A NEW PHASE DIAGRAM
FOR THE t-J MODEL

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Abstract

We study the so-called nonmagnetic phases (dimer and flux states) in the t-J model below half filling. We present a new phase diagram, at zero and finite temperature, that includes broad areas of phase coexistence (dimer-flux or flux-uniform), in accordance with experimental and numerical data on the possibility of separation into hole-rich and hole-poor regions. We also briefly comment on some techniques used in the literature to discuss phase separation in the t-J model.

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Since Anderson’s suggestion [1] that strongly correlated electron models might be relevant to describe the physics of high-Tc superconductors, much work, both numerical and analytical, has been done in order to understand the properties of the Hubbard model in 2-dimensions, in particular by examining simplified models that can be obtained from it in the strong coupling limit, such as the Heisenberg model or the t-J model [2] for the one-band version or the spin-fermion model [3] for the three-band case.

Still, the question of the ground state of these models has not been settled, at least away from half-filling. As candidate for the ground state, a variety of phases has been proposed, which include the long-range antiferromagnetically ordered (AF) state [4], the short-range antiferromagnetically ordered (RVB) state [5], as well as the so-called non-magnetic states, such as the dimer and the flux phase [6].

In this paper, we will concentrate on the t-J model, which has been extensively studied by means of different techniques and within different approaches, that include standard mean field theory [6-8], slave-boson techniques [9-12] and numerical simulations [13, 14].

At half-filling, i.e. at zero doping (δ = 0), when the model reduces to the well known spin 1/2 Heisenberg Hamiltonian, the instability of the other phases against the AF phase has been established beyond any reasonable doubt by analytical and numerical methods [15]. Within mean field theory, the lowest energy phase is not the AF but the dimer phase, either the columnar or the staggered one [16, 17] which are degenerate at this level of approximation. Even the inclusion of both classical and quantum quadratic fluctuations does not increase the energy of the dimer phase above the energy of the AF state [18]. It is known that this apparent contradiction is strictly related to the difficulty of taking into account the constraint of one electron per site in this approach. Indeed, in [18] it has been shown that at the mean field level, eventually corrected by quadratic fluctuations, the constraint is implemented exactly for the AF phase but not for the dimer phase. Thus, in the latter case we are effectively dealing with a larger space of states and hence it comes of no surprise the fact the energy gets substantially lowered.

For finite doping fraction (δ > 0), the major difficulty consists of developing good approximating techniques while dealing with the Gutzwiller (or below-half-filling) constraint. The experimental evidence and all the above mentioned theoretical studies confirm the intuitive idea that the presence of holes tends to disfavour a long-range antiferromagnetically ordered phase. However, there is still no complete agreement on the possible ground state at δ ≠ 0. Among the candidates for the ground state of the t-J model, the RVB and the flux states have been mainly considered. The former, first proposed by Anderson and coworkers [7], is characterized by a superconducting ordered parameter of
the kind $\Delta_{ij} = \langle c_i^\uparrow c_{j\uparrow} - c_i^\downarrow c_{j\downarrow} \rangle$, where $i, j$ are nearest neighborhood sites, which gives short-range antiferromagnetic correlations. The latter \cite{3} corresponds to a nonmagnetic complex order parameter $U_{ij} = \langle \sum_{\alpha=\uparrow,\downarrow} c_{i\alpha}^\dagger c_{j\alpha} \rangle$, whose phase originates a nonzero magnetic flux threading the elementary (square) plaquettes of the lattice in a staggered way. Whenever the flux is different from 0 or $\pi$ (mod $2\pi$), this phase breaks parity and time-reversal symmetries. This has been the starting point of a large number of works, in which it has been argued that the continuum limit effective action describing the low-energy excitations around the flux phase could contain a Chern-Simons term \cite{13}, which would impart fractional statistics to the quasiparticles, leading to the possibility of anyonic superconductivity \cite{20}. An analysis of this claim requires more sophisticated techniques than the one used in this paper and goes beyond our present scope. We remark here only that, while it exists for the AF phase \cite{21, 3}, a detailed study of the continuum limit around the flux phase, able to prove or disprove the presence of a topological term, is still missing in the literature. We plan to further discuss this point in some future work.

At half filling, the large-U limit of the Hubbard model admits an SU(2) gauge symmetry \cite{22}, which shows the equivalence between the apparently different RVB and flux states. This symmetry is broken at $\delta \neq 0$, so that these two states evolve into different phases, which nevertheless stay very close in energies. In this paper we will not address the problem of the competition between the RVB and the flux phase \cite{12, 23}. We will concentrate our analysis on the nonmagnetic phases only. This is because we seem to find a phase diagram in the temperature-doping (T-$\delta$) plane richer than the one considered in previous works \cite{3} within the same kind of mean field approximation. If, on one side, our pure mean field data confirm the hypothesis that the flux phase gives the ground state in the range of the doping fraction $\delta$ which is relevant for superconductivity, on the other side, we discover that, especially at low temperatures, there are wide regions of phase coexistence, corresponding to either dimer-flux or flux-uniform phase separation, depending on the value of $\delta$. This seems to go in the same direction of some experimental data on high temperature superconducting materials \cite{24, 25} and as well as of some perturbative and numerical studies of the t-J model \cite{26-30}, which find a tendency towards a separation of regions with different hole concentrations. We remark here that the presence of phase coexistence regions might also affect a stability analysis of the RVB vs. the flux phase.

Our starting point is the t-J Hamiltonian, which can be obtained as the strong coupling limit, $|t| \ll U$, of the one-band version of the Hubbard model for small values of the doping $\delta$ \cite{4}:

$$H_{eff} = \sum_{\langle ij \rangle, \alpha} t_{ij} (1 - n_{i\alpha}) c_{i\alpha}^\dagger c_{j\alpha} (1 - n_{j\alpha})$$

(1)
\[ H = \sum_{<ij>} J_{ij} \left\{ \vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_in_j \right\} \]

where \( c_{i\alpha}^\dagger \) is the creation operator of one electron with spin \( \alpha = \uparrow, \downarrow \) in the site \( i \) and \( \vec{S}_i = \frac{1}{2} \sum_{\alpha\beta} c_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{i\beta} \) (\( \vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3) \) being Pauli matrices) are the spin operators on the site \( i \). In addition, \( J_{ij} = \frac{4|t_{ij}|^2}{U} \), \( \alpha = -\alpha \) while the symbol \( \langle ij \rangle \) denotes a sum over nearest-neighbor (n.n.) lattice sites only. The operator expressions containing \( n_{i\alpha} \equiv c_{i\alpha}^\dagger c_{i\alpha} \) have the effect of enforcing the Gutzwiller projector.

At exact half-filling, when \( n_i \equiv n_{i\uparrow} + n_{i\downarrow} = 1 \), the first term of (1) vanishes identically, while the second line reduces to the spin \( \frac{1}{2} \) antiferromagnetic Heisenberg Hamiltonian. If we introduce holes in the system, so that the doping fraction is \( \delta \neq 0 \), we can no longer neglect the first term of (1) which describes a direct hopping of one electron from the site \( j \) to the (empty) n.n. site \( i \). Because of the presence of the number operators \( n_{i\alpha} \), the hopping term is the sum of products of up to six electron creation/annihilation operators and is therefore very difficult to analyze.

Thus, following Anderson and coworkers [7], we make the assumption that the main effect of the Gutzwiller projection is the renormalization of the hopping amplitude from its nominal value \( t_{ij} \) to \( \delta t_{ij} \). We recall that such assumption has been proven to be correct either within a slave boson approach at the mean field level [9, 31] and within a variational approach making use of the Gutzwiller approximation [32]. With the further assumption that \( t_{ij} = t \), up to nonrelevant constant factors, the Hamiltonian (1) becomes:

\[ \mathcal{H} = t\delta \sum_{<ij>} \sum_{\alpha} c_{i\alpha}^\dagger c_{j\alpha} - \frac{J}{2} \sum_{(ij)} \sum_{\alpha\beta} c_{i\alpha}^\dagger c_{j\alpha} c_{j\beta}^\dagger c_{i\beta} \].

(2)

We will also restrict our attention to 2-D square lattices.

To study the phase diagram of (2), we will follow the technique described in [16] to rewrite the partition function in the grand canonical ensemble \( Z = Tr \{ e^{-\beta (\mathcal{H} - \mu N)} \} \) as:

\[ Z = \int [\mathcal{D}\psi_{i\alpha}^* \mathcal{D}\psi_{i\alpha}] \exp \left\{ - \int_0^1 d\tau \left[ \sum_i \sum_{\alpha} \psi_{i\alpha}^* (\partial_\tau - \mu) \psi_{i\alpha} \right. \right. \]

\[ + \left. \beta t\delta \sum_{<ij>} \sum_{\alpha} \psi_{i\alpha}^* \psi_{j\alpha} - \frac{\beta J}{2} \sum_{<ij>} \sum_{\alpha\beta} \psi_{i\alpha}^* \psi_{j\alpha} \psi_{j\beta}^* \psi_{i\beta} \right\} \]

(3)

where we have introduced Grassmann fields \( \psi_{i\alpha} \) for the fermionic operators \( c_{i\alpha} \).

We can now decouple the quartic term in the exponential of (3) via
Hubbard-Stratonovich auxiliary fields $U_{ij}$ as follows:

$$Z = \int [\mathcal{D}\psi^*_{i\alpha} \mathcal{D}\psi_{i\alpha}] \int [\mathcal{D}U^*_{ij} \mathcal{D}U_{ij}] \exp \left\{ -\frac{2\beta}{J} \int_0^1 d\tau \sum_{<ij>} U^*_{ij} U_{ij} \right\} \int [\mathcal{D}\psi^*_{i\alpha} \mathcal{D}\psi_{i\alpha}]$$

$$\times \exp \left\{ -\int_0^1 d\tau \left[ \sum_i \sum_{\alpha} \psi^*_{i\alpha} (\partial_\tau - \mu_\beta) \psi_{i\alpha} + \beta \delta \sum_{<ij>} \sum_{\alpha} \psi^*_{i\alpha} \psi_{j\alpha} + \beta \sum_{<ij>} \sum_{\beta} U^*_{ij} \psi^*_{i\beta} \psi_{j\beta} \right] \right\} .$$

We will work in the static approximation: $U_{ij}(\tau) = U_{ij}$ (constant in the imaginary time $\tau$), so that, going to Fourier transform with respect to $\tau$, (4) can be rewritten as:

$$Z = \int [\mathcal{D}U^*_{ij} \mathcal{D}U_{ij}] \exp \left\{ -\frac{2\beta}{J} \sum_{<ij>} U^*_{ij} U_{ij} \right\} \int [\mathcal{D}\psi^*_{i\alpha} \mathcal{D}\psi_{i\alpha}]$$

$$\times \exp \left\{ \sum_{nn'} \sum_{ij} \sum_{\alpha} \psi^*_{i\alpha} (\omega_n) \left[ G^{-1} - \beta U \right]_{nn'}^{ij} \psi_{j\alpha} (\omega_{n'}) \right\} ,$$

where $\omega_n = (2n+1)\pi$ ($n \in \mathbb{Z}$) are Matsubara frequencies and

$$[G^{-1}]_{nn'}^{ij} = (i\omega_n + \mu_\beta) \delta_{ij} \delta_{nn'},$$

$$[U]_{nn'}^{ij} = \left\{ \begin{array}{ll} [t \delta + U_{ij}]_{nn'} & \text{if i.n.n. } j \\ 0 & \text{otherwise} \end{array} \right. \quad \text{(6)}$$

We can now perform the integral over the fermionic variables to get:

$$Z = \int [\mathcal{D}U^*_{ij} \mathcal{D}U_{ij}] \exp \left\{ -\frac{2\beta}{J} \sum_{<ij>} U^*_{ij} U_{ij} \right\} \exp \left\{ -S_{\text{eff}} \right\} \quad \text{(8)}$$

$$S_{\text{eff}} \equiv -2 \text{Tr} \left\{ \log \left[ -G^{-1} + \beta U \right] \right\} ,$$

where the factor 2 comes from spin summation and “Tr” stands for a trace over lattice sites and frequencies.

Following [6], we consider solutions of the saddle point equations, $\frac{\partial S_{\text{eff}}}{\partial U_{ij}} = 0$, that admit a symmetry for translations along the diagonal of elementary plaquette of the square lattice. In this case, the matrix $U$ depends only on four independent link variables $U_{ij}$ as shown in figure (a). Under this assumption, the corresponding Brillouin zone gets halved. The Reduced Brillouin Zone (RBZ) is given by the shaded area of figure (b).

In momentum space, the matrix $U$ can be easily diagonalized. It has eigenvalues:

$$E_k = \pm |\lambda_k|$$

$$\lambda_k \equiv \chi_1 e^{ik_x a} + \chi_2 e^{-ik_y a} + \chi_3 e^{-ik_x a} + \chi_4 e^{ik_y a}$$

$$\quad \text{(10)}$$
with $\chi_j \equiv t\delta + U_j$ and $k \in RBZ$, so that:

$$S_{\text{eff}} = -2 \sum_{k \in RBZ} \sum_n \log(-i\omega_n - \mu_\beta + \beta|\lambda_k|) + \log(-i\omega_n - \mu_\beta - \beta|\lambda_k|) .$$  

The sum over the Matsubara frequencies can now be performed, yielding the following expression for the partition function in the static approximation:

$$Z = \int [DU_j^*DU_j] e^{-\beta\Omega}$$  

$$\Omega = \frac{N}{J} \sum_{j=1}^4 |U_j|^2 - \frac{2}{\beta} \sum_{k \in RBZ} \left[ \log(1 + e^{\beta(\mu - |\lambda_k|)}) + \log(1 + e^{\beta(\mu + |\lambda_k|)}) \right] .$$

The stationary points of $\Omega$ are thus given by the saddle-point equations:

$$U_1 = \frac{J}{N} \sum_{k \in RBZ} e^{-ik_x a} \frac{\lambda_k}{|\lambda_k|} \left[ \frac{1}{1 + e^{-\beta(\mu + |\lambda_k|)}} - \frac{1}{1 + e^{-\beta(\mu - |\lambda_k|)}} \right] ,$$

$$U_2 = \frac{J}{N} \sum_{k \in RBZ} e^{-ik_y a} \frac{\lambda_k^*}{|\lambda_k|} \left[ \frac{1}{1 + e^{-\beta(\mu + |\lambda_k|)}} - \frac{1}{1 + e^{-\beta(\mu - |\lambda_k|)}} \right] ,$$

$$U_3 = \frac{J}{N} \sum_{k \in RBZ} e^{ik_x a} \frac{\lambda_k}{|\lambda_k|} \left[ \frac{1}{1 + e^{-\beta(\mu + |\lambda_k|)}} - \frac{1}{1 + e^{-\beta(\mu - |\lambda_k|)}} \right] ,$$
\[ U_4 = \frac{J}{N} \sum_{k \in RBZ} e^{ik_\alpha} \frac{\lambda_k^*}{|\lambda_k|} \left[ \frac{1}{1 + e^{-\beta(\mu + |\lambda_k|)}} - \frac{1}{1 + e^{-\beta(\mu - |\lambda_k|)}} \right], \] (16)

which must be supplemented by the equation determining the chemical potential \( \mu \):

\[ N(1 - \delta) = 2 \sum_{k \in RBZ} \left[ \frac{1}{1 + e^{-\beta(\mu - |\lambda_k|)}} + \frac{1}{1 + e^{-\beta(\mu + |\lambda_k|)}} \right]. \] (17)

We have already recalled that, at half filling, the Hamiltonian (4) admits an \( SU(2) \) gauge symmetry. As a special case, (2) is invariant under a local \( U(1) \) transformation mapping the operator \( c_{j\alpha} \) into \( e^{i\theta} c_{j\alpha} \). Such transformation changes the phases of the link variables \( U_{jk} = |U_{jk}| e^{i\theta_{jk}} \) by

\[ \theta_{jk} \to \theta_{jk} + \theta_k - \theta_j , \] (18)

but keeps the sum of the phases around an elementary plaquette (of vertices \( j, k, l, m \)) invariant: \( \Delta \theta = \theta_{jk} + \theta_{kl} + \theta_{lm} + \theta_{mj} = \text{cost} \). Indeed, \( \Delta \theta \) is a gauge invariant, hence observable, quantity and can be thought of as the flux associated to a magnetic field threading the plaquette. In addition, equations (13-17) with \( \delta = 0 \) are left invariant and hence the grand canonical potential \( \Omega \) will admit a set of degenerate minima, parametrized by \( U(1) \) and all corresponding to the same \( \Delta \theta \). For \( \delta \neq 0 \), this symmetry is explicitly broken by the hopping term and, in general, only one specific choice of the phases \( \theta_{jk} \), which are no longer pure gauge degrees of freedom, will correspond to a minimum of \( \Omega \).

We have chosen to study equations (13-17) numerically for the case of \( t/J = 1 \), a value that well approximates the experimental values for the hopping amplitude \( (t = 1 eV) \) and the Hubbard repulsion \( (U = 5 eV) \). We have found the following solutions yielding (local) minima of the grand canonical potential \( \Omega \):

1. **Uniform phase.**
   This is characterized by the choice:

   \[ U_1 = U_2 = U_3 = U_4 = U \in \mathbb{R}^+ . \] (19)

   This solution exists at all temperature and is the only minimum of \( \Omega \) at high temperature and/or high doping. At all value of the doping \( \delta \), the total flux per plaquette is \( \Delta \theta = 0 \).

2. **Dimer phase.**
   It corresponds to solutions of the form:

   \[ U_1 \neq U_2 = U_3 = U_4 , U_j \in \Phi \] (20)

   \[ U_1 = U_2 = U_3 = U_4 = U \in \mathbb{R}^+ . \] (19)
and with

\[ |U_1| \gg |U_2| \quad . \tag{21} \]

At \( \delta = 0 \), the \( U(1) \)-gauge symmetry mentioned above allows to choose the \( U_j \) real. In addition, in this case, \( U_2 = 0 \). For finite \( \delta \), gauge invariance is broken and the parameters \( U_j \) are in general complex. This is indeed the case for a range of temperature \( 0 < T < T_1 = 0.1J \), in which the parameters stay real only up to some value \( \delta_{c1}(T) \) and then acquire a phase increasing with \( \delta \). For \( T \geq T_1 \), on the contrary, the parameters are always real. In addition, for \( \delta > \delta_{c2}(T) \), \( \text{(20)} \) ceases to be a solution of the saddle point equations. This behaviour is shown in figure 2.

Figure 2:
The phase \( \phi_1 \) of the order parameter \( U_1 \) in the dimer phase as a function of the doping \( \delta \) at different temperatures.
The critical dopings \( \delta_{c1} \) and \( \delta_{c1} \) are shown for \( T = 0.02 \).

3. Kite phase.
This solution exists only in a very small region of the parameter space
and corresponds to the choice:
\[ U_1 = U_2 \neq U_3 = U_4 , \ U_j \in \mathbb{R} \ . \] (22)
The parameters \( U_3 \) and \( U_4 \) are zero at \( \delta = 0 \) and then increase while \( \delta \) increases.

4. Flux phase.
This phase corresponds to a sort of complex uniform phase and is given by the choice:
\[ U_1 = U_2 = U_3 = U_4 \equiv U \ e^{i\phi} , \ U \in \mathbb{R}^+ \text{ and } \phi \neq 0 \ . \] (23)
Because of the \( U(1) \) invariance, at \( \delta = 0 \), the phases of the four parameters do not need to be the same, as long as the total magnetic flux per plaquette is equal to \( 4\phi \). In figure 3, \( \phi \) is shown as a function of \( \delta \) at different values of the temperature. For any \( T < T_c^{(0)} \), \( \phi \) is \( \frac{\pi}{2} \) at exact half-filling and then decreases with continuity going to zero at some critical value of delta \( \delta_c(T) \). We will discuss the behaviour of the curve for \( T = 0.02 \) shortly below.

After having calculated and compared the free energy \( F = \Omega + \mu N (1 - \delta) \) corresponding to the different mean field solutions described above, we have obtained the phase diagram shown in figure 4. We remark that, contrary to what happens in going from the dimer to the kite or the flux phase, the transition from the flux to the uniform phase is continuous, the phases of the order parameters \( U_j \) going smoothly to zero as \( \delta \) increases.

We observe that, for \( T = 0 \), we recover the results of [3]. Indeed, since we have renormalized the hopping coefficient \( t \) by a factor of \( \delta \), our data have to be compared with the ones that can be read moving along the diagonal line \( t/J = \delta \) of the zero temperature phase diagram given in [3]. Also, we remark that the flux phase has been extensively studied [10, 11] by analyzing the Hamiltonian (2) within a slave boson approach. Apparently, some different results are obtained: the authors of references [10, 11] find a flux phase corresponding to a magnetic flux per plaquette which for small \( \delta \) is blocked to the value \( \pi \), decreasing towards zero only after a finite value of the doping. It is not difficult to show, however, that the Hubbard-Stratonovich fields \( U'_{ij} \) used in those papers differs from the \( U_{ij} \) we have used, the relationship being:
\[
U'_{ij} = U_{ij} - \frac{t}{2J} \langle b_i^\dagger b_j \rangle \\
\simeq U_{ij} - \frac{t}{2J} \delta , \tag{24}
\]
where $b_i$ ($b_i^\dagger$) is the creation (annihilation) operator of the slave boson and the last equality is valid in the mean field approximation. We have checked that our numerical data for the $U_{ij}$ in the flux phase, once corrected according to formula (24), yield a phase for the $U_{ij}'$ that does indeed reproduce the behaviour described in [12, 11]. Thus, as it should be, the two approaches give the same mean field results.

Our mean field calculations indicate the existence of a rather extended region of stability for the flux phase below half-filling, which coincides roughly with the region relevant for superconductivity. We notice also that, between dimer and flux as well as between flux and uniform phases, there is a rather strange receding of the phase boundary line. This is the cause of the behaviour of the $T = 0.02$ curve in figure 3.

The phase diagram shown in figure 4 has been constructed without taking into account the possibility of phase separation. However, this possibility cannot be overlooked. It is indeed a long-standing and still unresolved problem concerning the Hubbard model and its parent Hamiltonians, such as the t-J.
Let us recall that experiments on different copper oxide compounds have found a spatial separation between AFM hole-poor and superconducting hole-rich regions, happening either at a microscopic level \cite{24} or at a macroscopic level, such as in ordered striped phases \cite{25}. From a theoretical point of view, much work has been done to demonstrate that this phenomenon can occur for the Hubbard model in the strong coupling limit. In particular phase separation for the t-J model has been discussed by means of a high-temperature expansion by Puttika et al. \cite{26} and by Emery et al. \cite{27} by using variational arguments and exact diagonalization numerical studies. Its connections with the onset of high-temperature superconductivity has been considered in \cite{33}. Also, phase coexistence has been examined for other phases that might be relevant in the t-J model, such as the spiral ones \cite{28} or the ferromagnetic one \cite{29,30}, in the latter case for its relevance to the Nagaoka problem. Anticipating our results, we find, for nonmagnetic phases as well, an instability towards phase coexistence and separation between hole-rich and hole-poor regions. Since we work in a mean field approximation, we are however not able to say how spatially distributed the two different regions can appear.

Figure 4:
The phase diagram of the t-J model at pure mean filed level.
We have therefore inquired about the stability of our mean field solutions towards phase separation by studying:

1) The fluctuation matrix for the grand canonical potential $\Omega$ around the saddle point solutions, since the mean field solution is unstable whenever the fluctuation matrix has one or more negative eigenvalues.

2) The behaviour of the chemical potential $\mu$ as a function of doping $\delta$, since an instability towards phase separation is signaled by $\frac{\partial \mu}{\partial \delta} > 0$ \[2\]. In fact, if $\frac{\partial \mu}{\partial \delta} > 0$ then the isothermal compressibility $\kappa^{-1} = n^2 \frac{\partial^2 f}{\partial n^2} = n^2 \frac{\partial \mu}{\partial n}$ is negative and the system is clearly unstable. The stable state is given by the coexistence between two phases having different values of doping and the same chemical potential. These values of doping are given by the application of the Maxwell construction to the diagram $\mu(\delta)$ \[3\].

3) The convexity of the free energy density $f = F/V$ as a function of $\delta$, since an instability towards phase separation is indicated also by a region of concavity of the free energy $f$. It is easy to see that, when working within an approximation scheme that respects the thermodynamical equalities, the region of concavity of $f$ should coincide with that where $\frac{\partial \mu}{\partial \delta} > 0$, since $\kappa^{-1} = n^2 \frac{\partial^2 f}{\partial n^2} = n^2 \frac{\partial \mu}{\partial n}$. In this case it is also possible to check that the bitangent to the curve $f(\delta)$ gives an interpolation between two different phases which is equivalent to the Maxwell construction for $\mu(\delta)$.

As for 1), we have considered only fluctuations around the mean field solutions which preserve the symmetry under translations along the diagonal of the square elementary plaquettes. We have found that the fluctuation matrix develops a negative eigenvalue in two regions of the phase diagram: a) on the left of the boundary separating the flux and the uniform phase, below a certain temperature $T_c \sim 0.145 J$; b) on the left of the boundary between dimer and flux phase, below a given temperature $T_{c1} \sim 0.085 J$. We might therefore expect both a region of flux-uniform and a region of dimer-flux phase coexistence.

Such scenario is fully supported by the behaviour of the chemical potential $\mu$ as a function of $\delta$. Indeed, $\frac{\partial \mu}{\partial \delta}$ becomes positive exactly in the regions where the fluctuation matrix develops a negative eigenvalue. We will analyze in detail only the flux-uniform phase coexistence, the discussion for the dimer-flux case being completely analogous.

The function $\mu(\delta)$ for the flux and uniform phases is represented in figure 5: for $\delta$ below the critical $\delta_c(T)$ of the transition between the flux and the uniform, we have plotted the chemical potential of the flux phase, while for $\delta > \delta_c(T)$ we have plotted the chemical potential of the uniform phase (this explains the cusp at $\delta_c(T)$). While for $T > T_c \sim 0.145 J$ the chemical potential is always decreasing with $\delta$, when $T < T_c$ we have $\frac{\partial \mu}{\partial \delta} > 0$ in a region of doping...
Figure 5:
The chemical potential $\mu$ as a function of the doping $\delta$ for the flux and the uniform phases.

which extends from a certain $\delta_{c0}(T)$ up to $\delta_c(T)$. In this region the flux phase is, therefore, unstable and the system separates in a hole-rich part, which is in the uniform phase, and in a hole-poor part which is in the flux phase.

The thermodynamical identities would require the free energy to be concave only in the region of the $\delta - T$ diagram with $\delta_{c0}(T) < \delta < \delta_c(T)$ and $T < T_c$. But we have found that, for temperature above $T_0 \sim 0.12J$, the free energy of the flux phase is already concave at $\delta = 0$ and remains concave up to the critical $\delta_c(T)$. We believe that such thermodynamical inconsistency is entirely due to some shortcoming of the mean field approximation. In fact, let us note that the inclusion of thermal and quantum fluctuations might improve the consistency between the convexity of $f(\delta)$ and the monotonicity of $\mu(\delta)$, since it could substantially modify the behaviour of the free energy while keeping the chemical potential unchanged, the latter being uniquely determined by the saddle point equations. In the case we are dealing with, such inclusion is, however, nontrivial and somewhat problematic. Indeed, at $\delta = \delta_{c0}(T)$, one of the eigenvalues of the fluctuation matrix becomes zero, so that the integration of gaussian fluctuations would give actually a divergent result. In a similar way,
special care has to be taken in the region of small $\delta$: at $\delta = 0$ the fluctuation matrix has, for the flux-phase, three zero modes corresponding to the $U(1)$ gauge invariance discussed above. At exact half filling, one can get rid of these modes by the standard Faddev-Popov procedure. Below half filling this gauge invariance is broken, but for small $\delta$ the eigenvalues are almost zero and a simple gaussian integration would overestimate the fluctuations. It is clear that next to quadratic corrections would be required to obtain a meaningful result.

We have not found any mention to inconsistencies between the behaviour of the free energy and that of the chemical potential in literature. In all the previous articles discussing phase separation in the t-J model, people have considered only one of the two approaches, but we believe that, at least for the works dealing with the mean field approximation, problems like the ones considered above would have to be found. We have been able to explicitly check this in one example, by comparing the Maxwell construction on the free energy which is given in [30] with the behaviour of the chemical potential, whose analytic expression is also reported.

Let us remark also that, at temperature $T > T_0$, we find the free energy to be strictly concave in the range $0 \leq \delta < \delta_c(T)$, which does include the zero. It is easy to see that this problem cannot be overcome by going to negative values of the doping (i.e. above half filling), since two phases with $\delta$ of opposite sign cannot have the same chemical potential. Thus, in some papers [30, 28], the “bitangent construction” on the free energy is performed by drawing the tangent to the curve $f(\delta)$ from the point $(0, f(\delta = 0))$, forgetting the fact that this line is not really tangent at $\delta = 0$. But it is not difficult to check that this leads to considering the coexistence of two phases having different chemical potentials, which cannot therefore be in equilibrium.

For all the reasons explained above, we have decided to base our analysis of phase separation on the behaviour of the chemical potential only, which, besides being stable against the inclusion of fluctuations, is also in agreement with the data on the positivity of the eigenvalues of the fluctuation matrix. As we have already said, we find two regions of instability, corresponding to the possibility of coexistence between a) the flux and the uniform phases, b) the dimer and the flux phases. The Maxwell construction on the chemical potential and the evaluation of the free energy for the mixed phases lead to a new phase diagram, which is substantially different from the one of figure 4. At high temperatures, the phase separation instabilities disappear and hence figure 4 does not change. On the contrary, at low temperatures, the regions of dimer-flux and flux-uniform phase coexistence are quite broad, and for $T < 0.05J$ the pure flux phase is never a minimum of the free energy, for any value of the
Doping $\delta$ (units of $J$)

Figure 6:
The phase diagram for the $t - J$ model, after taking into account phase separation.

...doping. In addition, the kite phase is no more present, since it has a higher energy than the coexistence between the flux and the uniform phase. The final phase diagram, taking into account phase coexistence, is shown in figure 6. Notice that we do not find receding phase boundaries anymore.

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