Orissa Journal of Physics
ISSN 0974-8202

Vol. 24, No.1
February 2017
pp. 45-51

Theoretical study of next-nearest-neighbor electron hopping on Superconducting gap in cuprates

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Received: 1.12.2016 ; *Revised : 30.12.2016* ; *Accepted : 5.1.2017*

Abstract. We propose here a single band tight binding model Hamiltonian to describe the effect of next-nearest-neighbor (NNN) electron hopping on superconducting gap in cuprates. The Hamiltonian consists of nearest- and next- nearest- neighbor electron hopping between the copper sides. BCS type superconducting interaction is considered taking d-wave pairing symmetry. The total Hamiltonian is solved by Zubarev's Green function technique. The temperature dependent superconducting gap equation is derived from the correlation functions and are solved self-consistently technique 100×100 grid points of the electron momentum. The evolution of the order parameter is investigated by varying superconducting coupling, and next- nearest- neighbor electron hopping integrals.

Keywords: High-temperature superconductor, d-wave pairing symmetry, next- nearest-neighbor electron hopping.

1. Introduction

The understanding of the high-T_c superconductors is essentials to meet the requirement of fundamental research and their technological applications for the increase in superconducting transition temperature T_c. Recently the d-wave models have attracted a lot of attention over s-wave pairing as it provides the mechanism by which high-T_c superconductivity might be explained. The incoporation of d-wave symmetry in cuprates does not necessarily specify a high-T_c mechanism. It does not impose well defined constraints on possible models. While the spin fluctuation pairing mechanism leads naturally to an ordered parameter with d-wave symmetry, the conventional BCS electron-phonon pairing interaction give rise to s-wave superconductivity. The relevance of phonon in high-T_c superconductivity is still a topic of great controversy. However, there is much experimental evidence for significance involvement of phonon's in superconductivity of cuprates [1,2]. One key element of BCS mechanism of superconductivity is electron pairing [3]. Of course there are evidences of s-wave pairing near quarter filling that near quarter-filling *s*-wave pairing exists [4].However there is also evidence of the symmetry of pairs in high-T_c materials in the d_{x2-y2} channel [5] for doping near to half-filling. It is also a well-established fact that the inclusion of next-nearest-neighbor interactions have important effects [6]. It was shown rigorously by Tasaki [7] that when pure Hubbard model is extended by hopping of electrons between nearest- and next-nearest-neighboring sites with dispersive bands it exhibits ferromagnetism at zero temperature for finite Coloumb interaction.

Zs. Szabo in his analysis [8] investigated the ground state phase diagram of the extended Hubbard model containing nearest- and next-to-nearest-neighbor interactions in the thermodynamic limit using an exact method. It was found that both the local correlations and next-nearest-neighbour interactions have significant effects on the position of the phase boundaries. The importance of nearest- and next-nearest-neighbor off-site interactions (diagonal and off-diagonal) has also been emphasized both experimentally [9] and theoretically [10]. Though the values of these interactions between clusters associated to next-nearest- neighboring 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 strongly correlated electron systems. Hence, the study of the effect of next-nearest- neighbor interactions by an exact method is important for these materials.

In cuprates, SC is known to occur only in a narrow concentration range in the region of x=0.15 as against the hole doped predecessor like $La_{2-x} Sr_x CuO_4$ in which SC occurs for a fairly wide range of doping: $0.05 \leq x \leq 0.25$. Besides, SC has not been observed for $Gd_{2-x} Ce_xCuO_4$ although T^* structure forms in the range: $0 \leq x \leq 0.15$. It is not yet understood why many cuprates with familiar CuO_2 planes are not superconducting [11-13] although it is established that the CuO_2 planes play an important role in the SC of cuprates. The study of such cuprates is of particular interest because it is likely to offer important clues to the behaviour of their superconducting counterparts. However in recent studies [14-15] high-T_c superconductors such as ($R_{2-x} M_x CuO_4$) (R = Nd , Pr , ...,M = Sr , Ce , . . .) compounds have received a considerable attention, because they happened to be electron carrier superconductors. We would therefore like to undertake a theoretical study on the next-nearest neighbor electron hopping on superconducting gap in cuprates.

We proposed here a single band tight binding model with nearest neighbor (NN) and next- nearest –neighbour (NNN) electron hopping for quasi-square lattice. In order to study the effect of NNN electron hopping on superconducting gap for d-wave pairing symmetry. We describe the theoretical model in section 2 and the calculations for order parameter in section 3. The results and discussion are presented in section 4 and finally the conclusion is given in section 5.

2. Theoretical Model

We consider here a tight binding model Hamiltonian including tight binding terms which can be written as

$$H = H_C (\pm \eta) + H_{SC}$$

$$H = \sum_{k,\sigma} \varepsilon_k \, c^{+}_{k,\sigma} c_{k,\sigma} - \sum_{k,\sigma} \Delta_c(k)(c^{+}_{k,\uparrow} \, c^{+}_{-k,\downarrow} + c_{-k,\downarrow} c_{k,\uparrow}) \quad (1)$$

The first term in H describes the hopping of copper d- electrons between adjacent sites. Here $c^{+}_{k\sigma}$ ($c_{k\sigma}$) is the creation (annihilation) operator of the conduction electrons of copper atoms. The hopping takes place between the neighboring sites of copper with the band dispersion energy of conduction electrons .

$$\varepsilon_k = -2t_1 [(1 + \eta) \cos k_x + (1 - \eta) \cos k_y] - 4t_2 \cos k_x \cos k_y - \mu \quad (2)$$

Where ε_k is the single band dispersion energy of conduction e^- within tight – binding approximation in the orthorhombic lattice. Where t_1 and t_2 are the nearest-neighbor (NN) and next – nearest neighbor (NNN) hopping integrals of electrons with t_1 and t_2 as the NN and NNN hopping integrals in the square lattice and also k_x and k_y are the components of the electron momentum $\vec{k}$ and μ is the chemical potential.

The second term represents the s- wave BCS type mean field superconducting interaction present in the conduction band. The momentum dependent superconducting (SC) gap parameter Δ_C (k) is defined as

$$\Delta_C (k) = - \sum_{k'} V^s \left(\vec{k} - \vec{k'}\right) < c^{+}_{k',\uparrow} c^{+}_{-k',\downarrow} > \quad (3)$$

Where the effective superconducting potential $V^s\left(\vec{k} - \vec{k'}\right)$ = $V_0 f_k f_{k'}$, f_k = (cos k_x - cosk_y) for d- wave and superconducting gap is given by Δ_C (k) = $\frac{V_0(\mathrm{T})}{2} f_k$.

3. Calculation of order Parameters

In order to find the expression for superconducting order parameter, we have to calculate their corresponding correlation functions from the corresponding single particle electron Green's functions. We define four electron green's functions for conduction electrons are given as follows,

$$A_1(k, \omega) = \ll c_{k\uparrow};\, c_{k\uparrow}^{+} \gg_{\omega} \quad (4)$$

$$A_2(k, \omega) = \ll c_{-k\downarrow}^{+};\, c_{k\uparrow}^{+} \gg_{\omega} \quad (5)$$

$$A_3(k, \omega) = \ll c_{k\downarrow};\, c_{k\uparrow}^{+} \gg_{\omega} \quad (6)$$

$$A_4(k, \omega) = \ll c_{-k\uparrow}^{+};\, c_{k\uparrow}^{+} \gg_{\omega} \quad (7)$$

These conduction electron Green's functions are analytically solved separately. When the denominator terms in the Green's functions are equated to zero, we obtain two quasi-particle bands with energy dispersion written as,

$\omega_{1k} = E_{kc}$ and $\omega_{2k} = - E_{kc}$.

Where the superconducting dispersion band is written as $E_{kc}^2 = \varepsilon_k^2 + \Delta^2$.

The superconducting gap equation is calculated from the correlation functions obtained from the single particle superconducting Green's function and the SC gap equation is written as,

$$1 = \frac{g}{\pi^2} \iint_0^{\pi} dk_x\, dk_y \left[\frac{2\mathrm{t}_1 (f_k)^2}{E_{kc}} \tanh\left(\frac{\beta E_{kc}}{2}\right) \right] \quad (8)$$

where f_k = (cos kx − cos ky)

Different quantities involved in Eqs. (8) is made dimensionless by dividing them by the nearest neighbor hopping integral $2t_0$. Where W = $8t_0$ ≈ 1.0 eV ≈ 10,000 K is the width of the conduction band. The parameters are the SC parameter z = $\frac{\Delta_0}{2t_0}$, reduced temperature, t = $\frac{k_B \mathrm{T}}{2t_0}$, the SC coupling g = $\frac{J}{2t_0}$, u_m = $\frac{\mu}{2t_0}$.

4. Results and Discussion

Based on our model, SC gap equation for d-wave is calculated. The dimensionless SC parameter (z) and SC coupling (g) are involved and they are solved self-consistently. The figure 1. Shows the temperature-dependent SC gap

(z) for different values of SC coupling(g).With increase of g the magnitude of SC gap is enhanced.

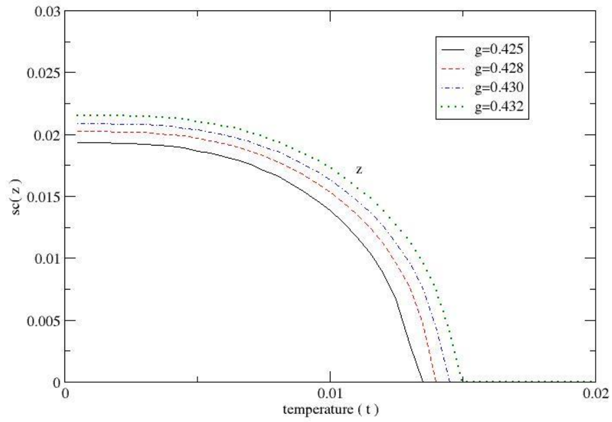

Fig. 1. The self-consistent plot of SC gap (z) vs. temperature (t) for different values of SC coupling g = 0.425, 0.428, 0.430 and 0.432.

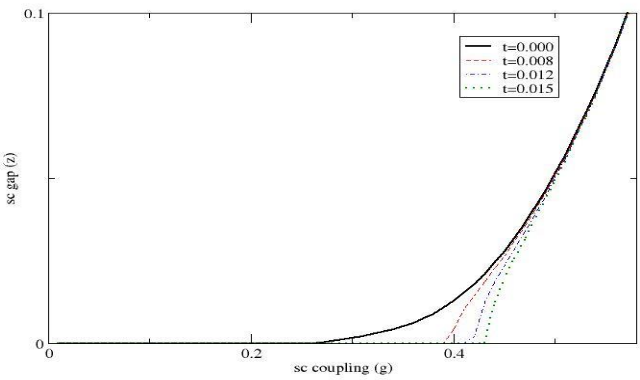

Fig. 2. The self-consistent plot of SC gap (z) vs. SC coupling (g) taking different temperature (t) = 0.000,0.008,0.012 and 0.015.

Figure 2 shows how the SC gap (z) varies with superconducting coupling g for different temperatures. By increasing temperature range t=0.00 to t=0.015, for a given value of SC coupling g =0.432, the SC gap increases. At each temperature there occurs a critical SC coupling below which there is no superconductivity.

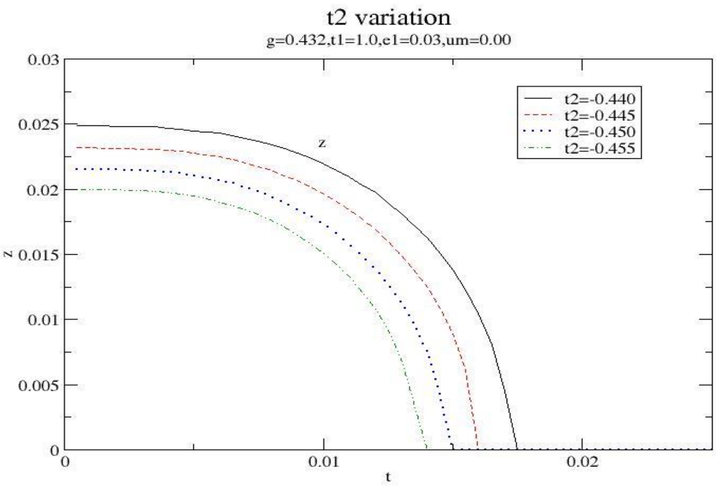

Fig. 3. The self-consistent plot of SC gap (z) vs. temperature taking different values of next- nearest-neighbor hopping integral (t_2) = - 0.440,- 0.445,- 0.450 and - 0.455.

Figure 3. shows the temperature dependence of SC gap (z) for different values of next- nearest- neighbor electron hopping integral. For a given value of nearest-neighbor hopping integral t1 = 1.0, the SC gap is suppressed with increase value of next- nearest-neighbor hopping integral t2.

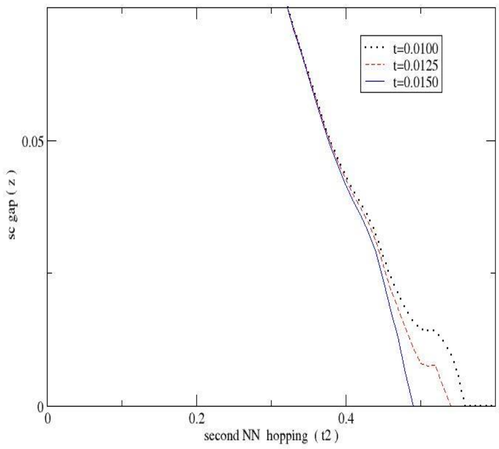

Figure 4. The self-consistent plot of SC gap (z) vs. next-nearest-neighbor hopping integral (t_2) taking different values of temperature (t) =0.0100,0.0125 and 0.0150.

The variation of SC gap (z) versus second NN hopping (t_2) taking different values of temperature is shown in Figure 4. The SC gap increases with decreasing temperature .For all temperatures the SC gap remains same for all higher values of SC coupling.

5. Conclusion

We have considered here a tight binding model Hamiltonian and reported the effect of next-neraest-neighbor hopping on superconducting gap in high-T_C Cuprates. We have considered here the mean field approximation for spin-spin interaction and found an expression for temperature dependent SC gap equation and solved self-consistently. It is observed the SC gap increases with decreasing temperatures. At each temperature there occurs a critical SC coupling below which there is no superconductivity.

Acknowledgement

The authors gracefully acknowledge the research facilities offered by the Institute of Physics, Bhubaneswar.

References

[1] M K. Crawfor, W.E. Farneth, E.M. McCarronn III, R.L. Harlow, A.H. Moudden, *Scienc*e **250**,1390 (1990).

[2] J.P. Franck, S. Harker, J.H. Brewer, *Phys. Rev. Lett.* **71**, 283 (1993).

[3] J Bardeen, L N Cooper and J R Schrifeer, *Phys. Rev.* **108**, 1175 (1957).

[4] E Dagotto, A Moreo, F Ortolani, D Poilblanc and J Riera, *Phys. Rev.* **B45**, 10741 (1992).

[5] E Dagotto and J Riera, *Phys. Rev. Lett*. **70**, 682 (1993).

[6] N S Mandal and N K Ghosh , *Pramana-J. Phys.*,**74**, 115(2010).

[7] H Tasaki, *Phys. Rev. Lett.* **75**, 4678 (1995).

[8] Zs Szabo, *Phys. Rev.* **B59**, 10007 (1999).

[9] C Verdozzi and M Cini, *Phys. Rev.* **B51**, 7412 (1995).

[10] Zs Szabo and Zs Gulacsi, *Philos. Mag.* **B76**, 911 (1997).

[11] H.B. Radousky , *J. Mater. Res.* **7**,1917 (1992).

[12] A. Schilling, F. Hulliger, S. Sawarappuli, H.R. Ott, *Mater. Lett.* **11**,217 (1991). [13] I.K. Gopalkrishnan,J.V.Yakhmi, *Physica C* **232**,127 (1994).

[14] Y Tokura, H Takagi, S Uchida, *Nature* **337**, 345 (1989).

[15] R Mohapatra, G C Rout, *Physica C* **512**,12 (2015).