

# Anisotropic superconductivity mediated by phonons in layered compounds with weak screening effects

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Anisotropic pairing interactions mediated by phonons are examined in layer systems. It is shown that the screening effects become weaker when the layer spacing increases. Then the anisotropic components of the pairing interactions increase with the screening length since the momentum dependence changes. As a result, various types of anisotropic superconductivity occur depending on the parameter region. For example,  $p$ -wave superconductivity occurs when the short-range part of Coulomb repulsion is strong and the layer spacing is large. Two kinds of interlayer pairing may occur when the layer spacing is not too large. Although the phonon contribution to the  $d$ -wave pairing interaction is weaker than the  $p$ -wave interaction, it increases with the layer spacing. The relevance of the present results to organic superconductors, high- $T_c$  cuprates, and  $\text{Sr}_2\text{RuO}_4$  is discussed.

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## I. INTRODUCTION

The anisotropy of the superconducting order parameter and the mechanism of pairing interactions in layered superconductors are recent subjects of much interest. In particular, high- $T_c$  cuprate superconductors, organic superconductors, and the  $\text{Sr}_2\text{RuO}_4$  compound have been studied by many authors.

There is some evidence that the order parameter has line nodes on the Fermi surface in high- $T_c$  cuprates. For example, an experiment and a theory on the Josephson junction gave evidence of a “ $d$ -wave” order parameter in a cuprate superconductor.<sup>1,2</sup> Linear temperature dependence of the penetration depth was observed at low temperatures.<sup>3</sup> An experiment of the Josephson junction by Li *et al.* in  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$  suggests that the order parameter include an isotropic  $s$ -wave component.<sup>4</sup>

On the other hand, superconductivity in  $\text{Sr}_2\text{RuO}_4$  is considered to be due to spin triplet pairing according to the results of a Knight shift measurement<sup>5</sup> and a  $\mu\text{SR}$  experiment.<sup>6</sup> Experimental results of the Josephson current between  $\text{Sr}_2\text{RuO}_4$  and  $s$ -wave superconductors do not seem to be settled. Jin *et al.* observed that the current vanishes along the  $c$  axis and discussed that it is of intrinsic origin.<sup>7</sup> On the contrary, Sumiyama *et al.* observed a finite current along the  $c$  axis.<sup>8</sup> In the absence of spin orbit coupling, the Josephson current between  $p$ -wave and  $s$ -wave superconductors does not occur, while in the presence of it, it might occur but the direction of the current is restricted by the  $\mathbf{d}$  vector of the triplet order parameter.<sup>7,8</sup> Rice and Sigrist suggested that the  $p$ -wave pairing might be due to a paramagnon mechanism in analogy to the superfluid  $^3\text{He}$ .<sup>9</sup> Mazin and Singh examined the same mechanism quantitatively on the basis of first principle calculations,<sup>10</sup> while they also suggested from the value of  $T_c$  that there is some room for the electron-phonon coupling in addition to the paramagnon contribution. However, it is difficult to prove the mechanism by a quantitative argument on superconducting transition tem-

perature  $T_c$ , because  $T_c$  is an extremely sensitive quantity as a function of the coupling constant. In the  $p$ -wave pairing, the full gap state is theoretically expected,<sup>9</sup> but some experimental results seem to indicate line nodes.<sup>11–13</sup>

In the high- $T_c$  cuprates, pairing interactions of magnetic origin, such as exchange of spin fluctuations and a superexchange interaction between nearest neighbor spins, have been discussed by many authors because of proximity to the antiferromagnetic phase. However, experimental results of the isotope effect suggest that there are contributions to the superconductivity from phonon-mediated interactions in many high- $T_c$  cuprates.<sup>14–20</sup> Absolute values of shifts of  $T_c$  are very large (0.2–0.7 K), but isotope effect exponents  $\alpha$  are small because of the high transition temperature.

Abrikosov proposed a theory based on weak screening of Coulomb interactions and phonon-mediated pairing interactions in which anisotropic  $s$ -wave order parameter was obtained.<sup>21</sup> In the presence of on-site Coulomb repulsion, an extremely anisotropic  $s$ -wave order parameter with nodes was obtained.<sup>22</sup> Bouvier and Bok also calculated an order parameter explicitly, and obtained anisotropic  $s$ -wave in the same model.<sup>23</sup> Recently, it has been shown that  $d$ -wave superconductivity is reproduced in a similar model with antiferromagnetic fluctuations.<sup>24,25</sup> Shen *et al.* showed that electron-phonon coupling plays an important role in pairing in the cuprate superconductors using angle-resolved photoemission data.<sup>26</sup>

On the other hand, Foulkes and Gyorfgy proposed that the electron-phonon interactions could give rise to a  $p$ -wave pairing in the presence of short-range Coulomb interactions.<sup>27</sup> We proposed in our previous paper<sup>28</sup> that triplet pairing superconductivity can be induced by phonon-mediated interactions in ferromagnetic compounds, where singlet pairing is suppressed by the Pauli paramagnetic effect.

The origin of the anisotropic components of pairing interactions mediated by phonons is briefly explained as follows. The screening effect limits electron-ion interactions within a range of the order of the screening length. Since the pairing interactions mediated by phonons are obtained by a second

order perturbation of the electron-ion interactions, they also have a range of the same order. For example, the screening effect is taken into account as vertex corrections within the diagrammatic technique.<sup>29</sup> When the screening length increases, the interactions are more localized in the momentum space. Hence, the anisotropic components of the interactions increase with the screening length.

In this paper, we examine layered superconductors with the phonon-mediated pairing interactions, extending it to systems with large layer spacing. The layered structure modifies the screening length and the pairing interactions significantly. It is shown that anisotropic components of the pairing interactions are large in the layered system. We discuss the possible relevance in the layered superconductors, such as  $\text{Sr}_2\text{RuO}_4$ , organics, and cuprates.

We study both the intralayer and interlayer pairings. Efetov and Larkin examined the influence of a magnetic field and electron hopping on the properties of the superconductors with those interactions.<sup>30</sup> Klemm and Liu examined this subject in detail for high- $T_c$  superconductors.<sup>31</sup> We examine how the coupling constants change when the layer spacing changes qualitatively.

We also study an effect of anisotropy of density of states in square lattice systems. Although the effect of the anisotropy must be most remarkable when the Fermi surface is near the van Hove singularities, we consider a system not necessarily near the van Hove singularity but a system with the density of states anisotropy within the layers.

In Sec. II, we define the model of the pairing interactions mediated by phonons. We derive expressions of the coupling constants for various types of anisotropic superconductivity. In Sec. III, we examine the dependence on the layer spacing of the screening length and the pairing interactions. In Sec. IV, we consider a situation in which interlayer coupling is of the order of intralayer coupling. In Sec. V, we examine an effect of the anisotropy in the electron dispersion in square lattice systems. Section VI is devoted to discussion and summary.

## II. SCREENING EFFECT AND PAIRING INTERACTIONS

First, we introduce a model of pairing interactions. Abrikosov examined an effective pairing interaction mediated by phonons of the form

$$V(\mathbf{q}) = g \left( \frac{q_s^2}{q^2 + q_s^2} \right)^n \frac{[\omega(\mathbf{q})]^2}{(\xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{q}})^2 - [\omega(\mathbf{q})]^2}, \quad (1)$$

with  $q = |\mathbf{q}|$  and  $q_s = l_s^{-1}$ , where  $l_s$  denotes the screening length.<sup>21,22</sup> A similar form corresponding to  $n = 1$  is obtained by taking into account the screening effect in electron-phonon interactions as explained in Ref. 29. If we put  $n = 1$  for simplicity and  $\xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{q}} = 0$  for the electrons near the Fermi surface in Eq. (1) according to Abrikosov,<sup>21</sup> we obtain a simplified form

$$V(\mathbf{q}) = - \frac{g q_s^2}{q^2 + q_s^2}. \quad (2)$$

We define lattice constants  $a$  within the layers and  $b$  between the layers. We take the  $x$  and  $y$  axes in the direction of the lattice vectors within the layers, and the  $z$  axis perpendicular to the layers.

When  $b \gg a$ , the discrete layered structure in the interlayer direction must be taken into account for shorter wavelength  $\lambda \sim q^{-1} \sim b$ . Therefore we extend Eq. (2) in the form

$$V(\mathbf{q}) = - \frac{g q_s^2}{|\mathbf{q}_{\parallel}|^2 + q_s^2} - \frac{g' q_s'^2}{|\mathbf{q}_{\parallel}|^2 + q_s'^2} \cos q_z b \quad (3)$$

including interlayer coupling  $g'$  for layer systems, where  $\mathbf{q}_{\parallel}$  is the momentum element in the layers. Here we have truncated the interaction at the nearest layers.

The gap equation of superconductivity is written as

$$\Delta(\mathbf{k}) = - \frac{1}{N} \sum_{\mathbf{k}'} V(\mathbf{k} - \mathbf{k}') W(\mathbf{k}') \Delta(\mathbf{k}'), \quad (4)$$

where

$$W(\mathbf{k}') = \frac{\tanh[E(\mathbf{k}')/2T]}{2E(\mathbf{k}')} \quad (5)$$

with  $E(\mathbf{k}) = \sqrt{\epsilon_{\mathbf{k}}^2 + [\Delta(\mathbf{k})]^2}$  and  $N$  the number of lattice sites.

We put the gap function

$$\Delta(\mathbf{k}) = \Delta_{\parallel}(\mathbf{k}_{\parallel}) \eta(k_z), \quad (6)$$

where  $\mathbf{k}_{\parallel} = (k_x, k_y)$  and  $\eta(k_z)$  is a normalized function of the momentum component  $k_z$ . From Eq. (3), the solution of the gap equation (4) at  $T = T_c$  has a form with  $\eta(k_z) = 1, \sqrt{2} \cos k_z b$ , or  $\sqrt{2} \sin k_z b$ . Then Eq. (4) is written as

$$\Delta_{\parallel}(\mathbf{k}_{\parallel}) = - \frac{1}{N_{\parallel}} \sum_{\mathbf{k}'_{\parallel}} V(\mathbf{k}_{\parallel}, \mathbf{k}'_{\parallel}) W(\mathbf{k}'_{\parallel}) \Delta_{\parallel}(\mathbf{k}'_{\parallel}), \quad (7)$$

where  $N_{\parallel}$  denotes the number of sites in a layer, and  $V(\mathbf{k}_{\parallel}, \mathbf{k}'_{\parallel})$  denotes the averaged pairing interaction defined by

$$V(\mathbf{k}_{\parallel}, \mathbf{k}'_{\parallel}) \equiv \frac{b^2}{(2\pi)^2} \int_{-\pi/b}^{\pi/b} dk_z \int_{-\pi/b}^{\pi/b} dk'_z \eta(k_z) V(\mathbf{k}, \mathbf{k}') \eta(k'_z). \quad (8)$$

Here we assume that the dispersion in the  $z$  direction can be neglected in  $\epsilon_{\mathbf{k}}$  in the gap equation.

We consider the cylindrically symmetric Fermi surface from now on. Hence we put  $|\mathbf{k}_{\parallel}| = |\mathbf{k}'_{\parallel}| = k_F$  in the pairing interactions Eq. (8) and obtain

$$V(\varphi - \varphi') \equiv V(\mathbf{k}_{\parallel}, \mathbf{k}'_{\parallel}) = - \frac{g(\alpha - 1)}{\alpha - \cos(\varphi - \varphi')}, \quad (9)$$

with

$$\alpha = 1 + \frac{q_s^2}{2k_F^2}, \quad (10)$$

for  $\eta(k_z)=1$ . On the other hand, for the order parameters with  $\eta(k_z)=\sqrt{2}\cos k_z b$  and  $\eta(k_z)=\sqrt{2}\sin k_z b$ , the expression for  $V(\varphi-\varphi')$  is obtained by replacing  $g$  and  $\alpha$  with  $g'$  and  $\alpha'=1+q_s'^2/2k_F^2$ , respectively, in Eq. (9).

We expand the averaged interaction  $V(\varphi-\varphi')$  as

$$\begin{aligned} V(\varphi-\varphi') &= \sum_{m=0}^{\infty} V_m n_m \gamma_m(\varphi-\varphi') \\ &= \sum_{m=0}^{\infty} V_m [\gamma_m(\varphi)\gamma_m(\varphi') + \bar{\gamma}_m(\varphi)\bar{\gamma}_m(\varphi')], \end{aligned} \quad (11)$$

and the gap function  $\Delta_{\parallel}(\varphi)=\Delta_{\parallel}(\mathbf{k}_{\parallel})$  as

$$\Delta_{\parallel}(\varphi) = \sum_{m=0}^{\infty} [\Delta_m \gamma_m(\varphi) + \bar{\Delta}_m \bar{\gamma}_m(\varphi)], \quad (12)$$

where

$$\begin{aligned} \gamma_m(\varphi) &= n_m \cos(m\varphi), \\ \bar{\gamma}_m(\varphi) &= n_m \sin(m\varphi), \end{aligned} \quad (13)$$

with normalization factors

$$n_m = \begin{cases} 1 & \text{for } m=0, \\ \sqrt{2} & \text{for } m \neq 0. \end{cases} \quad (14)$$

The expansion factor  $V_m$  is calculated by

$$V_m = \frac{1}{n_m} \int_0^{2\pi} \frac{d\theta}{2\pi} \gamma_m(\theta) V(\theta). \quad (15)$$

It is easy to perform the integration in Eq. (15). For  $\eta(k_z)=1$ , we obtain dimensionless coupling constants

$$\lambda_m = gN(0) \sqrt{\frac{\alpha-1}{\alpha+1}} [\alpha - \sqrt{\alpha^2-1}]^m. \quad (16)$$

Then the superconducting transition temperature  $T_c$  is obtained by

$$T_c = 1.13 \omega_D e^{-1/\lambda_m}, \quad (17)$$

with  $\lambda_m = -V_m N(0)$  from Eq. (4), where  $N(0)$  is the density of states per site of a given spin.

For  $\eta(k_z)=\sqrt{2}\cos k_z b$  and  $\sqrt{2}\sin k_z b$  we obtain a similar dimensionless coupling constant as

$$\lambda'_m = \frac{1}{2} g' N(0) \sqrt{\frac{\alpha'-1}{\alpha'+1}} [\alpha' - \sqrt{\alpha'^2-1}]^m \quad (18)$$

for nearest-neighbor layer pairings. The expression for  $T_c$  is the same as Eq. (17).

Here, we note that a contribution from the short-range part of the Coulomb repulsion must be subtracted from  $\lambda_0$

obtained above. For example, in the tight binding model, the on-site Coulomb energy is estimated by

$$U = \int \int d^3\mathbf{r} d^3\mathbf{r}' |w(\mathbf{r})|^2 \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}-\mathbf{r}'|} |w(\mathbf{r}')|^2, \quad (19)$$

where  $w(\mathbf{r})$  is the Wannier function. It is obvious that the energy  $U$  is not included in our interaction energy Eq. (3), since Eq. (19) depends on the profile of the Wannier function. Equation (3) describes the behaviors of pairing interactions of longer wavelength, while the energy  $U$  in Eq. (19) is characterized by the local states of electrons on each lattice site.

Therefore we must consider the on-site Coulomb repulsion in addition to the pairing interaction of Eq. (3). However, it reduces only the intralayer  $s$ -wave pairing interaction but not the other anisotropic pairing interactions because of the symmetry. We define a parameter  $\tilde{U}$  so that the  $s$ -wave interaction  $\lambda_0$  is reduced by  $\tilde{u} \equiv \tilde{U}N(0)$ . The value of the parameter  $\tilde{U}$  is not equal to  $U$ , because the retardation and spin fluctuation effects should be taken into account. We consider  $\tilde{U}$  as a given parameter without estimating it microscopically.

### III. DEPENDENCE ON THE LAYER SPACING OF THE ANISOTROPIC PAIRING INTERACTION

In this section, we calculate anisotropic components of the effective pairing interactions as functions of the layer spacing  $b$ . We concentrate on the case of intralayer pairing  $\eta(k_z)=1$  for a while.

The squared inverse of the screening length is

$$q_s^2 = \frac{e^2}{\epsilon_0} \rho(\mu), \quad (20)$$

in Thomas-Fermi approximation, where  $\rho(\mu)$  is total density of states of electrons per unit volume at chemical potential  $\mu$ . In layer systems, the total density of states per unit volume  $\rho(\mu)$  is written in terms of the total density of states per unit area  $\rho_{\parallel}^{2D}(\mu)$  in each layer as

$$\rho(\mu) = \rho_{\parallel}^{2D}(\mu)/b. \quad (21)$$

Here it is found that the screening becomes weaker when the layer spacing increases, because the volume density of electrons which contribute to screening decreases when the layer spacing increases. However, it should be noted that the screening length within a layer changes by the change of the interlayer spacing  $b$ , even when the lattice constant  $a$  in the layers is unchanged. Therefore the behavior of the screening length examined is not derived by a simple scale transformation in terms of  $a$  and  $b$  as the length scales.

We define a length scale  $b_0$  as

$$\alpha = 1 + \frac{q_s^2}{2k_F^2} \equiv 1 + \frac{b_0}{b}, \quad (22)$$

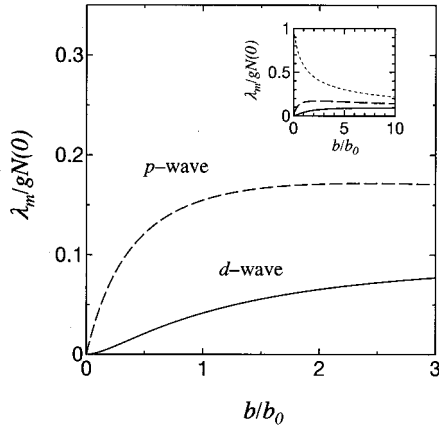


FIG. 1. The dimensionless coupling constants  $\lambda_m$  as a function of the layer spacing  $b$ . The solid and dashed lines show the results for the  $p$  wave ( $m=1$ ) and  $d$  wave ( $m=2$ ), respectively. In the inset, the short dashed line shows the result for the  $s$  wave ( $m=0$ ).

from Eqs. (20) and (21). In a simple case, the length scale  $b_0$  is estimated as follows. Assuming noninteracting two-dimensional electron gas in  $\rho_{\parallel}^{(2D)}(\mu)$ , we obtain

$$b_0 = \frac{a^2}{\pi n a_H}, \quad (23)$$

since  $\rho_{\parallel}^{(2D)}(\mu) = m/\pi\hbar^2$  and  $k_F a = \sqrt{2\pi n}$ , where  $n$  is the electron number per site. Here  $a_H$  denotes Bohr radius  $a_H = 4\pi\epsilon_0\hbar^2/me^2 = 0.5292 \text{ \AA}$ . As an example, if  $a \sim 4 \text{ \AA}$  and  $n \sim 1$  we have  $b_0 \sim 9.6 \text{ \AA}$  as a crude estimation. Since the basic length scale  $a_H$  which is independent of the lattice constants  $a$  and  $b$  comes in Eq. (23), changes not only of the ratio  $b/a$  but also of the absolute values of  $a$  and  $b$  give rise to changes in the qualitative results.

Figure 1 shows the result of  $\lambda_m$  as a function of the layer spacing  $b$ . It is seen that both  $p$ -wave and  $d$ -wave components of the pairing interactions increase with the layer spacing  $b$ . In particular, it is found that the  $p$ -wave components increase rapidly in the region  $0 < b \leq b_0$ . As the inset shows, the  $s$ -wave component  $\lambda_0/gN(0)$  is equal to 1 in the limit of  $b=0$  and decreases with  $b$ . It remains larger than the other anisotropic components, but if the additional short-range Coulomb energy  $U$  is sufficiently large so that  $\lambda_0 - \tilde{u} < \lambda_1$ ,  $p$ -wave pairing occurs instead of  $s$ -wave pairing.

Figure 2 is the phase diagram at  $T=0$  in the  $b$ - $\tilde{U}$  plane. It is found that  $p$ -wave superconductivity occurs in the region where the layer spacing  $b$  is larger and the short-range repulsion expressed by  $\tilde{U}$  is stronger. We will discuss the reality of such parameter values in the layered compounds in the last section.

On the other hand, for  $d$ -wave superconductivity to occur, some additional contribution to  $\lambda_2$  or a negative contribution to  $\lambda_1$  is needed, so that  $\lambda_2$  becomes larger than  $\lambda_1$ . We examine an enhancement of  $\lambda_2$  due to an anisotropy of the density of states later, and briefly discuss a contribution from the antiferromagnetic fluctuations in the last section.

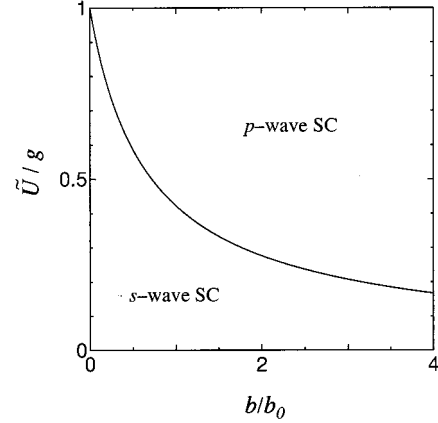


FIG. 2. The phase diagram at  $T=0$  in the  $b$ - $\tilde{U}$  plane. SC stands for superconductivity.

#### IV. INTERLAYER PAIRING

In this section we consider a situation in which the interlayer coupling constant  $g'$  is of the same order as the intralayer coupling constant  $g$ . The coupling constants would depend on the layer spacing  $b$ , but here we regard them as independent parameters. The condition  $g' \sim g$  would actually be satisfied when  $b$  is not too large. Then, we must consider the gap function of the form  $\Delta(\mathbf{k}) = \Delta_{\parallel}(\mathbf{k}_{\parallel})\eta(k_z)$  with  $\eta(k_z) = \sqrt{2} \cos k_z b$  or  $\sqrt{2} \sin k_z b$ . The expansion of  $\Delta_{\parallel}(\mathbf{k}_{\parallel})$  by Eq. (12) holds also in this case.

Figure 3 shows the dimensionless coupling constants  $\lambda'_m$ . A set of parameters,  $g' = 0.8g$ ,  $\tilde{U} = 0.4g$ , and  $q'_s = q_s$  are taken as an example. For  $b/b_0 \leq 0.6$  and  $b/b_0 \geq 2.2$ , intralayer pairing (of  $s$ -wave and  $p$ -wave in each region, respectively) is favored. On the other hand, for  $0.6 \leq b/b_0 \leq 2.2$ , interlayer pairing with  $m=0$  is favored. The gap function has a form such as

$$\Delta(\mathbf{k}) = \Delta_0 \sin k_z b,$$

$$\Delta(\mathbf{k}) = \Delta_0 \cos k_z b. \quad (24)$$

The former is an order parameter of triplet pairing, while the latter is that of singlet pairing. These gap functions have horizontal line nodes at  $k_z = 0, \pm\pi/b$  and at  $k_z = \pm\pi/2b$ , respectively, but they are isotropic in the layers. In the absence of additional pairing interactions, singlet and triplet order parameters of Eq. (24) have the same transition temperature. As Klemm and Liu examined, the horizontal line nodes vanish for coexistence of singlet and triplet order parameters in this case.<sup>31</sup>

#### V. EFFECT OF ANISOTROPY IN THE ELECTRON DISPERSION

In this section, we consider the square lattice systems, in which the electron dispersion depends on the direction of the momentum. We will show that the  $d$ -wave coupling constant  $\lambda_2$  is enhanced for  $d_{x^2-y^2}$  symmetry, but not for  $d_{xy}$  symmetry, due to the anisotropy of the density of single-particle

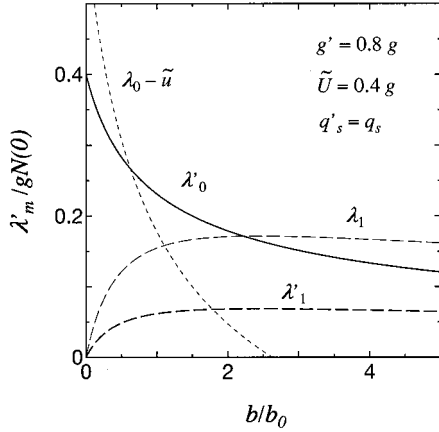


FIG. 3. The dimensionless coupling constants  $\lambda'_m$  of nearest-neighbor layer pairing as a function of the layer spacing  $b$ . The thick solid and dashed lines show the results of the interlayer pairing with  $m=0$  and  $m=1$ , respectively, while the thin dashed and short dashed lines show the results of intralayer pairing  $\lambda_1$  and  $\lambda_0 - \tilde{u}$ , respectively.

states. We define an angle-dependent density of states  $\rho(\epsilon, \varphi)$  as a density of single-particle states per unit energy and unit angle.

In the square lattice system, the angle-dependent density of states at the Fermi energy  $\rho(0, \varphi)$  can be approximated by

$$\rho(0, \varphi) \approx \rho_0 + \rho_4 \cos(4\varphi), \quad (25)$$

where  $\varphi$  is the angle between a momentum  $\mathbf{p}$  and  $p_x$  axis. In addition, we regard  $k_F$  as being constant, for simplicity.

Figure 4 shows a verification of this simplified model in the square lattice tight binding model with a nearest neighbor hopping energy  $t$  at  $\mu = -t$ . Although the Fermi surface is nearly isotropic, the density of states  $\rho(0, \varphi)$  varies with the direction  $\varphi$ . For example, when  $\mu = -t$ ,  $\rho_0 \approx 0.142$ , and  $\rho_4 \approx 0.040$  are estimated.

Regarding Eq. (25) as an expansion of  $\rho(\varphi, 0)$ , we could extend it into more general forms by adding terms  $\rho_{4n} \cos(4n\varphi)$  with  $n \geq 2$ . Then the terms of  $\rho_{4n}$  mix  $\Delta_m$  of a small  $m$  with  $\Delta_{m'}$  of a large  $m' = |m \pm 4n|$ . However, since  $V_m$  decreases rapidly with  $m$  as seen by Eq. (16),  $\Delta_{m'}$ 's of such large  $m'$  are small. Therefore the higher order terms in the expansion of  $\rho(\varphi, 0)$  can be omitted in practice.

In the gap equation, the anisotropic term proportional to  $\rho_4 \cos 4\varphi$  does not affect equations for  $\bar{\Delta}_m \sin m\varphi$ . Therefore we only consider equations for  $\Delta_m$ . For general  $m$ , we can write the gap equation at  $T = T_c$  as

$$\Delta_m = -\lambda_m^{(0)} \ln \frac{2e^\gamma \omega_D}{\pi T_c} \left[ \Delta_m + \frac{\rho_4}{2\rho_0} \left\{ \frac{n_m}{n_{m+4}} \Delta_{m+4} + \frac{n_m}{n_{|m-4|}} \Delta_{|m-4|} \right\} \right], \quad (26)$$

where we define  $\lambda_m^{(0)} \equiv V_m \rho_0 = V_m N(0)$  is the dimensionless coupling constant for the isotropic case.

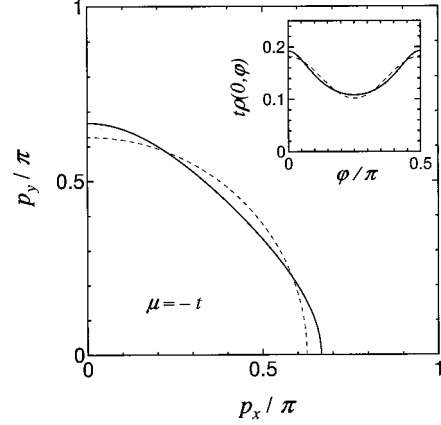


FIG. 4. The Fermi surface of a tight binding model with a chemical potential  $\mu = -t$  (solid line), and the averaged isotropic Fermi surface with  $k_F \approx 1.97/a$  (short dashed line). The inset shows the angle-dependent density of states  $\rho(0, \varphi)$  at the Fermi energy. The short dashed line in the inset shows the behavior of  $\rho(0, \varphi)$  approximated by Eq. (25) with  $\rho_0 = 0.142t$  and  $\rho_4 = 0.040t$ .

Since  $V_3, V_4, V_5, \dots$ , are much smaller than  $V_0$  and  $V_1$ , the terms proportional to  $\rho_4$  can be neglected in Eq. (26) for  $m=0$  and 1. Hence,  $\lambda_0$  and  $\lambda_1$  are not modified by  $\rho_4$ . On the other hand, for  $m=2$ , we cannot omit the term of  $\Delta_{|m-4|}$  in Eq. (26) since  $|m-4|=2$ . Neglecting the term of  $\Delta_{m+4} = \Delta_6$  because  $V_6 \ll V_2$ , we obtain

$$\Delta_2 = \lambda_2^{(0)} \left[ 1 + \frac{\rho_4}{2\rho_0} \right] \ln \frac{2e^\gamma \omega_D}{\pi T_c} \Delta_2 \equiv \lambda_2 \ln \frac{2e^\gamma \omega_D}{\pi T_c} \Delta_2, \quad (27)$$

where we define an effective coupling constant  $\lambda_2 \equiv \lambda_2^{(0)} (1 + \rho_4/2\rho_0)$ , which gives  $T_c$  by Eq. (17).

Therefore, it is found that  $d_{x^2-y^2}$ -wave pairing is favored more than  $d_{xy}$ -wave pairing by the enhancement factor  $(1 + \rho_4/2\rho_0)$ . The enhancement factor  $1 + \rho_4/2\rho_0$  is estimated to be 1.14 for  $\mu = -t$ , and 1.22 for  $\mu = -0.5t$ . On the competition with  $p$ -wave pairing, those values are not large enough to change the sign of  $\lambda_2 - \lambda_1$ . Therefore, another nonphonon contribution seems to be needed for  $d$ -wave pairing to occur.

## VI. DISCUSSION AND SUMMARY

We have examined pairing interactions mediated by phonons in the layer systems. The screening of Coulomb interactions becomes weaker when the layer spacing  $b$  increases. Then anisotropic components of the pairing interactions increase with the layer spacing  $b$  since the momentum dependence of the interactions changes. In particular,  $p$ -wave superconductivity occurs for large  $b$  and strong short-range Coulomb repulsion  $\tilde{U}$ , even in the absence of any additional nonphonon interactions.

It was found that the  $p$ -wave coupling constant  $\lambda_1$  increases rapidly with the layer spacing  $b$  in the region  $b \lesssim b_0$ , where  $b_0$  is a length scale defined by Eq. (22). For the rapid increase of  $\lambda_1$ , the condition  $\lambda_0 - \tilde{u} < \lambda_1$  is realized

more easily in layer systems than in usual three-dimensional systems, where  $\lambda_0$  denotes the  $s$ -wave coupling constant and  $-\tilde{u}$  is a negative contribution to  $s$ -wave pairing due to the short-range Coulomb repulsion discussed near Eq. (19). Hence triplet pairing superconductivity is favored in layered compounds.

We have also examined interlayer pairing. In some region of the parameter space, for example,  $0.6 \leq b/b_0 \leq 2.2$  for the parameters indicated in Fig. 3, the gap function may have horizontal line nodes parallel to the layers. In this case, the solutions of singlet pairing and triplet pairing of Eq. (24) degenerate. The horizontal line nodes vanish for coexistence of singlet and triplet order parameter.<sup>31</sup> If some effect due to spin fluctuations, ferromagnetic correlations, magnetic field, or spin-orbit coupling removes this degeneracy, interlayer triplet pairing may occur. In this case, the triplet order parameter has horizontal line nodes.

In  $\text{Sr}_2\text{RuO}_4$  compounds, existence of the line nodes was supported by some experiments such as temperature dependences of specific heat and NMR relaxation rate.<sup>11</sup> However, the direction of the line nodes does not seem clear at the present. Line nodes vertical to the layers were indicated by ultrasound attenuation,<sup>12</sup> whereas an almost isotropic state was indicated by thermal conductivity.<sup>13</sup> The isotropic state can be consistent with the specific heat and NMR experiments, if the horizontal line nodes are assumed.

The intralayer triplet pairing is a candidate for the vertical line nodes. However, we need some additional mechanism for the vertical line nodes to occur, for example, a multiband effect, because isotropic states such as  $p_x + ip_y$  have the lowest free energy in the present isotropic system. A consistent explanation of the experimental results within the present theory remains for a future study.

It is found in Figs. 1 and 3 that the coupling constant of the intralayer triplet pairing  $\lambda_1$  and that of the interlayer triplet pairing  $\lambda_0$  have a different layer spacing  $b$  dependence. The former increases with  $b$ , while the latter decreases with  $b$ . This difference might be useful for discriminating two kinds of order parameter experimentally, within the present theory.

In order to discuss the reality of the phonon-mediated anisotropic superconductivity, we crudely estimate the parameters for the  $\text{Sr}_2\text{RuO}_4$  compound and quasi-one-dimensional organic superconductors from the observed transition temperature  $T_c \sim 1.5$  K. We assume triplet pairing

here, although for the organics it might be rather controversial. The results of the parameter values do not strongly depend on the direction of the line nodes. Roughly speaking,  $b \geq b_0$  is satisfied in both kinds of compounds. If we assume  $\omega_D \sim 1000$  K and  $T_c \sim 1.5$  K, we have  $\lambda_1 \sim 0.151$  (or  $\lambda'_0 \sim 0.151$ ). Therefore, we obtain  $gN(0) \sim 1.0$  and  $0.69$ , respectively, from Figs. 1 and 3. For such choices of parameter values, in order to suppress the  $s$ -wave pairing, the on-site Coulomb repulsion must be larger than  $\sim 1/2N(0) \sim W/2$ , where  $W$  is the bandwidth. Although this estimation is crude, the value  $\sim W/2$  seems realistic as the order of the magnitude.

On the other hand, for  $d$ -wave superconductivity to occur in the present model,  $p$ -wave and  $s$ -wave pairing needs to be suppressed for some extra reason or some additional contributions to  $d$ -wave pairing. For this problem, we examined the effect of the anisotropy of the electron dispersion. It was found that the  $d$ -wave coupling constant  $\lambda_2$  is enhanced by the anisotropy for  $d_{x^2-y^2}$  symmetry, while not for  $d_{xy}$  symmetry and  $p_x$ ,  $p_y$  symmetries. However, the enhancement does not seem to be large enough to realize the  $d$ -wave superconductivity. This might suggest an existence of a non-phonon contribution to the  $d$ -wave pairing interaction in the cuprates, for example, antiferromagnetic spin fluctuations.

However, even if we assume that a nonphonon contribution is indispensable for high- $T_c$ , the present theory suggests that there is a large phonon contribution to the  $d$ -wave pairing interactions especially in layer systems for the weak screening. This result is consistent with the observed large shifts of  $T_c$  as absolute values due to the isotope effect.<sup>14-20</sup>

It was also found that the coupling constant  $\lambda_2$  increases with the layer spacing  $b$ . This behavior might be a reason why the transition temperature of  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$  is much higher than that of  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ . Since  $T_c$  is a sensitive function of  $\lambda_m$ , such a slight enhancement of  $\lambda_2$  may increase  $T_c$  considerably.

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