c-Axis Infrared Conductivity of a $d_{x^2-y^2}$-Wave Superconductor with Impurity and Spin-Fluctuation Scattering

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Abstract

Results of a calculation of the $c$-axis infrared conductivity $\sigma_c$ for a $d_{x^2-y^2}$-wave superconductor which include both elastic impurity and inelastic spin-fluctuation scattering are presented and compared with the $ab$-plane conductivity $\sigma_{ab}$ in the same model. In this model, the interlayer $c$-axis coupling is taken to be weak and diffusive. While in clean systems, inelastic scattering leads to a peak at $\omega = 4\Delta_0$ in $\sigma_{ab}$ for $T < T_c$, it has little effect on the corresponding $\sigma_c$, which exhibits structure only at $\omega \approx 2\Delta_0$ and is directly related to the single-particle density of states $N(\omega)$. The $c$-axis penetration depth $\lambda_c$ in the same model is predicted to vary as $T^3$ at low temperatures in clean samples. We discuss recent optical experiments on the cuprates and compare with these predictions.

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I. INTRODUCTION

In the superconducting state of optimally doped \(YBa_2Cu_3O_{7-\delta}\), a gap-like depression develops in the frequency dependence of the \(c\)-axis conductivity for \(T\) less than \(T_c\). As emphasized by Homes et al., this behavior is quite different from the in-plane \(ab\) conductivity observed in samples from the same source. We have recently developed a simple model for the \(ab\) conductivity which provided a qualitative fit to experimental data, and here we extend this model to see how well it can describe the \(c\)-axis conductivity. The model consists of BCS quasi-particles with a \(d_{x^2-y^2}\) gap and a lifetime determined by both elastic and inelastic scattering processes. The latter inelastic lifetime plays a key role in our model and was calculated from a spin-fluctuation interaction in which the quasi-particle \(d_{x^2-y^2}\) gap entered explicitly in determining the spectral weight of the spin-fluctuations. The elastic scattering, which is important at low frequencies, was treated in the resonant impurity scattering limit. Here, in discussing the \(c\)-axis conductivity, we will treat the interlayer transport as weak and diffusive. Our conclusion from this analysis is that a model of a \(d_{x^2-y^2}\) superconductor which includes inelastic as well as elastic scattering can provide a sensible fit of both the \(ab\) and the \(c\)-axis conductivities. In particular, it predicts the existence of absorption features at \(4\Delta_0\) in \(\sigma_{ab}\) and at \(2\Delta_0\) in \(\sigma_c\), where \(\Delta_0\) is the \(d\)-wave gap maximum; such features are apparently observed in a variety of materials. To the extent that the interlayer coupling can be treated as weak and diffusive, the \(c\)-axis conductivity provides direct information on the single particle density of states in a similar manner to SIS tunneling.

II. C-AXIS CONDUCTIVITY

The nature of \(c\)-axis transport in the cuprates is still controversial, but it is widely believed to be weak and incoherent. A simple model which describes this has \(H = H_0 + H_c\), where \(H_0\) describes free particles with residual \(d_{x^2-y^2}\) BCS pair interaction, and

\[
H_c = \sum_{i\sigma} V_i (c_{i1\sigma}^{\dagger} c_{i2\sigma} + h.c.),
\]
where the $V_i$ may be thought of as randomly placed static impurities mediating hopping between planes 1 and 2. We emphasize, however, that the end result of our treatment will yield a description in terms of a single $c$-axis relaxation time which must be similar to any weak diffusive transport model. The interplane paramagnetic current operator for a given configuration of the random potential is then

$$j_c^p = -ied \sum_i V_i (c_{i1\sigma} c_{i2\sigma} - h.c.). \quad (2)$$

The response to an applied electromagnetic field $\mathbf{A}$ is now determined by expanding the kinetic energy of the system up to second order in $\mathbf{A}$, yielding for the expectation value of the total current

$$\langle j_c(q, \omega) \rangle = [d^2 e^2 \langle H_c \rangle + \Lambda_{cc}(q, \omega)] A_z(q, \omega), \quad (3)$$

where $\langle j_c^p \rangle \equiv \Lambda_{cc} A_z$ to leading order.

We first examine the conductivity $\sigma_c(q = 0, \omega)$, assuming that $V$ is weak, thereby neglecting multiple scattering vertex corrections as well as self-energy corrections, since one power of $V$ is already contained in each of the $c$-axis current operators which enter $\Lambda_{cc}$. After impurity averaging, we find

$$\sigma_c(\omega) = -\frac{\text{Im}\Lambda_{cc}(\omega)}{\omega}, \quad (4)$$

with

$$\text{Im}\Lambda_{cc}(\omega) =$$

$$4\pi d^2 e^2 \int d\omega' \sum_{\mathbf{pp}' \mathbf{p}} |V_{\mathbf{p} - \mathbf{p}'}|^2 (f(\omega + \omega') - f(\omega')) \times (A(p, \omega + \omega') A(p', \omega') + B(p, \omega + \omega') B(p', \omega')) \quad (5)$$

Here the normal and anomalous spectral functions are defined as $A(p, \omega) = -\frac{1}{2\pi} \text{ImTr}\{\mathcal{G}(\mathbf{k}, \omega + i0)\}$, $B(p, \omega) = -\frac{1}{2\pi} \text{ImTr}\{\tau_1 \mathcal{G}(\mathbf{k}, \omega + i0)\}$, where $\mathcal{G}$ is the matrix Green’s function

$$\mathcal{G}(\mathbf{k}, \omega) = \frac{\tilde{\omega} \tau_0 + \xi_p \tau_3 + \Delta_0 \tau_1}{\tilde{\omega}^2 - \xi_p^2 - \Delta_p^2}. \quad (6)$$
The interlayer scattering matrix element $V_{p-p'}$ is defined by

$$V_i = \sum_m \mathcal{V}(R_i - R_m) = \sum_{p,m} V_p e^{ip \cdot (R_i - R_m)}, \quad (7)$$

where $m$ runs over all lattice sites and $i$ labels an impurity site. For simplicity we take a cylindrical Fermi surface with $\xi_p = (p^2/2m - \mu)$ and a $d_{x^2-y^2}$ gap $\Delta_p = \Delta_0(T) \cos 2\phi$.

The renormalized frequency $\tilde{\omega}$ includes the effects of scattering associated with the in-plane impurities and the lifetime effects due to dynamic spin fluctuations. In the resonant limit, the in-plane impurity scattering gives a renormalized quasi-particle energy $\tilde{\omega}$ determined by the self-consistent solution of

$$\tilde{\omega} = \omega - \Sigma_{imp}(\tilde{\omega}) = \omega + i\Gamma/\left(\frac{\tilde{\omega}}{\sqrt{\tilde{\omega}^2 - \Delta^2_k}}\right)_{\text{FS}}. \quad (8)$$

Here $\Gamma = n_i/\pi N_0$, with $n_i$ the impurity concentration and $N_0$ the Fermi level density of states.

We assume further that the inelastic scattering rate $\tau^{-1}_{\text{in}}(\omega, T)$ arising from spin fluctuations can be calculated separately, and take as a model the one-antiparamagnon self-energy calculated in a 2D Hubbard model by Quinlan et al. The momentum dependence of the full $1/\tau_{\text{in}}(p, \omega)$ has been neglected here in favor of a simpler effective relaxation rate for quasiparticles at the gap nodes, $1/\tau_{\text{in}}(\omega) \equiv 1/\tau_{\text{in}}(k_{\text{node}}, \omega)$ as discussed in Refs. At low temperatures $\tau^{-1}_{\text{in}}$ varies as $\omega^3$ for $\omega \lesssim 3 \Delta_0$, reflecting the usual $\omega^2$ dependence of an electron-electron scattering process along with a third factor of $\omega$ arising from the $d_{x^2-y^2}$ density of states. For $\omega \gtrsim 3 \Delta_0$, $1/\tau_{\text{in}}$ crosses over to the pseudo-linear behavior found in spin-fluctuation scattering calculations in the normal state. Although for concreteness we have chosen a particular model for $1/\tau_{\text{in}}$, we note that the behavior in the superconducting state is characteristic of any model based on electron-electron scattering with quasiparticles which are well-defined at sufficiently low temperatures, in the presence of gap line nodes.

Combining the elastic and inelastic contributions, we set

$$\tilde{\omega} = \omega - \Sigma_{imp}(\tilde{\omega}) + \frac{i}{\tau_{\text{in}}(\omega, T)}. \quad (9)$$
in Eqs. (8) and (9). The resulting lifetime for in-plane scattering is plotted in Fig. 1 for several values of the impurity concentration. Note the Hubbard parameters have been chosen so as to give a value of $1/\tau_m(\omega \to 0, T_c) = 2T_c$.

As discussed by Graf et al., setting $|V_{pp'-p'}|^2$ equal to a constant corresponds to diffuse transmission, while taking an extreme forward scattering form such that $\hat{p} = \hat{p}'$ (that is, $\phi = \phi'$) corresponds to specular transmission. In the diffuse transmission limit, the second term in Eq. (5), arising from pair transfers, vanishes for a $d$-wave gap. In the actual system, $|V_{pp'}|^2$ is anisotropic, and here we model this using the separable form

$$|V_{pp'}|^2 = |V|^2 + |V'|^2 \cos 2\phi \cos 2\phi'.$$

The interaction strength $V$ can be adjusted to fit the normal state $c$-axis conductivity

$$\sigma_{cn} = 2d^2e^2N_0/\tau_c$$

with $\tau_c^{-1} = 2n_c^\xi \pi N_0|V|^2$. Here $n_c^\xi \sim \mathcal{O}(1)$ is formally the density of scattering sites which allows the planes to communicate. The second term $V'$ can be used to fit the $c$-axis penetration depth $\lambda_c(0)$ (see below)

$$\frac{c}{4\pi \lambda_c^2(0)} = 0.480\sigma_{cn} \left| \frac{V'}{V} \right|^2 \Delta_0(0).$$

For $\sigma_n \sim 150 (\Omega \text{ cm})^{-1}$ and $\lambda_c(0) \sim 10^4 \text{ A}$, we find $|V'/V|^2 = \mathcal{O}(1)$.

With the form (10) for $|V_{pp'-p'}|^2$, the expression Eq. (4) for $\sigma_c(\omega)$ simplifies to

$$\frac{\sigma_c(\omega)}{\sigma_{cn}} = \frac{1}{\omega} \int d\omega' \left( f(\omega') - f(\omega' + \omega) \right)$$

$$\times \left( N(\omega + \omega')N(\omega') + \left| \frac{V'}{V} \right|^2 M(\omega + \omega')M(\omega') \right),$$

with

$$N(\omega) = \text{Re} \left\langle \sqrt{\tilde{\omega}^2 - \Delta_p^2} \right\rangle_{\text{FS}} = \frac{2}{\pi} \text{Re} \left\langle \frac{\Delta_0}{\tilde{\omega}} \right\rangle$$

and

$$M(\omega) = \text{Re} \left\langle \sqrt{\tilde{\omega}^2 - \Delta_p^2} \right\rangle_{\text{FS}}$$

$$= \frac{2}{\pi} \text{Re} \left\{ \frac{\Delta_0}{\tilde{\omega}} \left[ K(\Delta_0/\tilde{\omega}) - E(\Delta_0/\tilde{\omega}) \right] \right\}.$$
Here $K$ and $E$ are the complete elliptic integrals of the first and second kinds, respectively. Results for $\sigma_c(\omega)/\sigma_{cn}$ versus $\omega$ at different temperatures are shown in Fig. 2 under the assumption of isotropic diffusive scattering ($|V'/V|^2 = 0$).

The primary feature seen in the figure is the pseudogap of width $2\Delta_0$ which opens up below $T_c$. The low-frequency behavior can be estimated in this limit to be $\sigma_c(\omega)/\sigma_{cn} \simeq 2\omega^2/3\Delta_0^2$. Figure 3 illustrates the effects of adding anisotropy to the interplane scattering, as well as intraplane scattering effects. Because of the form of Eq. (12) as a convolution of normal and anomalous densities of states, the shoulder feature at $2\Delta_0(T)$ is quite robust.

While strongly scattering in-plane impurities ($\Gamma > 0$) can alter the very low-frequency behavior, the $2\Delta_0$ shoulder is essentially unaffected. The large intraplane relaxation rate near $T_c$ might be expected to change the behavior in an important way, but this is seen not to be the case, since the effect of a large $1/\tau$ is simply to smear out the density of states factors entering Eq. (12). Scattering anisotropy ($|V'/V|^2 > 0$) also does not lead to important qualitative differences from the results of Fig. 2, since the anomalous terms in the convolution give rise to a low-energy contribution to the conductivity of order $(\omega/\Delta_0)^4$. The results in these limits are therefore similar to those obtained earlier by Graf et al. In Fig. 4 we compare these results to the experimental data of Homes et al.; here we have chosen a parameter set which appears to give a reasonable fit to the $ab$ penetration depth and conductivity, but the $c$-axis conductivity is not terribly sensitive to this choice.

Due to the weak behavior of the anomalous density of states at low temperatures, we note that within this model a measurement of the $c$-axis conductivity provides a nearly direct measurement of the in-plane density of states $N(\omega)$. It will be interesting to compare $N(\omega)$ obtained in this way to results obtained, e.g., from tunneling measurements.

III. C-AXIS PENETRATION DEPTH

The real part of the current-current correlation function may also be calculated, yielding...
The diamagnetic term in Eq. (3) takes the form
\[ \langle H_c \rangle = 2n_i T \sum_{\omega_n} \sum_{p p' \sigma} |V_{pp'}|^2 \]
\[ \times \frac{1}{2} \text{Tr}[\tau_0 G_\sigma(p, \omega_n) \tau_0 G_\sigma(p', \omega_n)]. \]
which means that only the product of the anomalous Green’s functions survives in this approximation.

The remaining frequency sums and integrals may be evaluated in the diffusive limit treated above to find the London penetration depth, \( \lambda_c(T) \), as
\[ \frac{c}{4\pi \lambda_c(T)^2} = -\sigma_{cn} |V'/V|^2 \int d\omega \tanh(\frac{\omega}{2T}) \text{Im}[\Phi(\omega)^2] \]
\[ \simeq \sigma_{cn} |V'/V|^2 \Delta_0(T)[0.480 - \frac{6\zeta(3)}{\pi} \left( \frac{T}{\Delta_0(T)} \right)^3], \]
where \( \Phi = \frac{2}{\pi} \frac{\Delta_0}{\Delta_0}\left[K(\Delta_0/\bar{\omega}) - E(\Delta_0/\bar{\omega})\right] \) is the same angular average appearing in Eq. (14).

Note the last approximate equality is valid for \( T \ll T_c \) in the clean limit only. The expression (17) is equivalent to the result obtained by Radtke et al.\[6\] in the absence of direct interlayer tunneling. In Fig. 5 we have plotted the temperature dependence of \( \lambda_c(0)^2/\lambda_c(T)^2 \) for various values of the in-plane impurity scattering rate. As in the ab case\[13\] we expect a crossover to a \( \delta \lambda_c \sim T^2 \) behavior at low temperatures when the system becomes sufficiently dirty. Although the normalized superfluid density \( (\lambda_c(0)/\lambda_c(T))^2 \) is quite insensitive to the presence of planar impurities, as seen in Fig. 5, we note the peculiar result that in this model the penetration depth itself scales roughly with the c-axis conductivity, and should therefore be quite sensitive to disorder which affects c-axis transport.

IV. COMPARISON OF AB AND C-AXIS DATA

In constructing phenomenological theories of this kind, it is important to see if a consistent description of a wide class of experiments can be obtained, along with an understanding
of the effects of disorder. In this regard we would like to predict correlations among various quantities which should hold at least for all optimally doped materials, and possibly in the underdoped systems as well. The most important such correlation to emerge from the current analysis is the prediction of a clear shoulder in the $c$-axis conductivity at $\omega = 2\Delta_0$, a broad maximum in the $ab$ conductivity at $4\Delta_0$, and a shoulder-like feature in $1/\tau_{ab}(\omega)$ at $3\Delta_0$. Since the gap maximum $\Delta_0$ is not known for all materials, one can search for correlations of such features in optical experiments. While such a method will not provide the most accurate measure of the gap size, it will serve to confirm the general picture of a $d$-wave order parameter with nodal quasiparticles scattered by resonant defects of some kind at low energies, and strong spin-fluctuation scattering at higher energies. In Fig. 6, we show $\sigma_c$, $\sigma_{ab}$, and $1/\tau_{ab}$ together to illustrate the correlations we expect. In Fig. 7, we show data on $YBa_2Cu_3O_{6.95}$, $YBa_2Cu_3O_{6.6}$, and $YBa_2Cu_4O_8$ from recent work by Basov et al. Here we would like to note some similarities between the results for the optimally doped material below its $T_c$, and the behavior of the underdoped materials above their transition temperatures in the so-called pseudogap regime. The most distinct feature is the shoulder in $\sigma_c$ (upper panel of Fig. 7), which, as we have discussed, occurs at $2\Delta_0 \simeq 6 - 8T_c$ for $YBa_2Cu_3O_{6.95}$. In the underdoped compounds this shoulder, at what we will call “$2\Delta_0$”, becomes visible above $T_c$ in the pseudogap regime. In the underdoped compounds, “$2\Delta_0$” from this criterion is slightly reduced from its value in the optimally doped materials. The second panel in Fig. 7 shows $\sigma_{ab}(\omega)$. In Ref. 8, the absence of a $2\Delta_0$ structure and the broad rise at $4\Delta_0$ observed in the $ab$-plane conductivity of $YBa_2Cu_3O_{6.95}$ below $T_c$ at 1000 cm$^{-1}$ was attributed to a $4\Delta_0$ inelastic absorption threshold smeared by $d$-wave nodal quasiparticles. Now, as is well known, there is no gaplike structure in the $ab$ conductivity (second panel of Fig. 7) in the doping range for which the pseudogap is observed in the $c$-axis conductivity; there is, however, a narrowing of the Drude peak and a broad rise at higher frequencies near “$4\Delta_0$”. It could be that the appearance of the “$2\Delta_0$” in $\sigma_c$ but not in $\sigma_{ab}$ is similar to the behavior we have found for these quantities below $T_c$ in the model we have applied to $YBa_2Cu_3O_{6.95}$, in which the crucial factor is the direct relevance of the density of states
$N(w)$ to $c$-axis transport. Support for the correlation of the $c$-axis pseudogap and the density of state is found in studies by Homes et al.\textsuperscript{[1]} which found scaling of the pseudogap with the Knight shift in underdoped cuprates. Finally, as shown in the bottom panel of Fig. 7, that the in-plane relaxation rate for the underdoped materials shows a strong supression of the linear frequency dependence in the pseudogap regime even above $T_c$. In all cases shown, the crossover to stronger frequency dependence at sufficiently low temperatures occurs at an energy consistent with the “$3\Delta_0$” smeared threshold expected from the current model.

We turn finally to the comparison of the $c$-axis penetration depth with its $ab$ counterpart. The results are shown in Fig. 8 for the clean limit, and compared to the data of Hardy et al.\textsuperscript{[16]} on $YBa_2Cu_3O_{6.95}$. It is clear that the result agrees qualitatively with the much flatter temperature dependence of the $c$-axis penetration depth found at low temperatures. The low temperature behavior is not yet well characterized, however. The discrepancies result, in the intermediate temperature range, from the crude isotropic band structure assumed, and in the range close to $T_c$ from critical fluctuations not accounted for in the current model.

**V. CONCLUSIONS**

We have argued that a simple theory of $d$-wave superconductivity, together with impurity and spin fluctuation scattering, accounts for most of the qualitative aspects of both optical conductivity and London penetration depth measurements for currents along both the $a$ and $c$ axes. $c$-axis properties have been calculated under the further assumption that transport is primarily diffusive. The optical conductivities $\sigma_c$ and $\sigma_{ab}$ may then be correlated in this model, in that we expect a broad peak in $\sigma_{ab}$ at $\omega \approx 4\Delta_0$ and a shoulder-like feature in $\sigma_c$ at $\omega \approx 2\Delta_0$. This behavior indeed appears to be reproduced qualitatively in several materials, including underdoped materials, where a behavior qualitatively similar to that observed in the optimally doped materials below $T_c$ is seen significantly above $T_c$. If the phase coherence implicit in the BCS approach is ignored, the model considered here offers a natural interpretation of these results and an explanation of why the normal state $c$-axis
pseudogap does not manifest itself in planar transport properties. Further study is needed to put these speculations on a firmer basis.

Finally, we have calculated and compared the $c$-axis London penetration depth in the same model, and shown that in clean systems it will vary as $\delta \lambda_c \sim T^3$ at low temperatures. This temperature dependence is much stronger than the $ab$ result, $\delta \lambda_{ab} \sim T$ in the same model, in qualitative agreement with experiments on optimally doped $YBa_2Cu_3O_{7-\delta}$.

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FIG. 1. Normalized intraplane inelastic relaxation rate $\tau_{\text{in}}^{-1}(\omega)/\Delta_0(0)$ vs. $\omega/\Delta_0$. Solid line: $T = 0$; dashed-dotted line: $T = 0.8T_c$; dashed line: $T = T_c$. In all cases $\Delta_0(0)/T_c = 3$.

FIG. 2. Normalized $c$-axis conductivity $\sigma_c(\omega)/\sigma_{\text{cn}}$ vs. $\omega/\Delta_0(0)$. Solid line: $T = 0$; dashed-dotted line: $T = 0.5T_c$; dotted line: $T = 0.8T_c$; dashed line: $T = T_c$. Scattering anisotropy parameter $|V'/V|^2=0$, planar impurity scattering rate $\Gamma = 0$, $\Delta_0(0)/T_c = 3$. 

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FIG. 3. Normalized $c$-axis conductivity $\sigma_c(\omega)/\sigma_{cn}$ vs. $\omega/\Delta_0(0)$ for $T = 0$. a) $|V'|^2 = 0$ with scattering (dashed line, $\Gamma = 0.1T_c$ and inelastic scattering included) and without scattering (solid line, $1/\tau = 0$); b) $1/\tau = 0$ with $|V'|^2 = 1$ (dashed line) and $|V'|^2 = 0$ (solid line).
FIG. 4. Normalized c-axis conductivity $\sigma_c(\omega)/\sigma_{cn}$ vs. $\omega/\Delta_0(0)$, $|V'/V|^2 = 0$, $\Gamma = 0.02T_c$, inelastic scattering included, $T = T_c$ (dashed line), $T = 0.8T_c$ (dashed-dotted line), and $T = 0.1T_c$ (solid line), for $\Delta_0/T_c = 3$. Data from Homes et al. on $YBa_2Cu_3O_{6.95}$, solid line: $T=10$K, dashed line: $T=100$K. $\sigma_{cn}$ normalized to 100K data at 100 cm$^{-1}$.

FIG. 5. Inverse c-axis London penetration depth $\lambda_c(0)^2/\lambda_c(T)^2$ vs. normalized temperature $T/T_c$. Solid line: intraplane impurity scattering rate $\Gamma/T_c = 0$; dashed-dotted line: $\Gamma/T_c = 0.05$; dashed line: $\Gamma/T_c = 0.1$. Inelastic scattering included.
FIG. 6.  a) Normalized $c$-axis conductivity $\sigma_c(\omega)/\sigma_{cn}$ vs. $\omega/\Delta_0(0)$; b) $ab$-plane conductivity $\sigma_{ab}(\omega)/\sigma_0$ vs. $\omega/\Delta_0(0)$ (Note $\sigma_0 \equiv \sigma_{ab}(\omega = 0)$ at $T = T_c$); c) quasiparticle relaxation rate $\tau_{in}^{-1}(\omega)/\Delta_0$ vs. $\omega/\Delta_0(0)$. All panels show results for $\Gamma/T_c = 0.02$, $T = 0.1T_c$ (solid line), $0.8T_c$ (dashed-dotted line), and $T_c$ (dashed line).
FIG. 7. Data of Basov et al. for $YBa_2Cu_3O_{6.95}$, $YBa_2Cu_4O_8$, and $YBa_2Cu_3O_{6.6}$, in columns from left to right. Dashed-dotted lines: 300K, dashed lines: $T \simeq T_c$, solid lines: 10K. The $c$-axis conductivity of single crystals is taken from Homes et al. and multiplied by a factor of 4. Lines indicate position of shoulder ($2\Delta_0$) in $\sigma_c$, and twice this energy. (Lines not included in LANL archived preprint.)
FIG. 8. Inverse $c$-axis and $ab$-plane London penetration depth $\lambda_{c,ab}(0)^2/\lambda_{c,ab}(T)^2$ vs. normalized temperature $T/T_c$ for intraplane impurity scattering rate $\Gamma = 0$, no inelastic scattering included. Data from Hardy et al. on $YBa_2Cu_3O_{6.95}$.