Acoustic plasmons as a possible cause of the anomalous thermal conductivity peak in high-T_c superconductors below the critical temperature

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It is shown that the anomalies in the temperature dependence of the thermal conductivity $\kappa(T)$ in high-T_c superconductors below the critical superconducting transition temperature T_c are attributable to the existence of slowly damped Bose-type collective electron excitations with an acoustic dispersion law (acoustic plasmons) within the gap $2\Delta(T)$. This "plasmon" heat-conduction mechanism in layered cuprate metal oxide compounds accounts for the anomalous peak of $\kappa(T)$ in the plane of the CuO_2 layers, the quadratic dependence $\kappa(T) \propto T^2$ for $T \ll T_c$, the suppression of the maximum of $\kappa(T)$ at $T \approx T_c/2$ by allovalent impurities and a magnetic field, the reversal of the anisotropy of $\kappa(T)$ in the plane of the layers in single-domain $YBa_2Cu_3O_{7-\delta}$ crystals with ordered CuO chains in the transition from the normal state to the superconducting state, etc.

1. INTRODUCTION

As follows from the Bardeen–Cooper–Schrieffer (BCS) theory,[1] the phonon (lattice) contribution to the thermal conductivity of conventional low-temperature superconductors increases below the critical superconducting transition temperature T_c due to the "switching off" of the electronic mechanism for the absorption of phonons within the gap 2Δ in the spectrum of the quasiparticles,[2] and the electronic contribution to the thermal conductivity decreases rapidly as the temperature is lowered due to "freezing out" of the normal Fermi-type heat-transferring excitations.[3] As a result, the total thermal conductivity of a superconductor can either decrease or increase in the range $T<T_c$, depending on the purity of the samples, the structure of their electronic and phonon spectra, and other properties. In addition, at low temperatures in the range $T \ll \Delta$, at which the electronic contribution is exponentially small $[\sim \exp(-\Delta/T)]$, the heat-transfer processes in a crystal are determined mainly by the thermal conductivity of the Bose gas of acoustic phonons, which are characterized by a cubic temperature dependence of the thermal conductivity $\kappa_{ph}(T) \propto T^3$ as $T \to 0$.

High-T_c superconductors based on ceramic and crystalline samples of cuprate metal oxide compounds exhibit a sharp increase in the thermal conductivity below T_c (Refs. 4–13) followed by decay according to a T^2 law in the range $T \ll T_c$ (Refs. 4, 13, and 14). In BiSrCaCuO (Refs. 4 and 12), La(Ba, Sr)CuO (Ref. 6), and YBaCuO ceramics (Refs. 5–11 and 13) with the relatively low values of the normal-state thermal conductivity $\kappa \approx 1$–5 W/m·K, the increase in κ in the superconducting state is small (from 10 to 30%). In $YBa_2Cu_3O_{7-\delta}$ single crystals the value of the thermal conductivity for T above T_c is generally far greater: $\kappa \approx 10$–15 W/m·K, and the highest values of κ for $T<T_c$ are $\kappa \approx 25$–30 W/m·K in the plane of the two-dimensional (2D) CuO_2 conducting layers[10,11] (Figs. 1a and b).

At the same time, if the temperature gradient is directed along the **c** axis, $YBa_2Cu_3O_{7-\delta}$ crystals do not exhibit any appreciable increase in the thermal conductivity below T_c (Ref. 5–7), and its value along this axis κ_c can be an order of magnitude smaller than the values along the **a** and **b** axes, κ_a and κ_b (Ref. 6).

Moreover, in single-domain untwinned $YBa_2Cu_3O_{7-\delta}$ single crystals, which have one-dimensional (1D) CuO chains ordered along the b axis in the basal planes of the unit cell, there is appreciable anisotropy of the thermal conductivity in the a–b plane of the layers in both the normal and superconducting states. The difference $\kappa_b - \kappa_a$ is always greater than zero for $T>T_c$, and for $T<T_c$ it can be either greater or less than zero.[10,11]

A comparison of the values of the thermal conductivity for $T>T_c$ for superconducting phases of the cuprate metal oxide compounds $YBa_2Cu_3O_{7-\delta}$ (Refs. 5 and 13) and $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Ref. 12) with the lattice thermal conductivity of nonsuperconducting (insulating) phases of the same compounds reveals that the electronic contribution to the thermal conductivity in the normal (metallic) state of these high-T_c superconductors amounts to no more than 50%. The same estimate is obtained by subtracting the phonon contribution to the thermal conductivity, which was calculated in Ref. 11 for $YBa_2Cu_3O_{7-\delta}$ with consideration of the phonon–phonon relaxation mechanism.

The nature of the anomalous thermal conductivity below T_c in high-T_c superconductors cannot be regarded as conclusively established at the present time. For example, it was assumed in Refs. 5, 9, and 13 that the thermal conductivity maximum at $T \approx T_c/2$ is caused, as in conventional superconductors, by an increase in the phonon contribution to the thermal conductivity due to a decrease in the electronic absorption of phonons in the superconducting state because a gap occurs in the spectrum of the quasiparticles. However, as was shown in Ref. 15, despite the quasi-two-dimensional nature of the electronic spectrum and the strong anisotropy of the electron–phonon relaxation in layered cuprate metal oxide compounds, owing to the three-dimensional nature of the phonon spectrum, such a mechanism for enhancing the thermal conductivity should provide a significant increase in

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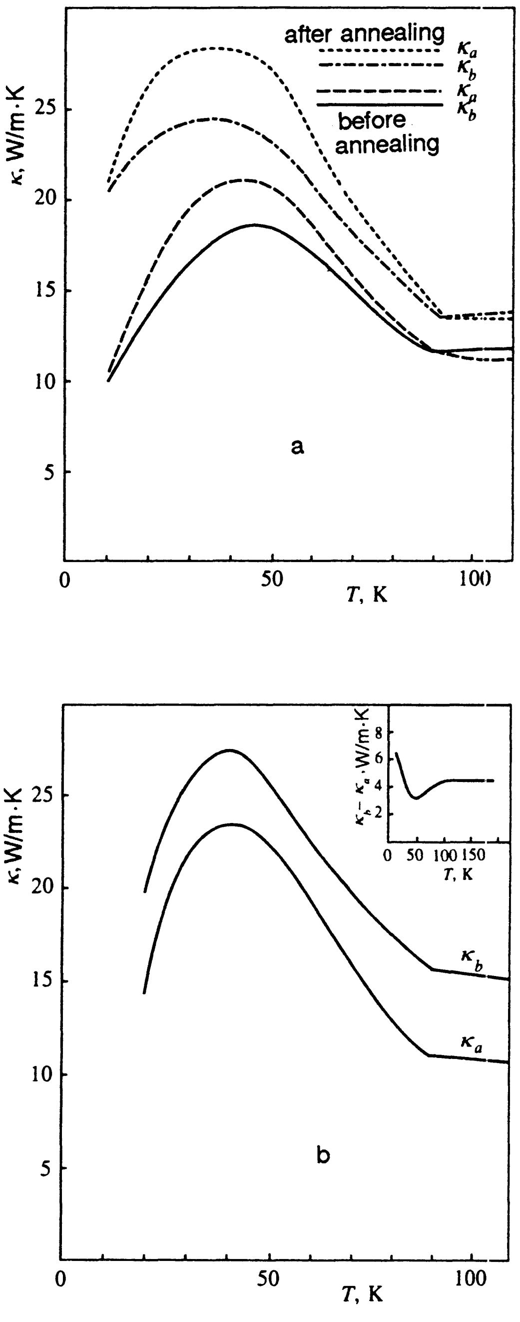

FIG. 1. Experimental plots of the temperature dependence of the thermal conductivity of $_{7-\delta}$ single crystals in the $a-b$ plane taken from Refs. 10 (a) and 11 (b). a) $\kappa_b-\kappa_a>0$ at $T>T_c$ and $\kappa_b-\kappa_a<0$ at $T<T_c$. The higher maxima of κ_a and κ_b correspond to samples which were additionally annealed in an oxygen atmosphere. b) $\kappa_b-\kappa_a>0$ both above and below T_c.

the thermal conductivity for $T<T_c$ not only in the $a-b$ plane of the layers, but also along the **c** axis, in contradiction to the experimental data.[5–7]

At the same time, in Refs. 4, 13, and 14 both ceramic and crystalline samples of BiSrCaCuO and YBaCuO exhibited a nearly quadratic temperature dependence of the thermal conductivity of the form $\kappa(T) \propto T^\alpha$, where $\alpha \approx 1.9-2.3$, at the low temperatures $T \lesssim 2-8$ K, while, as we know,[3,15] the phonon heat-conduction mechanism in the superconducting state leads to the cubic dependence $\kappa(T) \propto T^3$ at $T \ll T_c$.

Hence it follows that the anomalous behavior of the thermal conductivity in cuprate metal oxide compounds is apparently caused by a nonphonon heat-conduction mechanism (see Refs. 11 and 12). For example, in Ref. 13 the quadratic dependence $\kappa \propto T^2$ was attributed to the possible existence of two-well (two-level) systems with a transition to a state of the metallic-glass type as $T \to 0$ in ceramic samples of YBaCuO compounds. However, it should be noted that the dependence $\kappa \propto T^2$ has also been observed for $T<2$ K in a crystalline sample of $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Ref. 4).

Alexandrov and Mott[16] attributed the thermal conductivity maximum below T_c to the Bose condensation of a superfluid charged Bose gas of bipolarons using a previously proposed[17,18] model of the bipolaron mechanism of high-temperature superconductivity in cuprate metal oxide compounds. Moreover, it was postulated in Ref. 16 that the Coulomb interaction in layered crystals (just as in 2D systems) is described by the matrix element

$$V_{2D}(k)=2\pi e^2/k,$$

so that the Bogolyubov spectrum[19] of small-radius bipolarons has a square-root dependence $\omega_k \sim \sqrt{k}$ as $k \to 0$. According to Ref. 16, this produces singularities $k^{-3/2}$ at small k in the momentum dependence of the elastic scattering transport times. As a result, in the case of the bipolaron heat-conduction mechanism,[16] the increase in the thermal conductivity with decreasing T below the Bose condensation temperature (which is simultaneously the critical temperature of the transition to the superfluid and superconducting state) should follow a $(T_c-T)^{3/2}$ law with a derivative $\partial\kappa/\partial T$ that vanishes at $T=T_c$, and the decrease in the thermal conductivity in the low-temperature region $T \ll T_c$ should follow the cubic law $\kappa \propto T^3$, in analogy to the phonon contribution to the thermal conductivity. However, this dependence of $\kappa(T)$ is not consistent with the experimental data.[4–14]

On the other hand, it should be noted that in layered crystals the Coulomb interaction at $k \to 0$ (i.e., at large distances, greatly exceeding the distance between layers) is described by the three-dimensional (3D) matrix element

$$V_{3D}(k)=4\pi e^2/k^2,$$

so that the Bogolyubov spectrum of charged bosons (bipolarons) equals

$$E(k)=[\omega_{pl}^2+(k^2/2m_{BP}^*)^2]^{1/2}$$

(see Refs. 20 and 21) and has a finite gap in ω_{pl} at $k=0$ [where $\omega_{pl}=(4\pi e^2 n_{BP}/\varepsilon_0 m_{BP}^*)^{1/2}$ is the plasma frequency of the bipolarons with a density n_{BP} and an effective mass m_{BP}^* in an ionic crystal with a dielectric constant ε_0]. For this reason, no special features should appear in the transport properties, including the thermal conductivity of the superfluid (superconducting) Bose gas of bipolarons.

In this paper (see also Ref. 22) it is shown that all the main features and anomalies of the thermal conductivity of cuprate metal oxide compounds can be explained under the standard BCS theory[1] on the basis of a single hypothesis regarding the existence of a low-frequency branch of collec-

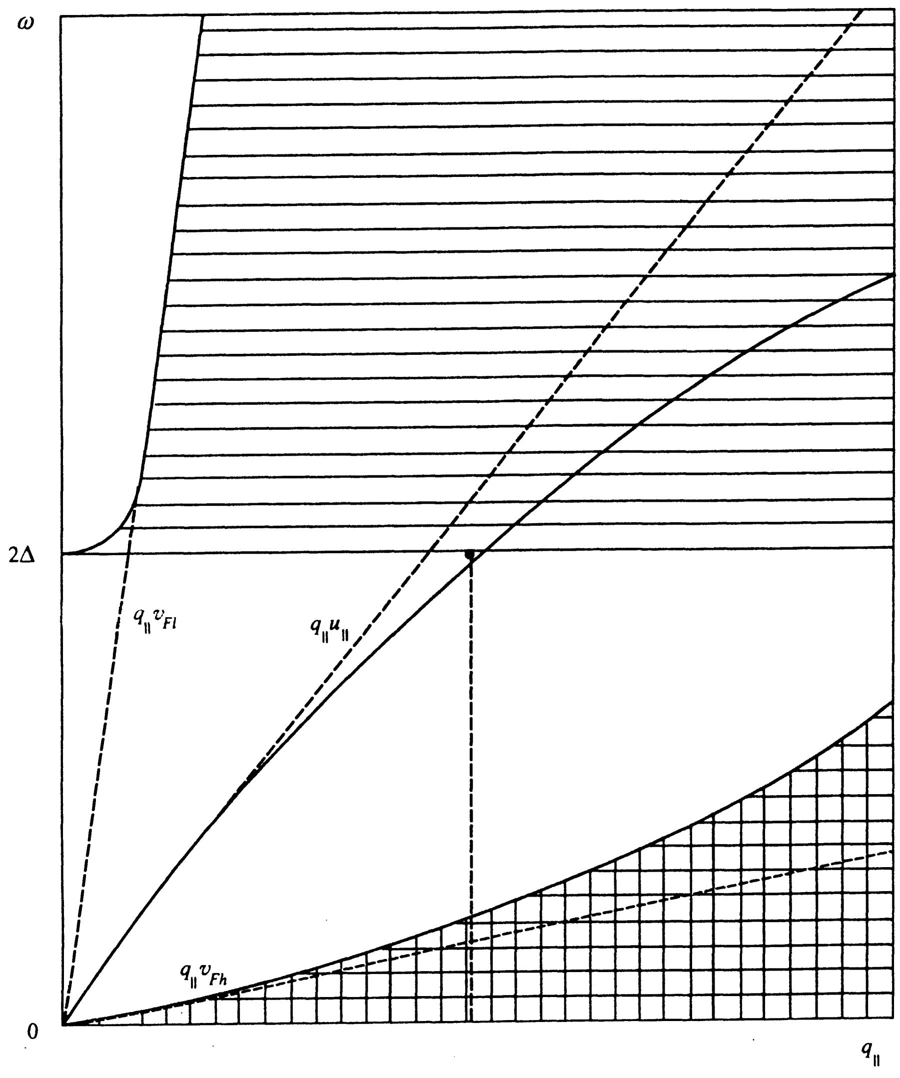

FIG. 2. Spectrum of the longitudinal acoustic plasmons in a layered two-band metal and regions of quantum Landau damping on l carriers (horizontal hatching) and on h carriers (cross hatching).

tive electron-density excitations with an acoustic dispersion law ($\omega_k \sim k$ at $k \to 0$), i.e., so-called acoustic plasmons,[23,24] which can exist as slowly damped, Bose-type quasineutral excitations in a two-component charged Fermi liquid with "light" (l) and "heavy" (h) charge carriers (electrons and holes). The sharp increase in the thermal conductivity in cuprate metal oxide compounds below T_c is caused by suppression of the quantum Landau damping of the long-wavelength acoustic plasmons within the gap $2\Delta(T)$ in the spectrum of the degenerate l carriers (see Fig. 2).

It is also shown in this paper that this a "plasmon" heat-conduction mechanism leads to a quadratic law for the decrease in the thermal conductivity with decreasing T at $T \ll T_c$ and to a nonzero value of $\partial\kappa/\partial T$ at T_c, in agreement with experiment[4–14] (we note that an "excitonic" mechanism for heat conduction in metals with localized electrons was previously considered in Ref. 25).

The anomalous contribution of the Bose gas of thermal acoustic plasmons to the thermal conductivity of layered crystals of cuprate metal oxide compounds exists only in the $a-b$ plane owing to the quasi-two-dimensional nature of the spectrum of acoustic plasmons, in complete agreement with the experimental data in Refs. 5–7. Moreover, in $YBa_2Cu_3O_{7-\delta}$ single crystals with CuO chains ordered along the b axis, the plasmon thermal conductivity is anisotropic in the $a-b$ plane. This is attributed to the anisotropy of the phase velocity and the damping rate of the acoustic plasmons (as well as Δ) and makes it possible to understand the results of the experiments in Ref. 10 and 11 (Fig. 1).

The plasmon contribution to the thermal conductivity decreases as the concentration of allovalent (charged) impurities and oxygen vacancies increases because the damping of the acoustic plasmons increases due to elastic Coulomb scattering of the h carriers (Drude damping). This can account for the experimental data indicating enhancement of the thermal conductivity peak when $YBa_2Cu_3O_{7-\delta}$ samples are annealed in an oxygen atmosphere[10] and suppression of the thermal conductivity maximum when the Pr and Zn concentration are increased in $Y_{1-x}Pr_xBa_2(Cu_{1-y}Zn_y)_3O_{7-\delta}$ (Ref. 13).

Finally, the suppression of the thermal conductivity maximum by a magnetic field observed in Ref. 26 at $T < T_c$ can be caused by enhancement of the Landau damping of the acoustic plasmons in the normal Abrikosov vortex "cores," which increase in number as the field strength increases.

2. SPECTRUM AND DAMPING OF ACOUSTIC PLASMONS IN LAYERED CUPRATE METAL OXIDE COMPOUNDS IN THE NORMAL AND SUPERCONDUCTING STATES

The hypothesis that layered cuprate metal oxide compounds have a branch of acoustic plasmons owing to the presence in their electronic spectra of overlapping broad and narrow 2D bands near the Fermi level, which are partially occupied by "light" (l) and "heavy" (h) charge carriers (electrons and holes) with strongly differing effective masses ($m_l^* \ll m_h^*$), was first advanced Refs. 17 and 27.

This hypothesis is indirectly supported, for example, by the weak dependence of the position of the Fermi level and the value of the optical plasma frequency in cuprate metal oxide compounds on the degree of doping,[28,29] which can be attributed to the predominant filling of the anomalously narrow 2D band with a high density of states by h holes (or h electrons). In this case the concentration N_l of degenerate l holes (or l electrons) in the broad 2D band with a low density of states remains almost unchanged in the doping process; therefore their Fermi energy $E_{Fl} \sim N_l$ and their plasma frequency $\Omega_l \sim \sqrt{N_l}$ remain almost constant. Since, according to the hypothesis, the plasma frequency of the h carriers satisfies $\Omega_h \ll \Omega_l$ in the region where the superconducting phase exists, according to the experiment in Ref. 29, the resultant plasma frequency satisfies $\omega_{\rm pl} = (\Omega_l^2 + \Omega_h^2)^{1/2} \approx \text{const}$ over the entire range of variation of the concentration of the dopant.

The direct observation of "flat" nondispersive to within 45 meV) portions of a 2D band near the symmetric points of the Brillouin zone in hole-type cuprate metal oxide BiSrCaCuO, YBaCuO (123), and 124 compounds by angle-resolved photoelectron spectroscopy (ARPES) was recently reported in Ref. 30. According to the experimental data in Ref. 30 and numerical calculations of the band spectrum (see, for example, Refs. 31–33), the open cylindrical or flattened Fermi surface of layered cuprate metal oxide compounds is a multiband (many-valley) surface, and the electronic states of the different bands (valleys) are separated in momentum space owing to the low carrier concentration.

In this case a good approximation for describing collective electron excitations is the model of a quasi-two-dimensional multicomponent charged Fermi liquid with l and h charge carriers. This model leads directly to the existence of a branch of acoustic plasmons[23,24] as a unique "Goldstone mode," which is associated with "spontaneous" violation of the principle of the indistinguishability of particles for electrons (holes) from different bands (valleys). We note that, as was shown in Ref. 34, when there are several equivalent extrema in the spectrum of the quasiparticles, a charged Fermi liquid has one more acoustic electronic mode, i.e., zero-point sound, with a phase velocity significantly greater than the velocity of an acoustic plasmon (see below).

In the case of a two-component Fermi liquid, the frequency and damping rate of the acoustic plasmons are determined from the condition that the complex dielectric constant vanish:

$$\varepsilon(\mathbf{q},\omega) = \varepsilon_0 - V_C(q_\parallel, q_z)[\Pi_l(q_\parallel,\omega) + \Pi_h(q_\parallel + \omega)], \quad (1)$$

where V_C is the Coulomb matrix element of a layered crystal:[35]

$$V_C(q_\parallel, q_z) = V_{2D}(q_\parallel)\frac{\sinh q_\parallel d}{\cosh q_\parallel d - \cosh q_z d},$$

$$V_{2D}(q_\parallel) = \frac{2\pi e^2}{q_\parallel}, \quad (2)$$

d is the distance between layers, $q_\parallel$ and q_z are the longitudinal (in the plane of the layers) and transverse (along the **c** axis) components of the wave vector **q**, and Π_l and Π_h are the polarization operators of the l and h carriers, which in the frequency range $q_\parallel v_{Fh} < \omega < q_\parallel v_{Fl}$ (v_{Fl} and v_{Fh} are the Fermi velocities of the l and h carriers). Taking into account the quasi-two-dimensional nature of the band spectrum, these are equal to

$$\Pi_l(q_\parallel,\omega) = -\frac{m_l^*}{\pi d}\left[1 + i\frac{\pi}{2}\frac{\omega}{q_\parallel v_{Fl}}\right],$$

$$\Pi_h(q_\parallel,\omega) = \frac{n_h q_\parallel^2}{m_h^* \omega(\omega + i/\tau_h)}. \quad (3)$$

Here n_h and τ_h are the density and characteristic time for elastic scattering of the h carriers in the narrow 2D band. Note that in order to combine the descriptions of the Landau and Drude damping mechanisms we should use a more precise expression for the polarization operator of the h-carriers, which conserves particle number (see, e.g., Ref. 51). It can be shown, however, that such a more rigorous (but also more elaborate) approach does not change the results obtained using the simple approximation (3).

From the condition $\varepsilon(q,\omega)=0$ we find the frequency $\omega(q_\parallel)$ and the damping rate $\gamma(q_\parallel)$ of the long-wavelength acoustic plasmons when $q_z=0$ and $q_\parallel d \ll 1$:

$$\omega(q_\parallel) = q_\parallel u_\parallel, \quad \gamma(q_\parallel) = \frac{\pi}{4}\frac{q_\parallel u_\parallel^2}{v_{Fl}} + \frac{1}{\tau_h}, \quad (4)$$

$$u_\parallel = \frac{1}{2}\Omega_h\sqrt{a_l^* d} \equiv v_{Fl}\left(\frac{m_l^*}{2m_h^*}\frac{N_h}{N_l}\right)^{1/2}. \quad (5)$$

Here $\Omega_h = (4\pi e^2 n_h / m_h^*)^{1/2}$ is the plasma frequency of the h carriers, $a_l^* = 1/e^2 m_l^*$ is the effective Bohr radius of the l carriers, and N_l and N_h are the two-dimensional (2D) densities of the l and h carriers in a layer.

For $q_z = \pi/d$ (but $q_\parallel d \ll 1$) the longitudinal group velocity of the acoustic plasmons equals

$$\bar{u}_\parallel = \frac{\Omega_h d}{\sqrt{2}(1 + 2d/a_l^*)^{1/2}} < u_\parallel. \quad (6)$$

We note that the group velocity of the acoustic plasmons across layers $u_z = \partial\omega/\partial q_z$ vanishes at $q_z = 0$ and $q_z = \pi/d$ and that it is negative for arbitrary q_z and small in absolute value in comparison with $u_\parallel$ (see Appendix).

Thus, long-wavelength acoustic plasmons propagate in a layered crystal practically in the plane of the layers, owing to the quasi-two-dimensional nature of the electronic spectrum and the small value of the 2D screening radius $R_s \equiv a_l^*/2 \ll d$.

In the transition to the superconducting state, as a result of the appearance of a gap in the spectrum of the quasiparticles, the quantum Landau damping of the acoustic plasmons decreases with decreasing temperature at the frequencies $\omega' < 2\Delta(T)$ according to an exponential law and tends to zero as $T \to 0$ (Fig. 2).

In this case the damping rate of the acoustic plasmons is given in the BCS model,[1] in analogy with the electronic damping of phonons,[3] by the expression (for $q_z=0$)

$$\gamma_s(q_\parallel,\Delta(T),T)=\frac{\pi}{4}\omega(q_\parallel)\frac{u}{v_{Fl}}g(\omega(q_\parallel),\Delta(T),T), \qquad (7)$$

where the function g for layered superconductors is practically the same as that for isotropic superconductors[3] (see Ref. 15). In particular, for $\omega \ll \Delta$ the function g does not depend on ω and equals[1]

$$g(\Delta(T),T)=2[\exp\{\Delta(T)/T\}+1]^{-1}. \qquad (8)$$

If the Drude damping of the acoustic plasmons due to elastic scattering of the h carriers on defects and impurities is sufficiently small ($\Delta\tau_h \gg 1$), in the transparency region (see Fig. 2)

$$\tau_h^{-1} \lesssim \omega(q_\parallel) \lesssim 2\Delta(T) \qquad (9)$$

the thermal acoustic plasmons can make a significant contribution to the thermal conductivity of the crystal (see below).

It should be stressed that expressions (4)–(7) are valid for layered BiSrCaCuO crystals with isotropic conductivity in the $a-b$ plane of the layers. However, in untwinned $YBa_2Cu_3O_{7-\delta}$ single crystals, when $\delta \ll 1$ holds, along with the cuprate 2D CuO_2 layers there are ordered 1D CuO chains (along the **b** axis) in the basal planes with a quasi-one-dimensional spectrum and a nearly flat Fermi surface (see Refs. 31–33). Then the ohmic conductivity and the electronic polarizability are anisotropic in the $a-b$ plane. In this case the spectrum of long-wavelength acoustic plasmons ($q \to 0$) is given by the equation

$$q_y^2/q_\parallel^2\Pi_1(q_y,\omega)+\Pi_l(q_\parallel,\omega)+\Pi_h(q_\parallel,\omega)=0. \qquad (10)$$

Here Π_1 is the polarization operator of the electrons in the 1D chains (in the y direction) with a longitudinal effective mass $m_1^* \sim m_l^* \ll m_h^*$ and a Fermi velocity $v_{F1} \gg v_{Fh}$, which at the low frequencies $\omega \ll q_y v_{F1}$ equals

$$\Pi_1=1/\pi v_{F1}a, \qquad (11)$$

where a is the distance between the CuO chains (in the x direction). The imaginary part of Π_1 equals zero, since the quantum Landau damping in a one-dimensional (chainlike) metal has a broad transparency window[36] at the frequencies $\omega < q_y v_{F1}(1-q_y/2k_{F1})$, where k_{F1} is the Fermi momentum of the electrons in the 1D chains.

From (10) and (11) we find the following expression for the anisotropic velocity of the acoustic plasmons in $YBa_2Cu_3O_{7-\delta}$ single crystals:

$$u_\parallel(\theta)=\left(\frac{\pi N_h}{m_h^* m_l^*}\right)^{1/2}\left[1+\frac{m_1^*}{m_l^*}\frac{\cos^2\theta}{k_{F1}a}\right]^{-1/2} \qquad (12)$$

where θ is the angle between the vector $q_\parallel$ and the **b** axis in the $a-b$ plane. Hence it follows that the group velocity u_b along the **b** axis ($\theta=0$) is smaller than u_a along the **a** axis ($\theta=\pi/2$).

3. PLASMON THERMAL CONDUCTIVITY IN LAYERED CRYSTALS OF CUPRATE METAL OXIDE COMPOUNDS

Let us consider the thermal conductivity of a Bose gas of slowly damped acoustic plasmons in a layered superconductor with an isotropic spectrum of acoustic plasmons in the plane of the layers. In analogy to the problem of the thermal conductivity of a Bose gas of acoustic phonons,[2] we write the Boltzmann kinetic equation for the small nonequilibrium perturbation $N_1(q_\parallel,T)$ associated with the temperature gradient ∇T to the equilibrium Bose–Einstein distribution function $N_0(\omega,T)=[e^{\omega/T}-1]^{-1}$ of the thermal acoustic plasmons, from which it follows that

$$N_1(q_\parallel,T)=-\mathbf{u}\nabla T\tau_{pl}(q_\parallel,T)\frac{\partial N_0}{\partial T}, \qquad (13)$$

where

$$\tau_{pl}^{-1}(q_\parallel,T)=\gamma_s(q_\parallel,\Delta,T)+\tau_h^{-1}, \qquad (14)$$

and $\mathbf{u}(u_\parallel,u_z)$ is the total group velocity vector of the acoustic plasmons.

The corresponding contribution of the nonequilibrium acoustic plasmons to the heat flux $\mathbf{Q}=-\kappa\nabla T$ is given by the expression

$$\mathbf{Q}_{pl}=\int\frac{d^3q}{(2\pi)^3}\mathbf{u}(\mathbf{q})\omega(\mathbf{q})N_1(\mathbf{q},T)$$
$$\cong-\frac{\nabla_\parallel T}{2T^2}\int\frac{d^3q}{(2\pi)^3}u_\parallel^2(\mathbf{q})\omega(\mathbf{q})\tau_{pl}(q_\parallel,T)\frac{e^{\omega(\mathbf{q})/T}}{[e^{\omega(\mathbf{q})/T}-1]^2}. \qquad (15)$$

The derivation of the last expression assumed $u_\parallel^2 \gg u_z^2$, so that the heat flux transferred by the Bose gas of acoustic plasmons can propagate only if the temperature gradient is parallel to the plane of the layers.

As follows from the expression for $u_\parallel(\mathbf{q})$ presented in the appendix, the dependence of $u_\parallel$ on $\mathbf{q}$ can be neglected for $q_\parallel d<1$ and $q_z d<1$. On the other hand, the main contribution to the integral (15) is made by the range of frequencies $\omega(\mathbf{q}) \lesssim T$ and the longitudinal momenta $q_\parallel \lesssim T/u_\parallel$. Both of these inequalities hold for $q_\parallel$, provided $T \lesssim u_\parallel/d$ holds (for $u_\parallel \approx 10^6$ cm/s and $d \approx 10^{-1}$ cm this corresponds to $T \lesssim 100$ K).

Assuming that this condition is satisfied and setting $u_\parallel=$const in (15), using (7) and (14) we arrive at the following expression for the thermal conductivity of the quasineutral Bose gas of acoustic plasmons in the plane of the layers (when Boltzmann's constant k_B and Planck's constant $\hbar$ are written explicitly):

$$\kappa_{pl}(T)=\frac{k_B^3T_c^2\tau_h}{4\pi\hbar^2 d}f(t), \qquad (16)$$

where

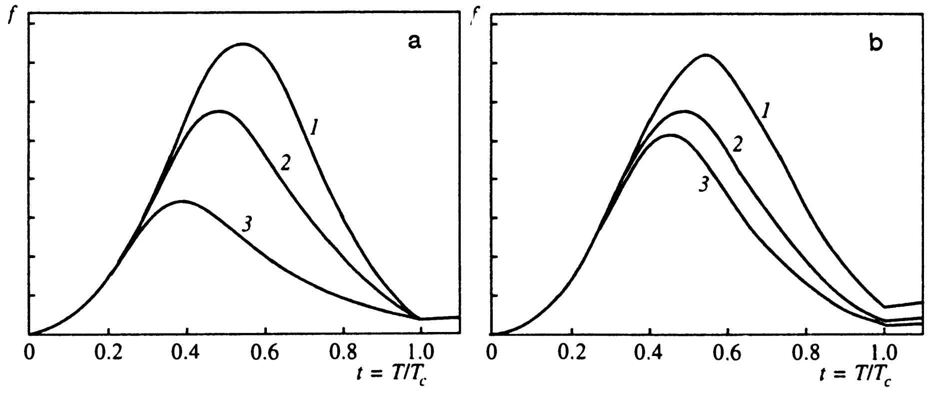

FIG. 3. a) Dependence of $f(t)$ on $t=T/T_c$ when $\beta/\nu=40$ for various values of $2\Delta_0/T_c$: 3.52 (*1*), 4.5 (*2*), 6 (*3*). b) Dependence of $f(t)$ for $2\Delta_0/T_c=4.5$ for various values of β/ν: 20 (*1*), 40 (*2*), 60 (*3*).

$$f(t)=t^2\int_0^\infty \frac{e^x x^3 dx}{[1+(\beta/\nu)txg(x,\delta(t),t)](e^x-1)^2}, \tag{17}$$

$$t=T/T_c, \quad \nu=\hbar/\tau_h k_B T_c,$$

$$\beta=u_\parallel/v_{Fl}, \quad \delta(t)=\Delta(T)/k_B T_c. \tag{18}$$

It follows from (17) that for $T\ll T_c$, when $\Delta\gg T$ holds and g is exponentially small [see (8)], the plasmon thermal conductivity (16) depends on T according to a quadratic law: $\kappa_{\rm pl}(T)\propto T^2$. This is consistent with the experimental data[4,13,14] and is attributed to the quasi-two-dimensional spectrum of the acoustic plasmons (in contrast to the three-dimensional spectrum of phonons).

On the other hand, the thermal conductivity as a function of the temperature has a kink at $T=T_c$ (the derivative $\partial\kappa_{\rm pl}/\partial T$ has a discontinuity), which is also consistent with experiment.[4–13]

Figure 3a shows plots of the dependence of $f(t)$ on t, calculated from (17) using the explicit expression for $g(\omega,\Delta,T)$ (see Refs. 3 and 14) with $\beta/\nu=40$ for various values of $2\Delta_0/T_c$, where Δ_0 is the superconducting gap at $T\to 0$.

Figure 3b shows plots of $f(t)$ for $2\Delta_0/T_c=4.5$ and various values of the ratio between β and ν, which can correspond to different values of the relaxation time τ_h of the h carriers and (or) different values of the group velocity $u_\parallel$ (at fixed values of T_c and v_{Fl}). In particular, as $\delta\to 0$, for a 2D density of the l carriers in $YBa_2Cu_3O_{7-\delta}$ of order

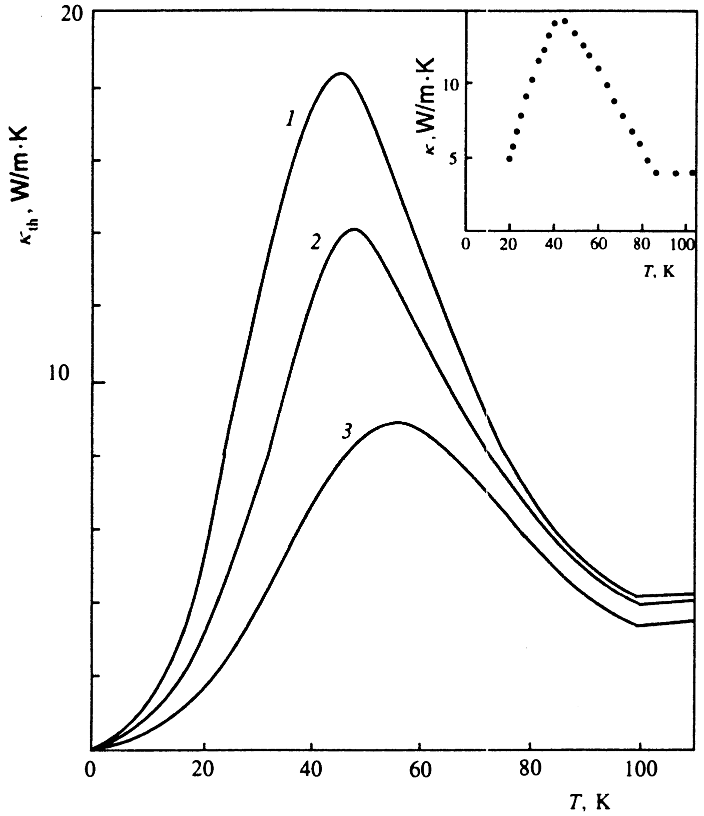

FIG. 4. Temperature dependence of the total thermal conductivity $\kappa(T)$ for the following parameters: $T_c=90$ K, $2\Delta_0/T_c=4.5$, $m_l^*=m_0$, $N_l=N_h=2\times10^{14}\,{\rm cm}^{-2}$, $d=10$ Å, $\tau_l=1.8\times10^{-3}$ s, $k_{Fl}=3.6\times10^7\,{\rm cm}^{-1}$, $v_{Fl}=4\times10^7$ cm/s, $\beta=0.04$, $u_\parallel=1.6\times10^6$ cm/s: *1*—$\nu=5\times10^{-4}$, $\tau_h=1.6\times10^{-10}$ s; *2*—$\nu=10^{-3}$, $\tau_h=8\times10^{-11}$ s; *3*—$\nu=2\times10^{-3}$, $\tau_h=4\times10^{-11}$ s.

$N_l \approx 2\times 10^{14}$cm^{-2} (in one CuO_2 layer) and for a longitudinal effective mass of the l carriers $m_l^* \approx m_0$ (where m_0 is the mass of the free electron) we obtain the estimates $k_{Fl}=\sqrt{2\pi N_l}\approx 3.6\times 10^7$cm^{-1} and $v_{Fl}=k_{Fl}/m_l^* \approx 4\times 10^7$ cm/s.

Figure 4 presents plots of the temperature dependence of the sum of the thermal conductivity of the Bose gas of thermal acoustic plasmons $\kappa_{\rm pl}$ for various values of τ_h (when $\beta=0.04$, $2\Delta_0/T_c=4.5$, $T_c=90K$, and $d=10$ Å) and the thermal conductivity of the Fermi gas of normal excitations (l carriers) in the broad 2D band κ_l, which is given in the BCS theory with consideration of the quasi-two-dimensional character of the electronic spectrum by the expression (compare with Ref. 2)

$$\kappa_l(T)=\frac{2N_l k_B^2 T\tau_l}{m_l^* d}\int_{\Delta(T)/k_BT}^{\infty}\frac{x^2dx}{\cosh^2(x/2)}, \qquad (19)$$

where τ_l is the effective relaxation time of the l carriers, which includes both elastic scattering on defects and impurities.

The insert in Fig. 4 shows the temperature dependence of the "electronic" thermal conductivity of a $YBa_2Cu_3O_{7-\delta}$ single crystal in the $a-b$ plane (parallel to the **a** axis) with the maximum value $\kappa_a \approx 14$ W/m·K at $T\approx 0.5T_c$ from Ref. 11. This plot was obtained in Ref. 11 by subtracting a certain model function $(w+vT)^{-1}$, which describes the lattice thermal conductivity caused by phonon–phonon scattering with consideration of the umklapp processes, from the experimentally measured thermal conductivity, the coefficients w and v being adjusted so as to most accurately describe the temperature dependence of the thermal conductivity for $T>T_c$.

4. DISCUSSION OF RESULTS AND COMPARISON WITH EXPERIMENT

As is seen from Fig. 4, the best agreement between theory and experiment with respect to the position and height of the thermal conductivity maximum is achieved at $\nu=10^{-3}$, i.e., for $\tau_h\approx 8\times 10^{-11}$ s (curve 2). For $T\geqslant T_c$ agreement between the theoretical and experimental curves is achieved for $\tau_l\approx 1.8\times 10^{-13}$ s. The large difference (more than two orders of magnitude) between the relaxation times of the l and h carriers is noteworthy. Its explantation calls for a separate discussion.

The value $\tau_l\approx 1.8\times 10^{-13}$ s for the relaxation times of the l carriers obtained by fitting the theoretical curves to the experimental value of the normal-state thermal conductivity[11] is twice smaller than the transport relaxation time $\tau_{\rm tr}\approx 3.5\times 10^{-13}$ s, which can be determined from the resistivity $\rho=4\pi/\Omega_l^2\tau_{\rm tr}\approx 100\mu\Omega\cdot$ cm at $T=100$ K for the same sample, if the plasma frequency is $\Omega_l=\sqrt{4\pi e^2 n_l/m_l^*}\approx 1.5$ eV (for $n_l=N_l/d\approx 2\times 10^{21}$ cm^{-3}). This points out the important role of the inelastic relaxation processes of quasiparticles both in the large number of optical phonon branches and in the low-frequency fluctuations of the charge density of the h carriers,[37,38] which is not included in (19). These processes can also cause the thermal conductivity to rise as the temperature falls in pure superconductors, with a peak $T\simeq 0.25\ T_c$ (cf. Ref. 52).

On the other hand, the anomalously large values $\tau_h\sim 10^{-10}$ can be associated with the strong localization of the h carriers near crystal-lattice sites in small regions of radius $r_0\lesssim a$, while the mean distance $\bar{l}$ between the defects and impurity atoms is far larger ($\bar{l}\gg a$). As a result, the elastic scattering of the h carriers in the narrow 2D band can be suppressed by a factor of $(\bar{l}/r_0)^2$ in comparison with the scattering of the almost free l carriers in the broad 2D band, i.e., $\tau_h\sim\tau_l(\bar{l}/r_0)^2\gg\tau_l$.

It should be noted in this context that the optimum value of the parameter $\beta\equiv u_\parallel/v_{Fl}=0.04$ for $v_{Fl}\approx 4\times 10^7$ cm/s corresponds to a longitudinal group velocity of the acoustic plasmons $u_\parallel\approx 1.6\times 10^6$ cm/s. According to (5), this leads to a very large value for the effective mass of the h carriers $m_h^*\approx 100m_0$ (for $N_h\approx N_l$), pointing out their strong localization and the importance of polaron effects. Setting $m_h^*\approx 4/a^2W_h$ for the narrow 2D band in the strong-coupling approximation, we find the width of the band $W_h\approx 25$ meV (for $a\approx 4$ Å), which is consistent with the experimental data[30,31] for "flat" bands (with a width less than 45 meV).

Curves *1* and *3* in Fig. 4 correspond to $\tau_h\approx 1.6\times 10^{-10}$ ($\nu=5\times 10^{-4}$) and $\tau_h\approx 4\times 10^{-11}$ s ($\nu=2\times 10^{-3}$), i.e., Drude damping of the acoustic plasmons due to elastic scattering of the h carriers, which are, respectively, weaker and stronger than for curve 2. It is generally known[39] that scattering on charged defects and impurities is more effective for current carriers with a large effective mass. Therefore, the time τ_h in (16) is determined mainly by Coulomb scattering of the h carriers and is inversely proportional to the concentration of charged centers (allovalent impurities and vacancies).

This circumstance allows us to attribute the experimental results in Ref. 13 indicating suppression of the thermal conductivity peak below T_c in $YBa_2Cu_3O_{7-\delta}$ as the concentration of charged substitutional impurities (Pr, Zn) increases, as well as the enhancement of the thermal conductivity maximum observed in Ref. 10 when $YBa_2Cu_3O_{7-\delta}$ samples were annealed in an oxygen atmosphere, to the tendency shown in Fig. 4 for lowering of the maximum of the plasmon thermal conductivity with decreasing τ_h.

In fact, when the Y^{3+} ions are partially replaced by Pr^{4+} ions, the probability of Coulomb scattering of the h carriers increases and τ_h decreases (ν increases) as the concentration of Pr atoms in $Y_{1-x}Pr_xBa_2Cu_3O_{7-\delta}$ rises. According to (16) and (17), this should lower the thermal conductivity maximum at $T<T_c$, as was observed in the experiments in Ref. 13. Note that an increase in x is accompanied by a decrease in the concentration of mobile holes in $Y_{1-x}Pr_xBa_2Cu_3O_{7-\delta}$, which should result in the lowering of T_c (Ref. 40). However, as $\delta\rightarrow 0$, the critical temperature can vary comparatively weakly over a broad range of variation of x near the maximum of T_c (Ref. 41), as was observed in Ref. 13 up to $x=0.2$.

The replacement of Cu^{2+} ions by Zn atoms in cuprate CuO_2 planes completely suppresses superconductivity even when the Zn content equals 9% (Ref. 42) (apparently as a result of local destruction of the quantum-chemical structure of these layers); therefore, even a small addition of Zn ($\sim 1\%$) has a significant influence on τ_h, T_c, and the height of the thermal conductivity maximum.[13]

On the other hand, the scattering of h carriers on neutral impurities is suppressed by a large effective mass.[39] This accounts for the weak dependence of the thermal conductivity in $Y_{1-x}Gd_xBa_{2-y}Al_yCuO_7$ on the concentration of the isovalent impurities Al and Gd.[13]

In pure $YBa_2Cu_3O_{7-\delta}$ single crystals with an oxygen deficiency ($\delta \neq 0$), Coulomb scattering of the h carriers on the positively charged oxygen vacancies dominates. Therefore, during annealing in an oxygen atmosphere, which is accompanied by a decrease in the number of oxygen vacancies in the crystal, the elastic scattering time should increase, and the maximum of the plasmon thermal conductivity should become higher, as was experimentally observed in Ref. 10.

The suppression of the thermal conductivity maximum for $T<T_c$ by a magnetic field as observed in Ref. 26 may occur because high-T_c superconducting materials are type-II superconductors and pass into a mixed (vortex) state in magnetic fields exceeding the lower critical field $H_{c1}(T)$. As the field strength increases, the number of Abrikosov vortices per unit area of the superconducting CuO_2 layers increases with resultant enhancement of the quantum Landau damping of the acoustic plasmons within the normal vortex cores, where the superconducting gap is suppressed.

In conclusion, we turn to the anisotropy of the thermal-conductivity observed in Refs. 10 and 11 in the $a-b$ plane in single-domain $YBa_2Cu_3O_{7-\delta}$ crystals (see Fig. 1). The anisotropy of the normal-state conductivity along and across the 1D chains ($\sigma_b>\sigma_a$) makes it possible to explain the anisotropy of the thermal conductivity for $T>T_c$ ($\kappa_b^N>\kappa_a^N$) on the basis of the Wiedemann–Franz law (although it can be violated when the role of the inelastic processes is significant, as noted in Ref. 12 for the case of BiSrCaCuO).

The anisotropy of the thermal conductivity of the same sign in the superconducting state ($\kappa_b^S-\kappa_a^S>0$) observed in Ref. 11 can be attributed to the anisotropy mentioned in Sec. 2 of the longitudinal group velocity of the acoustic plasmons ($u_a>u_b$) and consequently of the parameter β in Eq. (17), especially if we take into account the anisotropy observed in Ref. 43 of the Fermi velocities ($v_F^b>v_F^a$), so that $\beta_a>\beta_b$ and $\kappa_a<\kappa_b$.

The reversal of the sign of the anisotropy of the thermal conductivity for $T<T_c$ ($\kappa_b^S-\kappa_a^S<0$) observed in Ref. 10 can be caused by anisotropy of the gap parameter in the $a-b$ plane in pure $YBa_2Cu_3O_{7-\delta}$ single crystals, with $\Delta_a>\Delta_b$, and the function g is also anisotropic with $g_a<g_b$ [see (8)].

Recently performed *ab initio* numerical calculations[44] confirm the realization of anisotropy of the gap parameter of such a type ($\Delta_a>\Delta_b$) in $YBa_2Cu_3O_7$. In this case the appearance of the large gap Δ_a below T_c should result in more rapid growth and a higher maximum of κ_a^S than the growth and maximum of κ_b^S in the direction of the small gap Δ_b, i.e., $\kappa_a^S>\kappa_b^S$. Of course, such a situation can be realized only in pure superconductors, in which $\Delta_b\tau_l^{tr}\gg 1$ holds, where τ_l^{tr} is the transport elastic relaxation time of the l carriers with respect to the momentum.

In dirty superconducting YBaCuO crystals, in which the inequality $\Delta_a\tau_l^{tr}\lesssim 1$ holds, effective isotropization of the gap occurs during Cooper pairing, so that the anisotropy of the thermal conductivity at $T<T_c$ can be determined only by the anisotropy of the spectrum of the acoustic plasmons and l carriers. Here $\kappa_b>\kappa_a$ holds at all temperatures, but Yu *et al.*[11] observed a tendency for a decrease in the positive difference $\kappa_b-\kappa_a$ below T_c (see the insert in Fig. 1b), which can be caused by weak anisotropy of the gap.

5. CONCLUDING REMARKS

Thus, the foregoing treatment of the plasmon mechanism of heat conduction in cuprate metal oxide compounds proposed in Ref. 22, which is an alternative to the phonon mechanism[3,15] and is based on the hypothesis that such compounds have a low-frequency branch of collective electron-density excitations with an acoustic dispersion law (acoustic plasmons), has made it possible to qualitatively, and in some cases quantitatively, describe all the main features and anomalies of the heat-transfer processes in high-T_c superconductors both above and below T_c, including the quadratic dependence of the thermal conductivity on T for $T\ll T_c$, the kink on the plot of $\kappa(T)$ at $T=T_c$, the strong 2D anisotropy of the thermal conductivity in layered crystals of metal oxide compounds, the weaker anisotropy in the $a-b$ plane in single-domain untwinned $YBa_2Cu_3O_{7-\delta}$ crystals, suppression of the thermal conductivity maximum for $T<T_c$ by allovalent impurities and a magnetic field, etc. Note that the presence of a peak in the thermal conductivity in the **c** direction, associated with the phonons (see Ref. 15), can arise because the branch of acoustic photons lies in the region where Landau damping on the **h**-carriers is strong (see Fig. 2).

The existence of Bose-type quasineutral electron excitations with an acoustic spectrum $\omega_q=q_\parallel u_\parallel$ as $q_\parallel\to 0$ is caused by the specific many-valley structure of layered cuprate metal oxide compounds[30–33] with overlapping broad and narrow 2D bands (valleys) occupied by l and h charge carriers. Moveover, as was noted above, the presence of several equivalent extrema (valleys) in the broad 2D band should result in regeneration of zero-point sound with a phase velocity $\omega/q_\parallel>v_{Fl}$ in such a multicomponent charged Fermi surface.[34,45] Since in the normal state the branch of zero-point sound lies in the transparency region, its contribution to the thermal conductivity scarcely changes across the transition to the superconducting state and is small in comparison with the contribution of the acoustic plasmons due to the small value of the ratio $u_\parallel/v_{Fl}\ll 1$.

The reversal of the anisotropy of the thermal conductivity in the $a-b$ plane observed in $YBa_2Cu_3O_{7-\delta}$ (Ref. 10) in the transition from the normal state, with $\kappa_b^N>\kappa_a^N$ to the superconducting state, in which $\kappa_b^N<\kappa_a^N$ holds, is of special interest. Such reversal can be caused by the strong anisotropy of the gap parameter, for which $\Delta_a>\Delta_b$ holds, as is confirmed by numerical calculations.[44]

The character of the anisotropy of the gap is presently a key question in the problem of the mechanism of high-T_c superconductivity in connection with the debate regarding the possibility of d-wave singlet Cooper pairing of current carriers as a result of the exchange of virtual paramagnons in an almost antiferromagnetic quasi-two-dimensional Fermi liquid.[46] (We note, among other things, that the recently performed first-principles numerical calculations[47] of T_c based on magnon d pairing model gave very low values $T_c \sim 1$ K because repulsion dominated throughout the Brillouin zone.) Such Cooper pairing suggests strong anisotropy of the absolute value of the gap (with dips to zero along the diagonals of the Brillouin zone), as well as variation of the phase of the order parameter by π under rotation through an angle of $\pi/2$ (from the **a** axis to the **b** axis), as is confirmed by tunneling experiments in $YBa_2Cu_3O_{7-\delta}$ single crystals.[48,49]

However, it was recently shown in Ref. 50 that the same result can be produced by the multicomponent nature of the gap parameter on a multiply connected anisotropic Fermi surface, provided the gaps in the 2D CuO_2 layers and in the 1D CuO chains (or, more precisely, in the corresponding cylindrical and flat sheets of the Fermi surface) have different signs. Such a model is consistent with the observed reversal of the anisotropy of the thermal conductivity in pure single-domain $YBa_2Cu_3O_{7-\delta}$ crystals,[10] as well as the tendency for a decrease in the anisotropy of the thermal conductivity in less perfect crystals[11] below T_c. For this reason there is interest in precision experimental verification of the dependence of the anisotropy of the thermal conductivity in the $a-b$ plane on the degree of perfection and purity of YBaCuO crystals.

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APPENDIX

As follows from Eqs. (1)–(3) and the condition Re $\varepsilon(q,\omega)=0$, the dispersion law of the acoustic plasmons in the region $q_\| a \ll 1$ (where a is the lattice constant in the plane of the layers) has the form

$$\omega(\mathbf{q})=\frac{\Omega_h\sqrt{q_\| d/2}}{\left[\frac{\cosh q_\| d-\cos q_z d}{\sinh q_\| d}+\frac{2}{q_\| a_l^*}\right]^{1/2}}. \qquad \text{(A1)}$$

The longitudinal group velocity of the acoustic plasmons (in the plane of the layers) equals

$$u_\|(\mathbf{q})\equiv\frac{\partial\omega(\mathbf{q})}{\partial q_\|}=\frac{\omega(\mathbf{q})}{2q_\|}\left\{1-q_\| d\left[\frac{\cosh q_\| d\cos q_z d-1}{\sinh^2 q_\| d}-\frac{2}{q_\|^2 a_l^* d}\right]\left[\frac{\cosh q_\| d-\cos q_z d}{\sinh q_\| d}+\frac{2}{q_\| a_l^*}\right]^{-1}\right\}. \qquad \text{(A2)}$$

The transverse group velocity of the acoustic plasmons (along the $c\|z$ axis) equals

$$u_z(\mathbf{q})\equiv\frac{\partial\omega(\mathbf{q})}{\partial q_z}=-\frac{\omega(\mathbf{q}\, d\sin q_z d/\sinh q_\| d}{2\left[\frac{\cosh q_\| d-\cos q_z d}{\sinh q_\| d}+\frac{2}{q_\| a_l^*}\right]}. \qquad \text{(A3)}$$

As follows from (A3), $u_z=0$ holds for $q_z=0$ and for $q_z=\pi/d$.

The maximum absolute value of u_z at $q_z=\pi/2d$ for $q_\| d<1$ equals

$$|u_z|_{\max}=q_\| u_\| \frac{a_l^* d}{2(a_l^*+2d)}. \qquad \text{(A4)}$$

Hence it follows that under the condition $d \gg a_l^*$ we have $|u_z|/u_\| \lesssim q_\| a_l^*/4 \ll 1$ $(a_l^* < a)$, i.e., the energy of acoustic plasmons, unlike that of phonons, is transported in a layered crystal practically only in the plane of the layers.

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