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Two-Gap Superconductivity in MgB_2*

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Abstract—The recent discovery of the superconductivity of MgB_2 has attracted great interest in multigap superconductivity. We use our two-band model to explain the two coupled superconductivity gaps of MgB_2. To study the effect of the increased T_c in MgB_2 due to the enhanced interband pairing scattering, we propose a two-channel scenario of superconductivity: a conventional channel, connected with the BCS mechanism in different zones, and an unconventional channel that describes the transfer or tunneling of a Cooper pair between two bands. The critical temperature is defined and the possibility of increasing the critical temperature is demonstrated.

1. INTRODUCTION

The recent discovery of the superconductivity of MgB_2 with T_c = 39 K, the highest of any two-component system [1], has attracted great interest in multigap superconductivity [2]. Although multigap superconductivity had been discussed theoretically in 1958 [3–5], multigap superconductivity was first observed experimentally in the 1980s [6]. MgB_2 is the first material in which its effects were found to be so dominant and its implications were so thoroughly explored. Nature has challenged us by allowing us to glimpse a few of her multigap mysteries. Recent band calculations [7, 8] for MgB_2 that employ the McMillan formula for transition temperature indicate the *e–p* interaction mechanism of superconductivity. The possibility of two-band superconductivity has also been discussed in relation to two-gap functions, both experimentally and theoretically. Very recently, two-band or multiband superconductivity was theoretically investigated in relation to the superconductivity arising from coulomb repulsive interactions. The two-band model was first introduced by Kondo in [5]. We have also investigated anomalous phases in two-band model by using the Green function techniques [10–15]. We recently pointed out the importance of multiband effects in high-T_c superconductivity [10–14]. The expressions for the transition temperature have been derived for several phases, and the approach has been applied to superconductivity in molecular crystals by charge injection and field-induced superconductivity [11]. In previous papers [10–12], we investigated superconductivity by using the two-band model and the two-particle Green function techniques. We applied the model to an electron–phonon mechanism for the traditional BCS method, an electron–electron interaction mechanism for high-T_c superconductivity, and to a cooperative mechanism [9]. Within the framework of the two-particle Green function techniques, it was shown in [16] that the temperature dependence of the superconductivity gap for high-T_c superconductors is more complicated than predicted in the BCS approach. In [8], we investigated phase diagrams for two-band model superconductivity by using the renormalization group approach. We discussed the possibility of a cooperative mechanism in two-band superconductivity relative to high-T_c superconductivity, and of studying the effect of increased MgB_2 due to enhanced interband pairing scattering. In this paper, we investigate our two-band model for explaining 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 our two-band model for superconductivity.

2.1 Hamiltonian

We start from the Hamiltonian for the two bands *i* and *j*,

$$H = H_0 + H_{\text{int}}, \tag{1}$$

where

$$H_0 = \sum_{\mathbf{k},\sigma} [[\epsilon_i(\mathbf{k}) - \mu] a^\dagger_{i\mathbf{k}\sigma} a_{i\mathbf{k}\sigma} + [\epsilon_j(\mathbf{k}) - \mu] a^\dagger_{j\mathbf{k}\sigma} a_{j\mathbf{k}\sigma}], \tag{2}$$

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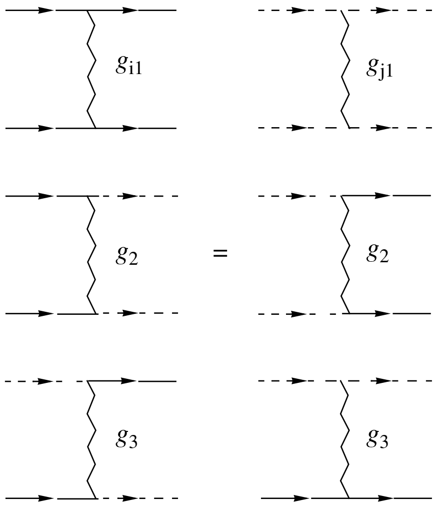

Fig. 1. Electron–electron interactions. Solid and dashed lines indicate π- and σ-bands, respectively; g_{i1}, g_{j1}, and g_2 contribute to the superconductivity.

$$H_{\rm int} = \frac{1}{4}\sum_{\sigma(\mathbf{p}_1+\mathbf{p}_2,\,\mathbf{p}_3+\mathbf{p}_4)}\ \sum_{\alpha,\beta,\gamma,\delta}[\Gamma^{iiii}_{\alpha\beta\gamma\delta}a^{\dagger}_{i\mathbf{p}_1\alpha}a^{\dagger}_{i\mathbf{p}_2\beta}a_{i\mathbf{p}_3\gamma}a_{i\mathbf{p}_4\delta} + (i\longleftrightarrow j) + \Gamma^{iijj}_{\alpha\beta\gamma\delta}a^{\dagger}_{i\mathbf{p}_1\alpha}a^{\dagger}_{i\mathbf{p}_2\beta}a_{i\mathbf{p}_3\gamma}a_{i\mathbf{p}_4\delta} + (i\longleftrightarrow j) + \Gamma^{ijij}_{\alpha\beta\gamma\delta}a^{\dagger}_{i\mathbf{p}_1\alpha}a^{\dagger}_{i\mathbf{p}_2\beta}a_{i\mathbf{p}_3\gamma}a_{i\mathbf{p}_4\delta} + (i\longleftrightarrow j)], \tag{3}$$

Γ is the bare vertex part

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

with

$$\langle i\mathbf{p}_1\alpha j\mathbf{p}_2\beta|k\mathbf{p}_3\beta l\mathbf{p}_4\alpha\rangle = \int dr_1 dr_2 \phi^*_{i\mathbf{p}_1\alpha}(r_1)\phi^*_{j\mathbf{p}_2\beta}(r_2)V(r_1, r_2)\phi_{k\mathbf{p}_3\beta}(r_2)\phi_{l\mathbf{p}_4\alpha}(r_1), \tag{5}$$

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 **p**. μ is the chemical potential. ϕ is a single-particle wave function. We suppose that the vertex function in Eq. (3) 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 on 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 Fig. 1).

Note that Γ's are given by

$$\begin{aligned}
\Gamma^{iiii}_{\alpha\beta\gamma\delta} &= g_{i1}(\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\gamma}\delta_{\beta\delta}),\\
\Gamma^{jjjj}_{\alpha\beta\gamma\delta} &= g_{j1}(\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\gamma}\delta_{\beta\delta}),\\
\Gamma^{iijj}_{\alpha\beta\gamma\delta} = \Gamma^{jjii}_{\alpha\beta\gamma\delta} &= g_2(\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\gamma}\delta_{\beta\delta}),\\
\Gamma^{ijij}_{\alpha\beta\gamma\delta} = \Gamma^{jiji}_{\alpha\beta\gamma\delta} &= g_3\delta_{\alpha\delta}\delta_{\beta\gamma} - g_4\delta_{\alpha\gamma}\delta_{\beta\delta},
\end{aligned} \tag{10}$$

where an antisymmetrized vertex function Γ is consid- 1
ered a constant independent of the momenta. The spectrum is elucidated by the Green's function method. Using Green's functions, which characterize the CDW, SDW, and SSC phases, we obtain a self-consistent equation by following the traditional procedure [10–17]. We can then obtain expressions of the transition temperature for certain cases.

The electronic phases of a one-dimensional system were investigated by using such approximation within the framework of the one-band model [10–17]. Within the framework of a mean field approximation and the two-band model, we derived expressions of the transition temperature for CDW, SDW, and SSC. In a previous paper [12–15], we investigated the dependence of T_c on hole or electron concentration for the superconductivity of copper oxides by using the two-band model and obtained a phase diagram of $Bi_2Sr_2Ca_{1-x}Cu_{2x}O_8$ (Bi-2212) by means of the above expressions for transition temperature.

For simplicity, we considered in [7] three cases: (1) $g_1 \neq 0$ and others = 0, (2) (1) $g_2 \neq 0$ and others = 0, and (3) g_{i1} and g_{j1}, and others = 0, using the two-particle Green function techniques. It was shown that the appearance of two superconductivity gaps is possible in case 3. The MgB_2 superconductivity arising from electron–phonon mechanisms $g_1 < 0$ and $g_1 < g_2$ falls within the two-gap region. On the other hand, the superconductivity of compounds such as copper oxides ($g_1 > g_2$) lies outside the two-gap region. These results indicate that we should be able to observe two gap functions for MgB_2 and only a single gap function for copper oxides.

2.2 Superconductivity in MgB_2

We use case (3) for g_{i1} and g_{j1}, $g_2 \neq 0$ and others = 0 for describing the superconductivity in MgB_2. We reduce the Hamiltonian

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

where

$$H_0 = \sum_{\mathbf{k},\sigma}[[\epsilon_i - \mu]a^{\dagger}_{i\mathbf{k}\sigma}a_{i\mathbf{k}\sigma} + [\epsilon_j - \mu]a^{\dagger}_{j\mathbf{k}\sigma}a_{j\mathbf{k}\sigma}], \quad (12)$$

$$H_{\text{int}} = \sum g_{1i}a^{\dagger}_{i\mathbf{k}}a^{\dagger}_{i-\mathbf{k}}a_{i-\mathbf{k}}a_{i\mathbf{k}} + \sum i \longrightarrow j + \sum g_2 a^{\dagger}_{i\mathbf{k}}a^{\dagger}_{i-\mathbf{k}}a_{j-\mathbf{k}}a_{j\mathbf{k}} \quad (13)$$

We now define the order parameters helpful in constructing the mean field Hamiltonian, defined as

$$\Delta_i = \sum_p \langle a^{\dagger}_{ip\uparrow}a^{\dagger}_{i-p\downarrow}\rangle, \quad (14)$$

$$\Delta_j = \sum_p \langle a^{\dagger}_{jp\uparrow}a^{\dagger}_{j-p\downarrow}\rangle. \quad (15)$$

The relation between two superconductivity gaps of the system is

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

where

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

with the coupled gap equation

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

We attempt to estimate the coupling constant of pair electron scattering process between π- and σ-bands of MgB_2 system. We calculate the parameters by using a rough numerical approximation. We focus on one π-band and one σ-band of MgB_2 and consider the electrons near the Fermi surfaces. We find value parameter g_1 = –0.4 eV by using the transfer integral between π-band and σ-band. We estimate the coupling parameter g_2 of pair-electron scattering process by the following expression:

$$g_2 = \sum_{k1,k2} V^{1,2}_{k1,k2}, \quad (19)$$

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

where labels 1 and 2 signify π-band and σ-band, respectively. $u_{i,r}(\xi)$ is the LCAO coefficient with the i-band and ξ moment [18, 19]. The variables $k1$ and $k2$ are summed over each Fermi surface. However, it is difficult to perform the summation exactly. We used a few points near the Fermi surface. The coupling constant of pair-electron scattering between the π-band and σ-band was around 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 used the density of states of π-band and σ-bands (ρ_i = 0.2 eV^{-1}, ρ_j = 0.14 eV^{-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).

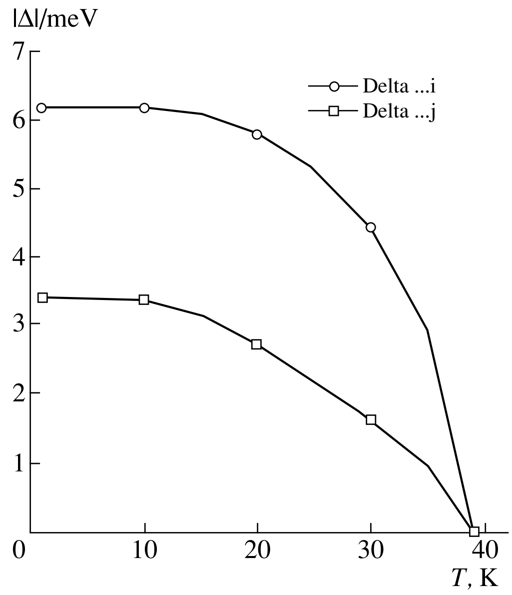

Fig. 2. Temperature dependence of two superconductivity gaps.

Our calculations are in qualitative agreement with the experiments in [20–22]. The expression for the superconductivity transition temperature is derived by a simple approximation:

$$T_{c+} = 1.13(\zeta - E_j)\exp(-1/g_+\rho), \quad (21)$$

where

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

and

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

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

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

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

Figure 3 shows a schematic diagram of the pairing mechanism for two gaps. The scenario is as follows: Electrons from the π and σ zones make up the sub-

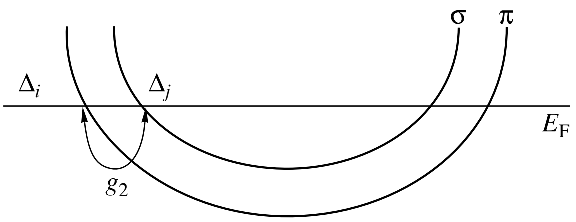

Fig. 3. Schematic diagram of the pairing mechanism for two gaps.

systems. If g_2, we have two independent subsystems with different superconductivity transition temperatures $T_{c\pi}$ and $T_{c\sigma}$ and two independent superconductivity gaps. In our model, we also have two coupled superconductivity gaps with relation (16) and one transition temperature of superconductivity T_{c+} that is in agreement with the experiments. In this model, we have two channels of superconductivity: a conventional channel (intraband g_1) and an unconventional channel (interband g_2). Two gaps similar to BCS gaps appear simultaneously in different zones. The gap in the π zone is bigger than that in the π zone, since the density of state is 0.25 eV in the σ zone and 0.14 eV in the σ zone. The current of the Cooper pair flows from the π zone into the σ zone, since the density of the Cooper pair in π zone is much higher. The tunneling of the Cooper pair also stabilizes the order parameter in the σ zone.

We thus can predict the physical properties of multigap superconductivity if we have superconductors with a multizone structure, as shown in Fig. 3.

3. CONCLUSIONS

We have presented our two-band model with intraband two-particle scattering and interband pairing scattering processes to describe the two-gap superconductivity in MgB_2. We have defined the parameters of our model and made numerical calculations for the temperature dependence of two gaps; these are in qualitative agreement with experiments. We propose a two-channel scenario of superconductivity: the first is a conventional channel (intraband g_1) associated with the BCS mechanism in different zones and an unconventional channel (interband g_2) that describes the Cooper pair tunnelling between the two bands. The tunneling of the Cooper pair also stabilizes the superconductivity order parameters [9–12] and raises the critical superconductivity temperature.

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