*Original Article*

*Bulletin of Pure and Applied Sciences.*
*Vol.37 D (Physics), No.2, 2018: P.158-162*
*Print version ISSN 0970 6569*
*Online version ISSN 2320 3218*
*DOI: 10.5958/2320-3218.2018.00021.0*

# Some Finite Temperature Characteristics of the High-$T_c$ Cuprates within *t-J-U* Model

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**Received on 27.06.218**
**Accepted on 22.11.218**

**Abstract**

The effects of nearest-neighbor (NN) antiferromagnetic (AF) exchange interaction (*J*) and temperature on high-$T_c$ cuprates have been studied using an eight-site frustrated *t-J-U* model. Average hole density is taken as $\langle h \rangle = 0.25$, appropriate for cuprates. Above a critical temperature, local moment decreases with temperature but increases with *J/t*. Corresponding double occupancy shows the reverse character. The system becomes more disordered with NN AF interaction. Low temperature specific heat curves show single peak structure where the peak-height decreases with *J/t*. The *t-J-U* model appears to be of non-Fermi liquid character.

**Keywords**: High-$T_c$ cuprates, *t-J-U* model, Thermodynamic properties

## 1. Introduction

The 2D *t-J* model has been accepted as one of the most successful models to describe cuprate superconductors [1,2]. The two essential features of the model are strong Coulomb repulsion at the Cu-sites and antiferromagnetic (AF) spin fluctuation in the ground state. However, a variety of newer interactions have been incorporated in the model to describe various anomalous properties of the high-$T_c$ superconductors. These interactions include next-nearest-neighbor (NNN) hopping of electrons or holes (depending on doping) [3], NNN inter-site Coulomb repulsion [4] and electron-phonon interaction [5].

This 2D *t-J* model is canonical for hole-doped copper oxide superconductors [6]. It reproduces the essential characteristics of the cuprates for the physical parameter range $J/t \sim 0.4$ [7]. The phase diagram of the $t$-$t'$-$J$-$J'$ model on the 2D Shastry-Sutherland lattice shows that the ground state characteristics largely depend on frustration and doping [8]. Employing slave-boson mean field theory, the calculation on the $t$-$t'$-$J$ model confirms the coexistence of AF and superconductivity in a broad doping regime [9]. The stability of the AF, superconducting and charge density wave states has been examined within *t-J-U-V* model [10]. They showed that charge ordering appears in a limited doping range and above a critical value of $V$. The effect of $V$ on AF state is negligible but it suppresses superconducting state. The interaction like correlated hopping has also been studied within *t-J-U* model [11]. They showed that correlated hopping interaction increases the possibility of pairing at the electron-doped side of the phase diagram. The influence of the interlayer effects on the superconducting state has been examined within a bilayer *t-J-U* model [12] with a number of interlayer dynamical processes within the Hamiltonian. The most significant contribution to the superconducting phase is from the interlayer pair hopping.

In this project, we have considered an 8-site tilted square cluster [13] to understand the temperature dependence of local moment, double occupancy, specific heat and entropy within the *t-J-U* model. The role of AF exchange interaction at finite temperature has also been studied. Lanczos exact diagonalization (ED) technique has been followed. All the calculations has been made at a hole doping <*h*> = 0.25, appropriate for cuprates.

Results obtained using ED technique is free from any error introduced by approximations assumed. However, we cannot perform our calculations in a larger cluster as the growth of the Hilbert space is exponential and this forbids diagonalization of the matrix. So, in our calculation, we can't ignore finite size effect. To minimize the effect, we have considered interactions up to NN sites only keeping it smaller than the dimension of the cluster. Calculations of thermal average of the parameters further reduce finite size effect as the calculations require averaging over large number of basis states. From all these considerations, we can say that finite size effect is minimal in the present calculation at finite temperature.

## 2. Formulations

We have considered the following model Hamiltonian in this problem

$$H = -t\sum_{<i,j>\sigma}[c_{i\sigma}^{+}c_{j\sigma} + H.c] + J\sum_{<i,j>}[\vec{S_i}\cdot\vec{S_j} - {}^{1}/_{4}\, n_i n_j] + U\sum_i n_{i\uparrow}n_{i\downarrow} \quad (1)$$

Where $t$ is the nearest neighbor (*NN*) hopping amplitude, $J$ is the antiferromagnetic exchange interaction between NN sites, $U$ is the on-site Coulomb interaction. <*i, j*> represents all pairs of nearest-neighbor *(NN)* sites. We have taken an 8-site tilted square cluster with periodic boundary conditions. *i* runs over all the sites. Also we set $S_z^{tot} = 0$.

We calculate here the local moment which is the zero separation value of the spin-spin correlation

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

Where $\delta = < n_{i\uparrow}n_{i\downarrow} >$ is the probability of double occupancy, which measures the localization of itinerant electrons.

The entropy per lattice site is ($N_S$ is the number of lattice sites.)

$$S = \frac{1}{N_S}\left(k_B lnZ + \frac{<H>}{T}\right) \quad (3)$$

The low temperature specific heat is given by

$$C_v = k_B\beta^2 \frac{\partial^2}{\partial\beta^2} lnZ \quad (4)$$

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 take unity to simplify our calculations.

## 3. Results and Discussions

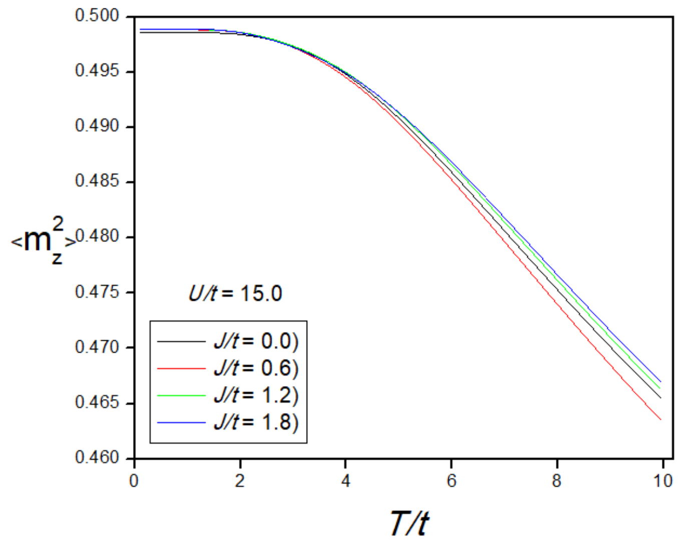


**Fig. 1**: Local moment vs. temperature for various NN antiferromagnetic interaction *J/t* with *U/t*=15.0

In Fig.1, we show the nature of local moment$<m_z^2>$ with temperature for various *J/t*. Initially, $<m_z^2>$ maintains a constant value up to a certain low temperature, then it decreases to lower values at higher temperatures. It is established that formation of doubly occupied sites is favored above a temperature $T = T(U)$ due to thermal excitation [14]. As a result, the local moment decreases with temperature above a critical temperature depending on $U$. Local moment increases with *J/t* except for *J/t* = 0.0 (which needs further investigation). The frustration induced by *J/t* may lead to unbind the hole pairs, increasing local moment.

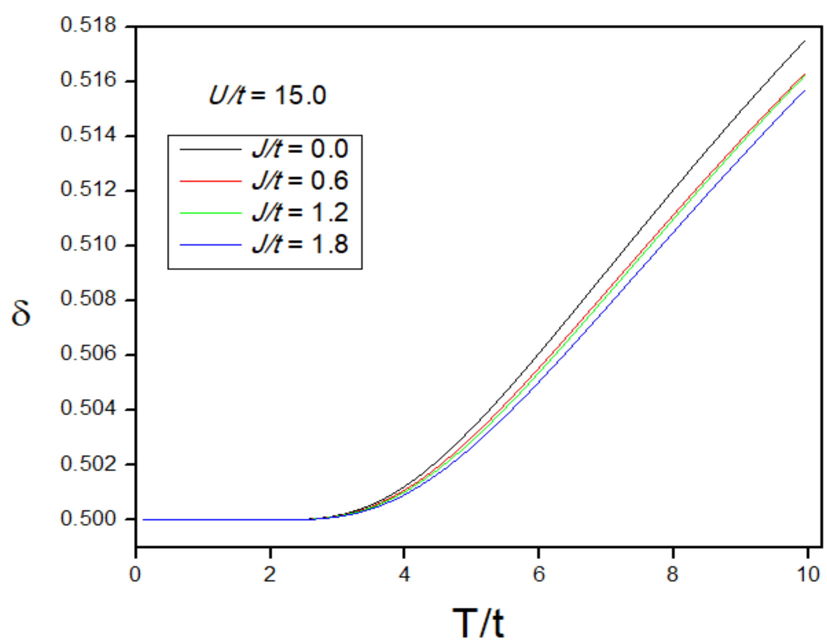


**Fig. 2**: Variation of double occupancy with temperature for different NN antiferromagnetic interaction *J/t* with *U/t*=15.0

We plot the related double occupancy $\delta$ with temperature for different *J/t* in Fig. 2. At a particular temperature, it decreases with *J/t* as frustration tends to unbind hole pairs. Double occupancy increases with $T$ above a particular temperature $T = T\ (U)$ as thermal excitation favors double occupancy. At very high temperatures, double occupancy may tend to 0.75 when any six of the sites are doubly occupied and two remaining empty.

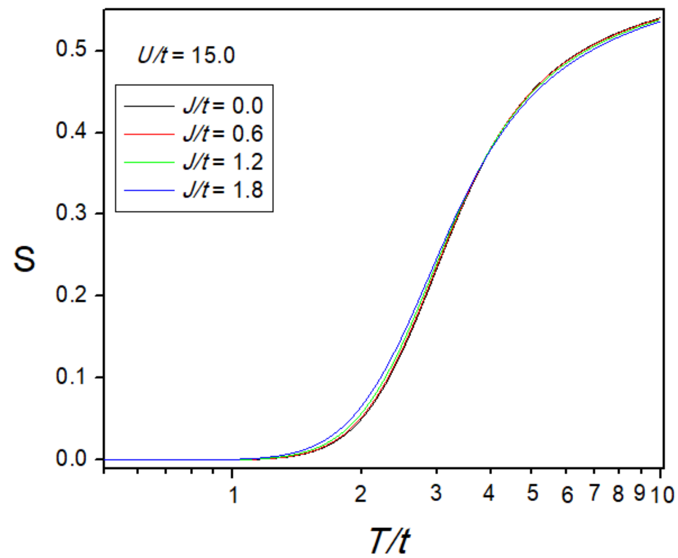


**Fig. 3**: Variation of entropy with temperature for different NN antiferromagnetic interaction *J/t* with *U/t*=15.0

Fig.3 shows temperature dependence of entropy $S$ for different values of *J/t* at low temperatures. Entropy is a measure of the disorder of the system. From the figure, it appears that entropy decreases with decreasing temperature and $S \rightarrow 0$ when $T \rightarrow 0$ [15]. This nature indicates that the ground state of this model is spin singlet and so residual entropy is absent. At low temperatures, entropy increases with *J/t*. Thus the system becomes more disordered with *J/t*. It may be concluded that frustration induced by *J/t* in the lattice tends to unbind hole pairs increasing entropy.

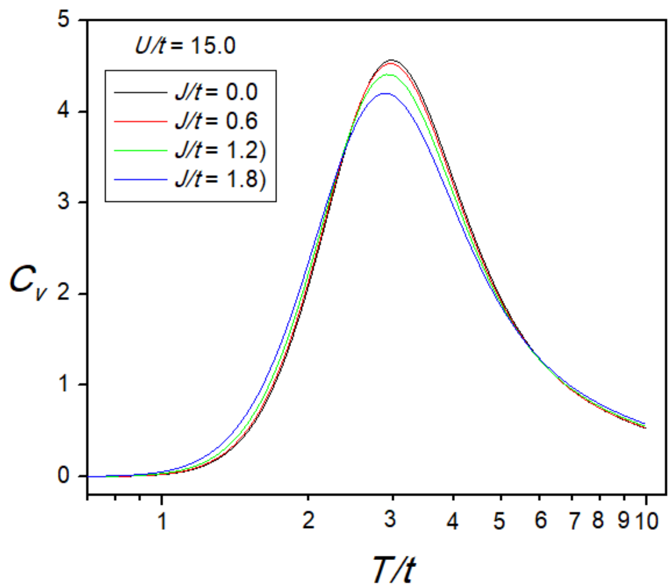


**Fig. 4**: Variation of specific heat with temperature for different NN antiferromagnetic interaction *J/t* with *U/t*=15.0

The variation of specific heat *($C_v$)* with temperature *T* for different *J/t* is shown in Fig. 4. At small temperatures, the specific heat is small and it follows $C_v \sim T^2$ (approximately). But, with the rise of temperature, specific heat increases and reaches maximum. The peak-height decreases with *J/t*. Thermal excitation of the spin degrees of freedom contributes to the peak in this doped system. So, NN AF interaction decreases effective energy. The *t-J-U* model appears to be of non-Fermi liquid character.

## 4. Conclusions

Finite temperature properties like local moment, double occupancy, entropy and specific heat have been studied within *t-J-U* model in an exact method. It appears that formation of doubly occupied sites is favored by thermal excitation which decreases local moment. Frustration induced by *J/t* increases local moment. Corresponding double occupancy δ behaves reversely. So far entropy is concerned; the system becomes more disordered with *J/t*. Specific heat curves show single peak structure where the peak-height decreases with *J/t*. Non-Fermi liquid character of the present system is confirmed here.

**Acknowledgment** We are thankful to University of Kalyani for infrastructural help.

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