

EXACT SOLUTION OF TWO-BAND SUPERCONDUCTIVITY IN ULTRASMALL GRAINS

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Abstract. We investigate two-band superconductivity in ultrasmall grain. The Richardson's exact solution is extended to two-band systems, and a new coupled equation is derived according to the procedure of Richardson's works. Parity gap and condensation energy of ultrasmall two-band superconducting grain are numerically obtained by solving the coupled equations. We discuss these properties in ultrasmall grain in relation to the correlation, interband interaction, and size dependence.

Key words: Two-band superconductivity, Ultrasmall grain, Richardson's exact solution

1. Introduction

Black et. al. have revealed the presence of a parity dependent spectroscopic gap in tunnelling spectra of nanosize Al grains (Black, 1996; Ralph, 1995). Many groups have theoretically investigated the physical properties, such as critical level spacing, condensation energy, parity gap, etc. of ultrasmall grains of conventional superconductors (Jankó, 1994; Delft, 1996; Smith, 1996; Matveev, 1997; Braun, 1998; Delft, 1999; Gladilin, 2002). The questions arising from the nanosize of superconducting grains have first been discussed by Anderson (Anderson, 1959). The standard BCS theory fails when the level spacing approaches the superconducting gap. To investigate

the properties in such nanosize systems, it is necessary to take more accurate treatment. Braun and von Delft (Braun, 1998; Delft, 1999; Braun, 1999; Sierra, 2000) have reintroduced the exact solution to the reduced BCS Hamiltonian developed by Richardson (Richardson, 1963; Richardson, 1964; Richardson, 1965; Richardson, 1966). It is noteworthy that the Richardson's solution is applicable at distributions of single-electron energy level. V. N. Gladioli et. al. (Delft, 1999) have investigated the pairing characteristics such as condensation energy, spectroscopic gap, parity gap, etc. by using the Richardson's exact solution for the reduced BCS Hamiltonian.

Recent discovery of superconductivity of MgB_2 (Nagamatsu, 2001) with $T_c = 39$ K has also been much attracted great interest for elucidation of its mechanism from both experimental and theoretical view points. Since this discovery, the possibility of two-band superconductivity has also been discussed in relation to two gap functions experimentally and theoretically. Two-band model has been introduced by several groups (Suhl, 1959; Moskalenko, 1959; Kondo, 1963). Recently, two-band or multi-band superconductivity has been theoretically investigated in relation to superconductivity arising from coulomb repulsive interactions and the possibility of new superconductivity arising from new mechanisms with higher transition temperature (Konsin, 1988; Yamaji, 1994; Combescot, 1995; Konsin, 1998; Nagao, 2000.2; Kondo, 2001; Kondo, 2002; Nagao, 1999; Nagao, 2002.1; Nagao, 2002.2; Nagao, 1997; Nagao, 1998; Nagao, 2000.1).

In this paper, we investigate two-band superconductivity in ultrasmall grain. The Richardson's exact solution is extended to two-band systems, and new coupled equation is derived according to the procedure of Richardson's works. Parity gap and condensation energy of ultrasmall two-band superconducting grain are numerically given by solving the coupled equation. We discuss these properties in ultrasmall grain in relation to the correlation, interband interaction, and size dependence.

2. Exact solution for two-band superconductivity

In this section, we derive an exact solution of two-band superconductivity for reduced BCS Hamiltonian.

2.1. HAMILTONIAN

We consider a Hamiltonian for two bands 1 and 2 written as

$$\begin{aligned}
 H = & \sum_{j\sigma} \varepsilon_{1j} a_{j\sigma}^\dagger a_{j\sigma} - g_1 \sum_{jk} a_{j\uparrow}^\dagger a_{j\downarrow}^\dagger a_{k\downarrow} a_{k\uparrow} + \sum_{j\sigma} \varepsilon_{2j} b_{j\sigma}^\dagger b_{j\sigma} - g_2 \sum_{jk} b_{j\uparrow}^\dagger b_{j\downarrow}^\dagger b_{k\downarrow} b_{k\uparrow} \\
 & + g_{12} \sum_{jk} a_{j\uparrow}^\dagger a_{j\downarrow}^\dagger b_{k\downarrow} b_{k\uparrow} + g_{12} \sum_{jk} b_{j\uparrow}^\dagger b_{j\downarrow}^\dagger a_{k\downarrow} a_{k\uparrow} . \tag{1}
 \end{aligned}$$

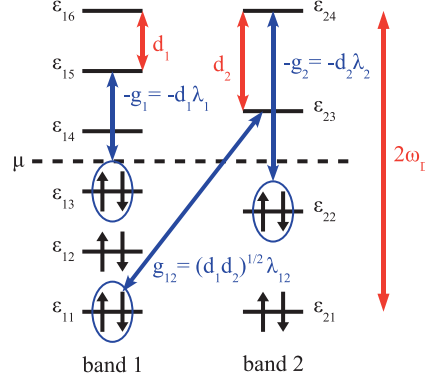


Figure 1. Two band system and parameters in Hamiltonian.

The first line of Eq. (1) corresponds to the reduced BCS Hamiltonian for bands 1 and 2. The third line means a coupling between them and corresponds to the pair scattering process between these two bands (see Fig.1). $a_{j\sigma}^\dagger$ ($a_{j\sigma}$) and $b_{j\sigma}^\dagger$ ($b_{j\sigma}$) are the creation (annihilation) operator in band 1 and 2 with spin σ and the single-particle levels ε_{1j} and ε_{2j} , respectively. The sums of j and k are over a set of N_1 states for band 1 with fixed width $2\hbar\omega_{1D}$ and a set of N_2 states for band 2 with fixed width $2\hbar\omega_{2D}$, respectively.

In this study, we assume that the Debye energies for two bands coincide with each other as

$$\omega_{1D} = \omega_{2D} = \omega_D . \quad (2)$$

The interaction constants g_1 and g_2 can be written as

$$g_1 = d_1\lambda_1 , \quad g_2 = d_2\lambda_2 , \quad (3)$$

where d_1 and d_2 mean the mean single-particle level spacing,

$$d_1 = 2\hbar\omega_D/N_1 , \quad d_2 = 2\hbar\omega_D/N_2 , \quad (4)$$

and λ_1 and λ_2 are dimensionality interaction parameters for two bands. We define the inter-band interaction constant as

$$g_{12} = \sqrt{d_1 d_2} \lambda_{12} . \quad (5)$$

The system we are considering consist of two half-filled bands, each of which has equally spaced N_n single-particle levels and $M_n (= N_n/2)$ doubly occupied pair levels ($n = 1, 2$). We take as our unit of energy the single-particle level spacing. Thus, the single-particle spectrum is given by

$$\varepsilon_{nj} = d_n j - \omega_D , \quad j = 1, 2, \dots, N_n \quad (n = 1, 2) . \quad (6)$$

Richardson had solved for the single band model for arbitrary set of single-particle levels. For simplicity, we assume that there are not singly occupied single-particle levels. As can be seen from Eq. (1), these levels are decoupled from the rest of the system. They are said to be blocked and contribute with their single-particle energies to the total energy. The above simplification implies that every single-particle level j is either empty (i.e. $|vac\rangle$), or occupied by a pair of electrons (i.e. $a_{j\uparrow}^\dagger a_{j\downarrow}^\dagger |vac\rangle$ and $b_{j\uparrow}^\dagger b_{j\downarrow}^\dagger |vac\rangle$). These are called as unblocked level.

2.2. EXACT SOLUTION

In order to extend Richardson's solution into the two-band system, we define two kind of hard-core boson operators as

$$c_j = a_{j\downarrow} a_{j\uparrow}, \quad c_j^\dagger = a_{j\uparrow}^\dagger a_{j\downarrow}^\dagger, \quad d_j = b_{j\downarrow} b_{j\uparrow}, \quad d_j^\dagger = b_{j\uparrow}^\dagger b_{j\downarrow}^\dagger. \quad (7)$$

The Hamiltonian Eq. (1) for the unblocked levels can be then written as

$$\begin{aligned} H_U = & 2 \sum_j^{N_1} \varepsilon_{1j} c_j^\dagger c_j - g_1 \sum_{jk}^{N_1} c_j^\dagger c_k + 2 \sum_j^{N_2} \varepsilon_{2j} d_j^\dagger d_j - g_2 \sum_{jk}^{N_2} d_j^\dagger d_k \\ & + g_{12} \sum_j^{N_1} \sum_k^{N_2} c_j^\dagger d_k + g_{12} \sum_j^{N_2} \sum_k^{N_1} d_j^\dagger c_k. \end{aligned} \quad (8)$$

We shall find the eigenstates $|M_1; M_2\rangle$ of this Hamiltonian with $M_1 + M_2$ pairs in the following form as

$$H_U |M_1; M_2\rangle_U = E(M_1; M_2) |M_1; M_2\rangle_U = \left(\sum_{J=1}^{M_1} E_{1J} + \sum_{K=1}^{M_2} E_{2K} \right) |M_1; M_2\rangle_U, \quad (9)$$

where $E(M_1; M_2)$ is the eigenvalue and

$$|M_1; M_2\rangle_U = \prod_{J=1}^{M_1} C_J^\dagger \prod_{K=1}^{M_2} D_K^\dagger |vac\rangle, \quad (10)$$

and

$$C_J^\dagger = \sum_j^{N_1} \frac{c_j^\dagger}{2\varepsilon_{1j} - E_{1J}}, \quad D_J^\dagger = \sum_j^{N_2} \frac{d_j^\dagger}{2\varepsilon_{2j} - E_{2J}}. \quad (11)$$

Now, we define C_0^\dagger and D_0^\dagger as

$$C_0^\dagger = \sum_j^{N_1} c_j^\dagger, \quad D_0^\dagger = \sum_j^{N_2} d_j^\dagger, \quad (12)$$

then, we can rewrite Eq. (8) as

$$H_U = 2 \sum_j^{N_1} \varepsilon_{1j} c_j^\dagger c_j - g_1 C_0^\dagger C_0 + 2 \sum_j^{N_2} \varepsilon_{2j} d_j^\dagger d_j - g_2 D_0^\dagger D_0 + g_{12} C_0^\dagger D_0 + g_{12} D_0^\dagger C_0. \quad (13)$$

Using these new operators, we find

$$\begin{aligned} H_U |M_1; M_2\rangle_U &= \left(\sum_{J=1}^{M_1} E_{1J} + \sum_{K=1}^{M_2} E_{2K} \right) |M_1; M_2\rangle_U \\ &+ C_0^\dagger \sum_{J=1}^{M_1} \left(1 - \sum_j^{N_1} \frac{g_1}{2\varepsilon_{1j} - E_{1J}} + \sum_{J' \neq J}^{M_1} \frac{2g_1}{E_{1J'} - E_{1J}} \right) |M_1(J); M_2\rangle_U \\ &+ D_0^\dagger \sum_{J=1}^{M_1} \left(\sum_j^{N_1} \frac{g_{12}}{2\varepsilon_{1j} - E_{1J}} - \sum_{J' \neq J}^{M_1} \frac{2g_{12}}{E_{1J'} - E_{1J}} \right) |M_1(J); M_2\rangle_U \\ &+ C_0^\dagger \sum_{K=1}^{M_2} \left(\sum_j^{N_2} \frac{g_{12}}{2\varepsilon_{2j} - E_{2K}} - \sum_{K' \neq K}^{M_2} \frac{2g_{12}}{E_{2K'} - E_{2K}} \right) |M_1; M_2(K)\rangle_U \\ &+ D_0^\dagger \sum_{K=1}^{M_2} \left(1 - \sum_j^{N_2} \frac{g_2}{2\varepsilon_{2j} - E_{2K}} + \sum_{K' \neq K}^{M_2} \frac{2g_2}{E_{2K'} - E_{2K}} \right) |M_1; M_2(K)\rangle_U, \end{aligned} \quad (14)$$

where

$$|M_1(L); M_2\rangle_U = \prod_{J=1}^{L-1} C_J^\dagger \prod_{J'=L+1}^{M_1} C_{J'}^\dagger \prod_{K=1}^{M_2} D_K^\dagger |vac\rangle, \quad (15)$$

$$|M_1; M_2(L)\rangle_U = \prod_{J=1}^{M_1} C_J^\dagger \prod_{K=1}^{L-1} D_K^\dagger \prod_{K'=L+1}^{M_2} D_{K'}^\dagger |vac\rangle. \quad (16)$$

Comparing Eq. (14) with Eq. (9), for arbitrary J and K we obtain

$$\begin{pmatrix} C_0^\dagger & D_0^\dagger \end{pmatrix} \begin{pmatrix} 1 + g_1 A_{1J} & -g_{12} A_{2K} \\ -g_{12} A_{1J} & 1 + g_2 A_{2K} \end{pmatrix} \begin{pmatrix} |M_1(J); M_2\rangle_U \\ |M_1; M_2(K)\rangle_U \end{pmatrix} = 0, \quad (17)$$

where

$$A_{nL} = - \sum_j^{N_n} \frac{1}{2\varepsilon_{nj} - E_{nL}} + \sum_{L' \neq L}^{M_n} \frac{2}{E_{nL'} - E_{nL}}. \quad (18)$$

Non-trivial solution of Eq. (17) is derived from a determinantal equation;

$$F_{JK} = (1 + g_1 A_{1J})(1 + g_2 A_{2K}) - g_{12}^2 A_{1J} A_{2K} = 0. \quad (19)$$

This constitutes a set of $M_1 + M_2$ couples equations for $M_1 + M_2$ parameters E_{1J} and E_{2K} ($J = 1, 2, \dots, M_1; K = 1, 2, \dots, M_2$), which may be thought of as self-consistently determined pair energies. Equation (19) is exact eigenvalue equation for two-band superconducting system, and can be regarded as a generalization of the Richardson's original eigenvalue equation.

2.3. PREPROCESSING FOR NUMERICAL CALCULATION

To remove the divergences from the second term of A_{nL} in Eq. (18), we make changes of energy variables.

$$E_{n2\lambda} = \xi_{n\lambda} + i\eta_{n\lambda}, \quad E_{n2\lambda-1} = \xi_{n\lambda} - i\eta_{n\lambda}, \quad \lambda = 1, 2, \dots, M_n/2, \quad (20)$$

where we assume that the number of pairs is even. Since complex pair energies appear in complex conjugate pairs, the total energy is kept in real.

A further transformation is necessary in order to remove the divergences from the first term of A_{nL} . We define new variables $x_{n\lambda}$ and $y_{n\lambda}$ as

$$\xi_{n\lambda} = \varepsilon_{n2\lambda} + \varepsilon_{n2\lambda-1} + d_n x_{n\lambda} \quad (x_{n\lambda} \leq 0), \quad (21)$$

$$\eta_{n\lambda}^2 = -\{(\varepsilon_{n2\lambda} - \varepsilon_{n2\lambda-1})^2 - d_n^2 x_{n\lambda}^2\} y_{n\lambda} \quad (y_{n\lambda} \geq 0). \quad (22)$$

Then, we can rewrite F_{JK} by using new variables and extract the real and the imaginary part as

$$F_{\lambda\lambda'}^+ = \frac{1}{2}(F_{\lambda\lambda'} + F_{\lambda\lambda'}^*), \quad F_{\lambda\lambda'}^- = \frac{1}{2i}(F_{\lambda\lambda'} - F_{\lambda\lambda'}^*). \quad (23)$$

Therefore, for arbitrary combination of λ and λ' we solve the following equations;

$$F_{\lambda\lambda'}^+ = 0, \quad F_{\lambda\lambda'}^- = 0 \quad (\lambda = 1, 2, \dots, M_1/2; \lambda' = 1, 2, \dots, M_2/2). \quad (24)$$

3. Results and discussion

We now apply the exact solution for two-band system to discuss properties of the two-band superconducting in ultrasmall grain. The single-particle level patterns of $(2M_1 + m) + 2M_2$ electron system ($m = 0, 1, \text{ and } 2$) that we are considering are represented in Figs. 2(a), (b), and (c), respectively. As seen these figures, the additional electrons first occupy the band 1, then the band 2. And numerical calculations given below are carried out under the condition that $N_1 : N_2 = 3 : 2$.

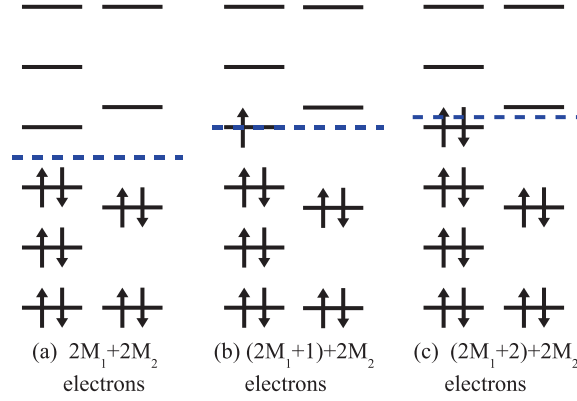


Figure 2. Single-particle levels near the Fermi level in a two band superconductivity. The dotted lines mean the chemical potential. The left and right bands are band 1 and 2, respectively. d_1 and d_2 are the mean level spacings. (a) $2M_1 + 2M_2$ electron system, where M_n is a number of pair levels. (b) $(2M_1 + 1) + 2M_2$ electron system. (c) $(2M_1 + 2) + 2M_2$ electron system.

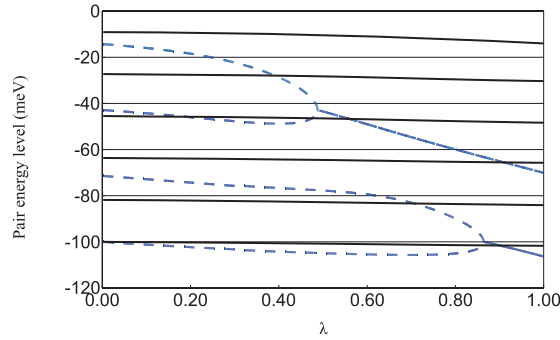


Figure 3. Typical behavior of pair energy levels of two bands for the ground state. Parameters used in calculation are $N_1 = 12$, $N_2 = 8$, $M_1 = 6$, $M_2 = 4$, $\hbar\omega_D = 50$, $0 < \lambda = \lambda_1 = \lambda_2 \leq 1.0$, and $\lambda_{12}/\lambda = 0.2$. Solid and broken lines are correspond to the pair energy levels of the band 1 and the band 2, respectively.

3.1. PAIR ENERGY LEVEL

By minimizing the sum of squares of Eq. (24) for various interaction parameters, we obtain a behavior of pair energy levels E_{nJ} of two bands as shown in Fig. 3.

As seen in the figures, the band 2 condenses into degenerate levels, but the band 1 does not. In general, we can expect that the single-particle levels in band of which mean level spacing d is larger than the other band degenerate faster. The behavior of the condensing band is qualitatively the same as that

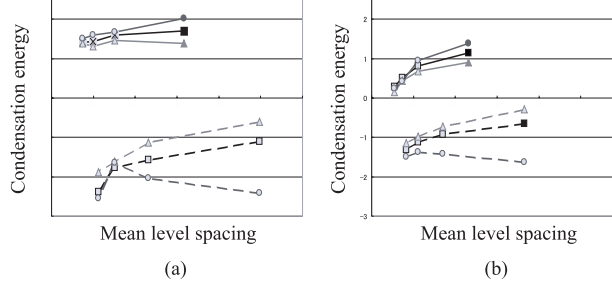


Figure 4. Condensation energy. Parameters used in the calculations are $\hbar\omega_D = 50$, and $\lambda = \lambda_1 = \lambda_2 = 0.5$. Values are normalized by the bulk gap, $\Delta = \omega_D \sinh^{-1} \left(\frac{\lambda}{\lambda^2 - \lambda_{12}^2} \right)$. The solid and broken lines correspond to the condensation energy for the band 1 and 2, respectively. Lines plotted by squares, by triangles and by circles are for $2M_1 + 2M_2$ electron system, for $(2M_1 + 1) + 2M_2$ electron system, and for $(2M_1 + 2) + 2M_2$ electron system, respectively. (a) The condensation energy for the interband coupling parameter $\lambda_{12} = 0.01$. (b) The condensation energy for $\lambda_{12} = 0.1$.

for the case of calculation for the single band (Delft, 1999). The co-existence of the normal band and the condensed one may be reflected in the opposite phase of the gaps of these bands (Nagao, in press).

3.2. CONDENSATION ENERGY

The condensation energy of band n for $(2M_1 + m) + 2M_2$ electron system can be defined as

$$E_n^C(2M_1 + m, 2M_2) = E_n(2M_1 + m, 2M_2) + \left(M_n + \frac{m}{2} \right) g_n - E_n^0(2M_1 + m, 2M_2), \quad (25)$$

where $E_n(2M_1 + m, 2M_2)$ and $E_n^0(2M_1 + m, 2M_2)$ are the ground state energy and the sum of the single-particle energy, respectively.

We calculate the condensation energies and show in Figs. 4(a) and (b). As seen in the figures, we can understand that the band 2 condenses, but the band 1 does not because of the sign of values. This difference of sign may also be reflected in the opposite phase of the gaps of these bands. The behaviors of the results for the condensed band (band 2) are qualitatively the same result as the case of the single band calculation. That of the condensation energy of band 2 for $(2M_1 + 2) + 2M_2$ electron system is, however, different from the others. We can also see that the condensation energy is affected by the interband interaction λ_{12} (Nagao, in press).

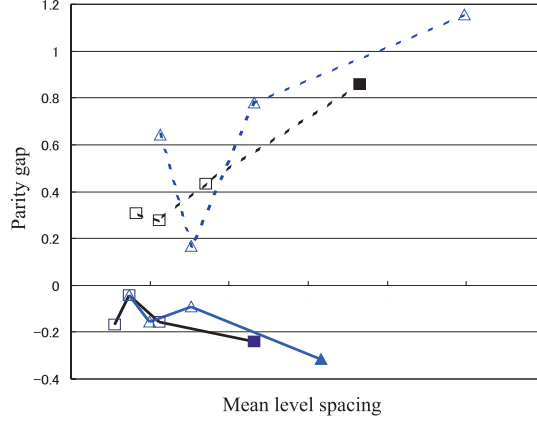


Figure 5. Parity gap. Parameters used in calculation are $\hbar\omega_D = 50$, and $\lambda_1 = \lambda_2 = 0.5$. The solid and broken lines correspond to the parity gap for the band 1 and 2, respectively. Lines plotted by triangles and by squares are for the interband coupling parameter $\lambda_{12} = 0.01$ and for $\lambda_{12} = 0.1$, respectively. Values are normalized by the bulk gap.

3.3. PARITY GAP

The parity gap of band n is defined as

$$\Delta_n^p = E_n(2M_1 + 1, 2M_2) - \frac{1}{2} \{E_n(2M_1, 2M_2) + E_n(2M_1 + 2, 2M_2)\}, \quad (26)$$

which has been introduced by Matveev and Larkin and characterizes the even-odd ground state energy difference (Matveev, 1997).

The parity gaps we have calculated are shown in Fig. 5. For the condensed band, we obtain qualitatively the same result as the case of the single band calculation, i.e. there is a minimal point and a tendency toward 1 for $d \rightarrow 0$. The mean level spacing giving the minimal point is, however, much less than that for the single band. The parity gap is almost independent upon the interband interaction λ_{12} . This is also mentioned in our previous work (Nagao, in press).

4. Conclusions

We have extended the the Richardson's exact solution to the two-band system, and have derived a new coupled equation. To investigate the properties of the two-band superconductivity, we have solved the equation numerically, and have given the behavior of pair energy levels, the condensation energy, and the parity gap.

The band of which mean level spacing is larger than the other band degenerates and condenses faster. The behavior of the condensing band is qualitatively the same as that for the case of calculation for the single band. The co-existence of the normal band and the condensed one may be reflected in the opposite phase of the gaps of these bands. This phase character appears in every results of numerical calculations. Therefore, the phase of gap is important to stabilize the two-band superconductivity.

We have also calculated the condensation energy and the parity gap for two-band superconductivity. The result suggest that the interband interaction λ_{12} affects on the condensation energy, but not on the parity gap.

In summary, an expression of Richardson's exact solution for two-band superconductivity has been presented, and has been solved numerically. Then, the behavior of pair energy levels, the condensation energy, and the parity gap have presented. The results for the condensed band is almost qualitatively the same as those for the calculation of single band, and the co-existence of the normal band and the condensed one may be originated from the opposite phase of the gaps of these bands.

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