Thermal Transport in a Charged Bose Gas and in High-T_c Oxides

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Transport properties of two-dimensional charged bosons in the normal and superconducting state are derived. The Wiedemann-Franz law and the Lorentz number are obtained for the normal state. A strong suppression of the quasiparticle scattering rate and a strong enhancement of the thermal conductivity in the superconducting state are found. Temperature dependence of the in-plane thermal conductivity of YBCO crystals is explained.

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The physics of charged Bose liquids has become of particular interest recently in the context of theories of high-temperature superconductors. Some microscopic models [1–3] suggest that charged bosons, formed by strong electron-phonon and electron-electron exchange interactions (lattice and spin bipolarons), might be responsible for the puzzling thermodynamic and kinetic properties of high-T_c oxides. Such characteristic features of high-T_c copper-based superconductors as the curious absence of coherent effects and of the Korringa law in the nuclear spin relaxation rate, the unexpected peak of low-frequency conductivity, linear in T resistivity are indicative of charged bosons [4]. One should add here the heat capacity [5,6], which is reminiscent of He-4 and the unusual temperature dependencies of lower and upper critical fields which, however, can be expected for charged bosons [5]. The approach based on the hypothesis of preformed $2e$ bosons has been used even for the insulating state to explain the physics of the insulator-superconductor transition in the CuO_2-based materials [7].

Among other properties, thermal conductivity shows an unusual temperature behavior [8], which is just opposite to that predicted by the standard BCS theory. The well known in-plane thermal conductivity enhancement in the superconducting state, which is a general property of high-T_c oxides, is commonly attributed to the lattice contribution, which is limited by the phonon-electron scattering. However, in view of the recent measurements on high-quality crystals [9,10] this explanation is now rejected [10]. Unlike previous analyses, Yu *et al.* [10] attributed the observed rapid rise in the superconducting-state thermal conductivity to the electronic contribution with a strongly suppressed scattering rate. A power-law scattering rate within this phenomenological approach is compatible with the d-wave pairing as it is expected in the nearly antiferromagnetic Fermi-liquid theory [11]. However, the normal-state thermal conductivity poses a problem. With the electronic Lorentz number and the experimental value of resistivity one obtains a sizable electronic contribution to the normal-state thermal conductivity, approximately half of the measured value. This clearly contradicts the near equality of the in-plane thermal conductivity above 100 K in the insulating and 90-K crystals, suggesting the more radical viewpoint that the electronic contribution is negligible in both systems [12]. This would be the case according to the Wiedemann-Franz ratio if the carriers have charge $2e$.

In this Letter we derive transport relaxation times for near-two-dimensional charged bosons in the normal and superconducting states and propose a possible microscopic explanation of the main puzzling features of the normal- and superconducting-state thermal conductivity of high-T_c oxides. Our explanation is quite compatible with the phenomenological model proposed by Yu *et al.* [10]. The fundamental difference is that the carriers in our model are bosons with charge $2e$. We find the infinite thermal conductivity of near-2D bosons, scattered by a short-range potential, which is of general interest.

The excitation spectrum of a Bose gas is described within the Bogoliubov approximation by the following expression:

$$\omega(\mathbf{k}) = \sqrt{k^4/4m^2 + V(\mathbf{k}) n_0(T) k^2/m}\ . \tag{1}$$

Here $V(\mathbf{k})$ is the Fourier component of the boson-boson interaction, m is the boson effective mass, and $n_0(T)$ is the superfluid density. For 2D charged bosons $V(\mathbf{k}) = 8\pi e^2/k\epsilon_0$, with ϵ_0 being the dielectric constant of the background, $2e$ being a bosonic charge, and Eq. (1) may be written as [13,14]

$$\omega(\mathbf{k}) = E_s\sqrt{k/q_s + k^4/q_s^4}\ , \tag{2}$$

with $E_s = q_s^2/2m$ and $q_s = q_d[n_0(T)/n]^{1/3}$. Here $q_d = (32\pi e^2 nm/\epsilon_0)^{1/3}$ is a two-dimensional screening wave number. The boson density is n.

The Bogoliubov approximation is valid for a weak interaction such that [13,14]

$$r_s = \sqrt{16m^2e^4/\pi n\epsilon_0} < 1\ , \tag{3}$$

and for a restricted temperature range close to $T=0$. However, one can extend the mean-field expression Eq. (1) up to $T=T_c$ in a qualitative analysis taking into account the depletion of the superfluid component with temperature. For weakly interacting near-2D bosons one obtains with logarithmic accuracy (for details see [4,15,16])

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$$k_B T_c = \pi n/mL \,, \tag{4}$$

$$n_0 = n(1-t) \,, \tag{5}$$

where L is a large logarithm, depending on the scattering amplitude [15,16] and (or) on the interplane hopping if 3D corrections to the energy spectrum are taken into account [4], $t = T/T_c$ is a reduced temperature, k_B is the Boltzmann constant, and $\hbar = 1$.

The elastic scattering of excitations is described by the Hamiltonian

$$H_s = \sum_{\mathbf{k},\mathbf{k}'} v(\mathbf{k},\mathbf{k}') \alpha^\dagger_{\mathbf{k}'} \alpha_{\mathbf{k}} \,, \tag{6}$$

with $b_{\mathbf{k}} = (\alpha_{\mathbf{k}} + A_{\mathbf{k}} \alpha^\dagger_{-\mathbf{k}})/\sqrt{1-A_{\mathbf{k}}^2}$ is a free boson annihilation operator, $A_{\mathbf{k}} = [\omega(\mathbf{k}) - k^2/2m]/V(\mathbf{k}) n_0 - 1$ a coefficient of the Bogoliubov transformation, and

$$v(\mathbf{k},\mathbf{k}') = \frac{v_0(\mathbf{k}-\mathbf{k}')(1+A_{\mathbf{k}}A_{\mathbf{k}'})}{\epsilon(\mathbf{k}-\mathbf{k}',0)\sqrt{(1-A_{\mathbf{k}}^2)(1-A_{\mathbf{k}'}^2)}} \tag{7}$$

a screened scattering potential. Here $v_0(\mathbf{q})$ is a Fourier component of a bare (unscreened) single boson-impurity or boson-acoustic phonon interaction. The latter can be treated as practically elastic [4] if the temperature is not extremely low: $T > T^*$, where $k_B T^* = ms^2/2$ with s being the sound velocity. T^* is less than 10 K even for relatively heavy bosons with $m = 10 m_e$. The RPA static dielectric function of a 2D Bose condensate ($T=0$) was derived by Pines and Frankel [13]. We slightly improve their result here by replacing the free energy spectrum by the normalized one, Eq. (2), in the polarization loop:

$$\epsilon(q,0) = 1 + V(q) \sum_{\mathbf{k}} \frac{f_{\mathbf{k}+\mathbf{q}} - f_{\mathbf{k}}}{\omega(\mathbf{k}) - \omega(\mathbf{k}+\mathbf{q})} \,. \tag{8}$$

With the free energy spectrum in the denominator of Eq. (8) one obtains an even stronger suppression of the relaxation rate in the superconducting state. The screening by superfluid bosons ($f_{\mathbf{k}} = n_0 \delta_{\mathbf{k},0}$) yields

$$\epsilon(q,0) = 1 + q_s E_s / q\omega(q) \,. \tag{9}$$

The contribution of excitations to the screening is negligible compared with that of the superfluid component for small $q < q_s$. In the normal state one can take $\epsilon(q,0) \simeq 1$ because the relevant momentum transfer q is of the order of the boson momentum itself, which is large compared with q_d for $T > T_c$ while r_s is small, Eq. (3).

With the Fermi "golden rule" and the Boltzmann equation one obtains the elastic transport relaxation rate for excitations in the usual way:

$$1/\tau(k) = 2\pi \sum_{\mathbf{k}'} \frac{k_x - k'_x}{k_x} v^2(\mathbf{k},\mathbf{k}') \delta(\omega(\mathbf{k}) - \omega(\mathbf{k}')) \,. \tag{10}$$

Substitution of Eqs. (2) and (7) into Eq. (10) yields

$$\frac{1}{\tau(k)} = \frac{k}{\pi} \frac{dk}{d\omega(k)} \left(\frac{1+A_k^2}{1-A_k^2} \right)^2 \int_0^\pi d\phi [1-\cos(\phi)] \frac{v_0^2(k\sqrt{2[1-\cos(\phi)]})}{\epsilon^2(k\sqrt{2[1-\cos(\phi)]},0)} \,. \tag{11}$$

First we calculate the integral, Eq. (11), in the normal state or for the high-energy excitations with $k > q_s$ in the superconducting state. In these cases $\epsilon(q,0) = 1$ and $\omega(k) = k^2/2m$. For the scattering by acoustic phonons [4] (or by point defects) v_0 is q independent ($v_0^2 = C_{\mathrm{ac}} t$) and τ_{ac} is k independent:

$$\tau_{\mathrm{ac}} = 1/mC_{\mathrm{ac}} t \,, \tag{12}$$

where C_{ac} is a temperature-independent constant. This result, Eq. (12), can explain the linear resistivity of doped Cu-based oxides [4]. For charged impurities $v_0^2(q) = C_{\mathrm{im}}/q^2$ and the relaxtion time shows a canonical Coulomb-scattering behavior, increasing with energy

$$\tau_{\mathrm{im}}(k) = \frac{2k^2}{mC_{\mathrm{im}}} \,, \tag{13}$$

with C_{im} being proportional to the number of impurities. In the superconducting state for low-energy Bogoliubov excitations with $k < q_s$ and $\omega(k) = E_s\sqrt{k/q_s}$ we can put $\epsilon(q,0) = (q_s/q)^{3/2}$ and $A_k^2 = 1 - 4(k/q_s)^{3/2}$ to obtain from Eq. (11)

$$\tau^s_{\mathrm{ac}}(k) = \frac{15\pi}{256} \left(\frac{q_s}{k} \right)^{3/2} \tau_{\mathrm{ac}} \tag{14}$$

and

$$\tau^s_{\mathrm{im}}(k) = \frac{3\pi}{32} \left(\frac{q_s}{k} \right)^{3/2} \tau_{\mathrm{im}}(k) \,. \tag{15}$$

Both τ_{ac} and τ_{im} show a sharp enhancement in the superconducting state for low-energy excitations, compared with the normal state. This enhancement (proportional to $k^{-3/2}$) is explained by the small phase volume, proportional to k, which is accessible for the scattering, and by a large group velocity of the 2D Bogoliubov mode, $d\omega/dk$, which is divergent as $k^{-1/2}$ in the long-wave limit.

One can see from Eq. (14) that in the superconducting state the acoustic relaxation time is strongly divergent in the long-wave limit. The charged impurity relaxation time, Eqs. (13) and (15), falls down linearly with the energy lowering both in the normal and in the superconducting state. As a result the total relaxation time

$$\tau = \frac{\tau_{\mathrm{ac}} \tau_{\mathrm{im}}}{\tau_{\mathrm{ac}} + \tau_{\mathrm{im}}} \tag{16}$$

has a rather sharp maximum in the superconducting state of good quality crystals at $k_{\max} = q_d \sqrt{5C_{\mathrm{im}}/48 q_d^2 C_{\mathrm{ac}} t}$:

$$\tau^s(k)=\frac{15\pi}{256}\tau_{\rm ac}\frac{q_s^{3/2}\sqrt{k}}{k^2+5C_{\rm im}/16C_{\rm ac}t} . \tag{17}$$

To calculate the thermal conductivity due to carriers in the normal state, K_n, one can apply the standard kinetic theory, developed for metals and semiconductors, replacing the Fermi-distribution function by the Bose distribution. As a result one obtains the Wiedemann-Franz law:

$$K_n=L_B\sigma T , \tag{18}$$

where $\sigma=4e^2n\tau_{\rm ac}/m$ is the normal-state conductivity and

$$L_B=\left(\frac{k_B}{2e}\right)^2\frac{3B_0(z)B_2(z)-4B_1^2(z)}{B_0^2(z)} \tag{19}$$

is a bosonic Lorentz number, and

$$B_\nu(z)=\int_0^\infty\frac{x^\nu dx}{\exp(x-z)-1} , \tag{20}$$

with zk_BT being a chemical potential. The scattering by acoustic phonons is assumed. In the classical high-temperature limit, $T\gg T_c$, we obtain

$$L_B=2\left(\frac{k_B}{2e}\right)^2 . \tag{21}$$

The same numerical coefficient ($=2$) is obtained for three-dimensional nondegenerate carriers, scattered by acoustic phonons. The bosonic Lorentz number, Eq. (21), should be compared with the electronic one, $L_e=\pi^2k_B^2/3e^2$, which does not depend on the scattering mechanism and on the dimensionality for degenerate carriers. Their ratio is very small mainly due to the double elementary charge of a boson and is given by

$$L_B/L_e=6/4\pi^2 , \tag{22}$$

which is approximately 0.152.

This fact can explain the near equality of the thermal conductivity of superconducting and insulating crystals of YBCO in the temperature range above 100 K, as has been discussed by one of us [17]. With the electronic Lorentz number one obtains the carrier temperature-independent contribution of approximately 4 W/mK (a direction), which is half of the total one [10]. On the other hand, with the bosonic Lorentz number the carrier contribution is negligible. The mean free path of phonons in both crystals might be of the same value, because the thermal phonons practically are not scattered by bosons. The number of bosons which can scatter thermal phonons is exponentially small, being proportional to $\exp(-T/T^*)$. We note that the near equality of thermal conductivity of superconducting and insulating crystals above 100 K also eliminates the possibility of bosonic excitations with charge e such as holons.

With decreasing temperature the bosonic Lorentz number falls. At $T=T_c$, the chemical potential $z=0$ and $B_0(z)=\infty$ in Eq. (19). If one takes into account three-dimensional corrections, then $B_0(0)=L$, and L_B is logarithmically small at $T=T_c$.

The situation changes drastically in the superconducting state. Because of the above-mentioned singularity of the group velocity, which is a common feature of surface waves, the 2D Bogoliubov mode is a perfect heat carrier. In fact, its thermal conductivity is infinite, if the short-range potential including phonons is operating alone. The scattering by charged impurities restricts the 2D bosonic thermal conductivity in the superconducting state. To show this we write the expression for the heat flow, taking into account that in the superconducting state both the chemical and the electrical potentials equal zero:

$$Q=-\sum_{\mathbf{k}}\frac{d\omega(k)}{d\mathbf{k}}\omega(k)\frac{\partial f_{\mathbf{k}}}{\partial T}\tau^s(k)\left[\frac{d\omega(k)}{d\mathbf{k}}\nabla T\right] , \tag{23}$$

where $f_{\mathbf{k}}$ is the Bose-Einstein distribution with zero chemical potential. Substitution of Eqs. (2) and (17) into Eq. (23) finally yields the superconducting-state thermal conductivity:

$$K_s=K_{s0}\frac{(1-t)^2}{t^2}\int_0^\infty\frac{dx x^4}{\sinh^2(x)[x^4+\eta(1-t)^2/t^5]} , \tag{24}$$

where $K_{s0}=K_n15\pi(Lr_s)^2/1024$ with K_n determined by the classical expression, Eq. (18), with $L_B=2(k_B/2e)^2$. We replaced the upper limit in the integral of Eq. (24), which is E_s/k_BT, by the infinity, because the integration region is restricted by the distribution function and by the power-law singularity of the integrated function if parameter η is small:

$$\eta=5C_{\rm im}L^2(Lr_s)^2/64\pi C_{\rm ac}n . \tag{25}$$

Thus in a perfect crystal with $\eta=0$ two-dimensional bosons show infinite thermal conductivity ($K_s=\infty$). This is quite unexpected compared with the usual s-wave BCS superconductor, which has exponentially suppressed thermal conductivity due to a gap in the excitation spectrum. (As we have mentioned above this is not applied to a d-wave BCS pairing.)

The low-temperature behavior of K_s is given by ($t\ll 1$)

$$\frac{K_s}{K_{s0}}=\frac{96\zeta(5)t^3}{\eta}=\frac{100t^3}{\eta} . \tag{26}$$

Close to T_c we obtain from Eq. (24) ($1-t\ll 1$)

$$\frac{K_s}{K_{s0}}=\frac{(1-t)^{3/2}}{\eta^{1/4}} . \tag{27}$$

In the intermediate temperature region K_s has a maximum, Fig. 1, the height of which depends on the charged impurity concentration. The position of the maximum also depends on the quality of the crystal (η), but this dependence is very weak. These findings are in global qualitative agreement with the experimental data [9, 10,12]. For a quantitative comparison we need to subtract the lattice contribution, which is less than 30% of the total value in the superconducting region, as one can

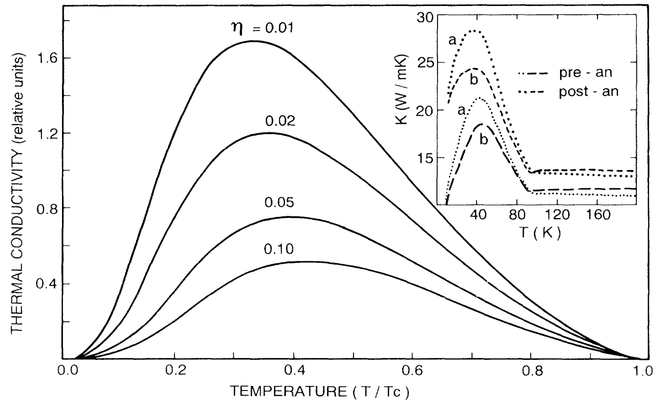

FIG. 1. Temperature dependence of the thermal conductivity of near 2D bosons in the superconducting state for different concentrations of charged impurities, η. $K_s = \infty$ in a perfect crystal with $\eta = 0$. Inset: Experimental results after Ref. [9].

estimate using the measurements by Hagen, Wang, and Ong (see Fig. 3 of Ref. [12]) on insulating crystals of YBCO. This contribution is a smooth function slowly decreasing with temperature decreasing below 50 K. Thus it does not influence the main unusual features of the superconducing heat transport, a sharp rise just below T_c with a maximum approximately at half T_c and a power-law fall in the low-temperature region, which are in good agreement with our theoretical result, Eq. (24), and Fig. 1.

Of course, the enhancement effect of thermal conductivity in a good quality quasi-two-dimensional crystal discussed above is not influenced by the approximation made. As an example, bosons must have hard core and this boundary condition in 2D leads to physics that is not present in the Bogoliubov approximation. However, the effect under discussion is due to long-wave excitations, which are not influenced by hard core. The 3D corrections to the energy spectrum restrict the maximum value of K_s as well. We assume in our discussion that the scattering by charged impurities is more important.

We should also mention that two-dimensional plasmon excitations of a normal and superconducting charged Fermi liquid show the divergent behavior of their group velocity, identical to that of the Bogoliubov mode of a 2D Bose gas. However, different from the Bogoliubov mode, they are not one-particle excitations but the poles of a two-particle propagator. In general they are dumped by one-particle excitations.

The good overall agreement between our theoretical predictions and numerous experimental results (see also Refs. [1–5] and for a recent review [17,18]) reinforces the supposition that the charge carriers in the new high-T_c materials are charged ($2e$) bosons below and *above* T_c as they must be if the BCS analysis is carried into the strong-coupling region [18]. However, some experimental observations remain to be explained with the Bose-liquid ground state, among them a "Fermi edge" measured with angle-resolved photoemission spectroscopy and the de Haas–van Alphen effect in pulsed magnetic fields. Their possible interpretation within the proposed model was already discussed by us in Ref. [19].

In summary, we derive the transport relaxation times of charged bosons in the normal and superconducting state. We find a strong suppression of the relaxation rate and an enhancement of the thermal conductivity in the superconducting state. In a perfect crystal with a low charged impurity concentration this enhancement might be huge. We predict the infinite thermal conductivity of near-two-dimensional bosons, scattered by a short-range potential, including phonons. The normal-state thermal conductivity of charged bosons (charged $2e$) is many times smaller than that of electrons with the same electrical conductivity. We explain the main puzzling features of the thermal conductivity of metal oxides, in particular, the near equality in insulating and superconducting crystals above 100 K and the pronounced maximum below T_c.

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