Thermodynamics of the two-dimensional *t-J* model

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We present results for the thermodynamics of the two-dimensional *t-J* model on finite square lattices in the grand canonical ensemble. The specific heat has a double-peak structure independent of J. The susceptibility shows antiferromagnetic behavior above a critical value J_c where for $J<J_c$ the ground state of the one-hole sector has maximal spin. We give evidence that phase separation observed in the ground state of the *t-J* model at large J may be suppressed at any finite, nonzero T.

Stimulated by the discussion of whether electron-electron interactions give rise to high-temperature superconductivity, the two-dimensional (2D) *t-J* model as the simplest model containing electron-hopping and spin-exchange interactions has received renewed interest.[1,2] The *t-J* model can be obtained either from the one-band Hubbard model for a large, positive Hubbard U or from the two-band Emery model.[3] Although both derivations lead us to believe that J is usually smaller than t in the copper oxides, the *t-J* model is theoretically interesting as a model of strongly interacting electrons even for large values of J.[4] Apart from a few analytical results concerning the Nagaoka limit,[5] most work on the *t-J* model has been done using numerical techniques such as exact-diagonalization and variational calculations, both of which address ground-state properties, and Monte Carlo simulations which unfortunately cannot be extented to very low temperatures due to the sign problem. Finite-lattice calculations can, in principle, close this gap, but the computational effort increases greatly since, at finite temperatures, all or at least a considerable number of low-lying eigenvalues must be obtained. In order to reduce finite-size effects,[6] we performed a study of the *t-J* model on a ten-site lattice in the grand canonical ensemble. Working in the grand canonical (GC) ensemble also allows for a continuous variation of the average electron number $\bar{N}_e$ even for small lattices by solving the equation $\bar{N}_e=\beta^{-1}\partial_\mu \ln Z_{\rm GC}$ for the chemical potential μ. $Z_{\rm GC}$ is the grand canonical partition function defined as

$$Z_{\rm GC}=\sum_{N_e=0}^{2N} e^{\beta\mu N_e} Z_C(N_e) \tag{1}$$

with the canonical partition function $Z_C=\sum_{\mathbf{k},S_z}\sum_{m(\mathbf{k},S_z)} g_m e^{-\beta\Lambda_m}$ and g_m being the degeneracy of the eigenvalue Λ_m.

The Hamiltonian of the *t-J* model is

$$H=-t\sum_{\langle ij\rangle,\sigma}(\tilde{c}^\dagger_{i\sigma}\tilde{c}_{j\sigma}+\text{H.c.})+J\sum_{\langle ij\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j-\tfrac{1}{4}n_i n_j)\ , \tag{2}$$

where $\tilde{c}^\dagger_{i\sigma}=(1-n_{i-\sigma})c^\dagger_{i\sigma}$ are creation operators in the Hilbert space without doubly occupied sites. The sum goes over all nearest-neighbor pairs of a ten-site square lattice with periodic boundary conditions. In contrast to conventional exact diagonalization studies, where only the ground state is calculated, grand canonical thermodynamics requires the calculation of all eigenvalues for all numbers of holes. We first used as good quantum numbers S_z and $\mathbf{k}$ to block diagonalize the Hamiltonian. The resulting blocks were then diagonalized using an EISPACK routine.

The finite-size dependence has been checked by comparing against the results of the eight-site lattice. For small hole densities, thermodynamic quantities are relatively size independent.[6,7] When the hole concentration approaches quarter-filling, the results become more size dependent due to the small number of eigenvalues for the few-electron systems. Therefore, we restrict our calculation to electron densities larger than quarter-filling. At very low temperatures there are always finite-size gaps which lead to an activated shape of the specific heat.[7]

The chemical potential μ as a function of electron density n is plotted in Fig. 1 for three different temperatures. For $J=0.4$ at higher temperatures, the variation of μ with n is smooth. At very low temperatures, μ jumps at densities corresponding to integer electron numbers closely resembling the zero-temperature variation. At $J=4.0$, we have a smooth curve for all temperatures approaching a constant chemical potential as a function of electron density for $T=0$ which indicates phase separation (see below). First of all this shows that the grand canonical calculation allows for a continuous variation of particle concentration for temperatures larger than the ones set by the scale of finite-size gaps [cf., Fig. 1(a)]. Note, however, that the finite-size dependence, which is seen as $T\to 0$ for $J=0.4$, is reduced compared to a free-electron case as reported in Ref. 8. The second point to be emphasized is that the abrupt change of n with μ for $J=4.0$ as $T\to 0$ is not caused by finite-size effects because it extends over the whole concentration regime. The smaller plateau seen for $J=0.4$ up to $n=0.2$ is a different case caused by the low energy of the two-hole ground state and will disappear as the system increases.

We have qualitative agreement with the $n(\mu)$ curves obtained by Ref. 9 for the Hubbard model using the Quantum Monte Carlo on larger lattices. Their zero-temperature plateau corresponds to the sharp drop of μ from the Heisenberg value ($\mu_{\rm HSB}=\infty$).

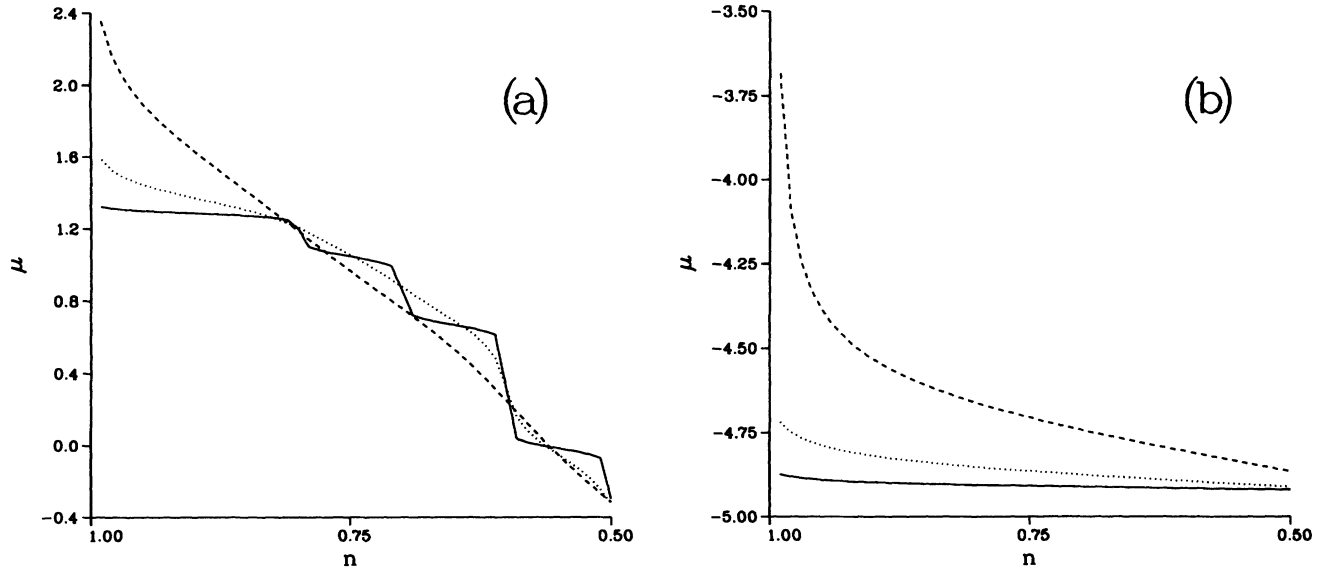

FIG. 1. The chemical potential μ as a function of electron density for (a) $J=0.4$ and (b) $J=4.0$ and $T=0.025$ (solid line), $T=0.1$ (dotted line) and $T=0.25$ (dashed line). All energies are measured in units of the hopping matrix element t. All figures were calculated from data for the ten-site lattice.

Having obtained the chemical potential for a given concentration of holes and for a given temperature, we show the specific heat per site

$$c_v/k_B=\beta^2\left[(\overline{H^2}-\overline{H}^2)-\frac{(\overline{HN_e}-\overline{H}\,\overline{N_e})^2}{(\overline{N_e}-\overline{N_e})^2}\right] \tag{3}$$

for $J=0.4$ (strong correlation limit of the Hubbard model $t/J\gg 1$) and $J=4.0$ (strong antiferromagnetic spin interaction[4]) in Figs. 2(a) and 2(b). Here overbars denote averages in the grand canonical ensemble. The second part in (4) arises from fluctuations in the particle number which are inherent in the grand canonical approach. The qualitative peak structure remains the same apart from a rescaling of the temperature axis by $J=4t^2/U$. It consists of two peaks: one around J and one around $J/4$. The peak around J survives in the Heisenberg limit and is caused by spin-wave-like excitations as shown by Ref. 7 with a renormalized coupling constant. The height of the peak around $J/4=t^2/U$ is proportional to the concentration of holes. It is not due to the term $(J/4)n_in_j$ since we see the same two-peak structure if we set this term to

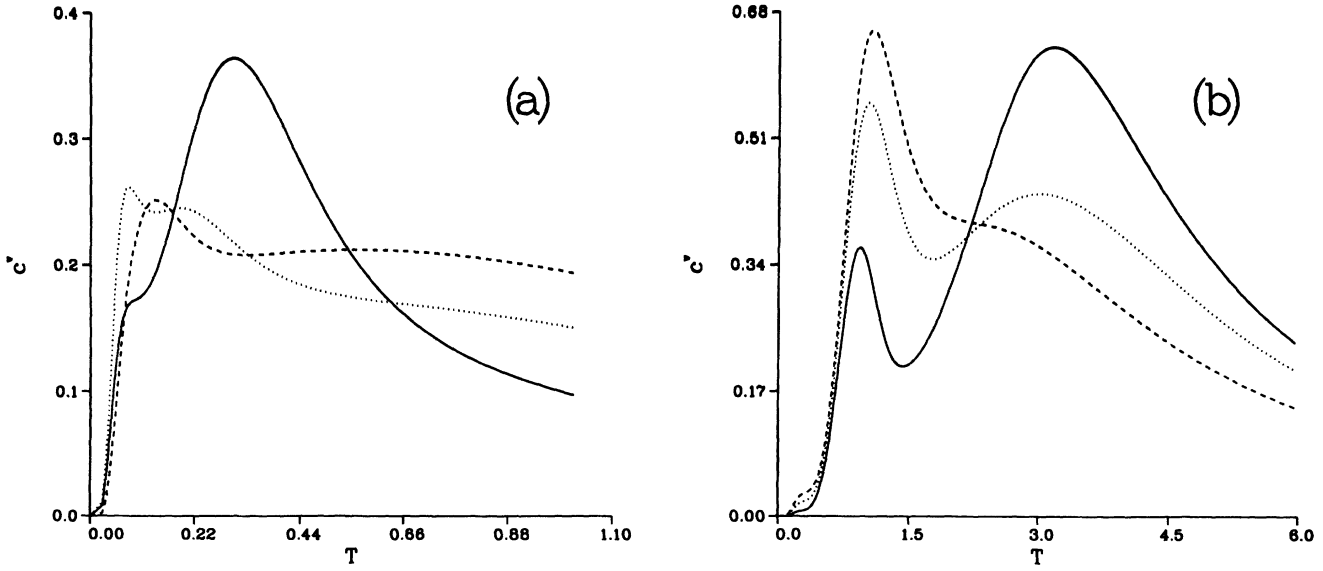

FIG. 2. The specific heat per site as a function of temperature for (a) $J=0.4$ and (b) $J=4.0$ and electron densities $n=0.95$ (solid line), $n=0.85$ (dotted line), and $n=0.75$ (dashed line).

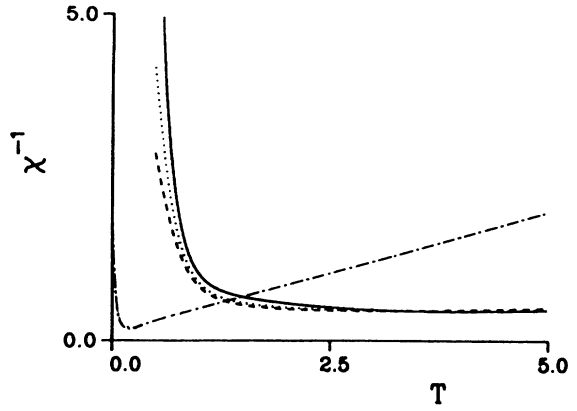

FIG. 3. The inverse susceptibility per site as a function of temperature for $J=4.0$ and electron densities $n=0.95$ (solid line), $n=0.85$ (dotted line), and $n=0.75$ (dashed line), and for $J=0.2$ at $n=0.95$ (dash-dotted line).

zero. It may be caused by the correlated motion of holes because its position is proportional to $1/U$, or due to local spin rearrangements[10] (of course, in the t-J model we do not see the excitations across the Mott-Hubbard gap).

In the magnetic susceptibility per site we find, for $J>J_c$, a tendency towards antiferromagnetic behavior, i.e., the paramagnetic Curie temperature Θ_D obtained by a fit to the high-temperature points is negative and decreases with increasing J (see Fig. 3). Here $J_c=0.138(1)$ denotes the Nagaoka value for the ten-site cluster. For $J<J_c$, the ground state of the one-hole sector has maximal total spin S. Due to the use of the grand canonical ensemble, our data are smooth as a function of hole density and do not jump as erratically as seen in the canonical calculation of Ref. 11. For very small values of J, smaller than the Nagaoka value, the susceptibility shows a tendency towards ferromagnetic behavior around $0.85<n<0.95$, i.e., Θ_D becomes positive. Finite-size effects, however, become large, maybe indicating the existence of a phase of quasi-non-interacting particles like spinless fermions. Therefore, we cannot decide on the existence of ferromagnetic phases apart from the one-hole Nagaoka limit.

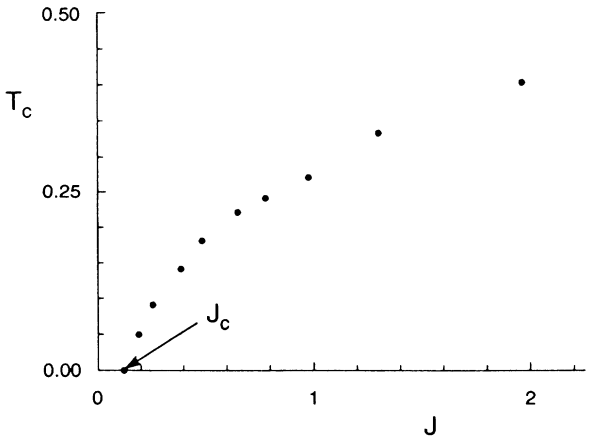

FIG. 4. The curve $T_c(J)$ as defined in the text. J_c is the Nagaoka value for the ten-site system.

At finite, nonzero temperature, the question of phase separation into a hole-rich and an antiferromagnetic phase arises again. It is not clear whether the phase separation observed in the t-J model at $T=0$ (Refs. 12 and 13) extends to nonzero temperature. In a finite-size study, the results for various thermodynamic quantities (i.e., the free energy) may differ using the canonical or the grand canonical description. The grand canonical description, however, represents the thermodynamic limit much better.[6]

Using the canonical ensemble, the natural extension of the function $e(x)$ (x being the concentration of holes) defined by Ref. 13 is $e(x,T)=[f_C(x,T)-f_C(0,T)]/x$,

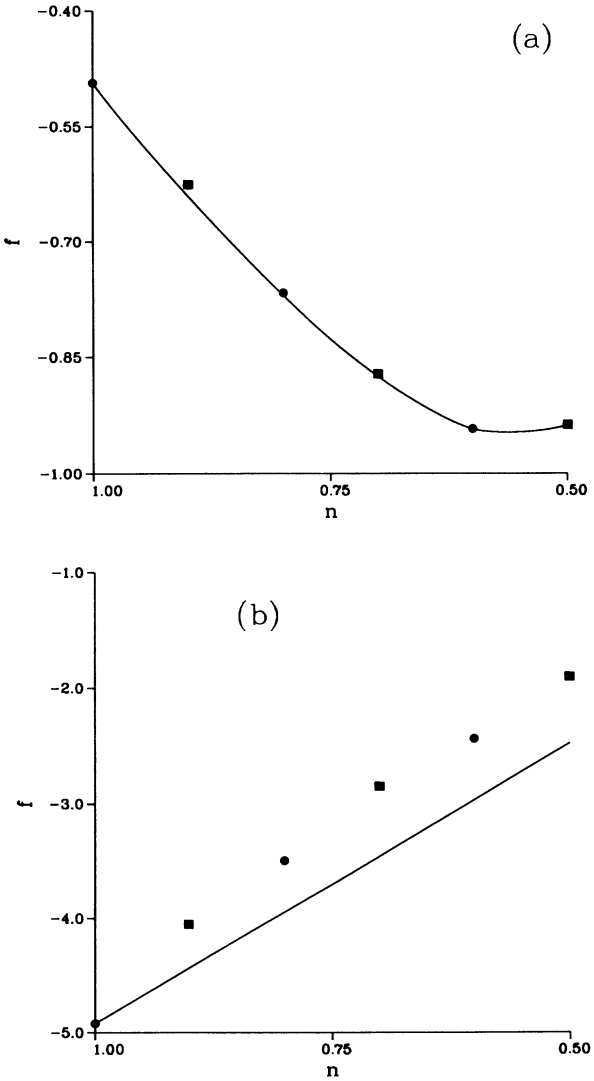

FIG. 5. The free energy per site as a function of electron density for (a) $J=0.4$, (b) $J=4.0$, and $T=0.1$. The circles (squares) are the values of f_C for even (odd) numbers of electrons; the solid line is f_{GC}.

where f_C is the canonical free energy per site. Assuming a homogeneous finite system, a minimum in $e(x)$ corresponds to a concave f_C (or negative compressibility) below a critical concentration. We use this as an indication of phase separation to relate our results to the work of Emery *et al.*[13] At low T, we indeed find a minimum of $e(x,T)$ as a function of x which disappears at a J-dependent temperature T_c. In Fig. 4 we show the variation of T_c with J. At $T=0$, phase separation vanishes at the Nagaoka value of J. Below $T_c(J)$, a phase-separated state gives a lower value than the f_C's of the homogeneous phases. In order to allow for fluctuations in the particle number, we calculated $e(x,T)$ with a grand canonical free energy $f_{GC}=\Omega/N+\mu n$, i.e., via a Legendre transform of the grand canonical potential $\Omega=-\beta^{-1}\ln Z_{GC}$. We could not find a minimum at any finite temperature even for $J=4$. To further investigate this, we note that f_{GC} in the phase-separated state is the free energy obtained from the canonical ones using the Maxwell construction. Therefore, it should be a straight line as a function of concentration. In Figs. 5(a) and 5(b) we show both f_C and f_{GC} for $J=0.4,4$ and at low temperatures. For $J=0.4$ we see the instability of f_C due to the two-hole state. f_{GC} is just convex, which shows that there is no phase separation. For $J=4$, f_C is concave and therefore unstable, whereas f_{GC} is nearly a straight line over the *whole* concentration axis. Here we discuss the free energy to show the dependence on the mean electron density. The related grand canonical potential as a function of μ exhibits a discontinuity in slope, which is related to the abrupt change of $n(\mu)$ [cf., Fig. 1(b)]. The system therefore exhibits phase separation into a Heisenberg antiferromagnet and a hole-rich phase without electrons. The slight convexity of f_{GC} gives additional indication that phase separation may be unstable at any *finite* temperature. As $T\to 0$, we have, for f_{GC},

$$f_{GC}(\overline{N_e}) = \inf_{l^-,l^+}\left[E_0(l^-)+\frac{E_0(l^+)-E_0(l^-)}{l^+-l^-}(\overline{N_e}-l^-)\right], \quad (4)$$

where $E_0(l)$ is the ground-state energy per site for a system with l electrons. At *zero* temperature we need only the ground state and hence the calculations can be extented to larger systems up to $N=20$. The main result is that one observes phase separation if J is sufficiently large. One can use Eq. (5) to determine the critical value J_{PS} above which phase separation becomes complete. We get $J_{PS}=1.5$, 2.2, 2.0, and 2.2 for system sizes $N=10$, 16, 18, and 20, respectively.

Summarizing, we have used the grand canonical ensemble to calculate thermodynamic properties of the 2D t-J model on a ten-site lattice. This allowed us to vary the density continuously. The specific heat was shown to exhibit a double-peak structure rescaled by J. One peak could clearly be identified as being due to usual antiferromagnetic spin-wave-like excitations, the other may be caused by the correlated motion of holes. Antiferromagnetic behavior of the susceptibility was found for all concentrations apart from J larger than the Nagaoka value. Phase separation was shown to be indicated by a straight-line behavior of f_{GC}. Finally, we have given the crossover values of J from a homogeneous to a totally phase-separated state for lattices up to 20 sites.

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