Quantum Fluctuations in the spiral phase of the Hubbard Model

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Abstract

We study the magnetic excitations in the spiral phase of the two-dimensional Hubbard model using a functional integral method. Spin waves are strongly renormalized and a line of near-zeros is observed in the spectrum around the spiral pitch $\pm Q$. The possibility of disordered spiral states is examined by studying the one-loop corrections to the spiral order parameter. We also show that the spiral phase presents an intrinsic instability towards an inhomogeneous state (phase separation, CDW, ...) at weak doping. Though phase separation is suppressed by weak long-range Coulomb interactions, the CDW instability only disappears for sufficiently strong Coulomb interaction.

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The proximity of superconductivity and antiferromagnetism observed in the copper–oxide superconductors has led to intensive studies on the magnetic properties and their interplay with charge dynamics in the CuO$_2$ planes. The insulating (half–filled) compounds are Néel antiferromagnets, and upon doping strong antiferromagnetic fluctuations persist both in the normal and superconducting phases of the copper oxides. In particular, recent neutron data on La$_{2-x}$Sr$_x$CuO$_4$ have revealed incommensurate fluctuations peaks in the dynamical susceptibility $\chi''(q,\omega)$. The effect of finite doping in the antiferromagnetic background has thus been extensively studied within the framework of the Hubbard model or its strong–coupling derivations.

Within the Hartree–Fock approximation, doping induces an incommensurate magnetic order since the magnetic susceptibility then peaks at incommensurate wave vectors instead of $Q_0 = (\pi, \pi)$ as in the half filling. In particular, it has become clear that doping initially gives rise to an (inhomogeneous) antiferromagnetic insulator before a conducting phase is eventually reached upon further doping. For strong correlations, mean field theories based on the t–J model propose a spiral magnetic order. Nevertheless, the mean field solutions contradict the fact that no magnetic order has ever been observed in the doped copper oxides. From the theoretical point of view, it is then very important to study fluctuation effects in order to determine whether the models concerned are really relevant to the physics of high temperature superconductors. Based on a phenomenological long–wavelength approach for both the spin and charge degrees of freedom Shraiman and Siggia investigated fluctuations in the spiral phase. They proposed short–range spiral order based on a dynamical mixing of charge and (out–of–plane) spin fluctuations introduced phenomenologically.

In this paper the issue of quantum fluctuations in the spiral magnetic phase will be addressed on a microscopic basis, using a functional integral method. We provide a systematic investigation of the mechanism which couples the spin and charge fluctuations in a doped Hubbard antiferromagnet. The renormalized spin waves are found to be strongly anisotropic in momentum space. However, despite of a line of near–zero energies observed in the Goldstone modes, we show that the spin waves alone are not sufficient to destroy the
long–range order, and the possibility of disordered phases depends crucially on the incoherent particle–hole excitations. We shall also demonstrate that the Hubbard model presents an intrinsic instability towards an inhomogeneous state (phase separation, CDW, ...) at weak doping, due to strong coupling between charge fluctuations and in–plane–spiral fluctuations. Although phase separation is suppressed by long–range Coulomb interactions, a possible inhomogeneous (CDW) state can only be suppressed for sufficiently strong Coulomb interactions.

We start by writing the action for the Hubbard model in two dimensions using a local spin reference axis

$$S(\bar{\Phi}, \Phi, R) = \int_0^\beta d\tau \left\{ \sum_r \bar{\Phi}_r (\partial_\tau - \mu + \bar{R}_r \dot{R}_r) \Phi_r + H(\bar{\Phi}, \Phi, R) \right\} ,$$

$$H(\bar{\Phi}, \Phi, R) = -t \sum_{\langle rr' \rangle} (\bar{\Phi}_r \bar{R}_{r'} R_{r'} \Phi_{r'} + c.c.)$$

$$+ \frac{U}{4} \sum_r [(\Phi_r \Phi_r)^2 - (\Phi_r \sigma_z \Phi_r)^2] ,$$

where $R$ defines the SU(2) rotation from the original electron operators $\Psi = (\psi_{r\uparrow}, \psi_{r\downarrow})^T$ to the new operators $\Phi$ via $\Psi = R \Phi$. $R$ satisfies $R_r(\tau) \sigma_z R^+_r(\tau) = \Omega_r(\tau) \cdot \sigma$, where $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices, and $\Omega_r(\tau)$ is a dynamical variable that defines the local spin reference axis varying in time and space.

By the saddle point approximation, we can readily identify the spiral phase as favored among homogeneous candidates. In particular, it is the diagonal spiral phase with $Q = (Q, Q)$ which minimizes the free energy in the strongly correlated regime ($U \gg t$). The spiral pitch $p = \cos \frac{Q}{2}$ varies continuously from one at half–filling to zero in the ferromagnetic limit above some critical doping. Close to half filling, we can write $p = 2tx/J$, where $J = 4t^2/U$ and $x$ is the hole concentration. Within the framework of the Hubbard model, the formation of the spiral state makes it possible for the charge carriers to propagate freely, and the quasiparticle structure is determined by a single parameter $\gamma = \frac{J}{t} (p^{-1} - p)$, which measures the relative strength between intra– and inter–sublattice hoppings ($tp$ vs $J(1 - p^2)$). As a consequence, once holes are introduced the Fermi surface immediately shrinks to a single
small pocket around \( \mathbf{k}_m = (\pi/2, \pi/2) \). The quasiparticle mass satisfies \( m_-/m_+ = 1 + 2\gamma \) within the weakly doped regime, and thus shows an important anisotropy. Typically, the mass along \((1, 1)\) direction \( m_+ \approx 1/J \), much smaller than the mass in its perpendicular direction \( m_- \).

To explore the stability of the spiral phase, we have studied the low energy (transverse) spin excitations within the one–loop scheme. Assuming \( b_r = (\alpha_r + i\beta_r)/2 \), with \( \beta_r (\alpha_r) \) describing the local angular spin deviations within (out of) the spiral spin plane, the effective spin action becomes

\[
S_{\text{eff}} = \frac{1}{4} \sum_{\mathbf{q}, \nu} \begin{pmatrix} h_{\mathbf{q}} + \Delta_{\mathbf{q}} + S_+(\mathbf{q}, i\omega_\nu) & i\omega_\nu + S_z(\mathbf{q}, i\omega_\nu) \\ i\omega_\nu + S_z(\mathbf{q}, i\omega_\nu) & h_{\mathbf{q}} - \Delta_{\mathbf{q}} + S_-(\mathbf{q}, i\omega_\nu) \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{q}} \\ \beta_{\mathbf{q}} \end{pmatrix}
\]

where

\[
h_{\mathbf{q}} = \sum_k f_k \{-g(\mathbf{k}, \mathbf{q}) + \frac{2\tau^2}{U} - \frac{g^2(\mathbf{k}, \mathbf{q})}{U}\},
\]

\[
\Delta_{\mathbf{q}} = 2 \sum_k f_k \frac{\varepsilon_{\mathbf{k}+\mathbf{q}}}{U},
\]

with \( f_k \) the Fermi distribution function of the lower Hubbard band, \( \varepsilon_{\mathbf{k}} = 2t \sin \frac{Q}{2}(\sin k_x + \sin k_y) \) and \( g(\mathbf{k}, \mathbf{q}) = 2tp(\cos(k_x + q_x) + \cos(k_y + q_y) - \cos k_x - \cos k_y) \). \( S_\pm(\mathbf{q}, i\omega_\nu) \), \( S_z(\mathbf{q}, i\omega_\nu) \) contain the renormalization of the spin wave propagator by particle–hole excitations within the lower Hubbard band. Without giving detailed expressions, we only mention that (i) \( S_z(\mathbf{q}, i\omega_\nu) \) is an odd function of \( \omega \) and vanishes in the static limit; (ii) more importantly, a strong anisotropy exists in the interaction vertices \( U_\pm(\mathbf{k}, \mathbf{q}) \), which couple particle–hole excitations across the Fermi surface to the out–of– (in–)plane spin fluctuations respectively. In particular, for small doping the coupling is maximal (minimal) for excitations propagating along (perpendicular to) the spiral twisting.

The spin wave spectrum is determined by zeros of the determinant of the \( 2 \times 2 \) matrix in eq.(3). The spectrum contains three Goldstone zeros at \( \mathbf{q}_0 = 0, \pm Q \), as would be expected from symmetry considerations. In agreement with previous findings, to correctly account for the spin wave structure in the spiral state, it is crucial to take into account the dynamical effects of particle–hole excitations (\( h_{\mathbf{q}} + \Delta_{\mathbf{q}} = -S_+(\mathbf{q}, 0) \neq 0 \) at \( \mathbf{q}_0 = \pm Q \)).
Fig. 1 shows the numerical results for the spin wave spectrum within the Brillouin zone. In comparison with the half-filled case where particle–hole excitations are absent in the lower Hubbard band, the overall spectral structure has changed drastically for even the slightest doping. Summarizing the numerical results, we find: (i) spin waves are observed in the $q \to 0$ limit only for very weak doping, they are completely dissolved into the particle–hole excitation spectrum as doping further increases. On the other hand, the spin wave velocity is always slightly above the half filling value of $\sqrt{2}J$ when the mode is not overdamped, which disagrees with the result derived from t–J model but agrees qualitatively with Chubukov and Frenkel (ii) around $\pm Q$, spin wave excitations are strongly renormalized. In particular, they have very low energies along the diagonal direction for wave vectors between $\pm (Q, Q_0)$, a region of length $\sim 4Ux/t$. These excitations will certainly dominate the low energy properties in the spiral state; (iii) more surprisingly, an extra zero is found in the spectrum immediately after the spin waves reemerge from the the particle–hole pair spectrum (at $q' \neq 0$). This unexpected result will be seen to signal the instability of the spiral state against an inhomogeneous state.

Things are rather transparent in the long wavelength limit. Increasing doping raises the Fermi velocity, which in turn pushes up the upper bound of the pair spectrum. The spin wave excitations near $q = 0$ then become overdamped as doping exceeds a certain threshold. Below the threshold the leading correction $S_-(q \to 0, \omega \to 0)|_{\omega/q|<c}$ has its origin in the coupling between spin fluctuations within the spiral plane and particle–hole excitations just across the Fermi surface, which scales as $x^{1/4}$ as doping approaches zero. Correspondingly, the spin wave velocity has approximately the form:

$$c = \sqrt{2}J + J \sqrt{\frac{2\pi t}{J}} \left( \frac{q_x + q_y}{\sqrt{q_x^2 + q_y^2}} \right)^3 x^{1/4}$$

(6)

This disagrees with Gan et al. who find a leading correction of $O(x)$. From eq.(6), it is clear that renormalization in the spin wave velocity is maximal along (1, 1) direction, and minimal in its perpendicular direction.

For the dynamical spin susceptibility near $\pm Q$, out–of–plane spin fluctuations dominate.
Here, mixing with charge excitations is crucial in determining the low-lying spin excitations. We have already indicated that the Goldstone modes at \( \pm Q \) appear as the direct consequence of the spin–charge coupling. Around \( \pm Q \), \( S_\pm(q,\omega) \) dominates the selfenergy correction, and the spin wave spectrum can be approximated by:

\[
\omega^2_{q}/J^2 = \left(1 + \frac{4}{\gamma}x\right)(\delta q_x - \delta q_y)^2 + 4x\left(1 + \frac{1}{\gamma}\right)(\delta q_x + \delta q_y)^2
\]

provided that the hole concentration is small but finite (such that \( tp \) or \( \gamma \) remains finite).

Eq. (7) corresponds to the so-called torsion mode in Shraiman and Siggia’s description.\(^8,11\)

We emphasize the strong anisotropy observed in the spin wave spectrum (see also Fig.1b). In particular, the characteristic velocity is \( O(\sqrt{x}J) \) in the \((1,1)\) direction where the renormalization is maximal and \( O(J) \) otherwise.

Finally, the unexpected extra zero in the spin wave spectrum (at \( q' \)) belongs, in fact, to an imaginary mode existing for \( q \in (0, q') \),\(^13\) which certainly implies the instability of the spiral phase. However, what is remarkable here is its simultaneous presence with the Goldstone modes.

That in-plane and out-of-plane spin fluctuations are decoupled in the static limit helps in determining both the nature of this instability and the offending fluctuations. In Fig.2 we have plotted the variation of \( S_-(q,0) \) for a given \( U/t \) and a hole density. The presence of a sharp peak in \( S_-(q,0) \) easily explains the qualitative change in the nature of spin fluctuations within the spiral plane at sufficiently low doping. In this regime, since \( hq - \Delta_q \) is a smooth function and approaches zero in the limit \( q \to 0 \), we readily find that under the condition:

\[
U\rho(0) > \frac{q_x^2 + q_y^2}{(q_x + q_y)^2}
\]

the spin propagator \( \langle \beta_q \tilde{\beta}_q \rangle_{\omega \to 0} \) changes sign for wavevectors \( q \in (0, q') \), and correspondingly the spin stiffness becomes negative for fluctuations inside the spiral plane. Here \( \rho(0) \) is the quasiparticle density of states at the Fermi energy.

The nature of the instability at \( q = 0, q' \) is further clarified by studying the charge response to the corresponding spin fluctuations. A RPA calculation for the density–density
response function $\chi(q,\omega)$ reveals that the static charge susceptibility couples only to the spin fluctuations within the spiral plane. The divergence in $\langle \beta_q \tilde{\beta}_q \rangle_{\omega \to 0}$ then leads to a similar behavior in the charge susceptibility. As a result we find in the limit $q \to 0$ a negative compressibility under exactly the same condition, eq.(8), which predicts phase separation. This has been realized in earlier studies of the compressibility based on mean field solutions. Further, the divergence of $\chi(q,0)$ at a finite wavevector clearly indicates a CDW instability. Contrary to phase separation which is often overemphasized, we note that this second instability has received little attention in previous studies. On the other hand, for the wide parameter region we have examined, we have not seen any indication of a non–coplanar phase claimed by Chubukov and Musaelian.

Of course, phase separation would hardly survive in real materials in view of long–range interactions neglected in the Hubbard model. We have therefore reexamined the problem in the presence of a $1/r$ potential. We find that, in the static limit, Coulomb interactions modifies only the spin fluctuations within the spiral plane, (and along with them, the charge density response function). The screened spin propagator $\langle \beta_q \beta_{-q} \rangle_{\omega \to 0}$ now becomes:

$$\langle \beta_q \beta_{-q} \rangle_{\omega \to 0} \approx \frac{-2}{h_q - \Delta_q + \frac{1}{2} U_{f-}^2 \chi_0(q,0)/\epsilon(q,0)}$$

where $\chi_0(q,0)$ is the bare charge susceptibility in the lower Hubbard band, and $\epsilon(q,0) = 1 - V_q \chi_0(q,0)$ is the dielectric constant in the presence of the Coulomb potential $V_q$. Eq.(9) has been obtained by assuming that the interaction vertex $U_{f-}(k,q)$ can be approximated by its value on the Fermi surface, $U_{f-}(q)$, which is correct at sufficiently weak doping. From eq.(9) we easily see that even weak Coulomb interactions stabilize against phase separation. On the other hand, the instability against a CDW state can only be eliminated for sufficiently strong Coulomb interactions. In the intermediate regime, a possible compromise can be established by forming a modulated spiral phase, or domain walls, as suggested by Dombre.

A physically interesting possibility is the disordering of the long–range ordered spiral state induced by low–lying (torsion) modes, as suggested by Shraiman and Siggia. In what follows, we assume the instabilities discussed above to be absent in real systems, and
for that purpose suppress by hand the corresponding vertex $U_-(k, q)$\cite{22}. Then one can verify that the imaginary mode and hence the extra zero in the spin wave spectrum disappear. Otherwise, the low–lying Goldstone modes remain nearly unchanged\cite{13}. We have calculated the renormalized spin amplitude (per electron) $m = 1/2 - |b|^2$ in the presence of these zero point fluctuations. In general, $|b|^2 \equiv (|\alpha|^2 + |\beta|^2)/4$ consists of contributions from the spin wave modes as well as the incoherent particle–hole excitations due to their coupling with spin fluctuations. By analogy with the half–filled case we concentrate on the spin–wave corrections. Fig.\[3\] shows $m$ as a function of doping for two values of $U/t$. The variation of $m$ reflects the magnetic frustration of the system upon doping. Starting from the Néel state at half filling, where $m = S - 0.197$, doping initially induces frustration leading to the spiral phase and to an increase in zero–point spin fluctuations. However, after reaching a maximum (where $m$ is minimized), frustration reduces continuously until the ferromagnetic limit, where no zero–point fluctuations are expected and $m$ remains unchanged at its saturation value. The $U/t$ dependence of $m$ can also be understood. Provided that the maximal frustration is reached at a certain spiral pitch $p_c$, the optimal doping $x_c$ where $m$ is minimized decreases as $U/t$ increases. In particular, $x_c$ varies inversely proportional to $U/t$ in the weak doping regime. From the above calculation we have learned that even in the most frustrated case where zero–point spin fluctuations are the most violent they are not sufficient to destabilize the spiral phase in favor of a disordered state.

To conclude, our analysis on the quantum fluctuations in a spiral phase reveals an intrinsic instability in the weakly doped Hubbard model. Phase separation is suppressed by the long–range Coulomb interactions in a real material, however, we emphasize that an inhomogeneous state may well persist provided the long–range interactions were not too strong. A possible scenario is then the formation of a structure similar to the domain walls found in the weak correlation regime\cite{20} before the system eventually conducts. We remark that such a scenario may be relevant the recent observations in La$_2$NiO$_{4+y}$\cite{22}. Within the present framework, we have further examined the possibility of disordered spiral phases. We have shown that zero–point spin wave excitations alone are not sufficient to destroy
the long-range magnetic order. Nevertheless, the contribution from the incoherent excitations in the system grows as one further dopes the system. We expect that above a critical doping, an inhomogeneous state should finally give way to a disordered state with strong incommensurate correlations. Finally, the hole dynamics in such doped systems is far from being understood.
FIGURES

FIG. 1. (a) Spin wave spectrum in the (1, 1) spiral state. for $U/t = 10$ and $x = 1.5\%$ (above), $x = 7.5\%$ (below). The region between dotted lines stands for the continuum for particle–hole excitations. (b) The spectrum near $\pm \mathbf{Q}$ for $U/t = 20$ and 2% doping.

FIG. 2. The selfenergy correction for the static spin propagator within the spiral plane, $S_q(\mathbf{q}, 0)$, for $U/t = 20$ and $x = 5\%$.

FIG. 3. Renormalized spin amplitude $m$ as a function of doping in the presence of spin wave excitations.
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$S_-(\mathbf{q}, 0)$
