Thermodynamic Properties of the Planar t-J Model

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Several thermodynamic quantities within the planar t-J model are calculated using the $T > 0$ Lanczos method on clusters of up to 26 sites. The hole density $c_h(\mu, T)$ shows a non-Fermi-liquid behavior as a function of T and suggests a transition from small to large Fermi surfaces at $c_h \sim 0.15$. The specific heat reveals a maximum at the exchange energy scale up to $c_h = 0.2$, where it becomes almost T independent for $T \gtrsim 0.15t$. At constant T the entropy has maximum for $c_h \sim 0.15$ with large values at low T, consistent with experiments on cuprates. In the underdoped regime the spin susceptibility $\chi_0(T)$ exhibits a maximum at finite $T = T^*$, with T^* decreasing with doping and disappearing for $c_h > 0.15$. [S0031-9007(96)00800-9]

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The normal state of the superconducting cuprates, in particular, the character of the low-energy excitations, still lacks proper understanding. Although there appears to be a consolidation of experimental results probing their transport [1], magnetic [2], thermodynamic [3], and single-electron [4] properties, on the theoretical side several important questions about the nature of the corresponding quantum liquid remain open. While undoped cuprates are well understood in terms of a two-dimensional (2D) $S = 1/2$ antiferromagnet (AFM), it is less clear what changes are induced on doping the AFM with mobile holes. Besides the questionable existence of quasiparticles (QP) in the sense of some type of Fermi liquid, the character of the QP and the associated Fermi surface (FS) in doped AFM are also controversial. While at low doping, theoretical studies [5,6] as well as experimental findings [7] seem to favor the interpretation in terms of hole QP in a rigid band and related hole-pocket FS, the situation at larger doping is more consistent with the usual large electronic FS [4,8,9]. Nevertheless, several normal-state dynamical properties of cuprates have recently been reproduced by using unbiased numerical techniques with strong correlations taken fully into account [10,11]. It is the aim of this paper to present results on relevant thermodynamic properties of correlated electrons, which could help in finding a proper concept for such systems, but also in establishing the relevant model for cuprates.

In the following we address some of the questions above by studying finite-T static properties of the 2D t-J model as a prototype model for strongly correlated electrons and cuprates, in particular [12],

$$H = -t \sum_{\langle ij \rangle s} (c^{\dagger}_{js} c_{is} + \text{H.c.}) + J \sum_{\langle ij \rangle} (\vec{S}_i \cdot \vec{S}_j - \tfrac{1}{4} n_i n_j) . \quad (1)$$

Here $c^{\dagger}_{is}$, c_{is} are projected fermionic operators, excluding the states with doubly occupied sites. To investigate the regime of cuprates we set $J/t = 0.3$.

Although there have been so far extensive numerical studies of the ground-state properties of the t-J model [13], its finite-T properties are less explored. At $T > 0$ a fruitful technique in addressing several thermodynamic properties proved to be the high-T series expansion [9,14,15]. In the present study we aim at the calculation of the finite-T static properties of the model Eq. (1) with a recently introduced method, combining the Lanczos diagonalization technique and random sampling [10], which has been so far applied to the study of several dynamical responses [11]. We concentrate on calculating the quantities, which are related to the expectation values of the conserved operators, commuting with the Hamiltonian, Eq. (1). Such operators are, e.g., total number of electrons N_e, total energy H, and S_z, the z component of the total spin operator. In terms of them some interesting thermodynamic quantities can be expressed, in particular, chemical potential μ, entropy S, specific heat C_V, and the uniform susceptibility χ_0. The reason to limit our treatment only to commuting operators is technical, since in this case we can avoid time and memory consuming computations of wave functions and their scalar products. This in turn enables us to study larger clusters with up to 20 sites at all doping concentrations.

We follow the method for the evaluation of $T > 0$ static quantities [10]. To calculate the quantity of the type $\mathrm{Tr}[f(N_e, S_z, H) e^{-\beta(H - \mu N_e)}]$, the trace is expanded in terms of an arbitrary orthonormal set of basis functions $|n\rangle$, $n = 1, \ldots, K$, with good quantum numbers N_e and S_z. Each state $|n\rangle$ is used as initial function $|\phi^n_0\rangle$ for the M-step Lanczos procedure [13], yielding a subspace spanned by functions $|\phi^n_j\rangle$, $j = 0, \ldots, M$. The Hamiltonian is diagonalized in this subspace to obtain the eigenvalues E^n_j and corresponding eigenvectors $|\psi^n_j\rangle$, which are used to evaluate $\langle f \rangle$

$$\langle f \rangle \approx \frac{N_{\mathrm{st}}}{K\Omega} \sum_{n=1}^{K} \sum_{j=0}^{M-1} |\langle n | \psi^n_j \rangle|^2 \times f(N^n_e, S^n_z, E^n_j) e^{-\beta(E^n_j - \mu N^n_e)}, \quad (2)$$

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where $\Omega = \mathrm{Tr}[e^{-\beta(H-\mu N_e)}]$ is the grand-canonical partition function. Clearly, the expression (2) is exact for $K = M = N_{\mathrm{st}}$, where N_{st} is the dimension of the complete basis. In practice $K, M \ll N_{\mathrm{st}}$ are used, with states $|n\rangle$ sampled randomly. More detailed discussions of the method and tests are given elsewhere [10,11]. In the present application it is essential that scalar products $\langle n|\psi_j^n\rangle$ are trivially evaluated, since this is the component of the function $|\phi_0^n\rangle$ in the wave function $|\psi_j^n\rangle$, i.e., can be obtained from the eigenvectors of the $M \times M$ tridiagonal matrix without storing $|\phi_j^n\rangle$. Typically, also small $M \lesssim 100$ is used, thus reorthogonalization of the Lanczos functions can be avoided. The computational effort in the present case is then equal to a ground-state Lanczos procedure, repeated K times. We employ in the following typically $K \sim 200-1000$ in every N_e sector.

We have calculated a few static quantities above using the approximation (2) on clusters with $N = 16$, 18, and 20 sites, thus having control over the finite-size effects through comparison of the results. We also treated the undoped system with $N = 26$ sites. In general, the results are quite free of finite-size effects for temperatures $T > T_{\mathrm{fs}}(N, c_h)$, which amounts to $T_{\mathrm{fs}} \sim 0.1t$ for $N = 20$ and $c_h \leq 0.3$.

We first analyze the hole density $c_h = 1 - \langle N_e\rangle/N$ as a function of T and μ. In Fig. 1(a) we present curves $c_h(T)$ for several μ_h, where the chemical potential for holes is $\mu_h = -\mu$. Clearly, for $\mu_h < \mu_h^0$ the ground state of the system contains no holes. Here $\mu_h^0 = -1.99t$ [13] is related to the minimum energy of a single hole added into the undoped system. The corresponding curves for $\mu_h < \mu_h^0$ are denoted with dashed lines. In Fig. 1(a) we, in general, do not find a T^2 dependence of c_h at low T, as expected for a normal Fermi liquid, except within the extreme overdoped regime $c_h > 0.3$. In particular, in a broad range $0.15 < c_h < 0.3$ very unusual linear variation of $c_h(T)$ is observed at lowest T. Moreover, a remarkable feature is a nonmonotonous $c_h(T)$ dependence as the value $c_h(0)$ is varied. There exists a doping concentration c_h^* such that derivative dc_h/dT at low T is positive for curves with $c_h(T \sim 0) < c_h^*$ and negative for curves with $c_h(T \sim 0) > c_h^*$. The marginal doping $c_h^* \sim 0.15$ seems to be system independent, as checked quantitatively for systems with $N = 16$, 18, and 20.

In Fig. 1(b) we plot the variation of c_h with μ_h at several chosen temperatures T. We include also $T = 0.05t < T_{\mathrm{fs}}$, since in this case it shows less pronounced finite-size effects. As $T \to 0$ clearly $c_h(\mu_h < \mu_h^0) \to 0$, while $c_h(\mu_h > \mu_h^0)$ remains finite. The slope $dc_h/d\mu_h$, being proportional to the compressibility κ of the hole fluid, is finite for $T > 0$, indicating the absence of the phase separation in the system at chosen J/t [15]. On the other hand, Fig. 1(b) reveals that for $T \to 0$ κ is increasing and becoming large on approaching $\mu_h \sim \mu_h^0$, consistent with large (polaron) mass enhancement of individual holes at vanishing doping. Moreover, we cannot exclude a singular behavior (divergence) of κ, as deduced from analogous results for the Hubbard model [16].

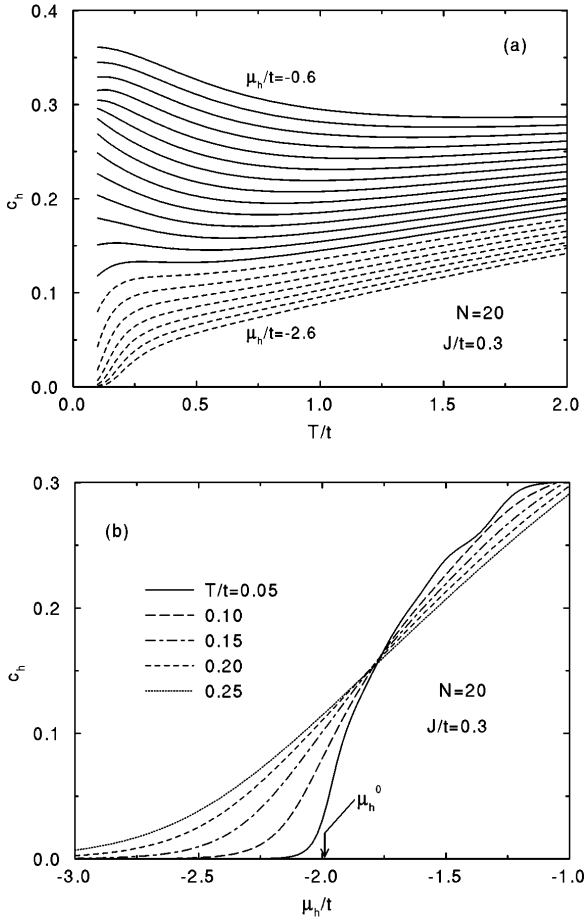

FIG. 1. (a) Hole density c_h as a function of T at several values of hole chemical potential μ_h in steps of $0.1t$. Dashed lines denote $\mu_h < \mu_h^0$. (b) c_h as a function of μ_h at various T.

Next we find remarkable a feature appearing at the hole density of $c_h \sim c_h^*$, where μ_h is essentially pinned at the value $\mu_h \sim -1.8t$, i.e., does not vary with T. This pinning is active in a wide range of T and is again almost not dependent on the system size. It is tempting to interpret the marginal concentration c_h^* as a change of the character of the FS. To establish the relation, we still have to rely on arguments which apply to the gas of noninteracting fermions. Denoting by $g(\varepsilon)$ the density of the single-fermion states, a simple Sommerfeld expansion yields that the number of particles at fixed chemical potential μ is given by $c_e(T) = c_e(T = 0) + (\pi^2/6)(k_B T)^2 g'(\mu)$. Therefore the prefactor of the T^2 term is just proportional to the derivative of the density of states. Indirectly, this gives information about the character of the FS, since one would plausibly associate $g'(\mu) > 0$ for $c_e \lesssim 1$ with a

large electron FS, and oppositely $g'(\mu) < 0$ with holelike FS or small hole pockets vanishing for $c_e \to 1$. For 2D it is straightforward to represent $g'(\mu)$ more explicitly as a line integral

$$g'(\mu) = \frac{1}{2\pi^2} \int_{L_\mu} \frac{dl_{\vec{k}}}{|\nabla\varepsilon(\vec{k})|^2} \left[\frac{1}{K} - \frac{\hat{K} \cdot \mathbf{m}^{-1} \hat{K}}{|\nabla\varepsilon(\vec{k})|} \right] \quad (3)$$

over the curve $L_\mu = \{\vec{k};\ \varepsilon(\vec{k}) = \mu\}$. Here $1/K$ is the curvature of L_μ (positive for electronlike orbits and vice versa), $\hat{K}$ the unit vector perpendicular to L_μ, and $\mathbf{m}^{-1} = \partial^2\varepsilon(\vec{k})/\partial\vec{k}\partial\vec{k}$ the inverse effective mass tensor. Apart from the effective mass term, this is similar to the expression for the Hall resistivity in terms of the curvature of the FS [17]. From Eq. (3) it follows that at least in the region of the $\vec{k}$ space, where the effective-mass tensor is positive definite, $g'(\mu) > 0$ implies also that the average curvature K^{-1} of the FS L_ε is positive. Although the observed nonquadratic T dependence in Fig. 1(a) questions above arguments, we may still interpret $dc_h/dT < 0$ (i.e., $dc_e/dT > 0$) in Fig. 1(a) as an indication for $g'(\mu) > 0$, i.e., positive average curvature of the FS for $c_h \gtrsim c_h^*$. This in turn implies a transition from the hole-pocket picture [5–7], existing at low doping, to an electronlike FS [8,9] at $c_h \sim c_h^*$.

Next we consider the entropy

$$S = k_B \ln \Omega + (\langle H \rangle - \mu \langle N_e \rangle)/T\,. \quad (4)$$

As a test we have checked and found agreement of our entropy data with available results from the high-T series [18]. In Fig. 2 we show the doping dependence of the entropy density (per site) at different $T \leq J$ and $N = 16-20$. As expected, finite-size effects are most pronounced at lowest $T = 0.1t \sim T_{\rm fs}$. Nevertheless, at all $T < J$ the entropy has a broad maximum at $c_h \sim 0.15$, indicating the highest density of many-body states in this "optimum" doping regime.

The magnitude of the entropy in the optimum regime appears very large, i.e., at $T = 0.1t = J/3$ the entropy per site is $s \sim 0.39 k_B$, which is almost 40% of $s(T = \infty)$ for the same doping c_h, although $T \ll J, t$. In other words, introducing the degeneracy temperature by $s(T_{\rm deg}) = s(T = \infty)/2$, for intermediate dopings of $c_h \sim 0.15$ we get $T_{\rm deg} \sim 0.17t$, being very small in comparison with any reasonable QP bandwidth W, e.g., $W = 8t$ of the noninteracting electrons. It is remarkable that the entropy of such magnitude has been deduced from the electronic specific heat measurements in $YBa_2Cu_3O_{6+x}$ materials [3]. For example, for the optimally doped material with $x = 0.97$ at $T = 300$ K it was found $\Delta s = 0.35 k_B$ per planar copper site ($\Delta s = 0.7 k_B$ per unit cell) relative to the undoped $x = 0$ sample. We find the corresponding value $s(c_h = 0.15) - s(c_h = 0) \sim 0.30 k_B$ at $T = 0.1t \sim 450$ K (assuming $t = 0.4$ eV [12]).

In Fig. 3 we present the T dependence of the specific heat $C_V = T(\partial S/\partial T)_\mu/N$ at different dopings. For the undoped AFM we have not observed any appreciable size dependence on systems with 16–26 sites, and our results seem to be even superior to those obtained by other methods [19]. C_V is strongly T dependent in the observed interval $T = 0-3.3J$, with a maximum at $T \sim 2J/3$, and approximately $C_V \propto T^2$ at low T. As the system is doped, $C_V(T)$ still exhibits a maximum, which is, however, strongly suppressed and gradually moves to lower T with increasing c_h. The peak can be attributed to the thermal activation of the spin degrees of freedom with an exchange energy scale persisting in the doped system, as observed already in dynamical spin correlations [11]. The presence of the exchange energy scale, however, disappears in the "overdoped" regime $c_h \geq 0.3$.

It is characteristic (and consistent with the vanishing role of J) that in the optimally doped regime $c_h \sim 0.2$ we find $C_V(T) \sim$ const for $0.15t < T < t$, being far from the Fermi liquid behavior. The anomalous behavior in this regime implies $\Omega \propto T$, as follows from Eq. (4), as well as a constant (flat) density of many-body states $D(E) \sim$ const, as defined through $\Omega = \int D(E) e^{-\beta E} dE$, at least in a broad intermediate region of energies. It

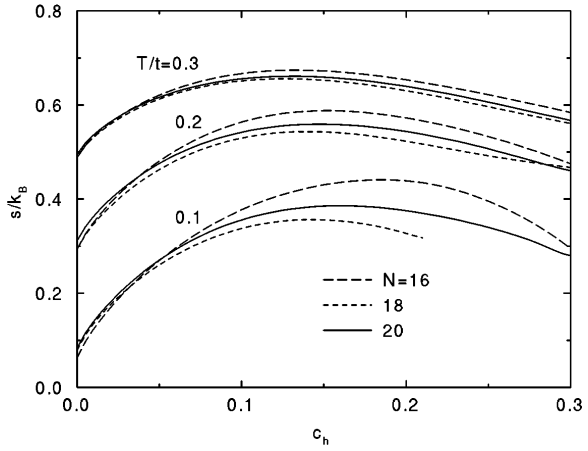

FIG. 2. Entropy density $s = S/N$ vs hole concentration c_h at several T.

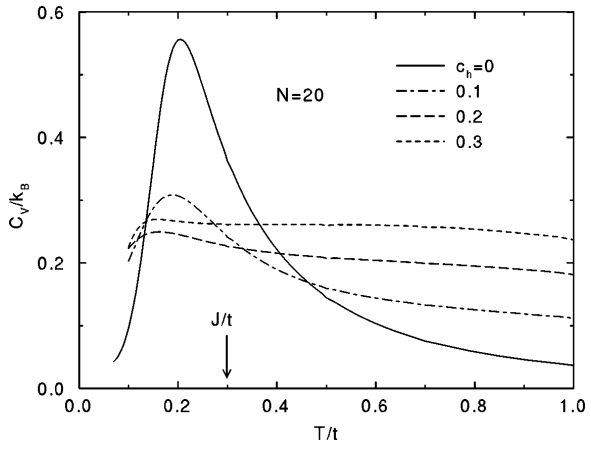

FIG. 3. Specific heat per site vs T at several c_h. $c_h = 0$ was obtained for $N = 26$.

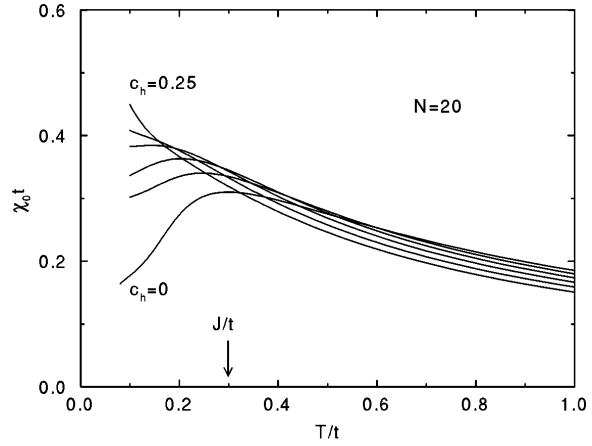

FIG. 4. Uniform susceptibility χ_0 vs T at several c_h in steps of 0.05. $c_h = 0$ was obtained for $N = 20$.

seems natural to connect this phenomenon with the observed universality of dynamical response in the optimum doping regime [11].

Only at extreme overdoping $c_h > 0.5$ (low electron density) we were able to see indications of the Fermi-liquid-like $C_V \propto T$ behavior in a broad interval $T \lesssim t$. On the other hand, we have indications for a different $C_V \sim \gamma T$ behavior at lowest $T_{\rm fs} < T < 0.15t$, as deduced from a drop of C_V in Fig. 3, which would be closer to the experimental results [3] and the QP picture. Such interpretation would be again difficult, since it would require $T_{\rm deg} \sim 800$ K. On the other hand, it is puzzling that obtained γ in the low $T < 0.15t$ regime can be matched with the value for noninteracting fermions at $c_e \lesssim 1$ in a tight-binding band renormalized only by a modest factor $t/\tilde{t} \sim 2.5$, as noted previously [3].

At last we consider the uniform spin susceptibility $\chi_0 = \langle (S_z)^2 \rangle / N k_B T$, which is shown in Fig. 4 at several c_h. Again for $c_h = 0$ our results agree with other calculations [14] down to $T \sim 0.3J$. In the undoped system χ_0 exhibits a maximum at $T = T^* \sim J$, which gradually shifts to lower T with doping and finally disappears at $c_h > 0.15$. χ_0 at $T \to 0$ increases with doping, in agreement with experiments [2] and some previous results [13,14]. The existence of such maximum at $T = T^*$ in undoped cuprates has been interpreted in terms of a pseudogap [1]. At doping $c_h = 0.15$ we observe a monotonous, Pauli-like χ_0 for $T < 0.2t$, which could signify an onset of a QP low-T behavior. On the scale of temperatures of the order of t, however, we do not find the Fermi liquid behavior $\chi_0 = \text{const}$ up to $c_h > 0.6$.

To conclude, we have calculated several thermodynamic properties of strongly correlated electrons within the t-J model and found essentially non-Fermi-liquid behavior in a wide range of doping concentrations, up to $c_h > 0.3$. Non-Fermi-liquid temperature dependence is observed in chemical potential, specific heat, and uniform spin susceptibility, at least in the region of intermediate temperatures $0.15t < T < t$, while at very low $T < 0.15t$ we cannot exclude a possible QP character of low-energy excitations, as signified by nearly constant $\chi_0(T)$ and $C_V \propto T$. We observe in addition a very nonmonotonous $c_h(\mu, T)$ dependence, which we relate to a transition from a small hole-pocket-like to a large electronlike FS around doping $c_h^* \sim 0.15$. Entropy was found to be consistent in magnitude with experiments on cuprates, again showing maximum at $c_h \sim c_h^*$. Finally, the calculated $\chi_0(T, c_h)$ is consistent with experiments, confirming the t-J model as a suitable one for the explanation of normal-state properties of cuprates.

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