Anomalies of the elastic moduli and their manifestation in the properties of high-temperature superconductors

V. M. Zverev, V. P. Silin, and S. A. Uryupin

P.N. Lebedev Physics Institute, Academy of Sciences of the USSR, Moscow
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An interpretation is given of the experimentally established change in the velocity of sound on transition to the superconducting state. This interpretation is based on a thermodynamic analysis of the bulk modulus. Within the framework of this interpretation it is shown that the change in the sound velocity can be attributed approximately to a corresponding change in the Debye temperature, proportional to the square of the superconducting energy gap, which leads to a similar dependence of the phonon free energy. It is demonstrated that an allowance for the change in the free energy of phonons in the superconducting state accounts for the observed experimental deviations of the ratio of the energy gap to the critical temperature, of the specific heat jump, and of the isotopic effect from the predictions based on the BCS theory. The changes in the parameters of the Ginzburg–Landau phenomenological theory due to the influence of the superconductivity on the free energy of phonons are determined. Such changes lead, in particular, to a modification of the thermodynamic critical magnetic field and of the depth of penetration of an electromagnetic field into a superconductor.

Experimental investigations of high-temperature superconductors have revealed considerable changes in the temperature dependence of the velocity of sound v_s on transition to the superconducting state in $YBa_2Cu_3O_7$ (Refs. 1–6) and in $La_{2-x}Sr_xCuO_4$ ($x \geqslant 0.15$).[7] In the case of $La_{2-x}Sr_xCuO_4$ a considerable abrupt reduction in the velocity of sound occurs at the superconducting transition temperature T_c and this is followed by an increase in the velocity of sound as a result of cooling. The behavior of $YBa_2Cu_3O_7$ is somewhat different. In fact, an abrupt change in the velocity of sound at T_c is reported only in Ref. 6 and the magnitude of this change is small compared with an anomalously large increase in the velocity of sound during the subsequent cooling reported by many authors (see, for example, Refs. 1, 3, 5, and 8). One should mention also the result of Ref. 1 indicating that an increase in the correction to the velocity of sound below T_c is proportional to Δ^2, i.e., it is proportional to the square of the width of the superconducting energy gap. The dependence of the velocity of sound on Δ is predicted by the theory of Ref. 9.

We shall present those consequences that follow from the experimentally established dependence of the velocity of sound on the superconducting gap and which may be regarded as accounting for the nature of the deviations from the BCS theory exhibited by the experimental data on the isotropic effect, on the jump in the specific heat ΔC at the superconducting transition, and on the ratio of the width of the superconducting gap at zero temperature Δ_0 to the superconducting transition temperature.

Using the simplest model in which the relative change in the velocity of longitudinal sound $\Delta v_s/v_s$ is governed by the relative change of the bulk modulus $\Delta K/2K_0$, where K_0 is the value of the modulus in the normal state, we shall give (in Sec. 1 of the present paper) simple expressions derived from the electron free energy and describing the dependences of the bulk modulus on the superconducting gap. We shall use these expressions to interpret the experimental temperature dependences of the velocity of sound reported for LaSrCuO and YBaCuO. The large value of the superconducting gap is responsible for the anomalously large change in the velocity of sound exhibited by high-temperature superconductors. After separation of the contribution to the bulk modulus made by the jump at the phase transition point, we can then account for the temperature dependence of the velocity of sound simply using the following dependence of the bulk modulus $K = K_0 + K'\Delta^2$, where $K' = (6–10)\times 10^{36}$ erg$^{-1}\cdot$cm^{-3} for LaSrCuO and $K' = (2–33)\times 10^{36}$ erg$^{-1}\cdot$cm^{-3} for YBaCuO.

In our approach, based on the experimental results, we shall regard the Debye temperature as dependent on the superconducting gap in accordance with the law $\Theta(\Delta) = \Theta + \Theta'\Delta^2$. Such a dependence gives rise to a dependence of the phonon free energy on Δ^2. It is this dependence that accounts for the deviation of the result of our approach from the usual BCS theory results. We must mention straight away why such a change in the Debye temperature can give rise to significant effects. We recall first of all that the energy per electron representing the change in the superconducting state (per electron) relative to the energy of the normal state amounts to $\sim\Delta^2/\varepsilon_F$, where Δ is the energy gap of electrons in the superconducting state and ε_F is the Fermi energy. The phonon energy, per degree of freedom, is of the order of $\varkappa\Theta$, where $\varkappa$ is the Boltzmann constant. The change in the phonon energy, governed similarly by the dependence of the velocity of sound on Δ^2, can be estimated to the nearest order of magnitude from $\varkappa\Theta\Delta^2 K'/K_0$. Therefore, the parameter that determines the influence of the phonon energy dependence on the superconducting gap is $(K'/K_0)\varepsilon_F\varkappa\Theta N_p/N_e$, where N_e is the number of electrons and N_p is the number of phonon degrees of freedom. In estimates of the effects associated with thermal phonons we can use the power-law approximations $N_p(T/\Theta)^p$ where, for example, in the Debye model we have $1 \leqslant p \leqslant 4$. Such estimates are rough, but they give us some idea of the role of the anomalies of the elastic moduli in the problem of the properties of high-temperature superconductors.

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In Sec. 2 we shall show how the influence of the superconductivity on the phonon free energy modifies the equation describing the temperature dependence of the superconducting gap, how it modifies the temperature of the superconducting transition and the width of the energy gap at zero temperature, and how it alters the expression describing the jump in the specific heat at the superconducting transition and the expressions describing the isotopic effect, the thermodynamic critical magnetic field, and the depth of penetration of an electromagnetic field into a superconductor. We shall show that in the case of superconducting LaSrCuO the freezeout of phonons means that only zeroth phonon fluctuations are important. On the other hand, in the case of superconducting $YBa_2Cu_3O_7$ the relatively high temperature of the superconducting transition means that thermal phonons are also manifested.

1. The change in the velocity of sound on transition to the superconducting state is well known from the theory of superconductivity.[9] This change can easily be demonstrated using the following expression for the electron free energy:[10]

$$F_e=\nu V\int_0^{\varkappa\theta} d\varepsilon\left\{\frac{\Delta^2}{2\varepsilon}\operatorname{th}\frac{\varepsilon}{2\varkappa T_0}-\varkappa T\ln\frac{1+\operatorname{ch}((\varepsilon^2+\Delta^2)^{1/2}/\varkappa T)}{1+\operatorname{ch}(\varepsilon/\varkappa T)}\right\}, \tag{1}$$

where V is the volume; ν is the density of the electron energy states at the Fermi level; T is the absolute temperature; T_0 is the superconducting transition temperature predicted by a theory that does not allow for the change in the velocity of sound; Θ is the Debye temperature. Differentiation of Eq. (1) gives the following expression for the electron correction to the bulk modulus:

$$V\left(\frac{\partial^2 F_e}{\partial V^2}\right)_T=\delta K_1(\Delta)+\delta K_2(\Delta), \tag{2}$$

where

$$\delta K_1(\Delta)=V\left(\frac{\partial^2 F_e}{\partial V^2}\right)_{\Delta,T}=\frac{F_e}{V}\left[\frac{d\ln\nu}{d\ln V}+\frac{1}{\nu}\frac{d^2\nu}{d(\ln V)^2}\right]$$
$$-\frac{1}{2}\nu\Delta^2\left[\frac{d^2\ln T_0}{d(\ln V)^2}+\frac{d\ln T_0}{d\ln V}\left(1+2\frac{d\ln\nu}{d\ln V}\right)\right],$$
$$\delta K_2(\Delta)=V\left(\frac{\partial^2 F_e}{\partial V\,\partial\Delta}\right)_T\left(\frac{\partial\Delta}{\partial V}\right)_T=-\nu\left(\frac{d\ln T_0}{d\ln V}\right)^2 \tag{3}$$

$$\times\left\{\int_0^{\varkappa\theta}\frac{d\varepsilon}{(\varepsilon^2+\Delta^2)^{1/2}}\left[\operatorname{th}\frac{(\varepsilon^2+\Delta^2)^{1/2}}{2\varkappa T}-\frac{((\varepsilon^2+\Delta^2)^{1/2}/2\varkappa T)}{\operatorname{ch}^2((\varepsilon^2+\Delta^2)^{1/2}/2\varkappa T)}\right]\right\}^{-1}. \tag{4}$$

In the vicinity of the superconducting transition when $\Delta\ll\varkappa T$ Eqs. (3) and (4) become

$$\delta K_1(\Delta)=K_1'\Delta^2, \tag{5}$$
$$\delta K_2(\Delta)=\delta K_2(0)+K_2'\Delta^2, \tag{6}$$

where

$$K_1'=-\frac{\nu}{2}\left\{\left[\frac{d\ln\nu}{d\ln V}+\frac{1}{\nu}\frac{d^2\nu}{d(\ln V)^2}\right]\ln\frac{T_0}{T}+\frac{d\ln T_0}{d\ln V}\left(1+2\frac{d\ln\nu}{d\ln V}\right)+\frac{d^2\ln T_0}{d(\ln V)^2}\right\}, \tag{7}$$

$$K_2'=-\frac{3}{4}\frac{A_5}{A_3^2}\nu\left(\frac{d\ln T_0}{d\ln V}\right)^2,\qquad A_3=1{,}05,\qquad A_5=1{,}0, \tag{8}$$

$$\delta K_2(0)=-\frac{\nu}{2A_3}(\pi\varkappa T)^2\left(\frac{d\ln T_0}{d\ln V}\right)^2. \tag{9}$$

The last expression for $\delta K_2(0)$ describes a jump in the bulk modulus at the superconducting transition point. An estimate of this expression in accordance with the BCS model, when T_0 is the superconducting transition temperature, is in agreement with the experimental values (see, for example, Refs. 11–14).

By way of illustration, we shall give the results of a comparison for tin and lead, when $[\delta K_2(0)/K_0]_{\exp}(\mathrm{Sn})\approx-1.5\cdot10^{-6}$ (Ref. 11) and $[\delta K_2(0)/K_0]_{\exp}(\mathrm{Pb})\approx-4\cdot10^{-6}$ (Ref. 13). In the case of tin, when following Refs. 15 and 16 we assume that $\nu=1.7\times10^{34}$ states·erg^{-1}·cm^{-3}, $T_c=3.7$ K, $K_0=4.5\times10^{11}$ dyn/cm^2, and $d\ln T_c/d\ln V=5.6$, Eq. (9) gives $\delta K_2(0)/K_0\approx-1.4\cdot10^{-6}$. Similarly, in the case of lead if following Refs. 15 and 16 we assume that $\nu=2.7\times10^{34}$ states·erg^{-1}·cm^{-3}, $T_C=7.2$ K, $K_0=4.3\times10^{11}$ dyn/cm^2, and $d\ln T_c/d\ln V\approx3.2$, we find that Eq. (9) gives $\delta K_2(0)/K_0\approx-3\cdot10^{-6}$.

At low temperatures, when $\Delta\gg\varkappa T$, Eqs. (3) and (4) become:

$$\delta K_1(\Delta)=-\frac{1}{2}\nu\Delta^2\left\{\left[\frac{1}{2}-\ln\frac{\gamma\Delta}{\pi\varkappa T_0}\right]\left[\frac{d\ln\nu}{d\ln V}+\frac{1}{\nu}\frac{d^2\nu}{d(\ln V)^2}\right]+\frac{d^2\ln T_0}{d(\ln V)^2}+\left(\frac{d\ln T_0}{d\ln V}\right)\left(1+2\frac{d\ln\nu}{d\ln V}\right)\right\}, \tag{10}$$

$$\delta K_2(\Delta)=-\nu\Delta^2\left(\frac{d\ln T_0}{d\ln V}\right)^2. \tag{11}$$

A comparison of the dependences (10) and (11) with the experimental data of Refs. 11 and 13, allowing for the values of $\delta K_2(0)$ gives $\delta K_1\sim\delta K_2$, whereas for lead we obtain $\delta K_1\sim2\delta K_2$. In other words, the two contributions to the bulk modulus are comparable.

If we assume that Eqs. (5)–(11) apply to high-temperature superconductors, we can use these expressions to interpret the experiments on the velocity of sound in such superconductors as $La_{2-x}Sr_xCuO_4$ ($x\geqslant0.15$) and $YBa_2Cu_3O_7$. We shall use a simple relationship between the relative changes in the velocity of longitudinal sound and the bulk modulus $\Delta v_s/v_s\sim(\delta K_1/2K_0)+(\delta K_2/2K_0)$. We shall first consider the case of LaSrCuO. A strong reduction in the velocity of sound as a result of the superconducting transition corresponds to "softening" of the bulk modulus. According to Ref. 7, the experimentally observed softening leads to $(\delta K_2(0)/2K_0)_{\exp}\sim(\Delta v_s/v_s)_{\exp}\sim-0.8\cdot10^{-4}$. A similar value of $\delta K_2(0)/2K_0\sim-10^{-4}$ is obtained from estimates based on Eq. (9) if we use the experimental data: $\nu=2\times10^{34}$ states·erg^{-1}·cm^{-3} (Ref. 17), $K_0=1.8\times10^{12}$ dyn/cm^2 (Ref. 7), $T_0\approx T_c=37$ K (Ref. 7), and $d\ln T_c/d\ln V=-12$ (Ref. 18). According to Ref. 7, at low temperatures the velocity of sound rises: $\Delta v_s/v_s\approx1.4\times10^{-4}$. Bearing in mind that the contribution to $\Delta v_s/v_s$ made by $\delta K_2/2K_0$ is, according to Eq. (11), $\approx-0.6\times10^{-4}$ and corresponds to a reduction in the velocity of sound, we may conclude that in the case of $La_{2-x}Sr_xCuO_4$ the contribution to $\Delta v_s/v_s$ made by

$\delta K_1/2K_0$, corresponding to Eq. (10), is the largest. It should be positive and the absolute values should be 3–4 times greater ($\delta K_2/2K_0$).

The latter property is manifested even more strikingly in the case of YBaCuO, because it is found that the relative softening of the bulk modulus as a result of the superconducting transition is relatively small. The corresponding reduction in the velocity of sound was reported only in Ref. 6, whereas other investigations[1,3,5] failed to detect a jump in the velocity of sound and instead there was a monotonic rise in this velocity. According to Eqs. (10) and (11), such a behavior of the velocity of sound can be understood if we regard the contribution δK_1 to the bulk modulus to be positive and much greater than δK_2. According to Refs. 1 and 3, an increase in the bulk modulus (or in the velocity of sound) amounts to $(1\text{–}4)\times 10^{-3}$, i.e., in high-temperature superconductors the effect under discussion is between two and three orders of magnitude stronger than in the case of the conventional superconductors. It follows from Eqs. (5)–(11) that such a great increase in the change in the velocity of sound is due to a large gap in high-temperature superconductors. Another difference is related to the relatively small softening contribution to the elastic modulus. Bearing in mind these properties, we shall assume that the dependence of the modulus on the superconducting gap $K = K_0 + K'\Delta^2$ can be regarded as approximately established experimentally and we shall see how such a dependence affects certain typical properties of high-temperature superconductors.

2. The dependence of the bulk modulus on the square of the order parameter leads us to the assumption of a similar dependence of the Debye temperature $\Theta(\Delta) = \Theta + \Theta'\Delta^2$. In its turn the dependence of the Debye temperature on Δ^2 makes the following contribution to the free energy dependent on the order parameter F_p. In the Grüneisan model of corresponding states, when $F_p = \Theta(\Delta) f[T/\Theta(\Delta)]$ (Ref. 19), if we allow for the smallness of the correction to Θ proportional to Δ^2, we have approximately[20]

$$F_p=\Theta f(T/\Theta)+\Delta^2\Theta'\varphi(T/\Theta), \tag{12}$$

where $\varphi(x) = f(x) - xf'(x)$ and $f(0) > 0$ describe the contributions of zero-point vibrations to the free energy F_p. We shall give here the expressions used by us to estimate the functions $f(x)$ and $\varphi(x)$ in terms of the experimentally determined lattice specific heat in the normal state $C_p(T/\Theta) = -(T/\Theta)f''(T/\Theta)$:

$$f(x)=f(0)-x\int_0^x \frac{dz}{zp(z)} C_p(z), \tag{13}$$

$$\varphi(x)=\varphi(0)+\frac{x}{p(x)}C_p(x), \qquad p(x)=\frac{d}{d\ln x}\ln[\varphi(x)-\varphi(0)], \tag{14}$$

where $\varphi(0) = f(0)$. Then, describing a minimum of the sum $F_e + F_p$ [Eqs. (1) and (12)] as a function of the parameter Δ, we obtain an equation for the temperature dependence of the superconducting gap:

$$\int_0^{\varkappa\Theta} d\varepsilon\left[\frac{\mathrm{th}(\varepsilon/2\varkappa T_c)}{\varepsilon}-\frac{\mathrm{th}((\varepsilon^2+\Delta^2(T))^{1/2}/2\varkappa T)}{(\varepsilon^2+\Delta^2(T))^{1/2}}\right] = \frac{2\Theta'}{\nu V}\left[\varphi\left(\frac{T_c}{\Theta}\right)-\varphi\left(\frac{T}{\Theta}\right)\right]. \tag{15}$$

In writing out this equation we shall introduce the superconducting transition temperature T_c, related to its value T_0, which is realized on neglect of the phonon contribution to the free energy, by the expression

$$\frac{2\Theta'}{\nu V}\varphi\left(\frac{T_c}{\Theta}\right)=\int_0 \frac{d\varepsilon}{\varepsilon}\left[\mathrm{th}\left(\frac{\varepsilon}{2\varkappa T_c}\right)-\mathrm{th}\left(\frac{\varepsilon}{2\varkappa T_0}\right)\right]\approx \ln\frac{T_0}{T_c}. \tag{16}$$

Such an introduction of T_c naturally is meaningful only if Eq. (16) has the solution. According to Eq. (16) renormalization of the superconducting transition temperature depends on the value of the function $\varphi(T/\Theta)$ at $T = T_c$. The hardening (softening) of the bulk modulus, leading to $\Theta' > 0$ ($\Theta' < 0$) reduces (increases) T_c and the gap $\Delta_0 = \Delta(T = 0)$. This can be demonstrated by subtracting Eq. (16) from Eq. (15) at $T = 0$, which gives

$$\Delta_0=\frac{\pi}{\gamma}\varkappa T_0\exp(-\Xi), \qquad \Xi=2\Theta' f(0)/\nu V, \tag{17}$$

where $\gamma = 1.78$. According to Eqs. (16) and (17), renormalization of T_c, like that of Δ_0, depends on the contribution of the zero-point vibrations to the free energy of a superconductor. On the other hand, it is clear from Eq. (15) that the ratio $2\Delta_0/\varkappa T_c$ depends on the zero-point vibrations only via the dependence $\varphi(T_c/\Theta)$ on the temperature T_c in accordance with the equation

$$\frac{2\Delta_0}{\varkappa T_c}=\frac{2\pi}{\gamma}\exp[\Lambda(T_c/\Theta)]=3{,}52\exp(\Lambda), \tag{18}$$

where

$$\Lambda=\Lambda(T_c/\Theta)=(2\Theta'/\nu V)[\varphi(T_c/\Theta)-\varphi(0)].$$

The explicit temperature dependence of the superconducting gap described by Eq. (15) is readily obtained at near-zero temperatures when $\Delta_0 \gg \varkappa T$ and also near the superconducting transition temperature when $\varkappa T_c \gg \Delta$. At low temperatures ($\varkappa T \ll \Delta_0$) we find from Eqs. (15)–(17) that

$$\frac{\Delta(T)}{\Delta_0}=1-\left[2\pi\frac{\varkappa T}{\Delta_0}\right]^{1/2}\exp\left(-\frac{\Delta_0}{\varkappa T}\right)-\Lambda(T/\Theta), \tag{19}$$

where in addition to the usual exponential temperature dependence associated with the creation of quasiparticles, we have an additional dependence due to the change in the phonon spectrum (or in the Debye temperature) when the number of phonons exhibits a power-law increase with increasing temperature. In the other case, when $\varkappa T_c \gg \Delta$, an expansion of the left- and right-hand sides of Eq. (15) in terms of a small parameter $(T_c - T)/T_c \ll 1$ gives

$$\Delta(T)=\frac{\pi}{A_3^{1/2}}\varkappa T_c(1+p\Lambda)^{1/2}(1-T/T_c)^{1/2}, \tag{20}$$

where $p = p(T_c/\Theta)$ of Eq. (14) is the power exponent describing the rise of the function $\varphi(T/\Theta) - \varphi(0)$ at the superconducting transition temperature. According to the Debye theory, the power exponent p can vary within the range $1 \leqslant p \leqslant 4$. It is clear from Eq. (20) that the influence of phonons alters the slope of the dependence $\Delta(T)$ in the vicinity of T_c. The change in the temperature dependence of the superconducting gap $\Delta(T)$ because of renormalization of the

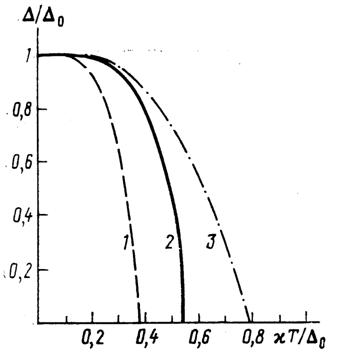

FIG. 1. Temperature dependences of the superconducting gap in the Debye model. The calculations were carried out assuming that $\Theta/T_c = 4$ and using three values of Λ: 1) $\Lambda = 0.35$ ($2\Delta_0/\varkappa T_c = 5.5$; $\Delta C/C_{\rm en} = 6.2$); 2) $\Lambda = 0$ ($2\Delta_0/\varkappa T_c = 3.5$; $\Delta C/C_{\rm en} = 1.4$); 3) $\Lambda = -0.35$ ($2\Delta_0/\varkappa T_c = 2.5$; $\Delta C/C_{\rm en} \simeq 0$); $C_{\rm en} = E_{\rm en}(T_c)$ is the electron specific heat at $T = T_c$.

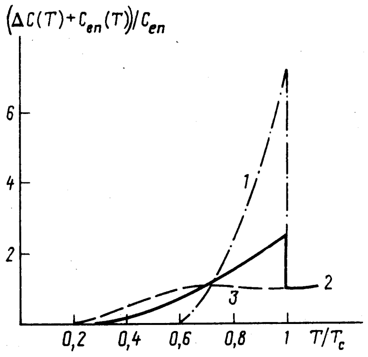

FIG. 2. Temperature dependence of the specific heat $[\Delta C(T) + C_{\rm en}(T)]/C_{\rm en}$ in the Debye model. The calculations were made for $\theta/T_c = 4$ and three values of Λ: 1) 0.35; 2) 0; 3) -0.35.

phonon spectrum is illustrated in Fig. 1, which gives the numerical solution of Eq. (15) obtained using the interpolation Debye model[19] according to which the specific heat is $C_p(x) = C_d(x)$, where

$$C_d(x) = 9\varkappa N_A p(x) x^3 \int_0^{1/x} dz\, z^3/(e^z - 1)$$

and N_A is the number of atoms. According to Fig. 1, hardening of the bulk modulus ($\Lambda > 0$) makes the curve $\Delta(T)$ steeper and increases the ratio $2\Delta_0/\varkappa T_c$ of Eq. (18) compared with that predicted by the BCS theory. Conversely, when softening ($\Lambda < 0$) occurs, the curve $\Delta(T)$ becomes flatter and the ratio $2\Delta_0/\varkappa T_c$ decreases.

We shall now consider the temperature dependence of the specific heat. By definition, we have

$$C_s = -T\left(\frac{\partial^2 F}{\partial T^2}\right)_{\Delta,V} - T\left(\frac{\partial^2 F}{\partial \Delta\, \partial T}\right)_V \left(\frac{\partial \Delta}{\partial T}\right)_V, \qquad (21)$$

where $F = F_{\rm en} + F_e + F_p$ and $F_{\rm en}$ is the free energy of electrons in the normal state. Hence, using Eq. (1) for F_e, Eq. (12) for F_p, and also Eq. (15) for the energy gap $\Delta(T)$, we obtain the following expression for the difference between the specific heats in the superconducting C_s and normal C_n states:

$$\Delta C(T) = C_s - C_n$$

$$= \frac{\nu}{2\varkappa T^2} \int_0^{\varkappa\Theta} d\varepsilon \left[\frac{\varepsilon^2 + \Delta^2}{\mathrm{ch}^2((\varepsilon^2+\Delta^2)^{1/2}/2\varkappa T)} - \frac{\varepsilon^2}{\mathrm{ch}^2(\varepsilon/2\varkappa T)} \right]$$

$$- \frac{\nu \Delta^2}{2\Theta^2} T \Lambda''(T/\Theta) + 2\nu\varkappa \left[\int_0^{\varkappa\Theta} \frac{d\varepsilon/2\varkappa T}{\mathrm{ch}^2((\varepsilon^2+\Delta^2)^{1/2}/2\varkappa T)} \right.$$

$$\left. + \frac{T}{\Theta} \Lambda'\left(\frac{T}{\Theta}\right) \right]^2$$

$$\times \left\{ \int_0^{\varkappa\Theta} \frac{d\varepsilon}{\varepsilon^2+\Delta^2} \left[\frac{2\varkappa T}{(\varepsilon^2+\Delta^2)^{1/2}} \mathrm{th} \frac{(\varepsilon^2+\Delta^2)^{1/2}}{2\varkappa T} \right.\right.$$

$$\left.\left. - \frac{1}{\mathrm{ch}^2((\varepsilon^2+\Delta^2)^{1/2}/2\varkappa T)} \right] \right\}^{-1}. \qquad (22)$$

Here, the functions $\Lambda'(x)$ and $\Lambda''(x)$ are determined by the lattice specific heat as follows:

$$\Lambda'(x) = \frac{2\Theta'}{\nu V} C_p(x), \qquad (23)$$

$$\Lambda''(x) = \frac{2\Theta'}{\nu V} C_p'(x). \qquad (24)$$

The temperature dependence of the specific heat deduced from the Debye model on the assumption that $C_p(x) = C_d(x)$ (Fig. 1) is plotted in Fig. 2. We can see from Fig. 2 that if $\Lambda > 0$, the specific heat jump is greater than that projected by the BCS theory, whereas for $\Lambda < 0$ it is smaller. Assuming that $\Theta \gg T_c$, we find that the jump in the specific heat at the superconducting transition temperature, deduced from Eq. (22), is

$$\Delta C = \frac{\pi^2}{2A_3} \nu \varkappa^2 T_c (1 + p\Lambda)^2 = \frac{\pi^2}{2A_3} \nu \varkappa^2 T_c \left[1 + p \ln \frac{\gamma \Delta_0}{\pi \varkappa T_c} \right]^2. \qquad (25)$$

We shall now give an expression which describes the influence of the change in the Debye temperature at the superconducting phase transition on the isotopic effect:

$$\alpha = -\frac{d \ln T_c}{d \ln M_i} = \frac{1}{2}\{1 - (\Lambda + \Xi)(1 + p\Lambda)^{-1}\}, \qquad (26)$$

where M_i is the mass of an ion. Equation (26) is derived on the assumption that the functions $f(0)$ and Θ'/Θ are independent of the ion mass. If the elastic moduli are increased by the superconductivity, when $\Theta' > 0$ and $\Lambda > 0$, Eqs. (25) and (26) describe an increase in the specific heat jump and the reduction in the isotopic effect. Consequently, when softening occurs, the specific heat jump decreases and the isotopic effect is enhanced provided $\Lambda > -1/p$.

It follows from Eqs. (18), (25), and (26) that the deviations of the ratio Δ_0/T_c [Eq. (18)], of the specific heat jump ΔC [Eq. (25)], and of the isotopic effect α [Eq. (26)] from the predictions of the BCS theory depend on the values of the parameters p, Λ, and Ξ. We shall consider a possible way of estimating these parameters for LaSrCuO and YBaCuO. We shall consider LaSrCuO first; in this case it follows from Refs. 17 and 21 that $T_c = 37$ K, $\Delta_0 = 0.9 \times 10^{-14}$ erg, $N_A/V = 4 \times 10^{22}$ cm^{-3}, $\Theta = 280$ K,

$\nu = 2\times 10^{34}$ states·erg^{-1}·cm^{-3}; according to Ref. 7, we then have $(\Theta'\Delta_0^2/\Theta)\sim 3\cdot 10^{-4}$. Since for this compound the ratio $T_c/\Theta \approx 1/7$ is relatively small, we can estimate the temperature-dependent parameters p and Λ using the Debye model. We then find that $p = 4$ and $\Lambda \sim 10^{-2}$. The small value of Λ is due to the low level of thermal excitation of phonons when $T_c/\Theta \approx 1/7$. The smallness of Λ means that the change in the bulk modulus of LaSrCuO due to the phase transition does not affect the ratio Δ_0/T_c of Eq. (18) and the specific heat jump ΔC of Eq. (25). The situation is different in the case of the isotopic effect whose magnitude depends strongly on zero-point vibrations whose energy is independent of temperature.

It is not easy to obtain a reliable estimate of the parameter Ξ governing the change in the zero-point vibrational energy on transition to the superconducting phase. The difficulty is due to the fact that we have to know the number of the phonon modes that change under the influence of the superconducting electrons and what is the contribution of these modes to the zero-point vibrational energy. For this reason, by way of demonstration of the possible order of the effect, we shall confine ourselves to an estimate of the parameter Ξ within the framework of the Debye model. We can then speak of overestimated Ξ_l and underestimated Ξ_s values of Ξ. The value of Ξ_l corresponds to the case when the frequencies of all the vibrational modes in a crystal change and we have $f(0) = \frac{9}{8}\varkappa N_A$, whereas the value of Ξ_s is obtained if only the acoustic modes change, which corresponds to $f(0) = \frac{9}{8}\varkappa N$, where N is the number of unit cells. Using the data of Refs. 7, 17, and 21 given above, we find that $\Xi_l \sim 0.7$ and $\Xi_s \sim 0.1$. The corresponding values of the isotopic effect α of Eq. (26) are $\alpha_l \approx 0.15$ and $\alpha_s \approx 0.45$. For comparison, we shall also give the values of α found experimentally for $La_{2-x}Sr_xCuO_4$, if $x = 0.15$ then $\alpha \sim 0.16$ (Ref. 22), whereas for $x > 0.15$, it is reported that $\alpha \sim 0.1$ (Ref. 23).

We shall now consider whether we can predict a quantitative manifestation of changes in the elasticity in the case of $YBa_2Cu_3O_7$. It follows from the experimental results that $T_c = 90$–95 K, $\Delta_0 = (2.5$–$5)\times 10^{-14}$ erg, $N_A/V = 7\times 10^{22}$ cm^{-3}, $V_{\text{mol}} = 104$ cm^3, $\Theta = 360$–400 K, $\nu = 1.5\times 10^{34}$ states·erg^{-1}·cm^{-3}, (Refs. 17 and 21), and $(\Theta'\Delta_0^2/\Theta)\sim(1$–$4)\cdot 10^{-3}$ (Refs. 1 and 3). In contrast to LaSrCuO, the ratio $T_c/\Theta \approx 1/4$ is large and, therefore, the level of thermal excitation of phonons is considerably higher. At temperatures greater than or of the order of $T_c = 90$–95 K the specific heat of a crystal is governed by the lattice, so that in estimating the parameter Λ of Eq. (18) we can use the experimental data on the specific heat in the normal state slightly above T_c.

In fact, since according to Eq. (14) we have $\Lambda = (2T_c/\nu pV)(\Theta'/\Theta)C_p$, where $C_p = (\Theta/T_c)p[\varphi(T_c/\Theta) - \varphi(0)]$, it follows that if we use $C_p \sim 1.5\times 10^5$ mJ·K^{-1}·mole^{-1} from Ref. 24 and the values of T_c, ν, $(\Theta'\Delta_0^2/\Theta)$ given above for $p\sim 2.7$ and $\Delta_0 \sim 3\times 10^{-14}$ erg, we obtain $\Lambda \sim 0.1$–0.4. For comparison, we should mention that similar values of the parameter Λ are obtained from the interpolation Debye model if we use real values of T_c/Θ and N_A/V (see above). For these values of Λ Eqs. (18) and (25) give $2\Delta_0/\varkappa T_c = (4$–$6)$ and $\Delta C/T_c \sim 20$–60 mJ·K^{-2}·mole^{-1}, which is not in conflict with the experimental values $[2\Delta_0/\varkappa T_c]_{\text{exp}} \sim (4$–$8)$ (Ref. 21) and $[\Delta C/T_c]_{\text{exp}} \sim (30$–$60)$ mJ·K^{-2}·mole^{-1} (Refs. 17 and 24). Finally, Eq. (26) predicts a considerable reduction in the isotopic effect, which can be demonstrated by estimating the limiting values Θ_l and Θ_s: $\Theta_l \sim 0.6$–2.4, $\Theta_s \sim 0.05$–0.2, which correspond to $\alpha_l < 0.2$ and $\alpha_s \sim 0.4$–0.3. The experiments yield $\alpha \sim 0.03$–0.05 (Ref. 25) and $\alpha \sim 0.05$–0.15 (Ref. 26). A comparison of our theoretical estimates of α with the experimental values of YBaCuO and LaSrCuO leads to the conclusion that the observed values are close to the estimate of the isotopic effect given by α_l.

We shall conclude by considering those changes which appear in the expression for the free energy near the phase transition point:[27,28]

$$F_s - F_n = aV|\psi|^2 + {}^1/_2 bV|\psi|^4. \tag{27}$$

Here, the square of the modulus of the wave function is related in the usual way to the superconducting energy gap

$$|\psi|^2 = A_3 N_e (\Delta/\pi\varkappa T_c)^2, \tag{28}$$

whereas the coefficients of the expansion a and b are given by:

$$a = \beta\tau, \quad \beta = \frac{\nu}{2N_e A_3}(1 + p\Lambda)(\pi\varkappa T_c)^2, \tag{29}$$

$$b = \frac{\nu}{2A_3 N_e^2}(\pi\varkappa T_c)^2. \tag{30}$$

In Eqs. (28)–(30) the electron density is denoted by N_e and we have $\tau = (T - T_c)/T_c$. Therefore, we can say that the changes in the elastic properties of high-temperature superconductors alter the coefficient a by a factor of $(1 + p\Lambda)$. The superconducting transition temperature is then also modified, because of the change in the elasticity, in accordance with Eq. (16).

It is appropriate to consider once again the problem of the reason why small changes in the velocity of sound and, therefore, small changes in the free energy of phonons produce a considerable effect. However, it is known also that the difference between the electron free energy of a superconductor from the free energy of the normal state is also small. In fact, if we ignore the change in the velocity of sound we find that, for example,

$$aV|\psi|^2 = aVA_3 N_e\left(\frac{\Delta}{\pi\varkappa T_c}\right)^2 \approx \frac{1}{2}\nu V\Delta^2\tau.$$

The corresponding change in the temperature-dependent contribution to the free energy of Eq. (12) is described by

$$\Delta^2\Theta'[\varphi(T/\Theta) - \varphi(0)] = (\Theta'\Delta^2/\Theta)TC_p/p,$$

where C_p is the phonon specific heat in the normal state at $T = T_c$. Therefore, the effective comparison parameter can be represented in the form $(\Theta'\Delta^2/\Theta)C_p/C_{\text{en}}$, where $C_{\text{en}} = (\pi^2/3)\cdot\nu\varkappa^2 T_c V$ is the electron specific heat. In view of the large value of the ratio $C_p/C_{\text{en}} \gg 1$ for high-temperature superconductors, this parameter exceeds considerably the small parameter encountered initially $(\Theta'\Delta^2/\Theta)$.

Next, since a minimum of the function $(F_s - F_n)_0$ is reached for

$$|\psi_0|^2 = -\frac{a}{b} = -N_e(1 + p\Lambda)\tau > 0, \tag{31}$$

it follows that determination of the function $(F_s - F_n)_0$ at the minimum allows us to find the thermodynamic critical field H_{cm}:

$$(F_s-F_n)_0=-\frac{a^2}{2b}V=-\frac{H_{cm}^2}{8\pi}V,$$
$$H_{cm}=\pi(2\pi\nu/A_3)^{1/2}\varkappa(T_c-T)(1+p\Lambda). \quad (32)$$

Following the definitions taken from, for example, Ref. 29, we shall give here also the expressions for the Ginzburg–Landau parameter $\varkappa_{GL}$ and for the depth δ of penetration of an electromagnetic field into a superconductor:

$$\delta^2=\frac{\delta_L^2(0)}{2|\psi_0|^2}N_e=\frac{\delta_L^2(0)}{2(1+p\Lambda)}\frac{T_c}{T_c-T}, \quad (33)$$

$$\varkappa_{gL}=2^{1/2}\frac{\delta^2}{\hbar c}eH_{cm}=2\pi\left(\frac{\pi}{A_3}\nu\right)^{1/2}\frac{e}{\hbar c}\varkappa T_c\delta_L^2(0)\approx 0{,}96\frac{\delta_L(0)}{\xi_0}, \quad (34)$$

where e is the electron charge; $\hbar$ is the Planck constant; c is the velocity of sound; $\delta_L(0)=(m_ec^2/4\pi N_ee^2)^{1/2}$ is the London depth of penetration of the field; m_e is the electron mass;

$$\xi_0=(\gamma/\pi^2)(\hbar c/e\varkappa T_c\delta_L(0))(3/4\pi\nu)^{1/2}$$

is the correlation length. It follows from Eqs. (32) and (33) that a change in the lattice elasticity on transition to the superconducting state results, for example in the case of $YBa_2Cu_3O_7$, in an increase in the thermodynamic critical magnetic field of Eq. (32) by a factor of $(1+p\Lambda)$ and it reduces the depth of penetration of the field into a superconductor by a factor $(1+p\Lambda)^{1/2}$. However, the parameter $\varkappa_{GL}$ of Eq. (34) change in our analysis only to the extent of a change in the superconducting transition temperature [see Eq. (16)].

We can summarize these results by concluding that in order to understand the number of properties of high-temperature superconductors we must consider not only the change in the electron energy spectrum of electrons fundamental to superconductivity described, for example, by the BCS theory, but also allow in a self-consistent manner for the change in the crystal lattice itself due to superconductivity.

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