Thermodynamic Properties of the $t$-$J$-$U$ Model in the Context of High-$T_c$ Cuprates

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Abstract. Some thermodynamic properties of the high-$T_c$ cuprates have been studied using $t$-$J$-$U$ model at different doping ($<h>$) by an exact method on a tilted square cluster. Low temperature specific heat curves show single-peak structure where the peak-height decreases with increasing $<h>$. The system becomes more disordered with decreasing hole occupancy. The extrapolation of all reciprocal susceptibility ($\chi^{-1}$) curves intercept at a negative temperature $\Theta_N$ which suggests an antiferromagnetic correlation in the system.

INTRODUCTION

The 2D $t$-$J$ model is considered as a basic model which is important for the description of anomalous properties of cuprate superconductors [1,2]. Subsequently, this model has been enriched with the incorporation of various new and justified interactions. To mention, the extended $t$-$J$ models contain NNN inter-site Coulomb repulsion [3], electron-phonon interaction [4] and next-nearest-neighbor (NNN) hopping of electrons or holes (depending on doping) [5].

The 2D $t$-$J$ model has been originally designed for hole-doped cuprates [6], but it has the ingredients to reproduce the essential characteristics of other cuprates for the physical parameter range $J/t$~0.4 [7]. Ground state characteristics of the $t$-$t'$-$J$-$J'$ model on the 2D Shastry-Sutherland lattice show that frustration and doping of the system largely control these characteristics [8]. The stability of the AF, superconducting and charge density wave states has been examined within $t$-$J$-$U$-$V$ model [9]. A slave-boson mean field theory calculation on the $t$-$t'$-$J$ model confirms the coexistence of antiferromagnetism (AF) and superconductivity in a broad doping regime [10]. The stability of the $t$-$J$-$U$ model extended by correlated hopping has also been studied[11]. It is observed that correlated hopping increases the possibility of pairing at the electron-doped side of the phase diagram. Within a bilayer $t$-$J$-$U$ model [12] with a number of interlayer dynamical processes, it is shown that the most significant contribution to the superconducting phase is from the interlayer pair hopping.

In this communication, the temperature dependence of specific heat, entropy and reciprocal susceptibility has been investigated within the $t$-$J$-$U$ model on an 8-site tilted square cluster [3]. All the calculations have been performed for different doping of the system employing Lanczos exact diagonalization (ED) technique. Finite size effect on the results has been minimized by considering interactions up to NN sites (smaller than the dimension of the cluster). Further, to calculate thermal properties, averaging over large number of basis states is required which effectively reduces finite size effect.
HAMeLTONIAN AND FORMULATION

The t-J-U Hamiltonian used in this investigation is given as follows

\[
H = -t \sum_{i,j>\sigma} [c_i^\dagger_{\sigma} c_j_{\sigma} + H.c] + J \sum_{i,j>\sigma} \left[ S_i^z S_j^z - \frac{1}{4} n_i n_j \right] + U \sum_i n_{i\uparrow} n_{i\downarrow}
\]  

(1)

Where the nearest-neighbor (NN) hopping amplitude is \(t\), \(J\) is the antiferromagnetic exchange interaction between NN sites, \(U\) represents the on-site Coulomb interaction, \(<i, j>\) includes all pairs of nearest-neighbor (NN) sites. Periodic boundary conditions have been implemented in the calculations. \(i\) runs over all the sites. Also we set the z-component of the total spin \(S^z_{\text{tot}} = 0\).

The expression of the entropy per lattice site is given as

\[
S = \frac{1}{N_S} \left( k_B \ln Z + \frac{<H>}{T} \right)
\]

(2)

We calculate the low temperature specific heat defined as

\[
C_v = k_B \beta^2 \frac{\partial^2}{\partial \beta^2} \ln Z
\]

(3)

Where \(Z = \sum_{\alpha} e^{-\beta E_{\alpha}}\), the sum exists over all the eigenstates, \(E_{\alpha}\)'s represent the eigenvalues, and \(\beta = \frac{1}{k_B T}\), \(k_B\) being the Boltzmann constant which we set as unity for simplification.

The local moment which is the zero separation value of the spin-spin correlation is given by the following relation

\[
< m_z^2 > = < (n_{i\uparrow} - n_{i\downarrow})^2 > = (< n > - 2\delta)
\]

(4)

Where \(\delta = < n_{i\uparrow} n_{i\downarrow} >\) is a measure of the probability of double occupancy.

Finally, the spin magnetic susceptibility is calculated by using the formula,

\[
\chi = \beta < m_z^2 >
\]

(5)

We have used translational symmetry to reduce the number of basis states. Throughout our calculation we take \(t=1.0\) and \(k_B=1.0\).

RESULTS AND DISCUSSIONS

We plot specific heat \((C_v)\) against temperature \(T\) for various values of hole occupancy \(<h>\) in Fig. 1. From the figure it appears that at low temperatures, the specific heat increases sharply with \(T\) and attains a peak due to thermal excitation of the spin degrees of freedom. The peak-height increases with decreasing hole occupancy. At low temperatures, \(C_v \sim T^2\) (approximately) indicating non-Fermi liquid nature of the system.

To understand the dependency of entropy \(S\) on hole-doping \(<h>\) and temperature \(T\) at low temperatures, we have plotted entropy characteristics in Fig.2. Entropy increases with temperature and after a certain \(T\), it is almost parallel to \(T\)-axis. It is also apparent that \(S \rightarrow 0\) when \(T \rightarrow 0\) [13]. This absence of residual entropy when \(T \rightarrow 0\) indicates that the ground state is spin-singlet. The system becomes more disordered with decreasing hole occupancy.

The variation of the reciprocal magnetic susceptibility \(\chi^{-1}\) with temperature \(T\) is shown In Fig.3. At the low temperature region, curves are almost linear. The extrapolation of the curves intercept at a negative temperature \(\Theta_N\) (Curie temperature) which is different for different hole-doping \(<h>\). The significance of the negative Curie temperature lies in the fact that antiferromagnetic correlation is present in the system [14].
CONCLUSIONS

Summarizing, the exact diagonalization study of the $t$-$J$-$U$ model shows that specific heat characteristics has a sharp peak at low temperature and the peak height increases with decreasing hole doping. Entropy variation establishes that the system described by the Hamiltonian is a spin-singlet state. The extrapolation of all $\chi^{-1}$ curves intercept at a negative temperature $\Theta_N$ suggesting the presence of antiferromagnetic correlation in the system.
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REFERENCES

5. N. S. Mondal and N. K. Ghosh, Pramana. 74, 115-121 (2010).