Simple model of a temperature-dependent resistivity anisotropy of layered systems

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For electrons scattering on a bosonic mode we calculate within standard transport theory the in-plane and out-of-plane resistivities ρ_{ab} and ρ_c of a layered system. We show that, for dominant forward scattering on a quasi-two-dimensional mode, ρ_c / ρ_{ab} increases (and may even diverge) with decreasing temperature. $[S0163-1829(99)04029-1]$

I. INTRODUCTION

The transport properties of the cuprates remain the subject of intensive study, since it is believed that their understanding shall provide a key to solving the whole high- T_c problem. Both the in-plane¹ and out-of-plane² transport is strongly doping dependent and anomalous.

For optimally doped materials, the in-plane transport is characterized by a resistivity ρ_{ab} scaling linearly with temperature *T* down to the superconducting transition temperature, and also the Hall effect and in-plane magnetoresistance exhibit simple power laws of *T*. There is no consensus regarding the origin of the anomalous in-plane transport. Two broad classes of theories attribute the anomalies either to singular forward³ or large-momentum⁴ scattering. There are also attempts to describe the phenomenology of the cuprates by collective-mode-dominated transport,⁵ but this latter possibility shall not be discussed here.

The out-of-plane transport is equally mysterious.² Overdoped samples are characterized by a temperatureindependent ratio ρ_c / ρ_{ab} as in standard anisotropic metals. On the other hand, underdoped materials exhibit a divergent out-of-plane resistivity ρ_c as *T* decreases, even if their inplane resistivity ρ_{ab} is metallic. When compared to the inplane transport, the *c*-axis data are not as universal between different cuprate families. This is not so surprising since the blocking layers between the $CuO₂$ planes are very different for different families.

There exists an extensive literature on the *c*-axis transport. 2 Here we shall take the point of view that the divergence of ρ_c at low *T* in underdoped materials is due to the opening of a pseudogap in the electron spectral function, as suggested in Ref. 6. In order to study the *c*-axis transport of the strange metal phase, it is crucial to concentrate on the optimally doped samples. Here the experimental situation is not so clear. Experiments on Bi2212 suggest² that for optimally doped samples $\rho_c \propto T^{\gamma}$ with $\gamma \approx 0$.

Very recently, the poor *c*-axis conductivity has been discussed within a particularly attractive model with an in-plane anisotropy of the electron lifetime, namely within the coldspot model of Ioffe and Millis.⁷ In Ref. 7 it was shown that, if a plausible assumption is made about the dominant interplane hopping path of an electron,⁸ the cold-spot model predicts a divergent ρ_c / ρ_{ab} as $T \rightarrow 0$. It is the purpose of this paper to show (within the framework of standard transport theory) that the hypothesis of a strong forward scattering also yields a divergent ρ_c / ρ_{ab} and no further assumptions need to be made.

II. STANDARD TRANSPORT THEORY

Let us start with a formulation of the standard transport theory. In the presence of an electric field **E**, the electron distribution function f_k is shifted from its equilibrium value $f_{\mathbf{k}}^0$ according to $f_{\mathbf{k}} = f_{\mathbf{k}}^0 + \Phi_{\mathbf{k}} \delta(\varepsilon_{\mathbf{k}})$, where the function $\Phi_{\mathbf{k}}$ $= e\mathbf{E} \cdot \mathbf{v}_{\mathbf{k}} \tau_{\mathbf{k}}^{\text{tr}}$ describes the local displacement of the Fermi surface. \mathbf{v}_k is the group velocity of the electron and τ_k^{tr} is the transport lifetime to be determined from the solution of the Boltzmann equation.

Consider electrons scattering on a bosonic mode with spectral function $\text{Im}\chi(\mathbf{q},\omega)$. Let us discuss only tetragonal materials with lattice constants *a* and $a₁$ in the *x*,*y* and *z* directions, respectively. Furthermore, let us discuss only electric fields within the *x*,*y* plane or along the *z* direction, for which the current is parallel to **E**. In that case, the resistivity ρ can be found by minimizing the functional^{9,10}

$$
\frac{\rho}{\rho_0} = \min \frac{\oint d^2k \oint d^2k' A_{\mathbf{k},\mathbf{k'}} [\mathbf{n} \cdot (\mathbf{l}_{\mathbf{k'}} - \mathbf{l}_{\mathbf{k}})]^2}{\left[\oint d^2k l_{\mathbf{k}} (\mathbf{n} \cdot \mathbf{n}_{\mathbf{k}})^2\right]^2},\qquad(1)
$$

where $\rho_0 = \hbar a_1 / e^2$ is the inverse of the elementary conductivity, **n** and \mathbf{n}_k are unit vectors in the directions of **E** and \mathbf{v}_k , respectively, $\mathbf{l}_k = l_k \mathbf{n}_k$ and $l_k = v_k \tau_k^{\text{tr}}$ is the electron mean free path. The integrals are taken along the Fermi surface. The minimization is to be done with respect to the function l_k . The dimensionless function $A_{\mathbf{k},\mathbf{k}'}$ which characterizes the scattering between the points \bf{k} and \bf{k}' on the Fermi surface is given by

$$
A_{\mathbf{k},\mathbf{k'}} = \frac{g_{\mathbf{k},\mathbf{k'}}^2 a^2}{T v_{\mathbf{k}} v_{\mathbf{k'}}} \int_0^\infty d\omega \omega n(\omega) [n(\omega) + 1] \text{Im}\chi(\mathbf{k'} - \mathbf{k}, \omega),
$$
\n(2)

where $g_{\mathbf{k},\mathbf{k}'}$ is an appropriate coupling constant.

Recently, the following approximate solution of the variational problem Eq. (1) has become quite popular in the literature on the in-plane transport properties of the cuprates. In the nominator of Eq. (1) , there is an expression

$$
[\mathbf{n} \cdot (\mathbf{l}_{\mathbf{k}'} \!-\! \mathbf{l}_{\mathbf{k}})]^2 \!=\! (\mathbf{n} \!\cdot\! \mathbf{l}_{\mathbf{k}'})^2 \!+\! (\mathbf{n} \!\cdot\! \mathbf{l}_{\mathbf{k}})^2 \!-\! 2 (\mathbf{n} \!\cdot\! \mathbf{l}_{\mathbf{k}'}) (\mathbf{n} \!\cdot\! \mathbf{l}_{\mathbf{k}}).
$$

$$
\frac{\rho}{\rho_0} = \frac{4\pi^3}{a_\perp} \min \left[\frac{\oint d^2k l_{\mathbf{k}}^2 (\mathbf{n} \cdot \mathbf{n}_{\mathbf{k}})^2 / L_{\mathbf{k}}}{\oint d^2k l_{\mathbf{k}} (\mathbf{n} \cdot \mathbf{n}_{\mathbf{k}})^2} \right]^2,
$$

where we have introduced a single-particle mean free path $L_{\bf k}$

$$
\frac{1}{L_{\mathbf{k}}} = \frac{a_{\perp}}{2\pi^3} \oint d^2k' A_{\mathbf{k},\mathbf{k'}}.
$$
 (3)

It is easy to see that in this approximation the variational problem is solved by $l_{\mathbf{k}}=L_{\mathbf{k}}$ and the conductivity $\sigma=\rho^{-1}$ reads

$$
\sigma = \frac{e^2}{4\pi^3 \hbar} \oint d^2 k L_{\mathbf{k}} (\mathbf{n} \cdot \mathbf{n}_{\mathbf{k}})^2.
$$
 (4)

Equation (4) is very natural and this is probably the cause of its wide use in the literature. However, especially in strongly anisotropic situations as in the hot-spot⁴ and cold-spot⁷ models, it should be obvious from the above discussion that such an approximation provides at most qualitative answers.

III. QUASI-TWO-DIMENSIONAL METALS

Until now, our discussion was quite general. In this section, we shall discuss quasi-two-dimensional metals. Our key assumption is that the scattering of electrons is dominated by an in-plane collective mode with a weak dispersion in the *z* direction. Furthermore, we assume that the scattering takes place within a given two-dimensional plane,

$$
H' = \sum_{n} \sum_{\mathbf{k}_{\parallel}, \mathbf{k'}_{\parallel}} g_{\mathbf{k}_{\parallel}, \mathbf{k'}_{\parallel}} c_{n\mathbf{k'}_{\parallel}}^{\dagger} c_{n\mathbf{k}_{\parallel}} (b_{n\mathbf{q}_{\parallel}} + b_{n-\mathbf{q}_{\parallel}}^{\dagger}), \tag{5}
$$

where *n* is the layer index, $\mathbf{q}_{\parallel} = \mathbf{k}'_{\parallel} - \mathbf{k}_{\parallel}$, and $\mathbf{k} = (\mathbf{k}_{\parallel}, k_z)$, etc. $b_{n\mathbf{q}_{\parallel}}$ annihilates a bosonic excitation with in-plane momentum q_{\parallel} in the layer *n*. After Fourier transformation, Eq. (5) becomes

$$
H' = \sum_{\mathbf{k},\mathbf{k}'} g_{\mathbf{k}_{\parallel},\mathbf{k}'} c_{\mathbf{k}'}^{\dagger} c_{\mathbf{k}} (b_{\mathbf{q}} + b^{\dagger}_{\mathbf{q}}),
$$

where $\mathbf{q} = \mathbf{k}' - \mathbf{k}$. Thus $g_{\mathbf{k},\mathbf{k}'}$ does not depend on k_z and k'_z . Since also v_k and Im $\chi(\mathbf{q},\omega)$ are weak functions of the *z* components of the momenta, $A_{\mathbf{k},\mathbf{k}'}$ depends on k_z and k_z' only weakly.

This property of $A_{\bf k,k'}$ enables us to simplify Eq. (1) considerably. The in-plane resistivity ρ_{ab} can be calculated from

$$
\frac{\rho_{ab}}{\rho_0} = \min \frac{2 \oint dk \oint dk' A_{\mathbf{k},\mathbf{k'}} (\mathbf{l}_{\mathbf{k'}} - \mathbf{l}_{\mathbf{k}})^2}{\left[\oint dk' k_{\mathbf{k}}\right]^2},
$$

where the integrals are taken along the (one-dimensional) Fermi line. It is easy to see that for the *z*-axis resistivity ρ_c the approximation leading to Eq. (4) is exact and therefore

$$
\sigma_c = \frac{e^2}{2\pi^2 \hbar a_\perp} \oint dk L_{\mathbf{k}} \langle n_{\mathbf{k}z}^2 \rangle,
$$

where $\sigma_c = \rho_c^{-1}$, $L_{\mathbf{k}} = \pi^2/dk' A_{\mathbf{k}',\mathbf{k}}$, $\langle n_{\mathbf{k}z}^2 \rangle = (a_\perp/\sqrt{a_\mathbf{k}^2})$

 $(2\pi) \int dk_z n_{\mathbf{k}z}^2$, and $n_{\mathbf{k}z}$ is the *z* component of $\mathbf{n}_{\mathbf{k}}$.

Now we want to discuss possible mechanisms for disparate behaviors of ρ_{ab} and ρ_c within standard transport theory. An interesting proposal has been made by Ioffe and Millis in the context of the cold-spot model.⁷ According to this model, L_k is modulated within the plane in such a way that it is small in nearly all directions, except for regions at 45° with respect to the *x* and *y* axes (cold spots), for which L_k is large. On the other hand, there are arguments based on the quantum chemistry of the cuprates that precisely in the cold spots $n_{\mathbf{k}z}$ vanishes.⁸ This causes the suppression of the conductivity in the *z* direction with respect to its in-plane value.

However, only electron paths of a certain type are considered in the discussion⁸ leading to the conclusion about the vanishing of $n_{\mathbf{k}z}$ in the cold spots. Other electron paths (although leading to weaker interplane hopping amplitudes, in general) yield a finite contribution to $n_{\mathbf{k}z}$ even in the cold spots, and the picture of Ioffe and Millis may break down. Therefore, it is worthwhile to look for independent mechanisms which enhance ρ_c with respect to ρ_{ab} .

Forward scattering

Remarkably, there does indeed exist a simple and quite general mechanism for the enhancement of the resistivity anisotropy. Namely, we shall argue below that if in addition to the above assumptions of in-plane scattering on a quasitwo-dimensional collective mode the electrons are scattered predominantly in the forward direction, the ratio ρ_c / ρ_{ab} may even diverge at low temperatures.

In fact, consider dominant forward scattering of electrons. Furthermore, in order to keep the discussion as simple as possible, let us discuss only systems which are isotropic within the *x*-*y* plane. In particular, $A_{k'k}$ is assumed to depend only on the angle Θ between the points \mathbf{k}' , \mathbf{k} on the circular Fermi line. In this case it is reasonable to take $l_{\bf k}$ $=$ const for the in-plane conductivity and, therefore,

$$
\frac{\rho_{ab}}{\rho_0} = \frac{2}{\pi} \int_0^{2\pi} d\Theta A(\Theta) (1 - \cos \Theta),
$$

$$
\frac{\rho_c}{\rho_0} = \left(\frac{v_F}{w}\right)^2 \frac{2}{\pi} \int_0^{2\pi} d\Theta A(\Theta), \tag{6}
$$

where v_F is the in-plane Fermi velocity and the out-of-plane velocity is taken to be $v_{kz} = w \sin(k_z a_1)$. Equation (6) shows that ρ_c / ρ_{ab} is enhanced with respect to the simple bandstructure estimate $\rho_c / \rho_{ab} = (v_F / w)^2$ because of the different efficiency of the scattering in relaxing the current in the two directions.

Equation (6) can be interpreted as $\rho_{ab} \propto \tau_{tr}^{-1}$ and $\rho_c \propto \tau^{-1}$, where τ_{tr} and τ are the transport lifetime and the singleparticle lifetime, respectively. Remarkably, an analogous result has been found by completely different methods by Kumar and Jayannavar¹¹ in the limit $w\tau \ll a_{\perp}$, which is complementary to the region of validity of our calculation based on standard transport theory.

In order to proceed we have to choose a specific form of the scattering function $A(\Theta)$. Let us consider first a diffusive mode Im $\chi(q,\omega) = \omega/(\omega^2 + \omega_q^2)$ with a dispersion ω_q . The frequency integral in Eq. (2) for such Im $\chi(q,\omega)$ has been done in Ref. 10. Using that result we can write

$$
A_{\mathbf{q}} = \frac{\pi^2}{3} \left(\frac{g_{\mathbf{q}} a}{v_F} \right)^2 \frac{T^2}{\omega_{\mathbf{q}} \left[\omega_{\mathbf{q}} + (2\pi/3)T \right]}.
$$

The transferred momentum q in the scattering process can be written $q=2k_F \sin(\Theta/2)$, where k_F is the (in-plane) Fermi momentum. If we assume that for $\Theta \rightarrow 0$ $\omega_q = \Omega \Theta^\alpha$ and g_q^2 $= G^2 \Theta^{\beta}$, we find for the resistivities at $T \leq \Omega$

$$
\frac{\rho_{ab}}{\rho_0} \sim \left(\frac{Ga}{v_F}\right)^2 \left(\frac{T}{\Omega}\right)^{(\beta+3)/\alpha} \quad \text{for} \quad 1 < \frac{\beta+3}{\alpha} < 2,
$$
\n
$$
\frac{\rho_c}{\rho_0} \sim \left(\frac{Ga}{w}\right)^2 \left(\frac{T}{\Omega}\right)^{(\beta+1)/\alpha} \quad \text{for} \quad 1 < \frac{\beta+1}{\alpha} < 2. \tag{7}
$$

If the resistivity exponents are ≥ 2 , then the resistivities are not dominated by forward scattering. For exponents ≤ 1 , the integrals diverge at $\Theta \rightarrow 0$. The former requirement obviously depends on the large- ω behavior of Im_{χ}(α). For instance, for $\text{Im}\chi(\mathbf{q},\omega) = \delta(\omega-\omega_{\mathbf{q}}) - \delta(\omega+\omega_{\mathbf{q}})$ the scattering function

$$
A_{\mathbf{q}} = \frac{1}{2} \left(\frac{g_{\mathbf{q}} a}{v_F} \right)^2 \frac{\omega_{\mathbf{q}}/2T}{\sinh^2(\omega_{\mathbf{q}}/2T)}
$$

.

One finds readily that in this case Eqs. (7) are valid for β $1+3>\alpha$ and $\beta+1>\alpha$, respectively, and there are no upper bounds on the resistivity exponents.

Equations (7) demonstrate explicitly that for forward scattering on an in-plane collective mode, the resistivity anisotropy of a quasi-two-dimensional system ρ_c / ρ_{ab} $\sim (v_F/w)^2(\Omega/T)^{(2/\alpha)}$ diverges as $T\rightarrow 0$. E.g., scattering on the deformation potential of 2D phonons ($\alpha = \beta = 1$) yields $\rho_c \propto T^2$ and $\rho_{ab} \propto T^4$.

IV. THREE-DIMENSIONAL METALS

In this section we consider a three-dimensional metal in which the electrons scatter on a two-dimensional bosonic mode.¹² Furthermore, we assume dominant forward scattering. The resistivity is given by Eq. (1) with $A_{k,k}$ which depends only on the in-plane component $\mathbf{q}_{\parallel} = \mathbf{k}'_{\parallel} - \mathbf{k}_{\parallel}$.

For simplicity, let us consider a spherical Fermi surface. Then a vector **k** on the Fermi surface can be parametrized by two angles θ and φ and the transferred momentum in a scattering between \bf{k} and \bf{k}' reads

$$
\left(\frac{q_{\parallel}}{k_F}\right)^2 = (\sin\theta' - \sin\theta)^2 + 2\sin\theta\sin\theta'[1 - \cos(\varphi' - \varphi)].
$$
\n(8)

There are two types of processes with $q \ll k_F$: either θ' $\approx \theta$ or $\theta' \approx \pi - \theta$. Moreover, $\varphi' \approx \varphi$ has to hold, unless θ $\approx 0, \pi$ when $q_{\parallel} \ll k_F$ is satisfied irrespective of φ', φ .

Processes with $\theta' \approx \theta$ relax the current in approximately the same way irrespective of the direction of the current flow. However, processes with $\theta' \approx \pi - \theta$ are much more effective in relaxing a current in the *c*-axis direction than in the *x*-*y* plane. Therefore, a *T*-dependent anisotropy of ρ_c / ρ_{ab} is to be expected even in this case.

Let us proceed with an explicit calculation. Assuming forward scattering we can write $\theta' = \theta + \alpha$ or $\theta' = \pi - \theta + \alpha$ and $\varphi' = \varphi + \beta$, where $\alpha, \beta \le 1$. Equation (8) simplifies in this case to

$$
\Theta^2 \approx \alpha^2 \cos^2 \theta + \beta^2 \sin^2 \theta \equiv \Theta_1^2 + \Theta_2^2,
$$

where $\Theta = q_{\parallel}/k_F$. The Fermi-surface integrals can be written as $\oint d^2k = k_F^2 \int d\Omega$ where $d\Omega = d\varphi d\theta$ sin θ . For forward scattering from \bf{k} to \bf{k}' we can write

$$
\int d\Omega' \approx \sin \theta \sum_{\theta'} \int d\alpha \int d\beta = \frac{2\pi}{|\cos \theta|} \sum_{\theta'} \int_0^\infty d\Theta \Theta,
$$

where $\Sigma_{\theta'}$ means that both $\theta' = \theta + \alpha$ and $\theta' = \pi - \theta + \alpha$ should be considered. The single-particle mean free path *L* can be found from Eq. (3) . It is evident that *L* is only a function of θ . For θ not too close to $\pi/2$ we find

$$
L_{\theta} = \frac{\pi^2}{2k_F^2 a} \frac{|\cos \theta|}{\int_0^{\infty} d\Theta \Theta A(\Theta)},
$$
(9)

where we have set $a_{\perp} = a$ and we have assumed that the integral over Θ converges sufficiently rapidly at the upper limit. Note that the scaling $L_{\theta} \propto |\cos \theta|$ reflects the simple geometrical fact that the area of a Fermi-surface segment whose projection in the *z* direction has a given area, scales like $|\cos \theta|^{-1}$. For $\theta \rightarrow \pi/2$ a lower bound on L_{θ} can be found by applying the quasi-two dimensional result

$$
L_{\pi/2} = \frac{\pi^2}{k_F} \frac{1}{\int_0^\infty d\Theta A(\Theta)}.
$$
 (10)

Note the more singular behavior at small Θ in Eq. (10) as compared with Eq. (9) .

The resistivity is given by Eq. (1) . If we make use of **n** \cdot ($\mathbf{l_k}$, $-\mathbf{l_k}$) \approx l_k **n** \cdot ($\mathbf{n_k}$, $-\mathbf{n_k}$), the variational problem is solved easily. We find $l_{\theta} \propto \sin^2 \theta \cos \theta$ for the in-plane transport and $l_{\theta} \propto |\cos \theta|$ for the *c*-axis transport. The corresponding resistivities are

$$
\frac{\rho_{ab}}{\rho_0} = 12 \int_0^\infty d\Theta \Theta^3 A(\Theta),
$$

$$
\frac{\rho_c}{\rho_0} = 8 \int_0^\infty d\Theta \Theta A(\Theta).
$$
 (11)

Note that Eqs. (11) are analogs of Eqs. (6) for a layered material. A comparison to Eq. (9) reveals that again, as in the quasi-two-dimensional case, $\rho_{ab} \propto \tau_{tr}^{-1}$ and $\rho_c \propto \tau^{-1}$.

Let the bosonic mode be described by a spectral function $\text{Im}\chi(\mathbf{q},\omega) = \delta(\omega-\omega_{\mathbf{q}}) - \delta(\omega+\omega_{\mathbf{q}})$. If we assume that for $\Theta \rightarrow 0$ $\omega_q = \Omega \Theta^\alpha$ and $g_q^2 = G^2 \Theta^\beta$, we find for the resistivities at $T \ll \Omega$

Thus the resistivity anisotropy $\rho_c / \rho_{ab} \propto (\Omega/T)^{2/\alpha}$ scales in the same way with *T* as for a quasi-two-dimensional system.

V. CONCLUSIONS

The temperature-dependent resistivity anisotropy found in this paper results from a scattering function $A_{\mathbf{k},\mathbf{k}'}$ which has a peak at small in-plane momentum transfers and is independent of k_z , k'_z . Our results for the resistivities ρ_{ab} , ρ_c remain valid also if the *c*-axis dispersion of the bosonic mode Ω _z is finite but smaller than the thermal smearing. In the opposite limit $T \ll \Omega_z$, we expect a conventional isotropic lifetime. If the bosonic mode is a collective mode of the electrons of a layered system, then the assumption of small Ω_z is quite natural and the region of anomalous resistivity anisotropy Ω ^{*z*} \ll *T* \ll *N* may become large.

A consistent description of the phenomenology of the cuprates requires a very singular scattering. If we entirely phenomenologically require that $\rho_{ab} \propto T$ and $\rho_c \propto T^{\gamma}$ with γ \approx 0 ascribing the divergence of ρ_c at low *T* to the spin-gap effect, then Eqs. (6) require that the function $A(\Theta)$ is substantial only for Θ smaller than a characteristic angle Θ_0 $\propto \sqrt{T}$ and there its value is $A(\Theta) \sim A_0$ with $A_0 \propto 1/\sqrt{T}$. For such a singular scattering, our use of standard transport theory is doubtful, since the very concept of an electronlike quasiparticle is dubious in that case. When applied to the cuprates, our calculation should be understood as a perturbative argument which demonstrates explicitly that singular forward scattering might lead to a confinement of electrons in the limit $T\rightarrow 0$, as suggested by Anderson in Ref. 3.

Thus an interesting question about the nature of the scattering in the cuprates is, whether the dominant contribution comes from small or large momentum transfers. In the latter case, anisotropic in-plane charge transport is expected and direct experimental tests of such anisotropy have been proposed recently.^{13,14} On the other hand, dominant forward scattering implies $\tau_{tr} \gg \tau$. It has been argued that since τ is expected to be comparable to the electron dephasing time τ_{ϕ} and since experimentally $\tau_{tr} \approx \tau_{\phi}$, the assumption $\tau_{tr} \gg \tau$ is hardly consistent with measurements.⁶ While such an argument is definitely plausible, we believe that the question about the ratio τ_{tr} / τ still lacks a convincing answer. A direct measurement of the T dependence of τ , e.g., from photoemission measurements, would be therefore of great value.

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