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Effect of Next-Nearest-Neighbor (NNN) Hopping and Exchange Interactions on High-Tc Superconductivity

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ABSTRACT To investigate the effect of next-nearest-neighbor (NNN) hopping (t') and exchange interactions (J') on pairing mode (s- or d-wave) and hole-binding, the t-t'-J-J' model has been considered within an 8-site square cluster (tilted). Using the Lanczos exact diagonalization method, the dominance of s-wave is identified. The formation of two-hole pair is observed at J'/t > 0.5. However, appearance of superconducting condensation is absent in the model.

KEYWORDS High-T_c superconductivity; t - t'- J - J' model; Hole pairing.

INTRODUCTION

Different characteristics of the high-T_c cuprates (HTC) are successfully explained within the two-dimensional *t-J* model [1, 2]. Various numerical and analytical methods [3-5] have been applied to investigate within *t-J* Hamiltonian. The model is specially designed to understand the ground state features of the hole doped cuprates. Quantum cluster method successfully explains various ground state properties, pairing mechanism [6, 7] and thermodynamic behaviour [8]. Entropy and thermo power calculations within *t-J* Hamiltonian show strong doping dependent characteristics [9]. Antiferromagnetic fluctuations dominate for electron density $< n > \geq 0.84$, but, d-wave pairing fluctuations dominate for $< n > \leq 0.8$.

Applying variational method to the 2D *t-J* model on a square lattice, a close competition between stripe phase and superconductivity has been observed [10]. At a doping $< h >= 0.25$, the *t-J* model extended by inter-site Coulomb repulsion (a *t-J-V* model) exhibits superconductivity [11]. Experimental observation of the high-T_c superconductors can be explained successfully within 2D *t-J* model for the physical parameter range J/t~0.4 [12]. Authors investigated the finite temperature properties of HTC using the model [8, 9, 13] and reproduced similarity with experimental observation. Non-Fermi liquid character of the system is confirmed for a wide range of doping strengths [13].

It has been established theoretically [14, 15] and experimentally [16] that next-nearest-neighbour (NNN) interactions play important role in the strongly correlated systems. In [15], authors showed that NNN hopping interaction t' controls double occupancy at a site, local moment, order of the system. *t-J* model extended by Coulomb repulsion and NNN hopping (a *t-t'-J-V* model) has been examined [7] to explore hole doping and ground state properties of the HTC [7].

Off-site antiferromagnetic exchange interaction is very much relevant in high-T_c cuprates [17, 18]. In [17], authors investigated the effect of this interaction on $d_{x^2-y^2}$- wave pairing state. This interaction is responsible for stable long range antiferromagnetic order. It appears that two hole tend to bind for larger values of the NNN exchange interaction J' [18]. They also studied the signatures of this interaction on various ground states and finite temperature properties of high-T_c superconductors [19].

As a consequence of the discussion made above, the effect of the NNN exchange interaction (J') in the presence of the NNN hopping interaction (t') on the ground state properties of the extended *t-J* model has been investigated in this project using exact diagonalization (ED) technique. Our calculations are based on an 8-site tilted square cluster with 2-holes [7]. The nature of the ground state excitations and superconducting pairing mechanism has been discussed to give more insight into the physical properties of the system.

METHODOLOGY

The *t-t'-J-J'* Hamiltonian is written 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*> and [*p, q*] extends over all pairs of nearest-neighbor (NN) and next-nearest-neighbors (NNN) sites respectively on a tilted 8-site square cluster; t and t' are the near neighbor NN and NNN hopping amplitudes, J and J' are the NN and NNN antiferromagnetic interactions respectively. $c_{i\sigma}(c_{i\sigma}^{\dagger})$ are the particle 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 doping is fixed at <h> = 0.25. We also apply periodic boundary conditions to obtain the basis states of the Hamiltonian. Without losing any generality, we set z-component of total spin i.e., $S_z^{tot} = 0$.

The singlet pairing operator indicates the pairing mode and is defined as

$$\Delta_\alpha(r_i) = c_{i\uparrow}\left(c_{i+x,\downarrow} + c_{i-x,\downarrow} \pm c_{i+y,\downarrow} \pm c_{i-y,\downarrow}\right), \quad (2)$$

Where + and – signs correspond to extended *s*-wave and *d*-wave respectively and α indicates the symmetry of pairing function. The pairing–pairing correlation function

$$P_\alpha(i,j) = \langle \Delta_\alpha^{\dagger}(r_i)\Delta_\alpha(r_j) + \Delta_\alpha(r_i)\Delta_\alpha^{\dagger}(r_j)\rangle, \quad (3)$$

The susceptibility as the sum of pairing correlations and is written as

$$\chi_\alpha = \frac{1}{N}\sum_{i,j} P_\alpha(i,j), \quad (4)$$

To track the onset of pair formation, we calculate the binding energy of holes. The binding energy between two holes

$$E_{B,2} = (E_2 - E_0) - 2(E_1 - E_0) \qquad (5)$$

And, the binding energy of four holes

$$E_{B,4} = (E_4 - E_0) - 2(E_2 - E_0) \qquad (6)$$

where E_n stands for the ground state energy of the system with n holes. Attraction between holes is indicated by negative values of hole-binding energy.

FINITE SIZE EFFECT

In the present calculation, no approximate method has been followed. We have used exact diagonalization method in an 8-site tilted square cluster along with periodic boundary conditions. This small size of the cluster may invite finite size effect. However, the next higher geometry for our calculation is an 18-site cluster. But, in this cluster with $\langle h \rangle = 0.25$, the calculation is quite impossible due to exponential growth of the Hilbert space. In our calculation, we have considered interactions up to NNN sites only to keep finite size effect as minimum. Hence, to keep the results free from perturbations by the approximations made, this small 8-site cluster is competent enough to describe ground state properties of HTC.

RESULTS AND DISCUSSIONS

In this calculation, $\langle h \rangle=0.25$ corresponding to 2-hole state and $J/t=0.3$ which are appropriate for the cuprates [21]. Considering spin-singlet ground state of the *t-J* model [22], $S_z^{tot} = 0.0$ has been followed. Also, we have restricted ourselves to no double occupancy in the Hilbert space.

The variation of the *s*- and *d*-wave pairing susceptibilities are shown in Fig.1 for t'/t = -0.3. It appears that for appropriate values of the parameters for the HTC, *s*-wave susceptibility dominates. This fact establishes an *s*-wave superconducting phase. We also observe a decrease in both χ_s and χ_d with J'/t. This is probably due to delocalization of spin polaron with the increase of J', which breaks the spin singlet. The result is in good agreement with our previous findings [19].

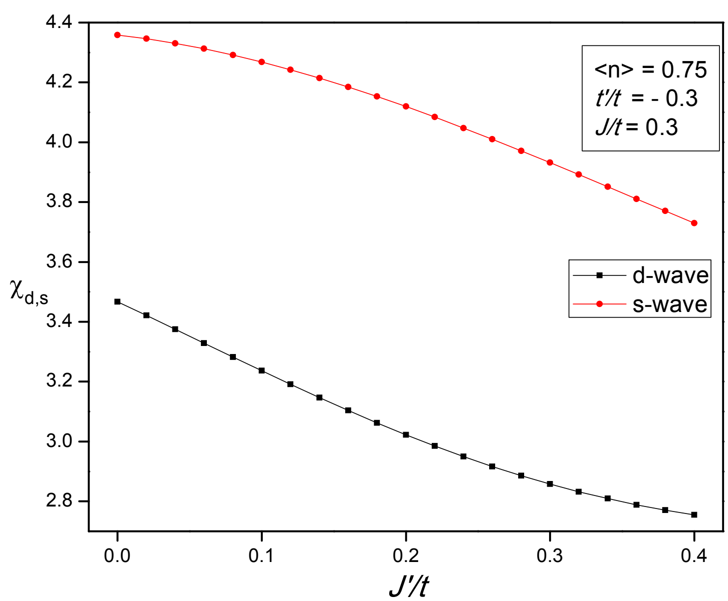

Figure 1: **d-wave and s-wave pairing susceptibilities vs. J'/t for t'/t=-0.3.**

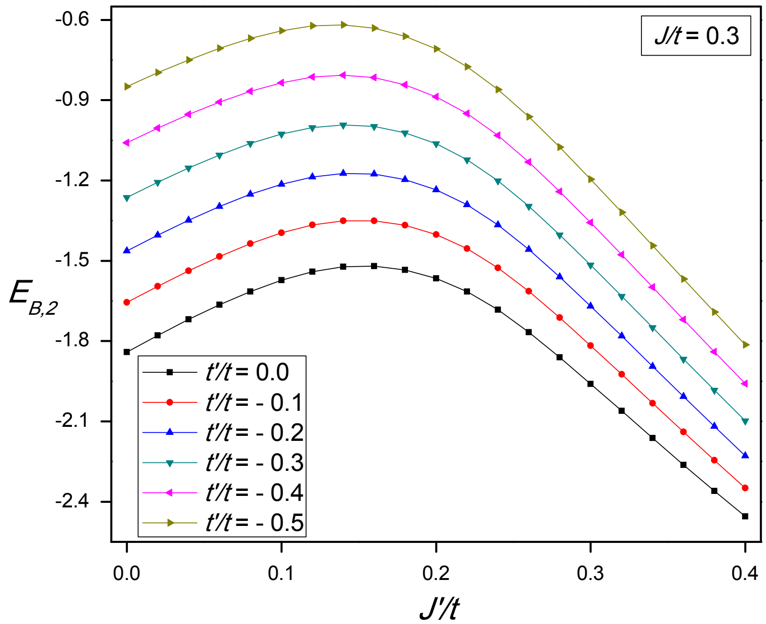

Figure 2: **Two-hole binding energy $E_{B,2}$ vs. J'/t for different values of t'/t.**

Two-hole binding energy is a good parameter to determine the superconducting phase. We have plotted $E_{B,2}$ as a function of J' and t' in Fig. 2. Initially, $E_{B,2}$ decreases with J'/t and reaches to a maximum (binding energy is minimum at this point J'/t = 0.15) and then decreases. Binding energy decreases with t'/t. Increase in NNN exchange interaction J'/t breaks the local singlets and the magnitude of binding energy decreases. For $J'/t \approx 0.15$, the holes are settled at NNN sites. These stable holes form singlets and magnitude of $E_{B,2}$ increases. With the increase of t'/t, the mobility of holes increases, decreasing the magnitude of $E_{B,2}$. This result using an 8-site tilted square cluster agrees well with that on a 4×4 square cluster [23]. We can further conclude that binding energy of 2-holes is small at lower values of J'/t, depending on t'/t. At larger J'/t, binding energy increases.

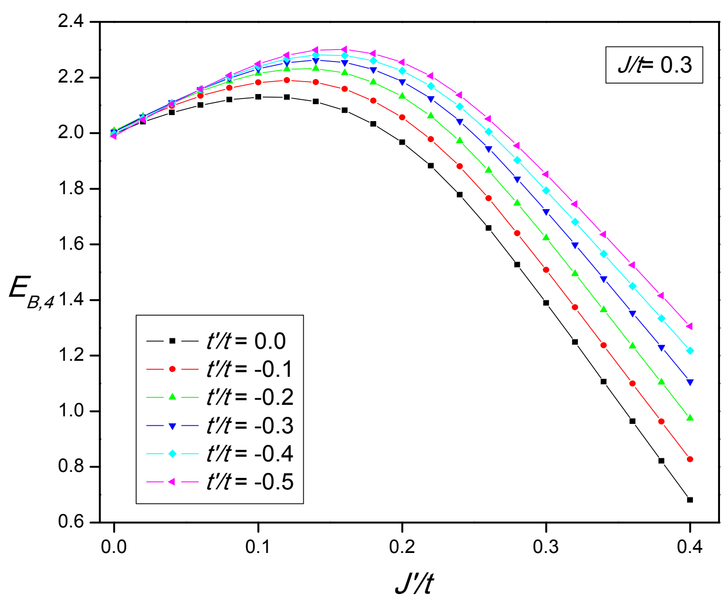

Figure 3: **Four-hole binding energy $E_{B,4}$ vs. J'/t for different values of t'/t.**

During superconducting condensation, droplets are formed. To trace any indication of the formation of superconducting condensation, we have shown the variation of the binding energy of two pairs of holes, $E_{B,4}$ with J'/t for different values of t'/t in Fig. 3. It is observed that for all values of J'/t and t'/t, in the parameter region of HTC, $E_{B,4}$ is always positive. Hence, superconducting condensation is not possible in the present system [7]. So, we can conclude that the two hole pairs repulse each other and t'/t increases the repulsion further. This requires further investigation in the matter.

CONCLUSIONS

The present investigation based on t-t'-J-J' Hamiltonian to explain ground state properties like *s*- and *d*-wave pairing susceptibilities, hole-binding energy etc. has the outcome as follows:

i) It appears that the pairing is in the *s*-wave channel, though *d*-wave pairing is not negligible.
ii) 2-hole binding energy calculation shows that pair formation is possible in the parametric region. However, stable bound pair formation of holes is more probable in the region $J'/t > 0.15$.
iii) Apparently, it is seen that superconducting condensation is not possible in the system.

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