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I.4

MULTI-GAP SUPERCONDUCTIVITY IN MgB_2

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Abstract: We using our two-band model for the explanation of two coupled superconductivity gaps for MgB_2.To study the effect of the increasing of T_c in MgB_2 due to the enhanced interband pairing scattering. We have proposed two channel scenario of superconductivity: the conventional channel which is connected with BCS mechanism in different zone and the unconventional channel which describes the transfer or tunneling of Cooper pair between two bands.

Key words: Multi-gap, Two-band model, Interband Pairing.

1. INTRODUCTION

Recent discovery of superconductivity of MgB_2 with T_c=39K, which is the highest as for intermetallics [1], has been recognized a multi-gap superconductor[2]. Although multi-gap superconductivity had been discussed theoretically [3-5] in the 1958, the multi-gap superconductivity has been observed experimentally [6] in the 1980s. MgB_2 is the first material in which its effects are so dominant and its implications so thoroughly explored. Nature has let us glimpse a few or her multi-gap mysteries and has challenged us. Recent band calculations [7,8] of MgB_2 cite with the

McMillan formula of transition temperature have supported the e-p interaction mechanism for the superconductivity. In this superconductivity, the possibility of two-band superconductivity has also been discussed in relation to two gap functions experimentally and theoretically. Very recently, two-band or multi-band superconductivity has been theoretically investigated in relation to superconductivity arising from coulomb repulsive interactions. Two-band model was first introduced by Kondo [5]. We have also investigated anomalous phases in two-band model by using the Green function techniques[10-15]. Recently, we have pointed out the importance of many-band effects in high-T_c superconductivity [10-14]. The expressions of the transition temperature for several phases have been derived, and this approach has been applied to superconductivity in molecular crystals by charge injection and field-induced superconductivity [11]. In the previous papers [10-12], we have investigated superconductivity by using the two-band model and a two-particle Green function techniques. We have applied the model to an electron-phonon mechanism for the traditional BCS method, an electron-electron interaction mechanism for high- T_c superconductivity [9], and a cooperative mechanism. In the framework of the two-particle Green function techniques [16], it has been shown that the temperature dependence of the superconductivity gap for high- T_c superconductors is more complicated than predicted in the BCS approach. In paper [8] we have investigated the phase diagrams for two-band model superconductivity, using the renormalization group approach. We have discussed the possibility of a cooperative mechanism in the two-band superconductivity in relation to high-T_c superconductivity and to study the effect of the increasing of T_c in MgB_2 due to the enhanced interband pairing scattering.

In this paper, we investigate our two-band model for the explanation the multi-gap superconductivity of MgB_2. We apply the model to an electron-phonon mechanism for the traditional BCS method, an electron-electron interaction mechanism for high- T_c superconductivity, and a cooperative mechanism in relation to multi-band superconductivity.

2. THEORETICAL BACKGROUND

In this section, we briefly summarize a two-band model for superconductivity.

2.1 Hamiltonian

We start from the Hamiltonian for two-bands i and j ;

$$H = H_0 + H_{\mathrm{int}} , \quad (1)$$

where

$$H_0 = \sum_{\mathbf{k},\sigma} \Big[\big[\varepsilon_i - \mu\big] a^{+}_{i\mathbf{k}\sigma} a_{i\mathbf{k}\sigma} + \big[\varepsilon_j - \mu\big] a^{+}_{j\mathbf{k}\sigma} a_{j\mathbf{k}\sigma} \Big], \quad (2)$$

$$\begin{aligned} H_{\mathrm{int}} = \frac{1}{4} \sum_{\delta(\mathbf{p}_1+\mathbf{p}_2,\mathbf{p}_3+\mathbf{p}_4)} \sum_{\alpha\beta\gamma\delta} \Big[& \Gamma^{iiii}_{\alpha\beta\gamma\delta} a^{+}_{i\mathbf{p}_1\alpha} a^{+}_{i\mathbf{p}_2\beta} a_{i\mathbf{p}_3\gamma} a_{i\mathbf{p}_4\delta} + (i \to j) \\ & + \Gamma^{iijj}_{\alpha\beta\gamma\delta} a^{+}_{i\mathbf{p}_1\alpha} a^{+}_{i\mathbf{p}_2\beta} a_{j\mathbf{p}_3\gamma} a_{j\mathbf{p}_4\delta} + (i \to j) \\ & + \Gamma^{ijij}_{\alpha\beta\gamma\delta} a^{+}_{i\mathbf{p}_1\alpha} a^{+}_{j\mathbf{p}_2\beta} a_{i\mathbf{p}_3\gamma} a_{j\mathbf{p}_4\delta} + (i \to j) \Big], \end{aligned} \quad (3)$$

Γ is the bare vertex part:

$$\Gamma^{ijkl}_{\alpha\beta\gamma\delta} = \langle i\mathbf{p}_1\alpha\, j\mathbf{p}_2\beta | k\mathbf{p}_3\gamma\, l\mathbf{p}_4\delta \rangle \delta_{\alpha\delta}\delta_{\beta\gamma} - \langle i\mathbf{p}_1\alpha\, j\mathbf{p}_2\beta | l\mathbf{p}_4\delta\, k\mathbf{p}_3\gamma \rangle \delta_{\alpha\gamma}\delta_{\beta\delta} , \quad (4)$$

with

$$\langle i\mathbf{p}_1\alpha\, j\mathbf{p}_2\beta | k\mathbf{p}_3\gamma\, l\mathbf{p}_4\delta \rangle = \int d\mathbf{r}_1 d\mathbf{r}_2 \phi^{*}_{i\mathbf{p}_1\alpha}(\mathbf{r}_1) \phi^{*}_{j\mathbf{p}_2\beta}(\mathbf{r}_2) V(\mathbf{r}_1,\mathbf{r}_2) \phi_{k\mathbf{p}_3\gamma}(\mathbf{r}_2) \phi_{l\mathbf{p}_4\delta}(\mathbf{r}_1) , \quad (5)$$

and $a_{i\mathbf{p}\sigma}{}^{+}$ ($a_{i\mathbf{p}\sigma}$) is the creation (annihilation) operator corresponding to the excitation of electrons (or holes) in i-th band with spin σ and momentum $\mathbf{p}$. μ is the chemical potential. $\phi_{i\mathbf{p}\alpha}{}^{*}$ is a single-particle wave-function. Here, we suppose that in Eq.(3), the vertex function consists of the effective interactions between the carriers caused by the linear vibronic coupling in the several bands and the screened coulombic interband interaction of carriers.

When we use the two-band Hamiltonian of Eq.(1) and define the order parameters for the singlet exciton, triplet exciton, and singlet Cooper pair, the mean field Hamiltonian is easily derived [10-17]. Here, we focus three electron scattering processes contributing to the singlet superconducting phase in the Hamiltonian of Eq.(1):

$$g_{i1} = \langle ii|ii\rangle, \quad g_{j1} = \langle jj|jj\rangle, \tag{6}$$

$$g_2 = \langle ii|jj\rangle = \langle jj|ii\rangle, \tag{7}$$

$$g_3 = \langle ij|ij\rangle = \langle ji|ji\rangle, \tag{8}$$

$$g_4 = \langle ij|ji\rangle = \langle ji|ij\rangle. \tag{9}$$

g_{i1} and g_{j1} represent the i -th and j –th intraband two-particle normal scattering processes, respectively. g_2 indicates the intraband two-particle umklapp scattering (See Figure 1.).

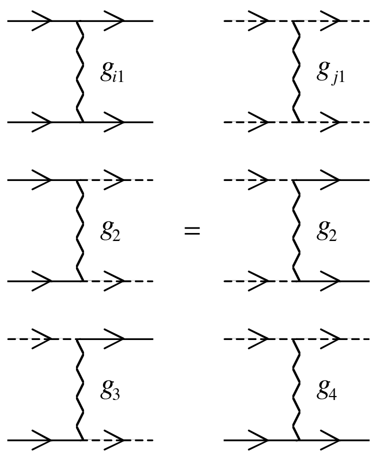

Figure I:4:1. Electron-electron interactions. Solid and dashed lines indicate π- and σ-bands, respectively. g_{i1}, g_{j1}, and g_2 contribute to superconductivity.

Note that Γ's are given by

$$\begin{aligned}
\Gamma^{iiii}_{\alpha\beta\gamma\delta} &= g_{i1}\left(\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\gamma}\delta_{\beta\delta}\right),\\
\Gamma^{jjjj}_{\alpha\beta\gamma\delta} &= g_{j1}\left(\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\gamma}\delta_{\beta\delta}\right),\\
\Gamma^{iijj}_{\alpha\beta\gamma\delta} = \Gamma^{jjii}_{\alpha\beta\gamma\delta} &= g_{2}\left(\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\gamma}\delta_{\beta\delta}\right),\\
\Gamma^{ijij}_{\alpha\beta\gamma\delta} = \Gamma^{jiji}_{\alpha\beta\gamma\delta} &= g_{3}\delta_{\alpha\delta}\delta_{\beta\gamma} - g_{4}\delta_{\alpha\gamma}\delta_{\beta\delta}\,,
\end{aligned} \tag{10}$$

where an antisymmetrized vertex function Γ is considered to be a constant independent of the momenta. The spectrum is elucidated by the Green function method. Using Green's functions, which characterize the CDW, SDW, and SSC phases, we obtain a self-consistent equation, according to the traditional procedure [10-17]. Then, we can obtain expressions of the transition temperature for some cases.

The spectrum is elucidated by the Green function method. Using Green's functions, which characterize the CDW, SDW, and SSC phases, we obtain a self-consistent equation, according to the traditional procedure [11-15]. Then, we can obtain expressions of the transition temperature for some cases. Electronic phases of a one-dimensional system have been investigated by using similar approximation in the framework of the one-band model [10-17]. In the framework of a mean field approximation with the two-band model, we have already derived expressions of the transition temperature for CDW, SDW, and SSC. In the previous paper [12-15], we have investigated the dependence of T_c on hole or electron concentration for superconductivity of copper oxides by using the two-band model and have obtained a phase diagram of $Bi_2Sr_2Ca_{1-x}Cu_{2x}O_8$ (Bi-2212) by means of the above expressions of transition temperature .

For simplicity, we consider in paper [7] three cases: (1) $g_1 \neq 0$ and others = 0, (2) $g_2 \neq 0$ and others = 0, and (3) g_{i1} and g_{j1}, $g_2 \neq 0$ and others = 0, using of the two-particle Green function techniques. It was shown that for case 3 possibly to arise two superconductivity gap. The superconductivity arising from electron-phonon mechanism $g_1 < 0$ and $g_1 < g_2$) such as MgB_2 is in the two-gap region. On the other hand, the superconductivity such as copper oxides ($g_1 > g_2$) is outside the two-gap region. These results predict that we may observe two gap functions for MgB_2 and only single gap function for copper oxides.

2.2 Superconductivity in MgB_2

We used case (3) for g_{i1} and g_{j1}, $g_2 \neq 0$ and others = 0 for description superconductivity in MgB_2. We will have reduced Hamiltonian :

$$H = H_0 + H_{\text{int}} \tag{11}$$

where

$$H_0 = \sum_{\mathbf{k},\sigma} \left[[\varepsilon_i - \mu] a^+_{i\mathbf{k}\sigma} a_{i\mathbf{k}\sigma} + [\varepsilon_j - \mu] a^+_{j\mathbf{k}\sigma} a_{j\mathbf{k}\sigma} \right] \tag{12}$$

$$H_{\text{int}} = \sum g_{1i} a^+_{ik} a^+_{i-k} a_{i-k} a_{ik} + \sum i \to j + \sum g_2 a^+_{ik} a^+_{i-k} a_{j-k} a_{jk} \,. \tag{13}$$

Now we define order parameter which are helpful to construct the mean field Hamiltonian , defined as

$$\Delta_i = \sum_p \left\langle a^+_{ip\uparrow} a^+_{i-p\downarrow} \right\rangle \tag{14}$$

$$\Delta_j = \sum_p \left\langle a^+_{jp\uparrow} a^+_{j-p\downarrow} \right\rangle \tag{15}$$

The relation between two superconductivity gaps of the system are

$$\Delta_j = \frac{1 - g_{i1} \rho_i f_i}{g_2 \rho_j f_j} \Delta_i \,, \tag{16}$$

where

$$f_i = \int_{\mu}^{\mu - E_c} \frac{d\xi}{\left(\xi^2 + \Delta_i^2\right)^{1/2}} \tanh \frac{\left(\xi^2 + \Delta_i^2\right)^{1/2}}{2T},$$
$$f_j = \int_{\mu - E_c}^{\mu - E_j} \frac{d\xi}{\left(\xi^2 + \Delta_j^2\right)^{1/2}} \tanh \frac{\left(\xi^2 + \Delta_j^2\right)^{1/2}}{2T} \tag{17}$$

with the coupled gap equation:

$$\left(1 - g_{i1}\rho_i f_i\right)\left(1 - g_{j1}\rho_j f_j\right) = g_2^2 f_i f_j . \tag{18}$$

We have tried to estimate the coupling constant of pair electron scattering process between π- and σ-bands of MgB_2 system. We have calculated the parameters by using roughly numerical approximation. We focus one π -band and σ-band of MgB_2 and consider electrons near Fermi surfaces. We find value parameter $g_1 =$ -0.4 eV , using transfer integral between π -band and σ-band .We estimate the coupling parameter g_2 of pair-electron scattering process by the following expression.

$$g_2 = \sum_{k1,k2} V_{k1,k2}^{1,2} \tag{19}$$

$$V_{k1,k2}^{1,2} = \sum_{r,s,t,u} u_{1,r}^*(k1)\, u_{1,s}^*(k1)\, v_{rs}\, u_{2,t}(k2)\, u_{2,u}(k2), \tag{20}$$

where label 1 and 2 mean π- and σ-bands, respectively. $u_{i,r}(ki)$ is LCAO coefficient with *i*-the band and *ki* moment [18,19]. The summation *k1* and *k2* sum over each Fermi surface. However, it is difficult to perform the sum exactly. In this case, we used few point near Fermi surface. The coupling constant of pair-electron scattering between π- and σ-bands is from about g_2=0.025 eV.

From numerical calculations of Eqs.(16)-(18), we can also obtain the temperature dependence of the two gap parameters as shown in Fig.2. We have used the density of states of π- and σ-bands (ρ_i=0.2 eV^{-1}, ρ_j=0.14eV^{-1}), chemical potential μ=-2.0, the top energy of σ-band E_j= -1.0, and fitting parameters (g_{i1}= -0.4 eV, g_{j1}= -0.6 eV, g_2= 0.02 eV).

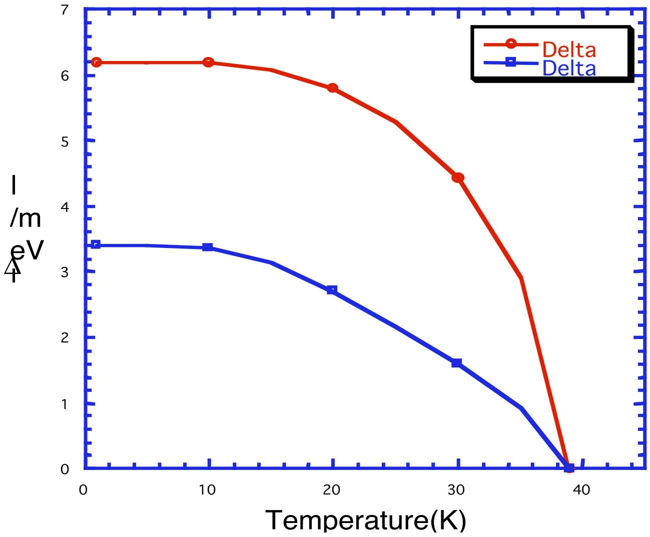

Figure I:4:2. Temperature dependent of two superconductivity gaps.

This calculations have qualitative agreement with experiments [20-22].

The expression of transition temperature of superconductivity is derived by a simple approximation :

$$T_{c_+} = 1.13(\zeta - E_j) \cdot \exp\left(-1 \big/ g_+ \rho \right) \tag{21}$$

where

$$g_+ = \frac{1}{24}\left(B + \sqrt{B^2 - 4A} \right) \tag{22}$$

and

$$A = g_{1i}g_{1j} - g_2^2 \quad (23)$$

$$B = g_{1i}g_{1j} + g_{1j} \quad (24)$$

$$\zeta = -\mu \quad (25)$$

We can see from expressions for T_{c+} the effect of increase of T_{c+} due to the enhanced interband pairing scattering (g_2)

Figure 3 shows a schematic diagram of mechanism of pairing for two gaps. Scenario is next. Electrons from π and σ zones make up the subsystems. If g_2=0 we have a two independent subsystems with different the transition temperature of superconductivity $T_{c\pi}$ and $T_{c\sigma}$ and two independently superconductivity gaps. In our model we have $g_2 \neq 0$ and two coupled superconductivity gaps with relation (16) and one transition temperature of superconductivity T_{c+} which has agreement with experiments. In our model, we have two channel of superconductivity: conventional channel (intraband g_1) and unconventional channel (interband g_2). Two gaps appear simultaneously in different zones which like BCS gaps. Gap in π zone is bigger to compare with σ zone, because the density of state in π zone is (0.25eV) and in σ zone (0.14eV). Current of Cooper pair gets from π zone in σ zone, because density of Cooper pair in π zone becomes much higher. The tunneling of Cooper pair also stabilizes the order parameter in σ zone.

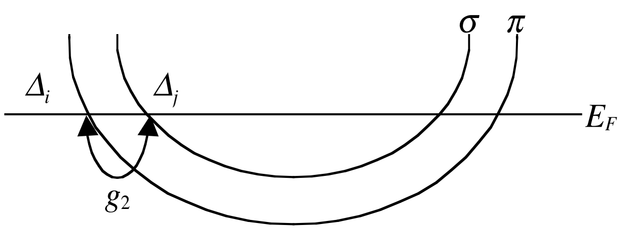

Figure I:4:3. Schematic diagram of mechanism of pairing for two gaps.

In this way, we can predict the physical properties of the multi-gaps superconductivity, if we have the superconductors with many zone structure as shown in Fig.3.

3. SUMMARY AND CONCLUSIONS

In conclusion, we have presented our two-band model with intraband two-particle scattering and interband pairing scattering processes to describing two-gap superconductivity in MgB_2.

We defined the parameters of our model and made numerical calculations of temperature dependent of two gaps. It is a qualitative agreement with experiments. We proposed a two channel scenario of superconductivity: first a conventional channel (intraband g_1) whichis is connected with BCS mechanism in different zone and a unconventional channel (interband g_2) which describes the tunneling of a Cooper pair between two bands. The tunneling of Cooper pair also stabilizes the order parameters of superconductivity [9-12] and increases the critical temperature of superconductivity.

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REFERENCES

1. J. Nagamatsu, N. Nakamura, T. Muranaka, Y. Zentani, and J. Akimitsu, *Nature*, 410, 63 (2001).
2. A. Bianconi, and M. Filippi, this volume Chapter 2; A. Bianconi, et al. *J. Phys.: Condens. Matter* 13, 7383 (2001); J. P.C. Canfield, S.L. Bud'ko and D.K. Finnemore, *Physica C,* 385, 1 (2003).
3. H. Suhl, B.T. Matthias, R.Walker, *Phys.Rev.Lett.,* 3, 552 (1959).
4. V.A. Moskalenko, *Fiz.Metalloved.*8, 25, (1959)
5. J. Kondo, *Prog . Theor. Phys.* 29, 1 (1963)
6. G. Binnig , A. Baratoff, Hoening, J.G. Bednorz , *Phys.Rev.Lett*. 45, 1352, (1980)
7. J. M. An and W. E. Picket, *Phys. Rev. Lett.* 86, 4366 (2001).
8. J. Kortus, I.I. Mazin, K.D. Belashenko, V.P.Antropov and I.L.Boyer, *Phys.Rev.Lett.* 86, 4656 (2001).
9. J. G. Bednorz and K. A. Müller, *Z. Phys. B* , **64**, 189 (1986).

10. H. Nagao, S.P. Kruchinin, A.M. Yaremko, and K.Yamaguchi, *Int. J. Mod. Phys. B,* **16,** 23, 3419 (2002) .
11. H. Nagao, M. Nishino, Y. Shigeta, Y. Yoshioka and K. Yamaguchi, *J. Chem. Phys.,* 113, 11237 (2000).
12. H. Nagao, H. Kawabe, S.P. Kruchinin, D.Manske , K. Yamaguchi, *Mod.Phys.Lett. B*, **17**, 10 , 423, (2003) .
13. H. Nagao, A.M. Yaremko, S.P. Kruchinin, and K.Yamaguchi, in J. Annett and S. Kruchinin (eds.), *New Trends in Superconductivity,* Kluwer Academic, Dordrecht, 155 (2002)
14. H. Nagao, S.P. Kruchinin , and K.Yamaguchi, in J.K. Srivastava and M. Rao (eds.), *Models and Methods of High-Tc superconductivity: Some Frontal Aspects,* Nova Science Publishers, Inc. Academic, 205 (2003)
15. H. Nagao, Y. Kitagawa, T. Kawakami, T. Yoshimoto, H. Saito, and K. Yamaguchi, *Int. J. Quantum Chem*., 85, 608 (2001).
16. A.M. Yaremko,E.V. Mozdor, and S.P. Kruchinin, *Int. J. Mod. Phys.* B **10**, 2665 (1996).
17. M. Yaremko, E.V. Mozdor, H. Nagao, and S.P. Kruchinin, in J. Annett and S. Kruchinin, (eds), *New Trends in Superconductivity ,* Kluwer Academic , Dordrecht , 329-339.
18. M. Yamamoto, K. Nishikawa, S. Aono, Bull. Chem. Soc. Jpn, 58, 3176, (1985)
19. M. Kimura, H. Kawabe, A. Nakajima, K. Nishikawa, S. Aono, Bull. Chem. Soc. Jpn., 61, 4239 (1988)
20. T. Örd , N. Kristoffel, and K. Rägo, in S. Kruchinin (eds.), *Modern Problems of superconductivity*, *Mod. Phys. Let.* B , 17, 667 (2003).
21. N. Kristoffel, T. Örd, K. Rägo, *Europhys. Lett.*, 61,109 (2003). P. Szabo et al., *Phys. Rev. Lett.* 87, 137005 (2001).