

Role of next-nearest-neighbour hopping in the internal structure of the ground state and finite temperature quantities of 2D t-J model

N S MONDAL* and N K GHOSH

Department of Physics, University of Kalyani, Kalyani 741 235, India

*Corresponding author. E-mail: nil16mon@gmail.com

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Abstract. An exact diagonalization calculation for a small cluster in the two-dimensional t-J model has been studied to calculate two-hole correlation. Calculations reveal dominant hole-hole correlation for holes sitting on next-nearest-neighbour (NNN) sites and critical coupling occurs at $J/t = 0.8$. With the increase in negative-type NNN hopping, correlation decreases at NNN sites whereas it increases at other sites. The thermodynamic properties such as entropy and specific heat are studied as functions of temperature with various NNN hopping strength. Results show that with the inclusion of negative NNN hopping, the system becomes more ordered. A qualitative transition temperature region has been estimated. It is shown that with the increase in NNN hopping strength, T_c increases. Specific heat results show non-Fermi liquid-type behaviour of the system. All our calculations establish the importance of negative-type NNN hopping.

Keywords. High-temperature superconductivity; t-J model; thermodynamic property; T_c .

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1. Introduction

It has been established that many physical properties of the strongly correlated electron systems and electronic models of materials exhibiting superconductivity at high temperatures (HTSC) can be described by 2D t-J model [1,2]. Various numerical methods ranging from Lanczos diagonalization [3,4] of small clusters to density matrix renormalization group studies [5,6] and quantum Monte Carlo (QMC) simulations of two-dimensional lattices [7,8] have been used to study Hubbard and t-J models. It is observed that the numerical studies with these basic models can exhibit antiferromagnetism, stripes, pseudogap behaviour and $d_{x^2-y^2}$ pairing. 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.

QMC method is most useful for the evaluation of static and some dynamical quantities at finite temperature. QMC method is also plagued by the minus sign problem in the most challenging regimes of correlated systems. On the other hand, the exact diagonalization of small correlated systems is free from the difficulties due to the fermionic sign problem. The deficiency of the method is in the relative smallness of the system sizes, though these small systems can also capture the ingredients of different models of strongly correlated electrons.

The inclusion of the next-nearest-neighbour interactions has important effects. QMC studies by Hlubina *et al* [9] confirmed this fact for finite temperatures too. The ground state phase diagram of the extended Hubbard model containing nearest and next-to-nearest-neighbour interactions has been investigated [10] and it is found that both the interactions have significant effects on the position of the phase boundaries. In our previous work [11], it has been shown that NNN hopping enhances the strength of $d_{x^2-y^2}$ pairing. Also, NNN antiferromagnetic interaction can be considered as an attractive interaction in the Hamiltonian.

Finite-temperature properties of the t-J model is a matter of intensive study [12–14]. In [12], authors evaluated finite-temperature static and dynamical quantities in small many-body quantum systems using the Lanczos diagonalization technique. They also investigated [13] the thermodynamic properties of the planar t-J model and observed non-Fermi liquid behaviour in a wide range of doping concentrations. In [14], authors studied the thermodynamic properties of the t-J model on the square lattice using numerical linked-cluster (NLC) algorithms. They suggested to combine NLC with Lanczos method to extend it to still lower temperatures.

The aim of the present paper is two-fold. First, we would like to extend the previous calculations of ref. [11] for the internal structure of the ground state. Second, the effect of NNN interaction on the finite-temperature quantities like entropy and specific heat is studied. An attempt has been made to compare our findings with a few existing results.

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 [2]

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

The summations extend over all pairs of nearest-neighbour sites on a simple two-dimensional square lattice. $c_{i\sigma}$ are the usual fermion operators ($\sigma = \text{spin}$), 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 in eq. (1).

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

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

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

$$|\psi_0\rangle = \sum_m c_m |\phi_m\rangle, \quad (3)$$

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

$$M \begin{pmatrix} c_1 \\ \vdots \\ c_N \end{pmatrix} = 0, \quad (4)$$

where N is the dimension of the Hilbert space and M is a symmetric matrix 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

$$\det M = 0. \quad (5)$$

To study the spatial distribution of mobile holes in the ground state, here we have calculated the hole-hole correlation function, defined as [15,16]

$$P_{hh}(d) = \frac{1}{N_h N_E(d)} \sum_{\langle i, j \rangle} \langle (1 - n_i)(1 - n_j) \delta_{|i-j|, d} \rangle, \quad (6)$$

where N_h is the total number of holes and $N_E(d)$ is the number of equivalent sites a distance d from some chosen site. Also, here we have calculated average hole-hole correlation over all lattice distances by $P_{hh}^{avg} = \frac{P_{hh}(d)}{5}$ (five different lattice distances in an 8-site square cluster).

In this paper, we consider the entropy per lattice site as

$$S = \frac{1}{N} \left(\ln Z + \frac{\langle H \rangle}{T} \right), \quad (7)$$

where N is the number of lattice sites.

Finally, we have calculated low-temperature specific heat defined as

$$C_v = k_B \beta^2 \frac{\partial^2}{\partial \beta^2} \ln Z, \quad (8)$$

where $Z = \sum_{\alpha} e^{-\beta E_{\alpha}}$, the sum is taken over all eigenstates, E_{α} s are the eigenvalues and $\beta = 1/k_B T$, k_B being the Boltzmann constant.

3. Results and discussions

To study the spatial distribution of mobile holes, we have considered the two-hole ground state of the 8-site square cluster. Figure 1 shows the variation of average

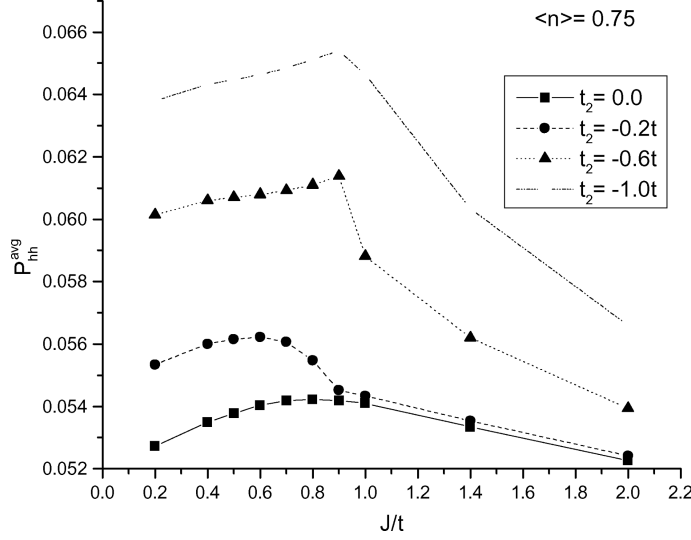


Figure 1. Average value of hole–hole correlation function as a function of J/t , over all lattice distances in the 8-site square cluster.

hole–hole correlation (P_{hh}^{avg}) with J/t for different values of NNN hopping. It is apparent from the figure that P_{hh}^{avg} increases with J/t at low temperature and has a peak at $J/t \sim 0.8$, suggesting the formation of a bound state in that region. This may be because each individual hole breaks four antiferromagnetic links in an otherwise undoped antiferromagnet, which cost some energy. Two holes stabilize the lost energy by sharing a common link and here critical coupling is $J/t \sim 0.8$. The hole–hole correlation increases with the increase of NNN hopping, confirming our previous result [11].

Figure 2 shows the variation of hole–hole correlation with $|t_2|/t$ for different distances between the holes in the lattice at $J/t = 0.8$. Without NNN hopping, hole–hole correlation is dominant at distance $\sqrt{2}$, but in general, the correlation decreases with distance. This is in good agreement with the previous data on 4×4 cluster [17,18]. So, in the parameter region believed to be appropriate for the high- T_c materials, the largest probability of finding two holes at a time is at the NNN sites. With the inclusion of t_2 , the increased diagonal mobility of the holes decreases the correlation between NNN sites but increases it between other sites. For large values of NNN hopping, the correlation becomes almost constant for $d = \sqrt{2}, 2, \sqrt{5}$. Strong correlation at distance 1 for large t_2 is unphysical.

We have discussed the dependence of entropy on temperature for different t_2 . This is shown in figure 3. At $\langle n \rangle = 0.5$ and $J/t = 2.4$, d -wave pairing correlation is maximum [1,11]. So here we have calculated entropy at these ranges. Figure 3 clearly shows that with the increase in $|t_2|$ up to a range of physical interest, we get more ordered phase. This result states the importance of the inclusion of NNN hopping term. With the increase in temperature, the difference between different t_2 curves becomes broad, and in the range $0.3 < T/t < 1.2$, the difference is maximum and after that all curves converge to the same curve. In figure 3 we

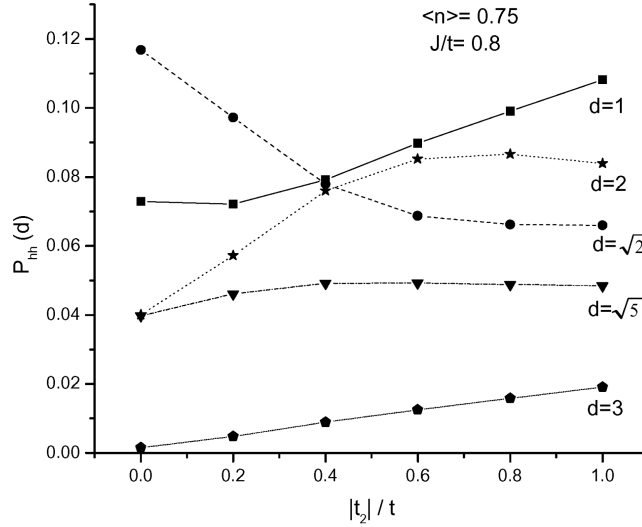


Figure 2. Hole-hole correlation function for two holes on 8-site square cluster. The separation between holes (d) is given in the units of lattice constant.

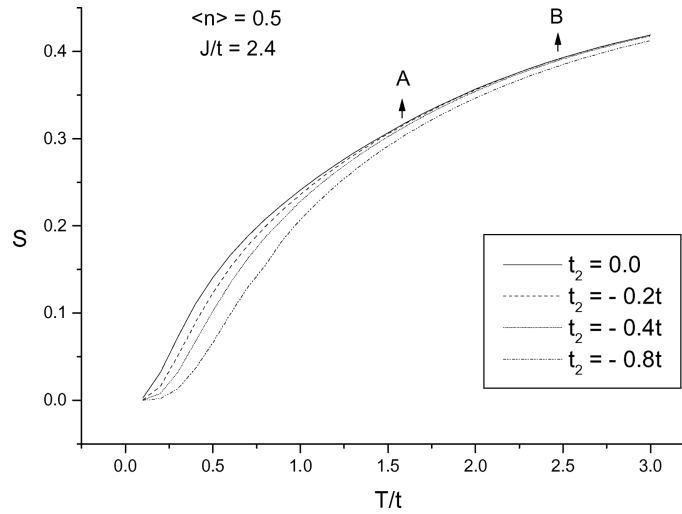


Figure 3. Entropy as a function of temperature for different values of NNN hopping strength. Here we have considered quarter filling case. Points A and B roughly represent the meeting point of two curves having $t_2 = -0.2t$ and $t_2 = -0.4t$ with $t_2 = 0.0$ curve.

have also marked two points A and B, from which we can identify that at $\langle n \rangle = 0.5$ filling transition temperature (T_c) is $T_c \sim 1.6t$ for $t_2 = -0.2t$ and for $t_2 = -0.4t$, T_c is $\sim 2.5t$ and for other higher values of t_2 , T_c takes higher values, i.e. with the increase in NNN hopping strength, transition temperature increases. This result might be interesting considering the experimental interest to increase transition temperature.

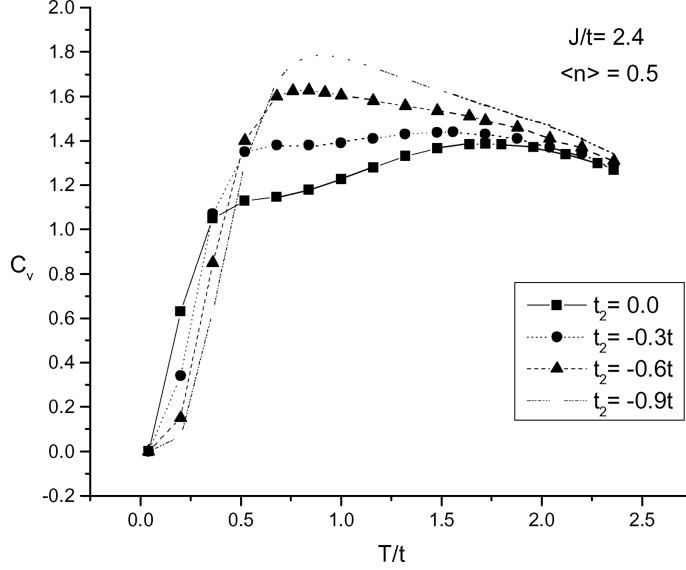


Figure 4. Specific heat as a function of temperature for different values of NNN hopping strength.

In figure 4 we present the temperature dependence of the specific heat C_v (k_B is taken as unity) at different NNN hoppings. In this calculation, J/t is taken as 2.4, where d -wave pairing correlation is maximum for $\langle n \rangle = 0.5$.

At low temperatures $C_v \sim T^2$ and exhibits a maximum which is prominent for higher NNN interaction. The peak is due to the thermal activation of the spin degrees of freedom with an exchange energy scale present in the doped system. Figure 4 clearly shows non-Fermi liquid behaviour of the t - J model in a small cluster.

Summarizing, our exact diagonalization calculations in the two-dimensional t - J model reveal dominant hole-hole correlation for holes situated in the next-nearest-neighbour (NNN) sites and critical coupling occurs at $J/t = 0.8$, and the region is quite near to the region believed to be appropriate for CuO_2 planes. With the increase in negative-type NNN hopping, correlation decreases at NNN sites whereas it increases at other sites. Results show that with the inclusion of negative NNN hopping, the system becomes more ordered. A qualitative transition temperature region has been estimated for different NNN hopping strength which shows that with the increase in NNN hopping strength, transition temperature increases. Specific heat results show non-Fermi liquid-type behaviour of the system. All our calculations establish the importance of negative-type NNN hopping interaction.

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