NANOSIZE TWO-GAP SUPERCONDUCTIVITY

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Abstract. We investigate properties of nanosize two-gap superconductivity by using a two-sublevel model in the framework of a mean field approximation. A model corresponding to a nanosize two-gap superconductivity is presented, and the partition function of the nanosize system is analytically derived by using a path integral approach. A definition of the critical level spacing of the two-gap superconductivity is also presented, and we discuss condensation energy and parity gap of the two-gap superconductivity in relation to the size dependence of those properties with two bulk gaps and effective pair scattering process between two sublevels.

Key words: Two-gap superconductivity, Ultrasmall grain

1. Introduction

The recent discovery of superconductivity of MgB_2(Nagamatsu et. al., 2001) has been much attracted great interest in the properties and for elucidation of its mechanism from both experimental and theoretical view points. A crucial role of the electron-phonon (e-p) interaction has been strongly suggested in the superconductivity of MgB_2(Liu et.al., 2001).Recent band calculations of MgB_2(Kortus et. al., 2001; An and Picket, 2001; Kato et. al., 2004) with the McMillan formula (McMillan, 1968) of transition temperature have supported the e-p interaction mechanism for the superconductivity. Since the discovery, the possibility of two-band superconductivity arising from other

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mechanisms has also been discussed in relation to two gap functions theoretically.

Recently, two-band or multi-band superconductivity has been theoretically investigated in relation to superconductivity arising from coulomb repulsive interactions (Konsin et. al., 1988; Yamaji and Shimoi, 1994; Combescot and Leyronas, 1995; Konsin and Sorkin, 1998; Nagao et. al., 2000; Kondo, 2001; konbo, 2002). The concept of the two-band model has been discussed in 1958 (Suhl et. al., 1959; Moskalenko, 1959; konbo, 1963). Recently, we have pointed out importance of many-band effects in superconductivity (Nagao et. al., 1999; Nagao and Yaremko et. al., 2002; Nagao and Kruchinin et. al., 2002; Nagao et. al., 2003; Kruchinin and Nagao, 2005). We have also investigated anomalous phases in two-band model by using the Green function techniques (Nagao et.al., 2000; Nagao, Kawabe and Kruchinin, to appear.). 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 (Nagao et. al., 1997; Nagao et. al., 1998; Nagao et. al., 2000).

Recent experiments (Black et. al., 1996; Ralph et. al., 1995) by Black et al. have also generated much interest in the size dependence of the superconductivity. Properties of ultrasmall superconducting grains have been theoretically investigated by many groups (Jankó et. al., 1994; von Delft et. al., 1996; Smith and Ambegaokar, 1996; Matveev and Larkin, 1997; Braun and von Delft, 1998; Gladilin et. al., 2002; Braun and von Delft, 1999). In such ultrasmall grains, the fundamental theoretical question for the size dependency of the superconductivity was noticed by Anderson (Anderson, 1959). The standard BCS theory gives a good description of the phenomenon of superconductivity in large sample. However, as the size of a superconductor becomes small, the BCS theory fails. In ultrasmall Al grains, the bulk gap has been discussed in relation to physical properties in ultrasmall grain such as the parity gap (Matveev and Larkin, 1997), condensation energy (Gladilin et. al., 2002), electron correlation (von Delft, 1996) etc. with the dependence of level spacing (Smith and Ambegaokar, 1996) of samples.

In this paper, we investigate properties of nanosize two-gap superconductivity by using a two-sublevel model in the framework of a mean field approximation. A model corresponding to a nanosize two-gap superconductivity is presented, and the partition function of the nanosize system is analytically derived by using a path integral approach. A definition of the critical level spacing of the two-gap superconductivity is also presented, and we discuss condensation energy and parity gap of the two-gap superconductivity in relation to the size dependence of those properties with two bulk gaps and effective pair scattering process between two sublevels.

2. Nanosize two-gap superconductivity

In nanosize grain of a superconductor, the quantum level spacing approaches the superconducting gap. In the case of two-gap superconductor, we can consider a model with two sublevels corresponding to two independent bands. In this section, we present a model for nanosize two-gap superconductivity and an expression of the partition function of the system.

2.1. HAMILTONIAN FOR NANOSIZE GRAINS

We consider a pairing Hamiltonian with two sublevels corresponding to two bands 1 and 2 written as

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

where

$$H_0 = \sum_{j,\sigma} \left[\varepsilon_{1j} - \mu\right] a^\dagger_{j\sigma} a_{j\sigma} + \sum_{k,\sigma} \left[\varepsilon_{2k} - \mu\right] b^\dagger_{k\sigma} b_{k\sigma} \ , \tag{2}$$

$$H_{\rm int} = -g_1 \sum_{j,j' \in I} a^\dagger_{j\uparrow} a^\dagger_{j\downarrow} a_{j'\downarrow} a_{j'\uparrow} - g_2 \sum_{k,k' \in J} b^\dagger_{k\uparrow} b^\dagger_{k\downarrow} b_{k'\downarrow} b_{k'\uparrow}$$
$$+ g_{12} \sum_{j \in I, k \in J} a^\dagger_{j\uparrow} a^\dagger_{j\downarrow} b_{k\downarrow} b_{k\uparrow} + g_{12} \sum_{j \in I, k \in J} b^\dagger_{k\uparrow} b^\dagger_{k\downarrow} a_{j\downarrow} a_{j\uparrow} \ . \tag{3}$$

$a^\dagger_{j\sigma}(a_{j\sigma})$ and $b^\dagger_{j\sigma}(b_{j,\sigma})$ are the creation (annihilation) operators in sublevels 1 and 2 with spin σ and energies ε_{1j} and ε_{2j}, respectively. The operators for each sublevel satisfy the anticommutation relations, and the operators between sublevels are independent. μ is the chemical potential. The second term in Eq.(1) is the interaction Hamiltonian. g_1 and g_2 are the effective interaction constant for sublevels 1 and 2. g_{12} is an effective interaction constant, which corresponds to the pair scattering process between two bands. The sums with respect to j and k in Eq.(3) are over the set I of N_{1I} states corresponding to a half-filled band 1 with fixed width $2\omega_{1D}$ and the set J of N_{2J} states for band 2, respectively.

In this study, we assume that the Deby energies for the two sublevel systems are the same $\omega_{1D} = \omega_{2D} = \omega_D$. With this assumption, the ratio of N_{1I} and N_{2J} can be related to the (constant) densities of state (DOS) ρ_1 and ρ_2 for two bands as follows: $N_{1I}/N_{2J} = \rho_1/\rho_2$. We write the interaction constants g_1 and g_2 as $d_1\lambda_1$ and $d_2\lambda_2$, respectively. $d_1 = 2\omega_D/N_{1I}$ and $d_2 = 2\omega_D/N_{2J}$ are the energy level spacings, and λ_1 and λ_2 are dimensionless parameters. In(3) we have introduced a pairing interaction $g_{12} = \sqrt{d_1 d_2}\lambda_{12}$. between the two sublevel systems. In summary, we have a relation of $\rho_1/\rho_2 = N_{1I}/N_{2J} = d_2/d_1$.

2.2. PATH INTEGRAL APPROACH

It is convenient to introduce a path integral approach for treatment of the fluctuations of the order parameters. This approach gives an exact expression for the grand partition function of a superconductor. $Z(\mu, T) = Tr \exp\left[-(H - \mu N)/T\right]$, where T is the temperature, and N is the number operator in the grain. The idea of the path integral approach is to replace the formulation for system of the problem in terms of electronic operators by equivalent formulation in terms of the superconducting order parameter.

By the path integral approach, we obtain an expression of the grand partition function for the Hamiltonian of Eq. (1).

$$Z(\mu, T) = \int D\Delta_1 D\Delta_1^* D\Delta_2 D\Delta_2^* e^{-S[\Delta_1, \Delta_2]} \quad , \tag{4}$$

where the action $S[\Delta_1, \Delta_2]$ is defined as

$$\begin{aligned} S[\Delta_1, \Delta_2] = &- \sum_j \left[Tr \ln G_{1j}^{-1} - \frac{\xi_{1j}}{T} \right] - \sum_k \left[Tr \ln G_{2k}^{-1} - \frac{\xi_{2k}}{T} \right] \\ &+ \int_0^{1/T} d\tau \frac{1}{g_1 g_2 - g_{12}^2} \left[g_2 |\Delta_1(\tau)|^2 + g_1 |\Delta_2(\tau)|^2 \right. \\ &\left. + g_{12} \left(\Delta_1(\tau) \Delta_2(\tau)^* + \Delta_1(\tau)^* \Delta_2(\tau) \right) \right] \quad . \end{aligned} \tag{5}$$

Δ_1 and Δ_2 are bulk gaps for sublevels 1 and 2, respectively. Here, $\xi_{1j} = \varepsilon_{1j} - \mu$ and $\xi_{2k} = \varepsilon_{2k} - \mu$, and the inverse Green functions

$$G_{aj}^{-1}(\tau, \tau') = \left[-\frac{d}{d\tau} - \xi_{aj} \sigma^z - \Delta_a(\tau) \sigma^+ - \Delta_a^*(\tau) \sigma^- \right] \delta(\tau - \tau') \quad , \tag{6}$$

where $a = 1, 2$ for band label, $\sigma^{\pm} = \sigma^x \pm i\sigma^y$, and $\sigma^{x,y,z}$ are the Pauli matrices. G_1^{-1} and G_2^{-1} satisfy antiperiodic boundary conditions.

In the case of stronger interaction, $\Delta_1 \gg d_1$ and $\Delta_2 \gg d_2$, we consider a mean field approximation for the order parameters in the path integral approach. Substituting a time-independent order parameters into the action of Eq. (5), we have

$$\begin{aligned} \Omega(\mu) \;=\; &\sum_j \left(\xi_{1j} - \epsilon_{1j} \right) + \sum_k \left(\xi_{2k} - \epsilon_{2k} \right) \\ &+ \frac{1}{g_1 g_2 - g_{12}^2} \left[g_2 \Delta_1^2 + g_1 \Delta_2^2 + g_{12} \left(\Delta_1^* \Delta_2 + \Delta_1 \Delta_2^* \right) \right] \quad , \end{aligned} \tag{7}$$

where $\epsilon_{1j} = (\xi_{1j}^2 + \Delta_1^2)^{1/2}$, and $\epsilon_{2k} = (\xi_{2k}^2 + \Delta_2^2)^{1/2}$. In Eq.(7), the values of Δ_1 and Δ_2 must be chosen in a way which minimizes Ω. From the minimization of Ω, we obtain a coupled gap equation at zero temperature for the two-gap system:

$$\begin{pmatrix} \Delta_1 \\ \Delta_2 \end{pmatrix} = \begin{pmatrix} g_1 \sum_j \frac{1}{2\epsilon_{1j}} & -g_{12} \sum_k \frac{1}{2\epsilon_{2k}} \\ -g_{12} \sum_j \frac{1}{2\epsilon_{1j}} & g_2 \sum_k \frac{1}{2\epsilon_{2k}} \end{pmatrix} \begin{pmatrix} \Delta_1 \\ \Delta_2 \end{pmatrix} \quad . \tag{8}$$

From the coupled gap equation of Eq.(8), we formally obtain an expression of bulk gap for two-gap superconductivity at zero temperature:

$$|\Delta_a| = \omega \sinh^{-1}\left(\frac{1}{\eta_a}\right) \quad , \quad (a = 1, 2) \quad , \tag{9}$$

where

$$\frac{1}{\eta_1} = \frac{\lambda_2 + \alpha_\pm [\eta_1, \eta_2] \lambda_{12}}{\lambda_1 \lambda_2 - \lambda_{12}^2} \quad , \quad \frac{1}{\eta_2} = \frac{\lambda_1 + \alpha_\pm^{-1} [\eta_1, \eta_2] \lambda_{12}}{\lambda_1 \lambda_2 - \lambda_{12}^2} \quad , \tag{10}$$

and $\alpha_\pm [\eta_1, \eta_2] = \pm \sinh\left(\frac{1}{\eta_1}\right) / \sinh\left(\frac{1}{\eta_2}\right)$ In two-band superconductivity, we can consider two cases for phase of the gaps: $\mathrm{sgn}(\Delta_1) = \mathrm{sgn}(\Delta_2)$, and $\mathrm{sgn}(\Delta_1) = -\mathrm{sgn}(\Delta_2)$. For the same phase, α_+ is used in Eqs.(10), and we use α_- for the opposite phase. Note that $\Delta_1 = -\Delta_2$ in the limit of strongly positive intersublevel coupling λ_{12}, that is, opposite phase. On the other hand, we find the same phase for negative λ_{12}. The transition temperature is defined from the absolute value of the gap functions. In $\lambda_{12} = 0$, we find the same results of two bulk gaps derived from conventional BCS theory for two independent sublevels.

3. Discussion

In this section, we discuss properties such as condensation energy, critical level spacing, and parity gap of nanosize two-gap superconductivity by using the partition function derived in previous section.

3.1. CONDENSATION ENERGY

In nanosize superconductivity, the condensation energy can be defined as $E_{N,b}^C(\lambda) = E_{N,b}^G(0) - E_{N,b}^G(\lambda) - n\lambda d$, where $E_{N,b}^G$ is the ground state energy of N-electron system in the interaction band. b is the number of electron on single occupied levels, and λ and n are the dimensionless coupling parameter and the number of pair occupied level, respectively. In the case of nanosize two-band system, the condensation energy can be written as $E_{N_1,b_1;N_2,b_2}^C(\lambda_1, \lambda_2, \lambda_{12}) =$

$E^G_{N_1,b_1;N_2,b_2}(0,0,0) - E^G_{N_1,b_1;N_2,b_2}(\lambda_1,\lambda_2,\lambda_{12}) - n_1\lambda_1 d_1 - n_2\lambda_2 d_2$, where $E^G_{N_1,b_1;N_2,b_2}(\lambda_1,\lambda_2,\lambda_{12})$ means the ground state energy of (N_1+N_2)-electron system. From Eq. (7), the condensation energy of two-sublevel system can be expressed by the condensation energy of independent single level systems:

$$E^C_{N_1,b_1;N_2,b_2}(\lambda_1,\lambda_2,\lambda_{12}) = E^C_{N_1,b_1}(\lambda_1) + E^C_{N_2,b_2}(\lambda_2) - \frac{\lambda_{12}^2}{\lambda_1\lambda_2-\lambda_{12}^2}\left(\frac{\Delta_1^2}{d_1\lambda_1}+\frac{\Delta_2^2}{d_2\lambda_2}+\frac{2\left(\Delta_1^*\Delta_2+\Delta_1\Delta_2^*\right)}{\sqrt{d_1 d_2}\lambda_{12}}\right) , \tag{11}$$

where $E^C_{N_1,b_1}(\lambda_1)$ and $E^C_{N_2,b_2}(\lambda_2)$ correspond to the condensation energy for single band case. In the same phases of Δ_1 and Δ_2, the condensation energy of Eq. (11) decreases, that is, appearing the instabilization by coupling constant λ_{12}. On the other hand, in the opposite phases, the condensation energy becomes larger, because $\Delta_1^*\Delta_2+\Delta_1\Delta_2^*<0$. We can expect that the condensation energy of two-gap superconductivity becomes more stable than that of two independent systems due to the intersublevel coupling λ_{12} and the opposite phases.

3.2. CRITICAL LEVEL SPACING

To discuss the critical level spacing for two-gap system, which means both gap functions vanish at a level spacing, $\Delta_1 = \Delta_2 = 0$, we start from the coupled gap equation of Eq. (8). For the case of the critical level spacing of two-gap system, we have

$$1 = \lambda_1\sum_j \frac{1}{2|\tilde{\xi}_{1j}|} + \lambda_2\sum_k \frac{1}{2|\tilde{\xi}_{2k}|} - (\lambda_1\lambda_2-\lambda_{12}^2)\sum_j \frac{1}{2|\tilde{\xi}_{1j}|}\sum_k \frac{1}{2|\tilde{\xi}_{2k}|} , \tag{12}$$

where $\tilde{\xi}_i = \xi_i/d_i$ for sublevel $i = 1,2$. For the odd or even electron number parity in the grain, Eq. (12) can be approximately solved by using the digamma function: For odd case, the critical level spacing becomes

$$d^o_{1c} = \omega_D e^\gamma \exp\left[-\frac{1}{\lambda}\right] , \quad d^o_{2c} = \frac{d_2}{d_1}d^o_{1c} , \tag{13}$$

and for even case,

$$d^e_{1c} = 4\omega_D e^\gamma \exp\left[-\frac{1}{\lambda}\right] , \quad d^e_{2c} = \frac{d_2}{d_1}d^e_{1c} . \tag{14}$$

Here, we use

$$\frac{1}{\lambda} = \frac{1}{2x}\left[\lambda_1+\lambda_2-ax+\sqrt{(\lambda_1-\lambda_2-ax)^2+4\lambda_{12}^2}\right] \tag{15}$$

with

$$x = \lambda_1\lambda_2 - \lambda_{12}^2 \quad , \quad a = \log\frac{d_1}{d_2} \quad . \tag{16}$$

From these expressions, we find some relations:

$$d_{1c}^e = 4d_{1c}^o \; , \quad d_{2c}^e = 4d_{2c}^o \quad . \tag{17}$$

and

$$d_{1/2c}^o \approx \frac{e^\gamma}{2}\exp\left[\frac{1}{\eta_{1/2}} - \frac{1}{\lambda}\right]\tilde{\Delta}_{1/2} \quad . \tag{18}$$

In the case of $|\lambda_1 - \lambda_2| \gg \lambda_{12}$, Eq. (18) can be approximately rewritten as

$$d_{1/2c}^o \approx \frac{e^\gamma}{2}\exp\left[\frac{\lambda_2 - \lambda_1 + 2\alpha\lambda_{12}}{\lambda_1\lambda_2 - \lambda_{12}^2}\right]\tilde{\Delta}_{1/2} \quad . \tag{19}$$

On the other hand, in the limit of $|\lambda_1 - \lambda_2| \ll \lambda_{12}$, we have

$$d_{1/2c}^o \approx \frac{e^\gamma}{2}\exp\left[\frac{(1+\alpha)\,\lambda_{12}}{\lambda_1\lambda_2 - \lambda_{12}^2}\right]\tilde{\Delta}_{1/2} \quad . \tag{20}$$

For case of $\lambda_{12} = 0$, Eq. (18) can be rewritten as $d_{1/2c}^o \approx \exp[\gamma]/2\exp[1/\lambda_1 - 1/\lambda_2]\tilde{\Delta}_{1/2}$. Therefore, when the coupling constants λ_1 and λ_2 become same value, we have a similar relation to that for single level system; $d_{1/2c}^o \approx 0.89\tilde{\Delta}_{1/2}$. These results suggest the critical level spacing strongly depend upon λ_{12} and the difference between the effective interaction constants for sublevels. The relation in Eq. (17) is the same relation in the conventional nanosize BCS theory.

3.3. PARITY GAP

In this subsection, we consider the parity gap in the case of two-gap superconductivity in ultrasmall grains. The parity gap in a single band system is the difference between the ground state energy of a grain containing $2n + 1$ electrons (odd parity) and the average ground state energy of grains containing $2n$ and $2n + 2$ electrons (even parity). It is a measure for the cost in energy of having one unpaired electron. In the case of two sublevel spacings, the chemical potential lies halfway between the highest occupied and the lowest unoccupied levels of smaller level spacing in the half-filled case as shown in Fig. 1(a). We assume that $d_1 < d_2$ and that the numbers of occupied levels corresponding to each sublevel are n_1 and n_2, respectively. Then, the total number of electron becomes $N = 2n_1 + 2n_2$. When we consider $N = 2n_1 + 2n_2 + 1$, the chemical potential lies on the level ε_{1n_1+1} as shown in

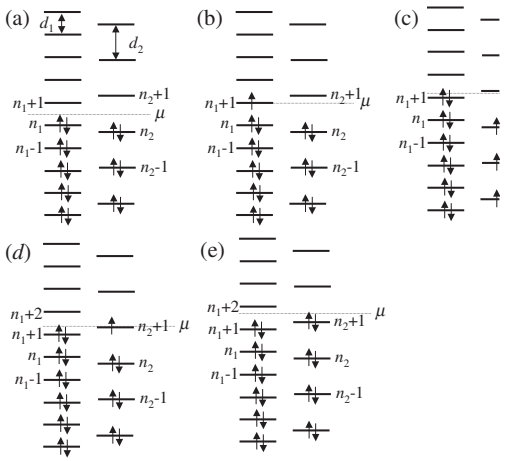

Figure 1. Positioning of the chemical potential relative the electronic energy levels in a two-gap superconducting grain. Solid and dotted lines mean two sublevels. (a) Half-filled system with $2n_1 + 2n_2$ electrons. (b) $2n_1 + 1 + 2n_2$-electron system. (c) $2(n_1 + 1) + 2n_2$-electron system. (d) $2(n_1 + 1) + 2n_2 + 1$-electron system. (e) $2(n_1 + 1) + 2(n_2 + 1)$-electron system.

Fig. 1(b). Figure 1(c) shows the position of the chemical potential in the case of $N = 2n_1 + 2n_2 + 2$. The parity gap of nanosize two-gap superconductivity is written as

$$\Delta_p^1 = E^G_{2n_1+1+2n_2,1} - \frac{1}{2}\left(E^G_{2n_1+2n_2,0} + E^G_{2(n_1+1)+2n_2,0}\right) \quad . \tag{21}$$

From Eq. (7) and the ground state energy as $E^G_{N,b} = \Omega_{\mu_N} + \mu_N N$, we obtain

$$\Delta_p^1 = \Delta_1 - \frac{d_1}{4}\left(\frac{\rho_1}{\rho_2} - 1\right) \quad . \tag{22}$$

From Figs. 1(c), (d), and (e), we can define another parity gap:

$$\Delta_p^2 = E^G_{2(n_1+1)+2n_2+1,1} - \frac{1}{2}\left(E^G_{2(n_1+1)+2n_2,0} + E^G_{2(n_1+1)+2(n_2+1),0}\right) \quad . \tag{23}$$

From the latter definition of Eq. (23), we have

$$\Delta_p^2 = \Delta_2 - \frac{d_2}{4}\left(\frac{3\rho_2}{\rho_1} - 1\right) \quad . \tag{24}$$

The present results suggest two kinds of the dependence of the parity gap on the level spacing. The parity gap does not depend upon the effective interaction λ_{12}. The structure around Fermi level plays an important role of the contribution to the size dependence on the parity gap.

3.4. CONCLUDING REMARKS

We have investigated properties of nanosize two-gap superconductivity by using a two-sublevel model in the framework of a mean field approximation. From the discussion for the condensation energy in nanosize two-gap superconductivity, the phases of the gaps is very important to stabilize the superconductivity. In the same phases, the two-gap superconductivity instabilizes by coupling constant λ_{12}. On the other hand, in the opposite phases, the superconductivity becomes stable. We can expect that the condensation energy of two-gap superconductivity becomes more stable than that of two independent systems due to the intersublevel coupling λ_{12} and the opposite phases.

We have also discussed the critical level spacing for two-gap superconductivity in ultrasmall grain. These results suggest the critical level spacing strongly depend upon λ_{12} and the difference between the effective interaction constants for sublevels. These results suggest that the relation between the critical level spacing and the bulk gaps is modified to compare with the result obtained in the ultrasmall grain of Al superconductivity.

In the parity gap in two-gap superconductivity, the present results suggest two kinds of the dependence of the parity gap on the level spacing and that the structure around Fermi level plays an important role of the contribution to the size dependence on the parity gap. The prity gap does not depend upon the effective interaction λ_{12}.

In the case of cluster system, we have to treat a more accurate approach for investigating these physical properties beyond the mean field approximation presented in this study, and we have also to consider the contribution of the surface of samples to the level structure around Fermi level. We will present these problems elsewhere (Kawabe, Nagao and Kruchinin, to appear.). From the present results, we might expect the possibility of a new multi-gap superconductivity arising in nanosize region with higher critical transition temperature.

In summary, a model corresponding to a nanosize two-gap superconductivity has been presented, and an expression of the partition function of the nanosize system has been analytically derived by using a path integral approach. A definition of the critical level spacing of the two-gap superconductivity has been also presented, and we discuss condensation energy and parity gap of the two-gap superconductivity in relation to the size dependence of those properties with two bulk gaps and effective pair scattering process between two sublevels.

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