Stability of homogeneous magnetic phases in a generalized $t - J$ model

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We study the stability of homogeneous magnetic phases in a generalized $t - J$ model including a same-sublattice hopping $t'$ and nearest-neighbor repulsion $V$ by means of the slave fermion-Schwinger boson representation of spin operators. At mean-field order we find, in agreement with other authors, that the inclusion of further-neighbor hopping and Coulomb repulsion makes the compressibility positive, thereby stabilizing at this level the spiral and Néel orders against phase separation. However, the consideration of Gaussian fluctuation of order parameters around these mean-field solutions produces unstable modes in the dynamical matrix for all relevant parameter values, leaving only reduced stability regions for the Néel phase. We have computed the one-loop corrections to the energy in these regions, and have also briefly considered the effects of the correlated hopping term that is obtained in the reduction from the Hubbard to the $t - J$ model.

Two-dimensional antiferromagnets doped with mobile holes have been extensively studied in the last decade in order to understand the physics of superconducting cuprates. Most often these studies have been carried out by considering the so called $t - J$ model,

$$H_{tJ} = -t \sum_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \frac{J}{2} \sum_{i} S_i \cdot S_j,$$

where $i, j$ are nearest-neighbor sites on a square lattice, the operator $c_{i\sigma}^\dagger$ creates a particle on a vacuum where all sites carry a Zhang-Rice singlet, and double occupancy is forbidden ($c_{i\sigma}^\dagger n_i = 0$). When this Hamiltonian is derived from a realistic three-band Hubbard model for the CuO$_2$ planes, the hopping integral $t \approx 2.5$ in units of the coupling $J = 1$. At half filling ($\delta = 0$) reduces to the Heisenberg antiferromagnet, which displays quantum Néel order at $T = 0$. The introduction of mobile holes disrupts the magnetic order, and eventually melts it. The description of this quantum phase transition has lead to the consideration of two related questions: i) the existence of an intermediate spiral magnetic phase for small doping, and ii) the possibility of phase separation in the ground state of the $t - J$ model. The existence of a spiral phase is very appealing in view of the incommensurate peaks in the magnetic susceptibility found in real materials. This incommensurability seems to appear only in superconducting samples, which lends support to the idea that is related to hole mobility. Phase separation is possible since for $J < t$ the $t - J$ model is related to the large repulsion limit of the Hubbard model, which only accounts for local on-site interactions. Consideration of the true long-range Coulomb interaction, even if strongly screened, could then prevent phase separation.

Shraiman and Siggia were the first to discuss the existence of a spiral phase in the $t - J$ model. In a semiclassical approach, they showed that for infinitesimal doping $\delta = 1 - n$, where $n$ is the particle density, the lowest-energy spin configuration is a spiral with pitch $Q \approx \delta t/J$. Since then, many authors have considered this problem using a variety of methods. One of the most elegant approaches is the slave fermion-Schwinger boson (SF-SB) theory, in which the physical particle is replaced by a product of a spinless fermion $f$ and a bosonic spinor $b^\dagger = (b^\dagger_1, b^\dagger_4)$:

$$c_{i\sigma} \rightarrow b_{i\sigma} f_i, \quad c_{i\sigma}^\dagger \rightarrow f_i^\dagger b_{i\sigma}.$$

This replacement, together with the site-occupation constraint $\sum_{\sigma} b_{i\sigma}^\dagger b_{i\sigma} + f_i^\dagger f_i = 1$, is a faithful representation of the original Fermi algebra. Thus, the spins can be written in terms of the Schwinger bosons as $S_i = \frac{1}{2} b_{i\uparrow}^\dagger \sigma_{\uparrow\downarrow} b_{i\downarrow}$, while the slave fermion $f_i$ accounts for the charge degrees of freedom. This representation naturally enforces the $t - J$ model restriction to a single particle per site. Moreover, at half filling it correctly reproduces the spin-wave results for the magnetization and spectrum, unlike the alternative fermionic description of spins. Using the representation, Jayaparakash, Krishnamurthy and Sarkar found a $T = 0$ phase diagram with four phases: a metallic phase with long-range ferromagnetic order for $t\delta > J$, an insulating phase with antiferromagnetic correlations for $t << J$ and $\delta$ not too large, a disordered ”spin-liquid” insulating phase with only short-range antiferromagnetic correlations for $t << J$ and $\delta$ large, and a spiral metallic phase with incommensurate spin order when $t\delta \approx J$. About the same time, Kane et al. argued that the incoherent processes that renormalize the hole spectrum in an antiferromagnetic background may be treated by including an effective same-sublattice hopping term $t'$. They considered several homogeneous spin configurations (Néel, canted, $(Q, Q)$ and $(Q, \pi)$ spirals, double spiral) within the same SF-SB mean-field theory $\lambda$.

For small doping ($\delta \approx 0$) these authors found that the spiral and Néel orders are favored, with their relative stability depending on the value of $t'$. They also found that for both
\( \delta \) and \( t/J \) large a state with uniform chiral order is favored. This state is similar to the flux phase obtained near half filling in the alternative slave-boson approach, and violates parity and time-reversal symmetries.

Antiferromagnetic systems are highly susceptible to local deformations of the spin order in the presence of holes. Their homogeneous magnetic states are thus inherently unstable due to the large compressibility of the holes, since the system wishes to enhance the spin deviations by locally increasing the hole density. This tendency to phase separation in the \( t - J \) model was observed by Auerbach and Larson (AL) by studying the SF-SB mean-field states by means of a expansion in \( \delta \). At the mean-field level, the most important result of this is the negativity of the compressibility \( \kappa \) for all values of \( t/J \) and very small \( \delta \). This negative \( \kappa \) suggests that phase separation between a hole-rich and a Néel phase takes place, provided the energy is minimized by homogeneous states at finite doping. Alternatively, the system could form local defects or spin polaron.\(^5\) Other works using different techniques lead to similar results.\(^6\) However, Mori and Hamada\(^7\) showed that the inclusion of the \( t' \) term can stabilize a Néel phase for small \( \delta \). Furthermore, Sarker\(^8\) found that in the presence of a Coulomb interaction (screened to a simple nearest-neighbor repulsion \( V \)) the incommensurate spiral states and also the antiferromagnetic order are favored over the flux states of\(^9\) and, more importantly, that they are stable against hole condensation for \( \delta \) larger than some \( \delta_c \).

Except for\(^10\) all the works mentioned above using the SF-SB representation are mean-field in character. The subtle differences among them correspond only to the several ways that the exact form of the constraint is used to simplify terms in the Hamiltonian. Since the constraint is later relaxed, all this equivalent Hamiltonians lead to slightly different results and, as a consequence, the relative stability of the magnetic phases changes. The more interesting question of the general stability of the mean-field picture due to order-parameter fluctuations was partially considered by AL, who found that for infinitesimal \( \delta \) the spiral phases are unstable for all values of \( t/J \). This instability appears as a negative eigenvalue of the dynamical matrix — the Hessian of the ground-state energy as a function of the order parameters —. They also considered the effects of the intrasublattice correlated hopping term of \( O(t'^2/U) \) that comes from the large \( U/t \) transformation of the Hubbard model — which was taking into account by the \( t' \) hopping term of very small \( \kappa \).\(^6\) In the following we will investigate this question by the consideration of order-parameter fluctuations. In particular, the novel features introduced in our calculations are the following: i) since the theory presents a local \( U(1) \) gauge symmetry we will use collective coordinate methods — as developed in the context of relativistic lattice gauge theories — to handle the infinitely-many zero modes associated to the local symmetry breaking in the saddle-point expansion. Contrary to what happens in the radial gauge, in this case the dynamical matrix explicitly displays the zero modes, which allows to check the calculations at intermediate steps; ii) unlike in\(^11\) here we will consider finite densities and will evaluate the fluctuations corrections in the region where the magnetic phases are stable; iii) we will include a nearest-neighbor repulsion \( V \) as considered by Sarker\(^12\) and also a second neighbor hopping \( t' \) in the spirit of\(^13\) We stress that the presence of a same-sublattice hopping has been frequently advocated as a stabilizing mechanism for spiral phases.\(^14\) The correlated hopping term considered by AL will be initially disregarded; its effects will be briefly discussed at the end of this work. We emphasize that these calculations are, to the best of our knowledge, the first complete evaluation of fluctuations corrections in the SF-SB theory reported in the literature.

After the Hamiltonian is written in terms of the new operators (\( \hat{B} \)), the partition function can be expressed as a functional integral over coherent Bose and Fermi states. Then, the different terms in \( H \) are decoupled by means of Hubbard-Stratonovich transformations according to the following scheme (indicated by a vertical bar):

\[
H_J \rightarrow \frac{J}{4} \sum_{ij} \left( \hat{B}_{ij}^+ \hat{B}_{ij} : \hat{A}_{ij}^+ \hat{A}_{ij} \right)
\]

\[
H_t \rightarrow - \sum_{ij} t_{ij} f_i f_j^\dagger \hat{B}_{ij}
\]

\[
H_V \rightarrow V \sum_{ij} f_i^\dagger f_i \hat{B}_{ij}^\dagger f_j
\]
In $H_f$ we wrote the Schwinger-boson spin-spin interaction in terms of the two $SU(2)$ invariants $\hat{B}^j_i = \sum_\sigma \hat{b}^{i\sigma}_j \hat{b}^{j\sigma}_i$ and $\hat{A}^j_{ij} = \sum_\sigma \sigma \hat{b}^{\sigma}_i \hat{b}^{\sigma}_j$. These operators describe the magnetic fluctuations in the ferromagnetic and antiferromagnetic channels respectively, and allow for a proper treatment of the incommensurate order upon doping. For the hopping term $H_V$ we just decoupled bosons from fermions (here the indices $i,j$ run also between next-nearest neighbors). Finally, for $H_V$ we indicated the Hartree factorization but we have also considered i) the alternative Fock decoupling, and ii) the contribution of this term when the nearest-neighbor repulsion is written in terms of bosons, i.e., $H_V = V \sum_{ij} B^j_i | B^j_i \rangle \langle B^j_i |$ in all these cases the results are qualitatively the same. According to the decompositions (3) of the interaction terms, in a saddle-point evaluation of the partition function the Hubbard-Stratonovich fields become the following self-consistent order parameters: 1) antiferromagnetic order: $A^j_{ij} = (\sum_\sigma \sigma \hat{b}^{\sigma}_i \hat{b}^{\sigma}_j)$, 2) ferromagnetic order: $B^j_{i-j} = (\langle \sum_\sigma \hat{b}^{\sigma}_i \hat{b}^{\sigma}_j \rangle$, 3) hopping: $F^j_{i-j} = (\langle \hat{f}^\dagger_j \hat{f}^j_i \rangle$, and 4) hole density $N_j = (\langle \hat{f}^\dagger_j \hat{f}^j_i \rangle$. The saddle-point Hamiltonian, quadratic in boson and fermion operators, can be diagonalized in the standard way. Here we only point out that in transforming to momentum space the boson operators we have defined $\hat{b}^{ij}_\sigma = \frac{1}{\sqrt{N}} \sum_{k} \hat{b}^{j\sigma}_{k} e^{ik\cdot r_i}$, with $k_\sigma = k + \sigma Q/2$.

The extra phase $\sigma Q/r/2$ is required to obtain the gapless (Goldstone) modes associated to the long-range magnetic order at the proper $k = 0, \pm Q$ points. The self-consistent order parameters are determined using a mesh of $100 \times 100$ points for the integrals in reciprocal space. Since our mean-field theory is not variational because it unphysically enlarges the configuration space, we cannot rely only on the energy-minimization criterion to seek for solutions of these consistency equations. Consequently, based on previous studies of the $t-J$ model, we considered solutions corresponding to magnetic wavevectors $(\pi - Q, \pi)$ and $(\pi - Q, \pi - Q)$, which in large regions of parameter space are very close in energy.

At the mean field level we computed the hole compressibility $\kappa \sim \frac{\partial^2 F_{FP}}{\partial n^2}$ to investigate indications of possible phase separation. In Fig. 1 we plot the energy of the $(Q, Q)$ spiral phase as a function of the density of holes for the standard $t-J$ model ($t' = 0 = V$). From this figure we see that, as found in several studies, the compressibility of holes is negative for small densities and all values of $t/J$, though it becomes positive for large to moderate doping and large $t/J$. The inclusion of a second-neighbour hopping $t'$ makes the spirals and Néel phases to be even closer in energy (less than 1% of difference) for all relevant parameter values. In Fig. 2 we give the energy of the Néel phase as a function of doping for different values of $t'/J$ and $V = 0$. We found that this energy does not depend on $t'$, since at mean-field order in the Néel phase the dominant processes correspond to coherent hopping in the same sublattice. Fig. 2 shows that for $t'/J > 0.05$ the compressibility becomes positive (the same is valid for the spiral phases and holds in general for $|t'|/J > 0.05$): the non-frustrating character of the second-neighbor hopping promotes hole mobility and prevents their segregation in real space. We have also verified that the inclusion of the nearest-neighbor repulsion $V$ further favors the stability of the homogeneous magnetic phases, as found by Sarker. Then, possible instabilities of these phases beyond mean-field order are not necessarily related to phase separation.

We turn now to the consideration of Gaussian fluctuation corrections to mean-field results, which can be obtained by extending the calculations described in [1]. The saddle-point expansion breaks the gauge invariance of the theory, leading to the existence of saddle-point solutions connected by the continuous $U(1)$ gauge group. This makes the dynamical matrix $D$ to have infinitely-many zero modes, which are the Goldstone bosons associated to the (spurious) local symmetry breaking. In particular, for translational-invariant saddle-point values of the decoupling fields, there is a zero mode $\varphi_i^0(k, \omega) = \delta \varphi(\theta) / \delta \theta_{|\varphi|} = 0$ in every $k-\omega$ subspace. Here $\varphi(\theta)$ is the vector of gauge-transformed fields, which depends on the set of local phases $\theta$, and the $\varphi_i^0(k, \omega)$ is shown to be right eigenvectors of the nonhermitian matrix $D$. To avoid the infinities associated to these modes without restoring forces we introduce collective coordinates along the gauge orbit. Exact integration of these coordinates eliminates the zero modes and restore the gauge symmetry (in the sense that noninvariant operators average to zero). This program can be carried out by enforcing in the functional integral for the partition function the so-called background gauge condition or “natural” gauge, $\varphi(\theta) \varphi^\dagger(\theta) = 0$. This condition can be introduced into the functional measure by means of the Faddeev-Popoff trick, and restricts the integration to fields fluctuations which are orthogonal to the collective coordinates. At $T = 0$, after carrying out these integrations on the genuine fluctuations, we obtain the one-loop correction to the ground-state energy per site,

$$E_1 = -\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \sum_k \ln \left( \frac{\Delta_{FP}(k, \omega)}{|\omega|\sqrt{\det D_k(k, \omega)}} \right). \tag{4}$$

Here $D_\perp$ is the projection of $D$ in the subspace orthogonal to the collective coordinates, and $\Delta_{FP}(k, \omega) = |\varphi^\dagger_i(k, \omega) \varphi_i^0(k, \omega)|$ is the Faddeev-Popoff determinant ($\varphi_i^0(k, \omega)$ is the left zero mode of $D$ in the $k-\omega$ subspace). More explicitly, $\Delta_{FP}(k, \omega) = [4 \sum_r J(1 + \cos k_\rho)] A_r^2 - 4 \sum_r (J B_r^2 + 4t_\rho B_r F_r)(1 - \cos k_\rho + \omega^2)^{1/2}$.

For spiral phases $D_\perp$ has always negative eigenvalues, which makes these phases unstable for all parameter values even in the presence of a large repulsion $V$. Only the Néel phase becomes stable in some regions of the $(\delta, t'/J)$ plane.
because of the intrasublattice hopping term, as shown in Fig. 3 for different values of $t/J$ and $V = 0$. Unlike the mean-field results, in this case the energy depends on $t/J$ since the fluctuations corrections incorporate the incoherent intersublattice hopping processes. Fig. 4 shows the corresponding stability diagram for $t/J = 2.5$, which is the value supposed to be relevant for the cuprates. The consideration of both positive and negative values of $t'$ is interesting in view of the proposal of Tohyama and Maekawa to explain the asymmetry in the behavior of superconducting cuprates doped with holes or electrons. According to this proposal, the asymmetry is related to the fact that in the generalized $t - J$ model for the CuO$_2$ planes one should have $t' > 0$ for systems doped with electrons and $t' < 0$ for those doped with holes. The results in Fig. 4 are qualitatively supporting this idea, since the magnetic order in systems with $t' > 0$ (corresponding to electron doping) are more stable than those with $t' < 0$ (hole doping), as observed experimentally. Notice, however, that there is also a region of stability for small negative $t'$ and medium to large $\delta$, but this could be an artifact of the approximation. This picture is not modified by the presence of the nearest-neighbor repulsion $V$. For completeness, in Fig. 5 we plot the mean-field and fluctuation-corrected energies in the Néel phase as a function of doping on the stable part of the line $t' = J$.

We have identified the unstable modes in the dynamical matrix. These modes have $\omega \approx 0$ and are distributed over most of the Brillouin zone, although they are more densely located near $k = 0$ and $(\pi, \pi)$. They couple the fluctuations of the intersublattice fermionic hopping $F_k$ and ferromagnetic order parameter $B_k$. This clearly shows that the tendency of the kinetic term $H_t$ in (1) to locally align the spins is responsible for the instabilities of the homogeneous magnetic phases, as previously found by AL. This effect of local distortions is very difficult to account for in mean-field theories, and requires the calculations of fluctuations to treat it. The inclusion of the $V$ term reduces the number of unstable modes near $k = 0$ (as expected, since this term acts against phase separation) but it is not able to stabilize the homogeneous phases, a result that had also been conjectured in.

Finally, we comment here on the effects of including the three-site correlated hopping term of $O(t^2/U)$ that can be obtained in the reduction of the Hubbard model to the $t - J$ one. After the replacement (2) this term becomes a product of eight boson and fermion operators, requiring a double Hubbard-Stratonovich transformations to be decoupled. Using the same order parameters as in (3), we found that its inclusion does not modify qualitatively the above results. In particular, it does not play any special roll in stabilizing or destabilizing the magnetic phases. In a previous work, we considered the alternative Bogoliubov factorization of the four slave-fermion operators in this term, which at mean-field order lead to a superconducting phase with some interesting properties, similar to those observed experimentally. Unfortunately, we found here that when the order-parameter fluctuations are considered this superconducting phase becomes unstable like the spiral phases in the magnetic state.

In this work we have considered, within the SF-SB theory, the general stability of homogeneous magnetic phases in a generalized $t - J$ model including a same-sublattice hopping $t'$ and nearest-neighbor repulsion $V$. At the mean-field level we found, in accordance with previous works, that the new terms help to stabilize the Néel and spiral phases against phase separation, since for small values of these parameters the compressibility $\kappa$ becomes positive (see Fig. 2). The correlated hopping term considered in (4) does not substantially modify these results. Beyond mean-field theory, the study of the dynamical matrix associated to the order-parameter fluctuations reveals that the homogeneous spiral phases are unstable in all regions of interest. On the other hand, the Néel phase becomes stable for reasonable values of $t' > 0$ or unphysically large $t' < 0$, as shown in Figs. 3 and 4. The consideration of moderate values of the nearest-neighbor repulsion $V$ does not modify these figures. We stress that Fig. 4 supports qualitatively the proposal in (5) that links the asymmetric behavior of hole-doped and electron-doped cuprates to the $t'$ sign in the corresponding effective $t - J$ model for the CuO$_2$ planes. Finally, we found that the consideration of Gaussian corrections to the mean-field picture of (6) unfortunately destroys the stability of the superconducting phase there obtained.

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1 S. W. Cheong, G. Aeppli, T. E. Mason, H. Mook, S. Hayden, P. C. Canfield, Z. Fisk, K. N. Clausen, and J. L. Martinez, Phys. Rev. Lett. 67, 1791 (1991); S. M. Hayden, G. Aeppli, H. Mark, D. Rytz, F. M. Hundley, and Z. Fisk, Phys. Rev. Lett. 66, 821 (1991); G. Shirane, R. Birgeneau, Y. Endoh, P. Gehring, M. Kastner, K. Kitazawa, H. Kojima, I. Tanaka, T. R. Thurton, and K. Yamada, Phys. Rev. Lett. 63, 330 (1989).

2 B. Shraiman and E. D. Siggia, Phys. Rev. Lett. 62, 1564 (1989).
Fig. 1: Mean-field energy $E(Q,Q)$ of the $(Q,Q)$ spiral phase as a function of doping $\delta$ for different values of $t/J$ and $t' = 0 = V$.

Fig. 2: Mean-field energy $E(\pi, \pi)$ of the Néel phase as a function of doping $\delta$ for different values of $t'/J$ and $V = 0$.

Fig. 3: Stability of the Néel phase for $t' > 0$, $V = 0$, and different values of $t/J$. The antiferromagnetic order is stable in the regions above the lines.

Fig. 4: Stability diagram of the Néel phase in the whole $(\delta, t'/J)$ plane for the physically relevant value $t/J = 2.5$.

Fig. 5: Mean-field and fluctuation-corrected energies in the Néel phase as a function of doping $\delta$ for the parameter values $t/J = 2.5$, $t' = J$, and $V = 0$, $J$. 

C. Jayaprakash, H. R. Krishnamurthy, and S. Sarker, Phys. Rev. B 40, 2610 (1989).
C. L. Kane, P. A. Lee, T. K. Ng, B. Chakraborty, and N. Read, Phys. Rev. B 41, 2653 (1990).
A. Auerbach and B. Larson, Phys. Rev. B 43, 7800 (1991).
A. Auerbach and B. E. Larson, Phys. Rev. Lett. 66, 2262 (1991).
T. I. Ivanov, Phys. Rev. B 44, 12077 (1991).
J. Igarashi and P. Fulde, Phys. Rev. B 45, 10419 (1992).
H. Mori and M. Hamada, Phys. Rev. B 48, 6242 (1993).
S. Sarker, Phys. Rev. B 47, 2940 (1993).
A. E. Trumper, L. O. Manuel, C. J. Gazza, and H. A. Ceccatto, Phys. Rev. Lett. 78, 2216 (1997).
A. J. Polyakov, Nucl. Phys. B120, 429 (1977); J. L. Gervais and B. Sakita, Phys. Rev. D 11, 2943 (1975).
B. Normand and P. A. Lee, Phys. Rev. B 51, 15519 (1995).
H. A. Ceccatto, C. J. Gazza, and A. E. Trumper, Phys. Rev. B 47, 12329 (1993).
E. Brezin and J. M. Drouffe, Nucl. Phys. B200, 93 (1982).
T. Tohyama and S. Maekawa, Phys. Rev. B 49, 3596 (1994).
C. D. Batista, L. O. Manuel, H. A. Ceccatto, and A. A. Aligia, Europhys. Lett. 38, 147 (1997).
FIG. 1.

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