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THEORETICAL STUDIES ON MANY-BAND EFFECTS IN SUPERCONDUCTIVITY BY USING RENORMALIZATION GROUP APPROACH

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We present a renormalization equations for two-band superconductivity by using a two-band model and present phase diagrams for the two-band superconductivity. In the framework of two-band model, the present results predict that superconductivity appears, even if electron-electron interaction is positive. We discuss the possibility of a cooperative mechanism in the two-band superconductivity in relation to high-T_c superconductivity.

1. Introduction

Since the discovery of high-T_c copper oxides,[1] many theoretical proposals have been presented by using theoretical models such as t–J model and so on. In these mechanisms, superconductivity arising from the electron-electron (e-e) interaction has been attracted great interest in relation to the possibility of the high-T_c superconductivity. Anderson[2] has indeed emphasized an important role of the e-e interaction. Past decade many non-BCS theories[3–10] have been proposed, but they do not converge as unified and well-accepted theory yet.

Recent discovery of superconductivity of MgB_2[11] has also been much attracted great interest for elucidation of its mechanism from both experimental and theoretical view points. A crucial role of the electron-phonon (e-p) interaction has been pointed out in the superconductivity of MgB_2. Recent band calculations of MgB_2[12,13] with the McMillan formula[14] of transition temperature have supported the e-p interaction mechanism for the superconductivity. In this superconductivity,

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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.[15–21] Two-band model was first introduced by Kondo.[22] Recently, we have pointed out importance of many-band effects in high-T_c superconductivity.[23–26] We have also investigated anomalous phases in two-band model by using the Green function techniques.[19] The expressions of the transition temperature for several phases have been derived, and the approach has been applied to superconductivity in several crystals by charge injection and field-induced superconductivity.[27–30]

In the previous paper,[25,26] we have investigated superconductivity by using the two-band model and a two-particle Green function techniques.[31–36] We have applied the model to an electron-phonon mechanism for the traditional BSC method, an electron-electron interaction mechanism for high-T_c superconductivity, and a cooperative mechanism. In the framework of the two-particle Green function techniques,[33] it has been shown that in electron-phonon system a class of new so-called coupled states arises. The numerical calculations for the model have shown that superconducting (SC) gap depends on the number of bands crossing the Fermi level and on the momenta $k_1 + k_2 \neq 0$ of interacting electrons and the temperature dependence of the SC gap for high-T_c superconductors is more complicated than predicted in the BSC approach.

In this paper, we investigate two- or many-band effects in superconductivity by using a two-band model with a renormalization group approach. Renormalization equations for the two-band superconductivity are derived from the response function and the vertex correction of the model. Phase diagrams numerically solved from the renormalization equations are presented. We discuss superconductivity arising from e-e repulsive interaction in relation to two-band superconductivity.

2. Theoretical Background

In this section, we briefly summarize a two-band model for the superconductivity and introduce a renormalization group approach.[37–39]

2.1. *Hamiltonian*

We consider a Hamiltonian for two bands i and j written as

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

where

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

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

Γ is the bare vertex part:

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

with

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

and $a^\dagger_{i\boldsymbol{p}\sigma}(a_{i\boldsymbol{p}\sigma})$ is the creation (annihilation) operator corresponding to the excitation of electrons (or holes) in i-th band with spin σ and momentum $\boldsymbol{p}$. μ is the chemical potential. $\phi^*_{i\alpha\boldsymbol{p}_1}$ 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.

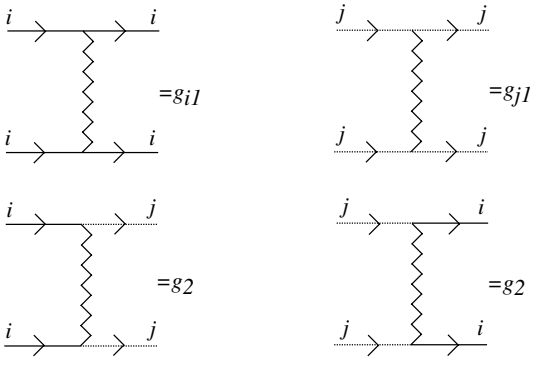

Fig. 1. Electron-electron interactions. Dependence of g on direction of momentum space is ignored in this model ($g_x(\boldsymbol{k}) \approx g_x$ $(x = i, j)$). We assume that g_x is constant.

We focus three electron scattering processes contributing to the singlet superconducting phase in the Hamiltonian of Eq. (1) as shown in Fig. 1.

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

$$g_{j1} = \langle jj|jj\rangle , \tag{7}$$

$$g_2 = \langle ii|jj\rangle = \langle jj|ii\rangle , \tag{8}$$

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. Note that Γ's are given by

$$\Gamma^{iiii}_{\alpha\beta\gamma\delta} = g_{i1}\left(\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\gamma}\delta_{\beta\delta}\right) ,$$

$$\Gamma^{jjjj}_{\alpha\beta\gamma\delta} = g_{j1}\left(\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\gamma}\delta_{\beta\delta}\right) ,$$

$$\Gamma^{iijj}_{\alpha\beta\gamma\delta} = \Gamma^{jjii}_{\alpha\beta\gamma\delta} = g_2\left(\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\gamma}\delta_{\beta\delta}\right) , \tag{9}$$

where we consider that an antisymmetrized vertex function Γ is a constant independent of the momenta in this study.

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.[23,30,19,24,39,40–42] 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.[39–42] 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,[23,19] 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 $Bi_2Sr_2Ca_{1-x}Y_xCu_2O_8$ (Bi-2212) by means of the above expressions of transition temperature.

2.2. *Renormalization group approach*

The Dyson equation is invariant under a multiple renormalization of Green's function and coupling parameters g. From this invariance for a scaling procedure, we obtain differential equations for the coupling parameters and the external vertex of Cooper pair.

$$y\frac{\partial}{\partial y}\tilde{g}_i(y,u,g) = \frac{\partial}{\partial \xi}\tilde{g}_i(\xi, u/y, \tilde{g}(t,u,g))|_{\xi=1} \ , \tag{10}$$

$$y\frac{\partial}{\partial y}\ln\Lambda(y,u,g) = \frac{\partial}{\partial \xi}\ln\Lambda(\xi, u/y, \tilde{g}(t,u,g))|_{\xi=1} \ , \tag{11}$$

where y and u are parameters with the dimension of energy. g means the set of original coupling, and Λ is the external vertex.

2.3. *Vertex correction and response function for Cooper pair*

To solve Eqs. (10) and (11), we estimate the right-hand side of Eq. (10) by using the perturbation theory. We consider the lowest order correction to the vertex for Cooper pair as shown in Fig. 2. From these diagrams, we obtain

$$\begin{pmatrix} \tilde{g}_{i1} \\ \tilde{g}_{j1} \end{pmatrix} = \begin{pmatrix} g_{i1} \\ g_{j1} \end{pmatrix} + \begin{pmatrix} -g_{i1}^2 & -g_2^2 \\ -g_{j1}^2 & -g_2^2 \end{pmatrix} \begin{pmatrix} L_i \\ L_j \end{pmatrix} , \tag{12}$$

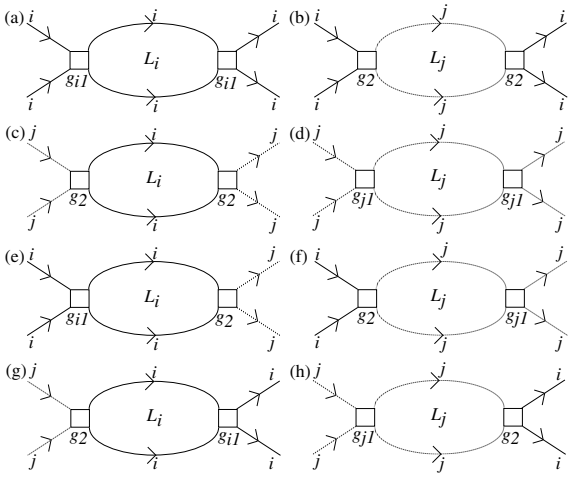

Fig. 2. Diagrams of the first order vertex correction. (a) and (b) contribute to $\tilde{g}_{i1}$. (c) and (d) are diagrams for $\tilde{g}_{j1}$. (e)-(h) for $\tilde{g}_2$.

$$\begin{pmatrix} \tilde{g}_2 \\ \tilde{g}_2 \end{pmatrix} = \begin{pmatrix} g_2 \\ g_2 \end{pmatrix} + \begin{pmatrix} -g_{i1}g_2 & -g_2 g_{j1} \\ -g_{j1}g_2 & -g_2 g_{i1} \end{pmatrix} \begin{pmatrix} L_i \\ L_j \end{pmatrix}, \tag{13}$$

where

$$L_i = \Pi_i(\boldsymbol{k}, \omega) = \frac{T}{N} \sum_{\boldsymbol{q}, \omega'} G_i(\boldsymbol{q}, \omega') G_i(\boldsymbol{k} - \boldsymbol{q}, \omega - \omega'),$$

$$L_j = \Pi_j(\boldsymbol{k}, \omega) = \frac{T}{N} \sum_{\boldsymbol{q}, \omega'} G_j(\boldsymbol{q}, \omega') G_j(\boldsymbol{k} - \boldsymbol{q}, \omega - \omega'). \tag{14}$$

G and T are the temperature Green function and temperature, respectively. For the special case $\omega = 0$, $\boldsymbol{k} = 0$, the above functions L_i and L_j become

$$L_i = -\left[\tanh\left(\frac{u_i/y}{2\xi}\right) + \tanh\left(\frac{u_i'/y}{2\xi}\right)\right] \ln \xi - 2A, \tag{15}$$

$$L_j = -\left[\tanh\left(\frac{u_j/y}{2\xi}\right) + \tanh\left(\frac{u_j'/y}{2\xi}\right)\right] \ln \xi - 2A, \tag{16}$$

where

$$A = \int dx \ln x \mathrm{sech}^2 \mathrm{x}. \tag{17}$$

u_i (u_j) and u_i' (u_j') are non-dimensional functions expressed by the chemical potential, cut-off energy, the top energy of j-th band, and the density of state for i-th (j-th) band.

Next, we consider a first order response function for singlet Cooper pair as shown in Fig. 3. Then, the first order vertex function Λ for i-th and j-th bands can be

written as

$$\begin{pmatrix} \Lambda_i + \Lambda_j \\ \Lambda_i - \Lambda_j \end{pmatrix} = \begin{pmatrix} 2 \\ 0 \end{pmatrix} + \begin{pmatrix} -g_1 & -g_2 \\ -g_1 & g_2 \end{pmatrix} \begin{pmatrix} L_i + L_j \\ L_i - L_j \end{pmatrix} \quad . \tag{18}$$

2.4. *Renormalization equation*

For simplicity, here and hereafter we assume $g_{i1} = g_{j1}$. From Eqs. (10), (12), and (13), we obtain differential equations written as

$$\frac{\partial}{\partial x}\tilde{g}_1 = -\left(\tilde{g}_1^2 + \tilde{g}_2^2\right) \ , \tag{19}$$

$$\frac{\partial}{\partial x}\tilde{g}_2 = -2\tilde{g}_1\tilde{g}_2 \quad . \tag{20}$$

In similar way, using Eqs. (11) and (18), we obtain differential equations written as

$$\frac{\partial}{\partial x}\ln\Lambda_+ = -\tilde{g}_1 - \tilde{g}_2 \, , \tag{21}$$

$$\frac{\partial}{\partial x}\ln\Lambda_- = -\tilde{g}_1 + \tilde{g}_2 \, , \tag{22}$$

where $\Lambda_+ = \Lambda_i + \Lambda_j$ and $\Lambda_- = \Lambda_i - \Lambda_j$.

3. Results and Discussion

In the previous section, we have derived basic equations of Eqs. (19)–(22) to find the low-temperature phases. For the special case of $g_2 = 0$, we obtain an analytic solution.

$$\tilde{g}_1 = \frac{1}{x + g_1^{-1}} \quad , \tag{23}$$

$$\tilde{g}_2 = 0 \quad , \tag{24}$$

$$\Lambda_i = \Lambda_j = \frac{1}{g_1 x + 1} \quad . \tag{25}$$

From these solutions, we find that the superconducting phase appears only when the intraband interaction g_1 is negative. In the case of the traditional superconductivity such as BCS theory, it is necessary that effective electron-electron interaction is negative ($g_1 < 0$) for realizing superconductivity. The present result agrees with that of the traditional theory for superconductivity expressed by one-band model.

For the case of $g_2 \neq 0$, phase diagrams numerically solved by the above renormalization equations are shown in Fig. 4. Figure 4(a) shows the phase diagram for the sum of superconductitivity for i-th and j-th bands. Thus, this phase implies that the sign of the superconducting state for i-th band and that of j-th band is the same. From this diagram, we find the superconductivity only in $-g_1 - g_2 > 0$ with negative g_2. On the other hand, the phase diagram for the difference between the superconducting states for i-th and j-th bands is shown in Fig. 3(b). In this case,

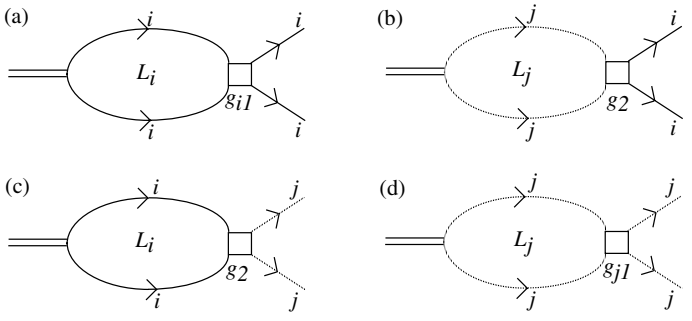

Fig. 3. Diagrams of the first order response function. (a) and (b) contribute to Λ_i. (c) and (d) show diagrams for Λ_j.

this phase means that the sign of the superconductivity for i-th band is different from that of j-th band. We can find that the superconductivity appears only in $-g_1 + g_2 > 0$ with positive g_2 from Fig. 4(b). Thus, the present results suggest that the two-band superconductivity appears, when the intraband umklapp repulsive scattering g_2 is larger than the normal repulsive scattering g_1. In the region of $g_2 > g_1$ with $g_2 < 0$ and $g_2 < -g_1$ with $g_2 > 0$ (two-gap region), we can expect that two gap functions are observed. In the former region, those superconducting gaps may be expressed by $|\Lambda_+| > |\Lambda_-|$ and the latter may be $|\Lambda_+| < |\Lambda_-|$. On the other hand, in the other region, we expect only single gap function. These results agree with the previous solutions[25,26] derived by using the two-particle Green function techniques. The superconductivity arising from electron-phonon mechanism ($g_1 < 0$ and $|g_2| < |g_1|$) such as MgB_2 is in the two-gap region. On the other hand, the superconductivity such as copper oxides ($|g_2| > |g_1|$) 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.

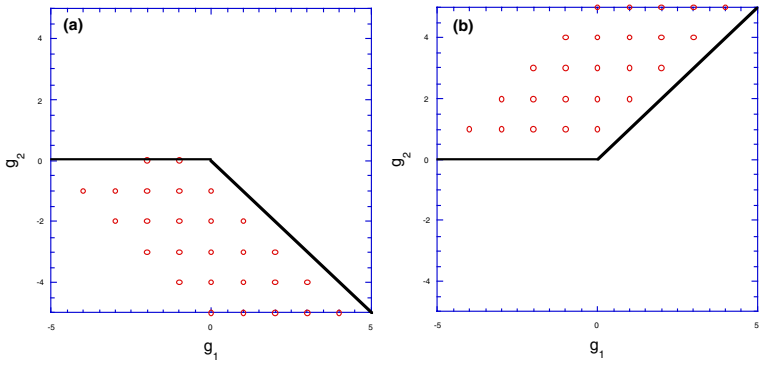

Fig. 4. Phase diagrams for superconductivity. (a) $\Lambda_i + \Lambda_j$. (b) $\Lambda_i - \Lambda_j$.

In a two-band model for negative g_1 with transfering or tunneling of Cooper pair between two bands, we can expect that transition temperature becomes higher than that derived from the single-band model. The tunneling of Cooper pair causes to stabilize the order parameter of superconductivity.[22,43] We can also expect higher T_c superconductivity than that of copper oxides in two regions of $g_1 < 0$, $g_2 < 0$ and $g_1 < 0$, $g_2 > 0$ by a cooperative mechanism. Phase diagrams for CDW, SDW, singlet superconductivity derived from more general Hamiltonian will be presented elesewhere.

In conclusion, we derive a renormalization equations for two-band superconductivity and present phase diagrams for the two-band superconductivity. In the framework of two-band model, the present results predict that superconductivity appears, even if electron-electron interaction is positive. We can expect that transition temperature becomes higher than that of copper oxides by a cooperative mechanism.

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