Effect of anisotropy on the energy gap and the critical temperature in a strongly coupled layered superconductor

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The Eliashberg theory is applied to study the critical temperature and a gap anisotropy of strongly coupled layered superconductors. The electron-ion pseudopotential, the electron, and the phonon energy spectra are proposed to be anisotropic in layered crystals with an open Fermi surface. The anisotropic electron-phonon spectral density $[\alpha^2F(z)]_{p_z}$ is found to be expanded in $\cos(np_zd)$ functions. Such an expression for $[\alpha^2F(z)]_{p_z}$ demands the energy gap $\Delta(p_z,\omega)$ to present also as an expansion in the harmonic functions. Therefore, the value of the energy gap along the c axis should display p_z dependence. The value of Δ differs from that obtained by in-plane measurements. By using McMillan's method we present each amplitude $\Delta_n(\omega)$ in the harmonic expansion of the energy gap $\Delta(p_z,\omega)$ by trial function. The infinite set of coupled homogeneous equations for Δ_0, Δ_1, Δ_2,... is obtained, the solution of which should yield the critical temperature. We estimate only those equations which include the three amplitudes, Δ_0, Δ_1, and Δ_2, in the harmonic expansion of the energy gap. An approximate calculation of T_c shows that the critical temperature must be enhanced due to the influence of anisotropy. [S0163-1829(96)05130-2]

I. INTRODUCTION

Experimental investigation of the energy gap shows considerable anisotropy for almost all high-temperature superconducting crystals.[1–4] Different values of the energy gap, when wave vector is directed along ($\mathbf{k}\perp\mathbf{c}$) and perpendicular ($\mathbf{k}\|\mathbf{c}$) to superconducting layers in $YBa_2Cu_3O_7$ crystals, have been obtained from far-infrared,[1] Raman,[2] and tunneling,[3] measurements. According to these data, the ratio $2\Delta(0)/T_c$ is about 8 for the in-plane, while it is 3 for the out-plane measurements. The energy gap anisotropy can also be observed inside the Cu-O superconducting planes,[4] which is directly associated with an in-plane anisotropy.

The gap anisotropy of the layered superconductors (SC's) has been theoretically investigated by many authors,[5] taking *a priori* the anisotropy of the pairing interaction, i.e., the internal spherical symmetry of pairs in isotropic SC's is phenomenologically destroyed according to the crystalline symmetry of anisotropic SC's. The orientational dependence of the gap parameter in the layered SC's has been also investigated in Ref. 6 in the framework of the excitonic mechanism of superconductivity. The anisotropic effects in the theory of strongly coupled superconductors have been studied by using the Fermi-surface harmonics.[7,8] According to this method, the physical quantities defined in the $\mathbf{k}$ space can be expanded in orthonormal functions on the Fermi surface, which are called the Fermi-surface harmonics.

In this paper we shall study the effects of anisotropy on the energy gap and on the critical temperature of strongly coupled layered SC's. Taking into account the anisotropies in the microscopic characteristics of superconducting crystals, the energy gap can be shown to be anisotropic and the transition temperature to be enhanced in the layered superconductors.

The anisotropy of the energy gap in layered SC's may be originated by the electron-phonon interaction anisotropy, also by the electron and phonon spectra anisotropies. Though the Coulomb pseudopotential in layered crystals should depend on the crystallographic axis, we shall not take into account this dependence and we shall admit the Coulomb pseudopotential as a constant for simplicity.

The major factor which reduces to the $\mathbf{k}$ dependence of the gap is an anisotropy of the electron-ion pseudopotential. We assume that the electron-ion interaction occurs not only inside a layer but also between nearest-neighboring layers. The general form of the electron-ion pseudopotential is given in Sec. II.

Since the current carriers in high-T_c superconductors exist inside the Cu-O layers, its energy spectrum is proposed to be

$$E(\mathbf{k},k_z)=\frac{\hbar^2}{2m^*}\,(k_x^2+k_y^2)+t_\perp(1-\cos k_zd); \qquad (1)$$

where, m^* is current carrier's effective mass, $t_\perp$ is the tunneling integral from plane to neighboring plane, and d is the interlayer distance. The one-particle properties' anisotropy is characterized by the small parameter, $t_\perp/\epsilon_F\ll 1$, where ϵ_F is the Fermi energy of particles inside the layers. The condition $t_\perp\ll\epsilon_F$ is satisfied for open Fermi surfaces. It should be noticed that an anisotropy which appears only in the one-particle characteristics of a system cannot reduce to the energy-gap anisotropy in superconducting materials.[9]

The phonon spectrum of the layered crystals is, generally speaking, anisotropic. The dispersion relations for longitudinal $\Omega_L(\mathbf{q},q_z)$ and transverse $\Omega_T(\mathbf{q},q_z)$ phonons are given by the following expressions:[10]

$$\Omega_L^2(\mathbf{q},q_z)=u_\|^2q^2+\frac{2}{d^2}\,u_\perp^2(1-\cos q_zd), \qquad (2)$$

$$\Omega_T^2(\mathbf{q},q_z)=\overline{u_\perp^2}q^2+\frac{2}{d^2}u_T^2(1-\cos q_z d). \tag{3}$$

The sound velocity components $u_\parallel$, $u_\perp$ and $\overline{u_\perp}$, u_T in anisotropic solids should satisfy the relations

$$u_\parallel \gg u_\perp \quad \text{and} \quad \overline{u_\perp} \gg u_T. \tag{4}$$

Such a form of phonon energy spectrum denotes that a lattice is most rigid with respect to vibrations of atoms inside the layers and the rigidity for vibrations of one layer relative to the others are very small.

The plan of this paper is as follows. In Sec. II we study the electron-phonon coupling constant for a layered superconductor. Starting from the anisotropic Eliashberg equations, written near the critical temperature T_c, we show in Sec. III that the k_z-dependent energy gap of layered SC's may be expressed as an harmonic expansion. In Sec. IV we derive the expression for the transition temperature T_c by using McMillan's trial functions method. The critical temperature is shown to be enhanced with respect to the isotropic value of T_c.

II. ELECTRON-PHONON INTERACTION

We shall use the electron-phonon interaction part of the Hamiltonian, written for a layered superconductor, in the following form:

$$\hat{H}_{\text{e-ph}}=\sum_{j,j'}\int d^2r\int d^2r'\,\psi_j^+(\mathbf{r})V_j[\mathbf{r}-\mathbf{R}_{j'}(\mathbf{r}')]\psi_j(\mathbf{r}), \tag{5}$$

which describes the interaction of an electron at the $\mathbf{r}$th point of the jth layer with ion at the $\mathbf{r}'$th point of the $\mathbf{j}'$th layer through the electron-ion interaction potential of $V_j[\mathbf{r}-\mathbf{R}_{j'}(\mathbf{r}')]$. By expressing an ion radius-vector $\mathbf{R}_{j'}(\mathbf{r}')$ as a sum of $\mathbf{R}_{j'}^0(\mathbf{r}')$ equilibrium position and $\delta\mathbf{R}_{j'}(\mathbf{r}')$ displacement radius vector, we can expand the electron-ion potential $V_j[\mathbf{r}-\mathbf{R}_{j'}(\mathbf{r}')]$ around $\mathbf{R}_{j'}^0(\mathbf{r}')$. Further we express $\delta\mathbf{R}_j(\mathbf{r})$ by phonon creation $b_\alpha^+(\mathbf{q},q_z)$ and destruction $b_\alpha(\mathbf{q},q_z)$ operators, as

$$\delta\mathbf{R}_j(\mathbf{r})=\left(\frac{1}{2NM}\right)^{1/2}\sum_{\alpha=L,T}\sum_{\mathbf{q},q_z}\frac{\mathbf{e}_\alpha}{[\Omega_\alpha(\mathbf{q},q_z)]^{1/2}}e^{i(\mathbf{q}\cdot\mathbf{r}+q_z jd)} \times[b_\alpha(q,q_z)+b_\alpha^+(-\mathbf{q},-\mathbf{q}_z)], \tag{6}$$

where the subscript α denotes the transverse (T) and longitudinal (L) phonons. The electron-ion pseudopotential $V_j[\mathbf{r}-\mathbf{R}_{j'}^0(\mathbf{r}')]\equiv V_{jj'}(\mathbf{r}-\mathbf{r}')$ is proposed to be the following form:

$$V_{jj'}(\mathbf{r}-\mathbf{r}')=V_1(\mathbf{r}-\mathbf{r}')\delta_{jj'}+V_2(\mathbf{r}-\mathbf{r}')[\delta_{j',j+1}+\delta_{j',j-1}], \tag{7}$$

In Eq. (7) the potentials $V_1(\mathbf{r})$ and $V_2(\mathbf{r})$ characterize the electron-ion interactions in the same and nearest-neighboring layers, respectively.

After substituting Eqs. (6) and (7) in Eq. (5) and transforming into an electron creation $a_{\mathbf{q},q_z}^+$ (destruction $a_{\mathbf{q},q_z}$) operator as

$$\psi_j^+(\mathbf{r})=\sum_{\mathbf{q},q_z}a_{\mathbf{q},q_z}^+e^{-i(\mathbf{q}\cdot\mathbf{r}+jdq_z)}, \tag{8}$$

we can obtain the following electron-phonon interaction Hamiltonian:

$$\hat{H}_{\text{e-ph}}=\sum_{\alpha=L,T}\sum_{\substack{\mathbf{q},q_z\\ \mathbf{k},k_z}}g_\alpha(\mathbf{k},k_z)(b_{\mathbf{q},q_z}^\alpha+b_{-\mathbf{q},-q_z}^{\alpha^+})a_{\mathbf{k}+\mathbf{q},k_z+q_z}^+a_{\mathbf{k},k_z} \tag{9}$$

with $g_L(\mathbf{k},k_z)$ and $g_T(\mathbf{k},k_z)$ being the ''bare'' electron-phonon coupling constants:

$$g_L(\mathbf{k},k_z)=-i\left(\frac{N}{2M\Omega_L(\mathbf{k},k_z)}\right)^{1/2}|\mathbf{k}| \times[V_1(\mathbf{k})+2V_2(\mathbf{k})\cos k_z d], \tag{10}$$

$$g_T(\mathbf{k},k_z)=-i\left(\frac{N}{2M\Omega_T(\mathbf{k},k_z)}\right)^{1/2}\frac{\sin k_z d}{d} \times[V_1(\mathbf{k})+2V_2(\mathbf{k})\cos k_z d]. \tag{11}$$

Now, we have to make the Coulomb renormalization of the ''bare'' electron-phonon coupling. Following the renormalization procedure, which has been carried out for an isotropic SC,[11] we must replace $g_\alpha(\mathbf{k},k_z)$ by the renormalized coupling constant $\overline{g_\alpha}(\mathbf{k},k_z)$. The expressions for $\overline{g_L}(\mathbf{k},k_z)$ and $\overline{g_T}(\mathbf{k},k_z)$ will be defined by Eqs. (10) and (11), but with replacing the ''bare'' electron-phonon pseudopotential $V(\mathbf{k},k_z)$ and the ''bare'' phonon-dispersion relation $\Omega_\alpha(\mathbf{k},k_z)$ by the renormalized ones $\nu(\mathbf{k},k_z)$ and $\omega_\alpha(\mathbf{k},k_z)$, respectively.

Expression (7) for the ''bare'' electron-ion pseudopotential permits electrons and ions to interact only on the same and nearest-neighboring layers. We believe that the Coulomb renormalization does not reduce to next-nearest-neighboring and further interactions in Eq. (7), i.e., the renormalization must ''dress'' only $V_1(\mathbf{r}-\mathbf{r}')$ and $V_2(\mathbf{r}-\mathbf{r}')$ potentials in Eq. (7), replacing them by the new renormalized potentials $\nu_{1,2}(\mathbf{r}-\mathbf{r}')$, as $V_{1,2}(\mathbf{r}-\mathbf{r}')\Rightarrow\nu_{1,2}(\mathbf{r}-\mathbf{r}')$ or $V_{1,2}(\mathbf{k})\Rightarrow\nu_{1,2}(\mathbf{k})$ in Eqs. (10) and (11).

The phonon-dispersion relation $\Omega_\alpha(\mathbf{k},k_z)$ for an anisotropic metal is renormalized by the real part of the electron dielectric function $\epsilon(\mathbf{k},k_z;0)$:[11]

$$\Omega_\alpha(\mathbf{k},k_z)\Rightarrow\omega_\alpha(\mathbf{k},k_z)=\Omega_\alpha(\mathbf{k},k_z)/[\epsilon_1(\mathbf{k},k_z;0)]^{1/2},$$

where $\epsilon_1(\mathbf{k},k_z;0)=\text{Re}[\epsilon(\mathbf{k},k_z;0)]$.

For a strongly anisotropic metallic system with electron spectrum $E(\mathbf{k},k_z)$, defined by Eq. (1), the polarization operator $\Pi(\mathbf{k},k_z;0)$, and consequently $\epsilon(\mathbf{k},k_z;0)$ has been calculated by us in Ref. 12. It was shown that $\Pi(\mathbf{k},k_z;0)$ remains constant, as it is in two-dimensional (2D) systems, for $0\leq k\leq 2k_F$ (k_F is Fermi momentum), and there are small corrections to $\Pi(\mathbf{k},0)$ only in the vicinity of $2k_F$. We propose that as a result of renormalization $\omega_\alpha(\mathbf{q},q_z)$ is reduced to the following form:

$$\omega_L^2(\mathbf{q},q_z)=u_\parallel^2(q)q^2+\frac{2}{d^2}u_\perp^2(q)(1-\cos q_z d), \tag{12}$$

$$\omega_T^2(\mathbf{q},q_z)=\overline{u_\perp^2}(q)q^2+\frac{2}{d^2}\,\overline{u_T^2}(q)(1-\cos q_z d). \quad (13)$$

The coefficients $u_\parallel$, $u_\perp$ and $\overline{u_\perp}$, u_T become dispersive due to the renormalization, but the relations (4) must be satisfied for an arbitrary q, i.e.,

$$\frac{u_\perp(q)}{u_\parallel(q)}\approx\frac{u_\perp}{u_\parallel}\ll 1 \quad \text{and} \quad \frac{u_T(q)}{\overline{u_\perp}(q)}\approx\frac{u_T}{u_\perp}\ll 1. \quad (14)$$

Expressions (2) and (3) for the dispersion relations actually mean that phonons can hop only between the nearest-neighboring layers. The Coulomb renormalization is not assumed to change the character of the interlayer phonon hopping that is reflected in Eqs. (12) and (13).

Thus, the dressed electron-phonon coupling $\overline{g_\alpha}(\mathbf{k},k_z)$ for layered SC's gets the following form:

$$\overline{g_L}(\mathbf{k},k_z)=-i\left(\frac{N}{2M\omega_L(\mathbf{k},k_z)}\right)^{1/2}|\mathbf{k}| \times[\nu_1(\mathbf{k})+2\nu_2(\mathbf{k})\cos(k_z d)], \quad (15a)$$

$$\overline{g_T}(\mathbf{k},k_z)=-i\left(\frac{N}{2M\omega_T(\mathbf{k},k_z)}\right)^{1/2}\frac{\sin(k_z d)}{d} \times[\nu_1(\mathbf{k})+2\nu_2(\mathbf{k})\cos(k_z d)], \quad (15b)$$

where ω_L and ω_T are defined by Eqs. (12) and (13), correspondingly, and $\nu_{1,2}(\mathbf{k})$ are the Fourier transforms of the dressed potentials $\nu_{1,2}(\mathbf{r}-\mathbf{r}')$. The obtained electron-phonon coupling $\overline{g_\alpha}(\mathbf{k},k_z)$ allows us to derive the $\mathbf{k}$ dependence of the gap function and the expression for the critical temperature from the Eliashberg equations.

III. ELIASHBERG EQUATIONS AND GAP ANISOTROPY

The linearized Eliashberg equations valid for temperatures T near the critical temperature T_c have the form[13,11,8,14]

$$[1-Z(p_z,\omega)]\omega=-\int_{-\pi}^{\pi}\frac{dp_z'}{2\pi}\int_{-\infty}^{\infty}dz'\int_0^{\omega_0}dz \times(\alpha^2F(z))_{p_zp_z'}K(z,z';\omega), \quad (16)$$

$$Z(p_z,\omega)\Delta(p_z,\omega)=\int_{-\pi}^{\pi}\frac{dp_z'}{2\pi}\int_{-\infty}^{\infty}dz'\int_0^{\omega_0}dz(\alpha^2F(z))_{p_zp_z'} \times K(z,z';\omega)\mathrm{Re}\,\frac{\Delta(p_z',z')}{z'} -\int_{-\pi}^{\pi}\frac{dp_z'}{2\pi}\,\mu_{p_zp_z'}\int_0^{\omega_c}dz'\tanh \times\frac{z'}{2T}\,\mathrm{Re}\,\frac{\Delta(p_z',z')}{z'}, \quad (17)$$

where the kernel of these integral equations $K(z,z';\omega)$ is given by

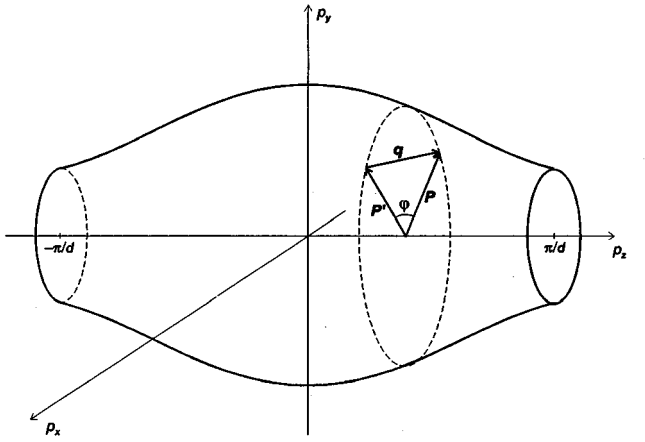

FIG. 1. The Fermi surface of the layered metals.

$$K(z,z';\omega)=\frac{1}{2}\left\{\frac{\tanh(z'/2T)+\coth(z/2T)}{z'+z-\omega-i\delta} -\frac{\tanh(z'/2T)-\coth(z/2T)}{z'-z-\omega-i\delta}\right\}. \quad (18)$$

Here we use the usual notation for the Eliashberg equations, i.e., $Z(p_z,\omega)$ is the renormalization parameter, $(\alpha^2F(z))_{p_zp_z'}$ is the electron-phonon spectral function, $\Delta(p_z,\omega)$ is the energy gap and $\mu_{p_zp_z'}$ is the anisotropic Coulomb pseudopotential. The anisotropic electron-phonon spectral density $(\alpha^2F(z))_{p_zp_z'}$ for scattering of an electron pair from the $(p_z,-p_z)$ state to the $(p_z',-p_z')$ state on the Fermi surface is defined by the following expression:

$$(\alpha^2(z)F(z))_{p_zp_z'}=\frac{N_{2d}(0)}{\pi}\int_0^{2p_F^*}\frac{dq}{\sqrt{(2p_F^*)^2-q^2}} \times\{|\overline{g_L}(q,p_z-p_z')|^2b_L(q,p_z-p_z';z) +|\overline{g_T}(q,p_z-p_z')|^2b_T(q,p_z-p_z';z)\}, \quad (19)$$

where $N_{2d}(0)=m/\pi\hbar^2$ is the density of the 2D electron states, $b_\alpha(q,p_z-p_z';z)$ is the phonon spectral weight, and

$$p_F^*=\sqrt{p_F^2-2mt_\perp(1-\cos p_z')}. \quad (19a)$$

The momentum integration in Eq. (19) has been carried out by changing 2D variables from $\mathbf{p}'=\{|\mathbf{p}'|,\varphi\}$ to the energy variable $E(p')$ and $q=|\mathbf{p}-\mathbf{p}'|$, (see Fig. 1). Since, we set both $|\mathbf{p}|$ and $|\mathbf{p}'|$ equal to p_F, q will denote the angular variation as $\mathbf{p}'$ moves on the Fermi surface and is related the angle φ by

$$\int_0^{2\pi}d\varphi\cdots=4\int_0^{2p_F^*}\frac{dq}{\sqrt{(2p_F^*)^2-q^2}}\cdots.$$

To study the gap anisotropy we expand the electron-phonon couplings $\overline{g_\alpha}$ in Eq. (19) over the small parameters

$$\frac{u_\perp^2}{u_\parallel^2(p_Fd)^2}\ll 1 \quad \text{and} \quad \frac{u_T^2}{\overline{u_\perp^2}(p_Fd)^2}\ll 1.$$

Then we get

$$\begin{aligned}(\alpha^2F(z))_{p_zp_z'}&=\frac{N_{2d}(0)}{\pi}\int_0^1\frac{dy}{\sqrt{1-y^2}}[\nu_1(y)+2\nu_2(y)\cos(p_z-p_z')]^2\Bigg\{\frac{b_L(y,z)}{u_\parallel^2(y)}\frac{y^2}{y^2+u_\perp^2/2u_\parallel^2(p_Fd)^2}+\frac{1}{2\overline{u_\perp^2}(y)(2p_Fd)^2}\\&\times\frac{1-\cos2(p_z-p_z')}{1-(t_\perp/\epsilon_F)(1-\cos p_z')}\frac{b_T(y,z)}{y^2+u_T^2/2\overline{u_\perp^2}(p_Fd)^2}+\frac{u_\perp^2b_L(y,z)}{2u_\parallel^4(p_Fd)^2}\frac{\cos(p_z-p_z')-(t_\perp/\epsilon_F)(1-\cos p_z')}{1-(t_\perp/\epsilon_F)(1-\cos p_z')}\frac{y^2}{(y^2+u_\perp^2/2u_\parallel^2(p_Fd)^2)^2}\\&+\frac{u_T^2}{16\overline{u_\perp^4}(p_Fd)^4}\cdot\frac{[1-\cos2(p_z-p_z')][\cos(p_z-p_z')-(t_\perp/\epsilon_F)(1-\cos p_z')]}{[1-(t_\perp/\epsilon_F)(1-\cos p_z')]^2}\cdot\frac{b_T(y,z)}{(y^2+u_T^2/2\overline{u_\perp^2}(p_Fd)^2)^2}+\cdots\Bigg\}.\end{aligned}\tag{20}$$

For simplicity we neglect the (p_z-p_z') dependence of the phonon spectral weight b_α in Eq. (20).

After integration of $(\alpha^2F(z))_{p_zp_z'}$ over p_z' in the first Brillouin zone we obtain from Eq. (20)

$$(\alpha^2F(z))_{p_z}\equiv\int_{-\pi}^{\pi}\frac{dp_z'}{2\pi}(\alpha^2F(z))_{p_zp_z'}=\sum_{n=0}^{\infty}\left(\frac{t_\perp}{\epsilon_F}\right)^n(\alpha^2F(z))_n\cos np_z=(\alpha^2F(z))_0+\frac{t_\perp}{\epsilon_F}(\alpha^2F(z))_1\cos p_z+\cdots,\tag{21}$$

where

$$\begin{aligned}(\alpha^2F(z))_0=&\frac{N_{2d}(0)}{\pi}\int_0^1\frac{dy}{\sqrt{1-y^2}}\Bigg\{\frac{y^2b_L(y,z)}{u_\parallel^2y^2+\dfrac{u_\perp^2}{2(p_Fd)^2}}[\nu_1^2+2\nu_2^2]+\frac{1}{8(p_Fd)^2}\frac{b_T(y,z)}{\overline{u_\perp^2}y^2+u_T^2/2(p_Fd)^2}[\nu_1^2+\nu_2^2]\\&+\frac{u_\perp^2}{2(p_Fd)^2}\cdot\frac{y^2b_L(y,z)}{(u_\parallel^2y^2+u_\perp^2/2(p_Fd)^2)^2}\left[2\nu_1\nu_2-\frac{t_\perp}{\epsilon_F}(\nu_1^2+2\nu_2^2-2\nu_1\nu_2)\right]\\&+\frac{u_T^2}{16(p_Fd)^4}\cdot\frac{b_T(y,z)}{(\overline{u_\perp^2}y^2+u_T^2/2(p_Fd)^2)^2}\left[\nu_1\nu_2-\frac{t_\perp}{\epsilon_F}(\nu_1^2+\nu_2^2)\right]\Bigg\},\end{aligned}\tag{22}$$

$$\begin{aligned}(\alpha^2F(z))_1=&-\frac{N_{2d}(0)}{8\pi(p_Fd)^2}\int_0^1\frac{dy}{\sqrt{1-y^2}}\Bigg\{\frac{b_T(y,z)}{\overline{u_\perp^2}y^2+u_T^2/2(p_Fd)^2}\nu_1\nu_2+\frac{2u_\perp^2y^2b_L(y,z)}{\left(u_\parallel^2y^2+\dfrac{u_\perp^2}{2(p_Fd)^2}\right)^2}[\nu_1^2+3\nu_2^2-4\nu_1\nu_2]\\&+\frac{u_T^2}{4(p_Fd)^2}\frac{b_T(y,z)}{(\overline{u_\perp^2}y^2+u_T^2/2(p_Fd)^2)^2}[\nu_1^2+2\nu_2^2-2\nu_1\nu_2]\Bigg\},\end{aligned}\tag{23}$$

$$\begin{aligned}(\alpha^2F(z))_2=&-\frac{N_{2d}(0)}{32\pi(p_Fd)^2}\int_0^1\frac{dy}{\sqrt{1-y^2}}\Bigg\{\frac{b_T(y,z)}{\overline{u_\perp^2}y^2+u_T^2/2(p_Fd)^2}\nu_1^2(y)+\frac{8u_\perp^2y^2b_L(y,z)}{(u_\parallel^2y^2+u_\perp^2/2(p_Fd)^2)^2}(\nu_2^2-\nu_1\nu_2)\\&-\frac{4u_T^2b_T(y,z)}{(\overline{u_\perp^2}y^2+u_T^2/2(p_Fd)^2)^2}\nu_1^2(y)\Bigg\},\end{aligned}\tag{24}$$

$$\begin{aligned}(\alpha^2F(z))_3=&\frac{N_{2d}(0)}{32\pi(p_Fd)^2}\int_0^1\frac{dy}{\sqrt{1-y^2}}\Bigg\{\frac{b_T(y,z)}{\overline{u_\perp^2}y^2+u_T^2/2(p_Fd)^2}\nu_1\nu_2-\frac{2u_\perp^2y^2b_L(y,z)}{(u_\parallel^2y^2+u_\perp^2/2(p_Fd)^2)^2}\nu_2^2\\&+\frac{1}{2(p_Fd)^2}\frac{u_T^2b_T(y,z)}{(\overline{u_\perp^2}y^2+u_T^2/2(p_Fd)^2)^2}[\nu_1^2+\nu_2^2-3\nu_1\nu_2]\Bigg\},\end{aligned}\tag{25}$$

$$(\alpha^2F(z))_4=-\frac{N_{2d}(0)}{128\pi(p_Fd)^2}\int_0^1\frac{dy}{\sqrt{1-y^2}}\frac{b_T(y,z)}{\overline{u_\perp^2}y^2+u_T^2/2(p_Fd)^2}\left\{\nu_2^2(y)-\frac{2u_T^2}{(p_Fd)^2}\frac{1}{(\overline{u_\perp^2}y^2+u_T^2/2(p_Fd)^2)^2}\left[\nu_2^2-\frac{5}{4}\,\nu_1\nu_2\right]\right\}. \tag{26}$$

It is seen from Eqs. (22)–(26) that the coefficients of the high harmonics in $(\alpha^2F(z))_{p_z}$ may be positive as well as negative, e.g., $(\alpha^2F(z))_0>0$, $(\alpha^2F(z))_3>0$ and $(\alpha^2F(z))_1<0$, $(\alpha^2F(z))_2<0$, $(\alpha^2F(z))_4<0$. But each term in the series (21) is smaller than the previous term by the parameter $t_\perp/\epsilon_F\ll1$.

Substituting the harmonic expansion Eq. (21) for $(\alpha^2F(z))_{p_z}$ into the first Eliashberg equation (16), we get

$$\begin{aligned}Z(p_z,\omega)&=\sum_{n=0}^{\infty}\left(\frac{t_\perp}{\epsilon_F}\right)^n\cos np_zZ_n(\omega)\\&=Z_0(\omega)+\frac{t_\perp}{\epsilon_F}\,Z_1(\omega)\cos p_z+\cdots,\end{aligned} \tag{27}$$

where

$$Z_n(\omega)=\delta_{n,0}+\frac{1}{\omega}\int_{-\infty}^{\infty}dz'\int_0^{\omega_0}dz(\alpha^2F(z))_nK(z,z';\omega). \tag{28}$$

To solve the second Eliashberg equation (17), we choose the gap function $\Delta(p_z,\omega)$ in the following form:

$$\begin{aligned}\Delta(p_z,\omega)&=\sum_{n=0}^{\infty}\left(\frac{t_\perp}{\epsilon_F}\right)^n\Delta_n(\omega)\cos np_z\\&=\Delta_0(\omega)+\frac{t_\perp}{\epsilon_F}\,\Delta_1(\omega)\cos p_z\\&\quad+\left(\frac{t_\perp}{\epsilon_F}\right)^2\Delta_2(\omega)\cos2p_z+\cdots.\end{aligned} \tag{29}$$

We substitute expressions (27), (29), and (20) for $Z(p_z,\omega)$, $\Delta(p_z,\omega)$, and $(\alpha^2F(z))_{p_zp_z'}$, respectively, into Eq. (17). After some simplifications, the left and the right sides of Eq. (17) can be expressed as an harmonic expansion with $\cos(np_z)$ being the basis functions. By equating the coefficients of the same basis functions we get an infinite set of coupled equations for $\Delta_n(\omega)$ as

$$\begin{aligned}&Z_0(\omega)\Delta_0(\omega)+\frac{1}{2}\sum_{n=1}^{\infty}\left(\frac{t_\perp}{\epsilon_F}\right)^{2n}Z_n(\omega)\Delta_n(\omega)\\&\quad=\int_0^{\infty}\frac{dz'}{z'}\int_0^{\omega_0}dz\;K(z,z';\omega)(\alpha^2F(z))_0\\&\qquad\times\left[\Delta_0(z')-\frac{1}{2}\left(\frac{t_\perp}{\epsilon_F}\right)^2\Delta_1(z')+\frac{1}{4}\left(\frac{t_\perp}{\epsilon_F}\right)^4\Delta_2(z')\mp\cdots\right]\\&\qquad-\mu_0\int_0^{\omega_c}\frac{dz'}{z'}\tanh\frac{z'}{2T}\,\Delta_0(z'),\end{aligned} \tag{30}$$

$$\begin{aligned}&Z_0(\omega)\Delta_1(\omega)+Z_1(\omega)\Delta_0(\omega)+\frac{1}{2}\left(\frac{t_\perp}{\epsilon_F}\right)^2[Z_1(\omega)\Delta_2(\omega)\\&\qquad+Z_2(\omega)\Delta_1(\omega)]+\cdots\\&\qquad=\int_0^{\infty}\frac{dz'}{z'}\int_0^{\omega_0}dz\;K(z,z';\omega)\left\{(\alpha^2F(z))_1\left[\Delta_0(z')-\Delta_1(z')+\frac{1}{2}\left(\frac{t_\perp}{\epsilon_F}\right)^2\Delta_2(z')-\frac{1}{4}\left(\frac{t_\perp}{\epsilon_F}\right)^4\Delta_3(z')\pm\cdots\right]\right.\\&\qquad\left.+\frac{N_{2d}(0)}{\pi}\int_0^1\frac{dy}{\sqrt{1-y^2}}\frac{y^2b_L(y,z)}{u_\parallel^2y^2+u_\perp^2/2(p_Fd)^2}\times2\nu_1(y)\nu_2(y)\Delta_1(z')\right\},\end{aligned} \tag{31}$$

$$\begin{aligned}&Z_0(\omega)\Delta_2(\omega)+\frac{1}{2}\,Z_1(\omega)\Delta_1(\omega)+Z_2(\omega)\Delta_0(\omega)\\&\qquad+\frac{1}{2}\left(\frac{t_\perp}{\epsilon_F}\right)^2[Z_1(\omega)\Delta_3(\omega)+Z_3(\omega)\Delta_1(\omega)]+\cdots\\&\qquad=\int_0^{\infty}\frac{dz'}{z'}\int_0^{\omega_0}dz\;K(z,z';\omega)\left\{(\alpha^2F(z))_2\right.\\&\qquad\times\left[\Delta_0(z')-\Delta_1(z')+2\Delta_2(z')-\left(\frac{t_\perp}{\epsilon_F}\right)^2\Delta_3(z')\right.\\&\qquad\left.+\frac{1}{2}\left(\frac{t_\perp}{\epsilon_F}\right)^4\Delta_4(z')\mp\cdots\right]+\frac{N_{2d}(0)}{\pi}\\&\qquad\left.\times\int_0^1\frac{dy}{\sqrt{1-y^2}}\frac{y^2b_L(y,z)}{u_\parallel^2y^2+u_\perp^2/2(p_Fd)^2}\,\nu_2^2(y)\Delta_2(z')\right\},\end{aligned} \tag{32}$$

$$\begin{aligned}&Z_0(\omega)\Delta_3(\omega)+\frac{1}{2}\,Z_1(\omega)\Delta_2(\omega)+\frac{1}{2}\,Z_2(\omega)\Delta_1(\omega)\\&\qquad+Z_3(\omega)\Delta_0(\omega)+\frac{1}{2}\left(\frac{t_\perp}{\epsilon_F}\right)^2\\&\qquad\times[Z_1(\omega)\Delta_4(\omega)+Z_4(\omega)\Delta_1(\omega)]+\cdots\\&\qquad=\int_0^{\infty}\frac{dz'}{z'}\int_0^{\omega_0}dz\;K(z,z';\omega)(\alpha^2F(z))_3\\&\qquad\times\left[\Delta_0(z')-\Delta_1(z')+2\Delta_2(z')-4\Delta_3(z')\right.\\&\qquad\left.+2\left(\frac{t_\perp}{\epsilon_F}\right)^2\Delta_4(z')\pm\cdots\right],\end{aligned} \tag{33}$$

etc. It must be noticed that the Coulomb pseudopotential $\mu_{p_zp_z'}$ in Eq. (30) is taken to be isotropic for simplicity, i.e., $\mu_{p_zp_z'}=\mu_0$.

IV. THE CRITICAL TEMPERATURE

The critical temperature for layered superconductors in the weak-coupling regime can be calculated by solving Eqs. (27), (28), and (30)–(33). We shall use McMillan's trial functions[15] for each components of the gap function:

$$\Delta_i^t(\omega)=\begin{cases}\Delta_i(0), & 0<\omega<\omega_0\\ \Delta_i(\infty), & \omega_0<\omega\end{cases} \tag{34}$$

and

$$Z_i(\omega)=\begin{cases}Z_i(0), & 0<\omega<\omega_0\\ Z_i(\infty), & \omega_0<\omega.\end{cases} \tag{35}$$

Inserting Eq. (35) into Eq. (28) we immediately obtain

$$Z_0(0)=1+\lambda_0;\quad Z_0(\infty)=1, \tag{36a}$$

$$Z_i(0)=1 \quad \text{and} \quad Z_i(\infty)=0 \quad \text{for} \quad i=1,2,3,\ldots, \tag{36b}$$

where

$$\lambda_1=2\int_0^{\omega_0}\frac{dz}{z}\,(\alpha^2F(z))_i,\quad i=0,1,2,3,\ldots. \tag{37}$$

Expressions (36a)–(37) show that the only zero harmonic λ_0 in the electron-phonon interaction renormalizes the electron mass, i.e., λ_0 is the usual mass-enhancement parameter. The high harmonic corrections, λ_i ($i=1,2,3,...$), to the electron-phonon coupling constant have no effects on $Z_i(\omega)$.

At high energies the Coulomb interaction has the contribution only to $\Delta_0(\infty)$ because of the simple form ($\mu_{p_zp_z'}=\mu_0$) of the Coulomb pseudopotential

$$\Delta_0(\infty)=-\mu^*\,\ln\left(\frac{\omega_0}{T_c}\right)\Delta_0(0) \tag{38a}$$

and

$$\Delta_1(\infty)=0,\quad i=1,2,3,\ldots, \tag{38b}$$

where

$$\mu^*=\frac{\mu_0}{1+\mu_0\,\ln(\omega_c/\omega_0)} \tag{39}$$

is the Coulomb pseudopotential of Morel and Anderson.[17] After substitution of the above obtained expressions (36a)–(38b) into the equations for the gap components written at low energies, we get an infinite set of homogeneous equations for $\Delta_i(0)$. The critical temperature is determined by the roots of the main determinant of this system of homogeneous equations. To calculate the critical temperature, for simplicity we study here only those equations, which include three harmonics, namely Δ_0, Δ_1, and Δ_2:

$$\Delta_0(0)\left[1+\lambda_0-\lambda_0\ln\frac{\omega_0}{T_c}+\mu^*\ln\frac{\omega_0}{T_c}+\mu^*\ln\frac{\omega_0}{T_c}\,\frac{\lambda_0\langle\omega\rangle_0}{\omega_0}\right]$$
$$+\frac{1}{2}\left(\frac{t_\perp}{\epsilon_F}\right)^2\Delta_1(0)\left[1+\lambda_0\ln\frac{\omega_0}{T_c}\right]+\frac{1}{2}\left(\frac{t_\perp}{\epsilon_F}\right)^4\Delta_2(0)$$
$$\times\left[1-\lambda_0\ln\frac{\omega_0}{T_c}\right]=0, \tag{40a}$$

$$\Delta_0(0)\left[1-\lambda_1\ln\frac{\omega_0}{T_c}+\mu^*\,\frac{\lambda_1\langle\omega\rangle_1}{\omega_0}\ln\frac{\omega_0}{T_c}\right]$$
$$+\Delta_1(0)\left[1+\lambda_0-\lambda_1^*\ln\frac{\omega_0}{T_c}\right]$$
$$+\frac{1}{2}\left(\frac{t_\perp}{\epsilon_F}\right)^2\Delta_2(0)\left[1-\lambda_1\ln\frac{\omega_0}{T_c}\right]=0, \tag{40b}$$

$$\Delta_0(0)\left[1-\lambda_2\ln\frac{\omega_0}{T_c}+\mu^*\,\frac{\lambda_2\langle\omega\rangle_2}{\omega_0}\ln\frac{\omega_0}{T_c}\right]$$
$$+\Delta_1(0)\left[\frac{1}{2}+\lambda_2\ln\frac{\omega_0}{T_c}\right]$$
$$+\Delta_2(0)\left[1+\lambda_0-\lambda_2^*\ln\frac{\omega_0}{T_c}\right]=0, \tag{40c}$$

where dimensionless coupling constants λ_i are defined by Eq. (37) and

$$\langle\omega\rangle_i=\frac{2}{\lambda_i}\int_0^{\omega_0}dz(\alpha^2F(z))_i;\quad i=1,2,3,\ldots, \tag{41}$$

$$\lambda_{10}=2\int_0^{\omega_0}\frac{dz}{z}\left\{\frac{2N_{2d}(0)}{\pi}\int_0^1\frac{dy}{\sqrt{1-y^2}}\,\frac{y^2}{u_\parallel^2y^2+u_\perp^2/2(p_Fd)^2}\right.$$
$$\left.\times b_L(y,z)\,\nu_1(y)\,\nu_2(y)\right\}, \tag{42a}$$

$$\lambda_{20}=2\int_0^{\omega_0}\frac{dz}{z}\left\{\frac{N_{2d}(0)}{\pi}\right.$$
$$\left.\times\int_0^1\frac{dy}{\sqrt{1-y^2}}\,\frac{y^2}{u_\parallel^2y^2+u_\perp^2/2(p_Fd)^2}\,b_L(y,z)\,\nu_2^2(y)\right\}, \tag{42b}$$

$$\lambda_1^*=\lambda_{10}-\lambda_1, \tag{42c}$$

$$\lambda_2^*=2\lambda_2+\lambda_{20}. \tag{42d}$$

We get approximately two values of the critical temperature from Eqs. (40a)–(40c):

$$T_{c1}=\frac{\omega_D}{1.45}\exp\left\{-\frac{1+\lambda_0}{\lambda_0+\lambda_1^*+\lambda_2^*-\mu^*-\mu^*(\lambda_0\langle\omega\rangle_0/\omega_0)}\right\}, \tag{43}$$

$$T_{c2}=\frac{\omega_D}{1.45}\exp\left\{-(1+\lambda_0)\times\frac{\lambda_0+\lambda_1^*+\lambda_2^*-\mu^*-\mu^*(\lambda_0\langle\omega\rangle_0/\omega_0)}{[\lambda_0-\mu^*-\mu^*(\lambda_0\langle\omega\rangle_0/\omega_0)](\lambda_1^*+\lambda_2^*)+\lambda_1^*\lambda_2^*}\right\}, \tag{44}$$

and

$$T_c=\max\{T_{c1},T_{c2}\}.$$

It should be noticed that the McMillan's prefactor $\omega_D/1.45$ in Eqs. (43) and (44) for T_c can be refined following Allen and Dynes,[16] by changing it from $\omega_D/1.45$ to $\omega_{\ln}/1.2$, where $\omega_{\ln}$ is a logarithmic average phonon frequency.

The positive parameters λ_1^* and λ_2^* are the first- and the second-harmonic corrections to the electron-phonon coupling constant. Equations (43) and (44) show that the higher harmonic corrections λ_1, λ_2, . . . should enhance the critical temperature of anisotropic SC's.

To obtain expressions (43) and (44) for T_c we are restricted by three harmonics in the infinite set of homogeneous equations (30)–(32) for $\Delta_n(\omega)$, $n=0,1,2,\ldots$. The further inclusion of the higher harmonics gives rise to renormalization of λ by the high harmonic parameters λ_3, λ_4, ... As a result, T_c should be enhanced.

V. CONCLUSIONS

In this paper we study an anisotropy of the energy gap in strongly coupled layered superconductors. The electron-ion pseudopotential, and the electron and phonon energy spectra are proposed to be anisotropic. We believe that such proposition is true for strong anisotropic layered structures like the Bi- and Tl-based high-temperature superconductors. The Eliashberg theory for a strongly coupled layered superconductor is applied to study the critical temperature of a system. The anisotropic electron-phonon spectral density $(\alpha^2F(z))_{p_z}$ is shown to be expanded in the $\cos(np_zd)$ functions [see Eq. (21)]. The leading term in this expansion is the zero harmonic $(\alpha^2F(z))_0$, which renormalizes the electron mass. The coefficients of the higher harmonics in the expansion of Eq. (21) are small and ~ 0 $((t_\perp/\epsilon_F)^n)$. Such a form of the electron-phonon spectral density demands the energy gap $\Delta(p_z,\omega)$ to be also expanded in the harmonic functions, as presented by Eq. (29). Expression (29) for the energy gap shows that the value of $\Delta(p_z,\omega)$ does not depend on the wave vector inside of SC layers. Nevertheless the value of Δ along the c axis should display p_z dependence. The value of the energy gap in the c direction differs from its in-plane value Δ_0 due to the contribution of such higher harmonic terms as $\Delta_1,\Delta_2,\Delta_3,\ldots\Delta_0$ in the c direction.

The Coulomb pseudopotential $\mu_{p_zp_z'}$ in the Eliashberg equations is chosen to be nondispersive and $\mu_{p_zp_z'}=\mu_0=\text{const}$. Therefore μ_0 has a contribution only to Δ_0. We expect that accurate calculation should give rise to harmonic expansion of $\mu_{p_zp_z'}$ as

$$\mu_{p_zp_z'}=\sum_{n=0}^{\infty}\mu_n(t_\perp/\epsilon_F)^n\cos[n(p_z-p_z')d].$$

The higher prefactors, μ_n $(n=1,2,3,\ldots)$, in this expansion must contribute to corresponding Δ_n and will slightly alter the expression for T_c.

To study the critical temperature we used McMillan's method,[15] by applying the trial functions for each amplitude Δ_n in the harmonic expansion Eq. (29) of the gap function. The larger of the obtained two expressions (43) and (44) is the actually observed critical temperature. It can be easily seen from Eqs. (43) and (44) that the critical temperature of layered SC's should be enhanced due to the high harmonic corrections $\lambda_1,\lambda_2,\lambda_3,\ldots$ to the electron-phonon coupling constant. It should be noticed that similar results, such as the harmonic expansion of the gap parameter and T_c enhancement in the layered SC's have been obtained in Ref. 6 (see, also Ref. 5) by using the excitonic mechanism of superconductivity.

The influence of anisotropy on T_c in a layered SC has been studied in Ref. 18 by using a Fermi-surface harmonic expansion. According to the Fermi-surface symmetry of a layered SC, a complete orthonormal set of expansion functions on the Fermi surface is chosen to be $\cos(np_zd)$ and the anisotropic electron-phonon interaction kernel $\lambda_{p_z,p_z'}$ is expanded over these cosine functions. Taking into account only two corrections in this expansion it was shown that the critical temperature should be enhanced. Unlike our study, where all terms in the harmonic expansion can be specified and expressed by the characteristic parameters of the system [see, e.g. Eqs. (21)–(26)], in the Fermi-surface harmonic method in Ref. 18 the undetermined coefficients of the harmonic expansion of $\lambda_{p_z,p_z'}$ are taken phenomenologically.

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