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Signatures of next-nearest-neighbor (NNN) Antiferromagnetic Exchange Interaction on High-T_c Superconductivity Within t-t'-J-J' Model

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Abstract

The influence of the next-nearest-neighbor (NNN) antiferromagnetic interaction J' has been examined within t - t' - J - J' model in an exact technique. An 8-site square cluster is chosen as the representative of the system. The effect of the next-nearest-neighbor (NNN) antiferromagnetic interaction on various ground state properties such as electron-electron correlation, spin-spin correlation, effective hopping amplitude etc. has been studied. Temperature variation of the susceptibility shows that J' suppresses short range antiferromagnetic order. Applying periodic boundary conditions, the calculations have been extended beyond the 8-site limit.

Keywords: High-Tc superconductivity; t-t'-J-J' model; Electronic structure; Thermodynamic properties.

1. INTRODUCTION

The two-dimensional (2D) t-J model has drawn the interest of the physicists to understand the basic features of the cuprates [1]. The experimental observations of the high-T_c cuprates can be well explained within the model in the physical parameter range $J/t \approx 0.4$ [2]. However, the calculations using t–J model based on different approximations reproduced diverse results. Here lies the importance of numerical studies where the results are not perturbed by approximations made [3].

The various extensions of the model have been investigated to explore the pairing mechanism and other properties of cuprates [4,5]. Next-nearest-neighbor (NNN) interactions have been successfully incorporated by many authors to give a fine touch in explaining the properties of high-T_c superconductors [6,7]. An exact diagonalization study of the 2D t - J model extended by phonon mediated interaction showed that phonon mediated attractive interaction has influence on the formation of d-wave pairing [8]. The coexistence of antiferromagnetism and superconductivity has been established in *t-t'-J* model applied to a honeycomb lattice [9]. *t–J* model extended by an effective density–density type interaction (a *t-J-V* model) has been successful to explain the experimental data of some cuprates in the optically doped cuprates [10].

Thermodynamic properties of the 2D *t-J* model have been extensively studied to understand the strongly correlated high-T_c cuprates [11-13]. The finite temperature properties of the planar *t-J* model have been investigated for a wide range of doping concentrations [11]. The non-Fermi liquid behavior of the system has been confirmed. Using numerical linked cluster (NLC) algorithms, the thermodynamic properties of the model on a square lattice have been examined [12]. The calculation can be extended to further lower temperatures using Lanczos method with NLC. In [13], authors observed strong electron density dependent behavior of entropy and thermo power in the 2D *t-J* model. Results showed that d-wave fluctuations dominate for n ≤ 0.8 but antiferromagnetic fluctuations dominate for n ≥ 0.84.

In this paper we study the 2D *t-J* model extended by NNN hopping (t') and NNN exchange interaction (J'). In our previous work [14], we have observed the coexistence of antiferromagnetism and $d_{x^2-y^2}$ wave superconductivity in presence of NNN antiferromagnetic interaction $J' \leq 0.4J$. Here we have examined the role of NNN exchange interaction (J') on some ground state and finite temperature properties of high-T_c superconductors. We have used an exact diagonalization technique on an 8-site tilted square cluster [15]. Observations have been compared with existing results.

2. FORMULATIONS

We consider the following t - t' - J - J' model Hamiltonian defined as

$$H = -t \sum_{<i,j>\sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + H.c.) - t' \sum_{<p,q>\sigma} (c_{p\sigma}^{\dagger} c_{q\sigma} + H.c.) + J \sum_{<i,j>} [\vec{S_i} \cdot \vec{S_j} - {}^1\!/_4\, n_i n_j]$$
$$+J' \sum_{<p,q>} [\vec{S_p} \cdot \vec{S_q} - {}^1\!/_4\, n_p n_q] \quad (1)$$

Where the summation over <*i,j*> extend over all pairs of nearest-neighbor (NN) sites and the summations over [*p,q*] extend over all pairs of next-nearest-neighbors (NNN) sites on a tilted 8-site square cluster; t is the near neighbor (NN) hopping amplitude, t' is the next to near neighbor (NNN) hopping amplitude, J is the NN antiferromagnetic interaction and J' is the NNN antiferromagnetic interaction. $c_{i\sigma}(c_{i\sigma}^{\dagger})$ denotes the electron annihilation (creation) operator for one electron at site I with spin $\sigma = \uparrow, \downarrow$; $\vec{S_i}$ is spin-1/2 operator at the site i. Average hole concentration is <h>=0.25 and periodic boundary conditions are applied to obtain the basis states of the Hamiltonian. Also, z-component of total spin $S_z^{tot} = 0$ is followed.

We measure the spatial distribution of electrons by observing the electron-electron (e - e) density correlation function [16] as

$$C_{el-el}(l) = \frac{1}{N_e N_E(l)} \sum_{<i,i+l>} \langle \psi_0 | n_i n_{i+l} | \psi_0 \rangle \quad (2)$$

where $n_i = n_{i\uparrow} + n_{i\downarrow}$. N_e is the number of electrons and $N_E(l)$ is the number of equivalent sites at a distance l from some reference site i. In order to determine the magnetic behavior (antiferromagnetic order) of the system between NN sites, we have calculated the spin-spin correlation function defined by,

$$C(l) = < (n_{i+l\uparrow} - n_{i+l\downarrow})(n_{i\uparrow} - n_{i\downarrow}) > \quad (3)$$

Where *C(l)* is calculated for all sites *i* and taken average. *C(l)* measures the extent of alignment of the z component of spin at site *i* with respect to that on a site at a distance *l* away. In this chapter, *l*=0 is for on-site correlation (local moment), *l*=1 for NN sites and *l*=√2 for NNN sites, *l*=2 for next to NNN sites and so on. Zero separation value of the spin-spin correlation function is termed as local moment and it is $C(0) = < (n_{i\uparrow} - n_{i\downarrow})^2 >$. Positive (negative) *C*(1) indicates ferromagnetic (antiferromagnetic) tendency.

The influence of NNN antiferromagnetic interaction on bare electron mobility can be followed by observing the nature of effective hopping amplitude defined as [17,18]

$$t_{eff} = \frac{\sum_{<i,j>\sigma}\left\langle \psi_0 \middle| (c^{\dagger}_{i\sigma}c_{j\sigma} + H.c.) \middle| \psi_0 \right\rangle}{\sum_{<i,j>\sigma}\left\langle \varphi_0 \middle| (c^{\dagger}_{i\sigma}c_{j\sigma} + H.c.) \middle| \varphi_0 \right\rangle} \quad (4)$$

where $|\psi_0>$ indicates ground state wave function of the total Hamiltonian H and $|\varphi_0>$ is the ground state wave function of the standard *t-t'-J* model.

The uniform spin susceptibility χ is given by the relation

$$\chi = \beta < m_z^2 > \quad (5)$$

where $< m_z^2 >$ is the local moment defined by the relation

$$< m_z^2 > = (n_{i\uparrow} - n_{i\downarrow})^2 = (< n > -2\delta) \quad (6)$$

where $\delta = < n_{i\uparrow} n_{i\downarrow} >$ is identified as the probability of double occupancy.

We have performed our calculations using exact diagonalization method [19] in a 8-site tilted square cluster applying periodic boundary conditions. The choice of the cluster for high-T_c superconductors has been made following Maier *et al*. [20]. To minimize finite size effect, interactions upto NNN sites (which are smaller than the cluster dimension) have been considered. So, we can argue that finite size effect is minimal in the present investigation.

3. RESULTS AND DISCUSSIONS

In our calculation, we have set <*h*>=0.25 corresponding to 2-hole (6-electron) states. We have taken *J/t*=0.3 which is appropriate for the cuprates [21]. Considering spin-singlet ground state of the *t-J* model [22], $S_z^{tot} = 0.0$ has been followed.

The variation of electron-electron correlation with antiferromagnetic exchange interaction *J'* for different site-distances is shown in Fig.1. The correlation is dominant for *l*=2 and *l*=√2, minimum for *l*=3. Previously, for frustrated Hubbard model, we have observed that maximum *el-el* correlation is between NNN sites [23]. So, the effect of exchange interaction can be associated with the delocalization of spin polarons which causes the maximum *el-el* correlation at *l*=2. The correlation is almost independent of *J'* for *l*=√2, but for other distances, either it decreases slightly (*l*=√5, *l*=3) or increases slightly (*l*=2, *l*=1) with NNN exchange interaction.

To observe the ground state magnetic behavior of the system, we plot spin-spin correlation *C(l)* with *J'/t* for different site distances in Fig.2. *C(1)* is always negative but increases with *J'*. *C(√2)* is zero at *J'*=0 and decreases slowly with *J'*. Thus we can say that a short range AF order is present in the system, which is suppressed with *J'*. With the increase of NNN antiferromagnetic interaction, local singlet breaks down resulting to an increase towards ferromagnetic tendency, which destroys superconductivity [14].

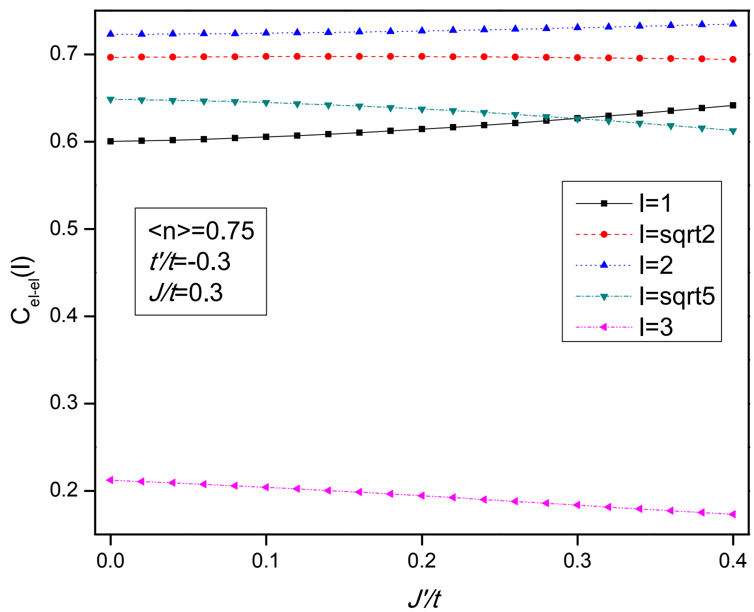

Figure 1: Variation of electron-electron correlation function $C_{el-el}(l)$ with NNN antiferromagnetic interaction for different site-distances. The distance $l = |i - j|$ is measured in the unit of lattice constant.

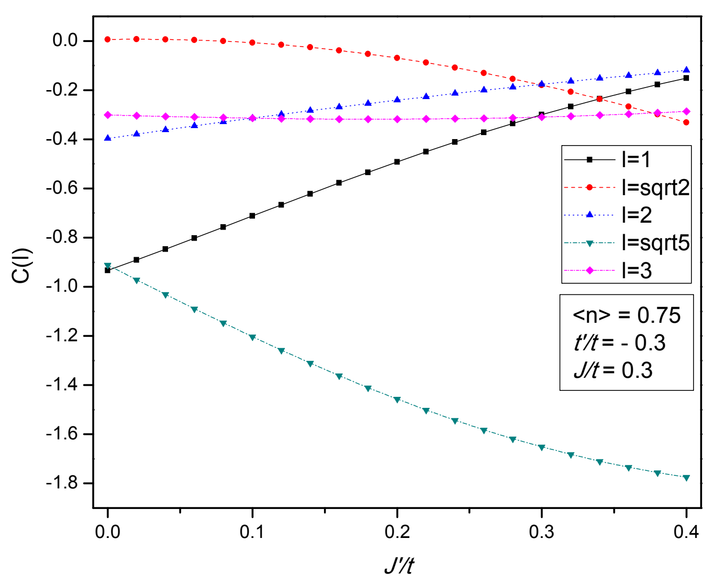

Figure 2: Variation of spin-spin correlation function $C(l)$ with NNN antiferromagnetic interaction for different lattice distances. The distance $l = |i-j|$ is measured in the unit of lattice constant.

Fig. 3 depicts the nature of the effective hopping amplitude with NNN antiferromagnetic interaction for different *J*. Initially, the amplitude increases with *J*' (*J*=0.3,0.4), reaches a maximum and then decreases sharply. The drop is faster for smaller *J*. So, it seems that NNN antiferromagnetic interaction increases the possibility of electron-hopping. A cross-over is found for *J*'/*t*=0.05. Here, NNN and NN antiferromagnetic interactions compete with each other.

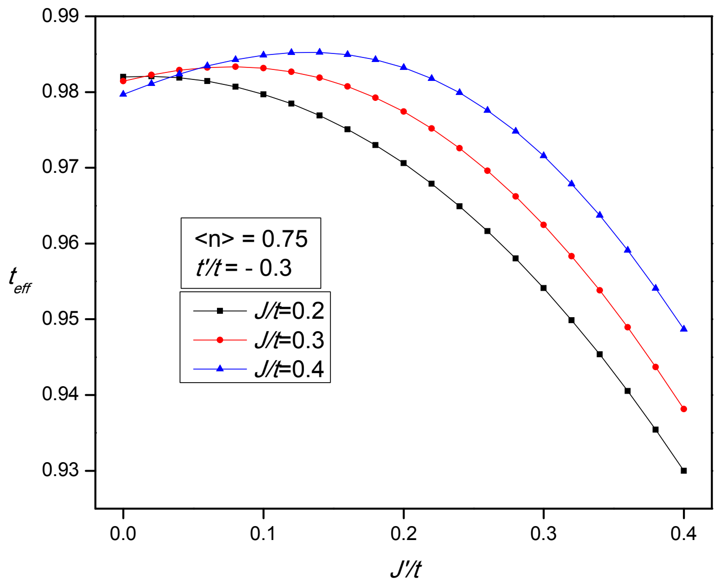

Figure 3: Variation of effective hopping amplitude (t_{eff}) as a function of *J*'/*t* for different NN antiferromagnetic interaction (*J*/*t*).

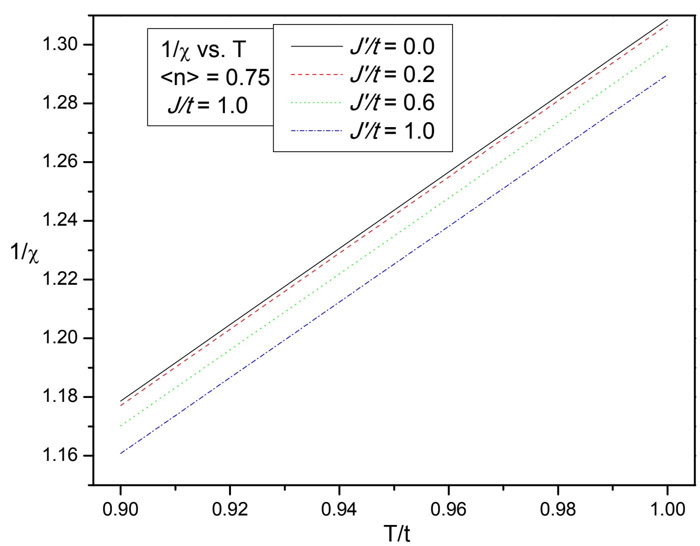

Figure 4: Variation of reciprocal susceptibility (χ^{-1}) with temperature for different values of NNN antiferromagnetic interaction (*J*'/*t*).

The dependence of reciprocal susceptibility χ^{-1} with temperature is shown in Fig.4. It appears from the figure that χ increases with J' and decreases with temperature. With the increase of NNN antiferromagnetic interaction, short range antiferromagnetic order is destroyed and ferromagnetic links grow which increases χ. As expected, with the increase of temperature, long range antiferromagnetic order due to super exchange interaction is destroyed and χ is decreased [24].

4. CONCLUSIONS

Ground state properties like electron-electron correlation, spin-spin correlation and effective hopping amplitude have been investigated within t - t' - J - J' model. It appears that *el-el* correlation is stronger between the site distance l=2. Short range antiferromagnetic order is suppressed with J'. J' increases the possibility of electron hopping. Ferromagnetic links grow with J' which increases χ. Results establish that NNN antiferromagnetic exchange interaction is very much relevant for high-T_c cuprates.

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