Lattice distortion and elasticity change in *s*-wave and *d*-wave superconductors

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The lattice anomaly, i.e., the lattice distortion and the elasticity change, caused by the appearance of superconductivity (SC) is studied by use of the BCS theory. The BCS Hamiltonian with any attractive interaction between electrons is introduced for crystals with the symmetry D_{4h}, so that the *s*-wave, $d_{x^2-y^2}$-wave, and d_{xy}-wave SC's may appear. The microscopic parameters in the Hamiltonian are expanded in powers of distortions u up to their first order, so as to make the Hamiltonian satisfy the crystal symmetry. The free energy of the system as a function of SC order parameters (SOP) and u's is obtained to reveal the properties of the lattice anomaly. The temperature dependence of the equilibrium distortion and the elastic constants in the SC phases with the different SOP's is calculated. The calculated distortion is shown to give its temperature dependence consistent with the observation. The elastic constants obtained can exhibit not only softenings but also hardenings below the transition temperature T_c, depending on the microscopic parameters. This behavior of elastic constant is just that observed in some high-T_c cuprates.

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I. INTRODUCTION

Since high-T_c superconductivities (SC) were found in some perovskite-type cuprates,[1] findings of new SC compounds have succeeded. In these SC compounds, not only the conventional SC but also unconventional SC 's have been observed. For example, the SC's in MgB_2,[2] Sr_2RuO_4,[3] and $PuRhGa_5$ (Ref. 4) are considered to be of *s*-wave, *p*-wave, and *d*-wave SC's, respectively. In experimental studies of SC's appearing in real compounds, various measurements such as those of NMR, thermal conductivity, specific heat, and others[5] have been done. Also measurements of bulk properties of crystal lattices, i.e., the lattice distortion and the elasticity change caused by SC have already been performed to clarify the properties of SC's and the role of SC-lattice coupling in the appearance of SC.[6,7] Unfortunately, however, it seems difficult at present to get full information on SC from the measurements on the lattice properties. In this paper, therefore, we aim to relate the lattice anomaly to microscopic quantities, so that the measurement on the lattice properties may be a more microscopic probe into SC's in real compounds.

Usually, the experimental results on the lattice anomaly caused by SC have been interpreted by use of the two theories, i.e., Ginzburg and Landau (GL)'s theory[8,9] and Testardi's theory.[10] In the former theory,[8,9] the free energy as a function of SC order parameter (SOP) Δ and distortions u is expanded near T_c in powers of Δ and u so as to conserve the symmetry of the SC-lattice system. This theory is helpful to analyze the experimental results, but cannot be suitable for description of the phenomena in a wide temperature region including absolute zero. Moreover, it is not easy to know from the analyses of experiments what happens in SC states in real compounds. In the latter theory,[10] on the other hand, the free energy is assumed to have a form as $\phi f(T/T_c)$ in the all temperature region, where ϕ and T_c are functions of stresses σ. This theory removed a difficulty at low temperatures in the GL theory and clarified relations between the lattice anomaly and some thermodynamic quantities, which supplied a helpful guide in analyses of observations. Nevertheless, it can hardly give detailed information about the origin of the lattice anomaly.

To get more insights into SC's from measurements on the lattice anomaly, we start with the BCS theory.[11] Here, we assume that any of the conventional and unconventional SC states result from formations of electron pairs by possible attractive interactions and are described by extended BCS Hamiltonians, irrespective of mechanisms of electron attraction. The microscopic parameters in the BCS Hamiltonian are introduced phenomenologically, but the Hamiltonian itself should satisfy the symmetry of the electron-lattice system. On the basis of the BCS Hamiltonian thus obtained, we see how the bulk distortion and the elastic change are caused by the appearance of SC and how those depend on the microscopic parameters in the BCS Hamiltonian. This theoretical procedure is made for both *s*-wave and *d*-wave SC states in order to compare their lattice anomalies.

In the next section, we introduce a model of the electron-lattice system in SC compounds. The Hamiltonian suitable for this model system is diagonalized in Sec. III to give the free energy as a function of Δ's and u's. Sections IV and V are devoted to derive the equilibrium distortions and the elastic changes for some different wave states of SC, respectively. Characteristics of the lattice anomaly are seen more explicitly in Sec. VI by making numerical calculations. The results are compared with experiments in Sec. VII. In the last section, VIII, concluding remarks and discussion are given.

II. MODEL SYSTEM AND ITS HAMILTONIAN FOR THE APPEARANCES OF THE *s*-WAVE AND *d*-WAVE SUPERCONDUCTIVITIES

Putting into mind cuprate superconductors, we consider compounds with tetragonal crystals whose structural symmetry is D_{4h}. In the compounds, the band electron system is assumed to be of the two-dimensional (2D) nature and to have a Fermi surface which has a cylindrical shape along the fourfold rotation axis, say the z axis, of the crystal. It is

further assumed that this electron system is able to make the appearance of the s-wave and d-wave SC's and the SC's couple to bulk distortions through various physical quantities. Without going into detail of mechanisms of attractive interaction, we construct the BCS Hamiltonian in the presence of bulk distortions under requirement of the symmetry of the starting crystal.[11] As the result, the total Hamiltonian of this electron-lattice system consists of the elastic energy $H_{\rm ela}$, the band electron energy $H_{\rm ele}$, and the energy of electron interaction $H_{\rm int}$:

$$H = H_{\rm ela} + H_{\rm ele} + H_{\rm int}. \tag{1}$$

When the s-wave and d-wave SC's appear in the present 2D electron system, it is sufficient to take into account the following normal modes of distortion:

$$u_1, u_3(A_{1g}); u_2(B_{1g}); u_6(B_{2g}), \tag{2}$$

where the irreducible representations of D_{4h} which each distortion mode belongs to are also given. Then, the first term in Eq. (1), $H_{\rm ela}$, is given by

$$H_{\rm ela} = \frac{1}{2} V(c_1 u_1^2 + c_2 u_2^2 + c_3 u_3^2 + c_6 u_6^2), \tag{3}$$

where V is the crystal volume in the absence of the distortions and c's are the elastic constants corresponding to each mode. The expressions of u's and c's in terms of the components of the strain tensor $e_{ii'}$ and the elastic stiffness constants $c_{jj'}$, respectively, are given in Appendix A.

For the electron band responsible for the appearance of SC, we introduce an effective band, which is parabolic in the k_x–k_y plane and has a sufficiently large mass in the k_z direction. The second term in Eq. (1), $H_{\rm ele}$, under the distortions is approximated to be

$$H_{\rm ele} = \sum_{\mathbf{k},\sigma} \tilde{\xi}_{\mathbf{k}} c^+_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}, \tag{4}$$

$$\tilde{\xi}_{\mathbf{k}} = \frac{\hbar^2}{2m_\perp}\{\tilde{\zeta}_1(k_x^2 + k_y^2) + \tilde{\zeta}_2(k_x^2 - k_y^2) + 2\tilde{\zeta}_6 k_x k_y\} - \tilde{\mu}, \tag{5}$$

where $c_{\mathbf{k}\sigma}$ is the annihilation operator of the electron with wave vector $\mathbf{k}$ and spin σ and $m_\perp$ is the electron mass in the k_x–k_y plane. In Eqs. (4) and (5), the constants $\tilde{\zeta}$ and the chemical potential $\tilde{\mu}$ are all defined to be quantities of distorted crystals.

The final term in Eq. (1), $H_{\rm int}$, on the other hand, can have the form

$$\begin{aligned} H_{\rm int} = -\frac{1}{V\tilde{k}_{F\perp}^4} {\sum_{\mathbf{k},\mathbf{k}'}}' \{ & \tilde{g}_1(k_x^2 + k_y^2)(k_x'^2 + k_y'^2) \\ & + \tilde{g}_2(k_x^2 - k_y^2)(k_x'^2 - k_y'^2) + 4\tilde{g}_6 k_x k_y k_x' k_y' \\ & + \tilde{g}_{12}[(k_x^2 + k_y^2)(k_x'^2 - k_y'^2) + (k_x'^2 + k_y'^2)(k_x^2 - k_y^2)] \\ & + 2\tilde{g}_{16}[k_x k_y(k_x'^2 + k_y'^2) + k_x' k_y'(k_x^2 + k_y^2)]\} \\ & \times c^+_{-\mathbf{k}'\downarrow} c^+_{\mathbf{k}'\uparrow} c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow}, \end{aligned} \tag{6}$$

where $\tilde{k}_{F\perp}$ is the Fermi wave number in the k_x–k_y plane and $\tilde{g}$'s are interaction constants, which are again defined for distorted crystals. One of $\tilde{g}_1$, $\tilde{g}_2$, and $\tilde{g}_6$, at least, should be positive for the appearance of SC. $\Sigma'_{\mathbf{k}}$ in Eq. (6) means a summation over $\mathbf{k}$ under $|\tilde{\xi}_{\mathbf{k}}| \leqslant \tilde{\epsilon}_c$, $\tilde{\epsilon}_c$ being a cut energy to exclude the energy region of normal electrons.

By taking into account the crystal symmetry, the constants $\tilde{\zeta}$'s and $\tilde{g}$'s can be expanded in powers of u's up to their first order as follows:

$$\begin{aligned} & \tilde{\zeta}_1 = 1 - \zeta_1 u_1 - \zeta_1' u_3, \quad \tilde{\zeta}_2 = -\zeta_2 u_2, \quad \tilde{\zeta}_6 = -\zeta_6 u_6, \\ & \tilde{g}_1 = g_1(1 + \gamma_1 u_1 + \gamma_1' u_3), \quad \tilde{g}_2 = g_2(1 + \gamma_2 u_1 + \gamma_2' u_3), \\ & \tilde{g}_6 = g_6(1 + \gamma_6 u_1 + \gamma_6' u_3), \\ & \tilde{g}_{12} = g_{12} u_2, \quad \text{and } \tilde{g}_{16} = g_{16} u_6. \end{aligned} \tag{7}$$

Here, ζ's, ζ''s, g's, γ's, and γ''s are new constants, which no longer depend on u's.

III. FREE ENERGY OF THE SUPERCONDUCTIVITY-DISTORTION SYSTEM

In order to derive the free energy of the system, we first diagonalize $H_{\rm ele}+H_{\rm int}$ by applying the mean field approximation to $H_{\rm int}$. The superconducting order parameters (SOP) that we are interested in are as follows:

$$\Delta_1 = \frac{g_1}{V\tilde{k}_{F\perp}^2} {\sum_{\mathbf{k}}}' (k_x^2 + k_y^2)\langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow}\rangle, \tag{8}$$

$$\Delta_2 = \frac{g_2}{V\tilde{k}_{F\perp}^2} {\sum_{\mathbf{k}}}' (k_x^2 - k_y^2)\langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow}\rangle, \tag{9}$$

$$\Delta_6 = \frac{2g_6}{V\tilde{k}_{F\perp}^2} {\sum_{\mathbf{k}}}' k_x k_y \langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow}\rangle, \tag{10}$$

where $\langle\ \rangle$ means the thermal average. We call in the following the SC's with Δ_1, Δ_2, and Δ_6 the s-wave, $d_{x^2-y^2}$-wave, and d_{xy}-wave SC's, respectively. Except for normal electrons with $|\tilde{\xi}_{\mathbf{k}}| > \tilde{\epsilon}_c$, the resultant mean-field Hamiltonian for $H_{\rm ele}+H_{\rm int}$ becomes $H_{\rm BCS}$, which is given by

$$\begin{aligned} H_{\rm BCS} = {\sum_{\mathbf{k}\sigma}}' \tilde{\xi}_{\mathbf{k}} c^+_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \frac{1}{\tilde{k}_{F\perp}^2} {\sum_{\mathbf{k}}}' \{ & [\tilde{\Delta}_1^*(k_x^2 + k_y^2) + \tilde{\Delta}_2^*(k_x^2 - k_y^2) \\ & + 2\tilde{\Delta}_6^* k_x k_y] c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} + \text{H.c.}\} + V\tilde{E}_s, \end{aligned} \tag{11}$$

where

$$\tilde{\Delta}_1 = \frac{\tilde{g}_1}{g_1}\Delta_1 + \frac{\tilde{g}_{12}}{g_2}\Delta_2 + \frac{\tilde{g}_{16}}{g_6}\Delta_6, \tag{12}$$

$$\tilde{\Delta}_2 = \frac{\tilde{g}_2}{g_2}\Delta_2 + \frac{\tilde{g}_{12}}{g_1}\Delta_1, \tag{13}$$

$$\tilde{\Delta}_6 = \frac{\tilde{g}_6}{g_6}\Delta_6 + \frac{\tilde{g}_{16}}{g_1}\Delta_1, \tag{14}$$

and

$$\tilde{E}_s = \frac{\tilde{g}_1}{g_1^2}|\Delta_1|^2 + \frac{\tilde{g}_2}{g_2^2}|\Delta_2|^2 + \frac{\tilde{g}_6}{g_6^2}|\Delta_6|^2 + \frac{\tilde{g}_{12}}{g_1 g_2}(\Delta_1^*\Delta_2 + \Delta_1\Delta_2^*) + \frac{\tilde{g}_{16}}{g_1 g_6}(\Delta_1^*\Delta_6 + \Delta_1\Delta_6^*). \tag{15}$$

By making the usual procedures, H_{BCS} is diagonalized to become

$$H_{\mathrm{BCS}} = \sum_{\mathbf{k}}{}' \tilde{E}_{\mathbf{k}}(\alpha_{\mathbf{k}\uparrow}^+\alpha_{\mathbf{k}\uparrow} + \alpha_{-\mathbf{k}\downarrow}^+\alpha_{-\mathbf{k}\downarrow}) + \sum_{\mathbf{k}}{}'(\tilde{\xi}_{\mathbf{k}} - \tilde{E}_{\mathbf{k}}) + V\tilde{E}_s, \tag{16}$$

where

$$\tilde{E}_{\mathbf{k}} = \{\tilde{\xi}_{\mathbf{k}}^2 + (1/\tilde{k}_{F\perp})^4|\tilde{\Delta}_1(k_x^2 + k_y^2) + \tilde{\Delta}_2(k_x^2 - k_y^2) + 2\tilde{\Delta}_6 k_x k_y|^2\}^{1/2}. \tag{17}$$

Equations (16) and (3) give the free energy $F(\Delta;u)$ of the SC state, which is subtracted by the electron free energy of the normal state, as

$$F(\Delta;u) = H_{\mathrm{ela}} - \sum_{\mathbf{k}}{}'\left\{\frac{2}{\beta}\ln\left[\frac{\cosh(\beta\tilde{E}_{\mathbf{k}}/2)}{\cosh(\beta\tilde{\xi}_{\mathbf{k}}/2)}\right]\right\} + V\tilde{E}_s, \tag{18}$$

where $\beta = 1/k_B T$ with the Boltzmann constant k_B, and temperature T. From Eq. (18), we see that the different SOP's cannot coexist in an equilibrium state with the crystal symmetry D_{4h}, but can if the crystal symmetry is lowered by distortions.

To avoid complications of various expressions, we first consider the case where only Δ_1 and Δ_2 can coexist under the distortions u_1 and u_2. Then, it is convenient to scale k_x and k_y by

$$\tilde{k}_x = \sqrt{\tilde{\zeta}_1 + \tilde{\zeta}_2}\, k_x, \quad \tilde{k}_y = \sqrt{\tilde{\zeta}_1 - \tilde{\zeta}_2}\, k_y, \tag{19}$$

so that the Fermi surface distorted by the lattice distortions becomes a circle in the $\tilde{k}_x$–$\tilde{k}_y$ plane. After the summation over $\mathbf{k}$ in Eq. (18) is replaced with the integrations over $\tilde{k}$ and θ defined by

$$\tilde{k} = \sqrt{\tilde{k}_x^2 + \tilde{k}_y^2}, \quad \theta = \tan^{-1}(\tilde{k}_y/\tilde{k}_x), \tag{20}$$

the free energy in the present case is shown to be expressed by

$$F(\Delta_1,\Delta_2;u_1,u_2) = \frac{1}{2}V(c_1u_1^2 + c_2u_2^2) + V\tilde{E}_s - 2V\tilde{D}\int_0^{\tilde{\epsilon}_c} d\xi \times \int_0^{2\pi}\frac{d\theta}{2\pi}\left\{\frac{2}{\beta}\ln\left[\frac{\cosh(\beta\tilde{E}(\xi,\theta)/2)}{\cosh(\beta\xi/2)}\right]\right\}. \tag{21}$$

Here, $\tilde{D}$ is the electronic density of states per unit volume at the Fermi energy in the presence of the distortions. We expand $\tilde{D}$ in powers of u's as

$$\tilde{D} = D(1 + \lambda_1 u_1), \quad D = m_\perp/2\pi c\hbar^2, \tag{22}$$

where λ_1 is assumed to be another expansion coefficient to take into account the u dependence of the density of states[12] and c is the lattice constant along the z axis. In the following, $\tilde{\epsilon}_c$ is replaced with the cut energy in the absence of the distortions, ϵ_c, by assuming that the difference $\tilde{\epsilon}_c - \epsilon_c$ gives only a minor contribution to $\tilde{E}_s$, as shown in Appendix B. $\tilde{E}(\xi,\theta)$ in Eq. (21) can be found by substituting Eqs. (12), (13), and (19) into Eq. (17) to be

$$\tilde{E}(\xi,\theta) = \sqrt{\xi^2 + |\tilde{\Delta}_1' + \tilde{\Delta}_2'\cos 2\theta|^2}, \tag{23}$$

$$\tilde{\Delta}_1' = \Delta_1\{1 + (\zeta_1 + \gamma_1)u_1 + (\zeta_1 + \gamma_1)\zeta_1 u_1^2 + (\zeta_2 + \eta_1)\zeta_2 u_2^2\} + \Delta_2\{(\zeta_2 + \eta_2)u_2 + (2\zeta_1\zeta_2 + \zeta_1\eta_2 + \zeta_2\gamma_2)u_1u_2\}, \tag{24}$$

$$\tilde{\Delta}_2' = \Delta_2\{1 + (\zeta_1 + \gamma_2)u_1 + (\zeta_1 + \gamma_2)\zeta_1 u_1^2 + (\zeta_2 + \eta_2)\zeta_2 u_2^2\} + \Delta_1\{(\zeta_2 + \eta_1)u_2 + (2\zeta_1\zeta_2 + \zeta_1\eta_1 + \zeta_2\gamma_1)u_1u_2\}, \tag{25}$$

where terms up to the second order of u's are retained in the expansion of $\tilde{\Delta}'$'s, and η_1 and η_2 are defined by

$$\eta_1 = \frac{g_{12}}{g_1}, \quad \eta_2 = \frac{g_{12}}{g_2}. \tag{26}$$

The free energy in the case where Δ_1 and Δ_6 coexist in the presence of u_1 and u_6, $F(\Delta_1,\Delta_6;u_1,u_6)$, is derived from $F(\Delta_1,\Delta_2;u_1,u_2)$ obtained above. When θ is replaced by $\theta - (\pi/4)$ in Eq. (20), $2\tilde{k}_x\tilde{k}_y$ is changed to $(\tilde{k}_x^2 - \tilde{k}_y^2)$. By use of this fact, $F(\Delta_1,\Delta_6;u_1,u_6)$ is easily obtained by replacing all subscripts 2 of quantities in $F(\Delta_1,\Delta_2;u_1,u_2)$ given by Eqs. (21)–(26) with the subscripts 6.

The free energies in the presence of u_3 instead of u_1 are also obtained as follows: Since u_1 and u_3 have the same symmetry properties, the two couple to the SC in the same way but with different coupling constants. Therefore, $F(\Delta_1,\Delta_2;u_3,u_2)$ and $F(\Delta_1,\Delta_6;u_3,u_6)$ are derived by the replacements

$$u_1 \to u_3, \quad c_1 \to c_3, \quad \zeta_1 \to \zeta_1', \quad \gamma_1 \to \gamma_1', \quad \gamma_2 \to \gamma_2', \quad \gamma_6 \to \gamma_6', \quad \text{and } \lambda_1 \to \lambda_1', \tag{27}$$

in $F(\Delta_1,\Delta_2;u_1,u_2)$ and $F(\Delta_1,\Delta_6;u_1,u_6)$, respectively.

In general, the SOP's can have different phases. In the following, however, we consider the case where they have the same phases even when different SOP's coexist through H_{int}. This simplification results only in discarding one of the + and − signs of u_2 or u_6 induced by coexisting SOP's.

IV. DISTORTIONS CAUSED BY THE *s*-WAVE AND *d*-WAVE SUPERCONDUCTIVITIES

First, we study the case of the s-wave SC state, where $\Delta_1 \neq 0$ and $\Delta_2 = \Delta_6 = 0$. Then, the linear terms of u's other

than those of u_1 and u_3 vanish in the free energy given by Eqs. (21) and (23), so that only the distortions u_1 and u_3 can be caused by the SC. Therefore, the free energy $F(\Delta_1,\Delta_2;u_1,u_2)$ with $\Delta_2=0$ and $u_2=0$ is sufficient to find the equilibrium u_1, u_{10}. By minimizing this free energy with respect to u_1, u_{10} is found to be

$$u_{10}=\frac{1}{c_1}\left\{(2\zeta_1+\gamma_1)\frac{|\Delta_{10}|^2}{g_1}+2D\lambda_1\int_0^{\epsilon_c}d\xi\frac{2}{\beta}\ln\left[\frac{\cosh(\beta E_1(\xi)/2)}{\cosh(\beta\xi/2)}\right]\right\}. \quad (28)$$

The equilibrium Δ_1, Δ_{10}, in the above equation should satisfy the gap equation:

$$\Delta_{10}=Dg_1\Delta_{10}\int_0^{\epsilon_c}d\xi\frac{1}{E_1(\xi)}\tanh\left(\frac{\beta}{2}E_1(\xi)\right), \quad (29)$$

where

$$E_1(\xi)=\sqrt{\xi^2+|\Delta_{10}|^2}. \quad (30)$$

Equation (29) gives the well-known transition temperature of the s-wave SC phase as

$$T_c=\frac{2e^\gamma}{\pi k_B}\epsilon_c\exp\left(-\frac{1}{g_1D}\right), \quad (31)$$

with Euler's constant γ.

Secondly, we study the case of the $d_{x^2-y^2}$-wave SC state, where $\Delta_2\neq 0$ and $\Delta_1=\Delta_6=0$. Also in this case, u_1 and u_3 can be caused by the SC. The equilibrium distortion u_{10} can be found by minimizing $F(\Delta_1,\Delta_2;u_1,u_2)$ with $\Delta_1=0$ and $u_2=0$ with respect to u_1 to be

$$u_{10}=\frac{1}{c_1}\left\{(2\zeta_1+\gamma_2)\frac{|\Delta_{20}|^2}{g_2}+2D\lambda_1\int_0^{\epsilon_c}d\xi\int_0^{2\pi}\frac{d\theta}{2\pi}\frac{2}{\beta}\ln\left[\frac{\cosh(\beta E_2(\xi,\theta)/2)}{\cosh(\beta\xi/2)}\right]\right\}. \quad (32)$$

The equilibrium Δ_2, Δ_{20}, in Eq. (32) should satisfy the gap equation:

$$\Delta_{20}=Dg_2\Delta_{20}\int_0^{\epsilon_c}d\xi\int_0^{2\pi}\frac{d\theta}{2\pi}\frac{\cos^2 2\theta}{E_2(\xi,\theta)}\tanh\left(\frac{\beta}{2}E_2(\xi,\theta)\right), \quad (33)$$

where

$$E_2(\xi,\theta)=\sqrt{\xi^2+|\Delta_{20}|^2\cos^2 2\theta}. \quad (34)$$

Equation (33) gives the transition temperature of the $d_{x^2-y^2}$-wave SC phase:

$$T_c=\frac{2e^\gamma}{\pi k_B}\epsilon_c\exp\left(-\frac{2}{g_2D}\right). \quad (35)$$

Thirdly, we mention the case of the d_{xy}-wave SC state, where $\Delta_6\neq 0$ and $\Delta_1=\Delta_2=0$. u_{10} in this case is obtained by replacing all subscripts 2 of quantities in Eqs. (32)–(34) with the subscripts 6.

In all cases, the distortions u_{30} can also occur in addition to u_{10}'s. They are easily found by the replacement $u_{10}\rightarrow u_{30}$ together with the replacements given by (27) in Eqs. (28) and (32).

V. ELASTICITY CHANGE CAUSED BY THE *s*-WAVE AND *d*-WAVE SUPERCONDUCTIVITIES

We confine ourselves to the isothermal elastic constants of the SC-lattice system at the static limit of applied stresses. Such constants are to be derived from the free energies, which have already been given in Sec. III. Considerable effects of SC on the elastic constants are expected in the case where the equilibrium SOP is deviated by distortions through linear couplings of distortions to the SC. Before going into detail of its calculation, the procedure for obtaining the elastic constants is outlined on a representative SC state where Δ_1 and Δ_2 coexist in the presence of u_1 and u_2, and $F(\Delta_1,\Delta_2;u_1,u_2)$ given by Eq. (21) is appropriate. When any stress is applied to give rise to further distortions δu_1 and δu_2 from their equilibrium distortions as

$$u_1=u_{10}+\delta u_1,\quad u_2=\delta u_2, \quad (36)$$

the SOP's deviate from their equilibrium values through the SC-lattice couplings as

$$\Delta_1=\Delta_{10}+\delta\Delta_1,\quad \Delta_2=\Delta_{20}+\delta\Delta_2. \quad (37)$$

For obtaining the elastic constants, it can be assumed that $\delta\Delta_1$ and $\delta\Delta_2$ are proportional to the distortions as

$$\delta\Delta_1=\Delta_{10}\chi_{11}\delta u_1+\Delta_{20}\chi_{22}\delta u_2, \quad (38)$$

$$\delta\Delta_2=\Delta_{20}\chi_{21}\delta u_1+\Delta_{10}\chi_{12}\delta u_2, \quad (39)$$

where χ's are the proportional constants depending on quantities in the equilibrium state. We substitute Eqs. (36)–(39) into Eq. (21) to obtain a new free energy as a function of δu_1 and δu_2. After this free energy is expanded in powers of δu_1 and δu_2, the resultant energy increases quadratically with δu_1 and δu_2.

When the above procedure is extended to SC states with any SOP's subjected to any distortions δu_j with $j=1$, 2, 3, and 6, the total increase of the free energy by the distortions should have the form

$$\delta F(\delta u_1,\delta u_2)=\frac{V}{2}\{C_{11}(T)(\delta u_1)^2+C_{22}(T)(\delta u_2)^2+C_{33}(T)\times(\delta u_3)^2+C_{66}(T)(\delta u_6)^2+2C_{13}(T)(\delta u_1)(\delta u_3)\}. \quad (40)$$

The coefficients $C(T)$ in this equation are the elastic constants which are affected by SC.

A. Elastic constants in the *s*-wave SC state

We derive $C_{11}(T)$ by use of $F(\Delta_1,\Delta_2;u_1,u_2)$ with $\Delta_2=0$ and $u_2=0$. The condition $\partial F/\partial\Delta_1=0$ gives the gap equation for Δ_1 in the presence of u_1 as

$$\frac{1}{g_1}(1+\gamma_1 u_1) = D\{1+(2\zeta_1+2\gamma_1+\lambda_1)u_1\} \times \int_0^{\epsilon_c} d\xi \frac{1}{\tilde{E}_1(\xi)} \tanh\left(\frac{\beta}{2}\tilde{E}(\xi)\right), \quad (41)$$

with

$$\tilde{E}_1(\xi) = \sqrt{\xi^2 + |\Delta_1|^2[1+2(\zeta_1+\gamma_1)u_1]}. \quad (42)$$

From Eqs. (41) and (36)–(38), χ_{11} is obtained to be

$$\chi_{11} = -\left\{\frac{(2\zeta_1+\gamma_1+\lambda_1)}{K_{11}(\Delta_{10})} + (\zeta_1+\gamma_1)\right\}, \quad (43)$$

where we have defined $K_{11}(\Delta_{10})$ by

$$K_{11}(\Delta_{10}) = g_1 D|\Delta_{10}|^2 \int_0^{\epsilon_c} d\xi \left(\frac{1}{E_1(\xi)}\right)^2 \times \left\{-\frac{1}{E_1(\xi)}\tanh\left(\frac{\beta}{2}E_1(\xi)\right) + \frac{\beta}{2}\,\mathrm{sech}^2\left(\frac{\beta}{2}E_1(\xi)\right)\right\}. \quad (44)$$

Substituting Eqs. (37) and (38) with Eq. (43) into $F(\Delta_1,0;u_1,0)$ known from Eq. (21) and expanding the free energy thus obtained in powers of δu_1, we arrive at

$$C_{11}(T) = c_1 + \frac{2|\Delta_{10}|^2}{g_1}\left\{\frac{(2\zeta_1+\gamma_1+\lambda_1)^2}{K_{11}(\Delta_{10})} + (\zeta_1+\gamma_1)^2\right\}. \quad (45)$$

$C_{22}(T)$, on the other hand, is derived by use of $F(\Delta_1,\delta\Delta_2;,u_{10},\delta u_2)$ with $u_{10}\simeq 0$ by noting that δu_2 induces $\delta\Delta_2$ under $\Delta_{10}\neq 0$. The induced $\delta\Delta_2$ should satisfy the gap equation as

$$\left\{\frac{g_1}{g_2} - K_{12}(\Delta_{10})\right\}\delta\Delta_2 = \{[1+K_{12}(\Delta_{10})]\zeta_2 + K_{12}(\Delta_{10})\eta_1\}\Delta_{10}\delta u_2, \quad (46)$$

where $K_{12}(\Delta_{10})$ can be expressed by

$$K_{12}(\Delta_{10}) = \frac{1}{2}\{1+K_{11}(\Delta_{10})\}. \quad (47)$$

Equations (46) and (39) give

$$\chi_{12} = -\left\{\frac{g_2\zeta_2 + g_1(\zeta_2+\eta_1)}{g_2K_{12}(\Delta_{10}) - g_1} + (\zeta_2+\eta_1)\right\}. \quad (48)$$

Substitution of Eqs. (37) and (39) with Eq. (48) into $F(\Delta_{10},\delta\Delta_2;0,\delta u_2)$ known from Eq. (21) and its expansion in powers of δu_2 result in

$$C_{22}(T) = c_2 + \frac{2|\Delta_{10}|^2}{g_1 g_2}\left\{\frac{[g_1(\zeta_2+\eta_1)+g_2\zeta_2]^2}{g_2K_{12}(\Delta_{10}) - g_1} + g_1(\zeta_2+\eta_1)^2\right\}. \quad (49)$$

$C_{66}(T)$ also is affected by the SC, because $\delta\Delta_6$ is induced by δu_6 under $\Delta_{10}\neq 0$ to be proportional to δu_6. In a similar way as in $C_{22}(T)$, $C_{66}(T)$ is derived by use of $F(\Delta_{10},\delta\Delta_6;u_{10},\delta u_6)$ with $u_{10}\simeq 0$. As a result, C_{66} can be obtained by the replacements of all subscripts 2 of quantities in Eqs. (49) and (47) with the subscripts 6.

B. Elastic constants in the $d_{x^2-y^2}$-wave SC state

Parallel calculations of the elastic constants to those in Sec. V A are made for the case of $d_{x^2-y^2}$-wave SC state. $C_{11}(T)$ in this case is derived by use of $F(0,\Delta_2;u_1,0)$ known from Eq. (21). The equilibrium condition of Δ_2 gives the gap equation as

$$\frac{1}{g_2}(1+\gamma_2 u_1) = D\{1+(2\zeta_1+2\gamma_2+\lambda_1)\} \times \int_0^{\epsilon_c} d\xi \int_0^{2\pi} \frac{d\theta}{2\pi}\frac{\cos^2 2\theta}{\tilde{E}_2(\xi,\theta)} \tanh\left(\frac{\beta}{2}\tilde{E}_2(\xi,\theta)\right), \quad (50)$$

with

$$\tilde{E}_2(\xi,\theta) = \sqrt{\xi^2 + |\Delta_2|^2[1+2(\zeta_1+\gamma_2)u_1]\cos^2 2\theta}. \quad (51)$$

Equations (50) and (39) give

$$\chi_{21} = -\left\{\frac{(2\zeta_1+\gamma_2+\lambda_1)}{K_{21}(\Delta_{20})} + (\zeta_1+\gamma_2)\right\}, \quad (52)$$

where we have defined $K_{21}(\Delta_{20})$ by

$$K_{21}(\Delta_{20}) = g_2 D|\Delta_{20}|^2 \int_0^{\epsilon_c} d\xi \int_0^{2\pi} \frac{d\theta}{2\pi} \times \left(\frac{\cos^2 2\theta}{E_2(\xi,\theta)}\right)^2 \left\{-\frac{1}{E_2(\xi,\theta)}\tanh\left(\frac{\beta}{2}E_2(\xi,\theta)\right) + \frac{\beta}{2}\,\mathrm{sech}^2\left(\frac{\beta}{2}E_2(\xi,\theta)\right)\right\}. \quad (53)$$

Equations (37), (39), (52), and (21) give

$$C_{11}(T) = c_1 + \frac{2|\Delta_{20}|^2}{g_2}\left\{\frac{(2\zeta_1+\gamma_2+\lambda_1)^2}{K_{21}(\Delta_{20})} + (\zeta_1+\gamma_2)^2\right\}. \quad (54)$$

$C_{22}(T)$ is also affected by the SC, which is derived by use of $F(\delta\Delta_1,\Delta_{20};u_{10},\delta u_2)$ known from Eq. (21). The gap equation for $\delta\Delta_1$ under $\delta u_2\neq 0$ becomes

$$\frac{g_2}{g_1}\delta\Delta_1 = K_{22}(\Delta_{20})\{\delta\Delta_1 + \Delta_{20}(\zeta_2+\eta_2)\delta u_2\} + \Delta_{20}\zeta_2\delta u_2, \quad (55)$$

where we have defined $K_{22}(\Delta_{20})$ by

$$K_{22}(\Delta_{20}) = g_2 D \int_0^{\epsilon_c} d\xi \int_0^{2\pi} \frac{d\theta}{2\pi} \times \frac{1}{[E_2(\xi,\theta)]^2} \left\{ \frac{\xi^2}{E_2(\xi,\theta)} \tanh\left(\frac{\beta}{2} E_2(\xi,\theta)\right) + |\Delta_{20}|^2 \frac{\beta}{2} \cos^2 2\theta \, \mathrm{sech}^2\left(\frac{\beta}{2} E_2(\xi,\theta)\right) \right\} \simeq 2 + K_{21}. \tag{56}$$

The last relation in the above equation can be confirmed by making numerical integrations in Eqs. (53) and (56). Equations (55) and (38) give

$$\chi_{22} = -\left\{ \frac{g_1\zeta_2 + g_2(\zeta_2+\eta_2)}{g_1 K_{22}(\Delta_{20}) - g_2} + (\zeta_2+\eta_2) \right\}. \tag{57}$$

Expanding $F(\delta\Delta_1, \Delta_{20}; u_{10}, \delta u_2)$ with $u_{10} \simeq 0$ and Eqs. (38) and (57) in powers of δu_2, we obtain

$$C_{22}(T) = c_2 + \frac{2|\Delta_{20}|^2}{g_1 g_2} \left\{ \frac{[g_2(\zeta_2+\eta_2) + g_1\zeta_2]^2}{g_1 K_{22}(\Delta_{20}) - g_2} + g_2(\zeta_2+\eta_2)^2 \right\}. \tag{58}$$

Since δu_6 does not couple linearly to $|\Delta_{20}|\delta|\Delta_j|$ ($j=1$, 2, and 6), the equilibrium SC state cannot be changed by δu_6 through the electron interaction. Nevertheless, $C_{66}(T)$ is also affected by the SC. This is because δu_6 changes the band electron energies to distort the Fermi surface and this distorted Fermi surface becomes favorable for the anisotropic SC state. As a result, $C_{66}(T)$ is shown to be $\{c_6 - (2\zeta_6^2|\Delta_{20}|^2/g_2)\}$.

C. Elastic constants in the d_{xy}-wave SC state

The d_{xy}-wave SC state affects $C_{11}(T)$ and $C_{66}(T)$. The expressions of $C_{11}(T)$ and $C_{66}(T)$ are obtained by replacing all subscripts 2 of quantities in Eqs. (54) and (58) with the subscripts 6. Moreover, $C_{22}(T)$ also is affected by the SC for a similar reason to that described about $C_{66}(T)$ in Sec. V B.

D. Elastic constants $C_{33}(T)$ and $C_{13}(T)$ in the all wave states of SC

The distortion u_3 couples to the SC in the same way as u_1, so that the properties of $C_{11}(T)$ hold also for $C_{33}(T)$ except for different coupling constants. The expressions of $C_{33}(T)$ are obtained by making the replacements (27) in the expressions of $C_{11}(T)$ given by Eqs. (45) and (54). The elastic constant $C_{13}(T)$ also is affected by the SC, whose expression is omitted here.

VI. NUMERICAL CALCULATIONS OF THE LATTICE ANOMALY AND ITS CHARACTERISTICS

In order to see characteristics of the lattice anomaly, we calculate numerically the distortions and the elastic constants on the basis of the results obtained in the preceding sections.

Figures 1 and 2 show, respectively, the calculated temperature dependence of u_{10} in the s-wave SC state and that in the $d_{x^2-y^2}$-wave SC state for some sets of chosen values of the parameters. As seen from both the figures, the temperature dependence of u_{10} exhibits similar characteristics irrespective of the SC state. This holds also for the equilibrium distortion u_{30}. The sign of distortion depends on some microscopic parameters. This is seen from the expressions of u_{10}'s at absolute zero, which are found from Eqs. (28) and (32) to be

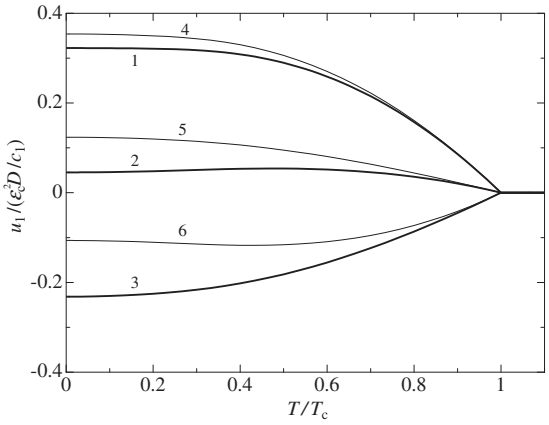

FIG. 1. Temperature dependence of the distortion u_{10} in the s-wave SC state. The parameter values $g_1 D = 0.41$ and $\epsilon_c/k_B = 300$ K have been assumed as an example, which give $T_c = 30$ K. The bold lines 1, 2, and 3 have been calculated for $\lambda_1 = 1$, -2, and -5, respectively, under common $(2\zeta_1 + \gamma_1) = 3$. The thin lines 4, 5, and 6 have been calculated for $(2\zeta_1 + \gamma_1) = 1$, -2, and -5, respectively, under common $\lambda_1 = 3$.

$$u_{10} \simeq \frac{|\Delta_{10}|^2}{c_1 g_1} \left\{ (2\zeta_1 + \gamma_1) + \lambda_1 g_1 D \left(\frac{1}{2} + \ln \frac{2\epsilon_c}{|\Delta_{10}|} \right) \right\}, \tag{59}$$

in the s-wave SC state, and

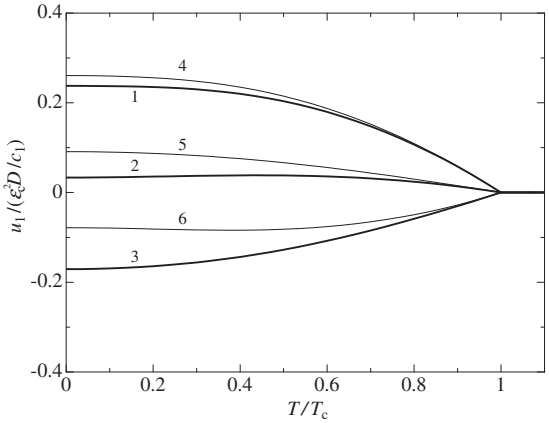

FIG. 2. Temperature dependence of the distortion u_{10} in the $d_{x^2-y^2}$-wave SC state. The parameter values $g_2 D = 0.82$ and $\epsilon_c/k_B = 300$ K have been assumed as an example, which give $T_c = 30$ K. The bold lines 1, 2, and 3 have been calculated for $\lambda_1 = 1$, -2, and -5, respectively, under common $(2\zeta_1 + \gamma_2) = 3$. The thin lines 4, 5, and 6 have been calculated for $(2\zeta_1 + \gamma_2) = 1$, -2, and -5, respectively, under common $\lambda_1 = 3$.

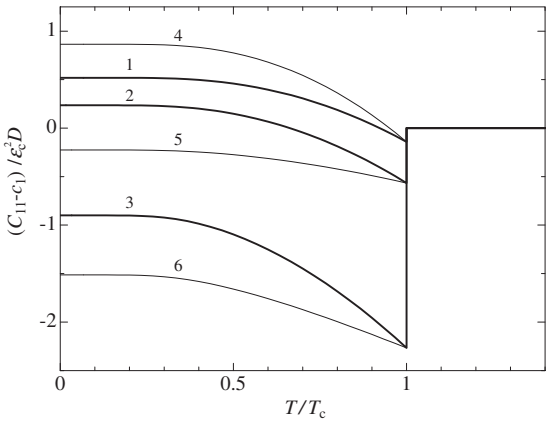

FIG. 3. Temperature dependence of the elastic constant $C_{11}(T)$ in the s-wave SC state. The assumed parameter values of $g_1 D$ and ϵ_c/k_B are the same as in Fig. 1. The bold lines 1, 2, and 3 have been calculated for $(\zeta_1+\lambda_1)=-2.5$, -1, and 0, respectively, under common $(\zeta_1+\gamma_1)=2$. The thin lines 4, 5, and 6 have been calculated for $(\zeta_1+\gamma_1)=-2.5$, -1, and 0, respectively, under common $(\zeta_1+\lambda_1)=2$.

$$u_{10} \simeq \frac{|\Delta_{20}|^2}{c_1 g_2}\left\{(2\zeta_1+\gamma_2)+\lambda_1\left(1+\frac{1}{4}g_2 D\right)\right\}, \qquad (60)$$

in the $d_{x^2-y^2}$-wave SC state. In addition, we see in the figures that the thermal expansion coefficients α, which are the T derivatives of u_{10} and u_{30}, always become zero at absolute zero and exhibit discontinuous changes at T_c. The sign of α can vary with temperature in some cases of the parameter values.

Figure 3 shows the calculated temperature dependence of $C_{11}(T)$ in the s-wave SC state for some sets of the parameter values chosen. As seen from this figure, $C_{11}(T)$ becomes soft just below T_c with a discontinuous change at T_c. This discontinuity at T_c arises from the fact that $K_{11}(\Delta_{10})$ in Eq. (45) becomes zero at T_c as shown in Fig. 4, or in other words, χ_{11}

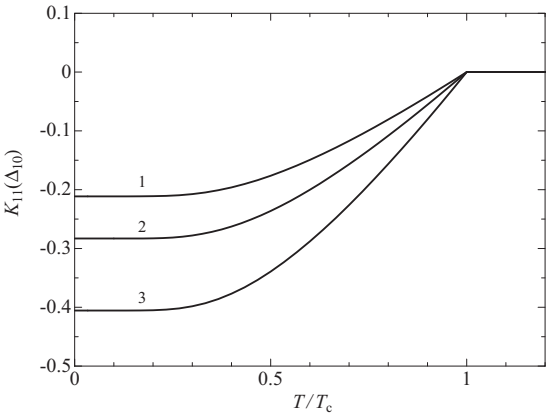

FIG. 4. Temperature dependence of $K_{11}(\Delta_{10})$ for different values of $g_1 D$. $\epsilon_c/k_B=300$ K has been assumed as an example. The lines 1, 2, and 3 have been calculated for $g_1 D=0.21$, 0.29, and 0.41, respectively. The sets of these parameter values give $T_c=3$, 10, and 30 K in the cases of the lines 1, 2, and 3, respectively.

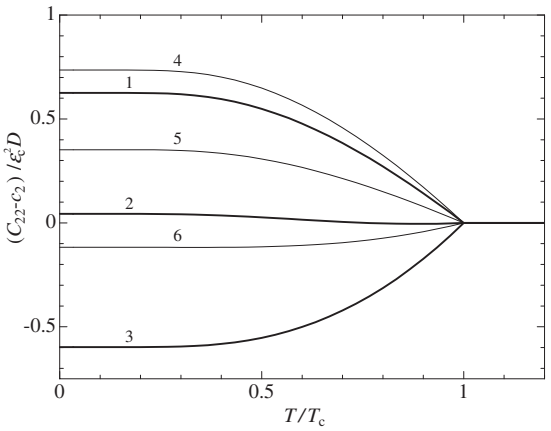

FIG. 5. Temperature dependence of the elastic constant $C_{22}(T)$ in the s-wave SC state. The same parameter values of $g_1 D$ and ϵ_c/k_B as in Fig. 1, and $g_2/g_1=-1.9$ have been assumed. The bold lines 1, 2, and 3 have been calculated for $\eta_1=1.5$, 0.5, and -0.5, respectively, under common $\zeta_2=-2.5$. The thin lines 4, 5, and 6 have been calculated for $\zeta_2=-2$, -1, and 0, respectively, under common $\eta_1=2$.

diverges at T_c. Equations (45) and (44) give the change at T_c in the case of the s-wave SC state as

$$C_{11}(T_c-0)-c_1=-2\left(\frac{k_B T_c}{g_1}\right)^2\frac{(2\zeta_1+\gamma_1+\lambda_1)^2}{D\kappa(\epsilon_c/k_B T_c)}, \qquad (61)$$

where $\kappa(y)$ has been defined by

$$\kappa(y)=\int_0^y \frac{1}{x^2}\left\{\frac{1}{x}\tanh\frac{x}{2}-\frac{1}{2}\,\mathrm{sech}^2\frac{x}{2}\right\}dx. \qquad (62)$$

The softening in $C_{11}(T)$ recovers partially with lowering temperature. When $\zeta_1=\lambda_1=0$ while $\gamma_1\neq 0$, or when $\gamma_1=0$ while $\zeta_1\neq 0$ and/or $\lambda_1\neq 0$, its recovery is not sufficient to cause a hardening at low temperatures, as seen from Eq. (45). When, however, $|2\zeta_1+\gamma_1+\lambda_1|$ is small but $|\zeta_1+\gamma_1|$ is large, $C_{11}(T)$ changes to show hardenings at low temperatures. These prove that the change of $C_{11}(T)$ from the softening to the hardening results from an interference of changes in the electron band and in the electron interaction. Figure 5 shows, on the other hand, the calculated temperature dependence of $C_{22}(T)$ in the s-wave SC state for some sets of parameter values. Usually, $C_{22}(T)$ becomes soft continuously below T_c. When $|(\zeta_2+\eta_1)+(g_2/g_1)\zeta_2|$ is sufficiently smaller (larger) than $|\zeta_2+\eta_1|$ for positive (negative) values of g_2, $C_{22}(T)$ changes to show hardenings at low temperatures, or, in the whole temperature region below T_c. In order to see a strong (g_2/g_1)-dependence of $C_{22}(T)$, we give in Fig. 6 the calculated temperature dependence of $C_{22}(T)$ in the same wave SC state for some different values of g_2/g_1. As seen from this figure, its softening is enhanced when $g_2(<2g_1)$ approaches to g_1. This is because the s-wave SC state can induce more easily the $d_{x^2-y^2}$-wave SC state through the cross term of the different SOP's, when the latent T_c of the $d_{x^2-y^2}$-wave SC state is closer to the real T_c of the s-wave SC state.

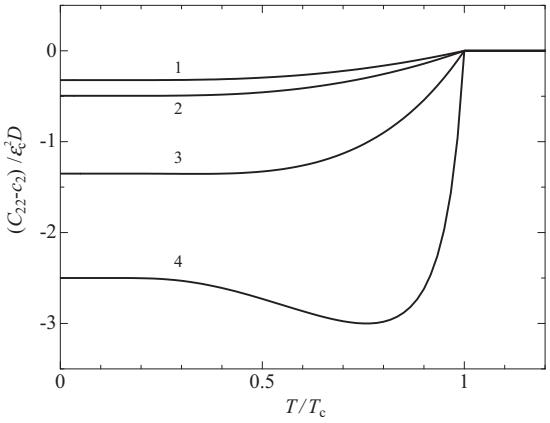

FIG. 6. Temperature dependence of the elastic constant $C_{22}(T)$ for different values of g_2/g_1 in the s-wave SC state. The same parameter values of $g_1 D$ and ϵ_c/k_B as in Fig. 1, $\zeta_2=1.0$ and $\eta_1=1.0$ have been assumed. The lines 1, 2, 3, and 4 have been calculated for $g_2/g_1=-1.9$, -1.0 1.0, and 1.9, respectively.

Similar calculations to those for the s-wave SC state can be made also for the $d_{x^2-y^2}$-wave SC state. Figure 7 shows the calculated temperature dependence of $C_{11}(T)$ in the $d_{x^2-y^2}$-wave SC state for some sets of parameter values. Also in this SC state, $C_{11}(T)$ becomes soft below T_c with a discontinuous change at T_c. This behavior is ascribed to the fact that $K_{21}(\Delta_{20})$ becomes zero at T_c, whose temperature dependence is shown in Fig. 8. Equations (54) and (53) give the discontinuous change at T_c in the $d_{x^2-y^2}$-wave SC state as

$$C_{11}(T_c-0)-c_1=-\frac{16}{3}\left(\frac{k_B T_c}{g_2}\right)^2\frac{(2\zeta_1+\gamma_2+\lambda_1)^2}{D\kappa(\epsilon_c/k_B T_c)}. \quad (63)$$

The softenings of $C_{11}(T)$ change to hardenings at low temperatures for $|2\zeta_1+\gamma_2+\lambda_1|$ sufficiently smaller than $|\zeta_1+\gamma_2|$.

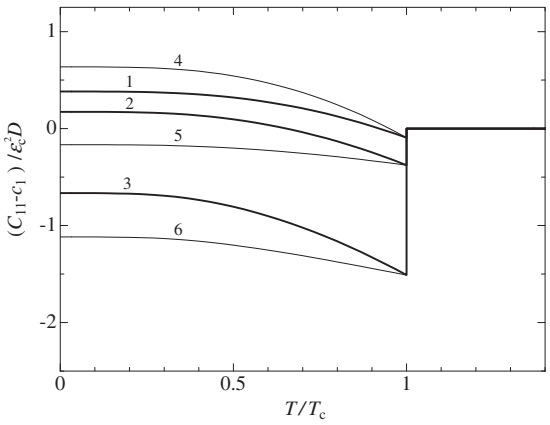

FIG. 7. Temperature dependence of the elastic constant $C_{11}(T)$ in the $d_{x^2-y^2}$-wave SC state. The assumed parameter values of $g_2 D$ and ϵ_c/k_B are the same as in Fig. 2. The bold lines 1, 2, and 3 have been calculated for $(\zeta_1+\lambda_1)=-2.5$, -1, and 0, respectively, under common $(\zeta_1+\gamma_2)=2$. The thin lines 4, 5, and 6 have been calculated for $(\zeta_1+\gamma_2)=-2.5$, -1, and 0, respectively, under common $(\zeta_1+\lambda_1)=2$.

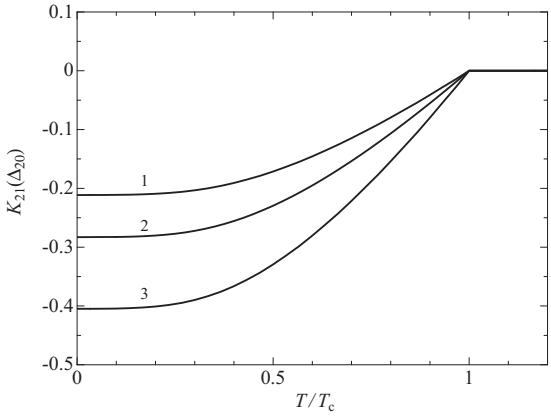

FIG. 8. Temperature dependence of $K_{21}(\Delta_{20})$ for different values of $g_2 D$. $\epsilon_c/k_B=300$ K has been assumed as an example. The lines 1, 2, and 3 have been calculated for $g_2 D=0.42$, 0.57, and 0.82, respectively. The sets of these parameter values give $T_c=3$, 10, and 30 K in the cases of the lines 1, 2, and 3, respectively. It is noticed that the temperature dependence of $K_{21}(\Delta_{20})$ is only slightly different from that of $K_{11}(\Delta_{10})$ shown in Fig. 4.

Figure 9 shows the calculated temperature dependence of $C_{22}(T)$ in the $d_{x^2-y^2}$-wave SC state. Again, $C_{22}(T)$ becomes soft continuously below T_c. The softenings of $C_{22}(T)$ change to hardenings at low temperatures or in the whole temperature region below T_c, when $|(\zeta_2+\eta_2)+(g_1/g_2)\zeta_2|$ is sufficiently smaller (larger) than $|\zeta_2+\eta_2|$ for positive (negative) values of g_1. As in the s-wave SC state, the temperature dependence of $C_{22}(T)$ in the $d_{x^2-y^2}$-wave SC state depends strongly on g_1/g_2, which is seen in Fig. 10. In the latter SC state, the $d_{x^2-y^2}$-wave SC state induces the s-wave SC state in the presence of the distortion u_2.

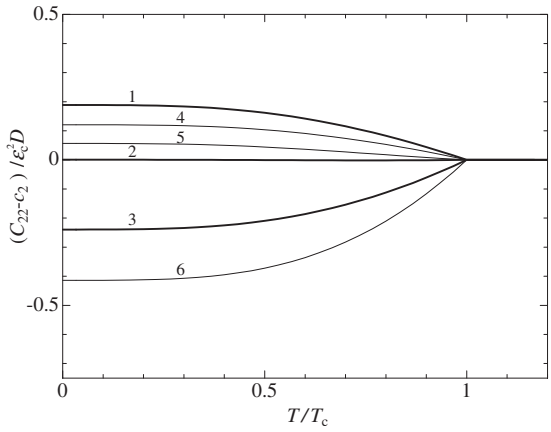

FIG. 9. Temperature dependence of the elastic constant $C_{22}(T)$ in the $d_{x^2-y^2}$-wave SC state. The same parameter values of $g_2 D$ and ϵ_c/k_B as in Fig. 2, and $g_1/g_2=-0.47$ have been assumed. The bold lines 1, 2, and 3 have been calculated for $\eta_2=2.5$, 2, and 1.5, respectively, under common $\zeta_2=-2.5$. The thin lines 4, 5, and 6 have been calculated for $\zeta_2=-2$, -1, and 0, respectively, under common $\eta_2=2$.

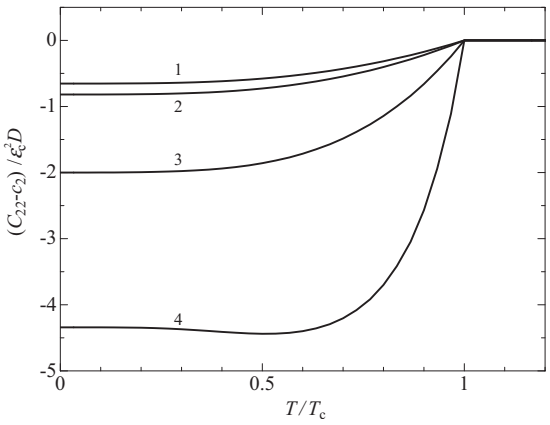

FIG. 10. Temperate dependence of the elastic constant $C_{22}(T)$ for different values of g_1/g_2 in the $d_{x^2-y^2}$-wave SC state. The same parameter values of $g_2 D$ and ϵ_c/k_B as in Fig. 2, $\zeta_2=1.0$ and $\eta_2=1.0$ have been assumed. The lines 1, 2, 3, and 4 have been calculated for $g_1/g_2=-0.45$, -0.25, 0.25, and 0.45, respectively.

VII. COMPARISON BETWEEN THE THEORY AND EXPERIMENTS

The results of the present theory are here compared with those of experiments performed on high-T_c cupurates. The theoretical analyses are done by assuming the $d_{x^2-y^2}$-wave SC state in these compounds.

$Bi_2Sr_2CaCu_2O_8$ has the crystal structure with the lattice constants $a \simeq b$ and $c \gg a, b$, and exhibits the SC with $T_c=90$ K. The prominent volume change caused by SC was observed on this compound by Asahi *et al.*[13] The measured temperature dependence of the volume change $v_S - v_N$ is shown in Fig. 11, where v_S and v_N are, respectively, the volumes of a unit cell in the superconducting and normal phases. If the small orthorhombicity of this compound is neglected, u_{10} obtained in the preceding sections can be compared with $v_S - v_N$ measured. Under the given T_c, we have

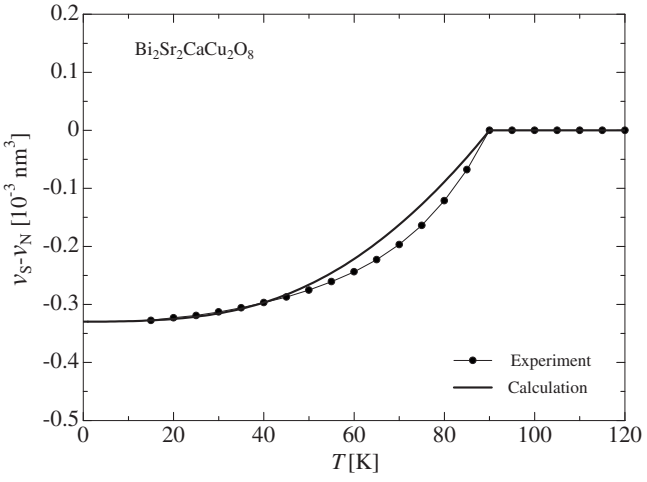

FIG. 11. Comparison between the theoretical and experimental temperature dependences of the volume change $v_S - v_N$ in $Bi_2Sr_2CaCu_2O_8$. The experimental data were taken from Ref. 13. For the parameter values used, see the text.

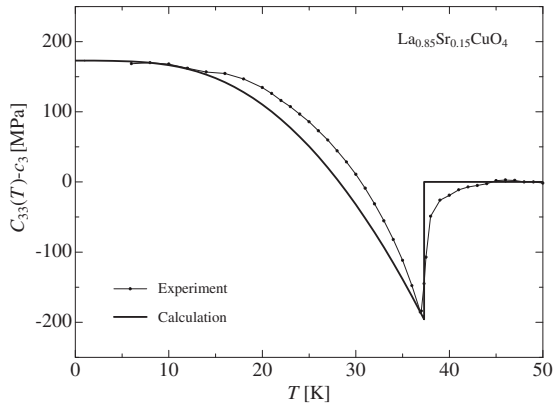

FIG. 12. Comparison between the theoretical and experimental temperature dependences of the elastic constant $C_{33}(T)-c_3$ in $La_{0.85}Sr_{0.15}CuO_4$. The experimental data were taken from Ref. 14. For the parameter values used, see the text.

the three parameters, ϵ_c, $D(2\zeta_1+\gamma_2)/c_1$, and $D\lambda_1/c_1$, whose values are chosen so as to fit the calculated curve to the measured one. The calculated u_{10} was found to depend on ϵ_c so weakly that the fitting could not determine uniquely the value of ϵ_c. When $\epsilon_c/k_B=300$ K was employed, the fitting gave

$$D(2\zeta_1 + \gamma_2)/c_1 = -8.3 \times 10^{-3}\, k_B^{-2}\, \mathrm{K}^{-2}, \tag{64}$$

$$D\lambda_1/c_1 = -1.7 \times 10^{-3}\, k_B^{-2}\, \mathrm{K}^{-2}. \tag{65}$$

The calculated curve by use of these parameter values also is shown in Fig. 11. When other values of ϵ_c/k_B, 100 K and 500 K, were employed, $D(2\zeta_1+\gamma_2)/c_1$ and $D\lambda_1/c_1$ had values near those given by Eqs. (64) and (65) and the curves were only slightly changed from the one in Fig. 11. As seen in Fig. 11, the agreement between the calculated and measured curves is fairly good. The deviation of the calculated curve from the measured one results partly from a difficulty in obtaining experimental values of v_N below T_c.[13]

Nyhus *et al.*,[14] on the other hand, measured the elastic constant $C_{33}(T)$ of $La_{0.85}Sr_{0.15}CuO_4$ with $T_c=37.3$ K. The temperature dependence of $C_{33}(T)-c_3$ measured[14] is shown in Fig. 12, c_3 being the elastic constant in the normal phase. In the calculation of $C_{33}(T)-c_3$, we have the three parameters, ϵ_c, $D(\zeta_1'+\gamma_2')^2$, and $D(2\zeta_1'+\gamma_2'+\lambda_1')^2$. When $\epsilon_c/k_B=300$ K was employed, the fitting of the calculated curve to the measured one gave

$$D(\zeta_1' + \gamma_2')^2 = 2.2 \times 10^{-2}\, k_B^{-2}\, \mathrm{K}^{-2}\, \mathrm{Mp}, \tag{66}$$

$$D(2\zeta_1' + \gamma_2' + \lambda_1')^2 = 4.4 \times 10^{-3}\, k_B^{-2}\, \mathrm{K}^{-2}\, \mathrm{Mp}. \tag{67}$$

The curve calculated by use of these parameter values also is shown in Fig. 12. As in the case of the calculation of u_{10}, other values of ϵ_c/k_B gave parameter values near those given by Eqs. (66) and (67) and curves very similar to the one in Fig. 12. As seen in Fig. 12, the present theory reproduced the observed discontinuous change of $C_{33}(T)-c_3$ at T_c and its hardenings observed at low temperatures. However, the agreement between the calculated and measured temperature

dependences of $C_{33}(T)-c_3$ is not quite sufficient. This result is again ascribed partly to the difficulty in obtaining experimental values of c_3 below T_c.[14]

VIII. CONCLUDING REMARKS AND DISCUSSION

In order to analyze the lattice anomaly accompanied by the appearance of superconductivities (SC), we have started with the BCS Hamiltonian, which is constructed for the system consisting of SC's and distortions u. The microscopic parameters have been introduced into the Hamiltonian so that itself may satisfy the crystal symmetry. By use of this Hamiltonian, we have derived a free energy as a function of the SC order parameters (SOP) and u's. The free energy thus obtained makes it possible to clarify how the distortions and the elastic change originate from the SC state. In the present analysis, we have taken into account the linear dependences of the microscopic parameters (7) and the electronic density of states $\tilde{D}$ in Eq. (22) on u's. In general, their quadratic dependences on u's also can contribute to the elastic changes.[11] In the usual SC compounds such as those with no strong electron-lattice coupling, we expect that the linear coupling terms play a major role in the lattice anomaly. Within this linear-coupling theory, we have obtained the same mode of distortion and the similar elastic properties in both the s-wave and d-wave SC states. Moreover, we have found that not only the softenings but also the hardenings of the lattice are possible in those SC states.

The results obtained in our theory are compared with those of the GL theory[9] and of Testardi's theory,[10] which were developed for the s-wave SC state. In the GL theory, the free energy of the system is expanded directly in powers of the SOP's and u's near T_c. As seen in Appendix C, a simplified GL theory gives the distortion $u \propto (T-T_c)$ near T_c and therefore gives a thermal expansion coefficient α independent of T. Testardi, on the other hand, considered the free energy proportional to $\{1-(T/T_c)^2\}^2$, which is assumed to hold at all temperatures below T_c.[10] This theory gave a temperature-dependent α, which has a nonzero slope at T_c but the zero slope at absolute zero, just as in the present theory. Such a temperature dependence of α agrees qualitatively with α's which were observed not only for $Bi_2Sr_2CaCu_2O_8$,[13] but also for $YBa_2Cu_3O_{7-\delta}$ (Ref. 15) and $HgBa_2Ca_2Cu_3O_{3+\delta}$.[16] However, the temperature dependence of the free energy used in Ref. 10 is different from that predicted by the BCS theory, even near T_c.

The elastic constants also were studied by use of the GL and Testardi's theories.[9,10] As shown in Appendix C, the GL theory gives an elastic modulus, which exhibits a discontinuous change at T_c but is constant below T_c. Testardi's theory gave the temperature-dependent elastic moduli of the longitudinal mode with a discontinuous change at T_c and of the shear mode with a continuous change. The global feature of these elastic moduli is somewhat analogous to that of ours, although not only the temperature dependence but also the microscopic quantities responsible for the elastic anomalies are different between the theories.

A pioneering work of the experiment on the elastic constants of the SC phase was reported by Alers and Waldorf.[17] They observed the clear change of the longitudinal and shear moduli by the conventional SC states of some $3d$ transition monatomic metals. Unfortunately, no detailed analysis of this elasticity change has been done from a theoretical point of view. The most conspicuous effect of SC on the elastic constants was found in some high-T_c compounds of A15-type such as V_3Si and Nb_3Sn.[18] In these compounds, both the SC and martensitic transitions occur, which interfere with each other. This interference originates the observed drastic change of elasticity in these compounds.[19,20] This phenomenon is not the subject of the present theory. More recently, extensive and detailed observations of elasticity on the cuprate compound system $La_{2-x}Sr_xCuO_4$ have been reported by Nohara *et al.*[21,22] They found the clear changes of elasticity by SC, which accompany the discontinuous or continuous changes at T_c as predicted. It was also found that the elastic behavior strongly depends on x and is very sensitive to external magnetic fields. Moreover, some elastic modes exhibited hardenings at low temperatures. This hardening was observed also for other high-T_c compounds.[23–25] Evidently, the elastic anomaly becomes more splendid in $La_{2-x}Sr_xCuO_4$ with a higher T_c. The whole behavior of elasticity observed in a wide region of x is too complicated to be systematically analyzed. Nevertheless, a thorough understanding of the lattice anomaly of the high-T_c compounds surely helps us to clarify the role of the electron-lattice interaction in the high-T_c of cuprates. Further experimental and theoretical studies on the interrelation between SC and lattice will be desirable.

APPENDIX A: NORMAL MODES OF ELASTIC DISTORTIONS IN CRYSTALS WITH D_{4h} SYMMETRY

When a crystal with the D_{4h} symmetry is subjected to the strains $e_{ii'}$ which can couple to the SOP's we are interested in, the elastic energy is expressed by

$$H_{\mathrm{ela}} = \frac{1}{2}V\{c_{11}(e_{xx}^2+e_{yy}^2)+c_{33}e_{zz}^2+c_{66}e_{xy}^2+2c_{12}e_{xx}e_{yy} + 2c_{13}(e_{xx}+e_{yy})e_{zz}\}, \tag{A1}$$

where c's are the elastic stiffness constants in the normal state. Here, we introduce the normal modes of distortion:

$$u_1 = \frac{1}{\sqrt{2+\nu^2}}\{e_{xx}+e_{yy}+\nu e_{zz}\}, \tag{A2}$$

$$u_2 = \frac{1}{\sqrt{2}}(e_{xx}-e_{yy}), \tag{A3}$$

$$u_3 = \frac{1}{\sqrt{2(2+\nu^2)}}\{-\nu(e_{xx}+e_{yy})+2e_{zz}\}, \tag{A4}$$

$$u_6 = e_{xy}, \tag{A5}$$

where

$$\nu = \frac{4c_{13}}{c'_{12} + \sqrt{(c'_{12})^2 + 8c_{13}^2}}, \quad c'_{12} = c_{11} + c_{12} - c_{33}. \tag{A6}$$

In terms of these normal modes, Eq. (A1) is shown to be written as Eq. (3), where c's have been defined by

$$c_1 = c_{11} + c_{12} + \nu c_{13}, \qquad c_2 = c_{11} - c_{12},$$

$$c_3 = c_{33} - \nu c_{13}, \quad \text{and } c_6 = c_{66}. \tag{A7}$$

APPENDIX B: EFFECT OF THE CHANGE IN THE CUT ENERGY BY THE DISTORTION

The cut energy $\tilde{\epsilon}_c$ in Eq. (21) is also affected by u_1 and u_3 up to the linear order of u's. Here, the contribution of this effect to the free energy per unit volume, $\tilde{E}'_s$, is derived. From Eq. (21), we see that $\tilde{E}'_s$ can be approximated as follows:

$$\tilde{E}'_s = -2D\int_{\epsilon_c}^{\tilde{\epsilon}_c} d\xi \int_0^{2\pi} \frac{d\theta}{2\pi}\frac{2}{\beta} \ln\left[\frac{\cosh(\beta E(\xi,\theta)/2)}{\cosh(\beta\xi/2)}\right]$$

$$\simeq -2D(\tilde{\epsilon}_c - \epsilon_c)\int_0^{2\pi}\frac{d\theta}{2\pi}\{E(\epsilon_c,\theta) - \epsilon_c\}$$

$$\simeq -\frac{1}{2}D\tau_1(2|\Delta_1|^2 + |\Delta_2|^2)u_1, \tag{B1}$$

for $\epsilon_c \gg |\Delta_1|$ and $|\Delta_2|$. In Eq. (B1), we have already expanded $\tilde{\epsilon}_c$ as

$$\tilde{\epsilon}_c = \epsilon_c(1 + \tau_1 u_1), \tag{B2}$$

where τ_1 is an expansion coefficient and u_3 is neglected. Comparison of Eq. (B1) with Eq. (15) suggests that $\tilde{E}'_s$ can be neglected when $g_1 D\tau_1$ and $g_2 D\tau_1/2$ are sufficiently small compared with 1.

APPENDIX C: A SIMPLIFIED GL THEORY OF THE LATTICE ANOMALY

In order to compare the results of the present theory with those of the GL theory, we give here a simplified GL theory of the lattice anomaly in a SC state. The SC state tested here has one component of SOP, Δ, which couples to a distortion u. Then, the GL free energy is assumed to be expressed by

$$F = V\left\{a\left(\frac{T}{T_c} - 1\right)|\Delta|^2 + \frac{1}{2}b|\Delta|^4 + \frac{1}{2}cu^2 - d|\Delta|^2 u\right\}, \tag{C1}$$

where a and b are positive constants, c is an elastic constant, and d is a coupling constant with any sign. Minimization of F with respect to $|\Delta|$ and u gives the equilibrium quantities $|\Delta_0|$ and u_0, which are obtained to be

$$|\Delta_0|^2 = \left(\frac{ca}{cb - d^2}\right)\left(1 - \frac{T}{T_c}\right), \tag{C2}$$

$$u_0 = \left(\frac{da}{cb - d^2}\right)\left(1 - \frac{T}{T_c}\right). \tag{C3}$$

Equation (C3) gives further a thermal expansion coefficient,

$$\alpha = \frac{\partial u_0}{\partial T} = -\frac{da}{(cb - d^2)T_c}, \tag{C4}$$

which is constant below T_c.

When a further distortion δu from u_0 is introduced, the SOP is changed as $|\Delta| = |\Delta_0| + \delta|\Delta|$. After that, the free energy is increased by

$$F - F_0 = V\left\{\left[a\left(\frac{T}{T_c} - 1\right) + 3b|\Delta_0|^2 - du_0\right](\delta|\Delta|)^2 - 2d|\Delta_0|\delta|\Delta|\delta u + \frac{1}{2}c(\delta u)^2\right\}. \tag{C5}$$

Another equilibrium condition of $\delta|\Delta|$ under δu gives

$$\delta|\Delta| = (d/2b|\Delta_0|)\delta u. \tag{C6}$$

Substituting Eq. (C6) into Eq. (C5), we arrive at the increase of the free energy due to δu and an elastic constant in the SC phase, C, as

$$F - F_0 = \frac{1}{2}C(\delta u)^2, \quad C = c - \frac{d^2}{b}. \tag{C7}$$

The above equations prove that the GL theory gives the elastic constant which becomes soft by a quantity independent of T below T_c.

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