Anisotropic normal-state transport properties predicted and analyzed for high-T_c oxide superconductors

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Electronic energy bands calculated from local-density-functional (LDF) theory are used to predict anisotropic transport properties of the oxide superconductors $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_7$. Calculations of the magnitude of the resistivity tensor $\rho_{\alpha\beta}$ (assuming only electron-phonon scattering) lead to results smaller than those given by current experiments, suggesting that LDF theory overestimates the Drude plasma frequency (or Fermi velocity), or else that another scattering mechanism dominates. Determinations of the Fermi velocity from critical-field measurements suggest, however, that it is close to the LDF value. Quantities which are independent of the scattering are calculated with more success: the resistivity anisotropy ρ_{zz}/ρ_{xx}, the Hall tensor $R^H_{\alpha\beta\gamma}$, and the thermopower $S_{\alpha\beta}$. It is predicted that R^H should appear "holelike" when electrons orbit in metallic planes but S should appear "electronlike" for thermal gradients in the plane. When fields are tipped 90°, all coefficients change sign. There are very little single-crystal data to compare with, but what exist are qualitatively consistent, including anomalous signs of the Hall tensor. Polycrystalline data for R^H seem completely at variance with the LDF results, so it is surprising how well single-crystal results agree.

I. INTRODUCTION

There are already nearly 100 papers reporting measurements of normal-state transport properties of oxide superconductors. In principle, these data reveal much about the still-mysterious electronic behavior of these compounds. This paper reports on analysis of normal-state transport based on local-density-functional (LDF) band theories, specifically the resistivity $\rho_{\alpha\beta}$, the Hall tensor $R^H_{\alpha\beta\gamma}$, and the thermopower $S_{\alpha\beta}$. The calculated anisotropy of these tensors is so large as to make comparisons with polycrystalline data nearly meaningless.

The normal state of ordinary superconductors such as Nb or Nb_3Sn is a Fermi liquid with quasiparticle energies $\varepsilon(k)$ which agree surprisingly well with eigenvalues obtained from LDF band theory. Transport properties[1] are described by the Bloch-Boltzmann theory,[2] and superconducting properties are described by Eliashberg theory.[3] Both of these theories rest on the Migdal approximation,[4] i.e., on the existence of a small parameter $N(0)\hbar\omega_D$ or $N(0)\hbar/\tau$ where $N(0)$ is the electron density of states at the Fermi level and τ is the scattering time, and they presume that the dominant interaction is electron-phonon. For the new oxide superconductors there is serious doubt that any of these conditions apply. Specifically, there are regions of the x,T (concentration, temperature) phase diagram exhibiting antiferromagnetism and Mott-insulating behavior. In these nonsuperconducting regions, conventional band theory does not apply. It is therefore plausible to assume that even in the metallic and superconducting regions, the physics may be dominated by a large on-site Hubbard U, and that the conventional band Fermi-liquid picture continues to fail. However, this is by no means certain. For example, Pd metal has a fraction of a d hole per atom and a significant on-site U, yet is quite well described as a band Fermi liquid. It might also be the case in copper oxide ceramics that screening of the Coulomb repulsion is sufficient to make the metallic regions relatively conventional metals. Our purpose is not to argue the merits of this view, but instead to offer a method to test it. We point out that conventional band Fermi-liquid theory applied to these materials makes some relatively robust and distinctive predictions about anisotropic transport properties, which can be tested by experiments on single crystals. Specifically, the Hall and thermoelectric tensors should have anomalous signs. There is already a limited amount of data, but not yet sufficient to make any firm conclusions about the success of these predictions.

Section II of this paper reviews the transport theory. Section III describes calculations of $\rho_{\alpha\beta}(T)$. The shape and anisotropy agree qualitatively with experiment, but theory has difficulty accounting for the magnitude. Section IV gives calculations of the Hall tensor R^H. Measurements on polycrystalline samples bear little resemblance to theory, but the few available single-crystal results agree much more closely. Section V gives predictions for the thermopower S. Polycrystalline data bear some resemblance. Predicted signs and approximate magnitudes of the numerous independent tensor components of R^H and S are all given. Experimental tests will require single crystals and should greatly clarify the nature of the normal state.

II. TRANSPORT THEORY

To obtain transport coefficients from a rigorous solution of the Boltzmann equation requires knowledge of the scattering operator, which is difficult to calculate. However, the variational principle[2] guides us toward accurate approximations, and many of the results obtained in first approximation do not depend on the scattering. In the presence of external **E** and **B** fields and a thermal gradient ∇T, the local distribution of electrons at point **r**, in steady state, is given in first approximation by

$$F(k,r)=f[T-\mathbf{v}(\mathbf{k})\tau\cdot\nabla T;\varepsilon(\mathbf{k}-\mathbf{F}_{\rm ext}\tau/\hbar)] , \quad (1)$$

$$f(T,\varepsilon)=\{\exp[(\varepsilon-\mu)/k_BT]+1\}^{-1} , \quad (2)$$

$$\mathbf{F}_{\rm ext}=-e\mathbf{E}-e\mathbf{v}(\mathbf{k}+e\mathbf{E}\tau/\hbar)\times\mathbf{B} , \quad (3)$$

where f is the Fermi-Dirac function, $\varepsilon(\mathbf{k})$ and $\mathbf{v}(\mathbf{k})$ are the energy and group velocity $\partial\varepsilon/\partial(\hbar\mathbf{k})$ of an electron with quantum numbers $(\mathbf{k},n,\sigma)$, and band and spin indices n,σ are suppressed. The "relaxation time" τ is the sole free variational parameter and should be chosen in such a way as to maximize the current for the particular scattering operator. If the only scattering mechanism is electron-phonon scattering, then this variational procedure when applied to a metal with $N(0)\hbar\omega_D\ll 1$ yields the result[5]

$$\hbar/\tau_{\rm ep}=4\pi k_BT\int_0^{\Omega_{\max}}\frac{d\Omega}{\Omega}\alpha_{\rm tr}^2F(\Omega)\left[\frac{\hbar\Omega/2k_BT}{\sinh(\hbar\Omega/2k_BT)}\right]^2 , \quad (4)$$

where $\alpha_{\rm tr}^2F(\Omega)$ is a close relative to $\alpha^2F(\Omega)$ which governs T_c in the Eliashberg theory.[3] The interpretation of Eq. (1) is quite simple: The number of electrons in state **k** and point **r** is the same as would have been found in equilibrium except "up-stream" by $\mathbf{l}=\mathbf{v}_k\tau$ where the temperature T was different by $-\mathbf{l}\cdot\nabla T$ and at momentum smaller than $\hbar\mathbf{k}$ by the amount $\mathbf{F}_{\rm ext}\tau$ which accounts for the acceleration since the previous collision.

We now use Eqs. (1)–(4) to evaluate the electrical current j:

$$j_\alpha=\sigma_{\alpha\beta}E_\beta+\sigma_{\alpha\beta\gamma}E_\beta B_\gamma+\nu_{\alpha\beta}\nabla_\beta T+\cdots \quad (5)$$

$$=-(e/\Omega_0)\sum_{\mathbf{k}}v_\alpha(\mathbf{k})F(\mathbf{k}) , \quad (6)$$

which enables us to get explicit approximate formulas for the transport coefficients[6]

$$\sigma_{\alpha\beta}=e^2\tau(n/m)_{\alpha\beta}\equiv(e^2\tau/\Omega_0)\sum_{\mathbf{k}}v_\alpha(\mathbf{k})v_\beta(\mathbf{k})[-\partial f/\partial\varepsilon(\mathbf{k})] , \quad (7)$$

$$\sigma^{\alpha\beta\gamma}=-(e^3\tau^2/\hbar\Omega_0)\sum_{k}v_\alpha(\mathbf{k})\{[\mathbf{v}(\mathbf{k})\times\nabla(\mathbf{k})]_\gamma v_\beta(\mathbf{k})\}\times[-\partial f/\partial\varepsilon(\mathbf{k})] , \quad (8)$$

$$\nu_{\alpha\beta}=(e\tau/\Omega_0T)\sum_{\mathbf{k}}v_\alpha(\mathbf{k})v_\beta(\mathbf{k})[\varepsilon(\mathbf{k})-\mu][-\partial f/\partial\varepsilon(\mathbf{k})] . \quad (9)$$

where Ω_0 is the normalization volume. The anisotropy in these expressions comes entirely from the anisotropy of the Fermi surface geometry. At a higher level of approximation, additional anisotropy enters from the anisotropy of the scattering, but in cases studied so far[1] this turns out to be a surprisingly small effect (a few percent), at least for electron-phonon scattering at $T\geq\Theta_D$. From the orthorhombic symmetry of the $YBa_2Cu_3O_7$ crystal we can deduce that each of the tensors (7)–(9) has three independent components. The conductivity $\sigma_{\alpha\beta}$ has $\sigma_{xx}\neq\sigma_{yy}\neq\sigma_{zz}\neq 0$ but all off-diagonal elements vanish when the Cartesian axes line up with the crystallographic axes. We use coordinates such that $\hat{\mathbf{z}}$ is the c axis, perpendicular to the metallic planes, and $\hat{\mathbf{y}}$ is the direction of the Cu–O chains lying between the Y layers. $\nu_{\alpha\beta}$ has the same symmetry as $\sigma_{\alpha\beta}$, whereas $\sigma_{\alpha\beta\gamma}$ vanishes unless all three axes are different. The three independent elements are σ_{xyz}, σ_{yzx}, and σ_{zxy}, with the other three fixed by the Onsager relations $\sigma_{yxz}=-\sigma_{xyz}$, etc. For the tetragonal structure of $La_{2-x}Sr_xCuO_4$ similar relations hold, except that the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions are equivalent.

It follows that the Hall coefficient tensor also has three independent components (two for the tetragonal structure)

$$R_{xyz}^H\equiv E_y/j_xB_z=\sigma_{xyz}/\sigma_{xx}\sigma_{yy} , \quad (10)$$

with R_{yzx}^H and R_{zxy}^H given by cyclic permutation. The scattering rate $1/\tau$ cancels out of Eq. (10), and the Fermi-Dirac function $-\partial f/\partial\varepsilon$ can be replaced by $\delta(\varepsilon-\varepsilon_F)$, yielding temperature independent numbers. In higher approximation, the scattering rate depends on both ε and $\mathbf{k}$, and this gives rise to some T dependence which can amount to $\sim 50\%$ but tends to be smaller when $T\geq\Theta_D$. However, unlike the case of $\sigma_{\alpha\beta}$, the effect of scattering anisotropy is not likely to be as small as a few percent at $T\geq\Theta_D$, because the variational principle guarantees errors of order δ^2 (where $\delta=\|F_{\rm exact}-F_{\rm var}\|$) only for the dissipative parts of σ, and not for the Hall tensor which retains an error of order δ. There is also a T-dependent correction arising from the difference between $(-\partial f/\partial\varepsilon)$ and $\delta(\varepsilon-\varepsilon_F)$, but it would not be consistent to attempt to include this without also improving the treatment of τ.

The thermoelectric tensor is defined by the condition $\mathbf{j}=0$ which means that a thermal gradient induces an E field (summation over repeated indices is implied)

$$E_\alpha=S_{\alpha\beta}\nabla_\beta T=-(\sigma^{-1})_{\alpha\gamma}\nu_{\gamma\beta}\nabla_\beta T . \quad (11)$$

Since $\underline{\sigma}$ and $\underline{\nu}$ are both diagonal, so is $\underline{S}$. The lowest-order approximation $-\partial f/\partial\varepsilon=\delta(\varepsilon-\varepsilon_F)$ causes $\nu_{\alpha\beta}$ to vanish, so the thermopower S_{aa} is a higher-order effect and less easy to compute. By inserting $1=\int d\varepsilon\delta[\varepsilon-\varepsilon(\mathbf{k})]$ inside Eqs. (7) and (8), S_{aa} can be written

$$S_{aa}(T)=-\frac{k_B}{e}\int d\varepsilon\left[\frac{\varepsilon-\mu}{k_BT}\right]\sigma_{aa}(\varepsilon)\left[-\frac{\partial f}{\partial\varepsilon}\right]\Big/\int d\varepsilon\,\sigma_{aa}(\varepsilon)\left[-\frac{\partial f}{\partial\varepsilon}\right] , \quad (12)$$

$$\sigma_{aa}(\epsilon)=(e^2/\Omega_0)\sum_{\mathbf{k}}v_a(\mathbf{k})^2\tau(\mathbf{k})\delta[\varepsilon(\mathbf{k})-\varepsilon] \quad (13)$$

$$=e^2N(\varepsilon)v_a^2(\varepsilon)\tau(\varepsilon) , \quad (14)$$

where we define

$$N(\varepsilon)=\Omega_0^{-1}\sum_{\mathbf{k}}\delta[\varepsilon(\mathbf{k})-\varepsilon] , \tag{15}$$

$$N(\varepsilon)v_a^2(\varepsilon)=\Omega_0^{-1}\sum_{\mathbf{k}}v_a^2(\mathbf{k})\delta[\varepsilon(\mathbf{k})-\varepsilon] , \tag{16}$$

and $\tau(\varepsilon)$ is defined by Eq. (14). In the lowest-order approximation, $\tau(\mathbf{k})$ in Eq. (13) is constant τ, so $\tau(\varepsilon)$ is also constant and cancels from Eq. (12). However, since S_{aa} vanishes in lowest order, it is appropriate to consider corrections to the constant τ approximation. This can be done approximately when $T\geq\Theta_D$ and phonon scattering becomes effectively elastic on the scale of the thermal smearing of the Fermi distribution. In this limit, Eq. (4) becomes

$$\hbar/\tau_{\rm ep}=2\pi\lambda_{\rm tr}k_BT , \tag{17}$$

where $\lambda_{\rm tr}$ is approximated reasonably well by λ which determines T_c in Eliashberg theory. Furthermore, $1/\tau_{\rm ep}(\varepsilon)$ is reasonably well approximated as proportional to $\lambda(\varepsilon)$, the value of λ appropriate to a material with a Fermi level altered from ε_F to ε.

This energy dependence can be estimated in two levels of sophistication. At the first level, variation in $\lambda(\varepsilon)$ is expected to follow variation $N(\varepsilon)$,

$$1/\tau_{\rm ep}(\varepsilon)\propto N(\varepsilon) . \tag{18a}$$

The virtue of this approximation is that it should also hold for impurity scattering. At the second level of sophistication we can take the energy variation of electron-phonon scattering approximately into account by the formula

$$1/\tau_{\rm ep}(\varepsilon)\propto\left[\sum_a\eta_a(\varepsilon)/M_a\right]\langle\omega^2\rangle^{-1} , \tag{18b}$$

where η_a is the McMillan-Hopfield parameter $N(\varepsilon)\langle I_a^2(\varepsilon)\rangle$ and M_a is the mass of atom a. The parameter η_a can be calculated in the rigid-muffin-tin model by the procedure of Gaspari and Gyorffy.[7] A third-level approximation for $1/\tau$, which is lower than the other two, is the choice

$$1/\tau(\varepsilon)=\text{const} , \tag{18c}$$

which represents the safest course if one feels totally ignorant of the ε dependence. We shall present calculations using all three levels of sophistication or ignorance; the range of answers obtained gives a fair indication of the degree of certainty of the theory.

III. RESISTIVITY

First we ask what can be learned from the shape of $\rho(T)$. For an ordinary metal, impurity and phonon scattering dominate, giving $\rho=\rho_0+\rho_{\rm ep}(T)$, where $\rho_{\rm ep}$ is given by Eqs. (4) and (7). The temperature dependence is all contained in $1/\tau_{\rm ep}$ given by Eq. (7). The expected shape of this temperature dependence is shown in Fig. 1, where inelastic neutron scattering data[8,9] for the cross-section-weighted density of states $G(\omega)$ have been used in place of $\alpha_{\rm tr}^2F(\omega)$. The part of $\rho(T)$ below T_c has been suppressed, and the remaining curves look surprisingly

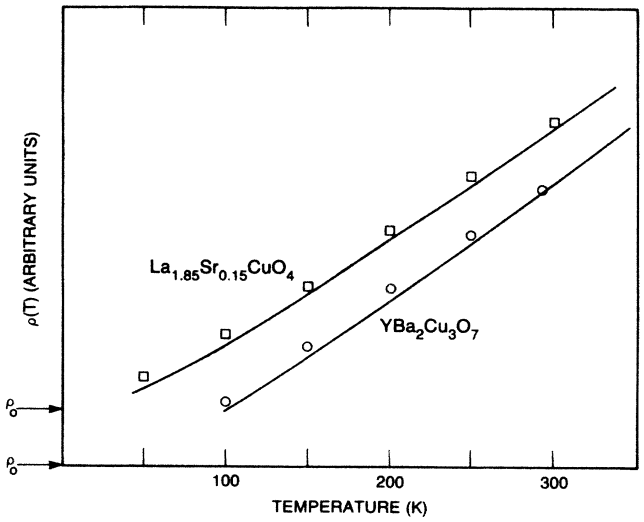

FIG. 1. Expected shape of the electron-phonon part of $\rho(T)$ according to the Boltzmann theory. These curves were obtained by numerical integration of Eq. (4) using neutron data from Refs. 8 and 9 in place of $\alpha_{\rm tr}^2F(\Omega)$. The curve for $La_{1.85}Sr_{0.15}CuO_4$ is displaced upwards by an arbitrary amount ρ_0.

linear, much like measured curves $\rho(T)$ for the best samples of oxide superconductors. Thus, there is no basis for the statement that the data are "too linear" for the electron-phonon mechanism.

The magnitude of $\rho(T)$ can be estimated theoretically if the coupling constant λ is known, from the formulas

$$\rho_{aa}^{\rm ep}=4\pi/(\Omega_{paa}^2\tau_{\rm ep}) , \tag{19}$$

$$1/\tau_{\rm ep}=(2\pi\lambda_{\rm tr}k_BT/\hbar)\times(1-\hbar^2\langle\omega^2\rangle_{\rm tr}/12k_B^2T^2+\cdots) , \tag{20}$$

$$\Omega_{paa}^2=4\pi e^2(n/m)_{aa} , \tag{21}$$

$$\lambda_{\rm tr}\langle\omega^n\rangle_{\rm tr}=2\int_0^\infty(d\Omega/\Omega)\alpha_{\rm tr}^2F(\Omega)\Omega^n , \tag{22}$$

where $(n/m)_{a\beta}$ is defined in Eq. (7). We have computed the Drude plasma frequencies Ω_{paa}^2 from linearized augmented plane wave (LAPW) electronic band structures.[10] Our results for $La_{2-x}Sr_xCuO_4$ were given in Ref. 11 for various values of x: the results at $x=0.15$ are repeated in Table I for comparison with our new results for $YBa_2Cu_3O_7$, also given in Table I, and in Fig. 2. In principle, experiment can determine Ω_p^2 and single-crystal values have now been reported for both systems. Schlesinger, Collins, Kaiser, and Holtzberg[12] have measured $\sigma_{ab}(\omega)$ in a twinned single crystal of $YBa_2Cu_3O_7$ and report $\hbar\Omega_p\sim3.1$ eV (which compares well with an rms average 3.7 eV of the xx and yy calculations of Table I). Bozović *et al.*,[12] doing infrared reflectance on oriented but polycrystalline films, obtained $\hbar\Omega_p\sim2.6$ eV. Tajima *et al.*[13] have reported $\hbar\Omega_{pxx}=2.35$ eV for single-crystal $La_{1.8}Sr_{0.2}CuO_4$ ($T_{c,\rm onset}\simeq30$ K) compared to our calculated value[11] of 2.8 eV for this composition. However, it is appropriate to be skeptical of infrared determination of Ω_p because of various factors,[14] such as the need to subtract interband contributions which occur[10] above ~0.8

TABLE I. Calculated band parameters for the high-temperature superconducting oxides.

	$La_{1.85}Sr_{0.15}CuO_4$	$YBa_2Cu_3O_7$	Unit
$N(\varepsilon_F)$	28.4	76.0	states/Ry cell (both spins)
$\langle v_x^2\rangle^{1/2}$	2.2	1.8	(10^7cm/s)
$\langle v_y^2\rangle^{1/2}$	2.2	2.8	
$\langle v_z^2\rangle^{1/2}$	0.41	0.7	
$\hbar\Omega_{pxx}$	2.9	2.9	(eV)
$\hbar\Omega_{pyy}$	2.9	4.4	
$\hbar\Omega_{pzz}$	0.55	1.1	
R^H_{xyz}	0.18	0.18	(10^{-9} m^3/C)
R^H_{yzx}	−0.94	−0.38	
R^H_{zxy}	−0.94	−1.07	

eV in $YBa_2Cu_3O_7$.

A somewhat riskier test of the parameters of Table I is the single-crystal coherence lengths $\xi_z(0)$ and $\xi_{x,y}(0)$, which have been estimated by Worthington, Gallagher, and Dinger[15] from anisotropic dH_{c2}/dT measurements in $YBa_2Cu_3O_7$. If we use the clean limit formula

$$\xi_a(0)=[\tfrac{7}{4}\zeta(3)]^{1/2}\frac{\hbar\langle v_a^2\rangle^{1/2}/(1+\lambda)}{2\pi k_B T_c}\ , \tag{23}$$

and neglect the mass enhancement factor (Ref. 16) $(1+\lambda)$ the approximate $\xi_a(0)$ values yield $\langle v_{x,y}^2\rangle^{1/2}=2.2\times10^7$ cm/s and $\langle v_z^2\rangle^{1/2}=0.5\times10^7$ cm/s, slightly smaller than numbers calculated in Table I, as if the missing mass enhancement λ were ~0.4. The uncertainties in this procedure are large so the good agreement cannot be taken too seriously, but the ratio $\langle v_{x,y}^2\rangle^{1/2}/\langle v_z^2\rangle^{1/2}$ is less risky and agrees very nicely with the experimental data.

In addition to Ω_p^2, it is necessary to have a value for $\lambda_{tr}\approx\lambda$ in order to predict ρ. For this purpose we use the formula

$$\lambda=\left[\sum_a \eta_a/M_a\right]\langle\omega^2\rangle^{-1}\ . \tag{24}$$

TABLE II. Electron-phonon parameters estimated from LDF bands, the Gaspari-Gyorffy expression for η, and using the neutron scattering spectral function $G(\omega)$ for $\alpha^2F(\omega)$. As discussed in the text, the use of the Gaspari-Gyorffy expression and $G(\omega)$ for $\alpha^2F(\omega)$ tend to lead to an underestimate of η and overestimate of ω^2, respectively, which translates into underestimates of λ and $\rho(295)$.

	$La_{1.85}Sr_{0.15}CuO_4$	$YBa_2Cu_3O_7$	Unit
$\sum_a\eta_a/M_a$	0.149	0.113	eV/Å^{2}amu
$\langle\omega^2\rangle^{1/2}$	31	38	meV
λ	0.65	0.32	
$\rho_{xx}^{cp}(295)$	80	37	$\mu\Omega$ cm
$\rho_{yy}^{cp}(295)$	80	16	
$\rho_{zz}^{cp}(295)$	2200	260	
$l(295)$	23	85	Å

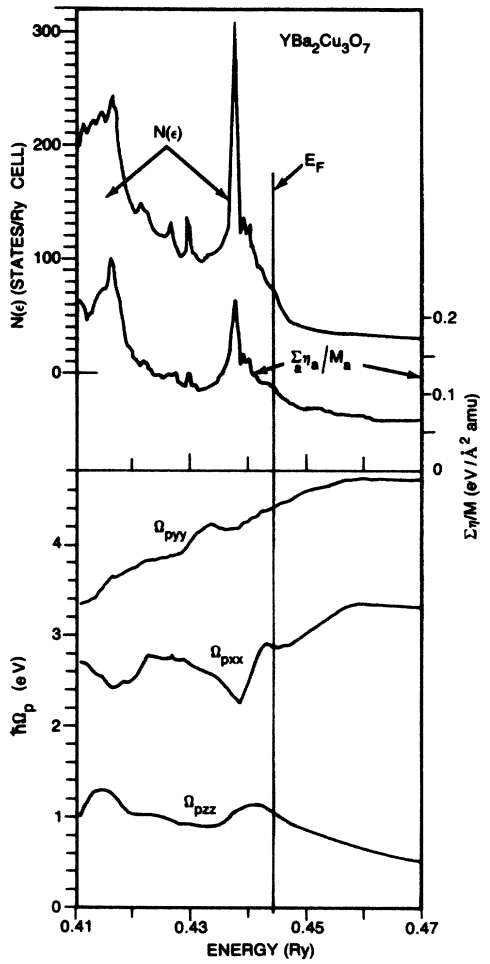

FIG. 2. Density of states, electron-phonon coupling η, and Drude plasma energies for $YBa_2Cu_3O_7$ as computed from the LAPW bands of Ref. 10, as a function of energy near ε_F.

The numerator $\sum_a\eta_a/M_a$ is calculated by the rigid-muffin-tin procedure in Ref. 10, and is shown in Fig. 2, along with $N(\varepsilon)$, as a function of energy for $YBa_2Cu_3O_7$. Our results for the numerator and denominator of Eq. (24), and for λ, are given in Table II. The denominator $\langle\omega^2\rangle$ is not known independently. Previous work[10] on $La_{1.85}M_{0.15}CuO_4$ showed that a low value of $\langle\omega^2\rangle^{1/2}\approx200$ K, such as could result from strongly coupled soft modes as predicted by Weber,[17] together with the calculated η/M sum would lead to $T_c\simeq35$ K. This estimate is no doubt an optimistic one. Another approach is to use the measured neutron scattering function $G(\omega)$ as the shape of $\alpha^2F(\omega)$, yielding estimates of $\langle\omega^2\rangle$ shown in Table II. The resulting values of λ, 0.65 and 0.32, represent moderate to weak coupling, and would predict $T_c=8$ and 0.4 K if McMillan's equation[18] were used with $\mu^*=0.1$, compared with experimental values of 40 and 95 K. These λ values have a large uncertainty, probably at least a factor of 2, partly from the uncertainty in $\langle\omega^2\rangle$. Additional uncertainty arises from the use of the rigid-muffin-tin model,[7] which has not been tested for oxides. Pickett *et al.*[19] have shown that "nonlocal" contributions to λ which are neglected in the rigid-muffin-tin model do occur

in these materials, but the size of the contribution to λ has not been determined. Given a fixed value of $\sum\eta_a/M_a$, a wide range of T_c is available in principle,[20] depending on μ^* and $\langle\omega^2\rangle$, namely

$$0 \le T_c \le (T_c)_{\max} = 0.18\left[\sum_a \eta_a/M_a\right]^{1/2} \quad (25)$$

the upper limit occurring when $\mu^* = 0$ and $\langle\omega^2\rangle \to 0$. The values of $(T_c)_{\max}$ predicted from these η calculations are 53 and 44 K for $La_{1.86}Sr_{0.14}CuO_4$ and $YBa_2Cu_3O_7$, respectively. Our calculations suggest the need for additional pairing mechanisms besides electron-phonon particularly for $YBa_2Cu_3O_7$, as do isotope effect measurements.[21] As mentioned above, there are contributions[19] to electron-phonon coupling which are not included in the rigid-muffin-tin formalism which will increase both λ and the limiting value $(T_c)_{\max}$.

These estimates of 0.65 and 0.32 for λ, which are probably underestimates, can be used to bound from below the magnitude of the electron-phonon part $\rho^{ep}_{\alpha\beta}(T)$. The results are shown in Table II, and are much smaller than anything seen experimentally so far. In particular, single-crystal data for $La_{1.94}Sr_{0.06}CuO_4$ by Suzuki and Murukami[22] have $\rho_{xx}(295) - \rho_{xx}(0) \sim 450\ \mu\Omega$ cm, compared with 80 predicted. For $YBa_2Cu_3O_7$, twinned single-crystal data by Tozer *et al.*[23] give $\rho_{ab}(295) - \rho_{ab}(0) \sim 380\ \mu\Omega$ cm and oriented film data by Bozović *et al.*[12] give $\sim 350\ \mu\Omega$ cm, compared with $\rho_{xx} = 37$ and $\rho_{yy} = 16$ predicted. There are at least four ways to understand this very large discrepancy between the lower bound and experiment: (1) increase λ by a factor of 5–10; (2) reduced Ω_p^2 by the same factor; (3) invoke an additional scattering mechanism; (4) blame the experiment (sample inhomogeneity, etc.). Option (1) was invoked by us in Ref. 11, and has the attractive aspect that it could account for the high T_c in $La_{2-x}Sr_xCuO_4$, but there are two difficulties. First, there is no good reason to expect that η values could be 5–10 times higher than the rigid-muffin-tin estimate. This was avoided in Ref. 12 by a much smaller choice of $\langle\omega^2\rangle$, an option not supported by the data of Ref. 8 (unless coupling to the lower frequency modes is very strongly favored). Second, as pointed out by Gurvitch and Fiory,[24] this will cause the high-T mean free path l to diminish to interatomic values ~ 3 Å, at which point resistivity saturation should be seen. This is inconsistent with the experimental observation[24] (in polycrystalline samples) that $\rho(T)$ continues to rise linearly.

The second option (reduce Ω_p^2) requires admitting a significant discrepancy between LDF bands and the true quasiparticle spectrum. An independent value of Ω_p^2 can be extracted from the London penetration depth $\lambda_L(T=0)$ which has been accurately measured by muon spin rotation (μSR). Kossler and co-workers[25] give $\lambda_L(T=0) \approx 2000$ Å in $La_{1.85}Sr_{0.15}CuO_4$ and ≈ 1300 Å in $YBa_2Cu_3O_7$; using $\Omega_p = c/\lambda_L$ this gives $\hbar\Omega_p = 1.0$ and 1.5 eV, respectively. These numbers must be interpreted as some kind of average over the tensor components $\Omega^2_{p\alpha\beta}$, which makes the further analysis somewhat uncertain. If we use the rms diagonal component, theory gives 2.4 and 3.1 eV, respectively. Then there is experimental support for reducing Ω_p^2 by a factor of ~ 5 although, as mentioned above, infrared measurements and ξ estimates favor our values. It will require single-crystal measurements of λ_L to make this unambiguous, but the suggestion is that Ω_p^2 or $(n/m)_{\text{eff}}$ is altered significantly from the LDF prediction. Such a reduction in Ω_p^2 will put the magnitude of $\rho(T)$ into decent alignment with our estimates of λ_{tr}. However, if LDF has failed for Ω_p^2 then there is no reason to trust the η or λ values, so the argument is not compelling. The mean-free-path dilemma is fairly well resolved, since reducing Ω_p^2 by a factor of 4–5 reduces the Fermi velocity by some fractional power of 4–5 (free-electron theory requires $\frac{1}{3}$ power) which could diminish values of l in Table II by as much as a factor of 2. This is safe and does not conflict with Ref. 24.

The third option, invoking an extra scattering mechanism, is also plausible, since we require an additional attractive interaction to account for T_c. Lee and Read[26] argue that conventional electron-electron Coulomb scattering may give T rather than T^2 behavior to $\rho(T)$ when the Fermi level is at a logarithmic $2d$ saddle-point singularity in $N(\varepsilon)$. Figure 2 and the dispersion curves of Refs. 10 and 11 show that dispersion in the z direction causes enough broadening of the $2d$ aspects to invalidate this suggestion. Also, the Fermi level in $YBa_2Cu_3O_7$ would only line up with a saddle point by accident, a situation which is not supported by the LDF bands. Magnetic fluctuations could provide a mechanism for additional scattering, and neutron scattering[27] on single crystals is giving support to this possibility.

The fourth option is to assert that the intrinsic magnitude of $\rho(T)$ will turn out to be lower than values measured so far, perhaps because of difficulties with contacts, or perhaps because samples are not yet homogeneous so that currents are only flowing through a portion of the sample, such as regions near the surface. We think that this should not be completely ruled out. However, the strong magnetic fluctuations in La_2CuO_4 make some combination of options 2 and 3 seem the most likely explanation.

A separate prediction of theory is the anisotropy of ρ_{aa}, a result which is independent of the scattering, in lowest order. For $La_{1.85}Sr_{0.15}CuO_4$, ρ_{zz}/ρ_{xx} is predicted to be 28, while for $YBa_2Cu_3O_7$, $\rho_{zz}/(\frac{1}{2}\rho_{xx} + \frac{1}{2}\rho_{yy}) = 10$ and $\rho_{zz}/(\frac{1}{2}\rho_{xx}^2 + \frac{1}{2}\rho_{yy}^2)^{1/2} = 9$ give two measures of the anisotropy. A direct measurement for $YBa_2Cu_3O_7$ by Tozer *et al.*[23] gave 30 at room temperature, with ρ_{zz} showing rather different T dependence from the conventional metallic behavior of ρ_{ab}. The mean free path $l \sim 85$ Å shown in Table II lies mostly in the *ab* planes; the mean free z distance traveled is predicted at 295 K to be 17 Å, not much larger than the cell dimension $c \sim 12$ Å. Thus the quasiparticle hypothesis underlying Boltzmann transport theory is predicted to be good for motion in the metallic planes, but not so good for motion perpendicular. The critical-field anisotropy $(H_{c2\parallel}/H_{c2\perp})^2$ is expected to equal ρ_{zz}/ρ_{ab} in lowest order. Shamoto, Onoda, and Sato[28] measured values 40–170 for La_2CuO_4-based systems, compared to our value of 28. For $YBa_2Cu_3O_7$, Iye, Tamegai, Takeya, and Takei[29] found $(H_{c2\parallel}/H_{c2\perp})^2 \sim 4$ near T_c (at 90 K) but increasing to ~ 25 at 86.5 K, while Worthington, Gallagher, and Dinger[15] found

$(H_{c2\parallel}/H_{c2\perp})^2 \sim 25$. These are qualitatively consistent with our calculated $\rho_{zz}/\rho_{ab} \sim 9$–$10$ from Table II.

IV. HALL COEFFICIENT

There appears to be considerable disparity between transport data on single crystals (only a few examples so far) and polycrystalline samples. Systematic studies of R^H in *polycrystalline* ceramic samples of $La_{2-x}Sr_xCuO_4$ as a function of x have been made by Penney, Shafer, Olson, and Plaskett[30] and Ong *et al.*[31] These measurements, as well as the measured resistivity by Birgeneau *et al.*[32] on a single crystal La_2CuO_4, flatly contradict the present picture obtained from LDF theory applied to *perfectly ordered, paramagnetic* materials. When $x \leq 0.05$, the samples are nonsuperconducting and probably also nonmetallic. Paramagnetic LDF band theory gives a metallic state when the symmetry is tetragonal, but strong Fermi surface nesting suggests that this should be unstable relative to a "Peierls" insulator and/or an antiferromagnetic (AFM) transition. Experiment shows no sign of Cu-O "breathing" modes going soft as expected in the Peierls state. The observed AFM order[27] suggests that the insulating behavior is associated either with the Fermi surface-driven AFM instability or with magnetic Coulomb correlations. Spin-density functional theory has not yet been able to find an antiferromagnetic ground state.[33] However, it is seen experimentally[34] only in the presence of $\sim 1\%$ oxygen vacancies. As x increases to ≥ 0.06, the orthorhombic distortion is greatly reduced, and metallic behavior and superconductivity are restored. There is little direct evidence concerning the origin of the magnetic behavior, or whether the magnetic fluctuations persist into the superconducting phase or disappear as metallic/superconducting behavior arises. Hall measurements,[30,31] and also electrochemical measures of the "$[Cu\text{-}O]^+$ concentration,"[30] suggest that the carrier density increases continuously with x up to $x \approx 0.15$ if a single, parabolic hole-band is assumed. For $x > 0.15$, T_c falls, and R^H jumps to smaller values consistent with the LDF metallic state. Wang *et al.*[35] have reported somewhat similar behavior in $YBa_2Cu_3O_{7-\delta}$, namely that as δ approaches 0.5 the Hall coefficient suddenly jumps suggesting a nonmetallic state. We shall not try to reconcile these polycrystalline results with LDF theory, but instead focus on the very limited single-crystal experiments.

Our predictions for the elements of the Hall tensor are given in Table I and Ref. 11 for $La_{2-x}Sr_xCuO_4$ and in Table I and Fig. 3 for $YBa_2Cu_3O_7$. There is a measurement by Suzuki and Murakami[22] in $La_{1.94}Sr_{0.06}CuO_4$ of R^H_{xyz} (300 K) $\approx +0.92\times10^{-9}$ m^3/C, while our rigid-band prediction is $+0.36\times10^{-9}$, and the polycrystalline value of Ref. 30 is 7.8×10^{-9}. (In Ref. 31, $R^H = 13\times10^{-9}$ was measured at $x = 0.05$.) Thus single-crystal data differ from polycrystalline data by an order of magnitude and agree much more closely with LDF theory than they do with polycrystalline data. This suggests that the polycrystalline results may be less amenable to a simple interpretation than has been assumed. The microscopic formulas (7), (8), and (10) and our band calculations offer *no* support for the notion that R^H is inversely related to carrier density, or that the labels "holelike" and "electronlike" have any ordinary meaning. The Hall tensor measures a complicated Fermi-surface average of the curvature which is not amenable to simple interpretation unless the surface is ellipsoidal, and current LDF bands are not ellipsoidal.

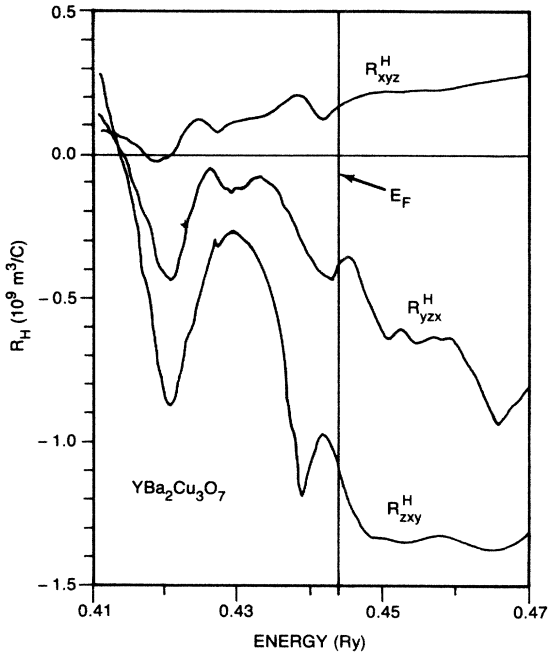

FIG. 3. The three elements of the Hall tensor for $YBa_2Cu_3O_7$ calculated as a function of energy near ε_F.

We make a striking prediction: The Hall tensor of $La_{2-x}Sr_xCuO_4$ should change sign if the **B** field is rotated to the *ab* (metallic) plane in a single crystal. This prediction also holds for $YBa_2Cu_3O_7$, and has been verified by Tozer *et al.*[23] Their crystal is twinned so that metallic *a* and *b* axes are mixed macroscopically. With **B** in the *ab* plane, they find an *electronlike value* $R^H \sim -0.8\times10^{-9}$ m^3/C; this should be some kind of average of R^H_{yzx} and R^H_{zxy}, which we predict to be -0.4×10^{-9} and -1.1×10^{-9}, respectively. The component R^H_{xyz} has not yet been measured. We predict $+0.2\times10^{-9}$. The uncertainty in our predictions arises mostly because we treat the scattering in the lowest-order approximation, where it cancels out, giving a T-independent answer. Higher-order effects are not suppressed by any variational principle and might be $\sim \pm 50\%$ or more and T dependent. For Cu and Nb Beaulac and co-workers[36] found the lowest-order theory accurate to $\pm 10\%$, but for Pd there was a factor-of-2 discrepancy with experiment. Polycrystalline data often show a strong decrease in R^H as T increases, bigger than normally expected from higher-order effects. In particular, Ref. 30 found a T^{-1} behavior of R^H in polycrystalline $YBa_2Cu_3O_7$. However, the single-crystal data on $YBa_2Cu_3O_7$ of Ref. 23 are nearly T independent, and those of Ref. 22 on $La_{1.94}Sr_{0.06}CuO_4$ show an intermediate T dependence. One possible source of complication in T

dependence arises from the situation that mean free paths in the x and y directions are long and have normal T^{-1} behavior, whereas in the z direction they are short and likely to exhibit weaker T dependence due to "saturation" effects. Thus, temperature need not cancel from ratios like $\sigma_{\alpha\beta\gamma}/\sigma_{\alpha\alpha}\sigma_{\beta\beta}$, and the measured T dependences in polycrystalline samples may reflect changes in current flow with temperature; i.e., a T-dependent averaging process.

V. THERMOPOWER

According to Eq. (12) the sign and magnitude of $S_{\alpha\alpha}(T)$ reflect the shape of the ε dependence of $\sigma_{\alpha\alpha}(\varepsilon)$. In the Migdal approximation,[4] $\hbar\omega_D$ and k_BT are the important energy scales, variations on a scale of ε_F are neglected, and $S(T)$ vanishes. The shape of $\sigma_{\alpha\alpha}(\varepsilon)$ for $YBa_2Cu_3O_7$ is shown in Fig. 4 for the three models of Eqs. (18) and the three crystallographic axes. Corresponding pictures for $La_{2-x}Sr_xCuO_4$ were given in Ref. 37. Clearly variations in $\sigma(\varepsilon)$ occur on a scale as small as 0.006 Ry = 1000 K. A Taylor series expansion around E_F does not represent $\sigma(\varepsilon)$ adequately, so $S(T)$ does not accurately follow the Mott formula $S \propto T\sigma'(\mu)/\sigma(\mu)$. We have done this integral in Eq. (12) numerically using an energy cutoff $> 10k_BT$. The results for $S_{\alpha\alpha}$ are given for $YBa_2Cu_3O_7$ in Fig. 5 and for $La_{2-x}Sr_xCuO_4$ in Ref. 37. The three models give significiant quantitative differences in magnitude of $S_{\alpha\alpha}(T)$, but preserve some common trends, specifically the ordering $S_{zz} > S_{yy} > S_{xx}$, and the tendency for $S(T)$ to flatten out or lose T dependence in the range $200 < T < 600$ K. The results of Ref. 37 are similar to the present results except that for $La_{2-x}Sr_xCuO_4$ the three models gave closer agreement with each other and there was a very clear indication that $S_{zz} > 0$ and $S_{xx} = S_{yy} < 0$. For $YBa_2Cu_3O_7$ we have $S_{xx} < S_{yy} < 0$ but the sign of S_{zz} is not predictable. It is amusing that like the Hall coefficient, the thermopower can switch from positive (holelike) to negative (electronlike) depending on orientation. Even more striking is our prediction that the "sign of the carriers" is opposite in R^H compared with S. When the **B** field is parallel to $\hat{\mathbf{z}}$, R^H measures orbits in the metallic xy planes and is holelike while S_{xx} and S_{yy} are electronlike. When **B** is in the xy plane and the orbit is open in the z direction, R^H is electronlike while S_{zz} tends to be holelike.

We are not aware of any single-crystal data for $S_{\alpha\alpha}(T)$. Extensive measurements of $S(T)$ polycrystalline samples have been reported by Ishii *et al.*[38] For $La_{2-x}Ba_xCuO_4$,

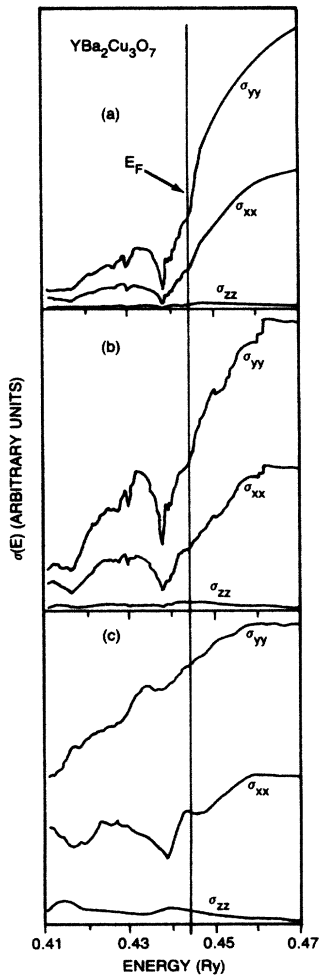

FIG. 4. Parts (a), (b), and (c) represent for $YBa_2Cu_3O_7$ the three models for $\sigma(\varepsilon)$ [Eq. (14)] represented by approximations (18a), (18b), and (18c), respectively, for $1/\tau(\varepsilon)$. Model (a) has $\sigma(\varepsilon) \propto v^2(\varepsilon)$ and model (c) has $\sigma(\varepsilon) \propto \Omega_p^2(\varepsilon)$.

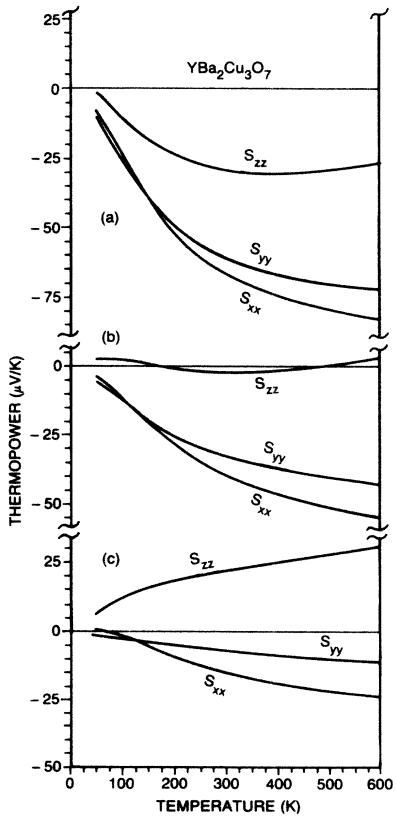

FIG. 5. The three elements of the thermopower tensor $YBa_2Cu_3O_7$ as calculated from the three models of Fig. 4.

$S(300\ \mathrm{K})$ is $\sim+25\ \mu\mathrm{V/K}$ at $x=0.15$ and $\sim+50\ \mu\mathrm{V/K}$ at $x=0.10$, with dS/dT small and negative at 300 K. There is no inconsistency with our predictions in Ref. 37, but no way to make a detailed comparison. For $YBa_2Cu_3O_{7-y}$, the smallest y reported (0.07) had $S(300\ \mathrm{K})=0$, and as y increased to 0.35, $S(300)$ increased to $\sim+35\ \mu\mathrm{V/K}$. The temperature derivative vanished at $y=0.07$ and became negative as y increased. These results are not easily compared with those of Fig. 5, but there is no inconsistency.

VI. CONCLUSIONS

Polycrystalline measurements[30,31,35] of R^H have been interpreted in terms of a picture where E_F lies near the top of a single holelike band below a Mott-Hubbard gap in a region dominated by Coulomb correlations, quite unlike LDF band theories. However, isolated measurements[22,23] of $R^H_{\alpha\beta\gamma}$ on single crystals are very different and much closer to the present picture based on LDF band theory. Further single-crystal data, on magnetic as well as transport properties, are essential to sort out the picture. The available single-crystal data for $\rho(T)$ are quantitatively at odds with a description in terms of the paramagnetic band structure and only phonon scattering. Including the effects of antiferromagnetic fluctuations on the band structure as well as in the transport theory may reconcile the LDF description with experimental data. A very good test will be single-crystal measurements of R^H_{xyz}, R^H_{yzx}, R^H_{zxy}, S_{xx}, S_{yy}, and S_{zz}. LDF theory makes quite striking predictions about the signs of these quantities, a few of which have been verified.

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