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Effect of next-nearest-neighbour interaction on $d_{x^2-y^2}$-wave superconducting phase in 2D t-J model

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Abstract. An exact diagonalization calculation of the t-J model on 2D square cluster has been studied for the ground state properties of HTSC. Effect of next-nearest-neighbour hopping and magnetic (both antiferromagnetic and ferromagnetic) interaction on $d_{x^2-y^2}$-wave pairing has been shown. Relative strength of the next-nearest-neighbour interaction with respect to that of near-neighbour interaction for the strongest $d_{x^2-y^2}$-wave pairing has been estimated. A schematic phase diagram is shown. It is shown that a two-sublattice model with antiferromagnetic interaction between them and a small intra-ferromagnetic-type interaction in one sublattice favours $d_{x^2-y^2}$-wave superconductivity and moderate negative type NNN hopping adds flavours to this phase.

Keywords. High-T_c superconductivity; t-J model; d-wave; local singlet.

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1. Introduction

After the discovery of high-T_c superconductors [1], a large number of theoretical and experimental works have been done to explain the phenomena [2–4] but many of the unusual properties are still unexplained. Theoretical studies in this context are in the channel where electrons correlate strongly [2]. There are two well-studied models, the Hubbard model and the t-J model, for strongly correlated electrons [3,5–8]. Different techniques, from analytic to numerical, have been applied to study these models for superconductivity. The importance of numerical studies lies in the fact that most of the realistic models of strongly interacting character use different approximations to give diverse results. In this class of systems the strength of the interactions between particles is comparable to or larger than their kinetic energy, i.e., any theory based on a perturbative expansion around the noninteracting limit is at the least questionable.

One key element of BCS mechanism of superconductivity is electron pairing [9]. There is evidence that the symmetry of pairs in high-T_c materials are in the $d_{x^2-y^2}$

channel [10] for doping near to half-filling. There are also evidences that near quarter-filling s-wave pairing exists [11]. The results are thus controversial. Most of the theoretical studies have been done for the single-band Hubbard model [12–14] (SHM) for its simplicity. Actual systems, however, inevitably have the orbital degeneracy. In the last few years the Hubbard model with orbital degeneracy has been extensively studied using various methods such as the Gutzwiller approximation [15,16], the slave-boson theory [17,18], the dynamical mean field approximation [19] etc.

Another well-accepted model is the two-dimensional (2D) t-J model [3,20]. It was shown that the two-dimensional t-J model, for the physical parameter range $J/t \approx 0.4$ reproduces the main experimental qualitative features of the high-T_c copper oxide superconductors [21]. Moreover, there are evidences of a close relation between phase separation and superconductivity in the t-J model [22,23].

It is also a well-established fact that the inclusion of next-nearest-neighbour interactions have important effects. It was shown rigorously by Tasaki [24] that the pure Hubbard model extended by hopping of electrons between nearest- and next-nearest-neighbouring sites with dispersive bands exhibits ferromagnetism at zero temperature for finite Coloumb interaction.

In [25], the ground state phase diagram of the extended Hubbard model containing nearest- and next-to-nearest-neighbour interactions has been investigated in the thermodynamic limit using an exact method. It has been found that taking into account local correlations and adding next-to-nearest-neighbour interactions both have significant effects on the position of the phase boundaries. The importance of nearest- and next-nearest-neighbour off-site interactions (diagonal and off-diagonal) has also been emphasized both from experimental [26] and theoretical sides [27]. Though the values of these interactions between clusters associated to next-nearest-neighbouring sites are not known, it is obvious that these interactions are present in real materials. The interaction values decrease with increasing interatomic distances in the lattice and have important consequences on the characteristics of the strongly correlated electron systems. Hence, the study of the effect of next-nearest-neighbour interactions by an exact method is important for these materials.

In this paper, we have studied 8-site square cluster using exact diagonalization method. Here we have considered both next-nearest-neighbour hopping and magnetic interaction. Our calculations are based on cluster with quarter filling.

2. Formulation

As the simplest model to describe the physics of CuO_2 planes, we have employed here the single band, two-dimensional t-J Hamiltonian [20]

$$H = J \sum_{\langle i,j \rangle} \left[\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j \right] - t \sum_{\langle i,j \rangle \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + \text{ H.c.}). \tag{1}$$

The summations extend over all pairs of nearest-neighbour site on a simple two-dimensional square lattice; $c_{i\sigma}$ are the usual fermion operators (σ = spin); t is the near-neighbour (NN) hopping amplitude; J is the near-neighbour antiferromagnetic interaction; $\vec{S}_i$ are spin-$\frac{1}{2}$ operators at the sites i and in the Hilbert space associated with the Hamiltonian double occupancy of a site is forbidden. To take the contribution of next-nearest-neighbour (NNN) hopping an extra term H_2 is also added with eq. (1).

$$H_2 = -t_2 \sum_{[p,q]} (c^{\dagger}_{p\sigma} c_{q\sigma} + \text{H.c.}). \tag{2}$$

For the contribution of next-nearest-neighbour magnetic interaction another extra term H_3 is also added with eq. (1).

$$H_3 = J_2 \sum_{p,q} \left[\vec{S}_p \cdot \vec{S}_q - \frac{1}{4} n_p n_q \right], \tag{3}$$

where $[p, q]$ denotes a pair of sites along the diagonals of the $\sqrt{8} \times \sqrt{8}$ cluster, t_2 the corresponding hopping amplitude and J_2 the corresponding magnetic interaction amplitude.

In our exact diagonalization study, the ground state is taken in the form

$$|\psi_0\rangle = \sum_m c_m |\phi_m\rangle, \tag{4}$$

where the basis are formed by defining S_z at every site, as $|\phi_k\rangle = |\uparrow 0 \downarrow \uparrow \downarrow 000\rangle$.

The coefficients c_m are the solutions of the system of equations

$$M \begin{pmatrix} c_1 \\ \vdots \\ c_N \end{pmatrix} = 0, \tag{5}$$

where N is the dimension of the Hilbert space and M is a symmetric matix with a typical element as $M_{mn} = [\langle \phi_m | H | \phi_n \rangle - \lambda \delta_{mn}]$; λ being the lowest solution of the eigenequation

$$\det M = 0. \tag{6}$$

To search for indications of superconductivity and the effect of next-nearest-neighbour interaction we have used the singlet pairing operator $\Delta_i = c_{i\uparrow}(c_{i+x,\downarrow} + c_{i-x,\downarrow} \pm c_{i+y,\downarrow} \pm c_{i-y,\downarrow})$; where + and − correspond to extended s- and $d_{x^2-y^2}$-waves respectively. The pairing–pairing correlation function $c(m) = \sum_i \langle \Delta^{\dagger}_i \Delta_{i+m} \rangle$ and susceptibility $X^{d,s}_{\text{sus}} = \sum_m c(m)$ have been calculated [3]; here d and s represent d-wave and extended s-wave respectively. $\langle \cdots \rangle$ denotes expectation values in the ground state, which is obtained by our exact diagonalization method.

In our calculations total projection of the spin $S^z_{\text{total}} = 0$ and we have implemented translation symmetry to reduce the number of basis.

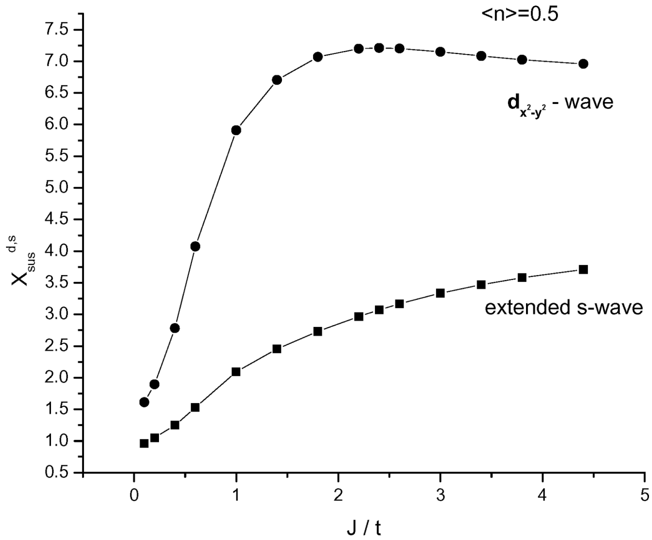

Figure 1. Comparison of $d_{x^2-y^2}$-wave and extended s-wave pairing susceptibilities as a function of J/t in an 8-site square cluster.

3. Results and discussions

Our calculations are on quarter filling ($\langle n\rangle = 0.5$). Figure 1 shows $d_{x^2-y^2}$-wave and extended s-wave susceptibilities with respect to J/t. It is apparent from the figure that $d_{x^2-y^2}$ pairing is the dominant channel of pairing and the susceptibility has a peak in the vicinity of $J/t = 2.4$, suggesting strong pairing correlations. The exchange interaction, J, stabilizes the local singlet (different from Zhang-Rice singlet) if two spins are coupled while leading to AF state in the bulk system of multiple spins [28]. The enhancement of $d_{x^2-y^2}$-wave with increased J confirms the coexistence of antiferromagnetism and superconductivity [29]. Our aims here are to investigate the effect of next-nearest-neighbour interaction in this coexisting phase.

Following the aim of this paper we now inspect the effect of next-nearest-neighbour interactions at $J/t = 2.4$. In figure 2 we have plotted $d_{x^2-y^2}$ susceptibility with respect to $|t_2|/t$ (in our calculations we have taken $t_2 < 0$; for hole-doped cuprate system NNN hopping is negative [30,31]). Figure 2 suggests that NNN hopping enhances the strength of $d_{x^2-y^2}$ pairing up to $|t_2| \sim t$. It has been shown [32] that two holes do not bind unless J exceeds a certain value. So, the possible contribution of NNN hopping is to increase the effective J/t, which might greatly enhance superconductivity. With the increase in t_2/t, mobility of the holes increases, and this diagonal movement of holes effectively accumulates those local singlets, hence coexistence of antiferromagnetism and superconductivity. When t_2/t is increased further, holes should become more mobile and the accumulation tendencies will diminish. This is quite similar to stripe stability [33].

Figure 3 shows the variation of $d_{x^2-y^2}$-wave pairing susceptibility with next-nearest-neighbor antiferromagnetic interaction (J_2). This result tells that

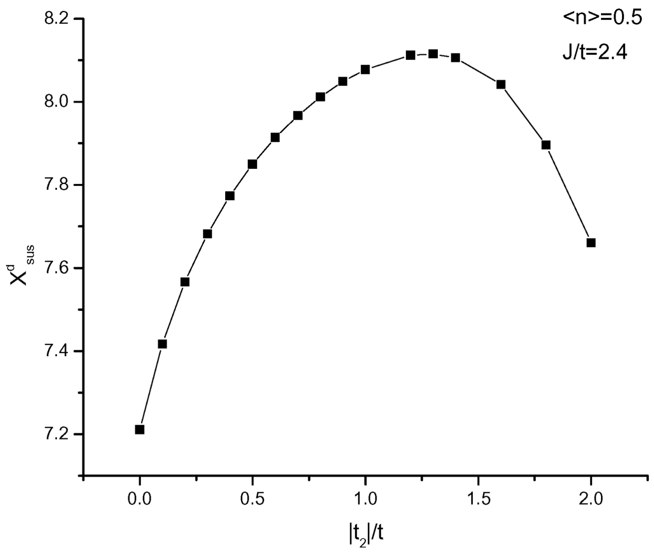

Figure 2. Variaton of $d_{x^2-y^2}$-wave susceptibility with NNN hopping.

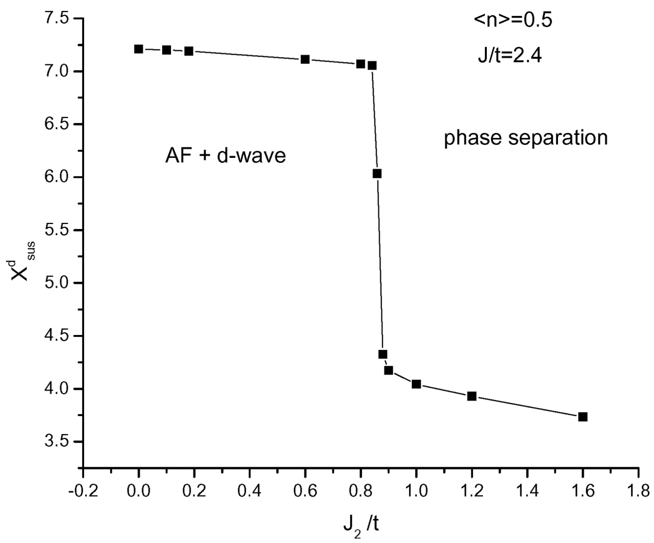

Figure 3. Phase diagram for the ground state of function J_2/t; J_2 is the next-nearest-neighbour antiferromagnetic interaction.

antiferromagnetic interaction above 40% of J, along the diagonals of the elementray plaquettes destroy the $d_{x^2-y^2}$ superconducting phase. As this type of interaction also destroys long-range AF order, it is natural to consider the coexistance of antiferromagnetism and $d_{x^2-y^2}$-wave superconductivity [28] in the region $J_2 \leq 0.4J$. This conclusion can be reached as, after that value of NNN antiferromagnetic

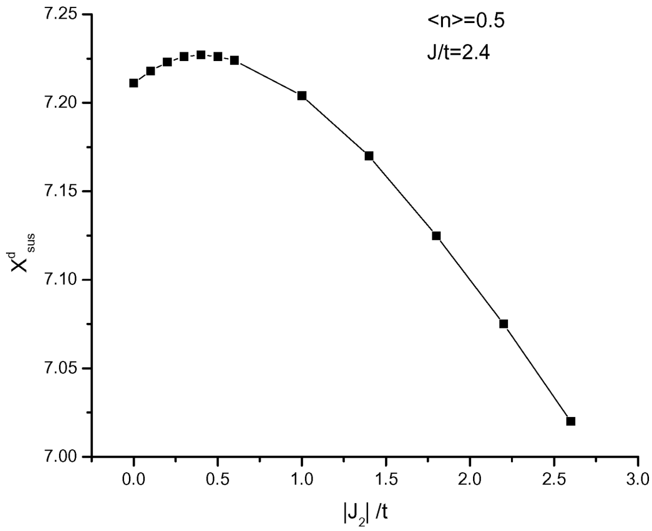

Figure 4. Pairing susceptibility for $d_{x^2-y^2}$-wave for different values of next-nearest-neighbour ferromagnetic-type interactions.

exchange interaction local singlet breaks down and ferromagnetic links grow which destroy superconductivity. So, it can be concluded here that NNN antiferromagnetic interaction can be considered as an attractive interaction in the Hamiltonian.

Figure 4 shows variation of $d_{x^2-y^2}$ susceptibility with ferromagnetic interaction along the plaquettes diagonal, i.e. considering the two sublattices independently, we find that a small ferromagnetic interaction (about 17% that of the nearest-neighbour AF interaction) favours $d_{x^2-y^2}$-wave state, as this kind of interaction stabilizes long-range antiferromagnetic order, i.e. accumulate local singlets. With larger values of ferromagnetic interaction, superconductivity diminishes because correlation between the two sublattices diminishes.

Summarizing, using our exact diagonalization study we shall say that the two-sublattice model with antiferromagnetic interaction between them and small intra-ferromagnetic-type interaction in one sublattice favours $d_{x^2-y^2}$-wave superconducting phase and negative-type NNN hopping adds flavour to this phase.

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