Three site hole hopping in high \( T_C \) superconductors

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Dynamics of holes containing three site hole hopping and parallel hopping has been studied. A new type of hole-hole correlation is discussed. The effect of three site term and parallel hopping term on hole-hole correlation has been investigated.

Keywords: High \( T_C \) superconductors, Superconductors, Three site hole hopping

1 Introduction

In high \( T_C \) superconducting oxides like \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) and \( \text{YBa}_2\text{Cu}_3\text{O}_{6+\delta} \), there appears antiferromagnetic insulating phase in the vicinity of superconducting phase. When holes are introduced into an antiferromagnetic (AF) insulator \( \text{La}_2\text{CuO}_4 \), AF phase rapidly disappears and gives rise to superconducting phase\(^1\). Pairing of holes is caused due to strong correlation on CuO\(_2\) plane. Schrieffer et al.\(^2\) have discussed spin bag pairing between holes. Anderson\(^3\) proposed a resonating valence bond state as the magnetic state after AF state disappears. It was suggested that the dynamics of holes is responsible for the mechanism of the high \( T_C \) superconductivity.

The model suitable for this mechanism is the t-J model, which is Hubbard model in strong correlation limit. Hole-hole correlation have been studied in a two dimensional t-J model by Bonca et al.\(^4\). They pointed out that this correlation is repulsive as well as attractive in nature depending on \( J \) values. The 2D Hubbard model was studied by Sorrela et al.\(^5\) and they found repulsive hole-hole correlation for \( U=0 \) to 60. The hole-hole correlation function in the 2D Hubbard model was investigated in low doping regime using Monte Carlo simulation and Lanczos diagonalisation. They pointed out that at \( U=4 \) correlations are relatively weak-coupling like, for large \( U \) they behave similar to hard core bosons.

In the present paper, different ways of hopping of holes situated on different sites have been studied. The hopping mostly takes place between oxygen and copper atomic sites and sometimes directly between oxygen atomic sites. Normally, hopping takes place between the nearest neighbour atomic sites. But in a doped superconductor higher order hopping and next nearest neighbour \((n-n)\) hopping also become important especially at low temperature. Three site hopping and next nearest hopping have been discussed by various researchers\(^5-7\). The possible various types of hopping of holes are shown in Fig. 1(a-e). Figure 1(a) is normal \( n-n \) hopping, Fig. 1(b) shows next \( n-n \) hopping, Fig. 1(c) shows three site hopping, Fig. 1(d) is four site hopping which is anticlockwise and cyclic and finally Fig. 1(e) shows parallel hopping. Here, we find that a new correlation function \( <(\hat{h}_i^+ \ h_k)> \) exists in the case of higher order hopping of holes. The nature of this correlation function is more or less opposite to the normal correlation \( <(\hat{h}_i^+ \ h_k)> \). It means that when \( <(\hat{h}_i^+ \ h_k)> \) is repulsive, \( <(\hat{h}_i^+ \ h_k)> \) shows attractive nature and vice versa. We have used Green function technique\(^8\) and low temperature series expansion method for two dimensional and half spin system.

2 Model Hamiltonian

Since we are interested in the dynamics of holes in high \( T_C \) superconductors, we will not discuss the anti-
ferromagnetic spin part of the model. Hamiltonian for such a system containing various types of interaction can be written as:

\[ H = T_1 + T_2 + T_3 \]  \hspace{1cm} \text{(1)}

where

\[ T_1 = -\alpha_1 \sum_{q=0}^{N} (h^+_i h^+_j - h^+_j h^+_i) \]

\[ T_2 = -\alpha_2 \sum_{q=0}^{N} (h^+_i h^+_j)^2 \]

\[ T_3 = \alpha_2 \sum_{q=0}^{N} (h^+_i h^+_j)(h^+_j h^+_k) \]

where \( h^+_i \) and \( h^+_j \) are hole operators at i and j sites, \( \alpha_1 \) and \( \alpha_2 \) are parameters. First term is standard bilinear hopping interaction between the nearest neighbours. Second term shows interaction between n-n sites i and j due to parallel hopping. The last term indicates three sites interaction for hopping of a hole. Terms \( T_2 \) and \( T_3 \) arise due to perturbation expansion of \( U/t \) where \( U \) is Coulomb term which is important for doped superconductors at low temperature. In general, pair hopping of holes takes place in three site interaction. The formation of hole pair indicates the attractive hopping of holes takes place in three site interaction. The attractive force between two n-n holes is based on the counting of numbers of destructed antiferromagnetic bonds of spins through the introduction of two holes. After Fourier transform, the above Hamiltonian can be written as:

\[ H = (t/\sqrt{N}) \sum_k h^+_k h^+_{-k} q_k \]

\[ + (\alpha_2 \frac{t}{\sqrt{N}} \sum_k (h^+_k h^+_{-k}) (h^+_{-k} h^+_k) q_k^2 \gamma_{k-k} \gamma_{k-k}^\ast \]  \hspace{1cm} \text{(2)}

where

\[ h^+_k = \frac{1}{\sqrt{N}} \sum_i h^+_i \exp(i \vec{k} \cdot \vec{R}_i) \]

\[ h_{-k} = \frac{1}{\sqrt{N}} \sum_j h_j \exp(i \vec{k} \cdot \vec{R}_j) \]

\[ t_q = \sum_{j} t_{ij} \exp(iq(\vec{R}_i - \vec{R}_j)) \]

\[ t_q = t z \gamma_q \]

where \( \gamma_q \) is the total number of sites.

\[ \gamma_q = (1/z) \sum_{\delta} \exp(iq\delta) \]

where \( \delta \) is the sum over nearest neighbours and \( z \) is the number of nearest neighbours.

F.T. \[ [t_{ij,k}] = \sum_{i,j,k} \{ \exp(iq(R_i-R_j) \times \exp(iq(R_j-R_k)) \]

or F.T. \[ [t_{i,j,k}] = \sum_{i,j,k} \gamma_q \gamma_{k-k} \gamma_{k-k} \]

or, F.T. \[ [t_{i,j,k}] = \alpha_2 \gamma_q \gamma_{k-k} \gamma_{k-k} \]

\( N \) is the total number of sites.

\[ \alpha_2 t = \sum_{i,j,k} \text{ for } q=0 \text{ and } k'-(k-q) = 0. \]

### 3 Green Function Approach

The equation of motion for a hole green function \( [h^+_k, h^+_q] \) is given by:

\[ E[h^+_k, h^+_q] = \frac{[h^+_k, h^+_q]}{2\pi} + [[h^+_k, H], h^+_q] \]  \hspace{1cm} \text{(3)}

Substituting the values of H from Eq. (2) into Eq. (3), we get:

\[ E[h^+_k, h^+_q] = 1/2 \pi - (tz/\sqrt{N}) \]

\[ \times \sum_{k} \sum_{k'} \sum_{k''} \sum_{k} \{ [h^+_k, h^+_q], [h^+_q, h^+_q], [h^+_q, h^+_q] \} \]

\[ \times \sum_{k} \sum_{k'} \sum_{k''} \sum_{k} \{ [h^+_k, h^+_q], [h^+_q, h^+_k], [h^+_k, h^+_k] \} \]

\[ \gamma_{k-k} \gamma_{k-k}^\ast \]  \hspace{1cm} \text{(4)}

where \( [h^+_k, h^+_k] = 1 \).

Using following Poissons bracket relation, commutation relations and decoupling of higher order Green’s function to the Eq. (4):

\[ [h^+_k, h^+_k] = 0, [h^+_k, h^+_q] = 0 \]

\[ [h^+_k, h^+_k h^+_q] = [h^+_k, h^+_k] h^+_q + h^+_k [h^+_k, h^+_q] \]

\[ [h^+_k, (h^+_k h^+_q)] h^+_k = [h^+_k, h^+_k] h^+_q h^+_k \]

\[ + h^+_k h^+_k h^+_q h^+_k \]

\[ [h^+_k, h^+_q h^+_k] = 0, [h^+_k, h^+_q] = 0 \]

\[ [h^+_k, h^+_q h^+_k] = \delta_{k-k} [h^+_k, h^+_k] = \delta_{k-k} \]

\[ \langle h^+_k, h^+_q h^+_q \rangle = \langle h^+_k, h^+_q \rangle \langle h^+_q, h^+_q \rangle \]

\[ \langle h^+_k, (h^+_k h^+_q) (h^+_k h^+_q) \rangle = \langle h^+_k, h^+_q \rangle \langle h^+_q, h^+_q \rangle \]

\[ \langle h^+_k, (h^+_k h^+_q) (h^+_q h^+_k) \rangle = \langle h^+_k, h^+_q \rangle \langle h^+_q, h^+_k \rangle \]

\[ \langle h^+_k, (h^+_k h^+_q) (h^+_k h^+_q) \rangle = \langle h^+_k, h^+_q \rangle \langle h^+_q, h^+_k \rangle \]
\[ \phi \text{=} h_k^+ > h_{k-q} > < h_k^+ h_{k-q} > \text{ for } k \not= k' \]

we get,

\[ \text{E} < h_k^+ h_{k-q} > = \frac{1}{2\pi} - \left( \frac{t \mathcal{Z}}{\sqrt{N}} \right) \sum \gamma_q \gamma_q' \]

\[ \text{where } \gamma_q = \gamma_q' \]

From Eq. (5), we have the expression for Green’s function:

\[ G(k) = \frac{1}{2\pi(E - E_q)} \]  

where \( E_q \) is the required hole energy which can be written as:

\[ E_q = -(t\mathcal{Z}) \sum \gamma_q \gamma_q' \]

\[ \times \sum (h_k^+ h_{k-q}^2) > a_2 (t/\sqrt{N}) \]

\[ \times \sum (h_{k-q}^2) > a_1 \gamma_q' \quad \gamma_q = -(a_2 t/\sqrt{N}) \sum < h_{k-q} > \]

\[ < h_k^+ h_{k-q} > > a \gamma_q > \]  

Hole-hole correlation-1 can be written in terms of \( qa \) at low temperature, hole-hole correlation can be approximately rewritten as:

\[ < h_k^+ h_{k-q} > = \frac{\exp(-E_q/kT)}{\exp(-E_q/kT) + \exp(-E_q/kT)} qa + (qa^2) + (qa^4) + ... \]  

where \( K \) is Boltzmann constant and \( T \) is absolute temperature.

Substituting the value of \( E_q \) from Eq. (8) and integrating one by one for two dimensional lattice in terms of \( qa \) at low temperature, hole-hole correlation can be approximately rewritten as:

\[ < h_k^+ h_{k-q} > \]

\[ \text{Occupation number } \phi(k) \text{ is given by the relation:} \]

\[ \phi(k) = (\exp(E_q/2kT))^{-1} \]  

Total occupation number of a system is given by:

\[ \Phi(K) = (1/N) \sum_k \phi(k) \]  

and hence

\[ \Phi^2(k) = (1/N) \sum_k \phi^2(k) = < h_k^+ h_{k-q} > \]
For small $k$, summation can be converted into integration and using Eqs (11) and (13), we get the relation for hole-hole correlation-2

$$<h^+_k h^+_q> = -a^2/2\pi \Sigma \exp(-nE_q/K'T) [(qa)^2/2! + (qa)^3/4! + (qa)^6 6! + ....]$$

substituting the value of $E_q$ from Eq. (8) into Eq. (14) and solving different integrals and finally arranging the equation for $<(h_k h_q)^2>$, we get the following relation:

$$<(h_k h_{-q})^2> = a^6/6\pi^{10} (6KT/T)^{5/3}$$

$$+ 0.1 \alpha^{9/10} (240KT/T)^{1/3} [\xi(1/2) - \xi(3/2)]$$

$$+ 2\alpha^{8}/(10\pi) (80\pi^2 KT/(T^2 \alpha^2))^{7/5}$$

$$+ (h_k h_{-q})^2 [\xi(1/2) - \xi(3/2)]$$

$$+ 3\alpha^{9}/4 (6KT/T)^{3/5} [\xi(3/2) - \xi(5/2)] + ....$$

Eqs (10) and (15) are solved by iteration method for different values of $\alpha_1$ and $\alpha_2$ together with different values of $KT/t$.

4 Results and Discussion

Figure 2 shows the variation of hole-hole correlation function $<h^+_k h^+_q>$ with $\alpha_2$, for $\alpha_1 = 0.1$ and $KT/t = 0.001$. We infer that hole-hole correlation contains the positive and negative values and it decreases sharply for smaller values of $\alpha_2 < 0.2$ and afterwards it decreases slowly up to $\alpha_2 = 0.5$ and finally, it increases from $\alpha_2 = 0.5$ to 0.9. Positive and negative values of correlation function depend on the type of sites which are under consideration. If the sites undertaken are the same, the hole-hole correlation will give out positive value otherwise its value will be negative. Since the sites have been taken at random, we get both the positive as well as negative values. Nearest neighbour hole-hole interaction is repulsive in nature while the three site interaction is attractive. When the two types of interactions are considered simultaneously, the nature of combined interaction is still repulsive hence, the value of $<h^+_k h^-_{-q}>$ increases with $\alpha_2$ up to a certain extent. When a large number of sites are considered to find the energy and hole correlation as well, three site interaction begins to dominate over $n-n$ interaction and hence, the nature of interaction becomes attractive and energy begins to increase with increase in $\alpha_2$. The decrease and increase in hole-hole correlation with increase in $\alpha_2 = \alpha j/t$ can be verified from the curves of pair structure factor $S_{nn}$ and the curves of hole-hole correlation $<n_j n_{-j}>$ for $L=16$, $N_0=2$ and $V=0$.

Figure 3 shows the variation of hole-hole correlation quadrupolar type parameter $<h_k^+ h_k>$ with $\alpha_2$ for $\alpha_1 = 0.8$ and $KT/t = 0.001$. In Fig. 3, circle (o) indicates the values of pair hole correlation for different values of $\alpha_2$ and triangle (Δ) due Ammon et al. Pair correlation and bond order correlation $<h_k^+ h_k>$ show moreover, the similar behaviour with respect to interaction parameter $\alpha_2$. Bond order correlation depends on the occurrence of two holes on the $n-n$ sites for parallel hopping. With the increase in interaction parameter, the probability of finding two holes increases and hence, the value of bond order correlation increases. Other interaction parameter $\alpha_1$ produces repulsion between hole pair and hence bond correlation.
decreases. Thus, the two interaction parameters have opposite effect on bond order correlation. For \( \alpha_2 < 0.3 \), the effect of parameter \( \alpha_1 \) on bond order correlation is dominating over \( \alpha_2 \). The effect of parameter \( \alpha_2 \) is dominating over \( \alpha_1 \) in the range \( 0.3 < \alpha_2 < 0.5 \). For \( 0.5 < \alpha_2 < 1 \) two interaction parameters nullify each other and hence, bond order correlation becomes constant.

Figure 4 indicates that hole-hole correlation-2 \( \langle h_k^+ h_k \rangle \) decreases with the increase of parallel hopping interaction parameter \( \alpha_2 \) in the range between 0.1 and 0.3 Afterwards, it changes the sign and increases up to \( \alpha_1 = 0.5 \). Finally, it decreases slowly for \( \alpha_2 \) from 0.5 to 0.6 and after that it becomes almost constant. Thus, we find that initially parameter \( \alpha_2 \) is much effective but later on its effect becomes insignificant.

Figure 5 shows the variation of \( \langle h_k^+ h_k \rangle \) with \( \alpha_1 \) for \( \alpha_2 = 0.01 \) and \( KT/t = 0.001 \). It is observed from Fig. 5 that the value of \( \langle h_k^+ h_k \rangle \) is negative and decreases linearly with the increase of \( \alpha_1 \). Fig. 6 shows temperature dependence of \( \langle h_k^+ h_k \rangle \) for \( \alpha_1 = 0.8, \alpha_2 = 0.5 \) and \( \alpha_1 = 0.8, \alpha_2 = 1.0 \) during initial period. The value of \( \langle h_k^+ h_k \rangle \) increases very slowly but in the range of \( KT/t \) between 0.008 and 0.01, the increase in more pronounced for \( \alpha_1 = 0.8 \) and \( \alpha_2 = 0.5 \) (Fig. 6). At the same time for \( \alpha_1 = 0.8 \) and \( \alpha_2 = 1.0 \), \( \langle h_k^+ h_k \rangle \) decreases sharply for \( KT/t \) between 0.001 and 0.005 and afterwards it increases rapidly up to \( KT/t = 0.01 \). Thus, three site interaction parameter \( \alpha_2 \) plays a significant role in the change of \( \langle h_k^+ h_k \rangle \) with reduced temperature \( KT/t \). Fig. 7 shows that hole-hole correlation-2 i.e. \( \langle h_k^+ h_k \rangle \) decreases almost linearly with the increase of temperature and the effect of \( \alpha_2 \) in this case seems to be negligible.

5 Conclusions

From the results and discussion of Figs (2-7), conclusions can be drawn which are as follows. Hole-hole correlation-1 i.e. \( \langle h_k^+ h_k \rangle \) contains repulsive as well as attractive nature in a doped superconductor. From the variation of \( \langle h_k^+ h_k \rangle \) with \( \alpha_2 \), one obtains that probability of finding hole pairs increases as well
as decreases. The decrease and increase in correlation function-1 with increases in reduced temperature KT/t shows that the nature of correlation changes from attractive to repulsive and vice-versa.

The decrease in hole-hole correlation-2 with increase in $\alpha_2$ indicates the reduction in probability of finding two holes due to parallel hopping. The decrease and increase in $<(h_k^+ h_k)^2>$ with $\alpha_2$ points out the change in its nature. Decrease in $<(h_k^+ h_k)^2>$ with increase in KT/t shows the reduction in finding the probability of parallel hopping.

References