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Theory of Multiband Superconductivity

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Superconductivity arising from coulomb repulsion between electrons has been studied for a multiband system. We consider on-site and inter-site coulomb integrals, inter-site exchange integrals and inter-site exchange-like integrals [K of eq. (42)]. We do not take account of the correlation effect caused by the interaction, such as spin fluctuation etc., and calculate the average of the interaction energy with the BCS wave function. We find that when K is so large that satisfies eq. (50), an s-type superconducting state is stable when there are two fermi surfaces. The gap functions on these fermi surfaces have different signs and so the pair transition between them gives us a negative energy for a positive K, leading to superconductivity.

KEYWORDS: superconductivity, multiband, exchange-like integral, theory
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1. Introduction

Superconductivity arising from coulomb repulsion has been a subject of many theoretical works. A point of interest for it is how a condensation energy (a negative energy) arises from a positive interaction energy.[1,2] The key is to devide the $\boldsymbol{k}$-space into two regions, where the sign of the gap function is either positive or negative. The pair transition from the positive region to the negative one or the reverse transition gives us a negative energy, if the matrix element of the transition is positive. When the $\boldsymbol{k}$-dependence of the matrix element is appropriate, this negative contribution overcomes the positive ones, which arise from the pair transition within each region and results in superconductivity. A bare coulomb repulsion incorporated with the BCS wave function is not appropriate for this scenario to be realized, and one must take the electron correlation into the BCS wave function to obtain an effective interaction which has an appropriate $\boldsymbol{k}$-dependence[3–8] or take the correlation directly by using something like the Gutzwiller projection.[9–11]

The aim to obtain a negative energy from a positive interaction may also be achieved when one treats a two-band or multi-band superconductivity. In this case the sign of the gap function within each band may be definite but different from each other. Then the pair transition between the bands of different signs of the gap may give us a negative energy when the transition matrix element is positive. This scenario was first proposed by the present author[12] and studied by several authors for realistic substances.[13–22] As we shall see later, such a pair transition between bands is induced by an exchang-like integral between atomic orbitals belonging to different bands. Our concern is that many other integrals, such as on-site or inter-site coulomb or exchange integrals, might destroy the superconductivity caused by the interband transition. This problem was not studied seriously in previous works and we here present some results of the study for the condition of realizing superconductivity from the interband transiton. We consider a bipartite lattice and first find a one-particle eigenstate (Bloch orbitals) by introducing intra- and inter-sublattice transfer integrals. Based on these Bloch states the interaction Hamiltonian is expressed in terms of many integrals involving four atomic orbitals. We keep only the on-site and inter-site coulomb integrals, the exchange and exchange-like integrals between orbitals belonging to different sublattices. With such a Hamiltonian we take its average by the BCS wave function extended to a multiband case. We do not take account of the electron correlation, which means we work in the lowest order of the interaction. Contrary to the single band case we find that superconductivity exists in a wide range of reasonable parameter values without invoking higher-order effects of the interaction. In most cases superconductivity exists when there are two fermi surfaces, on each of which the sign of the gap function is definite but different from each other. In some cases the gap function may have zeros even though it is essentially of the s-character.

2. The Model

We consider L atomic orbitals in the unit cell denoted by ϕ_λ^n with $\lambda = 1, \cdots, L$. Here, n specifies the unit cell, and the position vector of the n-th unit cell is denoted by $\boldsymbol{R}_n$ and that of the λ-th atomic orbital measured from $\boldsymbol{R}_n$ by ρ_λ, so we write as

$$\phi_\lambda^n(\boldsymbol{r}) = \phi_\lambda(\boldsymbol{r} - \boldsymbol{R}_n - \rho_\lambda). \tag{1}$$

Especially, we use the notation $\phi_\lambda^0 = \phi_\lambda(\boldsymbol{r} - \rho_\lambda)$. We construct L LCAO's from ϕ_λ^n as

$$u_\lambda^{\boldsymbol{k}} = \frac{1}{\sqrt{N}} \sum_n \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_n} \phi_\lambda^n, \tag{2}$$

from which we obtain the eigenstates of the one-particle Hamiltonian as

$$\psi_l^{\boldsymbol{k}} = \sum_\lambda \alpha_l^\lambda(\boldsymbol{k}) u_\lambda^{\boldsymbol{k}} \quad l = 1, \cdots, L. \tag{3}$$

Here N is the total number of the unit cells. The coefficient of the transformation, $\alpha_l^\lambda(\boldsymbol{k})$, has the property $\alpha_l^\lambda(\boldsymbol{k}) = \bar{\boldsymbol{\alpha}}_l^\lambda(-\boldsymbol{k})$.

We now take account of the electron-electron interaction. In the second quantization scheme, the electron field is described by

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$$\psi(\boldsymbol{r},\xi)=\sum_{l\boldsymbol{k}\sigma}a_{l\boldsymbol{k}\sigma}\psi_l^{\boldsymbol{k}}(\boldsymbol{r})\sigma(\xi), \tag{4}$$

where ξ denotes the spin coordinate and $\sigma(\xi)$ is either the up-spin (α) function or the down-spin (β) function. In this scheme the interaction takes the form

$$H'=\frac{1}{2}\sum_{\xi\xi'}\int\psi^\dagger(\boldsymbol{r},\xi)\psi^\dagger(\boldsymbol{r}',\xi')V(\boldsymbol{r},\boldsymbol{r}')\psi(\boldsymbol{r}',\xi')\psi(\boldsymbol{r},\xi)\mathrm{d}\nu\mathrm{d}\nu'. \tag{5}$$

Among terms involved in eq. (5), we retain only those which correspond to scattering of the Cooper pair. Thus we have

$$H'_{\mathrm{red}}=\frac{1}{2}\sum_{l\boldsymbol{k}l'\boldsymbol{k}'}V_{l\boldsymbol{k}l'\boldsymbol{k}'}\sum_{\sigma\sigma'}a^\dagger_{l\boldsymbol{k}\sigma}a^\dagger_{l-\boldsymbol{k}\sigma'}a_{l'-\boldsymbol{k}'\sigma'}a_{l'\boldsymbol{k}'\sigma}, \tag{6}$$

where

$$V_{l\boldsymbol{k}l'\boldsymbol{k}'}=\langle\psi_l^{\boldsymbol{k}}\psi_l^{-\boldsymbol{k}}|\psi_{l'}^{\boldsymbol{k}'}\psi_{l'}^{-\boldsymbol{k}'}\rangle. \tag{7}$$

In general we use the notation

$$\langle\phi_i\phi_j|\phi_l\phi_k\rangle=\int\bar{\phi}_i(1)\bar{\phi}_j(2)V(1,2)\phi_l(1)\phi_k(2)\mathrm{d}\nu_1\mathrm{d}\nu_2. \tag{8}$$

The right hand side of eq. (7), which involves $\psi_l^{\boldsymbol{k}}$'s, can be expressed in terms of ϕ_λ^n's by using eqs. (2) and (3). Among integrals involving ϕ_λ^n's, we retain only coulomb integrals, exchange integrals and exchange-like integrals, whose definitions will be shown presently. Thus we have

$$\begin{aligned}V_{l\boldsymbol{k}l'\boldsymbol{k}'}=&\frac{1}{N}\sum_{n\lambda\lambda'}\mathrm{e}^{\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}_n}\bar{\alpha}_l^\lambda(\boldsymbol{k})\alpha_l^{\lambda'}(\boldsymbol{k})\alpha_{l'}^\lambda(\boldsymbol{k}')\bar{\alpha}_{l'}^{\lambda'}(\boldsymbol{k}')\langle\phi_\lambda^0\phi_{\lambda'}^n|\phi_\lambda^0\phi_{\lambda'}^n\rangle\\&+\frac{1}{N}{\sum_{n\lambda\lambda'}}'\mathrm{e}^{\mathrm{i}(\boldsymbol{k}+\boldsymbol{k}')\cdot\boldsymbol{R}_n}\bar{\alpha}_l^\lambda(\boldsymbol{k})\alpha_l^{\lambda'}(\boldsymbol{k})\alpha_{l'}^{\lambda'}(\boldsymbol{k}')\bar{\alpha}_{l'}^\lambda(\boldsymbol{k}')\langle\phi_\lambda^0\phi_{\lambda'}^n|\phi_{\lambda'}^n\phi_\lambda^0\rangle\\&+\frac{1}{N}{\sum_{n\lambda\lambda'}}'|\alpha_l^\lambda(\boldsymbol{k})|^2\cdot|\alpha_{l'}^{\lambda'}(\boldsymbol{k}')|^2\langle\phi_\lambda^0\phi_\lambda^0|\phi_{\lambda'}^n\phi_{\lambda'}^n\rangle.\end{aligned} \tag{9}$$

The integrals in each line of eq. (9) are, from the above, the coulomb integral, the exchange integral and the exchange-like integral, respectively. All these integrals must be positive. The prime on the summation sign means to neglect the term with $n=0$ and $\lambda=\lambda'$. We naturally have $V_{l\boldsymbol{k}l'\boldsymbol{k}'}=\bar{V}_{l'\boldsymbol{k}'l\boldsymbol{k}}$. Furthermore we have $V_{l\boldsymbol{k}l'\boldsymbol{k}'}=V_{l'\boldsymbol{k}'l\boldsymbol{k}}$, if the atomic orbitals are real, which we assume to be the case. For simplicity we assume that all these atomic orbitals are of the s-type.

Now we take the BCS wave function extended to a multiband case

$$\Psi=\prod_{l\boldsymbol{k}}(u_{l\boldsymbol{k}}+v_{l\boldsymbol{k}}a^\dagger_{l\boldsymbol{k}\uparrow}a^\dagger_{l-\boldsymbol{k}\downarrow})|0\rangle, \tag{10}$$

and calculate the average of eq. (6) with it to find

$$\begin{aligned}\langle H'_{\mathrm{red}}\rangle=&\sum_{l\boldsymbol{k}l'\boldsymbol{k}'}V_{l\boldsymbol{k}l'\boldsymbol{k}'}u_{l\boldsymbol{k}}v_{l\boldsymbol{k}}u_{l'\boldsymbol{k}'}v_{l'\boldsymbol{k}'}\\=&\frac{1}{N}\sum_{n\lambda\lambda'}\langle\phi_\lambda^0\phi_{\lambda'}^n|\phi_\lambda^0\phi_{\lambda'}^n\rangle\left|\sum_{l\boldsymbol{k}}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_n}\bar{\alpha}_l^\lambda(\boldsymbol{k})\alpha_l^{\lambda'}(\boldsymbol{k})u_{l\boldsymbol{k}}v_{l\boldsymbol{k}}\right|^2\\&+\frac{1}{N}{\sum_{n\lambda\lambda'}}'\langle\phi_\lambda^0\phi_{\lambda'}^n|\phi_{\lambda'}^n\phi_\lambda^0\rangle\left|\sum_{l\boldsymbol{k}}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_n}\bar{\alpha}_l^\lambda(\boldsymbol{k})\alpha_l^{\lambda'}(\boldsymbol{k})u_{l\boldsymbol{k}}v_{l\boldsymbol{k}}\right|^2\\&+\frac{1}{N}{\sum_{n\lambda\lambda'}}'\langle\phi_\lambda^0\phi_\lambda^0|\phi_{\lambda'}^n\phi_{\lambda'}^n\rangle\sum_{l\boldsymbol{k}}|\alpha_l^\lambda(\boldsymbol{k})|^2u_{l\boldsymbol{k}}v_{l\boldsymbol{k}}\times\sum_{l\boldsymbol{k}}|\alpha_l^{\lambda'}(\boldsymbol{k})|^2u_{l\boldsymbol{k}}v_{l\boldsymbol{k}}.\end{aligned} \tag{11}$$

The first two terms, the coulomb term and the exchange term, are positive definite and superconductivity is not expected with only these terms, but the third therm, the exchange-like term, may be negative and its negative contribution to the energy may overcome the positive ones of the first two terms and result in superconductivity. We will study the condition for this scenario to be realized.

Before starting calculation, we rewrite eq. (11) as

$$\begin{aligned}\langle H'_{\mathrm{red}}\rangle=&\boldsymbol{E}'_0+\frac{1}{N}{\sum_{n\lambda\lambda'}}'[\langle\phi_\lambda^0\phi_{\lambda'}^n|\phi_\lambda^0\phi_{\lambda'}^n\rangle+\langle\phi_\lambda^0\phi_{\lambda'}^n|\phi_{\lambda'}^n\phi_\lambda^0\rangle]\\&\times\left|\sum_{l\boldsymbol{k}}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_n}\bar{\alpha}_l^\lambda(\boldsymbol{k})\alpha_l^{\lambda'}(\boldsymbol{k})u_{l\boldsymbol{k}}v_{l\boldsymbol{k}}\right|^2,\end{aligned} \tag{12}$$

where

$$\boldsymbol{E}'_0=N\sum_{\lambda\lambda'}c_{\lambda\lambda'}X_\lambda X_{\lambda'}, \tag{13}$$

$$X_\lambda=\frac{1}{N}\sum_{l\boldsymbol{k}}|\alpha_l^\lambda(\boldsymbol{k})|^2u_{l\boldsymbol{k}}v_{l\boldsymbol{k}},$$

$$c_{\lambda\lambda'}=\sum_n\langle\phi_\lambda^0\phi_\lambda^0|\phi_{\lambda'}^n\phi_{\lambda'}^n\rangle=c_{\lambda'\lambda}. \tag{14}$$

In a simple and useful approximation, we keep only $\boldsymbol{E}'_0$. It is a quadratic form and will be indefinite in sign when there is at least one negative eigenvalue of the matrix $c_{\lambda\lambda'}$. We will later study this problem for a simple example.

Let $\varepsilon_{l\boldsymbol{k}}$ be the one-particle energy of each band measured

from the fermi level μ. (We consider the ground state of the system.) Then the total energy with this energy included is written as

$$E = 2\sum_{lk} \varepsilon_{lk} v_{lk}^2 + \sum_{lkl'k'} V_{lkl'k'} u_{lk} v_{lk} u_{l'k'} v_{l'k'}. \tag{15}$$

Minimization of this expression determines the variation parameters u_{lk} and v_{lk} as

$$u_{lk}^2 = \frac{1}{2}\left(1 + \frac{\varepsilon_{lk}}{E_{lk}}\right), \tag{16}$$

$$v_{lk}^2 = \frac{1}{2}\left(1 - \frac{\varepsilon_{lk}}{E_{lk}}\right), \tag{17}$$

$$2u_{lk}v_{lk} = \frac{\Delta_{lk}}{E_{lk}}, \tag{18}$$

$$E_{lk} = \sqrt{\varepsilon_{lk}^2 + \Delta_{lk}^2}, \tag{19}$$

with the self-consistency equation

$$\Delta_{lk} = -\frac{1}{2}\sum_{l'k'} V_{lkl'k'} \frac{\Delta_{l'k'}}{E_{l'k'}}. \tag{20}$$

We set $\Delta_{lk} = \Delta \cdot z_{lk}$, where Δ represents the magnitude of the gap ($\Delta > 0$) and z_{lk} its angular dependence. We concentrate on the case of small Δ, when the following relation holds[1,2)]

$$\sum_{\boldsymbol{k}} \frac{F(\boldsymbol{k})}{E_{lk}} = -2\log\Delta \cdot \sum_{\boldsymbol{k}} F(\boldsymbol{k})\delta(\varepsilon_{lk}) + (\text{terms non-divergent as } \Delta \to 0).$$

Keeping only the first contribution, we find the self-consistency equation now reads

$$\frac{1}{\log\Delta} z_{lk} = \sum_{l'k'} V_{lkl'k'} \cdot \delta(\varepsilon_{l'k'}) \cdot z_{l'k'}. \tag{21}$$

This is a homogenous linear equation with the eigenvalue being $1/\log\Delta \equiv \rho$. It is not an Hermitian equation and one might wonder if the eigenvalue is real or not. That it is real can be seen by multiplying both sides of eq. (21) by $\bar{z}_{lk}\delta(\varepsilon_{lk})$ and summing over l and $\boldsymbol{k}$:

$$\frac{1}{\log\Delta}\sum_{lk} |z_{lk}|^2 \delta(\varepsilon_{lk}) = \sum_{lkl'k'} V_{lkl'k'} \bar{z}_{lk} z_{l'k'} \delta(\varepsilon_{lk})\delta(\varepsilon_{l'k'}).$$

Since both sums are real and the one on the left hand side does not vanish, we can conclude $1/\log\Delta \equiv \rho$ must be real. Since we are restricting ourselves to the weak coupling limit, a negative eigenvalue ρ assures a superconducting ground state.

We will obtain the expression for $V_{lkl'k'}$ from eq. (11) or eq. (12), but with E_0' we simply find

$$V_{lkl'k'} = \frac{1}{N}\sum_{\lambda\lambda'} c_{\lambda\lambda'} |\alpha_l^{\lambda}(\boldsymbol{k})|^2 |\alpha_{l'}^{\lambda'}(\boldsymbol{k}')|^2. \tag{22}$$

Hereafter we will tell about the results of keeping only E_0', but treatment of a more general case is straightforward and the results of that case will be mentioned when it is necessary. Since eq. (22) is the sum of the products of two functions depending only on $\boldsymbol{k}$ and $\boldsymbol{k}'$, the summation over $\boldsymbol{k}'$ in eq. (21) gives us a $\boldsymbol{k}$-independent factor, which we denote by x_λ:

$$x_\lambda = \frac{1}{N}\sum_{lk} |\alpha_l^{\lambda}(\boldsymbol{k})|^2 \delta(\varepsilon_{lk}) z_{lk}. \tag{23}$$

Then eq. (21) reads

$$\rho z_{lk} = \sum_{\lambda\lambda'} c_{\lambda\lambda'} |\alpha_l^{\lambda}(\boldsymbol{k})|^2 x_{\lambda'}. \tag{24}$$

Insertion of this expression into eq. (23) gives us

$$\rho x_\lambda = \sum_{\lambda'} a_{\lambda\lambda'} x_{\lambda'}, \quad \lambda = 1, \cdots, L \tag{25}$$

with

$$a_{\lambda\lambda'} \equiv \sum_{\lambda''} b_{\lambda\lambda''} c_{\lambda''\lambda'} \tag{26}$$

and

$$b_{\lambda\lambda'} \equiv \frac{1}{N}\sum_{lk} |\alpha_l^{\lambda}(\boldsymbol{k})|^2 |\alpha_l^{\lambda'}(\boldsymbol{k})|^2 \delta(\varepsilon_{lk}). \tag{27}$$

The dimension of the seqular equation has been reduced to L. We note that $b_{\lambda\lambda'}$ involves only the band parameters, whereas $c_{\lambda\lambda'}$ only the coulomb parameters. When eq. (25) has a negative eigenvalue, we conclude that a superconducting state is stable. The condition for a negative eigenvalue is closely related to the condition that the matrix $c_{\lambda\lambda'}$ has a negative eigenvalue and so E_0' is indefinite. This correlation is brought about by eq. (26). We will see an example of this correlation in the next section. After solving eq. (25) and finding x_λ within an arbitrary factor, we obtain angular dependence of the gap function from eq. (24). Without knowing details of the solution we see that the symmetry of the gap function is a_{1g}, because so is the symmetry of $|\alpha_l^{\lambda}(\boldsymbol{k})|^2$.

3. An Example of a Bipartite Square Lattice

As an example we consider a two-dimensional two-sublattice model as shown in Fig. 1, where $L = 2$. The LCAO's on sublattice 1 and 2 are

$$u_1^{\boldsymbol{k}} = \frac{1}{\sqrt{N}}\sum_n \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_n} \phi_1(\boldsymbol{r} - \boldsymbol{R}_n), \tag{28}$$

$$u_2^{\boldsymbol{k}} = \frac{1}{\sqrt{N}}\sum_n \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_n} \phi_2(\boldsymbol{r} - \boldsymbol{R}_n - \rho), \tag{29}$$

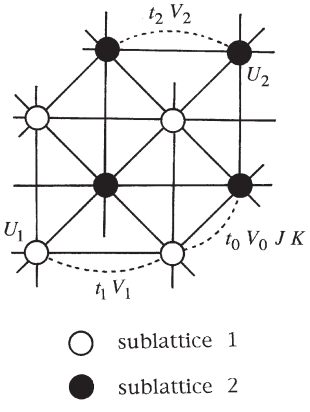

Fig. 1. Parameters of a two-dimensional bipartite lattice. U_1 and U_2 are on-site coulomb integrals and V_1 and V_2 are inter-site coulomb integrals on each sublattice, whereas t_1 and t_2 are transfer integrals in each sublattice. V_0, J and K are the coulomb, exchange and exchange-like integrals between the sublattices.

where $\rho = (1/2, 1/2)$. The lattice constant has been set to unity. The one particle energy of these LCAO's are

$$\zeta_{1\boldsymbol{k}} = e_1 + 2t_1(\cos k_x + \cos k_y) - \mu, \tag{30}$$

$$\zeta_{2\boldsymbol{k}} = e_2 + 2t_2(\cos k_x + \cos k_y) - \mu, \tag{31}$$

where t_1 and t_2 are the transfer integral in each sublattice and e_1 and e_2 are the energy level of ϕ_1 and ϕ_2, respectively.

We also consider transfer between nearest nighbouring ϕ_1 and ϕ_2:

$$\int \bar{u}_1^{\boldsymbol{k}} H_0 u_2^{\boldsymbol{k}} \mathrm{d}v = \zeta_{0\boldsymbol{k}} \mathrm{e}^{-\mathrm{i}\varphi_{\boldsymbol{k}}}, \tag{32}$$

$$\zeta_{0\boldsymbol{k}} = 4t_0 \cos(k_x/2)\cos(k_y/2), \tag{33}$$

$$\varphi_{\boldsymbol{k}} = (k_x + k_y)/2, \tag{34}$$

where t_0 is the relevant transfer integral (see Fig. 1).

The eigenstates, eq. (3), are now expressed by

$$\psi_1^{\boldsymbol{k}} = \alpha_1^1(\boldsymbol{k}) u_1^{\boldsymbol{k}} + \alpha_1^2(\boldsymbol{k}) u_2^{\boldsymbol{k}}, \tag{35}$$

$$\psi_2^{\boldsymbol{k}} = \alpha_2^1(\boldsymbol{k}) u_1^{\boldsymbol{k}} + \alpha_2^2(\boldsymbol{k}) u_2^{\boldsymbol{k}}, \tag{36}$$

with

$$\alpha_1^1(\boldsymbol{k}) = \cos\eta_{\boldsymbol{k}}, \qquad \alpha_1^2(\boldsymbol{k}) = -\mathrm{e}^{\mathrm{i}\varphi_{\boldsymbol{k}}} \sin\eta_{\boldsymbol{k}}, \tag{37}$$

$$\alpha_2^1(\boldsymbol{k}) = \mathrm{e}^{-\mathrm{i}\varphi_{\boldsymbol{k}}} \sin\eta_{\boldsymbol{k}}, \quad \alpha_2^2(\boldsymbol{k}) = \cos\eta_{\boldsymbol{k}}, \tag{38}$$

$$\tan 2\eta_{\boldsymbol{k}} = -\zeta_{0\boldsymbol{k}}/\Delta\zeta_{\boldsymbol{k}}, \qquad \Delta\zeta_{\boldsymbol{k}} = (\zeta_{1\boldsymbol{k}} - \zeta_{2\boldsymbol{k}})/2, \tag{39}$$

whereas the eigenvalues by

$$\varepsilon_{1\boldsymbol{k}} = \frac{1}{2}(\zeta_{1\boldsymbol{k}} + \zeta_{2\boldsymbol{k}}) + \sqrt{(\Delta\zeta_{\boldsymbol{k}})^2 + \zeta_{0\boldsymbol{k}}^2}, \tag{40}$$

$$\varepsilon_{2\boldsymbol{k}} = \frac{1}{2}(\zeta_{1\boldsymbol{k}} + \zeta_{2\boldsymbol{k}}) - \sqrt{(\Delta\zeta_{\boldsymbol{k}})^2 + \zeta_{0\boldsymbol{k}}^2}. \tag{41}$$

From now on we retain only the following integrals and equivalent ones:

$$\begin{aligned} U_1 &= \langle\phi_1^0\phi_1^0|\phi_1^0\phi_1^0\rangle, \quad U_2 = \langle\phi_2^0\phi_2^0|\phi_2^0\phi_2^0\rangle, \\ K &= \langle\phi_1^0\phi_1^0|\phi_2^0\phi_2^0\rangle. \end{aligned} \tag{42}$$

We then have $c_{11} = U_1$, $c_{22} = U_2$, $c_{12} = c_{21} = zK$, where $z = 4$ is the number of the nearest neighbours. We also find from eqs. (26) and (27)

$$\begin{aligned} a_{11} &= b_{11}U_1 + b_{12}zK, \quad a_{12} = b_{11}zK + b_{12}U_2, \\ a_{21} &= b_{21}U_1 + b_{22}zK, \quad a_{22} = b_{21}zK + b_{22}U_2, \end{aligned} \tag{43}$$

where

$$b_{11} = \frac{1}{N}\sum_{\boldsymbol{k}}[\cos^4\eta_{\boldsymbol{k}}\delta(\varepsilon_{1\boldsymbol{k}}) + \sin^4\eta_{\boldsymbol{k}}\delta(\varepsilon_{2\boldsymbol{k}})], \tag{44}$$

$$b_{22} = \frac{1}{N}\sum_{\boldsymbol{k}}[\sin^4\eta_{\boldsymbol{k}}\delta(\varepsilon_{1\boldsymbol{k}}) + \cos^4\eta_{\boldsymbol{k}}\delta(\varepsilon_{2\boldsymbol{k}})], \tag{45}$$

$$b_{12} = b_{21} = \frac{1}{N}\sum_{\boldsymbol{k}}\sin^2\eta_{\boldsymbol{k}}\cos^2\eta_{\boldsymbol{k}}[\delta(\varepsilon_{1\boldsymbol{k}}) + \delta(\varepsilon_{2\boldsymbol{k}})]. \tag{46}$$

From eq. (43) or eq. (26) one has

$$a_{11}a_{22} - a_{12}a_{21} = BC, \tag{47}$$

where

$$C \equiv c_{11}c_{22} - c_{12}c_{21} = U_1U_2 - (zK)^2, \tag{48}$$

$$\begin{aligned} B \equiv b_{11}b_{22} - b_{12}b_{21} &= \frac{1}{N^2}\sum_{\boldsymbol{k}\boldsymbol{k}'}(\cos^2\eta_{\boldsymbol{k}} - \sin^2\eta_{\boldsymbol{k}'})^2 \cdot \delta(\varepsilon_{1\boldsymbol{k}})\delta(\varepsilon_{2\boldsymbol{k}'}) \\ &+ \frac{1}{2N^2}\sum_{\boldsymbol{k}\boldsymbol{k}'}(\sin^2\eta_{\boldsymbol{k}} - \sin^2\eta_{\boldsymbol{k}'})^2 \cdot [\delta(\varepsilon_{1\boldsymbol{k}})\delta(\varepsilon_{1\boldsymbol{k}'}) + \delta(\varepsilon_{2\boldsymbol{k}})\delta(\varepsilon_{2\boldsymbol{k}'})] \geq 0. \end{aligned} \tag{49}$$

When $B > 0$, the condition that eq. (25) has a negative eigenvalue, namely $a_{11}a_{22} - a_{12}a_{21} < 0$, is equivalent to the condition that the E_0' is indefinite in sign, namely $C < 0$, or

$$(zK)^2 - U_1U_2 > 0. \tag{50}$$

On the other hand, when $B = 0$, the smallest eigenvalue of eq. (25) is zero and so the superconducting state cannot be stable. From eq. (49) we see that $B = 0$ when (i) there exists only a single fermi surface and (ii) $\sin^2\eta_{\boldsymbol{k}}$ is a constant on that surface. This criterion is very useful for later arguments. The negative eigenvalue of eq. (25) is obtained for $BC < 0$ as

$$\rho = (1/2)\left[U_1b_{11} + U_2b_{22} + 2zKb_{12} - \sqrt{(U_1b_{11} + U_2b_{22} + 2zKb_{12})^2 - 4BC}\right] \tag{51}$$

When $V_0 = \langle\phi_1^0\phi_2^0|\phi_1^0\phi_2^0\rangle$ and $J = \langle\phi_1^0\phi_2^0|\phi_2^0\phi_1^0\rangle$ are also kept, the second term of eq. (12) is found as

$$\begin{aligned} &\frac{4(V_0 + J)}{N}\left[\sum_{\boldsymbol{k}}\cos(k_x/2)\cos(k_y/2)\sin 2\eta_{\boldsymbol{k}}(u_{1\boldsymbol{k}}v_{1\boldsymbol{k}} - u_{2\boldsymbol{k}}v_{2\boldsymbol{k}})\right]^2 \\ &+ \frac{4(V_0 + J)}{N}\left[\sum_{\boldsymbol{k}}\sin(k_x/2)\sin(k_y/2)\sin 2\eta_{\boldsymbol{k}}(u_{1\boldsymbol{k}}v_{1\boldsymbol{k}} - u_{2\boldsymbol{k}}v_{2\boldsymbol{k}})\right]^2 \end{aligned} \tag{52}$$

Here we naturally assumed that $u_{1\boldsymbol{k}}v_{1\boldsymbol{k}}$ and $u_{2\boldsymbol{k}}v_{2\boldsymbol{k}}$ have the same even or odd parity. When the symmetry of the gap function is a_{1g}, the second line vanishes, but the first line does not because $\cos(k_x/2)\cos(k_y/2)\sin 2\eta_{\boldsymbol{k}}$ is also of the a_{1g}-symmetry. With the $V_0 + J$ term included we introduce

$$\xi_1 = \frac{1}{2N}\sum_{\boldsymbol{k}} \cos(k_x/2)\cos(k_y/2)\sin 2\eta_{\boldsymbol{k}}[z_{1\boldsymbol{k}}\delta(\varepsilon_{1\boldsymbol{k}}) - z_{2\boldsymbol{k}}\delta(\varepsilon_{2\boldsymbol{k}})]$$

beside x_1 and x_2 and solve the 3-dimentional eigenvalue problem. A term $4(V_0+J)\cos(k_x/2)\cos(k_y/2)\sin 2\eta_{\boldsymbol{k}}\xi_1$ should be added to the right hand side of eq. (24) for $l=1$ and subtracted from that for $l=2$.

4. Results

The results depend strongly on the band structure, which is determined by t_0, t_1, t_2, e_1, e_2. We discuss on two typical cases of the band parameters.

4.1 Case 1: $t_0 = 0.5$, $t_1 = -1$, $t_2 = -1$, $e_1 = 1$, $e_2 = -1$

This is the case of two paralel and displaced dispersion curves, which are repelled by the mixing t_0 between them. The resulting dispersion $\varepsilon_{1\boldsymbol{k}}$ and $\varepsilon_{2\boldsymbol{k}}$ are shown in Fig. 2. The bands are partially filled when the fermi level is between -6.2 are 5.0. There are two fermi surfaces, when the fermi level is between e_a and e_b of Fig. 2. Outside of this there is only a single fermi surface.

We have considered three cases for the choice of the interaction parameters:

A : $(U_1 = 5, U_2 = 0.4, K = 0.5)$,

B : $(U_1 = 5, U_2 = 0.4, K = 0.5, V_0 = 1, J = 0.5)$,

C : $(U_1 = 5, U_2 = 0.4, K = 0.5, V_1 = 2, V_2 = 3, J = 0.5)$,

in all of which $-C = 2$. In Case C we consider the inter-site coulomb integrals in the same sublattice, V_1 and V_2 (see Fig. 1). Minus of the eigenvalue ρ is shown in Fig. 3, from which we see that superconductivity exists only when the fermi level is between e_a and e_b, namely only when there exist two fermi surfaces. This is becasuse, outside of the region between e_a and e_b, $\sin^2\eta_{\boldsymbol{k}}$ is nearly constant on the fermi surface and so the second term of eq. (49) vanishes (the first term naturally vanishes when there is only a single fermi surface). The peaks at $\mu = -1$ and $\mu = 1$ are due to the van Hove singularities. Cases B and C involve fairly large coulomb integrals between sites, but still superconductivity is robust around the van Hove singularity, if $-C$ is not small (2 in this case).

We then discuss on the results of calculation of the gap function based on eq. (24) or similar one including the ξ_1 term. When the fermi level is between e_a and -1.0 and not close to the latter, the two fermi surfaces are nearly circular

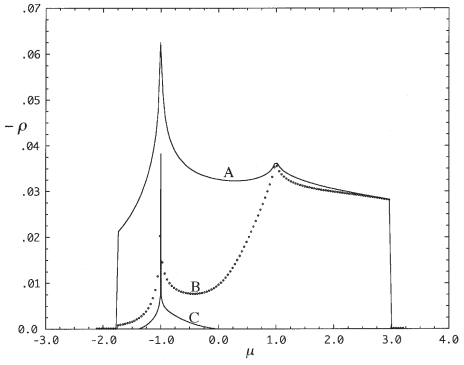

Fig. 3. Minus of the eigenvalue vs the fermi energy for the band parameters of Fig. 2 and the three choices of the interaction parameters (see text).

and the gap functions are almost constant on them, but have different signs for the different bands. This is what we expected: different signs of the gap function for the different bands and a positive scattering matrix element betwee them give us a negative contribution to the interaction energy and lead to superconductivity. We encounter a somewhat different situation near the van Hove singularity $\mu = -1$. Fig. 4 shows the fermi surfaces for the fermi level $\mu = -1.1$ and $\mu = -0.9$. A and C are those of the lower band and B and D those of the upper band. Fig. 5 shows the gap functions on these fermi surfaces with an arbitrary scale for Case B of the interaction parameters. One sees there are

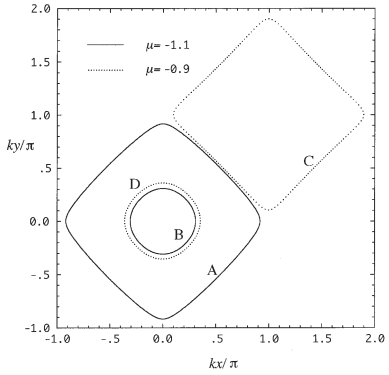

Fig. 4. The fermi surfaces for the dispersion curves of Fig. 2 for the fermi energy $\mu = -1.1$ and $\mu = -0.9$. The van Hove singularity is at $\mu = -1.0$.

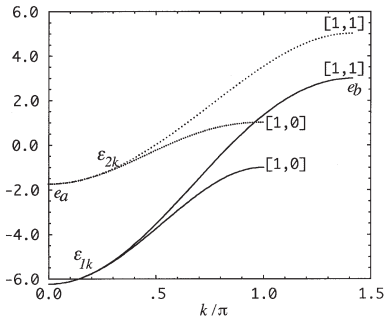

Fig. 2. The dispersion curves for case of $t_0 = 0.5$, $t_1 = -1$, $t_2 = -1$, $e_1 = 1$, $e_2 = -1$ drawn from (0,0) to $(\pi, 0)$ and from (0,0) to (π, π). When the fermi level is between e_a and e_b, there exist two fermi surfaces.

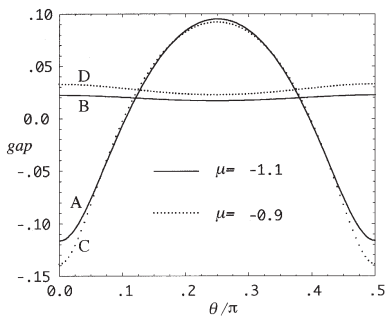

Fig. 5. The gap functions on A to D in Fig. 4 vs the angle θ between the k_x axis and the radius vector drawn from (0,0) or (π, π). The interaction parameters are Case B of §4.1.

eight zeros of the gap on the larger fermi surface. This is also the case for Case C but not the case for Case A, in which the gap function is nearly constant even close to the van Hove singularity.

4.2 *Case 2: $t_0 = 0.5$, $t_1 = -1$, $t_2 = 1$, $e_1 = 0$, $e_2 = 0$*

This is the case of the two crossing bands which are mutually repelled by the mixing t_0. The dispersion curves are shown in Fig. 6, from which one sees that in the regions between $\mu = -4.5$ and -4 and between $\mu = 4$ and 4.5 there exists only a single fermi surface. Figure 7 shows minus of the eigenvalue for the three cases of the interaction parameters as before. One finds that superconductivity does not exist in the regions mentioned above for the same reason as in §4.1. The van Hove singularities are at $\mu = -0.97$ and $\mu = 0.97$. When the fermi level is below -0.97, there are two fermi surfaces, one centered at (0,0) and the other at (π, π) (*e.g.*, A and B of Fig. 8). The gap functions have a constant sign on each of them, but have different signs from each other as in the case of §4.1. As the fermi level goes up above -0.97, a cross-over of the fermi surfaces results in C and D surfaces of Fig. 8. As one naturally sees from Fig. 8, each of the gap functions on C and D must have four zeros at the four edges. The gap functions calculated based on eq. (24) are shown in Fig. 9 for the interaction parameters of Case A. Results for Case B and Case C are similar. In the parts of the fermi surfaces A and C of the figure, *e.g.*, which are close to each other (denoted by+and+in Fig. 8), the values of the gap are almost the same. This is not apparent in Fig. 9, because the angle θ is not the same when the radius is drawn from the center of A and from that of C to a point on the fermi surface.

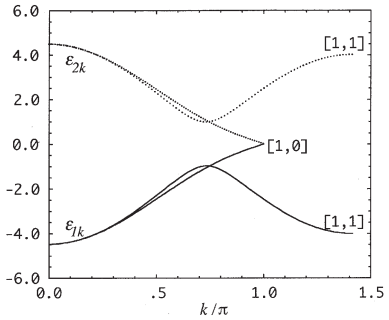

Fig. 6. The dispersion curves for case of $t_0 = 0.5$, $t_1 = -1$, $t_2 = 1$, $e_1 = 0$, $e_2 = 0$, drawn from (0,0) to $(\pi, 0)$ and from (0,0) to (π, π). When the fermi level is between -4.5 and -4.0 or between 4.0 and 4.5, there exists only a single fermi surface.

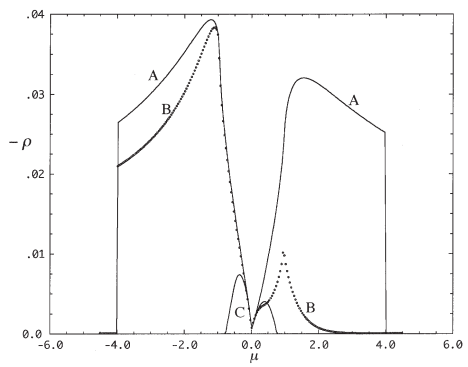

Fig. 7. Minus of the eigenvalue ρ vs the fermi energy for the band parameters of Fig. 6 and the same choices of the interaction parameters as in §4.1.

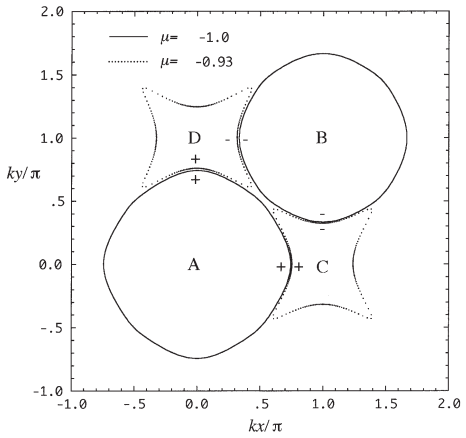

Fig. 8. The fermi surfaces for the dispersion curves of Fig. 6 for the fermi energy $\mu = -1.0$ and $\mu = -0.93$. The van Hove singularity is at $\mu = -0.97$ and $\mu = 0.97$. The gap functions are positive on A and negative on B, but change signs on C and D.

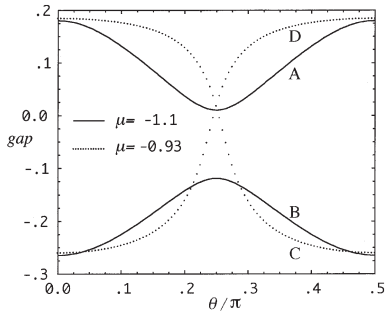

Fig. 9. The gap functions on A to D in Fig. 8 vs the angle θ between the k_x axis and the radius vector drawn from (0,0), (π, π), $(\pi, 0)$ or $(0, \pi)$. The interaction parameters are Case A of §4.1.

5. Discussion

We have seen an important role played by an exchange-like integral, such as $\langle \phi^0_\lambda \phi^0_\lambda | \phi^n_{\lambda'} \phi^n_{\lambda'} \rangle$, in leading to multi-band superconductivity. Its effect is enhanced by the factor z, the number of the nearest neighbours of a bipartite lattice as is seen in eq. (50). The negative effect of the on-site coulomb integrals is only cooperative, and if one of them is small, the effect is small even when the other is large. Thus the presence of a weakly correlated band favours for the superconductivity due to inter-band transition. Another point of interest of eq. (50) is that z is larger in three dimension and may be 6 at least. We may expect a more enhanced effect in three dimension. Superconductivity of MgB_2 may be a candidate to treat along this scheme.

We have not taken account of the electron correlation caused by the interaction. Thus the eigenvalue ρ of the self-consistency equation is linear in the interaction parameters. More precisely, when all the interaction parameters are multiplied by λ and all the band parameters and the chemical potential by ν, the eigenvalue is multiplied by λ/ν. This is easily seen in a special case, where only the parameter K is

retained. From eq. (51) we then have

$$\rho = -zK\left(\sqrt{b_{11}b_{22}} - b_{12}\right) \leq 0$$

where b's are inversely proportional to v.

The symmetry of the gap function is a_{1g} in the example of §4, so is essentially of the s-character. Then the effect of the on-site coulomb integrals is not suppressed, but superconductivity still exists when inequality (50) is satisfied. This is achieved by the gap function, which is positive in some part of the fermi surface and negative in the other part of it, while keeping the a_{1g} symmetry. Such a gap function takes advantage of the pair transition from the part of the positive gap function to the part of the negative one. In most cases such a gap function is realized when there are two fermi surfaces, in one of which it is positive and in the other it is negative. However it is also possible that the gap function changes its sign on a single fermi surface with several zeros, as we have seen in the example of §4.2. We can expect that there are several types of the specific heat vs temperature curve, when the present mechanism is relevant to the superconductivity.

We have not taken account of the correlation between electrons caused by the interaction. One of the important consequences of this approximation is that it is not the coulomb and exchange integrals but the exchange-like integrals that are responsible for superconductivity. Although this conclusion is quite general, the situation is changed when one takes account of the correlation by a perturbation theory or by a projection method. Even in this case it is certain that the exchange-like integrals help to enhance superconductivity.

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