``Enseigner la recherche en train de se faire”

COLLÈGE DE FRANCE
1530

Chaire de
Physique de la Matière Condensée

Seconde partie:
Quelques questions liées au transport dans les matériaux à fortes corrélations électroniques

Les mercredis dans l’amphithéâtre Maurice Halbwachs
11, place Marcelin Berthelot 75005 Paris
Cours à 14h30 - Séminaire à 15h45

Cycle 2011-2012
Partie II: 30/05, 06/06,13/06/2012

Antoine Georges

Séance du 30 mai 2012

- Séminaire : 15h45 –

Florence Rullier-Albenque, *SPEC, CEA-Saclay*

Multiband effects and electron-hole asymmetry in the transport properties of iron-pnictide compounds

- Séminaire: 16h45 -

Neven Barišić, SPEC, CEA-Saclay

Are there Quasi-Particles in the Normal State of Unconventional Superconductors?

ABSTRACT

These lectures aim at a description of some aspects of transport in materials with strong electron correlations, with a more phenomenological than formal perspective. I will first present some experimental results (on titanates, ruthenates, cuprates). Two issues will be raised: i) What sets the scale above which Fermi liquid behaviour (resistivity varying as T^2) is no longer valid ? ii) At which temperature is the Ioffe-Regel-Mott "limit" reached and what is its physical significance ? I will then introduce some theoretical notions (Boltzmann, Kubo). I will describe some very recent results on transport and optical conductivity of a simple model of a doped Mott insulator in which the questions above can be answered. I will show in particular that the range of temperature in which a Drude-like description is possible is far more extended than that in which Landau quasiparticles exist in a strict sense, and will explain why. Time permitting, the last lecture will be devoted to some thermoelectric properties of strongly correlated materials.

OUTLINE

- Today: Phenomenology, simple theory background. Mainly raise questions.
- Next lecture: Answer some of these questions for a doped Mott insulator (simplest 1-site DMFT description, recent results)
- June, 13 (time permitting): some notions on thermoelectric properties

"When exploring the physical properties of a material, the resistivity is the quantity that is often first measured, but last understood" (Neven Barisič, 2012)

Also implies that its hard to look at data without
any element of theoretical description in mind,
So lets start with the simplest one…

1. Drude description

$$\sigma_{dc} = \frac{ne^2\tau_D}{m} \quad , \quad \sigma(\omega) = \frac{\omega_p^2}{-i\omega + 1/\tau_D} \quad , \quad \omega_p^2 = \frac{ne^2}{m}$$

$$m\frac{d\vec{v}}{dt} = -e\vec{E} - \frac{m}{\tau_D}\vec{v}$$

$$m\left[\frac{1}{\tau_D} - i\omega\right]\vec{v}_\omega = -e\vec{E}_\omega$$

$$\vec{j} = -ne\vec{v}$$

Question: what are the charge carriers ? Mass m ? Density n ?
Scattering time ?

Ioffe-Regel [1960], Mott [1972]
When is a Drude description legitimate ?

→ When the mean-free path of the charge carriers is larger than the Fermi wavelength ?

$$l = v_F \tau_D \quad , \quad v_F = \frac{\hbar k_F}{m} \quad , \quad \sigma_{dc} = \frac{e^2}{\hbar} \frac{n}{k_F} l$$

Quasi-2D (layered) geometry:

$$n = \frac{N}{\Omega} = 2.\frac{1}{8\pi^3}.\pi k_F^2 \frac{2\pi}{c_0}$$

c_0: c-axis lattice spacing

3D isotropic geometry: $$n = 2.\frac{1}{8\pi^3}.\frac{4}{3}\pi k_F^3$$

IRM (cont'd):

Quasi 2D: $$\sigma_{dc} = \frac{e^2}{\hbar}\frac{1}{c_0}\frac{k_F l}{2\pi}$$

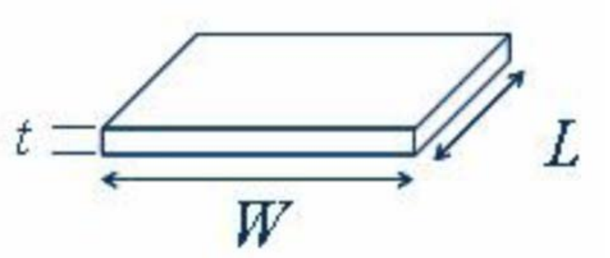
3D isotropic: $$\sigma_{dc} = \frac{e^2}{\hbar}\frac{1}{3\pi^2}k_F^2 l$$

IRM criterion – 2D – 1FS sheet

$$k_F l = 1 \rightarrow \rho_M = \frac{h}{e^2}c_0 = 0,25\,\mathrm{m}\Omega.\mathrm{cm} \times c_0[\mathrm{nm}]$$

IRM limit corresponds to sheet resistance = Resistance quantum per layer

$$R = \rho\frac{L}{tW} = R_s\frac{L}{W}$$



2. Some Phenomenology

a- Ruthenates (remember: 3 FS sheets)

ab-plane:

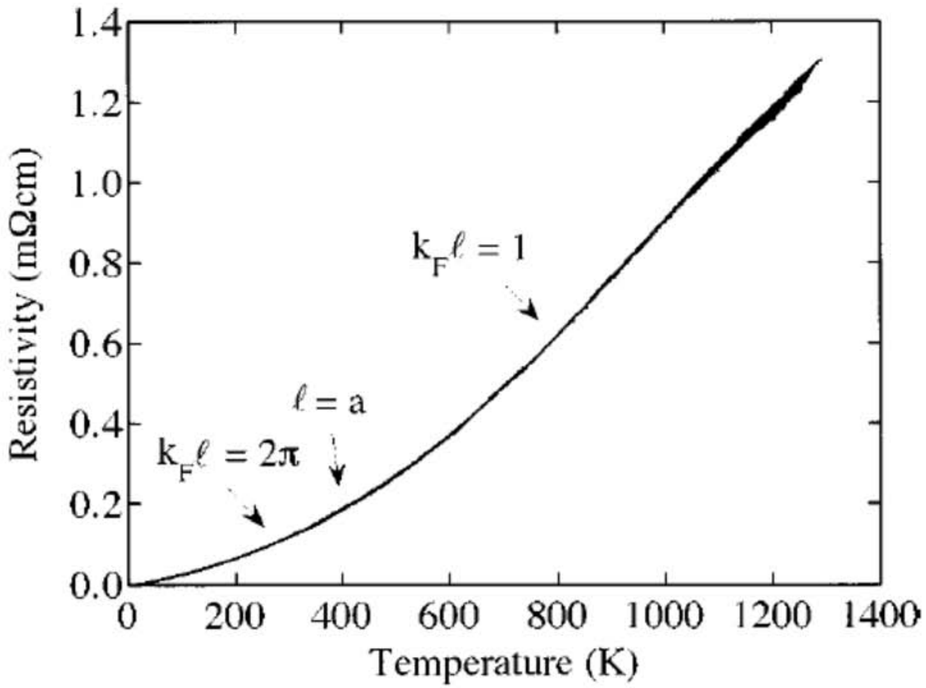


FIG. 1. The in-plane resistivity of Sr_2RuO_4 from 4 to 1300 K. Three criteria for the Mott-Ioffe-Regel limit are marked on the graph, and there is no sign of resistivity saturation, so Sr_2RuO_4 is a "bad metal" at high temperatures, even though it is known to be a very good metal at low temperatures.

- resistivity
does cross IRM value

- Nothing dramatic is seen
in ρ upon crossing IRM

Tyler,Maeno, McKenzie
PRB 58 R10107 (1998)

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Superconductivity in Bad Metals

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A number of the most interesting new materials discovered in the past few decades are "bad metals" in the sense that their resistance has a metallic (increasing) temperature dependence but, at sufficiently high temperatures, the mean free path l of a quasiparticle would be less than its de Broglie wavelength $\lambda_F = 2\pi/k_F$, were Boltzmann transport theory to apply. Among these materials are organic conductors, alkali-doped C_{60}, and high temperature superconductors. In this paper we show that, in a suffi-

``Bad metal'': resistivity exceeds IRM value at hi-T with no sign of saturation

Do `bad metals' necessarily fail to develop conventional quasiparticles at low-T ?

The failure of bad metals to exhibit resistivity saturation strongly suggests that any theory based on conventional quasiparticles with more or less well-defined crystal momenta suffering occasional scattering events does not apply. *Since there is no crossover in the temperature dependence of the resistivity as the temperature is lowered, this conclusion applies by continuity even at lower temperatures where the putative mean free path deduced from the measured values of the resistivity would not, of itself, rule out the possibility of quasiparticle transport.* In other words, a bad metal behaves as if it is a quasiparticle insulator which is rendered metallic by collective fluctuations [4].

Low-T state of ruthenates: a Fermi liquid

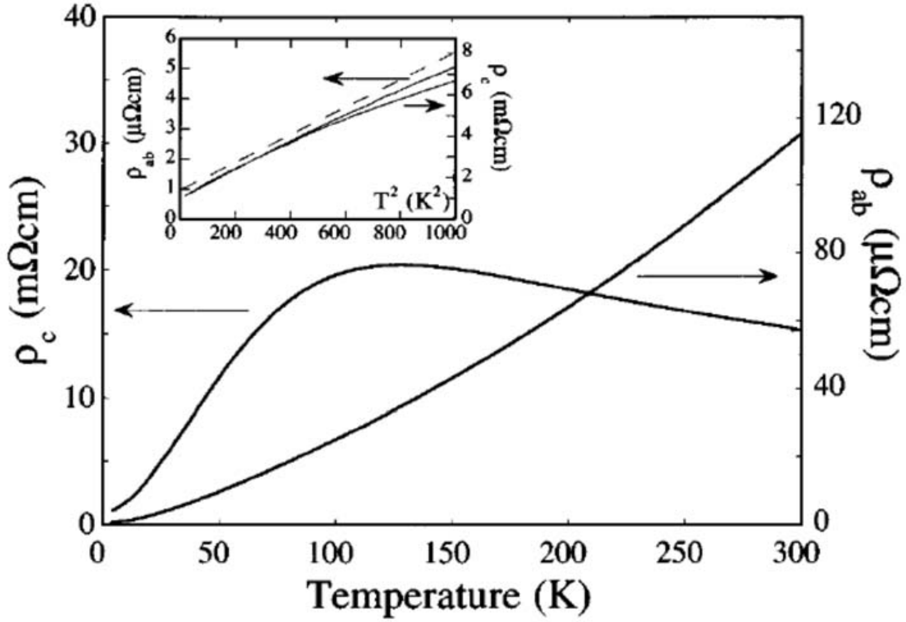


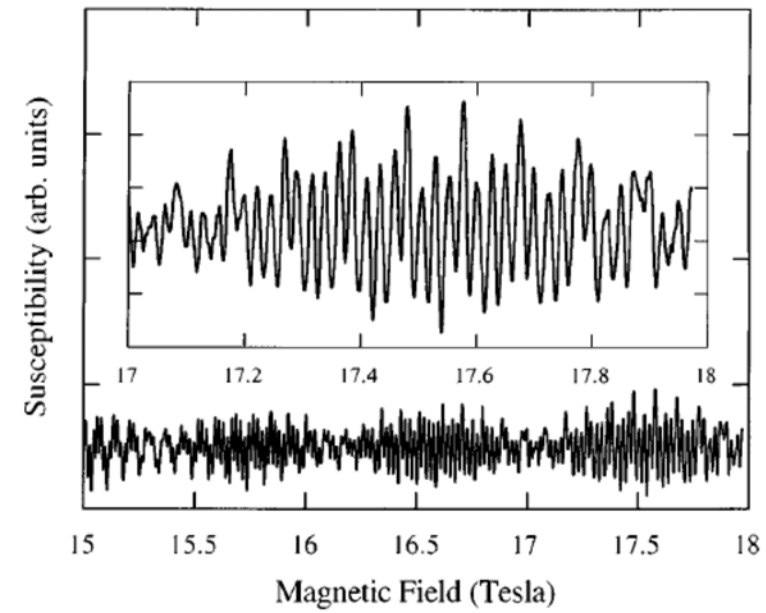
FIG. 1. Zero-field $\rho_{ab}(T)$ and $\rho_c(T)$ of Sr_2RuO_4. The inset shows $\rho_c(T)$ and $\rho_{ab}(T)$ below 32 K plotted against T^2. The dashed line is a guide to the eye.

KEY OBSERVATION:

still $\rho \ll \rho_M$ at $T \sim T_{FL}$

Hence large regime of T with non-T^2 (non FL) transport but still `good' metal

~ T^2 up to about T_{FL} ~ 20K



Tyler, Maeno and McKenzie PRB 1998:

The smooth increase of the in-plane resistivity through the Mott-Ioffe-Regel limit is particularly interesting. The fact that this kind of behavior can be observed in a material which is known to be a very good metal at low temperatures emphasizes that our current understanding of high-temperature conduction processes is very poor indeed. Other "bad metals" have ground states which are either superconducting with relatively high critical fields (e.g., the cuprates and alkali-doped C_{60}) or relatively poor metals with interesting magnetic behavior (e.g., manganites at some dopings or $SrRuO_3$). It has not been possible so far to confirm a conventional low-temperature metallic state by the observation of quantum oscillations in any of these materials, so the current observations on Sr_2RuO_4 clarify the problem that needs to be understood. There is now at least one example of a material in which a very smooth crossover from standard to highly nonstandard conduction processes is confirmed to exist.

Interesting action in c-axis:
maximum roughly where in-plane $k_F.l \sim 2\pi$

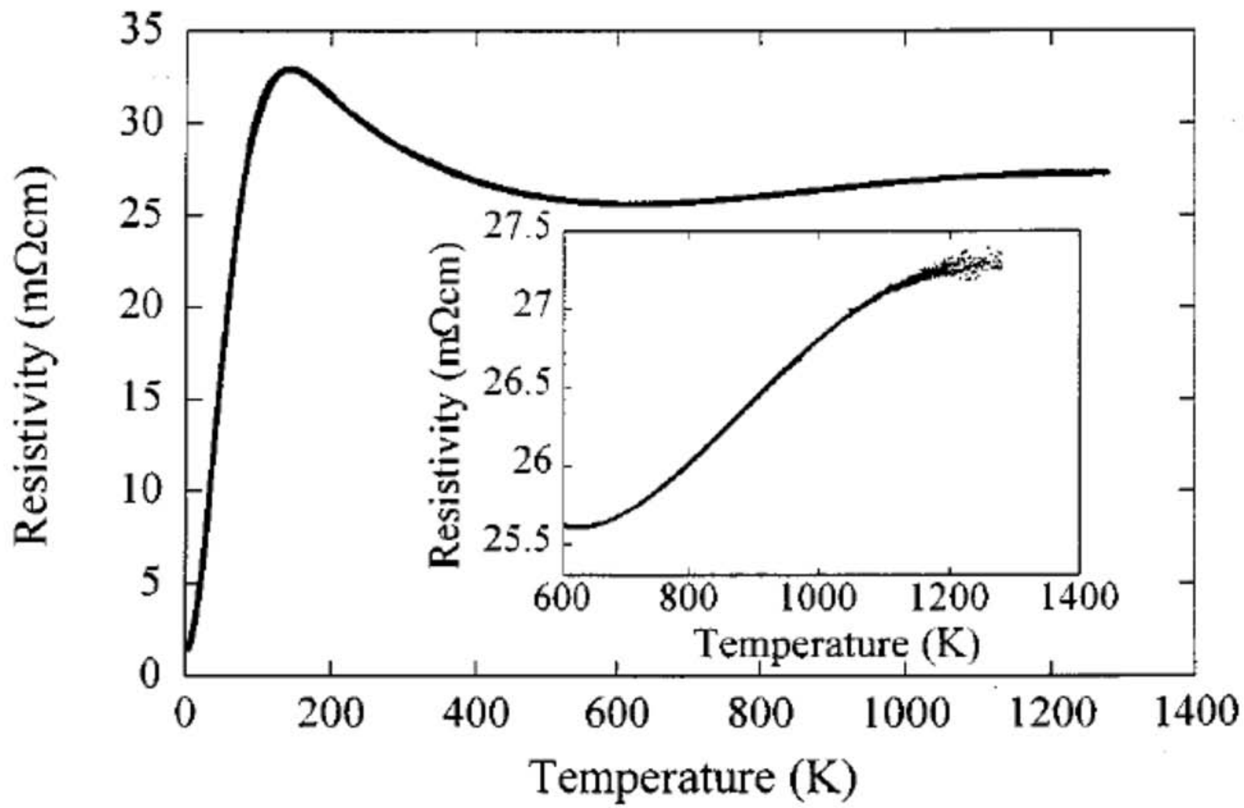


FIG. 3. The intrinsic out-of-plane resistivity of Sr_2RuO_4 from 4 to 1300 K. Although the high-temperature value is nearly 30 mΩ cm, the temperature derivative is positive between 700 and 1300 K, as shown in the inset.

Many strongly correlated materials are `bad metals' at hi-T

Gunnarsson Calandra Han
RMP2003

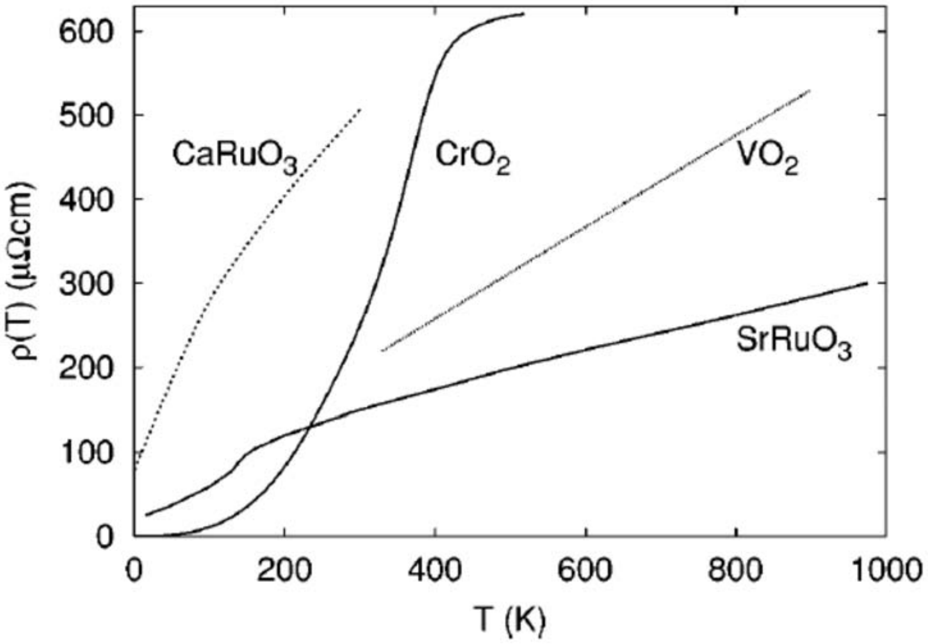


FIG. 6. Resistivity of $CaRuO_3$ (Klein *et al.*, 1999a, 1999b), CrO_2 (Rodbell *et al.*, 1966), VO_2 (Allen *et al.*, 1993), and $SrRuO_3$ (Allen *et al.*, 1996).

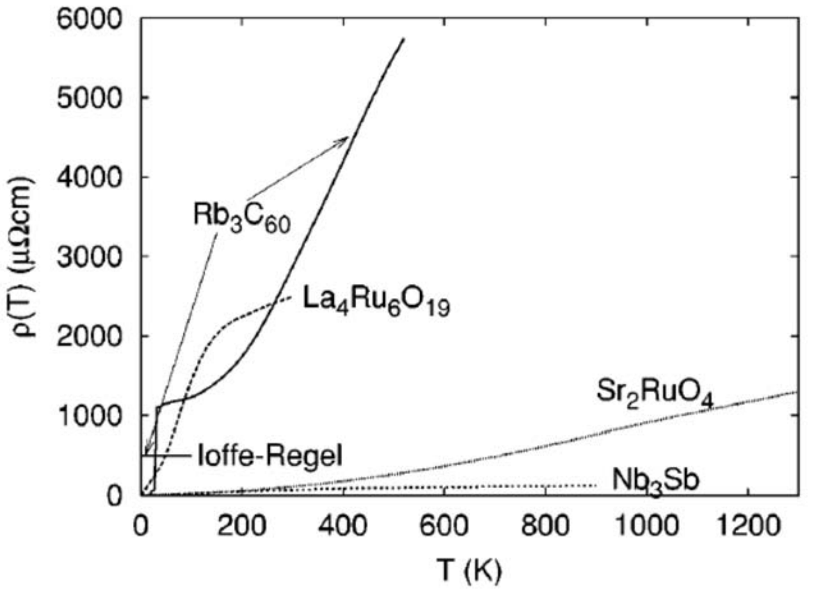


FIG. 3. Resistivity of Rb_3C_{60} (Hebard *et al.*, 1993), $La_4Ru_6O_{19}$ (Khalifah *et al.*, 2001), Sr_2RuO_4 (Tyler *et al.*, 1998), and Nb_3Sb (Fisk and Webb, 1976) and the Ioffe-Regel resistivity for Rb_3C_{60}. There is no sign of saturation at the Ioffe-Regel resistivity, but $La_4Ru_6O_{19}$ may saturate at a much larger resistivity.

LiV_2O_4: a ‘super-heavy’ oxide
- FL at low-T, bad-metal at hi-T

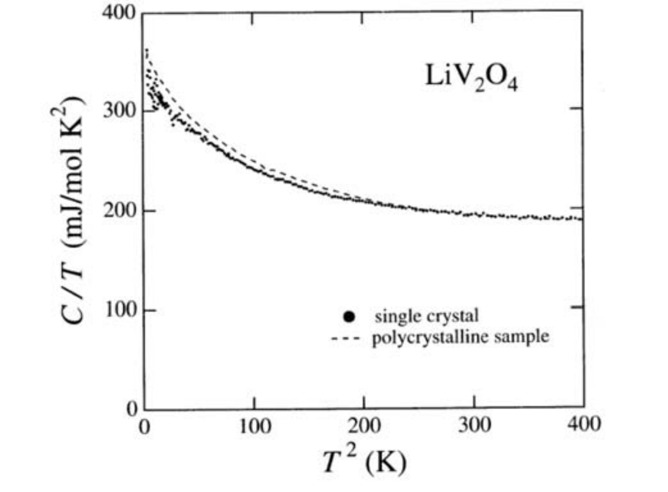


Fig. 2. The temperature dependence of specific heat of a 231 μg LiV_2O_4 single crystal (solid line), plotted as C/T vs. T^2. The result for polycrystalline sample is also shown (broken line) for comparison.

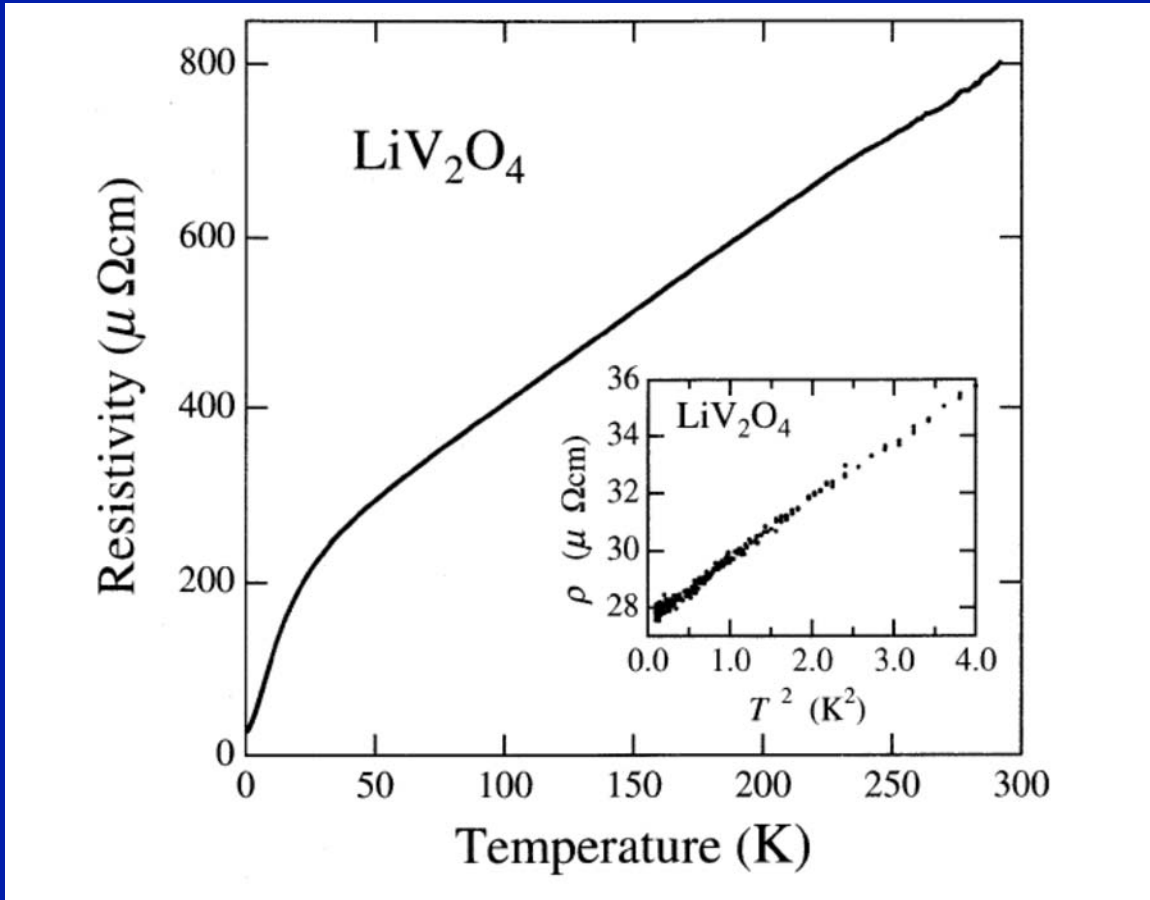


Fig. 4. The temperature dependence of resistivity for a LiV_2O_4 single crystal. The inset shows the resistivity vs. T^2 plot below 3 K.

T_{FL} ~ 2K

T_{IRM} ~ a few 100 K

CUPRATES

TABLE I. Resistivity $\rho(T)$ (in mΩ cm) of high-T_c cuprates. The measurement temperature T and the superconductivity transition temperature T_c are given in K.

Compound	T_c	T	$\rho(T)$	Reference
$HgBa_2Ca_0Cu_1O_{4+x}$	94	300	0.5	Daignere *et al.*, 2001
$HgBa_2Ca_1Cu_2O_{6+x}$	122	300	0.3	Yan *et al.*, 1998
$HgBa_2Ca_2Cu_3O_{8+x}$	125	500	0.6	Carrington *et al.*, 1994
$HgBa_2Ca_3Cu_4O_{10+x}$	130	400	0.5	Löhle *et al.*, 1996
$Tl_2Ba_2CuO_{6+y}$	80	300	1.3	Kubo *et al.*, 1991
$Tl_2Ba_2CuO_{6+y}$	80	270	0.6	Duan *et al.*, 1991
$TlSr_2CaCu_2O_{7-y}$	65	300	0.5	Kubo *et al.*, 1991
$Bi_2Sr_2CaCu_2O_{8+y}$	76	300	1.2	Chen *et al.*, 1998

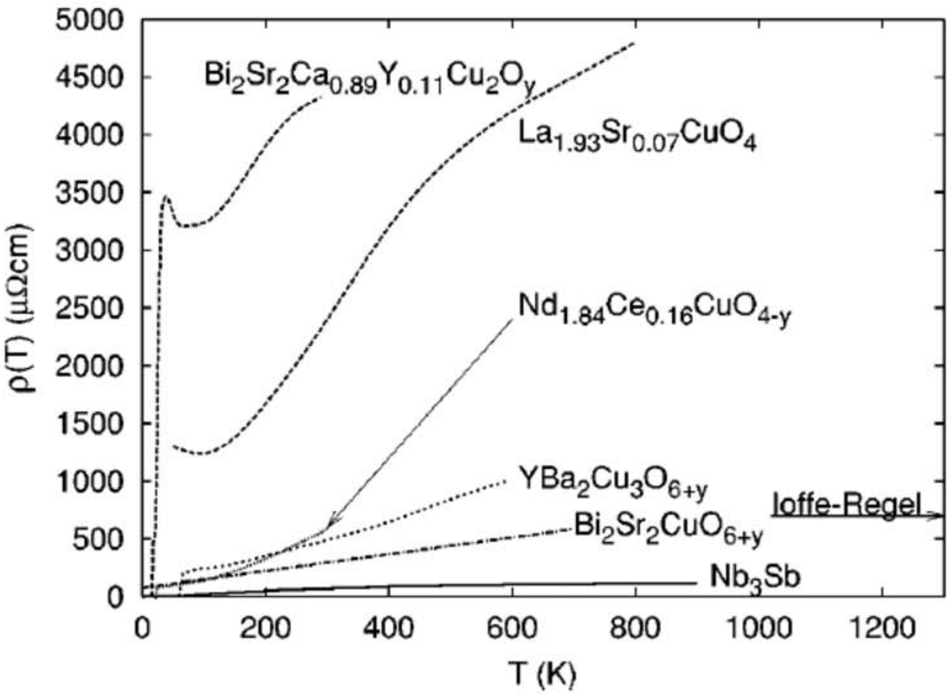


FIG. 2. Resistivity of $Bi_2Sr_2Ca_{1-x}Y_xCu_2O_{8+y}$ (T_c=30 K) (Wang, Geibel, and Steglich, 1996; Wang *et al.*, 1996), $La_{1.93}Sr_{0.07}CuO_4$ (Takagi *et al.*, 1992), $Nd_{1.84}Ce_{0.16}Cu_{4-y}$ (T_c =22.5 K) (Hikada and Suzuki, 1989), $YBa_2Cu_3O_{6+x}$ (T_c =60 K) (Orenstein *et al.*, 1990), $Bi_2Sr_2Cu_{6+y}$ (T_c=6.5 K) (Martin *et al.*, 1990), and Nb_3Sb (Fisk and Webb, 1976). The arrow shows the Ioffe-Regel resistivity of $La_{1.93}Sr_{0.07}CuO_4$. The figure illustrates that there is no sign of saturation at the Ioffe-Regel resistivity, but in some cases perhaps at much larger resistivities. Observe the magnitude compared with Nb_3Sb.

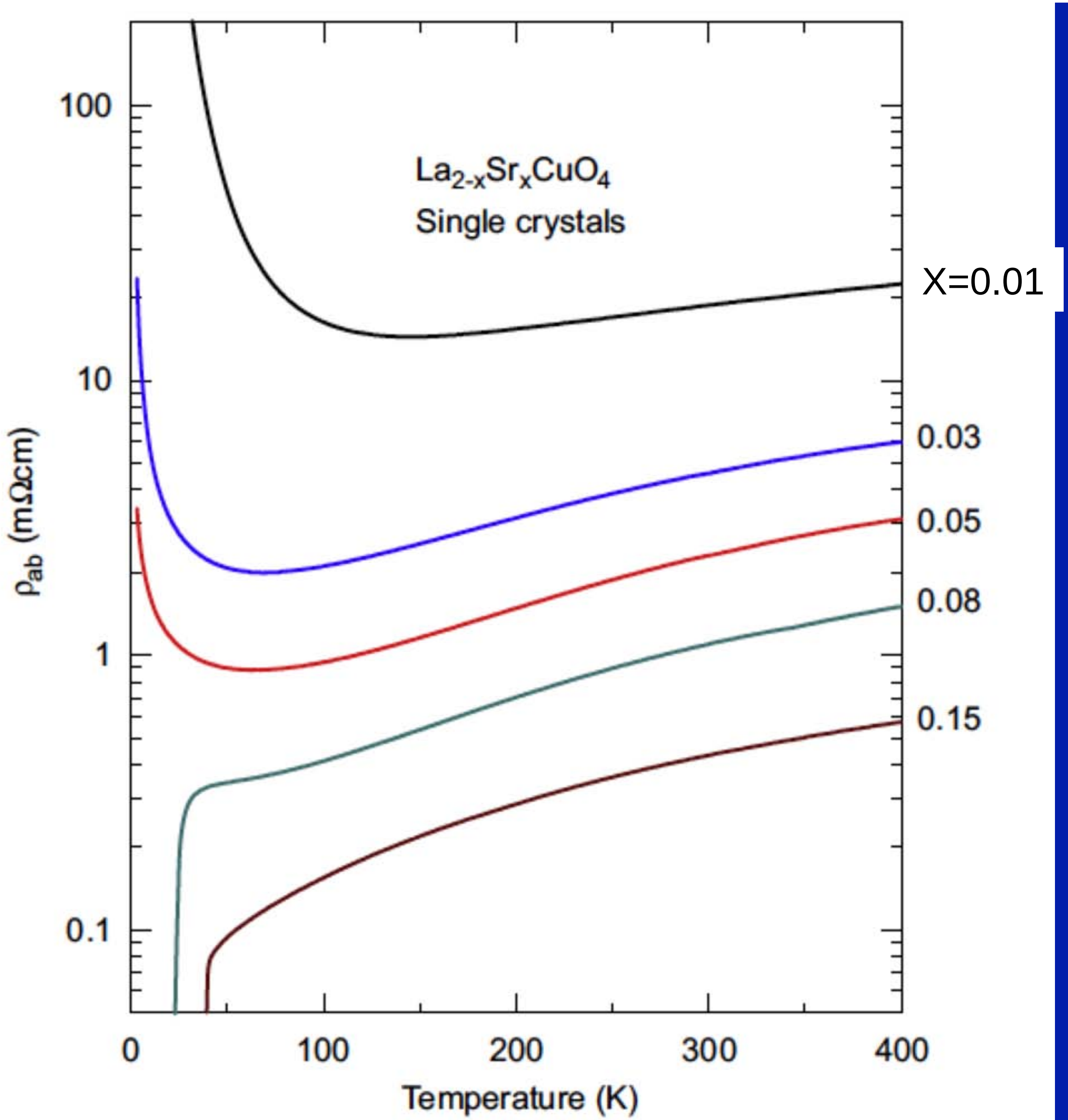


Fig. 2. Temperature dependences of ρ_{ab} of a series of high-quality LSCO single crystals measured up to 400 K. Note that a metallic behavior ($d\rho_{ab}/dT>0$) is observed at moderate temperature in all these samples, even for $x=0.01$.

Ando
Hi-quality
LSCO

In contrast, resistivity saturation often observed in materials for which e-phonon scattering dominates (e.g. A15)

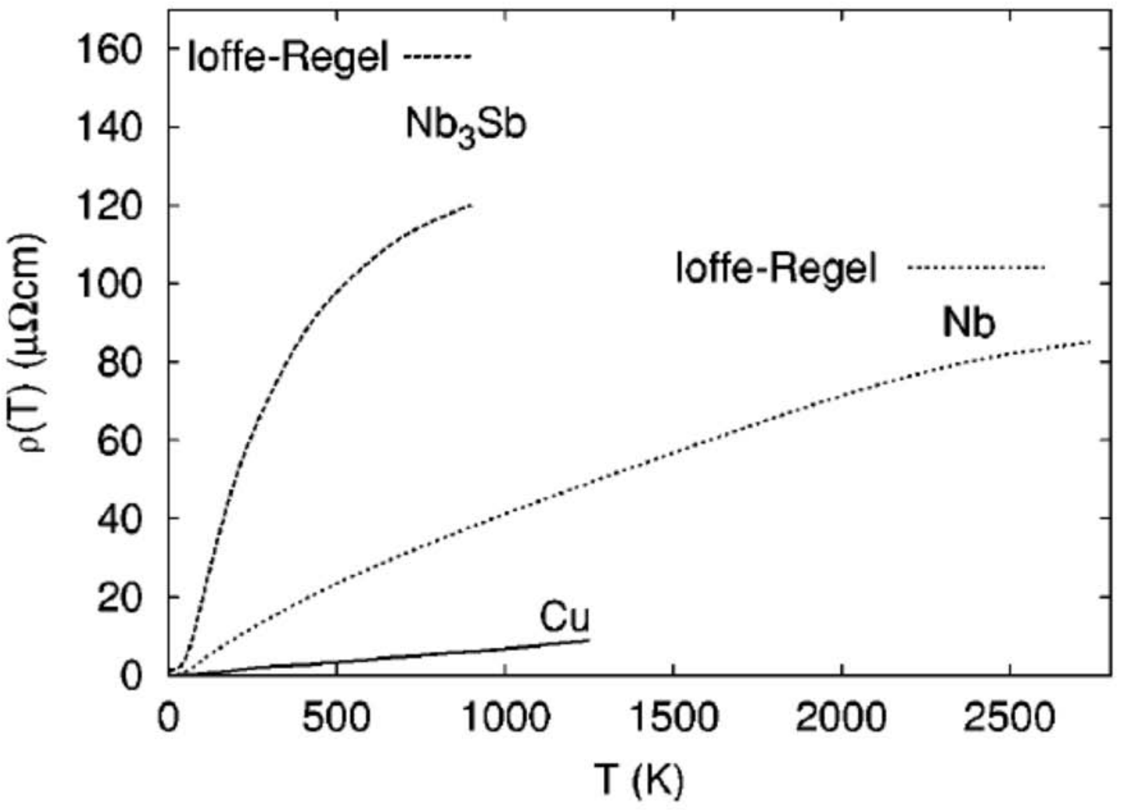


FIG. 1. Resistivity of Cu, Nb_3Sb (Fisk and Webb, 1976), and Nb (Abraham and Deviot, 1972). The figure also shows the Ioffe-Regel (Ioffe and Regel, 1960) saturation resistivities of Nb_3Sb and Nb [obtained by setting the mean free path l in Eq. (1) equal to the distance between the Nb atoms]. The corresponding value for Cu, 260 $\mu\Omega$ cm, falls outside the figure. The figure illustrates that for Nb_3Sb and Nb the resistivity saturates roughly as predicted by the Ioffe-Regel criterion, while $\rho(T)$ $\sim T$ for Cu at large T.

QUESTIONS :

- How low is T_{FL} and why ?
- What exactly happens to Landau quasiparticles at T_{FL} ?
- What are the current carrying entities for $T_{FL}<T<T_{IRM}$
- Is a Drude description applicable in this regime, despite the absence of Landau QPs ?
- Is there any signature of IRM in some physical observable (ARPES ? Optics ?)

Why are these questions timely ?

- There is increasing evidence that there are indeed well-defined QPs in cuprates, in nodal regions
- These QPs may even be FL-like at low-enough T, certainly in overdoped (Hussey) and perhaps also in underdoped (Barisic)
- Quantum oscillations !
- Move away from the quest of infra-red stable NFL fixed points !
- Understand crossover scales, possibly momentum dependent, and physics (e.g. transport, and more) above T_{FL}

A bit of theory: conductivity from Kubo formula

Linear response theory: consider a time-dependent perturbation V = F(t).B coupling to an operator B.

Influence of this perturbation on expectation value of some observable A:

$$\begin{aligned} \langle A(t)\rangle_V - \langle A(t)\rangle &= \int dt_1\,(-i)\theta(t-t_1)\left\langle\left[A(t),B(t_1)\right]\right\rangle * F(t_1) + \mathcal{O}(F^2) \\ &\equiv \int dt_1\,\chi_{AB}(t-t_1) * F(t_1) + \mathcal{O}(F^2). \end{aligned} \quad (6$$

Retarded (causal) correlation function:

$$\chi_{AB}(t) = -\frac{i}{\hbar}\theta(t)\left\langle\left[A(t),B(0)\right]\right\rangle = C^R_{AB}(t).$$

Time-dependent vector potential A(t), no scalar potential (choice of gauge).

Current ? (j: particle current ; electrical current: -e.j)

$$\hat{H} = \sum_i \frac{(\vec{p}_i - e\vec{A}_i)^2}{2m} + \hat{H}_{int}$$

$$j_\mu = -\frac{1}{e}\frac{\delta H}{\delta A_\mu} = j_p + j_d$$

$$j^p_{\vec{q}} = \frac{\hbar}{m}\sum_{\vec{k}\sigma}\left(\vec{k} + \frac{\vec{q}}{2}\right) c^\dagger_{\vec{k}\sigma} c_{\vec{k}+\vec{q}\sigma}$$

\`paramagnetic' current

$$j^d_{\vec{q}} = -\frac{e}{m}\frac{1}{\Omega}\sum_{\vec{k}\vec{k}'\sigma}\vec{A}(\vec{k}-\vec{k}')\, c^\dagger_{\vec{k}\sigma} c_{\vec{k}'+\vec{q}\sigma}$$

\`diamagnetic' current

Linear response applied to j^p

$$\langle j^p_\mu(\boldsymbol{r},t)\rangle^{(1)}_V = -e\int \frac{d\omega}{2\pi} e^{-i\omega t} \sum_\nu \int d\boldsymbol{r}'\, \mathscr{C}_{j^p_\mu(\boldsymbol{r}) j^p_\nu(\boldsymbol{r}')}(i\Omega_n \to \omega^+)\, \underbrace{A_\nu(\boldsymbol{r}',\omega)}_{\frac{1}{i\omega}E_\nu(\boldsymbol{r}',\omega)} .$$

j^d is already first-order in the perturbation A(t):

$$\langle j^d_\mu(\boldsymbol{r},t)\rangle^{(1)}_V = -\frac{e}{m} A_\mu(\boldsymbol{r},t)\langle n(\boldsymbol{r},t)\rangle = -\frac{e}{m}\langle n(\boldsymbol{r})\rangle \int \frac{d\omega}{2\pi}\, e^{-i\omega t}\, \underbrace{A_\mu(\boldsymbol{r},\omega)}_{\frac{1}{i\omega}E_\mu(\boldsymbol{r},\omega)} .$$

Conductivity tensor:

$$e\langle j_\mu(\boldsymbol{r},t)\rangle_V = \int \frac{d\omega}{2\pi} e^{-i\omega t} \sum_\nu \int d\boldsymbol{r}'\, \sigma_{\mu\nu}(\boldsymbol{r},\boldsymbol{r}',\omega) E_\nu(\boldsymbol{r}',\omega).$$

$$\sigma_{\mu\nu}(\vec{q},\omega) = \frac{ie^2}{\omega}\left[\hbar\chi_{jj}^{\mu\nu}(\vec{q},\omega+i0^+) + \delta_{\mu\nu}\frac{\langle n\rangle}{m}\right]$$

$$\chi_{jj}^{\mu\nu} \equiv -\frac{1}{\Omega}\langle j_\mu^p(\vec{q})\, j_\nu^p(-\vec{q})\rangle_{ret}$$

This expression was established for electrons in the continuum, with $\epsilon_{\vec{k}} = \hbar^2 \vec{k}^2/2m \ , \ v_{\vec{k}} = \hbar\vec{k}/m$

For a tight-binding band in a lattice model, appropriate changes have to be made, namely:

1. Current

$$j^p_{\vec{q}=\vec{0}} = \sum_{\vec{k}\sigma} v^\mu_{\vec{k}} \, c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma}$$

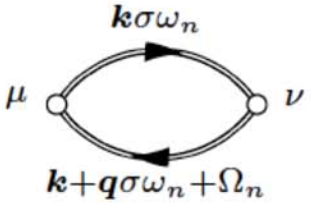
$$v^\mu_{\vec{k}} = \frac{1}{\hbar} \frac{\partial \epsilon_{\vec{k}}}{\partial k_\mu}$$

2. Diamagnetic term in $\sigma_{\mu\mu}$

$$\frac{ie^2}{\omega} \frac{n}{m} \rightarrow \frac{ie^2}{\omega} \int_{\mathrm{BZ}} \frac{d^d k}{(2\pi)^2} \frac{1}{\hbar^2} \frac{\partial^2 \epsilon_{\vec{k}}}{\partial k_\mu^2} n_{\vec{k}}$$

`Kubo-bubble', neglecting vertex (beware !)

$$\chi_{jj}^{\mu\nu}(\boldsymbol{q}, i\Omega_n) = -\sum_{\boldsymbol{k}\sigma} \frac{1}{\beta} \sum_{i\omega_n}$$



$$+ \quad \text{vertex corrections}$$

$$= \left(\frac{\hbar}{m}\right)^2 \sum_{\boldsymbol{k}\sigma} \left(k_\mu + \frac{q_\mu}{2}\right)\left(k_\nu + \frac{q_\nu}{2}\right) \int d\varepsilon_1 d\varepsilon_2\, A(\boldsymbol{k}, \varepsilon_1) A(\boldsymbol{k}+\boldsymbol{q}, \varepsilon_2)$$
$$\times \frac{f(\varepsilon_1) - f(\varepsilon_2)}{i\Omega_n + \varepsilon_1 - \varepsilon_2} \quad + \quad \text{vertex corrections.} \qquad (8.6)$$

Justified rigorously in single-site DMFT, at q=0:

<u>Local self-energy, local vertex</u>

Current matrix element is odd-parity

[Khurana PRL 64, 1990 (1990)]

In this context, interpreted as infinite-d limit,

consistent with all Ward identities and conservation laws.

Final expression for conductivity, Kubo-bubble :

$$\mathrm{Re}\,\sigma_{\mu\nu}(\vec{q}=\vec{0},\omega) = $$
$$= \frac{2\pi e^2}{\hbar} \int d\omega' \frac{f(\omega') - f(\omega'+\omega)}{\omega} \int d\epsilon\, \Phi_{\mu\nu}(\epsilon)\, A(\epsilon,\omega') A(\epsilon,\omega'+\omega)$$

Transport function contains information about **BARE** velocities:

$$\Phi_{\mu\nu}(\epsilon) = \int_{\mathrm{BZ}} \frac{d^d k}{(2\pi)^d} \frac{\partial \epsilon_{\vec{k}}}{\partial k_\mu} \frac{\partial \epsilon_{\vec{k}}}{\partial k_\nu} \delta(\epsilon - \epsilon_{\vec{k}}) \quad ,$$
$$\Phi(\epsilon) = \frac{1}{d} \sum_\mu \Phi_{\mu\mu}(\epsilon)$$

I hope I got factors of 2, π, e, h etc… right !
Dimensions are OK !

Transport function for quasi-2D free electrons :

$$\Phi(\epsilon) = \frac{1}{2}\int_{-\pi/c_0}^{+\pi/c_0} \frac{dk_z}{2\pi} \int \frac{dk_x dk_y}{4\pi^2} \left(\frac{\hbar^2}{m}\right)^2 (k_x^2 + k_y^2)\, \delta\left[\epsilon - \frac{\hbar^2}{2m}(k_x^2 + k_y^2)\right],$$

$$\Phi(\epsilon) = \frac{\epsilon}{2\pi c_0}$$

Hence, the IRM limit is naturally expressed in terms of $\Phi(\epsilon_F)/\epsilon_F$

Drude, quasi-2D:

$$\sigma_{dc} = \frac{e^2}{\hbar} \frac{\Phi(\epsilon_F)}{\epsilon_F} (k_F l)$$