Phase separation in the large-N limit of the t-J model

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We study the phase diagram of the SU(N) t-J model. The model has been investigated in the $N=\infty$ limit, analyzing various magnetic phases with cell doubling (dimer, flux, and uniform). We find a phase separation between a fully dimerized phase at half-filling and a hole-rich uniform phase supporting the occurrence of phase separation in the t-J model between a Fermi-liquid phase and an insulating magnetic phase.

The discovery of high-temperature superconducting oxides[1] revived the interest in lattice models of electrons with large on-site repulsion. In this context the t-J model has received considerable attention. The t-J Hamiltonian has three terms, an infinite local Hubbard repulsion, a nearest-neighbor hopping, and nearest-neighbor Heisenberg magnetic coupling. At half-filling this model describes a Mott insulator. The character of the ground state for very small doping is one of the most challenging problems in condensed-matter theory. Several non-Fermi-liquid phases with exotic magnetic order[2-6] have been conjectured to exist in this regime. A very different alternative was suggested many years ago by Visscher.[7] He proposed that the Hubbard model in the small-doping regime phase separates into a hole-rich phase and a hole-poor phase. This scenario has been recently revived as a generic feature of the t-J model close to half-filling.[8,9] This was demonstrated by an exact cluster diagonalization[8] and a field theoretic approach[9] using Hubbard projectors in the framework of a $1/N$ expansion. In this Brief Report we show that phase separation also takes place in the large-N limit of the t-J model[10] close to half-filling.

Phase separation is a rather common phenomenon in models with short-range interactions.[11] Recently a close connection between phase separation and superconductivity has been demonstrated in the Kondo-lattice model,[12] and in the three-band Hubbard model with nearest-neighbor repulsion.[13,14] The fact that phase separation is present in a region near where superconducting instabilities occur, lends further support to the idea that phase separation and superconductivity, two phenomena generally arising from attractive effective interactions, should be analyzed on the same footing. Since the large-N limit of the single-band t-J model undergoes a d-wave Cooper instability,[10] it is worthwhile to investigate whether a phase separation is also present in this limit.

We study the Hamiltonian

$$H=-\frac{t}{N}\sum_{\langle i,j\rangle,\sigma}\tilde{c}^{\dagger}_{i,\sigma}\tilde{c}_{j,\sigma}+\mu_0\sum_{i,\sigma}\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{i,\sigma}+\frac{J}{N}\sum_{\langle i,j\rangle,\sigma,\sigma'}\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{i\sigma'}\tilde{c}^{\dagger}_{j\sigma'}\tilde{c}_{j\sigma} \tag{1}$$

subjected to the constraint of no double occupancy $n_i\le q_0N$ (with $q_0=\frac{1}{2}$) due to the $U=\infty$ limit for the Hubbard repulsion. The constraint is then implemented via a standard slave-boson technique by means of the substitution $\tilde{c}\to b^{\dagger}c$ and $\tilde{c}^{\dagger}\to bc^{\dagger}$ leading to the following form of the constraint:

$$b_i^{\dagger}b_i+\sum_{\sigma}c^{\dagger}_{i\sigma}c_{i\sigma}=q_0N\ .$$

This constraint is enforced by a Lagrange multiplier field λ_i. In the $N=\infty$ limit the mean field is exact and static uniform solutions b and λ are assumed for the b_i and λ_i fields, respectively. The magnetic part of the Hamiltonian is instead decoupled by means of a Hubbard-Stratonovich transformation that introduces the bond variables $\tilde{\Delta}_{i,j}=(J/N)\sum_{\sigma}c^{\dagger}_{i,\sigma}c_{j,\sigma}$. The effective mean-field Hamiltonian is

$$H_{\rm mf}=-\frac{2tb^2}{N}\sum_{k,\sigma}(\cos k_x+\cos k_y)c^{\dagger}_{k,\sigma}c_{k,\sigma}+\mu\sum_{i,\sigma}c^{\dagger}_{i,\sigma}c_{i,\sigma}+\lambda(b^2-Nq_0)+\sum_{\langle i,j\rangle,\sigma}(\Delta_{i,j}c^{\dagger}_{i,\sigma}c_{j,\sigma}+\text{H.c.})+\frac{N}{J}\sum_{\langle i,j\rangle}|\Delta_{i,j}|^2\ , \tag{2}$$

where $\mu\equiv\mu_0+\lambda$ and $\Delta_{i,j}=\langle\tilde{\Delta}_{i,j}\rangle$. Notice that in this mean-field approach, b acts as a hopping multiplicative renormalization, while λ shifts the chemical potential.

The global minimization of Hamiltonian (2) for arbitrary values of t/J and doping is a very difficult problem. However at quarter filling progress has been made by Sachdev.[15] The local stability of the various minima has also been recently analyzed.[16] These investigations fo-

cused on the stability of the different phases at a fixed concentration of holes. Here we investigate the stability of the different phases at fixed chemical potential; phases which are absolutely stable when the concentration of holes is fixed, could in fact be unstable once we allow for density fluctuations if there is phase separation. We confine our analysis to mean-field solutions with at most double unit cell. Specifically we consider solutions where the average $\Delta_{i,j}$ has three different symmetries: uniform, dimer, and staggered flux. In the uniform (u) solution we set $\langle c_i^\dagger c_{i\pm x}\rangle = \langle c_i^\dagger c_{i\pm y}\rangle = \Delta$, while the dimerized ($d$) solutions for arbitrary value of doping are given by $\langle c_i^\dagger c_{i+x}\rangle = \Delta_1$; $\langle c_i^\dagger c_{i\pm y}\rangle = \Delta_2$; $\langle c_i^\dagger c_{i-x}\rangle = \Delta_3$ (here i has to be chosen on a sublattice), with Δ_i real. The staggered flux (f) phase is given by $\langle c_i^\dagger c_{i\pm y}\rangle = |\Delta| e^{\pm i\phi}$, $\langle c_i^\dagger c_{i\pm x}\rangle = |\Delta| e^{\pm i\phi}$.

The mean-field free energy per spin and per site is written as

$$F = g_s + \lambda\left[\frac{b^2}{N} - q_0\right] + \frac{T}{N_{\text{sites}}}\sum_k \ln(1+e^{[\mu - E^i(k)]/T}) \quad (3)$$

with $E^i(k)$ representing the eigenvalues of the Hamiltonian (2) and

$$g_{u,f} = \frac{2\Delta^2}{J}, \quad g_d = \frac{\Delta_1^2 + 2\Delta_2^2 + \Delta_3^2}{2J}.$$

The minimization of the mean-field free energy with respect to b, λ, Δ_i (and ϕ for the flux solution) leads to self-consistency equations which can be solved numerically together with the equation for the chemical potential μ, which fixes the average number of particles per unit cell and per spin n to the value $(1-\delta)/2$ (δ is the doping). The solution of the self-consistency equations yields the set of mean-field parameters (b, λ, Δ_i, and ϕ). Varying the doping and the coupling values of the Hamiltonian one obtains different mean-field solutions.

Comparing the energies of the different solutions one can identify which one is the most stable in the various regions of parameters. We obtained the phase diagram shown in Fig. 1.

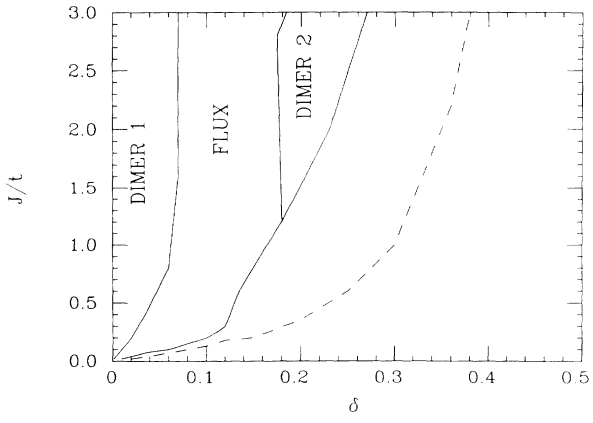

FIG. 1. Phase diagram for various values of J/t as a function of doping δ. The dashed line is the phase separation line. $J/t = 0.02$ is the minimum value here considered.

The phase diagram is qualitatively similar to the one obtained by Affleck and Marston,[4] who analyzed the Hubbard-Heisenberg model in the weak-coupling regime (U was scaled as $1/N$). We distinguish four different phases. The uniform one, stable for large doping, represents a Fermi liquid with AFM correlation. This phase was extensively discussed in Ref. 10. The intermediate flux region is given by the staggered flux phase with the parameter ϕ decreasing with doping starting from the $\pi/4$ value attained at half-filling.

The dimerized phase is, instead, split in two different regions where the dimerization has a different character. In the left region (dimer 1) the Δ_1 bond is always much greater than Δ_2 and Δ_3. In particular, at zero doping, $\Delta_1 = J/2$ and $\Delta_2 = \Delta_3 = 0$. The dimerized region to the right of the phase diagram (dimer 2) is, characterized by a remarkable one-dimensional character with $\Delta_1 = \Delta_3 > \Delta_2$. This solution bears some resemblance to the "kite" phase of Affleck and Marston.

The phases with nonuniform value of Δ_{ij} are the large-N analog of the Néel state. The presence of a dimer order breaks the translational invariance leading to the opening of a gap in the band structure at the boundary of the reduced Brillouin zone in strict analogy with the opening of a gap in a Slater insulator. At finite doping, however, the system is metallic due to the fact that the chemical potential is inside a band with finite dispersion ($\sim tb^2$ with $b^2 = \delta$).

In order to investigate the thermodynamic stability of the above phases we have analyzed the curvature of the free energy. Figure 2(a) shows the behavior of the free energy as a function of particle number (doping) for $J/t = 0.4$. The dashed line is the energy of the dimer 1 phase and is lowest at low doping ($\delta < 0.025$). The dotted

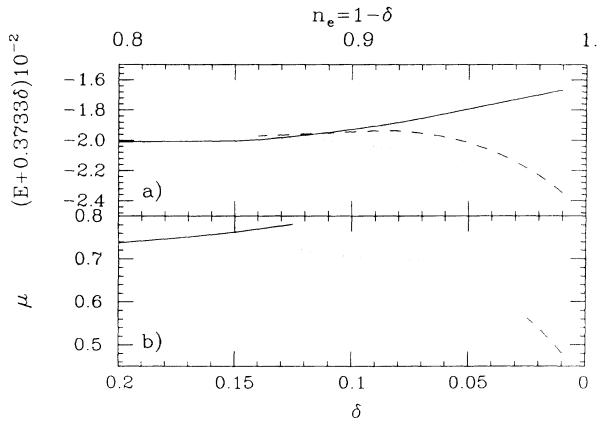

FIG. 2. (a) Free energy (in units $2t = 1$) as a function of particle number $n_e = 1 - \delta$ and doping δ for $J/t = 0.4$. The dashed line is the energy of the dimer 1 phase, the dotted line reports the energy of the system in the flux phase, while the uniform phase free energy is given by the continuous line. A common linear (0.3733δ) term has been added to the three curves in order to make the curvature more visible. (b) Chemical potential (in units $2t = 1$) of the most stable phase at different doping for $J/t = 0.4$. The jumps in the chemical potential signal the presence of the first-order phase transitions (dimer-flux and flux-uniform).

line reports the energy of the system in the flux phase, which is the most stable at slightly higher doping. At larger doping ($\delta > 0.125$) the uniform phase (continuous line) has the lowest energy.

A common linear ($0.3733\ \delta$) term has been added to the three curves in order to make the curvature more visible. It is then apparent that, whereas the uniform phase always has an upward curvature (positive compressibility), the dimer phase has a downward curvature (negative compressibility). Therefore this phase is unstable even in the small doping region ($\delta < 0.025$) although it has the lowest energy. The intermediate flux phase has an upward curvature only for very small doping $\delta < 0.0015$, which turns downward at larger doping. This latter behavior is not clearly distinguishable in Fig. 2(a), but is made clear in Fig. 2(b), where the chemical potential of the most stable phase at different doping is reported: whereas the chemical potential of the uniform (dimer) phase is always increasing (decreasing) with the particle number, the flux phase chemical potential has a negative slope throughout the doping range ($0.025 \leq \delta \leq 0.125$) where the flux phase has the lowest energy for this particular value of J/t.[17]

Figure 2(b) also shows the presence of jumps in the chemical potential at the first-order phase transitions (dimer-flux and flux-uniform). Both these facts, the wrong curvature in the free energy and the chemical potential jumps, lead to phase separation. Within the mean-field solutions here considered, the phase separation region is the one above the dashed line in Fig. 1. It was obtained using a standard Maxwell construction: for each doping the chemical potential of the stable solution was considered and a straight line was drawn in such a way that the areas above and below it were equal. With this procedure two values of doping were determined: at a given doping δ the system separates into regions with these two different concentrations of holes. In particular the system always separates into insulating fully dimerized regions at $\delta = 0$ and in uniform regions at rather large doping δ_u (e.g., $\delta_u \approx 0.2$ for $J/t = 0.4$). Thus phase separation preempts the formation of the intermediate flux and dimer phases. We find that for the minimum considered value $J/t = 0.02$ the dimer phase is still intrinsically unstable (it has negative compressibility) at least at low doping. Extrapolation of our analysis at lower J/t indicates that this feature is present at arbitrarily low J/t. At half-filling the hopping term vanishes leaving J as the only energy scale. Therefore at $\delta = 0$ the dimer phase is always the most stable no matter how large t is. If the dimer phase would be the global minimum even at $\delta = 0^+$, phase separation would take place irrespectively of the value of J/t.[18] Of course the extension and the form of the phase separation region may depend on the phases, which are the most stable at various doping for different J/t. Here we investigated magnetic phases with a simple unit-cell doubling only. Using larger unit cells would allow one to consider more complex (and perhaps richer) mean-field solutions, which could, in principle, have a lower energy than those here considered as well as a lower energy than the phase-separated solution. For instance, a solution with a quadruple unit cell was considered in Ref. 15 (many-hole bound state). This solution turned out to be more stable than the uniform at $\delta = 0.5$ for large values of J ($J > J_c = 3.333t$), thus surely leading to a modification of our phase diagram, which only includes dimer, flux, and uniform phases. However, the many-hole bound state solution was degenerate with the dimer one when $t = 0^+$ and $\delta = 0$, thereby indicating that at half-filling the dimer phase is in any case a good candidate as the mean-field ground state of the large-N t-J model. The analysis of Ref. 15 also showed that a first-order phase transition takes place at $\delta = 0.5$ between the many-hole bound state and the uniform phase at $J_c = 3.333t$. This suggests that this latter solution is a rather good candidate as the mean-field ground state of the system when $J < J_c$ and/or the doping is large.

Of course this consideration does not rule out the possibility that the many-hole bound state or some other state have a lower energy than the uniform phase at $\delta < 0.5$ and $J < J_c$, thus modifying the phase diagram of Fig. 1.

We finally notice that the region where the superconducting instabilities have been detected in Ref. 10 lie outside (but near to) the phase separation line determined in this paper.

In Ref. 8 a distinction was made between two distinct mechanisms leading to phase separation. When $J \gg t$ holes are segregated in order to spare antiferromagnetic bonds breaking. On the other hand, in the small-J regime ($J \ll t$), the holes polarize ferromagnetically the spin background in order to minimize their own kinetic energy and are, then, collected in large ferromagnetic bubbles. In our case, for $J \gg t$ and small doping, the wrong curvature of the free energy of the dimer phase arises from frustration of the magnetic energy of the bonds due to the holes added by doping. This is strictly analogous to the mechanism considered in Ref. 8. For $J \ll t$ the phase separation is mainly driven by the frustration of the kinetic energy in the magnetically correlated phases near half-filling, even though, contrary to Ref. 8, no ferromagnetic bubbles are allowed in our $1/N$ analysis. The spirit is however the same, the role of the ferromagnetic phase being played by the uniform phase, where the kinetic energy is best minimized.

Finally we comment on the effect of the long-range Coulomb force. If the phase separation would result in the formation of highly charged regions, the Coulomb force would surely prevent its occurrence. However, as first noticed in Ref. 8, phase separation could take place if negatively charged ions also phase separate compensating the hole-charge imbalance.[19]

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[18]The unstable region found within our approach at $J/t=0.02$ extends over a very narrow interval of doping $\delta \leq 0.002$, so that it would be impossible to detect it by means of a numerical analysis based on exact diagonalization of small clusters.
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