# Aspects of the Phase Diagram of the Two-Dimensional *t-J* Model

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(Received 9 September 1991)

The phase diagram of the 2D $t$-$J$ model is investigated using high-temperature expansions. Series for the Helmholtz free energy, the inverse compressibility, the chemical potential, and the uniform spin susceptibility through tenth order are calculated and analyzed. A region of phase separation is found at $T=0$ for $J/t$ lying above a line extending from $J/t=3.8$ at zero filling to $J/t=1.2$ at half filling. For very small $J/t$ near half filling where the Nagaoka effect is possible, we find a region of divergent uniform magnetic susceptibility at $T=0$.

PACS numbers: 74.65.+n, 71.10.+x, 74.20.−z, 74.70.Vy

A theoretical model describing the copper oxide planes common to all the high-temperature superconductors is of central importance to understanding the physics of these materials. The simplest description of the planes is the $t$-$J$ model on a square lattice [1,2]. As a result of the projection of doubly occupied states from the Hilbert space the $t$-$J$ model is inherently in the strong coupling limit. A wide variety of techniques have been used to study this problem: slave bosons, variational Monte Carlo, quantum Monte Carlo, and exact diagonalization methods [3], with varying success. In one dimension (1D) the $t$-$J$ model is now well understood. The ground-state properties have been calculated by the Bethe-ansatz technique [4] at $J/t=2$, and at other values of $J/t$ by Ogata *et al.* [5] using numerical diagonalization of sixteen-site chains. In two dimensions (2D) much less is known. In this Letter we investigate the phase diagram for the 2D $t$-$J$ model on a square lattice by means of high-temperature expansions.

High-temperature expansions have been used successfully for many years to investigate spin systems [6], but have not been widely applied to models of correlated electrons. For the Hubbard model with arbitrary $U$ only a fourth-order series has been calculated [7]. In the limit of infinite spatial dimensions Thompson and co-workers [8] derived a tenth-order expansion for the $U=\infty$ Hubbard model. For this case Kubo and Tada [9] generated ninth-order expansions for a number of 2D and 3D lattices. For bipartite lattices these expansions have only even terms, which makes the analysis difficult. The $t$-$J$ model for arbitrary $t$, $j$, and electron density $n$ does not have this problem so we can extract more information from a series of comparable length. In addition, $t$ and $J$ are of the same order of magnitude, unlike $t$ and $U$ for the strong coupling Hubbard model. Projecting out doubly occupied sites avoids having two widely separated energy scales. The series for the Heisenberg model [6] and those generated by Kubo and Tada [9] provide checks on our calculations.

We generate the high-temperature expansion of the thermodynamic potential $\Omega$ for the $t$-$J$ model by the finite cluster method [6], and by standard relations obtain the thermodynamic quantities in which we are interested. The Hamiltonian of the $t$-$J$ model in an applied uniform magnetic field is

$$H=-t\sum_{\langle ij\rangle\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c.})+J\sum_{\langle ij\rangle}\left(\mathbf{S}_i\cdot\mathbf{S}_j-\frac{n_in_j}{4}\right)-g\mu_Bh\sum_i S_i^z-\mu\sum_i n_i\,, \qquad (1)$$

with the constraint of no doubly occupied sites. After calculating $\Omega$ we use the thermodynamic relation $\bar{N}=-\partial\Omega/\partial\mu$ to find a series for $n$ at fixed $\mu$. Inverting this series allows us to substitute $n$ for $\mu$. All of the series considered later have coefficients which are homogeneous functions of $t$ and $J$ multiplied by exact polynomials in $n$: $C_i=\sum_{j=0}^{i}c_{ij}(n)t^{i-j}J^j$. Calculating the expansion through tenth order requires 679 clusters [10]. The clusters are evaluated by a Fortran program, requiring $\sim700$ h of CPU time on an IBM 3090. We then generate series for thermodynamic quantities with the symbolic manipulation program MAPLE [11], running on a Cray YMP.

We are interested in estimating properties of the $t$-$J$ model at $T=0$ and need the analytic continuation of the Taylor series in $1/T$ beyond their radius of convergence. The analytic continuations are obtained using Padé and integral approximants [6,12]. Estimating $T=0$ values is only possible if there is no intervening phase transition at $T>0$. In general the possibility of a phase transition at $T>0$ must be investigated before extending the series results to $T=0$. The minimum temperature we can extrapolate to varies with $J/t$, $n$, and the quantity being considered. The most accurate extrapolations can be made for the Helmholtz free energy $F$, where for $J/t\approx0.3$ and $n\approx0.9$ we can reach $T\sim t/5$. This is due to the monotonic temperature dependence and the entropy, $S=-\partial F/\partial T$, being zero at $T=0$. The complete series and further details of the cluster method and the analysis will be given in a future publication [13]. The entropy and a comparison of our estimates for the ground-state energy to numerical diagonalization will be given in Ref. [14].

We investigate phase separation for the $t$-$J$ model on a square lattice by calculating series for $F$, $\mu$, and the inverse compressibility, $1/n^2\kappa = \partial\mu/\partial n$. In 2D there is the possibility that phase separation occurs at $T>0$. One would expect the 2D $t$-$J$ model for large $J$ and high temperatures to behave like a lattice gas model, which is equivalent to the 2D Ising model [15] with $T_c>0$. In the limit $J/t \to \infty$ where phase separation is most favored we can approximate the $t$-$J$ model as a lattice gas model with an effective interaction between $\approx -J/2$ at low temperatures and $\approx -J/4$ at high temperatures, leading to a critical temperature $T_c \sim J/6$. The inverse compressibility goes to zero at the critical point and along the spinodal line. By considering both integral approximants for the compressibility series and Padé approximants for the logarithmic derivative of the compressibility series for $J/t \to \infty$ we find that the poles of the approximants do not give a well-converged value of the transition temperature. However, values of $T_c \lesssim J/5$ are difficult to detect with our current series. Since the estimated $T_c$ for $J/t \to \infty$ is in this range and increasing $t$ should lower $T_c$, we cannot determine reliable values for $T_c$.

To search for phase separation at $T=0$ we calculate integral approximants [12] for $F$, $\mu$, and $1/\kappa$ starting from small $J/t$ outside the region of phase separation. From the integral approximants we can estimate $T=0$ values for these thermodynamic quantities. Where phase separation takes places $F$ is linear in density, $\mu$ is independent of density for fixed $J/t$, and $1/\kappa$ is zero. As a test of our method we use tenth-order expansions to calculate the phase-separation line for the 1D $t$-$J$ model. In Fig. 1(a) the results are compared to those of Ogata *et al.* [5]. Our curve is a little more vertical, but the overall agreement is quite good. Using the same method for the 2D $t$-$J$ model we find the phase-separation line shown in Fig. 1(b).

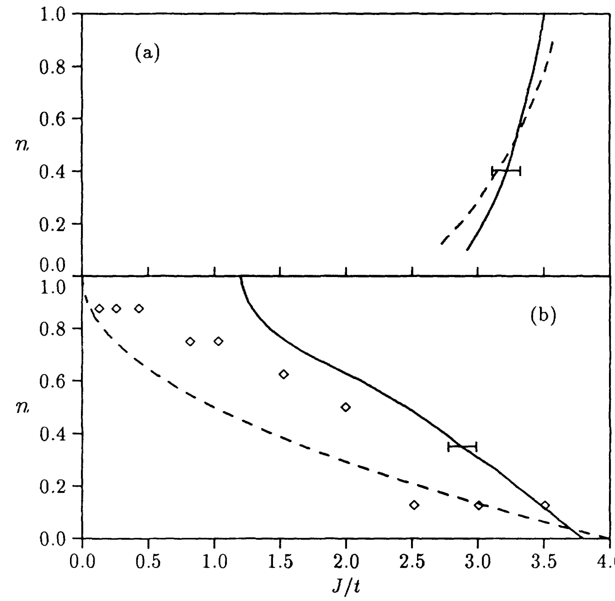


FIG. 1. (a) $T=0$ phase-separation line for the 1D $t$-$J$ model. The solid line is the high-temperature expansion result and the dashed line is the result of Ref. [5]. (b) $T=0$ phase-separation estimates for the 2D $t$-$J$ model. The solid line is the high-temperature expansion result. The points are from Ref. [16] and the dashed line is from Ref. [26]. Note that the dashed line is the boundary between a ferromagnetic region for small $J/t$ and a phase-separated region for large $J/t$.

Comparing phase separation in 1D and 2D we see that they are quite different. For the 1D $t$-$J$ model the phase-separation line is in the relatively narrow range between $J/t=2.7$ as $n\to 0$ and $J/t=3.5$ near half filling [5], while in 2D it extends from $J/t=3.8$ as $n \to 0$ to $J/t=1.2$ near half filling. The slope of the phase-separation line depends on which instability of the fully phase-separated state occurs first. If the phase-separated state is first unstable to inserting holes into the fully occupied region as $J/t$ is decreased, the slope is positive. Otherwise, if the phase-separated state is first unstable to electrons appearing in the empty region, the slope is negative. For the 1D $t$-$J$ model Ogata *et al.* [5] showed that the instability to insertion of holes into the Heisenberg chain occurs at a larger value of $J/t$ than the evaporation of pairs, which is consistent with the 1D phase-separation line having positive slope. In 2D Emery and co-workers [16] showed that at low densities the fully phase-separated state is first unstable to evaporation of pairs at $J/t=3.828$. We thus expect the slope of the phase-separation line to be negative, which agrees with our results shown in Fig. 1(b). For the 2D $t$-$J$ model in the phase-separated region one of the phases will always be the fully occupied phase. This difference between 1D and 2D is due to the larger spin disturbance around a hole in 2D. Prelovšek, Bonča, and Sega [17] have found that adding a longer-range spin exchange (chosen in a way to favor Néel order) in a 1D model causes much larger spin disturbances and changes the slope of the phase-separation line from positive to negative.

For values of $J/t$ less than 1.2 we find no tendency for the $t$-$J$ model to phase separate. In particular for $J/t \approx 0.3$ and $n \approx 0.8$, values of the phase diagram parameters of interest for the copper oxide planes, our method gives a finite value of $\kappa$ for all $T$. These results are consistent with recent quantum Monte Carlo calculations showing no phase separation for the 2D Hubbard model [18].

At $T=0$ for small $J/t$ and near half filling there is the possibility of long-range ferromagnetic order in the 2D $t$-$J$ model. For $J=0$ and one hole, Nagaoka [19] proved that the exact ground state is a fully polarized ferromagnet. It is not known if this state remains the ground state for finite hole density. For $J=0$ the instability of the Nagaoka state to a single spin flip has been investigated by variational wave functions [20]. In particular von der Linden and Edwards [20] obtained a lower bound on the density for the Nagaoka state of $n \approx 0.71$. Yedidia [21] has pointed out that near $n=\frac{8}{11}$ the high-temperature expansion for the spin susceptibility of the $U=\infty$ Hubbard model is approximately the same as free spins. Recently, Zhang, Abrahams, and Kotliar [22] have calculated by the quantum Monte Carlo method the average magnetization per electron for $J=0$. They find that the magnetization decays exponentially away from half filling.

We have calculated the high-temperature expansion for the uniform spin susceptibility $\chi_0$ through tenth order. Assuming a power-law singularity of the form $\chi_0=A(\beta t)^{\gamma}$ we can form the biased logarithmic derivative

$$(\beta t)\frac{d}{d(\beta t)}\ln\chi_0=\gamma. \qquad (2)$$

To estimate $\gamma$ we calculate diagonal Padé approximants for the resulting series. The part of the phase diagram where $\gamma\gtrsim 1$ is enclosed by the solid line in Fig. 2. Outside of this region we still find $\gamma>0$, but for smaller $\gamma$ the Padé approximants are not well converged and the $\gamma=0$ boundary is difficult to determine. Near half filling we can estimate the $\gamma=0$ line by the [5/5] Padé approximant, indicated by the dashed line in Fig. 2. At lower densities we do not have sufficient accuracy to estimate the $\gamma=0$ line. The largest value of $\gamma$ we observe is $\gamma\approx 1.2$, with $\gamma$ falling rapidly as $J/t$ is increased. For the 2D ferromagnetic Heisenberg model the calculations of Takahashi [23] give an exponential divergence for the susceptibility at $T=0$. The strength of the divergence we see is much weaker. In light of the results of Zhang, Abrahams, and Kotliar [22] this might be due to the average magnetization per electron being much less than 1. Another possibility is that we are not at low enough temperatures to see a decrease in the value of $\gamma$. However, our results are in agreement with a recent numerical diagonalization study of the Drude weight for the $t$-$J$ model [24] and variational Monte Carlo results [25]. Further calculations are underway to directly estimate the moment in this region.

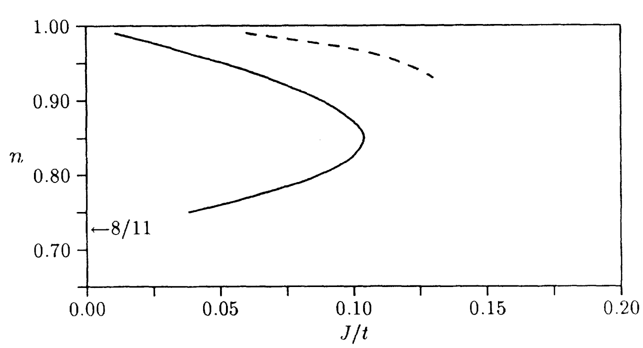


FIG. 2. The part of the phase diagram near half filling and at small $J/t$ showing the region of divergent uniform magnetic spin susceptibility at $T=0$ estimated by the logarithmic derivative of the high-temperature series. The solid line is $\gamma=1$ and the dashed line is an estimate of $\gamma=0$.

We now compare our results to previous calculations for the phase diagram of the 2D $t$-$J$ model. The line for phase separation has previously been estimated by Emery and co-workers [16] and by Marder, Papanicolaou, and Psaltakis [26]. Both groups find phase separation for all values of $J/t$. The latter calculation is a $1/S$ expansion modifying some of the commutation relations for the Hubbard operators. The effects of this modification are difficult to judge, but omitting the fermion sign of the electrons from the calculation of the high-temperature expansion we arrive at a phase diagram similar to Ref. [26]. Such an approximation greatly overestimates the size of the ferromagnetic region and gives phase separation at smaller $J/t$ than we find. Their Eq. (3.12) is plotted in Fig. 1(b).

The calculation of Emery and co-workers [16] is based on two parts: estimates of phase separation derived from exact diagonalization of a $4\times4$ cluster and the arguments of Visscher [27] and Ioffe and Larkin [28] at small $J/t$. The data points of Ref. [16] are shown in Fig. 1(b). For $J/t\gtrsim 1$ our results are in agreement with Ref. [16]. At small hole doping the odd-even effects on a $4\times4$ lattice are of the same size as the size of the minimum of the energy per electron so caution is needed in interpreting the results. For $J/t\ll 1$ and for a small density of holes Ioffe and Larkin [28] showed that it is not possible to have a uniform paramagnetic phase in equilibrium with a fully spin-polarized ferromagnetic phase. Their argument is based upon the thermodynamic requirement that $\mu$ and the pressure $P$ be the same in equilibrium. Since the bandwidth for the paramagnetic phase is smaller than for the ferromagnet most holes enter the ferromagnet to balance $\mu$. This gives a value $P\sim t$ in the ferromagnet and $P\sim J$ in the paramagnetic phase. Thus for $J\ll t$ equilibrium cannot be reached and the system phase separates with all the holes in the ferromagnetic phase. However, Ioffe and Larkin [28] also point out that this argument does not hold if there is an intervening ferrimagnetic phase. The system can then remain in equilibrium without phase separating. With the results of Zhang, Abrahams, and Kotliar [22] this may explain our inability to detect phase separation at $J/t\lesssim 1$ and $1-n\ll 1$.

In conclusion we have investigated the phase diagram of the 2D $t$-$J$ model by high-temperature expansions. A line of phase separation extends from $J/t=3.8$ as $n\to 0$ to $J/t=1.2$ near half filling. For the range of parameters of interest for the copper oxide planes we find no evidence for phase separation. At $J/t\ll 1$ and $1-n\ll 1$ we find a region of divergent uniform magnetic spin susceptibility. The detailed properties of this part of the phase diagram are not clear at present. The $t$-$J$ model parameters relevant for the high-temperature superconductors are in a part of the phase diagram where the uniform spin susceptibility is decreasing and the compressibility is increasing, indicating a crossover from predominantly repulsive interactions to attractive interactions as $J/t$ increases.

This work has been supported in part by a grant from the Swiss National Fund. The computations were done in part on the IBM 3090 of the Center for Computational Competence in Chemistry, ETHZ and the Cray YMP of the ETHZ. We are very grateful to G. A. Baker, Jr., for providing us with the data from Ref. [10] as computer files and the computer programs to extend the tabulated clusters. We thank W. P. Petersen for installing MAPLE on the Cray YMP. The authors thank N. Bonesteel, M. Ogata, and S. Sorella for many helpful discussions.

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