Uniform magnetic susceptibility of the t-J model on the 4×4 lattice

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We study the temperature and doping dependence of the uniform susceptibility, χ, for the t-J model by calculating exactly the low-lying states of the 4×4 system with periodic boundary conditions. We find that at low doping and temperatures around $J/3$ the susceptibility increases with doping. Furthermore the peak in its temperature dependence shifts to lower temperatures with doping. These features are in agreement with high-temperature expansions. At higher dopings (6 holes or larger) the susceptibility begins to decrease with increasing doping, again consistent with high-temperature expansions.

The two-dimensional t-J model[1,2] has emerged as a paradigm for studying the low-energy electronic properties of the copper-oxide-based high-temperature superconductors. Although the model appears very simple, it has been difficult to determine its low-temperature thermodynamic properties, in dimensionality greater than one. Some insight into the different phases and properties of the two-dimensional model has been gained by exact diagonalization of small systems,[3] and variational wave function studies.[4] More recently, high-temperature expansions,[5,6] and Monte Carlo simulations[7] have also been applied to the model. High-temperature expansions[6] suggest interesting low-temperature behavior for the magnetic susceptibility. It has been argued that the behavior looks remarkably like the experiments on doped cuprates.[8] However the high-temperature expansions do not show good convergence at temperatures much below J. Thus it is very important to study the low-temperature properties by other theoretical methods, which can provide complementary information.

Here we wish to use finite-size diagonalization to study this system at low temperatures. The Lanczos method is used to calculate exactly many low-lying states in different symmetry sectors of the Hilbert space for the 4×4 system with periodic boundary conditions. Thus the calculated low-temperature properties are essentially exact for the finite system under consideration. At high temperatures our results match on to the high-temperature expansions. At low temperatures they verify most of the qualitative features obtained in the high-temperature expansions. The main difficulty with the finite-size calculations are gaps in the spectra that arise due to the finite size, which cause the thermodynamic properties to vanish rapidly at low temperatures. Thus, while we do find a downturn in the susceptibility at low temperatures it is difficult to tell from this calculation alone if such a behavior will survive in the thermodynamic limit.

$$\mathcal{H}=-t\sum_{<i,j>,\sigma}P(c_{i\sigma}^{\dagger}c_{j\sigma}+c_{j\sigma}^{\dagger}c_{i\sigma})P+J\sum_{<i,j>}(\mathbf{S}_i\cdot\mathbf{S}_j-n_in_j/4)\ , \tag{1}$$

where the sums $\langle i,j\rangle$ run over nearest-neighbor pairs of sites on the square lattice, $c_{i\sigma}$ is the standard electron creation operator, $\mathbf{S}_i=\frac{1}{2}\boldsymbol{\sigma}_i$ is the electron-spin operator and n_i is the particle number operator on site i. The projection operators P ensure that no hopping causes any site to be doubly occupied.

The uniform susceptibility per lattice site, χ, is defined by the relation

$$N\chi=\frac{1}{T}\sum_{i,j}\langle S_i^zS_j^z\rangle\ . \tag{2}$$

Here the angular brackets refer to thermal averaging with respect to the canonical distribution. We can write this in terms of the total spin operator $\mathbf{S}_T$ as

$$N\chi=\frac{1}{3T}\langle\mathbf{S}_T\cdot\mathbf{S}_T\rangle\ . \tag{3}$$

In terms of the eigenstates of the Hamiltonian with eigenvalue E_n and the total spin s_n, this can be expressed as

$$N\chi=\frac{1}{3T}\frac{\sum_n e^{-\beta E_n}s_n(s_n+1)}{\sum_n e^{-\beta E_n}}\ . \tag{4}$$

Once the energy and total spin of the different eigenstates are known the susceptibility is readily calculated from (4).

The spectra of (1) for a given number of holes ($n_h=0,1,2,\ldots,16$) was calculated by using the Lanczos tridiagonalization algorithm. Using this method the lowest 15–20 eigenvalues, for each different sector of the Hilbert space (to be discussed below), were estimated. The numerical accuracy in these eigenvalues decreases as their relative position increases in the eigenspectrum. The numerical error in the finite temperature calculations such as Eq. (4) will be of order of $\exp-(E_{\rm neg}-E_{\rm gs})/kT$, where $E_{\rm neg}$ is the lowest neglected energy (i.e., not calculated in the Lanczos diagonalization and $E_{\rm gs}$ is the ground-state energy for the particular hole density.

In order to minimize this error we explore the symmetries of (1) by splitting the Hilbert space associated with (1) in the largest number of disjoint sectors possible.

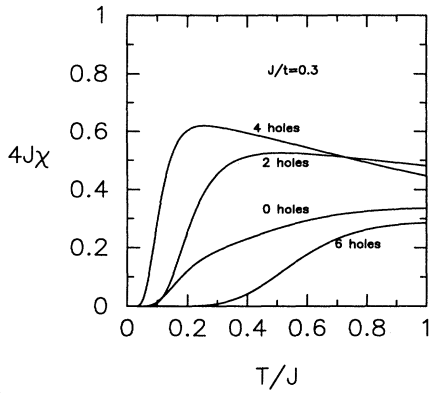

FIG. 1. Plots of the uniform susceptibility as a function of temperature for $t/J=0.3$ for 0, 2, 4, and 6 holes on the 4×4 lattice.

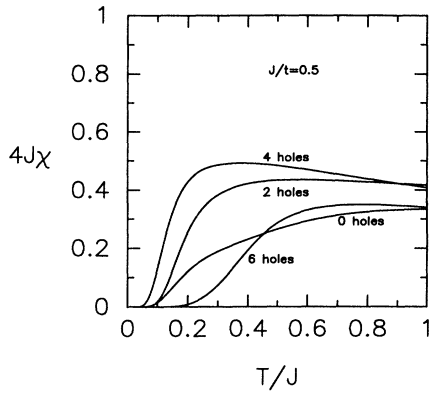

FIG. 2. Plots of the uniform susceptibility as a function of temperature for $t/J=0.5$ for 0, 2, 4, and 6 holes on the 4×4 lattice.

For a given number of holes n_h we separate the sectors according to the number of up spin ($n_u=0,1,2,\ldots 16-n_h$), momenta

$$\mathbf{K}=(2\pi l_x/4, 2\pi l_y/4)(l_x,l_y=0,1,2,3)\ ,$$

rotation quantum numbers $\omega=\exp(i2\pi r/4)$ ($r=0,1,2,3$), and in the sectors with equal number of up (n_u) and down (n_d) spins we also use the spin-reversal invariance.

The SU(2) symmetry of (1) can also be used to improve the precision of our numerical calculations. If a given eigenenergy occurs in a sector with z component of the spin $s_z=(n_u-n_d)/2$ and quantum numbers $\mathbf{K}$ and ω, then it should also occur in all the other sectors with lower s_z values and same quantum numbers $\mathbf{K}$ and ω. In this way, by matching the first few digits we can replace the eigenenergies appearing in the relatively higher position (lower precision) in the spectrum by those calculated in the sectors with high spin values and appearing in relatively lower position in the spectrum (higher precision). The spin of the eigenstates can also be determined by the largest s_z sector in which they appear.

Plots of the susceptibility as a function of temperature for 0,2,4, and 6 holes are shown in Figs. 1 and 2 for realistic values of J/t.[9] By comparing with the high-temperature expansions we find that the uncertainties in our calculations are of order 15%, at temperatures of order J. For the finite system itself, the errors are much smaller at lower temperatures. We observe the following. (a) The susceptibility around $T\approx J/3$ increases with doping at small doping. (b) This trend is reversed at larger dopings. (c) The susceptibility has a maximum as a function of temperature. This maximum occurs at a temperature around J for the Heisenberg model.[10] (d) This peak moves to lower temperature with doping. (e) The magnitude of the susceptibility increases with decreasing J/t for small number of holes. These features are in complete qualitative agreement with high-temperature expansions.[6] Many of these features are very similar to experiments on doped cuprates.[8]

One of the most intriguing experimental features is the downturn in the susceptibility as measured in the Knight-shift experiments, as one goes below room temperature in the metallic phase.[11] This behavior has been interpreted as an opening of a spin gap. In finite systems there is always a gap coming from the discreteness of the energy levels. Thus, although we see such a behavior in our calculations, we cannot disentangle a downturn caused by a finite-size gap from those that will survive in a thermodynamic system.

We have also calculated the free energy and specific heat for these systems. In principle, the specific heat can provide information on the critical points related to phase separation in the model.[12] Once again, however, the finite-size gap behavior dominates these functions at low temperatures and we are unable to draw any significant conclusion about the thermodynamic behavior.

To conclude, we have studied the finite temperature properties of the t-J model by calculating many low-lying states for the 4×4 system with periodic boundary conditions. Our most interesting result is the behavior of the uniform susceptibility. We find that at temperatures around $J/3$, the uniform susceptibility increases with doping at low doping and the peak in its temperature dependence shifts to lower temperatures. These features are in agreement with high-temperature expansions. We also see a "spin-gap"-like behavior in the calculated susceptibility. Unfortunately, there is also a large finite-size gap in these systems and it is not possible to disentangle the thermodynamic spin-gap behavior from the gap arising in finite systems.

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