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Effect of Interband Hopping and Density of States for Oxypnictide Superconductor for Two Band Model.

Vipul Singh[1] and Sarita Khandka[2]

[1,2]Department of Physics, Sam Higginbottom University of Agriculture Technology and Sciences, Allahabad – 211007, India.

Email: [1]vipul.singh@shiats.edu.in, [2]saritakh@rediffmail.com

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ABSTRACT

The two band model for oxypnictide system with interband interaction for single particle hopping and Cooper pair tunneling has been studied. It is assumed that phonon mechanism is operative within these interband interaction with intraband single particle hopping and Josephson tunneling is studied within two band model for oxypnictide superocnductors. Transition temperature T_c has been obtained and numerically solved. Dependence of T_c on various parameters is established from the expression. The transition temperature (T_c) is found to increase with density of states and it is found that the superconducting order parameter Δ decreases with increasing interband hopping (h) which has also been observed in cuprates. It is further found that Josephson tunneling is not contributing towards superconductivity.

Keywords: interband, hopping, density, states, two band, iron-pnictide, high T_c, superconducting order parameter.

1. Introduction

New class of superconductors composed of alternating $LnO_{1-x}F_x$ (Ln=La, Ce, Sm etc)[1] and FeAs layers were discovered[2]. The transition temperature values ranges from 25 – 52 K. Although these materials do not have high transition temperature as cuprates, but some properties of these materials are reminiscent of cuprates like superconductivity induced by doping a magnetic parent compound, layered basic structure and multi-band structure of the band structure[2].

Several experiments[3,4] and band structure calculations[5] suggests unconventional superconductivity in the paramagnetic Fe layer. Calculations indicate that superconductivity originates from the d orbitals of what would normally be expected to be pair-breaking magnetic Fe ions, suggesting that new non-phonon pairing mechanisms are responsible for the high-Tc superconducting state[6,7]. The reasonable parameters found for the angle-resolved photoemission spectra showed multiple gaps in oxypnictides. The calculations of the band structure of oxypnictides show that the Fermi surface (FS) is formed by disconnected hole-like pockets and electron-like pockets of the folded Brillouin zone of the FeAs planes[8].

Superconductivity in these materials is associated with FeAs layer, and that the density of states near Fermi level has maximum contribution from the Fe-3d orbitals[9]. It has been suggested that a minimal two band model[10] similar to that of MgB_2 will be useful for the study of iron based superconductors. Therefore in the present study two band extended Hubbard model is considered. The model Hamiltonian includes various intra and inter-bilayer interactions along with coupling of FeAs chains with FeO planes. The next section describes the model Hamiltonian of the problem. Theoretical calculation employing double time retarded Green's function formalism[11] has been employed. Transition temperature based on the two band model for iron pnictide has been calculated and its dependence on various parameters has been studied.

2. Mathematical Formulation

The Hamiltonian under consideration consists of the following terms

$$H = \sum_{k\sigma} E_{1k} C^{+}_{k\sigma} C_{k\sigma} + \sum_{k\sigma} E_{2k} D^{+}_{k\sigma} D_{k\sigma}$$
$$- \sum_{kk'} V^{11} C^{+}_{k\uparrow} C^{+}_{-k\downarrow} C_{-k'\downarrow} C_{k'\uparrow}$$
$$- \sum_{kk'} V^{22} D^{+}_{k\uparrow} D^{+}_{-k\downarrow} D_{-k'\downarrow} D_{k'\uparrow}$$
$$+ \tau \sum_{kk'} \left(C^{+}_{k\uparrow} C^{+}_{-k\downarrow} D_{-k'\downarrow} D_{k'\uparrow} + D^{+}_{k\uparrow} D^{+}_{-k\downarrow} C_{-k'\downarrow} C_{k'\uparrow} \right)$$
$$+ h \sum_{k\sigma} \left(C^{+}_{k\sigma} D_{k\sigma} + D^{+}_{k\sigma} C_{k\sigma} \right)$$
..(1)

The first and second terms are the kinetic energies (E_{1k} and E_{2k}) of the two bands. The third and fourth terms are the intraband interaction matrix elements (V^{11} and V^{22}) of the two bands. The fifth term represents the interband pair tunneling (τ) process between the bands and the sixth term represents the single particle hopping (h) between the bands.

Considering the following Green Functions[11]

$$G^{C\uparrow\uparrow}_{qq} = \left\langle \left\langle C_{q\uparrow}, C^{+}_{q\uparrow} \right\rangle \right\rangle$$
(3)

$$G^{C\downarrow\uparrow}_{-qq} = \left\langle \left\langle C^{+}_{-q\downarrow}, C^{+}_{q\uparrow} \right\rangle \right\rangle$$
(4)

$$G^{DC\uparrow\uparrow}_{qq} = \left\langle \left\langle D_{q\uparrow}, C^{+}_{q\uparrow} \right\rangle \right\rangle$$
(5)

$$G^{DC\downarrow\uparrow}_{-qq} = \left\langle \left\langle D^{+}_{-q\downarrow}, C^{+}_{q\uparrow} \right\rangle \right\rangle$$
(6)

Writing the equation of motion for equations 2-5 and taking Fourier transformation we get the following equations

$$\left(\omega - E_{1q}\right) G^{C\uparrow\uparrow}_{qq} + \left(\Delta^{11} - \frac{\tau}{V^{11}} \Delta^{22} \right) G^{C\downarrow\uparrow}_{-qq}$$
$$- \left(\tau\gamma + h\right) G^{DC\uparrow\uparrow}_{qq} = \frac{1}{2\pi}$$
(7)

$$\left(\omega + E_{1-q}\right) G^{C\downarrow\uparrow}_{-qq} + \left(\Delta^{11} - \frac{\tau}{V^{22}} \Delta^{22} \right) G^{C\uparrow\uparrow}_{qq}$$
$$+ \left(\tau\gamma + h\right) G^{DC\downarrow\uparrow}_{-qq} = 0$$
(8)

$$\left(\omega - E_{2q}\right) G^{DC\uparrow\uparrow}_{qq} + \left(\Delta^{22} - \frac{\tau}{V^{11}} \Delta^{11} \right) G^{DC\downarrow\uparrow}_{-qq}$$
$$- \left(\tau\gamma + h\right) G^{C\uparrow\uparrow}_{qq} = 0$$
(9)

$$\left(\omega + E_{2-q}\right) G^{DC\downarrow\uparrow}_{-qq} + \left(\Delta^{22} - \frac{\tau}{V^{11}} \Delta^{11} \right) G^{DC\uparrow\uparrow}_{qq}$$
$$+ \left(\tau\gamma + h\right) G^{C\downarrow\uparrow}_{-qq} = 0$$
(10)

Taking the following assumptions that $E_{1q} = E_{1-q} = E_{2q} = E_{2-q} = E_q$ and $\Delta^{11} = \Delta^{22} = \Delta$ and Substituting $\left(1 - \frac{\tau}{V^{11}}\right) = V$ where $V^{11} = V^{22}$; $W = \left(\tau\gamma + h\right)$ where $\gamma = \left\langle C^{+}_{-q\downarrow} D_{-q\downarrow} \right\rangle$.

Rewriting the equations (7-10)

$$\left(\omega - E_q\right)\mathrm{A} + \Delta V\overline{\mathrm{A}} - W\mathrm{B} = 1/2\pi \tag{11}$$

$$\Delta V\mathrm{A} + \left(\omega + E_q\right)\overline{\mathrm{A}} + W\overline{\mathrm{B}} = 0 \tag{12}$$

$$-W\mathrm{A} + \left(\omega - E_q\right)\mathrm{B} + \Delta V\overline{\mathrm{B}} = 0 \tag{13}$$

$$+W\overline{\mathrm{A}} + \Delta V\mathrm{B} + \left(\omega + E_q\right)\overline{\mathrm{B}} = 0 \tag{14}$$

On solving the four equations (11-14) we get

$$G_{-qq}^{C\downarrow\uparrow} = -\frac{\Delta V}{2\pi}\left[\frac{1}{\omega^2 - \xi^2} + \frac{1}{\omega^2 - \xi'^2}\right] \tag{15}$$

where $\xi = \left[\left(E_q + W\right)^2 + \left(\Delta V\right)^2\right]$ and $\xi' = \left[\left(E_q - W\right)^2 + \left(\Delta V\right)^2\right]$

The correlation function is expressed as

$$\left\langle C_{-q\downarrow}C_{q\uparrow}\right\rangle = -\frac{1}{i}\int_{-\infty}^{\infty}\frac{G_{-qq}^{\downarrow\uparrow}(\omega + i\varepsilon) - G_{-qq}^{\downarrow\uparrow}(\omega - i\varepsilon)}{e^{\frac{\omega}{KT}} - \eta} \tag{16}$$

Where $\eta = -1$ for fermions, K=Boltzmann constant and T=Temperature

Solving equation (16) using Green function (15) we get the superconducting order parameter as

$$\Delta = \left\langle C_{-q\downarrow}C_{q\uparrow}\right\rangle = \sum_q \frac{\Delta V}{2}\left[\frac{1}{\xi}\tanh\frac{\xi}{2KT} + \frac{1}{\xi'}\tanh\frac{\xi'}{2KT}\right] \tag{17}$$

Substituting that $T \rightarrow T_c$ as $\Delta \rightarrow 0$, Finally T_c can be expressed as

$$T_c = \frac{1}{2K}\left(\frac{\hbar\omega_D}{W} + 1\right)^{\frac{N_D}{2N_C}}\sqrt{\left(\left(\hbar\omega_D - W\right)W\right)}\exp\left(-\left(\frac{N'}{4} - 0.8185\right)\frac{1}{N_C}\right) \quad \text{... (18)}$$

where $W = \left(\tau\gamma + h\right)$ and $N' = \frac{1}{V^{11} - \tau}$.

3. Result & Discussion

The values of the variables in equation (17-18) have been taken as τ= -.005eV, γ=10^{-7}, h=0.01eV)[12] as cuprates and ironpnictide have similar properties.

On the basis of the above values the approximation that $W \approx h$ can also be taken since γ is very small. Also V^{11}=1and $N_C = N_0 = 0.2$.

Numerical analysis of equation (17 & 18) gives Tables – I & II which are plotted to obtain Figure 1 & 2.

Table – I. Variation of superconducting order parameter Δ(0) with interband hopping (*h*).

Δ(0) eV	***h* (eV)**
0.14095	0.001
0.14086	0.005
0.14060	0.010

0.14017	0.015
0.13956	0.020
0.13877	0.025
0.13780	0.030
0.13665	0.035
0.13531	0.040
0.13377	0.045
0.13203	0.050

Table – II. Variation of T_c with Ratio of Density of States

Density of States	T_c
0.1	46.2774
0.2	47.9717
0.3	49.7279
0.4	51.5485

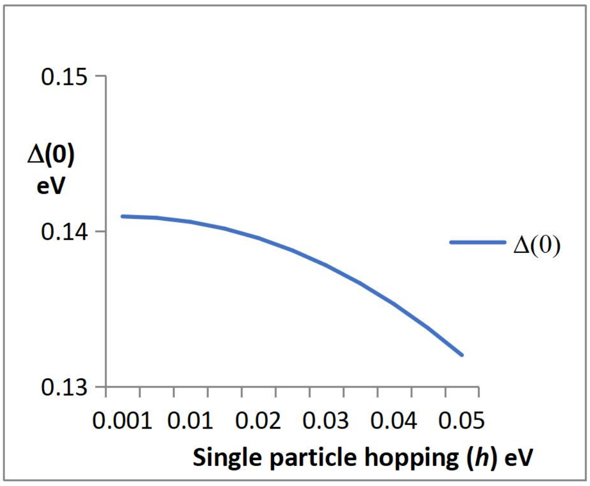

Figure 1. Variation of superconducting order parameter Δ(0) with interband hopping (*h*).

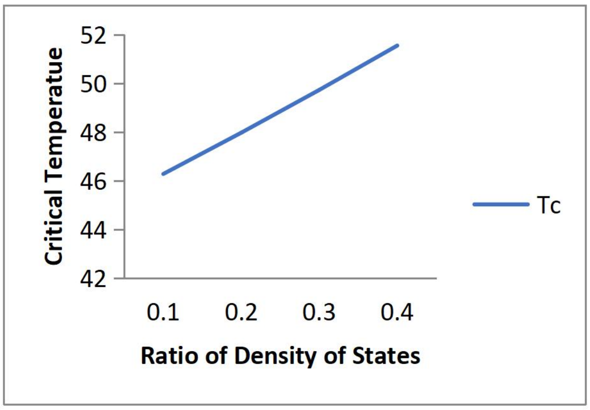

Figure 2. Variation of T_c with Ratio of Density of States

The expression for superconducting order parameter $\Delta(0)$ has been obtained from equation no. (17) by substituting T=0. Figure 1 shows that superconducting order decreases as the single particle hopping interaction increases. It shows that increasing hopping interaction across the physical parameter regime hardly modifies $\Delta(0)$. Further increasing single particle hopping to larger, unphysical values strongly suppresses T_c. Thus, our calculations support the hypothesis that a larger hopping range suppresses T_c which is in agreement with calculations on the multi band models. A similar result is also explained by C Weber et al.[14], which is in agreement to the above result.

It is evident from the Figure 2 that with increase of ratio of density of state the transition temperature also increases. Therefore for superconductors such as iron based superconductors, where two band model is applicable, the ratio of density of states for two band is crucial for obtaining higher values of Tc. also it has also been found that interband correlation parameter γ is very small, therefore its effect on interlayer hopping is negligible.

4. Conclusion

The transition temperature for iron-pnictides has been calculated using two band model using double-time retarded Green's function. The results based on two band model predict increase in T_C with increasing ratio of density of states. The transition temperature T_C is also found to be dependent on interband scattering and inter band hopping.

The superconducting order parameter $\Delta(0)$ decreases with increasing interband hopping (h) which has been observed in cuprates also. For physical plausible values of interband hopping (h) has little effect on superconducting order parameter $\Delta(0)$. But for higher values of h superconducting order parameter is suppressed significantly. Therefore channel for interband hoping have detrimental effect on the superconductivity of iron-pnictide superconductors.

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