Absence of anisotropic universal transport in YBCO

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There exists significant in-plane anisotropy between $a$ and $b$ axis for various properties in YBCO. However recent thermal conductivity measurement by Chiao et al. which confirms previous microwave conductivity measurement by Zhang et al., shows no obvious anisotropy in the context of universal transport. We give a possible explanation of why the anisotropy is seen in most properties but not seen in the universal transport.

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The topic of anisotropic superconductors is currently of great interest in relation to high-temperature superconductivity. For example, in the most studied material YBCO, due to the orthorhombic nature of its band structure, it exhibits strong in-plane anisotropy between some measurable quantities along the $a$ and $b$ axis. Anisotropic behavior is confirmed in the magnetic penetration depth $\lambda$, normal-state resistivity $\rho$, optical conductivity $\sigma(\omega)$, and thermal conductivity $\kappa$. Consistently a value of roughly two is found for the ratio of the carrier density to the effective electron mass (or the square of plasmon frequency) between the $b$-axis and the $a$-axis. This implies, in regard to YBCO, that the contribution from the CuO chain is crucial and of the same order as the CuO$_2$ plane contribution.

It is well known, following a Drude-like model, that the normal-state DC electrical conductivity is given by $\sigma_n = ne^2/\tau m$ with $n$ the carrier density, $m$ the effective mass of the carrier, and $\tau$ the average scattering time. When the system undergoes a phase transition into a superconducting $d_{x^2-y^2}$ state, a universal microwave conductivity $\sigma^{(0)} = ne^2/\tau m \Delta_0$ ($\Delta_0$ is the maximum gap on Fermi surface) is predicted at low temperatures. This universality arises due to the cancellation between the finite impurity-induced quasiparticle density of states at zero energy and the scattering time. Universal features have been confirmed in YBCO by Zhang et al. for the microwave conductivity and by Taillefer et al. for the thermal conductivity. Clearly $\sigma_n$ and $\sigma^{(0)}$ share a common dependence on $n/m$ so that one expects a similar in-plane $a$-$b$ axis anisotropy for them. Apart from the dependence on $n/m$, an anisotropic $\sigma_n$ can also arise from an anisotropic scattering time $\tau$, while the universal $\sigma^{(0)}$, by the meaning of “universal”, is independent of the scattering rate.

More recent thermal conductivity measurements of Chiao et al. which confirm previous microwave conductivity measurements of Zhang et al. on YBCO have observed the predicted low-temperature universality in both $a$ and $b$ directions, but observed no significant anisotropy between the two. This is in contradiction with the large anisotropy observed in many other quantities.

In this paper, we propose a scenario that resolves the discrepancy mentioned above. In reality, YBCO has three conducting layers (two CuO$_2$ plane and one CuO chain layer) within a unit cell. There is strong evidence that the gap in all three layers is mainly $d_{x^2-y^2}$-wave like with some small admixture of an $s$-wave component. The sub-dominant component arises because of the orthorhombic nature of YBCO. The Fermi surfaces are quite different in the different layers. For isolated layers, it is tetragonally two-dimensional for the two CuO$_2$ planes, while it is highly one-dimensional for the CuO chain layer.

![FIG. 1. Fermi surface for CuO$_2$ plane (a) and CuO chain (b) layers in YBCO. Frames (c) and (d) are the $d_{x^2-y^2}$ gaps seen on the Fermi surfaces for the plane and chain layers.](image-url)
open circular Fermi surface and simulates the highly one-dimensional nature of the chain band. The Fermi surface for chain band is shown in Fig. 1(b) with the CuO chain taken to be along the \( k_y \) axis. A cutoff angle, \( \phi_c > \pi/4 \), corresponds to the angular position where a minimum gap starts to appear on the Fermi surface of the chain layer. The measured properties will correspond to the sum of the contributions from the two plane layers (associated with a complete Fermi-surface integration) and the one chain layer (associated with an incomplete Fermi-surface integration).

Measurements on YBCO can be divided into two categories. The ones which are strongly dependent on seeing the gap nodes on Fermi surface (e.g., \( \sigma^0_t \)) and another which are not too dependent such as the value of the zero-temperature penetration depth \( \lambda(0) \). In the former case, due to the cutoff angle, the gap nodes may not cross anywhere on the entire Fermi surface for the chain band, and anisotropy is consequently suppressed because of the reduction of universal conductivity in the chain layer.

**Normal-State Transport.**— Assuming that the scattering rate is not dependent on the direction of the momentum \( \mathbf{k} \), the ratio of normal \textit{chain} conductivity along the \( a \) and \( b \) axis is then given by (\( v \) is the Fermi velocity)

\[
\frac{\sigma^a_n}{\sigma^b_n} = \frac{\langle v_y^2 \rangle_c}{\langle v_y^2 \rangle_c} = \frac{\langle \cos^2 \phi \rangle_c}{\langle \sin^2 \phi \rangle_c},
\]

where, \( \langle A \rangle_c \equiv (2/\pi) \int_{\phi_c}^{\pi/2} d\phi \ A \), denotes an incomplete Fermi-surface average for the chain layer. In Fig. 2, we plot the ratio, as a function of the cutoff angle \( \phi_c \), given in Eq. (1). It is seen, as expected, that \( \sigma^b_n > \sigma^a_n \) when an incomplete Fermi-surface integration is carried out because \( \langle v_y^2 \rangle_c \) has larger components than \( \langle v_y^2 \rangle_c \). When \( \phi_c \) is large corresponding to a flatter band, \( \sigma^b_n \gg \sigma^a_n \). For example in the case \( \phi_c = 45^\circ \), \( \sigma^b_n/\sigma^a_n \approx 4 \). This, in combination with the plane contribution, conforms with the large observed anisotropy between the the \( a \) and \( b \)-axis resistivities [3]. In a strictly 1D model for the chains, \( \sigma^a_n \) would be zero. Here it is finite but becomes small when \( \phi_c \) is large which approaches the chain case more closely and the model is good enough for qualitative arguments.

Similar arguments can be applied to the anisotropy exhibited in the zero-temperature value of the London penetration depth. Recent measurement of Basov et al. [2] showed for pure YBCO that \( \lambda(0) \) \( \approx \) 1600 Å and \( \lambda(0) \) \( \approx \) 1000 Å. In the pure limit, the square of the inverse penetration depth is given by

\[
\frac{1}{\lambda^2(0)} = \frac{8\pi e^2}{c^2} \frac{1}{\Omega} \sum \limits_k v_{k,\mu}^2 \left[ \frac{\partial f(E_k)}{\partial E_k} - \frac{\partial f(\epsilon_k)}{\partial \epsilon_k} \right]
\]

and is associated with the superfluid density. Here \( e \) is electron charge, \( c \) the velocity of light, \( v_{k,\mu} \) is \( \mu \) component of the Fermi velocity, and \( f \) the Fermi-Dirac distribution function. The electron energy in the normal state is \( \epsilon_k \) and \( E_k \) is the quasiparticle energy in the superconducting state with \( E_k = \sqrt{\epsilon_k^2 + \Delta_k^2} \). The zero-temperature value of \( \lambda(0) \) is determined solely by the second term in (1) and depends only on normal-state parameters. By considering an incomplete Fermi-surface integration for the chain layer, one obtains

\[
\frac{\lambda^2(0)}{\lambda^2_0} = \frac{\langle v_y^2 \rangle_c}{\langle v_y^2 \rangle_c} = \frac{\langle \cos^2 \phi \rangle_c}{\langle \sin^2 \phi \rangle_c}
\]

Thus, similar to Eq. (1) for the resistivity ratio, the introduction of a cutoff angle will naturally lead to the right ratio for the observed zero-temperature anisotropy of the penetration depths. (One must add in a plane contribution when comparison with experiment is made.)

**Superconducting-State Transport.**— Using the Kubo formalism, the zero-temperature microwave conductivity along the \( \mu \)-direction for the chain layer is given by

\[
\sigma_{\mu}(0) = c^2 \sum \limits_k \left[ \frac{v_{\mu}^2 \gamma^2}{(\gamma^2 + \epsilon_{\mu}^2 + \Delta_{k,\mu}^2)^2} \right]
\]

where \( c \) denotes an incomplete Fermi surface average, \( \gamma = i\Sigma_{\mu}(\omega = 0) \) is the impurity-induced scattering rate, and \( \Delta_{k,\mu} = \Delta_k + \Sigma_1(\omega = 0) \) is the impurity renormalized gap at zero frequency with \( \Sigma_1 \) the self-energies (see later). It is known that, for a gap with \( d_{x^2-y^2} \)-symmetry and a complete Fermi surface average, there will be no renormalization effect on the gap (\( \Sigma_1 = 0 \)), but this is no longer the case for a chain. After carrying out the energy integration, Eq. (4) is reduced to

\[
\sigma_{\mu}(0) = N(0) e^2 \left[ \frac{\gamma^2(\phi)\gamma^2}{(\gamma^2 + \Delta^2(\phi))^2} \right],
\]

where \( N(0) = m/(2\pi h^2) \) is the electronic density of states at the Fermi surface and \( m \) is the electron mass for the
band. For the a-axis, $\gamma_a(\phi) = \cos \phi$ and for the b-axis, $\gamma_b(\phi) = \sin \phi$.

To show the physics in a transparent way, we first ignore the gap renormalization, $\Delta(\phi) \rightarrow \Delta(\phi) = \Delta_0 \cos(2\phi)$, and manipulate Eq. (5) to obtain $\sigma_{a,b}(0) \equiv (ne^2/\pi m \Delta_0) I_{a,b}(\phi, \gamma)$, where $n = k_F^2/2\pi$ is the layer carrier density and

$$I_{a,b}(\phi, \gamma) \equiv 2 \int_{\phi_c}^{\pi/2} d\phi \frac{(\cos^2 \phi, \sin^2 \phi) \pi^2}{[\gamma^2 + \cos^2 2\phi]^{3/2}}.$$  (6)

Here, $\gamma \equiv \Delta_0/\Delta$ is the normalized scattering rate. The effect of impurities on the renormalization of the gap and on the effective scattering rate will be discussed later. In Fig. 3, we plot $I_{a,b}$ for two different choices of $\gamma$, namely $\gamma = 0.1$ and $0.01$ for small $\gamma$, the function $I_a$ is indistinguishable from $I_b$ at all values of $\phi_c$. Only when $\gamma$ is large, does $I_b$ starts to deviate from $I_a$ and, due to the fact that the chain Fermi surface mainly develops in the $\phi = \pm \pi/2$ region and has no contribution from the $\phi = 0, \pi$ region, $\sigma_0(0)$ is slightly larger than $\sigma_a(0)$. More importantly, $I_{a,b}$ almost vanish as long as $\phi_c > \phi_0$ (nodal angle) in the small $\gamma$ case. (In our present case for simplicity, we have $\phi_0 = \pi/4$.)

![FIG. 3. Values of $I_a$ and $I_b$ defined in Eq. (5) in terms of the cutoff angle $\phi_c$. The angle $\phi_0$ corresponds to the node. Top frame is for $\gamma/\Delta_0 = 0.01$ and bottom frame is for $\gamma/\Delta_0 = 0.01$.](image)

The small saturated low-temperature microwave conductivity in a $d_{x^2-y^2}$-wave superconductor is recovered from Fig. 3 in the case of $\phi_c \rightarrow 0$. As is clearly seen in Fig. 3, both $I_a$ and $I_b$ approach one and the conductivity is saturated to the value $\sigma_a(0) = \sigma_b(0) \rightarrow \sigma^0 \equiv ne^2/(\pi m \Delta_0)$, independent of $\gamma$, i.e., of the impurity concentration. It is worth emphasizing that both $\sigma_a(0)$ and $\sigma_b(0)$ are close to the saturated value $\sigma^0$ as long as $\phi_c < \phi_0$. The latter case means that the gap nodes cross pieces of the Fermi surface. In the opposite case $\phi_c > \phi_0$, the residual conductivity $\sigma_a(0)$ and $\sigma_b(0)$ (or $I_a$ and $I_b$) are both strongly suppressed. In this case, no gap nodes cross the one-dimensional chain Fermi surface. This is an effect due solely to the geometry of the chain Fermi surface and arises even though the gap used in our model calculation has pure $d_{x^2-y^2}$ symmetry. Moreover, when $\phi_c > \phi_0$ and a minimum gap $\Delta_{\min} \equiv \Delta_0 \cos(2\phi_c)$ is seen on the chain Fermi surface, one can show that $I_a < \pi (\cos^2 \phi_c \gamma^2 / (\gamma^2 + \Delta_{\min}^2))^{3/2}$ and $I_b < \pi (\sin^2 \phi_c \gamma^2 / (\gamma^2 + \Delta_{\min}^2))^{3/2}$. Here $\Delta_{\min} \equiv \Delta_{\min}/\Delta_0$. This means that both $I_a$ and $I_b$ are negligibly small when $\gamma \ll \Delta_{\min}$.

Thus, for the case of YBCO under consideration here, there is a possibility that the gap nodes do not cross the entire Fermi surface for the highly one-dimensional chain band ($\phi_c > \phi_0$) and, as a consequence, no saturation for $\sigma_a(0)$ occurs in the chain layer. In addition, for the same reason that the residual conductivity is strongly suppressed in chain layer (for both a and b-axes), there is no significant anisotropy in the residual microwave conductivity.

In order to understand what the temperature regime is, in which the universal value is valid for YBCO, one recalls that the low-temperature microwave conductivity, $\sigma(T) \simeq \sigma^0(1 + T^2/\gamma^2)$, as given by Hirschfeld et al. [3] for a $d_{x^2-y^2}$-wave superconductor with a complete circular Fermi-surface. Therefore, for the CuO$_2$ planes only, one needs to have $T \ll \gamma$ to achieve universality. For the chain layer in which the gap nodes do not cross the chain-band Fermi surface, a minimum gap $\Delta_{\min}$ is seen and a result similar to the s-wave case holds for the low temperature residual conductivity, namely $\sigma(T) \simeq \sigma_0(\Delta_{\min}/T) e^{-\Delta_{\min}/T}$ is predicted (see, for example, Ref. [13]). The chain residual conductivity is thus strongly suppressed until the temperature $T \gtrsim \Delta_{\min}$. The above picture corresponds exactly to the strong suppression of $\sigma_a(0)$ and $\sigma_b(0)$ for chain layer discussed before. Hence, the chain layer will have little effect on the temperature limit where universality holds if $\Delta_{\min}$ associated with the chain is larger than $\gamma$ associated with the plane.

Now we discuss the effect of impurity scattering on the zero-frequency effective scattering rate $[\gamma = i\Sigma_0(\omega = 0)]$ and gap renormalization $[\delta \Delta_k = \Delta_k - \Delta_k = \Sigma_3(1 + \omega)]$. In the usual t-matrix approximation, the self-energies $\Sigma_3(\omega) = n_i G_0 / (c^2 - G_0^2 + G_k^2)$ and $\Sigma_1(\omega) = -n_i G_1 / (c^2 - G_0^2 + G_k^2)$ with $n_i$ the impurity concentration, $c^2 \equiv 1/v_i^2$ ($v_i$ is the impurity potential), and the integrated Green’s function $G_k(\omega) \equiv \sum_k G_k(k, \omega)$. We note in general that the impurity renormalization effect should also be included in the band structure $\delta \Delta_k = \Sigma_3$ (in a general sense, $\phi_c$ will also be renormalized in our model). However, this is safely neglected.

In the unitary resonant scattering limit ($c = 0$), we obtain the coupled equations $[\delta \Delta_k \equiv \delta]$:

$$\gamma = \frac{n_i}{2\pi N(0)} \frac{I_0(\phi_c)}{I_0^2(\phi_c) + I_1^2(\phi_c)}$$
$$\delta = \frac{n_i}{2\pi N(0)} \frac{I_1(\phi_c)}{I_0^2(\phi_c) + I_1^2(\phi_c)}.$$  (7)
negative is because the highly 1D Fermi surface samples negative. The strong suppression of $\gamma$ wave superconductor towards an other hand, the result that the gap renormalization $\delta$ is decaying exponentially as $\gamma$ is noted in Fig. 4: (i) gap $\Delta_{\text{min}}$ proportional to $1/\sqrt{\phi_c}$ and gap renormalization $\delta$, (ii) the gap renormalization $\delta$ and $\gamma$ are given by Eqs. (7) and (8) respectively, (iii) the impurity-induced effective scattering rate $\gamma$ and gap renormalization $\delta$ scaled to $\Delta_0$ (gap maximum in the absence of impurity). Solid line is for $n_i/4N(0)\Delta_0 = 0.1$ and dashed line is for $n_i/4N(0)\Delta_0 = 0.01$ with $n_i$ the impurity concentration.

\[
I_0(\phi_c) = \left< \frac{\bar{\delta}}{\sqrt{\gamma^2 + \left(\cos 2\phi + \tau\delta\right)^2}} \right>_{c},
\]
\[
I_1(\phi_c) = \left< \frac{\cos 2\phi + \bar{\delta}}{\sqrt{\gamma^2 + \left(\cos 2\phi + \tau\delta\right)^2}} \right>_{c},
\]

with $\bar{\delta} = \delta/\Delta_0$. In Fig. 4 we show our self-consistent solutions for $\gamma$ and $\delta$ as a function of $\phi_c$ given by Eqs. (7) and (8). We have used two different impurity concentrations, namely $n_i/4N(0)\Delta_0 = 0.1$ and 0.01. Two features are noted in Fig. 4: (i) $\gamma$ is strongly suppressed in the large $\phi_c$ case and (ii) the gap renormalization $\delta$ is always negative. The strong suppression of $\gamma$ in the larger $\phi_c$ case is a natural consequence of the evolution of a $d$-wave superconductor towards an $s$-wave superconductor (i.e., a minimum gap $\Delta_{\text{min}}$ develops in the chain). On the other hand, the result that the gap renormalization $\delta$ is negative is because the highly 1D Fermi surface samples mainly the negative portion of the $d$-wave gap.

Analytical results are available in three different regimes. In the $\phi_c \to 0$ limit, one recovers the results for the complete Fermi surface case (appropriate for CuO$_2$ plane) that is $\gamma \sim (\Delta_0/\tau)^{1/2}$ [$\tau^{-1} \sim n_i/N(0)$ is the normal-state scattering rate] and $\delta = 0$ (i.e., no gap renormalization). When $\phi_c$ is small but finite (in the case that Fermi surface still sees nodes but the band structure has evolved from the tetragonal to the orthorhombic limit), we find $I_0 \simeq -\gamma \ln \gamma$ and $I_1 \simeq 1/\phi_c$. Consequently, $\gamma \sim \Delta_0 \exp(-\tau \Delta_0 \phi_c^2)$ and $\delta \sim 1/(\phi_c)$. Thus, $\gamma$ is decaying exponentially as $\phi_c$ increases and $|\delta|$ is proportional to $1/\phi_c$. When $\phi_c > \phi_0$ such that a minimum gap $\Delta_{\text{min}}$ develops on the Fermi surface, we find $\gamma$ is small (similar to the $s$-wave case), while $\delta \sim 1/(\tau(\pi/2 - \phi_c))$.

Therefore, $|\delta|$ increases as $\phi_c$ increases and diverges when $\phi_c$ approaches $\pi/2$. Of course, the latter case is an unphysical regime. The three different regimes for $\delta$ are seen most clearly in Fig. 4.

Since $\delta < 0$, the gap nodes will be effectively shifted downward (or equivalently $\phi_0 < \pi/4$). As a result, this effect increases the chance that the gap nodes will not cross the entire chain Fermi surface. In addition to the effect of impurity, the appearance of a negative $s$-wave admixture in the $d_{x^2-y^2}$-wave gap can naturally distort the gap nodes to be less than 45 degree and thus leads to a similar consequence. A finite minimum gap on the chain Fermi surface is therefore seen to be a robust feature of the one dimensional nature of the bands and of a $d$-wave gap. Recently, a detailed survey of the effect of Ni impurity (substitution for Cu) on YBCO has been carried out by Homes et al. using optical measurement. They concluded that the deposition of Ni is mainly situated in the chain layer. Hence the change with Ni impurity concentration can be used to test our model.

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