral phase is unstable contradicts the assumption made by Shraiman and Siggia that the subleading terms in the expansion over x stabilize the planar phase. On the contrary, our results indicate that they do not.

C. Uniform susceptibility

We conclude this section with a brief consideration of the uniform susceptibility of the spiral states. The key point here is that the spiral ordering in the XY plane away from half-filling couples the fluctuations along X and Y directions, which at half-filling constituted longitudinal and transverse fluctuations. We have found in

Sec. II that in the (π, π) state, longitudinal fluctuations acquire a correction proportional to the Pauli susceptibility, while transverse fluctuations do not. In a spiral phase, these fluctuations are coupled, and as a result, the uniform static susceptibility of the ordered state acquires a finite correction immediately away from half-filling,

$$\bar{\chi}^{+-}(0, 0) = \frac{1}{8J} + \frac{\tilde{\chi}_{2D}}{4}, \quad (37)$$

where

$$\tilde{\chi}_{2D} = \lim_{q \rightarrow 0} \frac{1}{N} \sum_{\substack{E_{k-Q}^d < \mu \\ E_{k-Q}^d > \mu}} \frac{1}{E_{k-Q}^d - E_{k+q}^d}. \quad (38)$$

For $\bar{Q} = (\pi, \pi)$, $\tilde{\chi}_{2D} = \chi_{2D} = \sqrt{m_{\parallel} m_{\perp}} / 2\pi$. However, for finite $\bar{q} = Ux/t$, the $t\bar{q}$ term in the denominator in (38) is the dominant one, and performing calculations we obtain

$$\tilde{\chi}_{2D} = \frac{1}{8J} \frac{2J^2}{t^2}. \quad (39)$$

We see, therefore, that the steplike correction to the uniform susceptibility is relatively small at $J \ll t$. Notice also that fluctuations in the Z direction are decoupled from the XY fluctuations, and hence $\bar{\chi}_{00}^{zz} = (1/8J) + O(x)$ without any steplike corrections.

We now proceed to the analysis of the states degenerate with the planar spiral to the lowest order in the hole density.

IV. NONCOPLANAR STATES

To specify the set of degenerate states, we first return to our results obtained to order $O(x^2)$ and observe that the zero modes in χ^{zz} are centered around (π, π) . A zero mode in the transverse susceptibility at (π, π) implies that the system is indifferent towards generation of a spontaneous commensurate antiferromagnetic order along the Z direction in addition to the incommensurate spin ordering in the XY plane (Fig. 2). We, therefore, consider a set of states having 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. Performing the mean-field decoupling of the interaction term and the diagonalization of the Hubbard Hamiltonian, we obtain

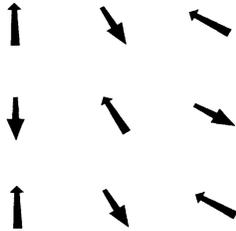


FIG. 2. Spin configuration of a noncoplanar state. Arrows with thick ends point out of the plane, while those with thick tails point into the plane. This configuration is different from the double spiral considered in Ref. 8(b).

$$H = \sum_k \bar{E}_k (c_k^\dagger c_k - d_k^\dagger d_k), \quad (40)$$

with the energy in the valence (d) and conduction (c) bands given by

$$\bar{E}_k = \sqrt{(E_+ + \sqrt{\Delta_{\parallel}^2 + E_-^2})^2 + \Delta_{\perp}^2}. \quad (41)$$

The ground-state energy, to order $O(x^2)$, is given by

$$E_{\Delta_{\perp}} = \frac{Ux^2}{z} - tq^*x + \frac{(q^*)^2 t^2}{2U}, \quad (42)$$

where $q^* = \bar{q}(\Delta_{\parallel}/\Delta)$ and $\Delta^2 = \Delta_{\perp}^2 + \Delta_{\parallel}^2$. For $U \gg t$ we indeed have $\Delta \approx U/2$. We also assumed in (42) that $\Delta_{\parallel} \gg x^{1/2}$.

Since we now have two order parameters, there are also two self-consistency conditions. The condition on the out-of-plane order parameter Δ_{\perp} is

$$\frac{1}{U} = \sum_k \frac{1}{2\bar{E}_k}, \quad (43)$$

and the condition on the in-plane order parameter Δ_{\parallel} is

$$\frac{1}{U} = \sum_k \frac{1}{2\bar{E}_k} \left(1 + \frac{E_+}{\sqrt{\Delta_{\parallel}^2 + E_-^2}} \right). \quad (44)$$

In the limit $\Delta_{\perp} \rightarrow 0$, the latter expression reduces to (11) as it should. However, for any nonzero Δ_{\parallel} , the two self-consistency conditions have to be satisfied simultaneously, which implies that the inverse pitch of the spiral is no longer a free parameter. Specifically, the compatibility of the two conditions requires that

$$\sum_k \frac{E_+}{\sqrt{\Delta_{\parallel}^2 + E_-^2} E_k} = 0. \quad (45)$$

However, solving this equation to order $O(x^2)$, we find that

$$q^* = \frac{U}{t}x, \quad (46)$$

which is exactly what one would obtain by simply minimizing the ground-state energy (42) with respect to q^* . As a result, substituting q^* into (42), we obtain that the ground-state energy *does not* depend on Δ_{\perp} ,

$$E_{\Delta_{\perp}} = Ux^2 \left(\frac{2}{z} - 1 \right) \equiv E^{(\pi, Q)}. \quad (47)$$

Clearly, then, all states with finite Δ_{\perp} are degenerate in energy with the planar spiral, and we have to go beyond the leading order in x to see which state actually has the lowest energy.

The calculations to order $O(x^3)$ proceed in the same way as in the previous section. We skip the details and focus on the results. For the inverse pitch of the spiral we obtained from the consistency condition (45)

$$q^* = \frac{U}{t} x \left[1 + 2x \left(1 - \frac{\Delta^2 + \Delta_{\parallel}^2}{2\Delta_{\parallel}^2} \frac{2}{z} \right) \right]. \quad (48)$$

Here we again assumed that $\Delta_{\parallel}/\Delta \gg x^{1/2}$. We see now that the values of \bar{q} at $\Delta_{\perp} = 0$ [Eq. (32)] and at $\Delta_{\perp} \rightarrow 0$ [Eq. (48)] are different to order $O(x^3)$. The reason is, of course, that in the case of a planar spiral there is only one self-consistency condition to satisfy. The energy of the noncoplanar phase, at $\Delta_{\parallel}/\Delta \gg x^{1/2}$, is given by

$$E_{\Delta_{\perp}} = E^{(\pi, Q)} + \frac{t}{2U} \left[q^* - \frac{Ux}{t} \right]^2 + Ux^3 \left(\frac{\Delta_{\perp}}{\Delta_{\parallel}} \right)^2 \left(1 - \frac{2}{z} \right), \quad (49)$$

where q^* is given by (48). Let us first discuss the second term in the right-hand side (rhs) of (49). This is a positive contribution to the energy related to the fact that q^* is no longer a free parameter. At $\Delta_{\perp} \rightarrow 0$, the last term in the rhs of (49) disappears and the energy of the noncoplanar state turns out to be larger than that of the (π, Q) state. Clearly, then, *very* close to $\Delta_{\perp} = 0$, a simple noncoplanar state that we consider is not the best choice. This in fact is consistent with the form of the susceptibility in the spiral phase which has a minimum at some momentum different from (π, π) [see Eq. (33)]. However, we also see that this energy difference is $O(x^4)$, and for all $\Delta_{\perp} \geq x^{1/2}$, the second term in the rhs of (49) can be neglected compared to the third term which is of the order x^3 and negative for $z < 2$ which we consider. This latter term increases with Δ_{\perp} . Moreover, Eq. (49) does not contain a restoring force (i.e., terms $\sim x^3 \Delta_{\perp}^4$). Therefore, by making Δ_{\perp} larger and larger, we can continuously decrease the ground-state energy as long as Eq. (49) remains valid, i.e., as long as $\Delta_{\parallel}/\Delta \gg x^{1/2}$. When Δ_{\perp} nearly reaches Δ , and $\Delta_{\parallel}/\Delta$ becomes comparable with $x^{1/2}$, the expression for the ground-state energy of the noncoplanar state becomes more complex. In this situation, we found

$$E_{\Delta_{\perp}} = \frac{Ux^2}{z} + \frac{Ux^2}{2} \left[(\alpha\beta)^2 + 2\beta^2 - \frac{\beta z}{6} f(\alpha) \right], \quad (50)$$

where

$$\alpha = \frac{\Delta_{\parallel}}{\Delta_{\perp} x^{1/2}}, \quad \beta = \frac{q^* t}{Ux} \frac{\Delta_{\perp} x^{1/2}}{\Delta_{\parallel}}, \quad f(\alpha) = \left(\alpha^2 + \frac{8}{z} \right)^{3/2} - \alpha^3. \quad (51)$$

For $\Delta_{\parallel}/\Delta \gg x^{1/2}$, $\alpha \gg 1$, and expanding in $1/\alpha$ in (51) we recover (49).

The solution of the self-consistency condition (45) is also more complex for $\Delta_{\parallel}/\Delta \sim x^{1/2}$. We found

$$\beta = \frac{z}{2} \left[\sqrt{\alpha^2 + \frac{4}{z}} - \alpha \right]. \quad (52)$$

At $\alpha \gg 1$ (but still, $\Delta_{\parallel} \ll \Delta$), this expression reduces to (48).

Substituting β into (51), we obtain the ground-state energy as a function of a single free parameter α . The equilibrium value of α (and, hence, of Δ_{\perp}) can now be obtained by a simple minimization of the energy. In a general case, the solution of $dE_{\Delta_{\perp}}/d\alpha = 0$ is rather involved, but for z close to 2, a simple analytical solution is possible. The point is that at $z \approx 2$, the equilibrium value of α is large [$\sim (2-z)^{-1/2}$], and so we can expand (51) in powers of $1/\alpha^2$. We then obtain

$$E_{\Delta_{\perp}} = E^{(\pi, Q)} + Ux^2 \left[\frac{1}{\alpha^2} \left(1 - \frac{2}{z} \right) + \frac{7}{24\alpha^4} \right]. \quad (53)$$

The energy has a minimum at

$$\alpha = \sqrt{\frac{7z}{12(2-z)}}. \quad (54)$$

For the equilibrium noncoplanar state we thus have

$$E_{\Delta_{\perp}} = \frac{Ux^2}{2z} (2-z) \left[1 - \frac{6}{7} (2-z) \right], \quad \bar{q} = \sqrt{\frac{12}{7} x \left(\frac{2}{z} - 1 \right)}, \quad \Delta_{\parallel} = \Delta \sqrt{\frac{7}{12} \frac{xz}{2-z}}. \quad (55)$$

We see that the energy of the noncoplanar state is substantially lower than that of the (π, Q) state. What is more, the energy gain in the equilibrium state scales as x^2 , instead of x^3 as in (49). This implies that the equilibrium state with $\Delta_{\parallel} \sim \sqrt{x}$, strictly speaking, does not belong to the original set of degenerate spin configurations, and could be selected already in the calculations to order $O(x^2)$. The discovery of the degenerate set of states and of the instability of the planar spiral gave us, nevertheless, a hint where to look for the minimum of the energy. Notice also that $\partial E_{\Delta_{\perp}}/\partial x^2 > 0$; i.e., there is no instability towards phase separation.

Another important point concerns the chirality of the novel state. Although the spin configuration in this state is noncoplanar, it is not chiral in the sense that there is no flux through a plaquette.²⁴ In other words, although the triple product of three adjacent spins along the Y direction, $\vec{S}_{i,j-1} \cdot (\vec{S}_{i,j} \times \vec{S}_{i,j+1}) \neq 0$, the triple product of spins lying in the vertices of a minimal triangle is always zero, since all spins along the rows in the X direction are parallel to each other. This fact distinguishes our noncoplanar state from the double spiral considered in Ref. 8(b), which has staggered chirality. We emphasize, however, that, at least in the SDW approximation, our noncoplanar state has *lower* energy than the double spiral.

V. MAGNETIC SUSCEPTIBILITY OF THE EQUILIBRIUM STATE

In the presence of a commensurate antiferromagnetism along the Z axis, the equation for magnetic instability becomes more complex as now bare susceptibilities with the momentum transfer (π, π) are also finite, and the total

susceptibility becomes an 8×8 problem. In view of this, we only computed the susceptibility to the leading order in Δ_\perp . We found that the compatibility condition (45) of the two self-consistent equations at $\Delta_\perp \rightarrow 0$ is equivalent [to order $O(x^3)$] to the condition that $\bar{\chi}^{zz}$ diverges at (π, π) (see Fig. 3). This extra zero mode exists because at $\Delta_\perp = 0$, the ground-state energy as a function of Δ_\perp has an extremum (maximum). We have not performed calculations at $\Delta_\perp \geq \Delta_\parallel$, but we believe it plausible that the spin susceptibility evolve with Δ_\perp as is shown in Fig 3. The equilibrium state is an energy minimum (at least, local), and we expect that the static susceptibility of this state is positive, diverging only at the Goldstone points. There exists, however, a subtlety in determining the locations of zero modes in this configuration, and so we will explicitly follow the recipe of the Goldstone theorem.²¹ This theorem states that if \hat{J} is a generator of a symmetry transformation, and the commutator $[\hat{A}, \hat{J}]$, where A is some operator, has a nonzero average value in the ground state, then the correlator $\langle TA^\dagger A \rangle$ diverges at $\omega = 0$. The residue of the quasiparticle pole near the Goldstone point is proportional to $[\hat{A}, \hat{J}]^2$. In our case the corresponding operators and correlators are the following.

(1) Rotation about the x axis: $\hat{J} = S_0^x$. If $\hat{A} = S_\pi^y$ [$\pi \equiv (\pi, \pi)$], then $[\hat{A}, \hat{J}] = -iS_\pi^z \sim \Delta_\perp$, and therefore $\chi_{st}^{xy}(\mathbf{q})$ diverges at $\mathbf{q} = \pi$. The residue of the pole is proportional to Δ_\perp^2 . If instead we choose $\hat{A} = S_{\pm\bar{Q}}^z$, then $[\hat{A}, \hat{J}] = iS_{\pm\bar{Q}}^y$, and we find a divergence in $\chi_{st}^{zz}(\mathbf{q})$ at $\mathbf{q} = \pm\bar{Q}$; the residue of the pole is proportional to Δ_\parallel^2 .

(2) Rotation about the y axis: $\hat{J} = S_0^y$. This case is analogous to the previous one. The divergences occur in $\chi_{st}^{xx}(\pi)$ with the residue of the pole $\propto \Delta_\perp^2$, and in $\chi_{st}^{zz}(\pm\bar{Q})$ with the residue $\propto \Delta_\parallel^2$.

(3) Rotation about the z axis: $\hat{J} = S_0^z$. Choosing $\hat{A} = S_{\bar{Q}}^+$ and $\hat{A} = S_{-\bar{Q}}^-$ we find divergences in $\chi_{st}^{+-}(\bar{Q})$ and $\chi_{st}^{-+}(-\bar{Q})$; in both cases the residue of the pole is proportional to Δ_\parallel^2 .

Combining these results, we find that in the equilibrium noncoplanar state, the in-plane static susceptibility

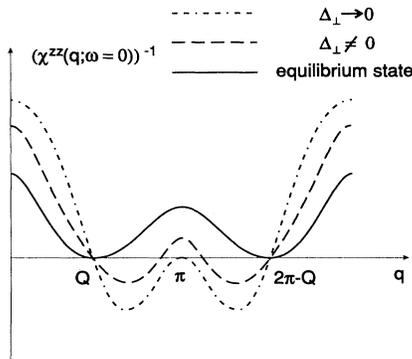


FIG. 3. The out-of-plane static susceptibility for three noncoplanar states: one with $\Delta_\perp \rightarrow 0$, another with an intermediate value of Δ_\perp , and the third with the equilibrium value of Δ_\perp .

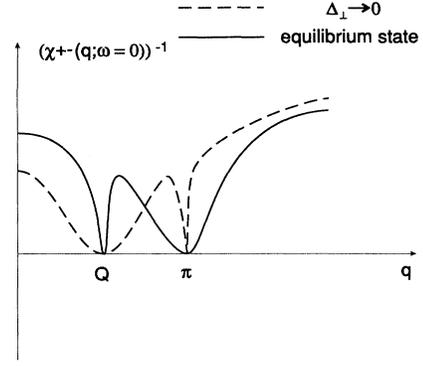


FIG. 4. The in-plane static susceptibility for the equilibrium noncoplanar state and a noncoplanar state with vanishing Δ_\perp .

χ^{+-} in fact has two poles, one at $q = (\pi, \pi)$ and the other at $q = -\bar{Q}$. Then, for q not too far from (π, π) , this susceptibility can be approximated as

$$\chi^{+-}(\mathbf{q}) \approx \frac{\chi_\pi}{(\mathbf{q} - \pi)^2} + \frac{\chi_{\bar{Q}}}{(\mathbf{q} + \bar{Q})^2}, \quad (56)$$

where the residues χ_π and $\chi_{\bar{Q}}$ are proportional to Δ_\perp^2 and Δ_\parallel^2 , respectively. Because $\Delta_\parallel \sim \sqrt{x}$, the residue of the pole at the incommensurate wave vector $\mathbf{q} = -\bar{Q}$ is suppressed with respect to the pole at the commensurate wave vector (π, π) , and the form of the static susceptibility is very similar to that for the (π, π) state (Fig. 4).

The out-of-plane static susceptibility χ^{zz} also has two poles,

$$\chi^{zz}(\mathbf{q}) \approx \frac{\chi_z}{(\mathbf{q} - \bar{Q})^2} + \frac{\chi_z}{(\mathbf{q} + \bar{Q})^2}, \quad (57)$$

but here both poles are suppressed as the residue χ_z is proportional to Δ_\parallel^2 and, therefore, to x . Again, the form of the susceptibility is very similar to that for the (π, π) state. On the contrary, in the planar spiral state, both transverse and longitudinal susceptibilities have Goldstone modes at $q = \pm\bar{Q}$ with the residue of the pole proportional to the total on-site magnetization (Fig. 3).

VI. CONCLUSIONS

Here we summarize the main results of this paper. We used spin-density-wave formalism and studied various magnetic phases of the 2D Hubbard model at low doping when a long-range magnetic order is still present. We found that the equilibrium spin configuration depends on the value of the dimensionless parameter $z = 4T\chi^{2D}$, where T is the scattering amplitude of two holes ($T = U$ in the mean-field approximation), and χ^{2D} is the Pauli susceptibility of holes which at low doping occupy pockets located at $(\pi/2, \pi/2)$ and symmetry-related points in the Brillouin zone. In 2D, Pauli susceptibility does not depend on the carrier concentration: $\chi^{2D} = \sqrt{m_\parallel m_\perp}/2\pi$.

We found that for $z < 1$, the commensurate antiferromagnetic state is stable. For $z > 2$, the spiral (Q, Q) phase is the equilibrium configuration at the mean-field level, but we found that this configuration has negative longitudinal stiffness and therefore is unstable against domain-wall formation. This result agrees with the macroscopic analysis in Ref. 9. The intermediate case, $1 < z < 2$, is the most interesting from a theoretical point of view. Here we found that the equilibrium configuration at the mean-field level is a (π, Q) spiral introduced by Shraiman and Siggia. The longitudinal stiffness in this configuration is positive, but the transverse stiffness vanishes to the leading order in hole density. This in turn implies that the spiral phase is degenerate in energy with many other spin configurations, and the equilibrium state only appears as an “order from disorder” effect. We performed calculations beyond the leading order in the hole density and found that the equilibrium state is not a planar spiral but rather a noncoplanar spin configuration which contains both (π, π) antiferromagnetism along one direction in spin space and a (π, Q) spiral in the orthogonal plane. The latter result suggests a scenario of spin reorientation with doping for $1 < z < 2$, different from the one suggested by Shraiman and Siggia. In their picture, upon doping spins remain in the same plane as at half-filling, but twist into a spiral with incommensurate momentum (π, Q) . In our scenario, the commensurate antiferromagnetic ordering (same as at half-filling) does not vanish, as doping only introduces a transverse component of the order parameter which forms a spiral in the plane perpendicular to the direction of the commensurate order. This transverse component is small to the extent of x , and the low- T behavior at finite doping remains nearly the same as in the commensurate antiferromagnet^{25,26}(Fig. 5).

It is essential that our analysis has been performed only for frequencies smaller than the energy scale ΔE associated with the lifting of the degeneracy. At larger fre-

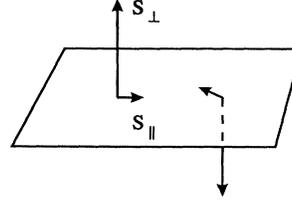


FIG. 5. Two adjacent spins in the equilibrium configuration. The in-plane component $S_{\perp} \sim x^{1/2}$ is small compared to the off-plane component, S_{\parallel} .

quencies, the static selection may be irrelevant, and one has to solve the full dynamical problem which presents a technical challenge.

The above analysis is valid for the magnetically ordered phase. We therefore cannot pretend to resolve the known discrepancy between neutron scattering and NMR experiments in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$,^{27,28} both of which have been performed well inside the metallic phase. We merely note that, as neutron data indicate, the incommensurability at (π, Q) observed at 7.5% and 14% doping *is not* correlated with the magnetic behavior in the ordered phase. This implies that our result, that in the ordered state susceptibility is always peaked at (π, π) , does not contradict the neutron data.

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APPENDIX A

In this appendix we present the results for the irreducible susceptibilities in the spiral phases. Each of the susceptibilities below was obtained by the standard SDW manipulations:

$$\begin{aligned} \chi_{q,-q}^{zz,\rho\rho} = & \frac{1}{8N} \sum_{E_k^d < \mu} \left[1 - \frac{\epsilon_k^- \epsilon_{k+q}^- \mp \Delta^2}{E_k^- E_{k+q}^-} \right] \left(\frac{1}{E_{k+q}^c - E_k^d - \omega} + \frac{1}{E_{k+q}^c - E_k^d + \omega} \right) \\ & + \frac{1}{8N} \sum_{\substack{E_{k+q}^d < \mu \\ E_k^d > \mu}} \left[1 + \frac{\epsilon_k^- \epsilon_{k+q}^- \mp \Delta^2}{E_k^- E_{k+q}^-} \right] \left(\frac{1}{E_k^d - E_{k+q}^d - \omega} + \frac{1}{E_k^d - E_{k+q}^d + \omega} \right) \end{aligned} \quad (\text{A1})$$

(upper sign for χ^{zz} and lower for $\chi^{\rho\rho}$); then

$$\begin{aligned} \chi_{q,-q}^{z\rho} = & \frac{1}{8N} \sum_{E_k^d < \mu} \left[\frac{\epsilon_k^-}{E_k^-} - \frac{\epsilon_{k+q}^-}{E_{k+q}^-} \right] \left(\frac{1}{E_{k+q}^c - E_k^d - \omega} - \frac{1}{E_{k+q}^c - E_k^d + \omega} \right) \\ & + \frac{1}{8N} \sum_{\substack{E_{k+q}^d < \mu \\ E_k^d > \mu}} \left[\frac{\epsilon_k^-}{E_k^-} + \frac{\epsilon_{k+q}^-}{E_{k+q}^-} \right] \left(\frac{1}{E_k^d - E_{k+q}^d - \omega} - \frac{1}{E_k^d - E_{k+q}^d + \omega} \right). \end{aligned} \quad (\text{A2})$$

Further,

$$\begin{aligned} \chi_{q,-q}^{+-} = & \frac{1}{4N} \sum_{\substack{E_{k-Q}^d < \mu \\ E_{k+q}^d < \mu}} \left[1 + \frac{\epsilon_{k-Q}^- \epsilon_{k+q}^-}{E_{k-Q}^- E_{k+q}^-} - \frac{\epsilon_{k-Q}^-}{E_{k-Q}^-} - \frac{\epsilon_{k+q}^-}{E_{k+q}^-} \right] \left(\frac{1}{E_{k+q}^c - E_{k-Q}^d - \omega} + \frac{1}{E_{k+q}^c - E_{k-Q}^d + \omega} \right) \\ & + \frac{1}{4N} \sum_{\substack{E_{k+q}^d < \mu \\ E_{k-Q}^d > \mu}} \left[1 - \frac{\epsilon_{k-Q}^- \epsilon_{k+q}^-}{E_{k-Q}^- E_{k+q}^-} - \frac{\epsilon_{k-Q}^-}{E_{k-Q}^-} + \frac{\epsilon_{k+q}^-}{E_{k+q}^-} \right] \left(\frac{1}{E_{k-Q}^d - E_{k+q}^d - \omega} + \frac{1}{E_{k-Q}^d - E_{k+q}^d + \omega} \right) \end{aligned} \quad (\text{A3})$$

and

$$\begin{aligned} \chi_{q,-(q+2\bar{Q})}^{++} = & -\frac{1}{4N} \sum_{\substack{E_{k-Q}^d < \mu \\ E_{k+q}^d < \mu}} \frac{\Delta^2}{E_{k-Q}^- E_{k+q}^-} \left(\frac{1}{E_{k+q}^c - E_{k-Q}^d - \omega} + \frac{1}{E_{k+q}^c - E_{k-Q}^d + \omega} \right) \\ & + \frac{1}{4N} \sum_{\substack{E_{k+q}^d < \mu \\ E_{k-Q}^d > \mu}} \frac{\Delta^2}{E_{k-Q}^- E_{k+q}^-} \left(\frac{1}{E_{k-Q}^d - E_{k+q}^d - \omega} + \frac{1}{E_{k-Q}^d - E_{k+q}^d + \omega} \right). \end{aligned} \quad (\text{A4})$$

Next,

$$\begin{aligned} \chi_{q,-(q+\bar{Q})}^{+z,\rho} = & \frac{\Delta}{8N} \sum_{\substack{E_{k-Q}^d < \mu \\ E_{k+q}^d < \mu}} \left[\frac{(E_{k+q}^- \pm E_{k-Q}^-) - (\epsilon_{k+q}^- \pm \epsilon_{k-Q}^-)}{E_{k+q}^- E_{k-Q}^-} \right] \left(\frac{1}{E_{k+q}^c - E_{k-Q}^d - \omega} \mp \frac{1}{E_{k+q}^c - E_{k-Q}^d + \omega} \right) \\ & + \frac{\Delta}{8N} \sum_{\substack{E_{k+q}^d < \mu \\ E_{k-Q}^d > \mu}} \left[\frac{(E_{k-Q}^- \mp E_{k+q}^-) - (\epsilon_{k-Q}^- \pm \epsilon_{k+q}^-)}{E_{k-Q}^- E_{k+q}^-} \right] \left(\frac{1}{E_{k-Q}^d - E_{k+q}^d - \omega} \mp \frac{1}{E_{k-Q}^d - E_{k+q}^d + \omega} \right). \end{aligned} \quad (\text{A5})$$

Again, the upper sign is for χ^{+z} , lower for $\chi^{+\rho}$. Finally,

$$\begin{aligned} \chi_{q,-(q+\bar{Q})}^{-z,-\rho} = & -\frac{\Delta}{8N} \sum_{\substack{E_{k-Q}^d < \mu \\ E_{k+q}^d < \mu}} \left[\frac{(E_{k+Q}^- \pm E_{k+q}^-) + (\epsilon_{k+Q}^- \pm \epsilon_{k+q}^-)}{E_{k+q}^- E_{k+Q}^-} \right] \left(\frac{1}{E_{k+q}^c - E_{k+Q}^d - \omega} \mp \frac{1}{E_{k+q}^c - E_{k+Q}^d + \omega} \right) \\ & + \frac{\Delta}{8N} \sum_{\substack{E_{k+q}^d < \mu \\ E_{k+Q}^d > \mu}} \left[\frac{(E_{k+q}^- \mp E_{k+Q}^-) - (\epsilon_{k+q}^- \pm \epsilon_{k+Q}^-)}{E_{k+Q}^- E_{k+q}^-} \right] \left(\frac{1}{E_{k+Q}^d - E_{k+q}^d - \omega} \mp \frac{1}{E_{k+Q}^d - E_{k+q}^d + \omega} \right). \end{aligned} \quad (\text{A6})$$

We also have $= \chi_{q+2\bar{Q},-q}^{--} = \chi_{q,-(q+2\bar{Q})}^{++}, \chi_{q+\bar{Q},-(q+2\bar{Q})}^{z,\rho+} = \chi_{q+2\bar{Q},-(q+\bar{Q})}^{-z,-\rho}, \chi_{q,-(q+\bar{Q})}^{+z,\rho} = \chi_{q+\bar{Q},-q}^{z,\rho-}$.

APPENDIX B

In this appendix, we show that the zero modes in the transverse susceptibilities of the two spiral phases exist, to order x^2 , independent of the ratio of t/U and t'/U . To see this, consider the transverse susceptibility right at $q = (\pi, \pi)$. We will show that $\chi^{zz} = 1/2U$; i.e., the total $\bar{\chi}_{\pi,-\pi}^{zz} = \chi^{zz}(1 - 2U\chi^{zz})^{-1}$ diverges despite the fact that for the spiral states, (π, π) is not the ordering momentum. For definiteness, we will perform the calculations for the (π, Q) phase. The calculations for the (Q, Q) phase proceed in the same way, and the final result is valid for both spiral states.

Expanding in (A1) to second order in $\bar{q} \sim x$ we obtain

$$\begin{aligned} \chi_{\pi,-\pi}^{zz} = & \frac{1}{2N} \sum_{E_k^d < \mu} \frac{1}{E_{k+\pi}^c - E_k^d} \\ & - \frac{1}{8N} \sum_{E_k^d < \mu} (\epsilon_k^- + \epsilon_{k+\pi}^-)^2 \frac{\Delta^2}{(E_k^-)^4} \frac{1}{E_{k+\pi}^c - E_k^d} \\ & + \frac{1}{8N} \sum_{\substack{E_{k+\pi}^d < \mu \\ E_k^d > \mu}} (\epsilon_k^- + \epsilon_{k+\pi}^-)^2 \frac{\Delta^2}{(E_k^-)^4} \frac{1}{E_k^d - E_{k+\pi}^d}, \end{aligned} \quad (\text{B1})$$

where π should be interpreted as the 2D momentum (π, π) , and as before, $\bar{q} = \pi - Q$. It is also convenient to redefine the momenta such that $\epsilon_k^{\pm} = (\epsilon_{k+Q} \pm \epsilon_k)/2$. For the (π, Q) spiral, we then have

$$\epsilon_k^- + \epsilon_{k+\pi}^- = 4|t'| \cos k_x \sin k_y \bar{q} \quad (\text{B2})$$

and also

$$\epsilon_{k+\pi}^+ - \epsilon_k^+ = -2t \bar{q} \sin k_y. \quad (\text{B3})$$

Substituting (B2) and (B3) into (B1), we find after some simple algebra

$$\begin{aligned} \chi_{\pi, -\pi}^{zz} = & \frac{1}{2U} + \frac{t^2 \bar{q}^2}{4N} \sum_k \frac{(\sin k_y)^2}{(E_k^-)^3} \\ & - \frac{(t')^2 \bar{q}^2}{N} \sum_k \frac{(\cos k_x \sin k_y)^2}{(E_k^-)^3} - \frac{t\bar{q}x}{4\delta^2}. \end{aligned} \quad (\text{B4})$$

In obtaining this result, we used the relation

$$\begin{aligned} & \frac{1}{2N} \sum_k \left(\frac{1}{E_{k+\pi}^- + E_k^-} - \frac{1}{2E_k^-} \right) \\ & = -2(t')^2 \bar{q}^2 \frac{1}{N} \sum_k \frac{(\sin k_y \cos k_x)^2 (\epsilon_k^-)^2}{(E_k^-)^5}, \end{aligned} \quad (\text{B5})$$

which can be derived by straightforward computations using (B2). In (B4) and (B5), the summation is over the whole Brillouin zone.

Notice that the pocket contribution [a term $\sim t\bar{q}x$ in (B4)] is the same as in the analysis in the bulk of the paper, where we assumed that $t', t \ll U$. This is simply related to the fact that the pockets are located at $(\pi/2, \pm\pi/2)$ where both ϵ_k^+ and ϵ_k^- are small compared to Δ independent of the ratio of the parameters.

We now need the exact relation between \bar{q} and x , valid to first order in x , but for arbitrary t , t' , and U . To find this relation, we again compute the ground-state energy of the (π, Q) spiral, but this time without assuming that U is large compared to the hopping integrals. Doing the same computations as in Sec. II, we find

$$\begin{aligned} E^{(\pi, Q)} = & -t\bar{q}x + t^2 \bar{q}^2 \frac{1}{N} \sum_k \left(\frac{2 \cos^2 k_y - \sin^2 k_y}{2E_k^-} \right. \\ & \left. + \frac{\sin^2 k_y (\epsilon_k^-)^2}{2(E_k^-)^3} \right) \\ & - 2(t')^2 \Delta^2 \bar{q}^2 \frac{1}{N} \sum_k \frac{\sin^2 k_y \cos^2 k_x}{(E_k^-)^3}. \end{aligned} \quad (\text{B6})$$

The equilibrium \bar{q} then satisfies

$$\begin{aligned} t\bar{q}x = & t^2 \bar{q}^2 \frac{1}{N} \sum_k \left(\frac{2 \cos^2 k_y - \sin^2 k_y}{E_k^-} + \frac{\sin^2 k_y (\epsilon_k^-)^2}{(E_k^-)^3} \right) \\ & - 4(t')^2 \Delta^2 \bar{q}^2 \frac{1}{N} \sum_k \frac{\sin^2 k_y \cos^2 k_x}{(E_k^-)^3}. \end{aligned} \quad (\text{B7})$$

Substituting this result into (B4), we obtain

$$\chi_{\pi, -\pi}^{zz} = \frac{1}{2U} + \frac{1}{2} t^2 \bar{q}^2 \Lambda, \quad (\text{B8})$$

where

$$\Lambda = \frac{1}{N} \sum_k \frac{\Delta^2 \sin^2 k_y}{(E_k^-)^3} - \frac{1}{N} \sum_k \frac{\cos^2 k_x}{E_k^-}. \quad (\text{B9})$$

Notice that all terms with t' are canceled out. Finally, to evaluate χ^{zz} to order x^2 , we actually need Λ only for $\bar{q} = 0$. In this case, $\epsilon_k^- = -2t(\cos k_x + \cos k_y)$, and integrating by parts in (B9), we immediately obtain that $\Lambda = 0$ is independent of the ratio of t/U . We thus find

$$\chi_{\pi, -\pi}^{zz} = \frac{1}{2U} + O(x^3). \quad (\text{B10})$$

This result implies that the zero modes in the transverse susceptibility exist at an arbitrary ratio of the parameters of the Hubbard model provided that the magnetic ordering at half-filling is commensurate, and doped holes form pockets at $(\pi/2, \pi/2)$ and symmetry-related points.

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