Anisotropic superconductivity in extended t-J models

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Anisotropic superconductivity in layered CuO_2 structures is theoretically examined by using extended t-J models. It is predicted that in multilayered structures the second transition can occur in superconducting states. The transition is between superconducting states belonging to different representations with respect to a symmetry operation of exchanging layers. Therefore, the transition is reduced to a sharp crossover when the layers are nearly equivalent. It is probable that above the crossover temperature the gap vanishes along lines on the Fermi surface in the three-dimensional Brillouin zone. However, around the crossover temperature the gap can start to open everywhere on the Fermi surface in multilayered structures distorted from tetragonal symmetry. The results can explain both the temperature dependences of the nuclear-magnetic relaxation time and the penetration depth in high-T_c superconductors, which appear to be inconsistent with each other.

I. INTRODUCTION

The discovery of high-T_c superconductors has stimulated research of strongly correlated electron systems. Anderson argued soon after their discovery that they must be close to the Mott-Hubbard metal-insulator transition, and that their essential physics must be included in the Hubbard model or in the t-J model.[1] Although it does not yet seem to be settled which is the simplest model including the essential physics, that is, whether oxygen p electrons should be explicitly included or not, we will follow Anderson in this paper; an argument is given in Sec. V for taking the t-J model.

In the large-U limit, the Hubbard model can be transformed into the t-J model:

$$\mathcal{H}_{t\text{-}J}=-t\sum_{\langle ij\rangle\sigma}d_{i\sigma}^{\dagger}d_{j\sigma}-\tfrac{1}{2}J\sum_{\langle ij\rangle}(\mathbf{s}_i\cdot\mathbf{s}_j-\tfrac{1}{4}n_in_j)\ , \qquad (1)$$

acting on the subspace with no doubly occupied sites, with $\mathbf{s}_i$ the electron spin, n_i the electron number, and $J=-4t^2/U$, U being the on-site repulsion in the Hubbard model. $|t/U|\ll 1$ is assumed, and the summation of $\langle ij\rangle$ is made over nearest-neighbor pairs of sites. Terms of three-site exchange interaction have been left out because they are not important in nearly half-filled cases. The last term in Eq. (1), which is the charge-charge coupling, can also be ignored because the charge fluctuations must be largely depressed in the t-J model due to the restriction of no doubly occupied sites.

The t-J model can be replaced by an auxiliary boson-fermion model. The local gauge symmetry with respect to auxiliary particles is necessarily required to guarantee the equivalence between the two models. The present author examined the auxiliary-particle model in keeping the local gauge symmetry.[2] Green functions of auxiliary particles must be site diagonal because of the local gauge symmetry, although the exchange between boson and fermion can occur; the exchange interaction corresponds to the transfer integral in the t-J model. Bosons and fermions can only move by the exchange processes. Physically this means that auxiliary particles are localized themselves, but that fermionic pair excitations between fermions and bosons are itinerant, and they correspond to electrons in the t-J model. His results in the case of $J=0$ are consistent with Hubbard's results[3] in the high-energy region, while the formation of heavy electrons at the top of the lower Hubbard band is predicted. The mass renormalization factor is evaluated as $\chi_m\approx 1/(1-n)$ in nearly half-filled cases, $n\approx 1$ and $n<1$, n being the electron number per site. Therefore he argued that a Fermi liquid is very probable in the case of vanishing exchange interaction, $J=0$. The formation of heavy electrons in the case of $J=0$ is assumed in the present paper.

The effects of the exchange interaction can be taken into account perturbatively, when the exchange interaction is small enough such as $|J|<(1-n)|8t|$. The opposite case of $|J|>(1-n)|8t|$ is out of scope in this paper. As far as the square lattice is concerned, anisotropic superconductivity with d symmetry is the most probable within the model.[4] The gap function of the d symmetry vanishes along lines on the Fermi surface in the three-dimensional Brillouin zone. This prediction seems to be confirmed by the temperature dependence of the nuclear-magnetic relaxation time.[5] However, it disagrees with the experiments of the penetration depth[6] and the tunneling,[7] which implies ordinary isotropic Bardeen-Cooper-Schrieffer (BCS) superconductivity where the gap is open everywhere on the Fermi surface. These experiments appear to be inconsistent with each other.

There are two ways of explaining the apparently inconsistent experiments. Because there are no chances of isotropic superconductivity in reasonable parameter spaces within the t-J model of the square lattice,[4,8] one simply discards the t-J model and tries to explain experiments with different models. However, we will take the other, which is to extend the t-J model. Actual high-T_c oxides usually have orthorhombic structures, where the s and the d symmetry should be coupled to each other. Be-

cause $YBa_2Cu_3O_7$ compounds have linear chains, for example, the effects of distortion can be expected to be large there. The other feature to be taken into account is that many high-T_c oxides have multiple layers of CuO_2 in a unit cell. One of the purposes of the present paper is to examine the effects of the distortion and multiple-layered structures within extended t-J models.

The plan of the present paper is as follows. Single-layered structures are examined in Sec. II by using a t-J model. An effective Hamiltonian of heavy electrons is proposed in Sec. III, which gives the same result as t-J models within the mean-field approximation of superconductivity. Multiple-layered structures are studied in Sec. III by using the effective Hamiltonian. Because it is hard work to solve the gap equation in the case of multiple-layered structures, superconductivity in multiple-layered structures is discussed in Sec. IV by using a phenomenological free energy. In Sec. V, we argue for taking the t-J models, and an application to actual high-T_c oxides is presented. A summary is given in Sec. VI. In the appendixes we examine impurity effects and the Meissner effect due to anisotropic Cooper pairs between Bloch electrons.

II. SINGLE-LAYERED STRUCTURES

A. Heavy electrons

First let us examine superconductivity in single-layered structures. The model Hamiltonian of Eq. (1) can be expressed in the momentum representation as

$$\mathcal{H}_{t\text{-}J}=\sum_{\mathbf{k}\sigma} e(\mathbf{k})d^{\dagger}_{\mathbf{k}\sigma}d_{\mathbf{k}\sigma}-\tfrac{1}{2}\sum_{\mathbf{q}} J(\mathbf{q})\mathbf{s}(\mathbf{q})\cdot\mathbf{s}(-\mathbf{q}) , \tag{2}$$

acting on the subspace with no doubly occupied sites. Here a small distortion from the square lattice is assumed:

$$e(\mathbf{k})=-(t_x+t_y)\phi_s(\mathbf{k})-(t_x-t_y)\phi_d(\mathbf{k}) , \tag{3}$$

with t_x and t_y the transfer integrals between nearest neighbors along the x axis and y axis, respectively:

$$\phi_s(\mathbf{k})=\cos(k_x a)+\cos(k_y b) \tag{4}$$

and

$$\phi_d(\mathbf{k})=\cos(k_x a)-\cos(k_y b) , \tag{5}$$

with a and b the lattice constants of the x axis and the y axis, respectively. Other form factors used in the following parts are defined here such as

$$\phi_0(\mathbf{k})=1 , \tag{6}$$

$$\phi_x(\mathbf{k})=\sqrt{2}\sin(k_x a) , \tag{7}$$

and

$$\phi_y(\mathbf{k})=\sqrt{2}\sin(k_y b) . \tag{8}$$

The exchange interaction is given by

$$J(\mathbf{q})=J_s\phi_s(\mathbf{q})+J_d\phi_d(\mathbf{q}) , \tag{9}$$

with

$$J_s=-\frac{4}{U}(t_x^2+t_y^2) \tag{10}$$

and

$$J_d=-\frac{4}{U}(t_x^2-t_y^2) , \tag{11}$$

U being the on-site repulsion in the Hubbard model:

$$s_+(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{k}} d^{\dagger}_{\mathbf{k}+\mathbf{q}\uparrow}d_{\mathbf{k}\downarrow} , \tag{12}$$

$$s_-(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{k}} d^{\dagger}_{\mathbf{k}+\mathbf{q}\downarrow}d_{\mathbf{k}\uparrow} , \tag{13}$$

and

$$s_z(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{k}\sigma} \tfrac{1}{2}\sigma d^{\dagger}_{\mathbf{k}+\mathbf{q}\sigma}d_{\mathbf{k}\sigma} \tag{14}$$

are the electron spins.

In the case of vanishing exchange interaction, single-particle Green functions of electrons are given by[9,2]

$$g_{\sigma}^{-1}(i\omega,\mathbf{k})=\chi_m[i\omega+\mu-\varepsilon(\mathbf{k})]+\sigma\chi_s\mu_B H , \tag{15}$$

in the presence of infinitesimally small magnetic fields, with $\chi_s\approx\chi_m\approx 1/(1-n)$, and $\varepsilon(\mathbf{k})=e(\mathbf{k})/\chi_m$ the dispersion relation of heavy electrons renormalized due to the restriction of no doubly occupied sites. The Ward identity tells us that χ_s is nothing but the vertex correction due to the restriction of no doubly occupied sites to the exchange interaction in the limit of small transferred energies and momenta.[9] Then the exchange interaction can be treated perturbatively for

$$|J(\mathbf{q})|(\chi_s/\chi_m)^2<W, \quad W=4(1-n)(|t_x|+|t_y|)$$

being the bandwidth of heavy electrons.

B. Gap equation

Because the exchange interaction is antiferromagnetic, only singlet Cooper pairs with even parity are possible. Single-particle Green functions of electrons in superconducting states are expressed as

$$g_s^{-1}(i\omega,\mathbf{k})=\begin{bmatrix} g_{\uparrow\uparrow}(i\omega,\mathbf{k}) & g_{\uparrow\downarrow}(i\omega,\mathbf{k}) \\ g_{\downarrow\uparrow}(i\omega,\mathbf{k}) & g_{\downarrow\downarrow}(i\omega,\mathbf{k}) \end{bmatrix}^{-1} =\chi_m\begin{bmatrix} i\omega+\mu-\varepsilon(\mathbf{k}) & -\Delta(\mathbf{k}) \\ -\Delta^*(\mathbf{k}) & i\omega-\mu+\varepsilon(\mathbf{k}) \end{bmatrix} , \tag{16}$$

where the basis $(d^{\dagger}_{\mathbf{k}\uparrow}, d_{-\mathbf{k}\downarrow})$ is taken. The gap function, the order parameter, or the self-energy can be determined self-consistently in an approximation shown in Fig. 1, which corresponds to the mean-field approximation of superconductivity:

$$\chi_m\Delta(\mathbf{k})=-T\sum_{\omega}\frac{1}{N}\sum_{\mathbf{p}}{}' [\tfrac{3}{4}J(\mathbf{k}-\mathbf{p})\chi_s^2 + U_{\uparrow\downarrow}\chi_m^2]g_{\uparrow\downarrow}(i\omega,\mathbf{p}) , \tag{17}$$

which leads to

FIG. 1. Diagrams of the self-energy of electrons. Solid lines are anomalous parts of the Green functions of electrons. A wavy line stands for the exchange interaction, and vertex corrections shown by hatched parts are put to the both ends of the exchange interaction. A double-dashed line is the T matrix caused by the restriction of no doubly occupied sites.

$$\Delta(\mathbf{k})=\frac{1}{N}\sum_{\mathbf{p}}{}'M(\mathbf{k}-\mathbf{p})\frac{1}{2E(\mathbf{p})}\tanh\left[\frac{E(\mathbf{p})}{2T}\right]\Delta(\mathbf{p}) , \quad (18)$$

with

$$E(\mathbf{k})=\{[\varepsilon(\mathbf{k})-\mu]^2+|\Delta(\mathbf{k})|^2\}^{1/2} \quad (19)$$

and

$$M(\mathbf{q})=-\tfrac{3}{4}I(\mathbf{q})-U_{\uparrow\downarrow} . \quad (20)$$

It should be noted that two vertex corrections, χ_s, are applied to both ends of the exchange interaction in obtaining Eq. (17) as shown in Fig. 1. Here $I(\mathbf{q})$ is the effective exchange interaction between heavy electrons, and it is calculated as

$$I(\mathbf{q})=I_s\phi_s(\mathbf{q})+I_d\phi_d(\mathbf{q}) , \quad (21)$$

with

$$I_s=J_s\left[\frac{\chi_s}{\chi_m}\right]^2<0 \quad (22)$$

and

$$I_d=J_d\left[\frac{\chi_s}{\chi_m}\right]^2 . \quad (23)$$

Electrons with antiparallel spins should show strong short-ranged repulsion to each other because of the restriction of no doubly occupied sites, and $U_{\uparrow\downarrow}\chi_m^2$ is the T matrix caused by the restriction of no doubly occupied sites. Although it is very difficult to evaluate $U_{\uparrow\downarrow}$, it must definitely be repulsive and presumably $U_{\uparrow\downarrow}=O(W)$. The summation over $\mathbf{p}$ in Eqs. (17) and (18) should be restricted to

$$|\varepsilon(\mathbf{p})-\mu|\ll W \quad (24)$$

because the quasiparticle or heavy-electron picture is not yet valid in the high-energy region.

The gap function or the order parameters of superconductivity can be expressed as

$$\Delta(\mathbf{k};T)=\Delta_0(T)\phi_0(\mathbf{k})+\Delta_s(T)\phi_s(\mathbf{k})+\Delta_d(T)\phi_d(\mathbf{k}) . \quad (25)$$

By using a relation

$$J(\mathbf{k}-\mathbf{p})=J_s\sum_{\alpha}\phi_\alpha(\mathbf{k})\phi_\alpha(\mathbf{p}) +J_d[\phi_s(\mathbf{k})\phi_d(\mathbf{p})+\phi_d(\mathbf{k})\phi_s(\mathbf{p}) +\phi_x(\mathbf{k})\phi_x(\mathbf{p})-\phi_y(\mathbf{k})\phi_y(\mathbf{p})] , \quad (26)$$

it can easily be found that

$$\begin{pmatrix} U_{\uparrow\downarrow}\Pi_{00}+1 & U_{\uparrow\downarrow}\Pi_{0s} & U_{\uparrow\downarrow}\Pi_{0d} \\ \tfrac{3}{4}I_s\Pi_{s0} & \tfrac{3}{4}I_s\Pi_{ss}+1 & \tfrac{3}{4}(I_s\Pi_{sd}+I_d\Pi_{dd}) \\ \tfrac{3}{4}I_s\Pi_{d0} & \tfrac{3}{4}(I_s\Pi_{ds}+I_d\Pi_{ss}) & \tfrac{3}{4}I_s\Pi_{dd}+1 \end{pmatrix}\begin{pmatrix}\Delta_0\\ \Delta_s\\ \Delta_d\end{pmatrix}=0 \quad (27)$$

should be satisfied, where

$$\Pi_{\alpha\beta}=\frac{1}{N}\sum_{\mathbf{p}}{}'\phi_\alpha(\mathbf{p})\phi_\beta(\mathbf{p})\frac{\tanh[E(\mathbf{p})/(2T)]}{2E(\mathbf{p})} , \quad (28)$$

with the restriction of Eq. (24). It should be noted that all $\Pi_{\alpha\beta}$ are real and that the matrix in Eq. (27) is a real matrix.

In the square lattice, $a=b$, $t_x=t_y$, and $I_d=0$; $\varepsilon(\mathbf{k})$ has the total symmetry of the lattice. In the presence of Cooper pairs with $\Delta_0\neq0,\Delta_s\neq0$, and $\Delta_d=0$, or Cooper pairs with $\Delta_0=\Delta_s=0$ and $\Delta_d\neq0$, $|\Delta(\mathbf{k})|$ has the total symmetry:

$$\Pi_{0d}=\Pi_{d0}=\Pi_{sd}=\Pi_{ds}=0 \quad (29)$$

in such a case. Cooper pairs can be classified into s symmetry and d symmetry.

It is argued that in the half-filled case the s symmetry and the d symmetry have the same superconducting critical temperatures T_c without $U_{\uparrow\downarrow}$ and the restriction of Eq. (24).[10] However, such a case ($|I_s|>W$) is outside the scope of this paper. Once holes are doped and the restriction of Eq. (24) is taken into account, T_c of the d symmetry is definitely higher than the s symmetry; the van Hove singularities lie at $\mathbf{Q}=(\pm\pi/a,0)$ and $(0,\pm\pi/a)$, and $\phi_d^2(\mathbf{k})$ has its maximum value of 4 at $\mathbf{Q}$.[4,8] If the effect of $U_{\uparrow\downarrow}>0$ is taken into account, T_c of the s symmetry is further reduced. Therefore T_c of d symmetry is definitely higher than that of s symmetry as long as $U_{\uparrow\downarrow}>0$.

The critical temperature and the gap function of d symmetry can be obtained by solving

$$\tfrac{3}{4}|I_s|\Pi_{dd}-1=0 . \quad (30)$$

This gap equation has already been solved numerically in Ref. 8. The gap function can be written as $\Delta(\mathbf{k})=\Delta_d(T)\phi_d(\mathbf{k})$, which vanishes at points on the Fermi surface in the two-dimensional Brillouin zone, or along lines in the actual three-dimensional Brillouin zone.

The temperature dependence of $4\Delta_d(T)$ is very close to its BCS dependence, although the size of the gap is significantly larger in this model than its BCS value; $2\varepsilon_G/T_c=3.53$ in BCS theory, while $4\Delta_d(0)/T_c=4.35$ in d symmetry. This unusual behavior is because of the sharp structure in the density of states due to the van Hove singularity.

C. Coexistence between s symmetry and d symmetry

When temperatures are enough lower than the critical temperature of s symmetry, the coexistence between s symmetry and d symmetry is possible. The gap function $|\Delta(\mathbf{k})|$ can have the total symmetry only when the order parameters have the following phases:

$$\Delta_0=\pm|\Delta_0|\exp(i\eta)\ , \tag{31}$$

$$\Delta_s=|\Delta_s|\exp(i\eta)\ , \tag{32}$$

and

$$\Delta_d=\pm i|\Delta_d|\exp(i\eta)\ . \tag{33}$$

Because the gap function can be written as

$$|\Delta(\mathbf{k})|^2=|\Delta_0+\Delta_s\phi_s(\mathbf{k})|^2+|\Delta_d\phi_d(\mathbf{k})|^2\ , \tag{34}$$

the gap is open everywhere on the Fermi surface. Because Eq. (29) holds in such a case, not only Eq. (30) but also

$$\begin{bmatrix} U_{\uparrow\downarrow}\Pi_{00}+1 & U_{\uparrow\downarrow}\Pi_{0s} \\ \frac{3}{4}I_s\Pi_{s0} & \frac{3}{4}I_s\Pi_{ss}+1 \end{bmatrix}\begin{bmatrix}\Delta_0\\ \Delta_s\end{bmatrix}=0 \tag{35}$$

should be satisfied below a critical temperature of the coexistence, that is, the second critical temperature. This solution corresponds to the so-called $s+id$ state.[10]

In other cases, the gap function cannot have the total symmetry. Therefore Eq. (29) does not hold; Eq. (27) should be treated instead of Eqs. (30) and (35). Because the matrix in Eq. (27) is a real matrix, the order parameters should have the same phase:

$$\Delta_0=\pm|\Delta_0|\exp(i\eta)\ , \tag{36}$$

$$\Delta_s=|\Delta_s|\exp(i\eta)\ , \tag{37}$$

and

$$\Delta_d=\pm|\Delta_d|\exp(i\eta)\ . \tag{38}$$

Since the gap equations are exactly the same in the limits $|\Delta_0|\to 0$ and $|\Delta_s|\to 0$, the second critical temperature of superconductivity should be the same in the two types of solutions. Because the gap function is given by

$$|\Delta(\mathbf{k})|^2=|\Delta_0+\Delta_s\phi_s(\mathbf{k})+\Delta_d\phi_d(\mathbf{k})|^2\ , \tag{39}$$

the gap presumably vanishes at points on the Fermi surface in the two-dimensional Brillouin zone or along lines in the actual three-dimensional Brillouin zone.

So far, we have confined ourselves to the square lattice. If a small distortion is introduced,

$$I_d\neq 0,\ \Pi_{0d}\neq 0,\ \Pi_{d0}\neq 0,\ \Pi_{sd}\neq 0,\ \text{and}\ \Pi_{ds}\neq 0\ , \tag{40}$$

in general. Therefore all the representations of even parity should be coupled to each other. Because the matrix in Eq. (27) is a real matrix, the order parameters should have the same phase in distorted lattices. The $s+id$ state can never be obtained in distorted lattices. The only possible solution is the second type. This implies that the $s+id$ state is unstable in an infinitesimally small distortion from the square symmetry or the tetragonal symmetry.

III. DOUBLE-LAYERED STRUCTURES

A. Effective Hamiltonian of heavy electrons

Double-layered structures are examined here as the simplest case because they include essential features of multiple-layered structures. It is straightforward to extend the t-J model to include two-layered structures. However, we take an effective Hamiltonian for heavy electrons following Ref. 11 for the sake of simplicity. It can be straightforwardly seen from two different calculations that the effective Hamiltonian gives the same results as the extended t-J model within the mean-field approximation, as far as superconductivity is concerned:

$$\mathcal{H}_{\text{eff}}=\mathcal{H}_0=\mathcal{H}_{\text{int}}\ , \tag{41}$$

with

$$\mathcal{H}_0=\sum_{ij}\sum_{\mathbf{k}\sigma}\varepsilon_{ij}(\mathbf{k})a^\dagger_{i\mathbf{k}\sigma}a_{j\mathbf{k}\sigma}\ , \tag{42}$$

and

$$\mathcal{H}_{\text{int}}=\tfrac{1}{2}\sum_i\sum_{\mathbf{q}}[-I(\mathbf{q})\mathbf{S}_i(\mathbf{q})\cdot\mathbf{S}_i(-\mathbf{q}) + U_{\uparrow\downarrow}N_i(\mathbf{q})N_i(-\mathbf{q})]\ , \tag{43}$$

where $a^\dagger_{i\mathbf{k}\sigma}$ is a creation operator of heavy electrons with band i or layer i, momentum $\mathbf{k}$, and spin σ:

$$\varepsilon_{ij}(\mathbf{k})=\begin{bmatrix}\varepsilon_1(\mathbf{k}) & \tau(\mathbf{k})\\ \tau^*(\mathbf{k}) & \varepsilon_2(\mathbf{k})\end{bmatrix}\ , \tag{44}$$

with $\chi_m\tau(\mathbf{k})$ the bare transfer integral between layers and $\chi_m\varepsilon_i(\mathbf{k})=e(\mathbf{k})$ the bare dispersion relation given by Eq. (3) without any interlayer-transfer integrals. Although $\varepsilon_1(\mathbf{k})=\varepsilon_2(\mathbf{k})$ in the present model, they are expressed differently in order to include more general cases:

$$S_{i+}(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{k}}a^\dagger_{i\mathbf{k}+\mathbf{q}\uparrow}a_{i\mathbf{k}\downarrow}\ , \tag{45}$$

$$S_{i-}(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{k}}a^\dagger_{i\mathbf{k}+\mathbf{q}\downarrow}a_{i\mathbf{k}\uparrow}\ , \tag{46}$$

$$S_{iz}(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{k}\sigma}\tfrac{1}{2}\sigma a^\dagger_{i\mathbf{k}+\mathbf{q}\sigma}a_{i\mathbf{k}\sigma}\ , \tag{47}$$

$$N_i(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{k}\sigma}a^\dagger_{i\mathbf{k}+\mathbf{q}\sigma}a_{i\mathbf{k}\sigma}\ , \tag{48}$$

and $I(\mathbf{q})$ is given by Eq. (21). The last term proportional to $U_{\uparrow\downarrow}$ in Eq. (43) is due to the restriction of no doubly occupied sites. Here any interlayer mutual interactions are assumed to be small enough to be ignored.

For vanishing exchange interaction, single-particle Green functions of heavy electrons in normal states are given by

$$G^{-1}(i\omega,\mathbf{k})=\begin{bmatrix} i\omega+\mu-\varepsilon_1(\mathbf{k}) & -\tau(\mathbf{k}) \\ -\tau^*(\mathbf{k}) & i\omega+\mu-\varepsilon_2(\mathbf{k}) \end{bmatrix} . \tag{49}$$

Since it is convenient to see where the Fermi surface is in the final results, let us use the representation to diagonalize Eq. (49). By introducing operators defined by

$$b_{1\mathbf{k}\sigma}=\cos[\lambda(\mathbf{k})]e^{i\kappa(\mathbf{k})}a_{1\mathbf{k}\sigma}+\sin[\lambda(\mathbf{k})]e^{-i\kappa(\mathbf{k})}a_{2\mathbf{k}\sigma} \tag{50}$$

and

$$b_{2\mathbf{k}\sigma}=\sin[\lambda(\mathbf{k})]e^{i\kappa(\mathbf{k})}a_{1\mathbf{k}\sigma}-\cos[\lambda(\mathbf{k})]e^{-i\kappa(\mathbf{k})}a_{2\mathbf{k}\sigma} , \tag{51}$$

with

$$\exp[i2\kappa(\mathbf{k})]=\frac{\tau(\mathbf{k})}{|\tau(\mathbf{k})|} \tag{52}$$

and

$$\tan[2\lambda(\mathbf{k})]=\frac{2|\tau(\mathbf{k})|}{\varepsilon_1(\mathbf{k})-\varepsilon_2(\mathbf{k})} , \tag{53}$$

it can be easily seen that single-particle Green functions can be diagonalized as

$$G^{-1}(i\omega,\mathbf{k})=\begin{bmatrix} i\omega+\mu-E_1(\mathbf{k}) & \\ & i\omega+\mu-E_2(\mathbf{k}) \end{bmatrix} , \tag{54}$$

with

$$E_1(\mathbf{k})=\tfrac{1}{2}(\varepsilon_1(\mathbf{k})+\varepsilon_2(\mathbf{k}) +\{[\varepsilon_1(\mathbf{k})-\varepsilon_2(\mathbf{k})]^2+4|\tau(\mathbf{k})|^2\}^{1/2})-\mu \tag{55}$$

and

$$E_2(\mathbf{k})=\tfrac{1}{2}(\varepsilon_1(\mathbf{k})+\varepsilon_2(\mathbf{k}) -\{[\varepsilon_1(\mathbf{k})-\varepsilon_2(\mathbf{k})]^2+4|\tau(\mathbf{k})|^2\}^{1/2})-\mu . \tag{56}$$

If three-dimensional features are ignored, $\tau(\mathbf{k})$ is independent of $\mathbf{k}$, and it can be assumed to be real. Here it is assumed that heavy electrons in the two layers have similar dispersion relations that

$$|\tan[2\lambda(\mathbf{k})]| \gg 1 \tag{57}$$

might be satisfied. When the two layers are equivalent such as $\varepsilon_1(\mathbf{k})=\varepsilon_2(\mathbf{k})$, $\tan[2\lambda(\mathbf{k})]=\infty$, which gives $\lambda(\mathbf{k})=\pi/2$. In such a case, the operator $b_{1\mathbf{k}\sigma}$ annihilates an electron in bonding states between two layers, and $b_{2\mathbf{k}\sigma}$ annihilates an electron in antibonding states, respectively.

B. Mean-field approximation

Let us confine ourselves to singlet superconductivity with even parity because the exchange interaction is antiferromagnetic. By assuming the broken gauge symmetry, $\mathcal{H}_{\rm int}$ can be reduced to a BCS-type Hamiltonian:

$$\begin{aligned}\mathcal{H}_{\rm red}&=\frac{1}{2N}\sum_i\sum_{\mathbf{k}\mathbf{p}\sigma}M(\mathbf{k}-\mathbf{p})(\langle a_{i-\mathbf{p}-\sigma}a_{i\mathbf{p}\sigma}\rangle a^\dagger_{i\mathbf{k}\sigma}a^\dagger_{i-\mathbf{k}-\sigma}+\text{H.c.})\\ &=\sum_{\mathbf{k}\sigma}\{[\Delta_1(\mathbf{k})b^\dagger_{1\mathbf{k}\uparrow}b^\dagger_{1-\mathbf{k}\downarrow}+\Delta_2(\mathbf{k})b^\dagger_{2\mathbf{k}\uparrow}b^\dagger_{2-\mathbf{k}\downarrow}+\Delta_3(\mathbf{k})(b^\dagger_{1\mathbf{k}\uparrow}b^\dagger_{2-\mathbf{k}\downarrow}+b^\dagger_{2\mathbf{k}\uparrow}b^\dagger_{1-\mathbf{k}\downarrow})]+\text{H.c.}\} ,\end{aligned} \tag{58}$$

with $M(\mathbf{q})$ given by Eq. (20). The gap equation is given by

$$\begin{aligned}\Delta_1(\mathbf{k})&=\frac{1}{N}\sum_{\mathbf{p}}M(\mathbf{k}-\mathbf{p})\{\cos^2[\lambda(\mathbf{k})]\langle a_{1-\mathbf{p}\downarrow}a_{1\mathbf{p}\uparrow}\rangle+\sin^2[\lambda(\mathbf{k})]\langle a_{2-\mathbf{p}\downarrow}a_{2\mathbf{p}\uparrow}\rangle\}\\ &=\frac{1}{2N}\sum_{\mathbf{p}}M(\mathbf{k}-\mathbf{p})\{\langle b_{1-\mathbf{p}\downarrow}b_{1\mathbf{p}\uparrow}+b_{2-\mathbf{p}\downarrow}b_{2\mathbf{p}\uparrow}\rangle+\cos[2\lambda(\mathbf{k})]\sin[2\lambda(\mathbf{p})]\langle b_{1-\mathbf{p}\downarrow}b_{2\mathbf{p}\uparrow}+b_{2-\mathbf{p}\downarrow}b_{1\mathbf{p}\uparrow}\rangle\} ,\end{aligned} \tag{59}$$

$$\begin{aligned}\Delta_2(\mathbf{k})&=\frac{1}{N}\sum_{\mathbf{p}}M(\mathbf{k}-\mathbf{p})\{\sin^2[\lambda(\mathbf{k})]\langle a_{1-\mathbf{p}\downarrow}a_{1\mathbf{p}\uparrow}\rangle+\cos^2[\lambda(\mathbf{k})]\langle a_{2-\mathbf{p}\downarrow}a_{2\mathbf{p}\uparrow}\rangle\}\\ &=\frac{1}{2N}\sum_{\mathbf{p}}M(\mathbf{k}-\mathbf{p})\{\langle b_{1-\mathbf{p}\downarrow}b_{1\mathbf{p}\uparrow}+b_{2-\mathbf{p}\downarrow}b_{2\mathbf{p}\uparrow}\rangle-\cos[2\lambda(\mathbf{k})]\sin[2\lambda(\mathbf{p})]\langle b_{1-\mathbf{p}\downarrow}b_{2\mathbf{p}\uparrow}+b_{2-\mathbf{p}\downarrow}b_{1\mathbf{p}\uparrow}\rangle\} ,\end{aligned} \tag{60}$$

and

$$\begin{aligned}\Delta_3(\mathbf{k})&=\tfrac{1}{2}\sin[2\lambda(\mathbf{k})]\frac{1}{N}\sum_{\mathbf{p}}M(\mathbf{k}-\mathbf{p})[\langle a_{1-\mathbf{p}\downarrow}a_{1\mathbf{p}\uparrow}\rangle-\langle a_{2-\mathbf{p}\downarrow}a_{2\mathbf{p}\uparrow}\rangle]\\ &=\tfrac{1}{2}\sin[2\lambda(\mathbf{k})]\frac{1}{N}\sum_{\mathbf{p}}M(\mathbf{k}-\mathbf{p})\sin[2\lambda(\mathbf{p})]\langle b_{1-\mathbf{p}\downarrow}b_{2\mathbf{p}\uparrow}+b_{2-\mathbf{p}\downarrow}b_{1\mathbf{p}\uparrow}\rangle .\end{aligned} \tag{61}$$

Here $\langle\cdots\rangle$ means the average in superconducting states. It can easily be seen that $\Delta_1(\mathbf{k})=\Delta_2(\mathbf{k})$, when the two layers are equivalent; the order parameter $\Delta_1(\mathbf{k})$ corresponds to Cooper pairs between bonding electrons and $\Delta_2(\mathbf{k})$ between antibonding electrons, respectively, while $\Delta_3(\mathbf{k})$ corresponds to Cooper pairs between bonding and antibonding electrons. A symmetry operation of exchanging layers can be defined, when the two layers are

exactly equivalent. Under this symmetry operation, $\Delta_1(\mathbf{k})$ and $\Delta_2(\mathbf{k})$ have even parity, while $\Delta_3(\mathbf{k})$ has odd parity.

By taking a basis of $(b^\dagger_{1\mathbf{k}\uparrow}, b_{1-\mathbf{k}\downarrow}, b^\dagger_{2\mathbf{k}\uparrow}, b_{2-\mathbf{k}\downarrow})$, the mean-field Hamiltonian is given by

$$\mathcal{H}_{\text{mean}}=\begin{bmatrix}\sigma_z E_1(\mathbf{k})+\sigma_x\Delta_1(\mathbf{k}) & \sigma_x\Delta_3(\mathbf{k}) \\ \sigma_x\Delta_3(\mathbf{k}) & \sigma_z E_2(\mathbf{k})+\sigma_x\Delta_2(\mathbf{k})\end{bmatrix}, \tag{62}$$

with σ_x and σ_z Pauli matrices. When $\tau(\mathbf{k})$ is real, $\Delta_i(\mathbf{k})$ can be made real in distorted lattices. By diagonalizing Eq. (62), the dispersion relation of quasiparticles is given by

$$E^2_\pm(\mathbf{k})=\tfrac{1}{2}[E^2_1(\mathbf{k})+E^2_2(\mathbf{k})+\Delta^2_1(\mathbf{k}) +\Delta^2_2(\mathbf{k})+2\Delta^2_3(\mathbf{k})\pm\sqrt{D(\mathbf{k})}], \tag{63}$$

with

$$D(\mathbf{k})=[E^2_1(\mathbf{k})-E^2_2(\mathbf{k})+\Delta^2_1(\mathbf{k})-\Delta^2_2(\mathbf{k})]^2 +4\Delta^2_3(\mathbf{k})\{[E_1(\mathbf{k})-E_2(\mathbf{k})]^2 +[\Delta_1(\mathbf{k})+\Delta_2(\mathbf{k})]^2\}. \tag{64}$$

C. Crossover between superconducting states

When the two layers are exactly equivalent, the critical temperatures are obtained by solving

$$\Delta_1(\mathbf{k})=\frac{1}{N}\sum_{i=1}^{2}{\sum_{\mathbf{p}}}' M(\mathbf{k}-\mathbf{p})\frac{1}{4E_i(\mathbf{p})}\tanh\left[\frac{E_i(\mathbf{p})}{2T}\right]\Delta_1(\mathbf{p}), \tag{65}$$

for even parity with respect to the symmetry operation of exchanging layers, while

$$\Delta_3(\mathbf{k})=\frac{1}{N}{\sum_{\mathbf{p}}}' M(\mathbf{k}-\mathbf{p})\frac{1}{E_1(\mathbf{p})+E_2(\mathbf{p})} \times\mathrm{Th}\left[\frac{E_1(\mathbf{p})}{T},\frac{E_2(\mathbf{p})}{T}\right]\Delta_3(\mathbf{p}), \tag{66}$$

with

$$\mathrm{Th}(x,y)=\frac{\exp(x+y)-1}{[\exp(x)+1][\exp(y)+1]}, \tag{67}$$

for odd parity. The restriction of Eq. (24) is assumed in Eqs. (65) and (66). Because $\mathrm{Th}(x,y\to x)=\tanh(x/2)$, Eqs. (65) and (66) should give similar critical temperatures for similar $E_1(\mathbf{k})$ and $E_2(\mathbf{k})$, that is, for small $|\tau(\mathbf{k})|$.

If the lattice has a tetragonal symmetry, Cooper pairs can be classified into *s* symmetry and *d* symmetry even in multiple-layered structures. As can easily be implied from weak interlayer couplings, the critical temperature of *d* symmetry should be much higher than that of *s* symmetry. In *d* symmetry states, all of the order parameters should be proportional to $\phi_d(\mathbf{k})$ such as $\Delta_i(\mathbf{k})\propto\phi_d(\mathbf{k})$. Therefore the energy gap should vanish along lines on the Fermi surface in the three-dimensional Brillouin zone.

Because *s* symmetry and *d* symmetry should be coupled to each other in distorted lattices, all the order parameters can be generally expressed as

$$\Delta_i(\mathbf{k})=\sum_\alpha c_{i\alpha}\phi_\alpha(\mathbf{k}). \tag{68}$$

There is no reason that $c_{1\alpha}$, $c_{2\alpha}$, and $c_{3\alpha}$ are the same in distorted lattices. Therefore, in general, three conditions of $\Delta_i(\mathbf{k})=0$ define different lines in the two-dimensional Brillouin zone, or different planes in the three-dimensional zone. In the following, distorted lattices are examined.

When the two layers are equivalent in distorted lattices, $\Delta_1(\mathbf{k})$ and $\Delta_2(\mathbf{k})$ have even parity with respect to the symmetry operation of exchanging layers, while $\Delta_3(\mathbf{k})$ has odd parity. However, their coexistence is possible below the second critical temperature, which is enough lower than both critical temperatures given by Eqs. (65) and (66). The situation is similar to the coexistence between *s* symmetry and *d* symmetry in Sec. II, and their coexistence is examined phenomenologically in Sec. IV. When the two layers are not equivalent, they should be mixed with each other, in general. The second transition is reduced to a crossover.

The gap presumably vanishes along lines on the Fermi surface in the three-dimensional zone above the crossover temperature. When the dispersion relations of the two bands are largely different, such as

$$|E^2_1(\mathbf{k})-E^2_2(\mathbf{k})|\gg|\Delta_i(\mathbf{k})|^2, \tag{69}$$

for $i=1$, 2, and 3, however, $\Delta_1(\mathbf{k})=0$ or $\Delta_2(\mathbf{k})=0$ is still the condition that the gap vanishes on the Fermi surface even below the crossover temperature. It can easily be seen from

$$E^2_+(\mathbf{k})\approx E^2_1(\mathbf{k})+\Delta^2_1(\mathbf{k})+2\Delta^2_3(\mathbf{k})\frac{E_1(\mathbf{k})}{E_1(\mathbf{k})-E_2(\mathbf{k})} \tag{70}$$

and

$$E^2_-(\mathbf{k})\approx E^2_2(\mathbf{k})+\Delta^2_2(\mathbf{k})+2\Delta^2_3(\mathbf{k})\frac{E_2(\mathbf{k})}{E_1(\mathbf{k})-E_2(\mathbf{k})} \tag{71}$$

and the relations of $E_1(\mathbf{k})=0$ or $E_2(\mathbf{k})=0$ on the Fermi surface. Therefore it is highly probable that the energy gap vanishes along lines on the Fermi surface in the three-dimensional Brillouin zone.

On the other hand, when the two dispersion relations are nearly the same such as

$$|E^2_1(\mathbf{k})-E^2_2(\mathbf{k})|\approx|\Delta_i(\mathbf{k})|^2 \tag{72}$$

or

$$|E^2_1(\mathbf{k})-E^2_2(\mathbf{k})|<|\Delta_i(\mathbf{k})|^2, \tag{73}$$

for $i=1$, 2, and 3, the situation is completely different. If the two layers are nearly equivalent, and if there exist only weak interlayer couplings, Eq. (72) or (73) is easily realized. In this case, all of $|\Delta_i(\mathbf{k})|$ are of the same order of magnitude. The gap can vanish on the Fermi surface, only when two set of points in the two-dimensional Brillouin zone defined by

$$\Delta_1(\mathbf{k})=\Delta_3(\mathbf{k})=0 \tag{74}$$

and

$$\Delta_2(\mathbf{k})=\Delta_3(\mathbf{k})=0 \tag{75}$$

are just on the Fermi surface. If $\Delta_1(\mathbf{k})=0$ and $\Delta_3(\mathbf{k})=0$ define the same lines in the two-dimensional zone, respectively, or if $\Delta_2(\mathbf{k})=0$ and $\Delta_3(\mathbf{k})=0$ define the same lines, respectively, the gap presumably vanishes at points on the Fermi surface in the two-dimensional zone. However, such situations cannot necessarily be satisfied. Even if the three-dimensional feature is taken into account, the same argument is still possible. It is very probable that the gap is open everywhere on the Fermi surface below the crossover temperature in highly distorted lattices with multiple-layered structures, if the admixture of s symmetry is significant.

IV. PHENOMENOLOGICAL THEORY OF TWO-LAYERED STRUCTURES

Because it is hard work to solve the gap equation given by Eqs. (59), (60), and (61), the model will be examined by a phenomenological argument. Let us take two order parameters, ρ_1 and ρ_2, which correspond to even parity and odd parity in Sec. III, respectively. The free energy can generally be written up to fourth order as

$$\begin{aligned}F(T;\rho_1,\rho_2)=T_0[&\tfrac{1}{2}A(\Theta-\Theta_0-\delta\Theta)\rho_1^2\\&+\tfrac{1}{2}A(\Theta-\Theta_0+\delta\Theta)\rho_2^2\\&-B\rho_1\rho_2+\tfrac{1}{4}C_0(\rho_1^4+\rho_2^4)+\tfrac{1}{2}C_2\rho_1^2\rho_2^2]\ ,\end{aligned} \tag{76}$$

with $A>0$, $C_0>0$, and $C_2>0$, T_0 as the unit in energy, Θ as temperature normalized by T_0, and $\Theta_0+\delta\Theta$ and $\Theta_0-\delta\Theta$ as the critical temperatures without any interlayer couplings, respectively; without loss of generality, $\delta\Theta>0$ and $B>0$. Here it is assumed that the two layers are equivalent or nearly equivalent.

When the two layers are equivalent, $B=0$ and $|\delta\Theta|\ll\Theta_0$. In this case, the condition of the free-energy minimum is given by

$$\frac{\partial F}{\partial\rho_1}=T_0\rho_1[A(\Theta-\Theta_0-\delta\Theta)+C_0\rho_1^2+C_2\rho_2^2]=0 \tag{77}$$

and

$$\frac{\partial F}{\partial\rho_2}=T_0\rho_2[A(\Theta-\Theta_0+\delta\Theta)+C_0\rho_2^2+C_2\rho_1^2]=0\ . \tag{78}$$

The superconducting critical temperature is obtained as

$$\Theta_{c1}=\Theta_0+\delta\Theta\ . \tag{79}$$

Because the order parameters are given by

$$\rho_1^2(\Theta)=\frac{A}{C_0}(-\Theta+\Theta_0+\delta\Theta)\ , \tag{80}$$

and $\rho_2^2(\Theta)=0$, the free energy is calculated as

$$F(\Theta)=-T_0\frac{A^2}{4C_0}(-\Theta+\Theta_0+\delta\Theta)^2\ . \tag{81}$$

If $C_0>C_2$, the second transition is possible: Its critical temperature is given by

$$\Theta_{c2}=\Theta_0-\frac{C_0+C_2}{C_0-C_2}\delta\Theta\ . \tag{82}$$

Below Θ_{c2} the order parameters are given by

$$\rho_1^2(\Theta)=\frac{A}{C_0+C_2}\left[-\Theta+\Theta_0+\frac{C_0+C_2}{C_0-C_2}\delta\Theta\right] \tag{83}$$

and

$$\rho_2^2(\Theta)=\frac{A}{C_0+C_2}\left[-\Theta+\Theta_0-\frac{C_0+C_2}{C_0-C_2}\delta\Theta\right]\ . \tag{84}$$

Therefore the free energy is given by

$$\begin{aligned}F(\Theta)=-\tfrac{1}{2}T_0A^2\Bigg[&\frac{1}{C_0+C_2}(-\Theta+\Theta_0)^2\\&+\frac{1}{C_0-C_2}\delta\Theta^2\Bigg]\ .\end{aligned} \tag{85}$$

Because the thermodynamic critical field, H_c, must be proportional to $|-F(\Theta)|^{1/2}$, H_c increases more rapidly with decreasing temperatures below Θ_{c2} than above Θ_{c2}. It can be easily seen that the total magnitude of the order parameters defined by $\rho_1^2+\rho_2^2$ also increases more rapidly with decreasing temperatures below Θ_{c2} than above Θ_{c2}.

When the two layers are not equivalent, then B is finite. In such a case, the second transition is reduced to a crossover. The crossover is very broad when the two layers are very different. On the other hand, the crossover is rather sharp for $B\ll A$, that is, when the two layers are nearly equivalent.

A superlattice structure can be made using a spontaneous distortion of lattices along the z axis in weakly coupled single-layered structures. In distorted lattices, parameter B is presumably linearly proportional to the distortion. If $A\delta\Theta$ is small enough there, a superlattice structure is stabilized by coexistence. It is possible that multiple-layered structures are made by spontaneous distortion.

V. APPLICATION TO HIGH-T_c SUPERCONDUCTIVITY

When the present results are applied to actual high-T_c superconductors, the first problem is whether the t-J models are correct models or not. Recent experiments of photoemission spectroscopy imply that holes should be mainly introduced into oxygen p orbits in the so-called hole-doped superconductors.[12] This simply means that the charge susceptibility of oxygen p electrons is much larger than that of Cu d electrons such as

$$\frac{d}{d\mu}n_{\mathrm{Cu}\,d}\ll\frac{d}{d\mu}n_{\mathrm{O}\,p}\ , \tag{86}$$

where $n_{\mathrm{Cu}\,d}$ is the number of Cu d electrons, and $n_{\mathrm{O}\,p}$ is the number of oxygen p electrons. If the correlation between Cu d electrons is large, such a situation is very reasonable. In general, it is a different problem which orbits are doped and of which electrons quasiparticles are made.

The formation of heavy electrons and the superexchange interaction are essential in the present theoretical framework of superconductivity. As far as heavy electrons and exchange interactions are concerned, no new ingredients appear even if the p orbits on oxygen ions are explicitly included.[2] For the sake of simplicity, therefore, we have not dealt with extended Hubbard models including oxygen p orbits explicitly, but rather we have confined ourselves to t-J models. The t-J models implicitly assume a strong hybridization between Cu d electrons and oxygen p electrons as implied by many band calculations.

Within the t-J model, d-symmetry Cooper pairs are the most probable as long as $|J|<(1-n)|8t|$. The condition is satisfied in actual high-T_c oxides because $|J|\approx 10^3$ K, $|8t|\approx 4\times 10^4$ K, and $(1-n)>0.1$. There is no chance of s symmetry without any other strong on-site attractions. Therefore one of the most promising choices is to try to explain experiments by assuming d-symmetry Cooper pairs.

However, it is implied by a number of experiments[6,7] that high-T_c superconductors are ordinary BCS superconductors, and that the gap should be open everywhere on the Fermi surface. The only exceptional observation is the nuclear magnetic relaxation time (NMR T_1).[5] No humps have been observed just below T_c in the dependence of $1/T_1$ as a function of T, and $1/T_1$ is proportional to T^3 below T_c. This dependence is consistent with the present results, which tell that the gap presumably vanishes along lines on the Fermi surface at temperatures not so far below the superconducting critical temperature. However, the theoretical results show that there should be a small hump even for d symmetry in clean systems,[8] and that a small number of impurities are needed to depress the hump.[13] Therefore the NMR T_1 data imply that impurities should exist in actual systems. It is usual that oxides include many defects, in particular, oxygen defects. The effects of impurities are examined in Appendix A.

The penetration depth was measured in $R\,\mathrm{Ba_2Cu_3O_7}$ compounds,[6] R being one of the rare-earth ions. Because they include linear chains between $\mathrm{CuO_2}$ layers, the admixture of s symmetry cannot be ignored as examined theoretically in Ref. 14, where a single layer and a single chain are assumed. Since the layers are nearly equivalent, superconducting critical temperatures must be nearly the same between different representations with respect to the symmetry operation of exchanging layers. Therefore it is highly probable that the two superconducting states start to coexist at the second critical temperature, or around the crossover temperature, and that the gap starts to open everywhere on the Fermi surface in $R\,\mathrm{Ba_2Cu_3O_7}$. Actually it has recently been reported that the lower critical field H_{c1} shows a rapid increase at a certain temperature below the superconducting critical temperature.[15] It is highly probable that the observed transition or crossover corresponds to that examined in this paper.

It is very interesting to observe the temperature dependence of the penetration depth in single-layered structures, or in multiple-layered structures with the tetragonal symmetry. The gap presumably vanishes along lines on the Fermi surface in the three-dimensional Brillouin zone.

VI. SUMMARY

It has been tried within extended t-J models to explain the temperature dependence of the penetration depth of the high-T_c superconductors, which is similar to ordinary isotropic BCS superconductors. Two extensions have been proposed such as multiple-layered structures of $\mathrm{CuO_2}$ planes, and the distortion from the tetragonal symmetry.

Anisotropic superconductivity in layered-$\mathrm{CuO_2}$ structures has been theoretically examined in the extended t-J models. Within the t-J models in square lattice or in tetragonal lattices, anisotropic Cooper pairs with d symmetry are the most probable. However, the coexistence between Cooper pairs with s symmetry and d symmetry has been investigated. The so-called $s+id$ state is unstable in infinitesimally small distorted lattices. A possible state is a mixed state with the same phase of the order parameters between s symmetry and d symmetry.

It has also been predicted that if layers are exactly equivalent to each other in multiple-layered structures, the second transition can occur in superconducting states. The transition is between superconducting states with different representations with respect to a symmetry operation of exchanging layers. If the layers are nearly equivalent, the transition is reduced to a sharp crossover.

It is most probable that at temperatures not so far below the superconducting critical temperature the gap vanishes at points on the Fermi surface in the two-dimensional Brillouin zone or along lines in the actual three-dimensional Brillouin zone. However, the gap can start to open everywhere at the second critical temperature or around the crossover temperature in multiple-layered structures with the orthorhombic symmetry, which are highly distorted from the tetragonal symmetry. Such a temperature dependence of the gap can explain both the temperature dependences of the penetration depth and the nuclear magnetic relaxation time in high-T_c superconductors, which appear to be inconsistent to each other.

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APPENDIX A: IMPURITY EFFECT

We will confine ourselves to the physical properties of anisotropic Cooper pairs with the d symmetry in single-layered structures examined in Sec. II. The admixture of Cooper pairs with the other symmetry is ignored. Because the gap function is given by $\Delta(\mathbf{k})=\Delta_d(T)\phi_d(\mathbf{k})$, the gap vanishes at $|k_x|=|k_y|$ on the Fermi surface. The density of states of heavy electrons vanishes linearly at small energies as

$$D_0(\omega)=-\frac{1}{\pi N}\sum_{\mathbf{k}}\chi_m \mathrm{Im}[g_{\uparrow\uparrow}(\omega+i0,\mathbf{k})] \propto |\omega/t\Delta_d(T)| , \tag{A1}$$

at $|\omega|\ll\Delta_d(T)$, t being $t_x=t_y$ and $g_{\uparrow\uparrow}(\omega+i0,\mathbf{k})$ being Green functions of electrons in superconducting state defined by Eq. (16).

Let us examine the effects of nonmagnetic impurities:

$$\mathcal{H}_{\mathrm{imp}}=v\sum_{i\sigma} d_{i\sigma}^{\dagger}d_{i\sigma} , \tag{A2}$$

with the impurity concentration n_{imp}. The decrease of T_c due to nonmagnetic impurities is similar to that of the BCS superconductors by magnetic impurities;[16] T_c in the presence of impurities is given by

$$\ln\left[\frac{T_{c0}}{T_c}\right]-\psi\left[\frac{1}{2}+\frac{\gamma_n}{2\pi T_c}\right]+\psi\left[\frac{1}{2}\right]=0 , \tag{A3}$$

with $\psi(x)$ the di-gamma function, T_{c0} the critical temperature in the absence of impurities, and γ_n the level broadening in normal states. Superconductivity is still possible for $\gamma_n/(2\pi T_{c0})<0.28$: If the mean free path l in normal states is longer than the coherent length ξ_{coh} in the absence of impurities, d-symmetry Cooper pairs are still possible in the presence of impurities. Here $l\gg\xi_{\mathrm{coh}}$ is assumed.

The level broadening γ at zero energy in superconducting states is determined in the self-consistent Born approximation:

$$\gamma=\pi n_{\mathrm{imp}}v^2\frac{1}{\chi_m}\int d\omega\, D_0(\omega)\Gamma(\omega) , \tag{A4}$$

with

$$\Gamma(\omega)=\frac{1}{\pi}\frac{\gamma}{\omega^2+\gamma^2} . \tag{A5}$$

Because of Eq. (A1), γ should be finite; otherwise the integration will be divergent. It is easy to see that γ decreases with decreasing T, and that

$$\gamma(T)\propto\Delta_d(T)\exp\left[-r\frac{\Delta_d(T)}{\gamma_n}\right] , \tag{A6}$$

at $T\ll T_c$ with $r=O(1)$. The temperature dependence of $\gamma(T)$ can be ignored at $T\ll T_c$, because $\Delta_d(T)$ is nearly constant at $T\ll T_c$. If γ at the zero energy is used approximately at general energies, the Green functions in superconducting states are given by

$$g_s^{-1}(i\omega,\mathbf{k})=\chi_m\begin{bmatrix} i\omega+i\gamma+\mu-\varepsilon(\mathbf{k}) & -\Delta(\mathbf{k}) \\ -\Delta^*(\mathbf{k}) & i\omega+i\gamma-\mu+\varepsilon(\mathbf{k})\end{bmatrix} . \tag{A7}$$

Impurities can make the density of states of heavy electrons finite at the zero energy, when the gap vanishes in the absence of impurities along lines on the Fermi surface in the three-dimensional Brillouin zone. Therefore a small linear specific-heat coefficient can appear even in superconducting states with the pure d symmetry.

APPENDIX B: MEISSNER EFFECT DUE TO BLOCH ELECTRONS

Let us consider the interaction between electromagnetic fields with small $\mathbf{q}$ ($|\mathbf{q}|a\ll 1$):

$$\mathcal{H}_{\mathrm{em}}=-\frac{1}{c}\sum_{\mathbf{q}} j(-\mathbf{q})A(\mathbf{q}) , \tag{B1}$$

with

$$j(-\mathbf{q})=\frac{e}{\hbar}\sum_{\mathbf{k}}\frac{\partial e(\mathbf{k})}{\partial\mathbf{k}}d^{\dagger}_{\mathbf{k}+(1/2)\mathbf{q}\sigma}d_{\mathbf{k}-(1/2)\mathbf{q}\sigma} . \tag{B2}$$

The current operator of the ξ component ($\xi=x$ or y) should be defined by

$$J_{\xi}(\mathbf{q})=\frac{e}{\hbar}\sum_{\mathbf{k}\sigma}\frac{\partial e(\mathbf{k})}{\partial k_{\xi}}d^{\dagger}_{\mathbf{k}-(1/2)\mathbf{q}\sigma}d_{\mathbf{k}+(1/2)\mathbf{q}\sigma} -\frac{e^2}{c\hbar^2}\sum_{\nu\mathbf{k}\sigma}\frac{\partial^2 e(\mathbf{k})}{\partial k_{\xi}\partial k_{\nu}}d^{\dagger}_{\mathbf{k}\sigma}d_{\mathbf{k}\sigma}A_{\nu}(\mathbf{q}) , \tag{B3}$$

with e the electron charge, in order to satisfy the gauge invariance:[17]

$$e\dot{n}(\mathbf{q})+i\mathbf{q}\cdot J(\mathbf{q})=0 , \tag{B4}$$

with

$$n(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{k}\sigma} d^{\dagger}_{\mathbf{k}+\mathbf{q}\sigma}d_{\mathbf{k}\sigma} . \tag{B5}$$

Therefore the current is calculated as

$$J_{\xi}(|\mathbf{q}|a\to 0)=-\frac{e^2}{c\hbar^2}\sum_{\nu} Q_{\xi\nu}(T)A_{\nu}(0) , \tag{B6}$$

with $Q_{\xi\nu}(T)=D_{\xi\nu}(T)+P_{\xi\nu}(T)$ given by

$$D_{\xi\nu}(T)=\frac{1}{N}\sum_{\mathbf{k}}\frac{\partial^2\varepsilon(\mathbf{k})}{\partial k_{\xi}\partial k_{\nu}}\int dx\, f(x)\frac{1}{2}\left[\left[1+\frac{\varepsilon}{E}\right]\Gamma(x-E)+\left[1-\frac{\varepsilon}{E}\right]\Gamma(x+E)\right] , \tag{B7}$$

$$P_{\xi\nu}(T)=-\frac{1}{N}\sum_{\mathbf{k}}\frac{\partial\varepsilon(\mathbf{k})}{\partial k_\xi}\frac{\partial\varepsilon(\mathbf{k})}{\partial k_\nu}\int\int dx\,dy\frac{f(x+E)-f(y+E)}{y-x}\Gamma(x)\Gamma(y) \tag{B8}$$

$$=\frac{4\pi}{\gamma N}\sum_{\mathbf{k}}\left[\frac{\partial\varepsilon(\mathbf{k})}{\partial k_\xi}\right]^2\int dx\,f(x+E)x\Gamma^2(x)\ , \tag{B9}$$

with $f(x)=[\exp(x/T)+1]^{-1}$ the Fermi distribution function, $\varepsilon=\varepsilon(\mathbf{k})-\mu$ and $E=E(\mathbf{k})$. Equation (B7) is a diamagnetic term, and Eq. (B8) or Eq. (B9) is a paramagnetic term. Because scatterers are of short range, impurity-ladder terms consistent with the Born approximation vanish in obtaining Eq. (B8). To obtain Eqs. (B7), (B8), and (B9), χ_m appearing in the Green functions have been replaced with the renormalization of current operators such as $\partial e(\mathbf{k})/\partial k_\xi\rightarrow\partial\varepsilon(\mathbf{k})/\partial k_\xi$.

It can easily be seen that $P_{\xi\nu}(T)\propto(T/T_c)^1$ at $T\ll T_c$ in the absence of impurities. However, impurities make $P_{\xi\nu}(0)$ finite; the Meissner current is reduced. Then let us examine the temperature dependencies of

$$\delta D_{\xi\nu}(T)\equiv D_{\xi\nu}(T)-D_{\xi\nu}(0)\ ,$$

$$\delta P_{\xi\nu}(T)\equiv P_{\xi\nu}(T)-P_{\xi\nu}(0)\ ,$$

and

$$\delta Q_{\xi\nu}(T)\equiv Q_{\xi\nu}(T)-Q_{\xi\nu}(0)$$

in the presence of impurities. By taking into account the chemical potential shift to keep the electron number constant, it can be found that $\delta D_{\xi\nu}(T)\propto(T/T_c)^\eta$ with $\eta\geq 2$ at $T\ll T_c$. If $\partial^2\varepsilon(\mathbf{k})/\partial k_\xi\partial k_\nu$ in Eq. (B7) is approximated by its averaged value on the Fermi surface, $\delta D_{\xi\nu}(T)=0$. It can be seen from Eq. (B9) that $\delta P_{\xi\nu}(T)\propto(T/\gamma)^2$ at $T\ll\gamma$. Therefore $\delta Q_{\xi\nu}(T)\propto(T/\gamma)^2$ at $T\ll\gamma$. This weaker dependence can be understood by a physical picture that any excitations of quasiparticles in the gapless region cannot cause a large reduction of the Meissner current, because the gapless region does not contribute to the current so much even at $T=0$ K as seen by finite $P_{\xi\nu}(0)$. On the other hand, $\delta Q_{\xi\nu}(T)\propto(T/T_c)^1$ at $\gamma\ll T\ll T_c$.

It can easily be proved as expected by a partial integration with respect to k_ξ in Eq. (B7) that the diamagnetic term and the paramagentic term cancel each other at $T>T_c$. The Meissner current vanishes at $T>T_c$.

Let us examine the penetration depth $\lambda(T)$ or its temperature variation $\delta\lambda(T)\equiv\lambda(T)-\lambda(0)$. In type-II superconductors with $\lambda(0)\gg\xi_{\rm coh}$, the penetration depth $\lambda(T)$ is roughly given by

$$\lambda(0)/\lambda(T)=[Q_{\xi\xi}(T)/Q_{\xi\xi}(0)]^{1/2}\ .$$

Therefore $\delta\lambda(T)\propto(T/\gamma)^2$ at $T\ll\gamma$, while $\delta\lambda(T)\propto(T/T_c)^1$ at $\gamma\ll T\ll T_c$.

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