Mixed Phases for the $t$-$J$ Model

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Abstract

We study the competition between non-magnetic (dimer or flux) states and short-range antiferromagnetically ordered RVB states in the $t$-$J$ model and present a finite temperature phase diagram. We show that, for a wide range of temperatures and dopings, the stable phase results to be a state in which both the flux and the RVB parameters are nonzero.

PACS: 71.27, 74.20.
In this paper we want to extend the analysis of the phase diagram of the $t$-$J$ model on a square lattice, started by some of the authors in ref. [1], where only the so called non-magnetic states (such as the dimer and the flux phase) were considered.

Our starting point is the $t$-$J$ Hamiltonian, as originally proposed in [2]:

$$
H = t \delta \sum_{(ij)} \sum_{\alpha} c_{i\alpha}^\dagger c_{j\alpha} - \frac{J}{4} \sum_{(ij)} \sum_{\alpha\beta} c_{i\alpha}^\dagger c_{j\alpha}^\dagger c_{j\beta} c_{i\beta},
$$

(1)

where $(ij)$ stands for a sum over ordered nearest-neighbor sites. This Hamiltonian incorporates the below-half-filling constraint only in average: the hopping coefficient $t$ of the first (kinetic) term gets renormalized by the doping factor $\delta$. At half filling ($\delta = 0$) the Hamiltonian reduces to the well-known Heisenberg Hamiltonian, with the spin operators written in a fermion representation.

As candidates for the ground state of the $t$-$J$ model, the RVB and the flux states have been mainly considered in literature. The former, first proposed by Anderson and coworkers [2], is characterized by a BCS-type order parameter of the kind $\Delta_{ij} = \langle c_{i\uparrow} c_{j\downarrow} - c_{i\downarrow} c_{j\uparrow} \rangle$, which gives short-range antiferromagnetic correlations. The latter [3] corresponds to a nonmagnetic complex order parameter $\chi_{ij} = \langle \sum_{\alpha = \uparrow, \downarrow} c_{i\alpha}^\dagger c_{j\alpha} \rangle$, whose phase gives rise to a nonzero magnetic flux threading the elementary (square) plaquettes of the lattice in a staggered way. It is well known [4] that the Heisenberg Hamiltonian, and hence the $t$-$J$ model (1) at half filling, is invariant under local $SU(2)$ transformations. One can exploit this symmetry [5] to show that the so called mixed-RVB and the flux phases are degenerate since they are related via one such gauge transformation. Thus, these apparently different phases actually represent the same physical state. Away from half filling, this $SU(2)$-gauge symmetry gets explicitly broken by the kinetic term. This means that the RVB and the flux phases are no longer equivalent so that the question of a possible competition between these two phases arises.

To start with, we want to reformulate the theory in a way that enables us to keep always track of the (broken) gauge symmetry. This can be done by introducing the $2 \times 2$ matrix operators:

$$
\Psi_i = \begin{pmatrix} c_{i\uparrow}^\dagger & c_{i\downarrow} \\ c_{i\downarrow}^\dagger & -c_{i\uparrow}^\dagger \end{pmatrix}
$$

(2)

and by defining:

$$
\Phi_{ij} = \Psi_i \Psi_j^\dagger
$$

(3)

For a detailed discussion of how to derive this formula in the strong-coupling limit of the Hubbard model at or below half-filling see [1] and references therein.
Then, with some algebra, one can easily show that (1) can be rewritten as:

\[ H = t \delta \sum_{ij} tr[\sigma_3 \Phi_{ij}] - \frac{J}{8} \sum_{ij} tr[\Phi_{ij}^\dagger \Phi_{ij}] , \]  

(4)

where \( \sigma_3 \) is the third Pauli matrix and \( tr \) stands for the trace over \( 2 \times 2 \) matrices. It is immediate to check that the second term in the Hamiltonian is gauge invariant under the following \( SU(2) \)-action:

\[ \Phi_{ij} \rightarrow g_i \Phi_{ij} g_j , \]  

(5)

g_i being any element of \( SU(2) \) possibly site-dependent, while the hopping term explicitly breaks such symmetry. Both the RVB and the nonmagnetic phases of the \( t-J \) can be studied in this context. Indeed, in the saddle point approximation, the mean value of the fields \( \Phi_{ij} \)'s is a function of \( \Delta_{ij} \) and \( \chi_{ij} \), namely:

\[ \langle \Phi_{ij} \rangle \propto \begin{pmatrix} -\chi_{ij}^* & \Delta_{ij} \\ \Delta_{ij}^* & \chi_{ij} \end{pmatrix} . \]  

(6)

where \( * \) denotes complex conjugation. Bearing this in mind, we study the \( t-J \) Hamiltonian by representing the partition function in the grand-canonical ensemble by means of a functional integral over Grassmann fields representing the fermionic operators and by decoupling the four-fermion Heisenberg interaction via a Hubbard-Stratonovich transformation over the auxiliary \( SU(2) \)-fields

\[ U_{ij} = \begin{pmatrix} -\chi_{ij}^* & \Delta_{ij} \\ \Delta_{ij}^* & \chi_{ij} \end{pmatrix} , \]  

(7)

Following [2] and [3] we will assume invariance under translations along the lattice for the parameters \( \Delta \)'s and along the diagonal for the \( \chi \)'s. We are then left with a total of six independent parameters, \( \Delta_{x,y} \) and \( \chi_{1,2,3,4} \), as shown in Fig. 1.

Due to the assumed translational symmetry, it is convenient to introduce a different notation for the fermionic fields living on odd and even sites (empty and full dots in the figure), say \( \psi \)'s and \( \phi \)'s. If we now go to momentum space – with \( k \) belonging to the Reduced Brillouin Zone (RBZ) and \( \omega_n \) denoting the fermionic Matsubara frequencies – the partition function in the static approximation (i.e. the auxiliary fields being time independent) can be rewritten as:

\[
Z = \int [\mathcal{D}\psi^*_{ka,n} \mathcal{D}\psi_{ka,n}] [\mathcal{D}\phi^*_{ka,n} \mathcal{D}\phi_{ka,n}] \int [\mathcal{D}\chi^* \mathcal{D}\chi] [\mathcal{D}\Delta^* \mathcal{D}\Delta] \\
\times \exp \left\{ -\frac{2M \beta}{J} \sum_{j=1}^{4} |\chi_j|^2 - \frac{4M \beta}{J} \sum_{j=x,y} |\Delta_j|^2 \right\}
\]
where
\[
\begin{align*}
\lambda_k &= (\chi_1 + t\delta)e^{ik_x} + (\chi_2^* + t\delta)e^{-ik_y} + (\chi_3 + t\delta)e^{-ik_x} + (\chi_4^* + t\delta)e^{ik_y} \\
\Delta_k &= 2(\Delta_x \cos k_x + \Delta_y \cos k_y)
\end{align*}
\] (9) (10)

and \( M \) is the number of lattice sites. The effective action in the functional integral (8) is now quadratic in the Grassmann fields \( \psi, \phi \), and it is actually a sum of independent quadratic forms acting separately in the four-dimensional subspaces spanned by \((\psi_{k\alpha,n}, \phi_{k\alpha,n}, \psi_{-k\alpha,-n}^*, \phi_{-k\alpha,-n}^*)\), for \( k \) in the RBZ, \( \alpha = \uparrow, \downarrow \) and \( \omega_n = (2n+1)\pi \), where they are represented by the matrices:

\[
\begin{pmatrix}
\mu & \lambda_k^* & 0 & -\Delta_k \\
\lambda_k & \mu & -\Delta_k & 0 \\
0 & -\Delta_k^* & -\mu & -\lambda_k \\
-\Delta_k^* & 0 & -\lambda_k^* & -\mu
\end{pmatrix}
\] (11)

Integrating then over the Grassmann fields, we arrive at the result:

\[
Z = \int [\mathcal{D}\chi_k^* \mathcal{D}\chi_k][\mathcal{D}\Delta_k^* \mathcal{D}\Delta_k] \exp\{-\beta \Omega\}
\] (12)
\[
\Omega = \frac{2M}{J} \left[ \sum_{j=1}^{4} |\chi_j|^2 + 2 \sum_{j=x,y} |\Delta_j|^2 \right] + S_{eff} - \mu M \tag{13}
\]

\[
S_{eff} = -\frac{1}{\beta} \sum_{n} \sum_{k \in RBZ} \sum_{j=1}^{4} (-i\omega_n - \beta \log E_k^j) \tag{14}
\]

\[
= -\frac{1}{\beta} \sum_{k \in RBZ} \sum_{j=1}^{4} \log \left( 1 + e^{\beta E_k^j} \right),
\]

where \( E_j^j (j = 1, 2, 3, 4) \) denote the eigenvalues of the matrix (11) multiplied by \( \beta \). Such matrix being \( 4 \times 4 \), it would be possible to give an analytic formula for the eigenvalues \( E_k^j \) and their dependence on the parameters \( \mu, \lambda_k, \Delta_k \), which is however very complicated and will not be presented here for the general case.

From (13) one can then derive the self-consistency equation that must hold for the parameters \( \chi \)'s and \( \Delta \)'s in the mean field approximation:

\[
\frac{\partial \Omega}{\partial \chi_j} = 0 \quad (j = 1, 2, 3, 4) \tag{15}
\]

\[
\frac{\partial \Omega}{\partial \Delta_j} = 0 \quad (j = x, y) \tag{16}
\]

which have to be supplemented by the equation fixing the chemical potential:

\[
\frac{\partial \Omega}{\partial \mu} = -M(1 - \delta) \tag{17}
\]

We have numerically investigated the solutions to this set of equations that also minimize the grand potential \( \Omega \), finding that all solutions belong to one of the following classes:

1) **Mixed-wave solutions**:

\[
\chi_1 = \chi_2 = \chi_3 = \chi_4 \equiv \chi, \quad \Delta_x \equiv \Delta, \quad \Delta_y = e^{i\tau} \Delta. \tag{18}
\]

2) **Dimer solutions**:

\[
\chi_j \text{ real, } |\chi_1| >> |\chi_2| = |\chi_3| = |\chi_4|, \quad \Delta_x = \Delta_y = 0. \tag{19}
\]

Under this assumptions it is possible to give a nice formula for the eigenvalues \( E_k^j \) and hence for the grand potential.

The effective action for the mixed-wave solution reads:

\[
S_{eff} = -\frac{2}{\beta} \sum_{k \in RBZ} \left[ \log \cosh \frac{\beta E_k^+}{2} + \log \cosh \frac{\beta E_k^-}{2} + 2 \log 2 \right] \tag{20}
\]

\[
E_k^\pm = \sqrt{(\mu \pm |\lambda_k|)^2 + |\Delta_k|^2}
\]

\[
\lambda_k = 2[(\chi + t\delta) \cos k_x + (\chi^* + t\delta) \cos k_y]
\]

\[
\Delta_k = 2\Delta(\cos k_x + e^{i\tau} \cos k_y)
\]
For the dimer solution one finds:

\[
S_{\text{eff}} = -\frac{2}{\beta} \sum_{k \in RBZ} \left[ \log(1 + e^{\beta(-E_k)}) + \log(1 + e^{\beta(E_k)}) \right]
\]

\[
E_k = |\lambda_k| = (\chi_1 + t\delta)e^{ikx} + (\chi_2^* + t\delta)e^{-iky} + (\chi_3 + t\delta)e^{-ikx} + (\chi_4^* + t\delta)e^{iky}
\]

It is among these classes of solutions that one has to look for the absolute minimum of the free energy \( F = \Omega + \mu M(1 - \delta) \) as the temperature \( T \) and the doping \( \delta \) vary. But, before presenting the phase diagram in the \( \delta - T \) plane, we need to understand some more properties of such solutions.

1) The solution we call mixed-wave can actually represent different phases already studied in literature, depending on the relative values of the two independent complex parameters \( \chi \) and \( \Delta \):

a) Uniform phase: it corresponds to \( \Delta = 0 \) and \( \chi \) real. As we will see this is the stable phase at high doping and high temperature.

b) Flux phase: it corresponds again to \( \Delta = 0 \) but now \( \chi \) has a nonvanishing imaginary part. If we write \( \chi = |\chi|e^{i\phi} \) we have that \( 4\phi \) might be seen as a magnetic flux threading the elementary square plaquette. One can check that, at fixed \( T \), the value of the phase \( \phi \) increases while \( \delta \) decreases, going from \( \phi = 0 \) at high doping (uniform phase) to \( \phi = \pi/4 \) at half filling (\( \delta = 0 \)).

c) RVB-d phase: it is obtained when \( \chi = 0 \) and \( \tau = \pi \). The actual value of the parameter \( \Delta \) depends, at fixed \( T \), on the doping \( \delta \).

d) RVB-mixed phase: it is given by \( \chi = 0 \) and \( \tau = \pi/2 \). Again the value of the parameter \( \Delta \) depends on the doping \( \delta \).

e) It is important to notice that, at half filling, the \( \pi \)-flux and the RVB-mixed phases are equivalent via an \( SU(2) \) transformation, and hence are degenerate in energy and actually represent the same physical state. It is only away from half filling that these two phases become independent. Still, one expects them to remain very close in energy, at least for low doping.

2) In the dimer solution, the relative values of the two independent order parameters \( \chi_1 \) and \( \chi_2 \) change with \( \delta \), for fixed \( T \). In particular, at any temperature, \( \chi_2 = 0 \) at half filling, so that only one link variable per plaquette is nonzero, giving rise to the so called staggered dimer configuration.

As for solutions of type (1), our analysis has shown that none of the above mentioned “pure solutions” is the actual absolute minimum of the free energy.
At not too small values of $\delta$, the latter is indeed minimized by a phase in which both the $\chi$ and the $\Delta$ parameters are different from zero. Precisely we obtain a sort of mixture between the uniform and the RVB-d phases, which we would like to call the mixed phase:

$$\chi \text{ real and } \tau = \pi.$$ (22)

The values of $|\chi|$ and $|\Delta|$ change with $T$ and $\delta$. Above a critical temperature $T_c = J/8$ we find $\Delta = 0$ and hence recover the uniform solution. At any $T < T_c$, there is a critical doping $\delta_c$ above which the stable solution is again the uniform phase. Below $\delta_c$, the parameter $\Delta$ increases continuously (second order transition) while $\delta$ decreases, in such a way that for $\delta = 0$ one also has $|\chi| = |\Delta|$. It is interesting to notice that the solution we find at half filling, where the $SU(2)$ symmetry is restored, is indeed equivalent via a gauge transformation to the RVB-mixed phase, or to the $\pi$-flux phase. This means that the introduction of the kinetic term breaks the $SU(2)$-degeneracy in favour of a state where all the $\chi$’s are equal and real, while the $\Delta$’s differ just for a phase of $\pi$.

At low dopings, it is the dimer phase that becomes stable. The transition from the dimer to the mixed phase is a first order transition.

The phase diagram is shown in Fig. 2 for $t/J = 1$. For different values of $t/J$ one obtains diagrams that look qualitatively the same: what changes slightly is only the position of the transition lines.

We have also investigated the stability of the mean field solutions around the lines of transition, by looking at the behaviour of the chemical potential $\mu$ as a function of doping $\delta$, since an instability towards phase separation is signaled by $\partial \mu / \partial \delta > 0$ (see the first paper in [1] for a discussion).

While no instability develops at the mixed/uniform line of transition, we find that the coexistence of the dimer and the mixed phases is favoured at all temperatures $0 < T < T_c$ around the original line of transition. Such effect is pretty strong especially at low temperatures, so that the pure dimer phase survives only very close to half filling. This is shown in Fig. 3.

We would like now to compare these results with our previous work [1]. Even if the starting Hamiltonian and the formalism we adopted are the same, and despite the fact that in the present paper we have enlarged the class of allowed mean field solutions, we find here a much simpler phase diagram. In particular we notice that the flux phase is no longer present, at any value of the doping and temperature, being substituted by the mixed phase (22). This is in agreement to and extends the findings of Zhang at zero temperature [7]. Also, our mean field Hamiltonian and self-consistency equations coincide, but

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**This phase is simply referred to as the “dimer phase” in [3]**
for some normalization coefficients, with the one given in [8] and obtained through an auxiliary-boson approach, originally formulated by Kotliar and Ruckenstein [9] for the Hubbard model, in which an empty site is described by a bosonic creation operator $b^\dagger_i$, whose density gets to be proportional to the doping in the mean field approximation:

$$\langle b^\dagger_i b_j \rangle = \delta.$$

On the contrary, the authors of ref. [6] find some wide region where the flux phase is stable and a small area of the phase diagram where there is a coexistence of the flux and the superconducting phases. They represent the $t$-$J$ model via the so-called Hubbard $X$-operators, which allow for the enforcement of the below-half filling constraint, and perform a $1/N$ expansion to extrapolate then to the case $N = 2$.

Our phase diagram is also substantially different from the one presented by Ubbens and Lee in [10] and obtained within a slave boson approach that differs from the one mentioned above [8] by the way the hopping term is treated. The free energy and hence the self-consistency equations found in [10] have an additional contribution coming from all the (infinite) bosonic states. As a result, the mean-field phase diagram shows a finite region, close to half filling, where the flux solution (either $\pi$ or staggered) is favoured against all other phases. A similar result is obtained, at zero temperature, also by Sheng et al. in [11]. They work again within the slave boson approach by introducing now

\[ t \sum_{(ij)} \sum_{\alpha} c^\dagger_{i\alpha} c_{j\alpha} b^\dagger_i b_i \]

Parenthetically, we notice that this explains also why the hopping Hamiltonian, which is written as $t \sum_{(ij)} \sum_{\alpha} c^\dagger_{i\alpha} c_{j\alpha} b^\dagger_i b_i$ in this approach, becomes $t\delta \sum_{(ij)} \sum_{\alpha} c^\dagger_{i\alpha} c_{j\alpha}$ in the mean field approximation as we wrote in [8].
Figure 3:
The phase diagram of the $t$-$J$ model, including the occurrence of phase separation.

an additional statistical gauge field that describes the hard-core nature of holes. In this case the free energy gets minimized, at low dopings, by a staggered flux phase combined with a nonzero statistical field yielding a uniform flux per plaquette.

As we have also noticed in the second paper of ref. [1], our calculations (à la Anderson) and the slave boson techniques seem to lead to very different results, in particular close to half filling. We are investigating why this discrepancy occurs. Even if we do not have a final answer to this question, we believe that the problem has to do with the way the below-half filling constraint is treated within the different approaches. Indeed, at the mean field level such constraint is respected only in some average sense and differences in the way this is implemented can result in different phase diagrams, especially close to half filling when the high density of electrons enhances the probability of including configurations with double occupied sites.

Finally, we want to comment on the possibility that, at a fixed temperature, phase separation might disappear when $J/t$ is lowered below a critical value $J_c/t$. In the second paper of ref. [1], we studied how this happens when considering non-magnetic phases only, showing that $J_c/t$ varies linearly with $T$ according to $J_c/t \approx 8T$. This results is confirmed in our present calculations, where we have also included RVB states. There is a difference however: now phase separation occurs as soon as the temperature is lower than the critical one $T_c = J/8$, whereas in our previous paper at temperatures close to the critical one only pure phases were present.
Acknowledgments
The authors would like to thank P. Pieri for the many helpful discussions.

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