``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 6 juin 2012

- **Séminaire : 15h45 –**

Nigel Hussey (University of Bristol)

High-temperature superconductivity and the Catch-22 conundrum

OUTLINE

- May, 30: Phenomenology, simple theory background. Mainly raise questions.
- June, 6: 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

In memoriam Bernard Coqblin

Directeur de Recherche au CNRS, LPS-Orsay
Honorary Professor, Polish Academy of Sciences, Wroclaw
Dr Honoris Causa, Univ. Federal do Rio Grande do Sul, Brasil

PHYSICAL REVIEW VOLUME 185, NUMBER 2 10 SEPTEMBER 1969

Exchange Interaction in Alloys with Cerium Impurities*

B. COQBLIN† AND J. R. SCHRIEFFER
Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania 19104
(Received 4 March 1969)

Ex: Ruthenates (remember: 3 FS sheets)

ab-plane:

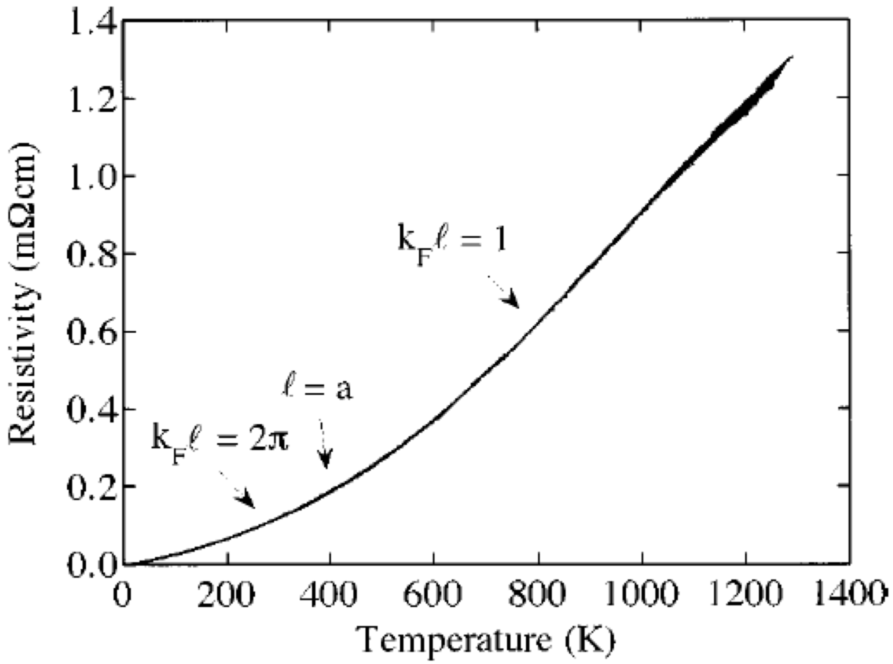


FIG. 1. The in-plane resistivity of Sr_2RuO_4 from 4 to 1300 K. Three criteria for the Mott-Ioffe-Regel limit are marked on the graph, and there is no sign of resistivity saturation, so Sr_2RuO_4 is a "bad metal" at high temperatures, even though it is known to be a very good metal at low temperatures.

- resistivity does cross IRM value

- Nothing dramatic is seen in ρ upon crossing IRM

Tyler, Maeno, McKenzie
PRB 58 R10107 (1998)

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}

Some answers in a precise context: Doped Mott insulator with single-site DMFT

Recent results by: Xiaoyu Deng (EP), Jernej Mravlje (EP&CDF)
Rok Zitko (Ljubljana) & AG



Building up on previous work by several authors, see e.g. G.Palsson et al. PRL 80, 475 (1998) and PhD Rutgers; Merino & McKenzie PRB 61, 7996 (2000), Limelette et al. PRL and Science 2003, Uhrig et al. recent papers, etc.

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 !

Why now ?

- Could have been done 20 years ago… in principle (part of it has been explored, some key points were missed though)
- In practice:
- Need highly accurate impurity solvers down to low-T, with excellent resolution at low frequency (calculation of transport is exceedingly delicate)
- Need to handle real frequencies: a challenge to QMC methods

Algorithms

- NRG (à la Wilson)
- CT-QMC (mostly HYB, also U-exp at hi-T)

E.Gull et al.

REVIEWS OF MODERN PHYSICS, VOLUME 83, APRIL–JUNE 2011

Continuous-time Monte Carlo methods for quantum impurity models

Allows for analytic continuation using Pade approximants !!
(M.Ferrero)

TRIQS – a Toolbox for Research on Interacting Quantum Systems

ÉCOLE POLYTECHNIQUE

XHTML 1.0

TRIQS

a Toolbox for Research on Interacting Quantum Systems

http://ipht.cea.fr/triqs/

UNITS

Energy, Temperature, Frequency:

½ bandwidth D (=1). Think of D= 1eV = 12000 K

Note: $\beta \equiv \dfrac{D}{k_B T}$

Resistivity

Ioffe-Regel-Mott value $\sigma_M = \dfrac{e^2}{\hbar} \dfrac{\Phi(\epsilon_F)}{\epsilon_F} \quad , \quad (k_F l = 1)$

Most calculations shown for U/D=4 (> Mott MIT ~ 3)

Transport function for quasi-2D free electrons :

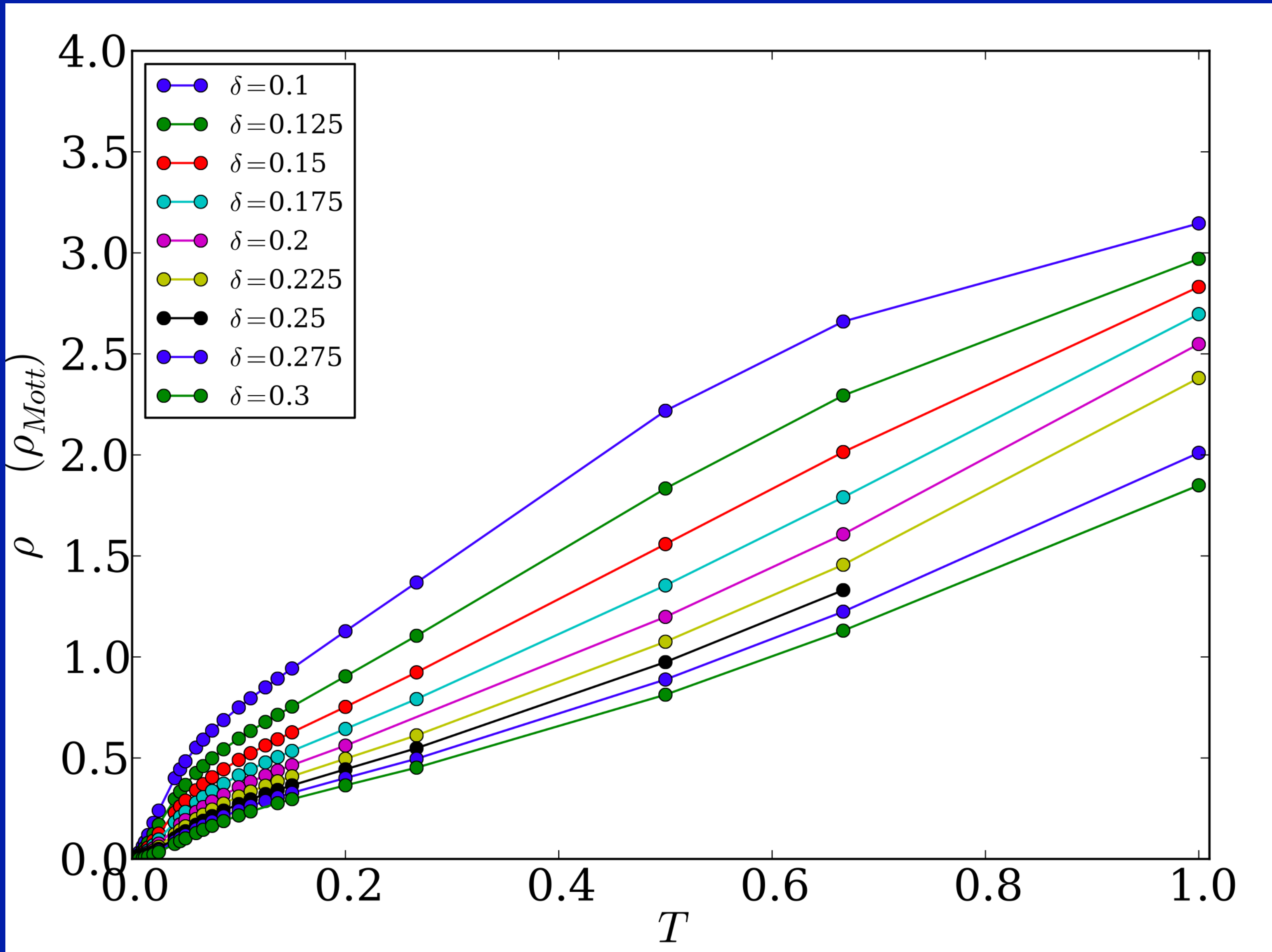
$$\Phi(\epsilon) = \frac{1}{2}\int_{-\pi/c_0}^{+\pi/c_0} \frac{dk_z}{2\pi} \int \frac{dk_x dk_y}{4\pi^2} \left(\frac{\hbar^2}{m}\right)^2 (k_x^2 + k_y^2)\, \delta\left[\epsilon - \frac{\hbar^2}{2m}(k_x^2 + k_y^2)\right],$$

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

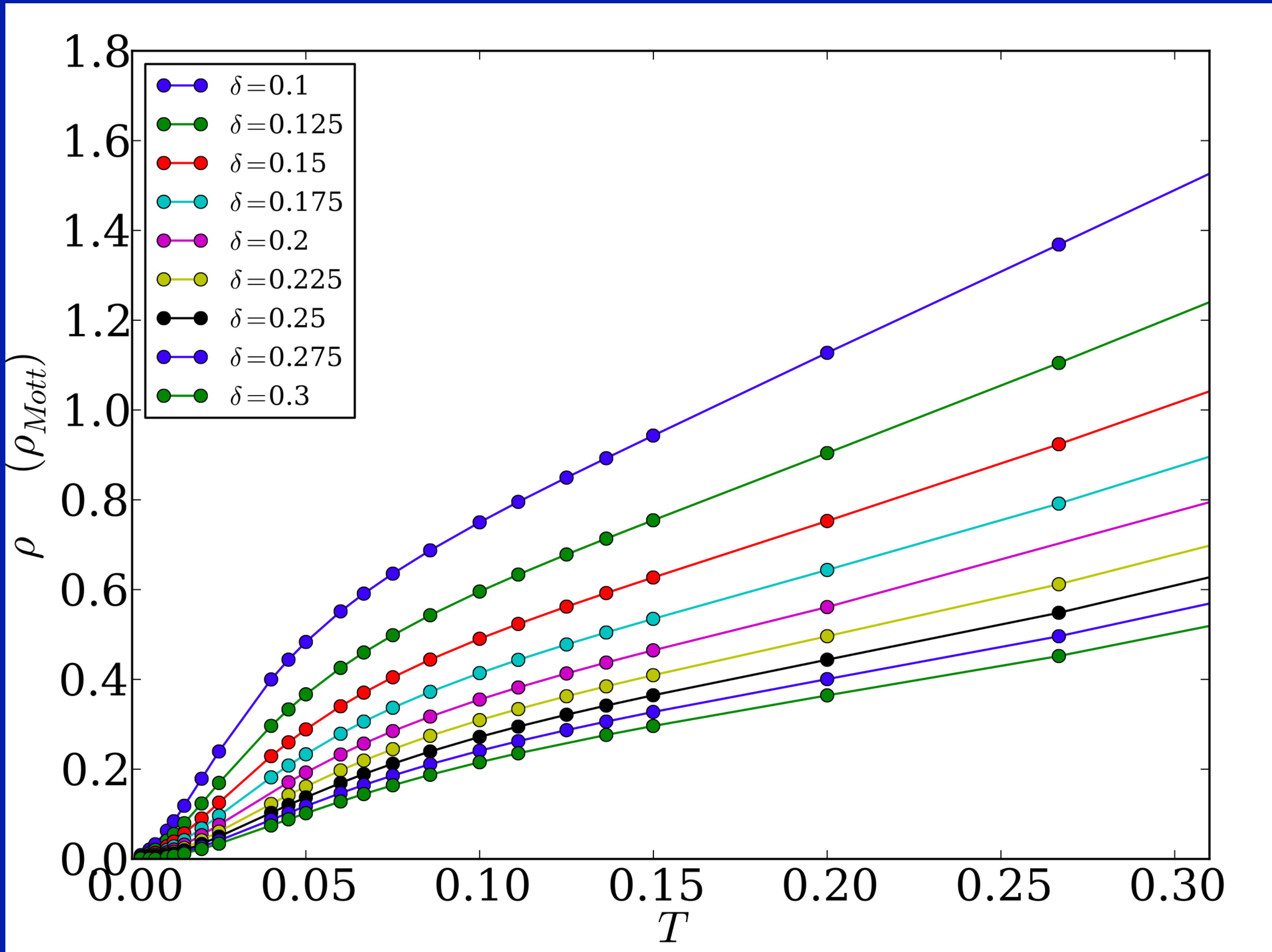
Hence, the IRM limit is naturally expressed in terms of $\Phi(\epsilon_F)/\epsilon_F$

Drude, quasi-2D:

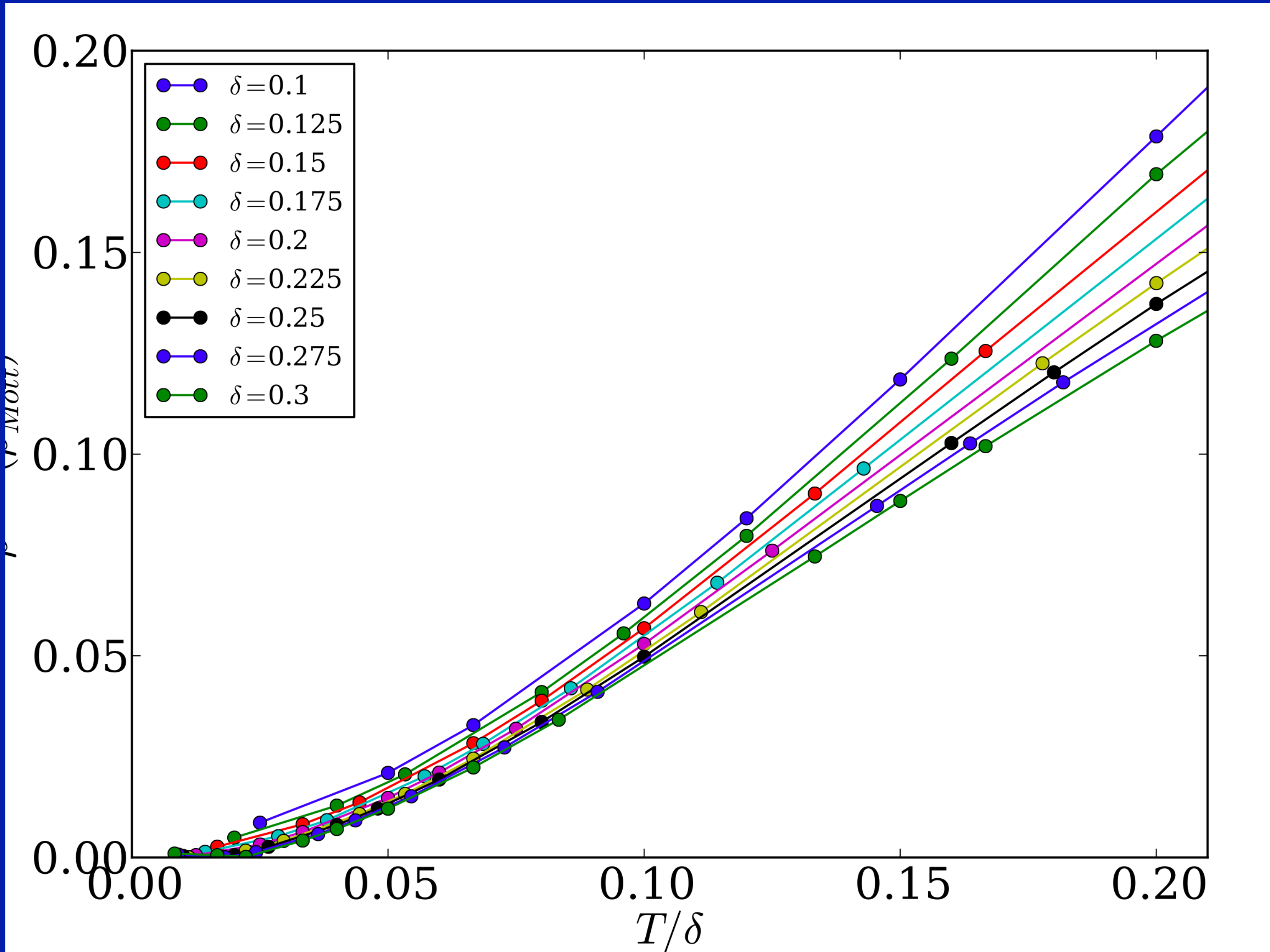
$$\boxed{\sigma_{dc} = \frac{e^2}{\hbar}\,\frac{\Phi(\epsilon_F)}{\epsilon_F}\,(k_F l)}$$



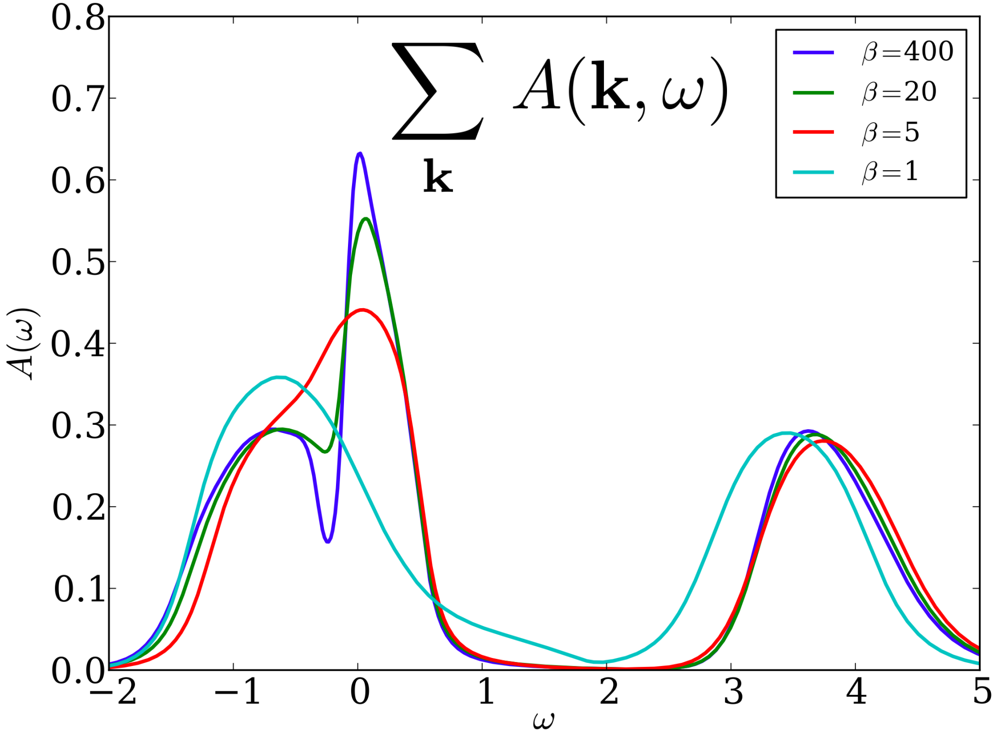
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0.0
0.2
0.4
0.6
0.8
1.0
T
$\rho \quad (\rho_{Mott})$
$\delta = 0.1$
$\delta = 0.125$
$\delta = 0.15$
$\delta = 0.175$
$\delta = 0.2$
$\delta = 0.225$
$\delta = 0.25$
$\delta = 0.275$
$\delta = 0.3$



$\delta=0.1$
$\delta=0.125$
$\delta=0.15$
$\delta=0.175$
$\delta=0.2$
$\delta=0.225$
$\delta=0.25$
$\delta=0.275$
$\delta=0.3$
$\rho \quad (\rho_{Mott})$
T
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
0.00
0.05
0.10
0.15
0.20
0.25
0.30



$\delta = 0.1$
$\delta = 0.125$
$\delta = 0.15$
$\delta = 0.175$
$\delta = 0.2$
$\delta = 0.225$
$\delta = 0.25$
$\delta = 0.275$
$\delta = 0.3$
0.00
0.05
0.10
0.15
0.20
T/δ

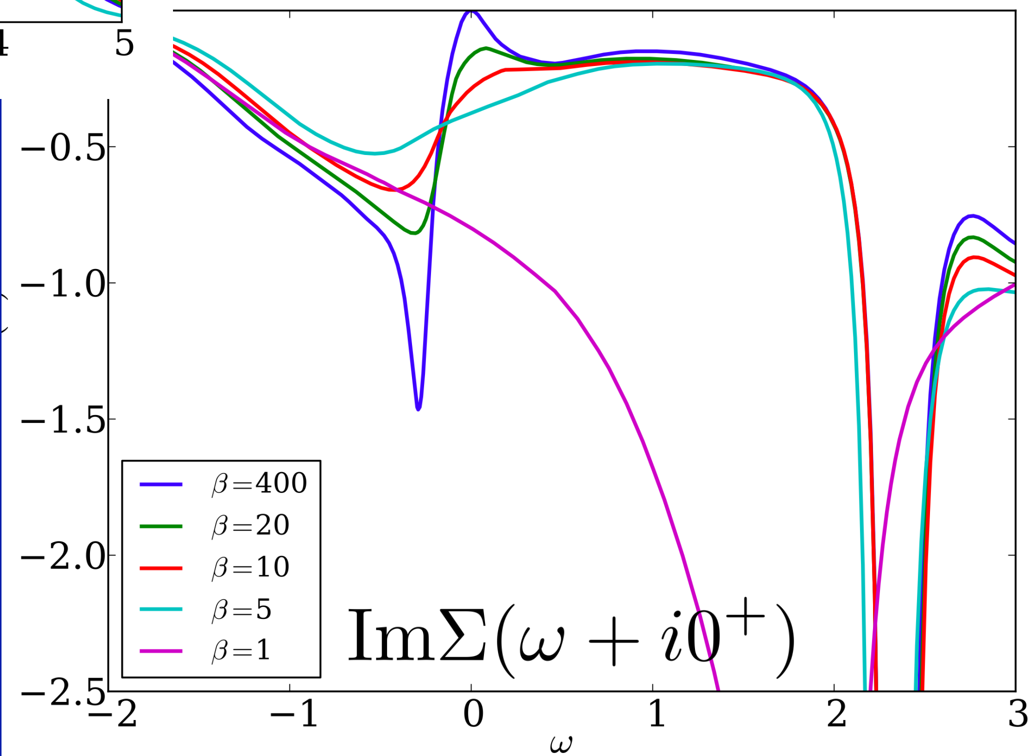


Doping: 20%

- Rich frequency dependence
- A lot of action in spectral properties as T is varied !

Total DOS

Self-energy
``scattering rate”



1. The Fermi-Liquid regime

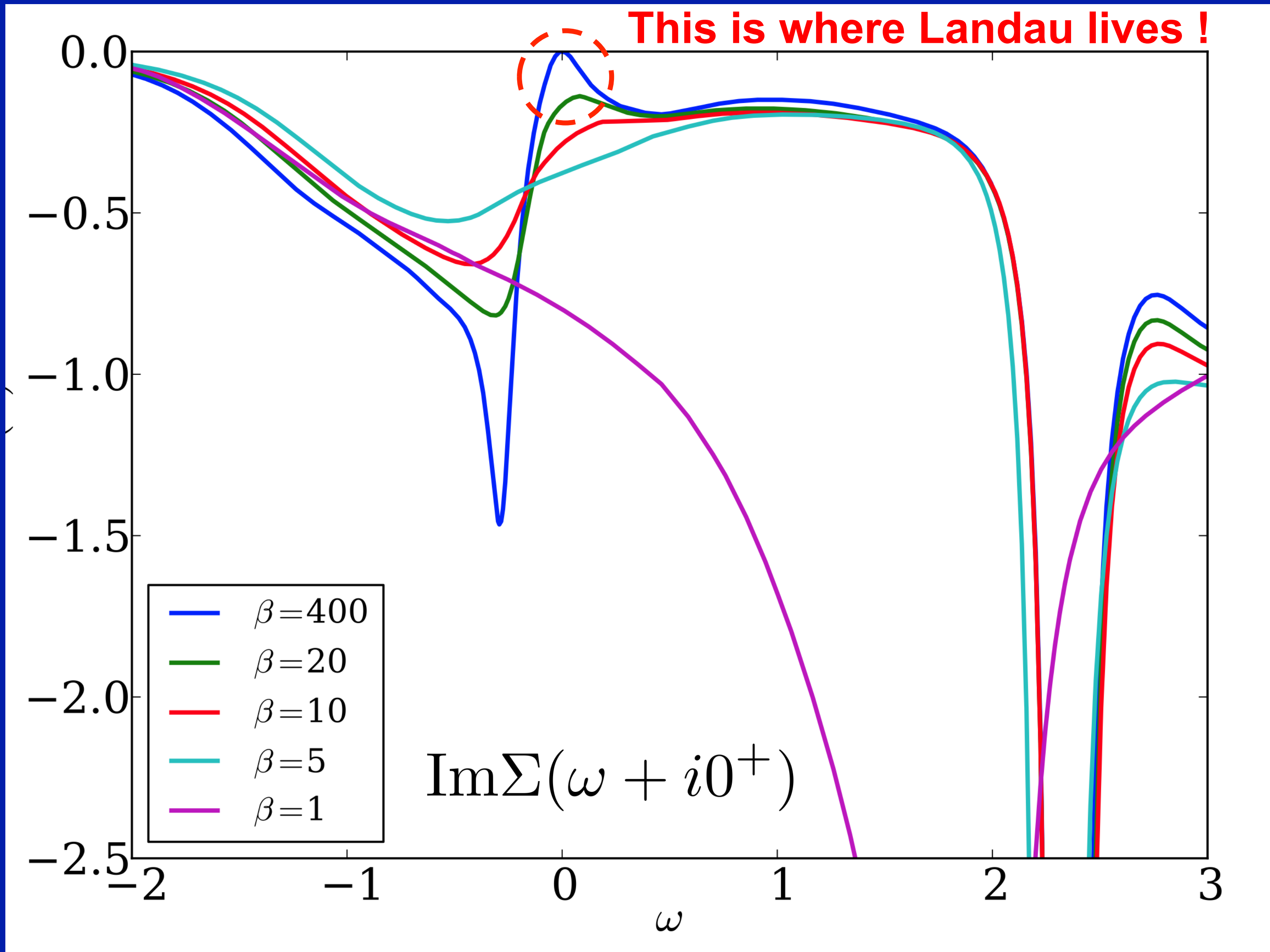
Local Fermi-liquid/Landau Theory description
A self-consistent Kondo-like screening problem
DMFT (lattice) self-consistency → intermediate coupling

$$\mathrm{Re}\Sigma(\omega + i0^+) = \Sigma_0 + (1 - \frac{1}{Z})\omega + \cdots$$

$$-\mathrm{Im}\Sigma(\omega + i0^+) = \frac{c}{D}\left[\omega^2 + (\pi T)^2\right]$$

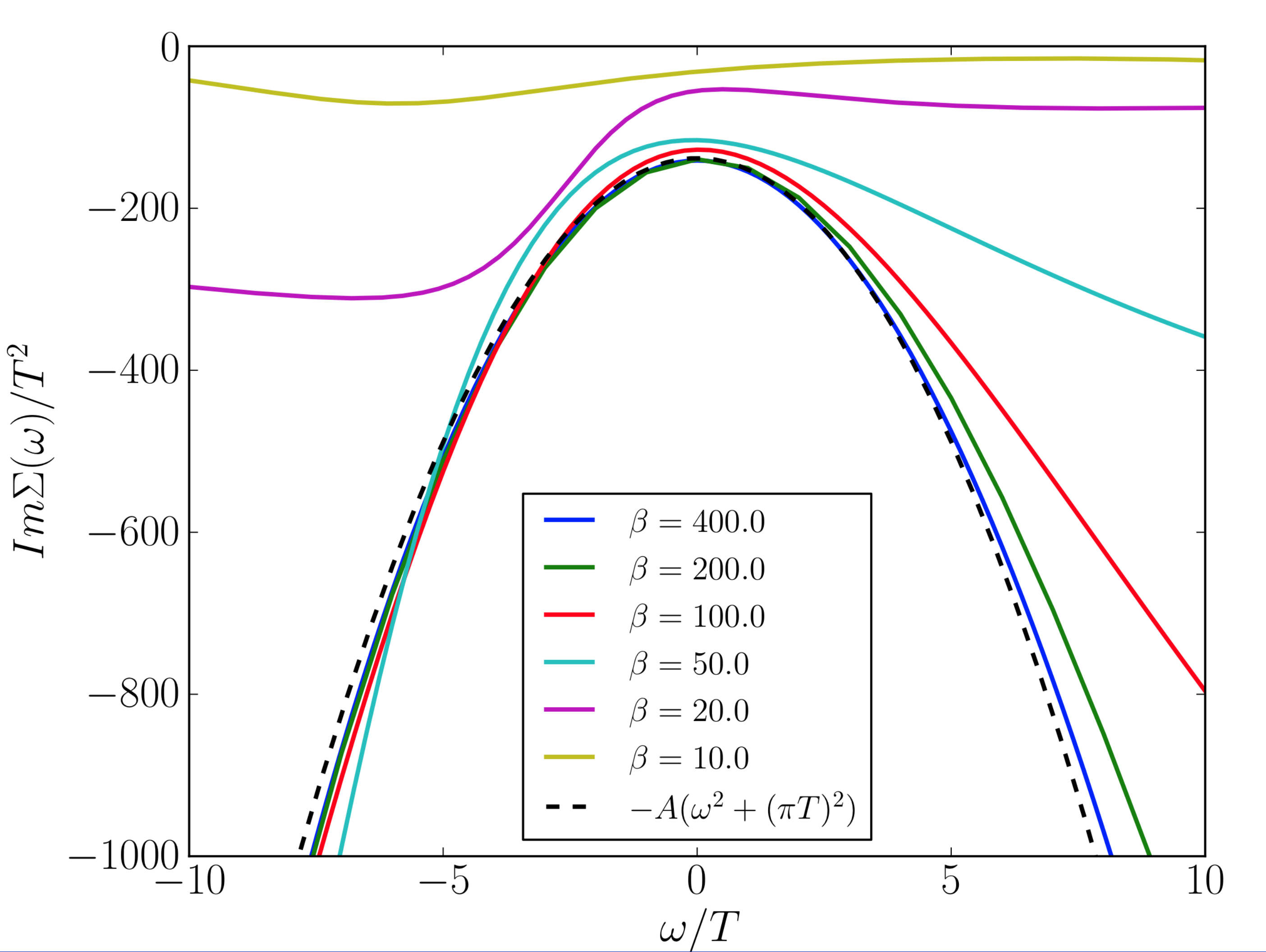
Luttinger theorem (large FS):

$$\mu - \Sigma_0(T=0) = \mu_{U=0}(n) \equiv \epsilon_F$$

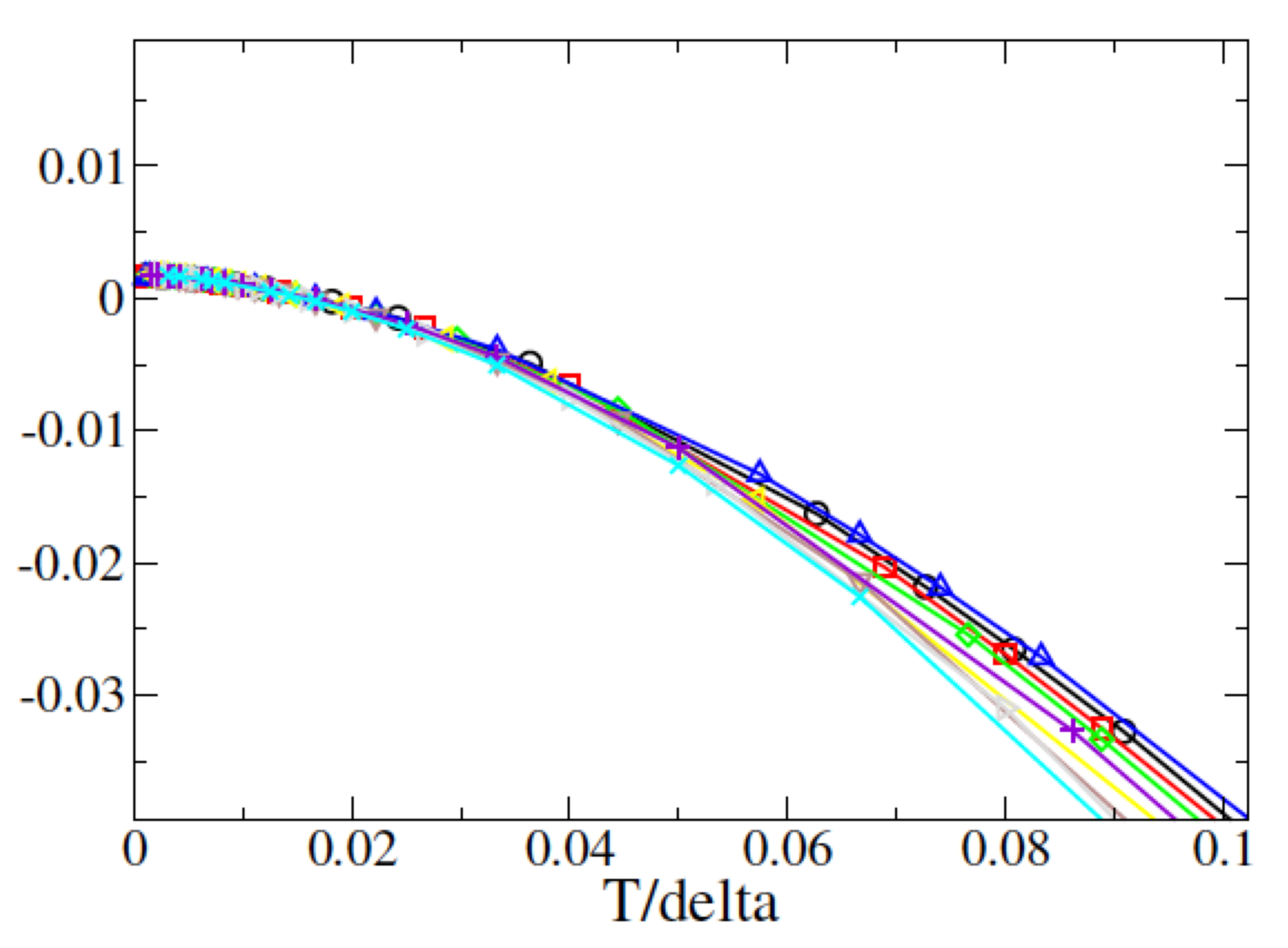


This is where Landau lives !
0.0
−0.5
−1.0
−1.5
−2.0
−2.5
−2
−1
0
1
2
3
ω
β=400
β=20
β=10
β=5
β=1
ImΣ(ω + i0+)

Identifying the Fermi Liquid scale
a. From ω^2+$(\pi T)^2$ scaling (Pade)

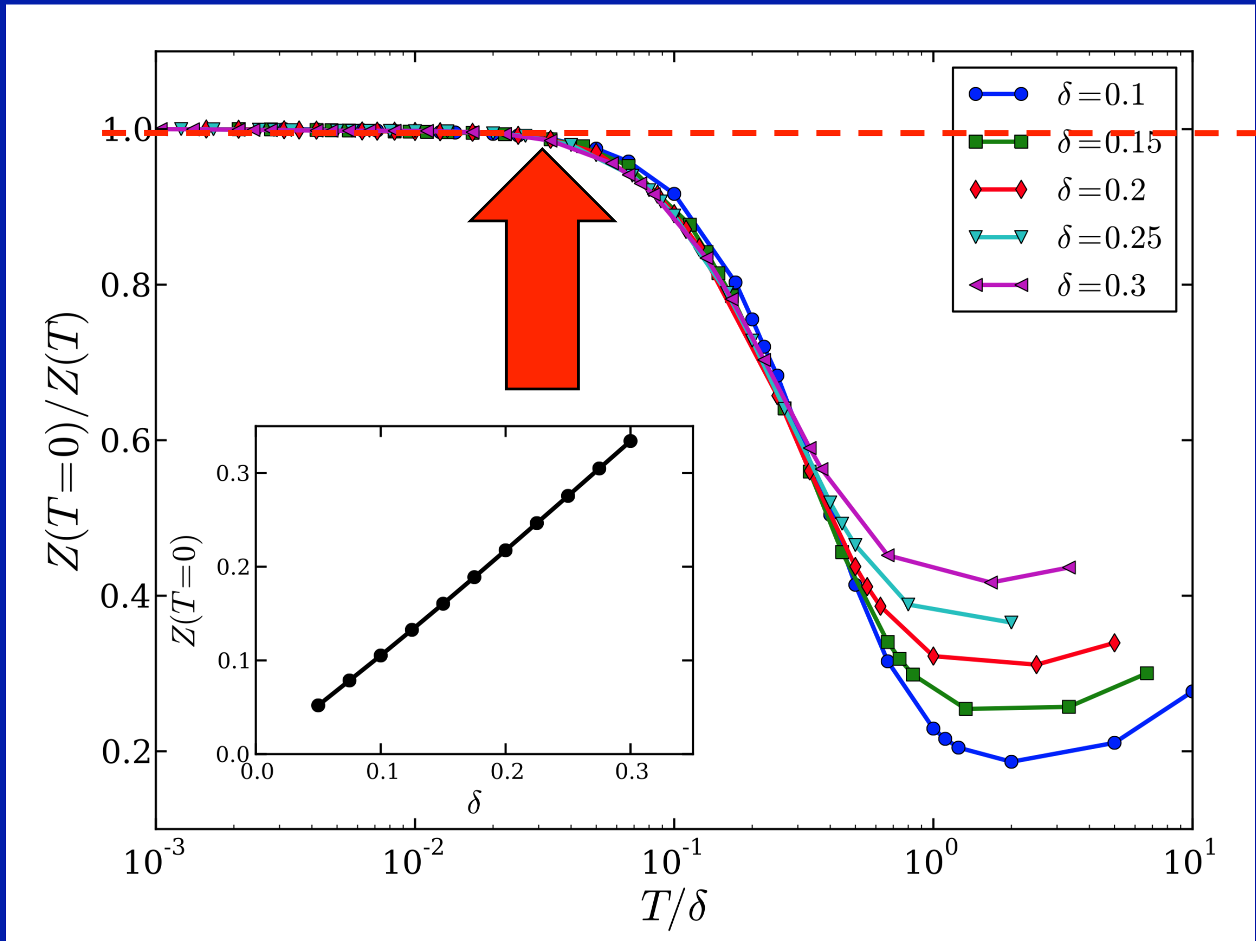


b. From ImΣ(0,T) vs. T/δ



c. From T-dep of ``effective mass''
(useful: Matsubara…)

$Z(0)/Z(T)$ = const. for $T < T_{FL}$



Brinkman-Rice Behaviour of

$$\frac{m^*}{m} = \frac{1}{Z} = \frac{1}{\delta}$$

Fermi Liquid scale (U/D=4)

$$\boxed{T_{\mathrm{FL}}/D \simeq 0.05\,\delta}$$

* A very low scale
(as compared to bare electronic scales) !
e.g. D=1eV, δ=10% → 60 K

* Scales ~ doping
but <u>much lower</u> than `Brinkman-Rice' scale ~ δD
(by 1/20)

Resistivity in the FL regime: analytics

Low ω,T scaling form of scattering rate:

$$-\,\mathrm{Im}\Sigma/D = a\left[\left(\frac{\omega}{\pi\delta}\right)^2 + \left(\frac{T}{\delta}\right)^2\right] + \cdots$$

$$a(U/D=4) \simeq 5.5$$

→ On blackboard

$$\frac{\rho(T)}{\rho_M} = 1.22a\left(\frac{T}{\delta D}\right)^2 + \cdots \simeq 0.017\left(\frac{T}{T_{FL}}\right)^2$$

$$\rho(T_{FL}) << \rho_M$$

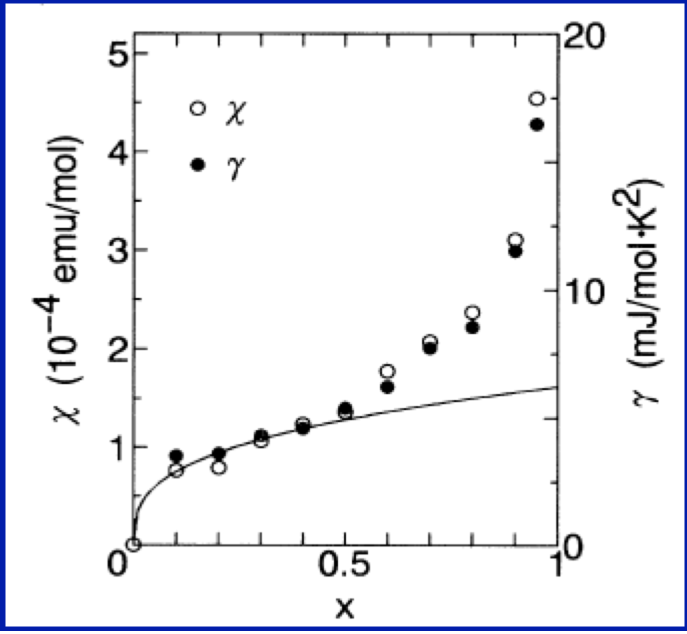
Note: Z~δ drops out from A/γ^2 = NON-UNIVERSAL constant

`Kadowaki Woods' 1986, TM Rice 1968

cf. N.Hussey JPSJ 74 (2005) 1107; B.Powell et al. Nature Physics 2009

$Sr_{1-x}La_xTiO_3$

Tokura et al. PRL 1993



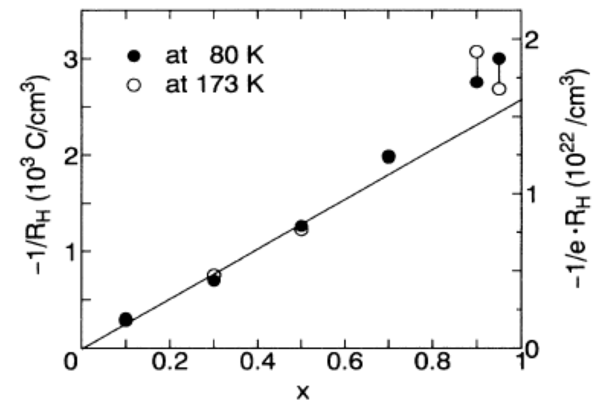
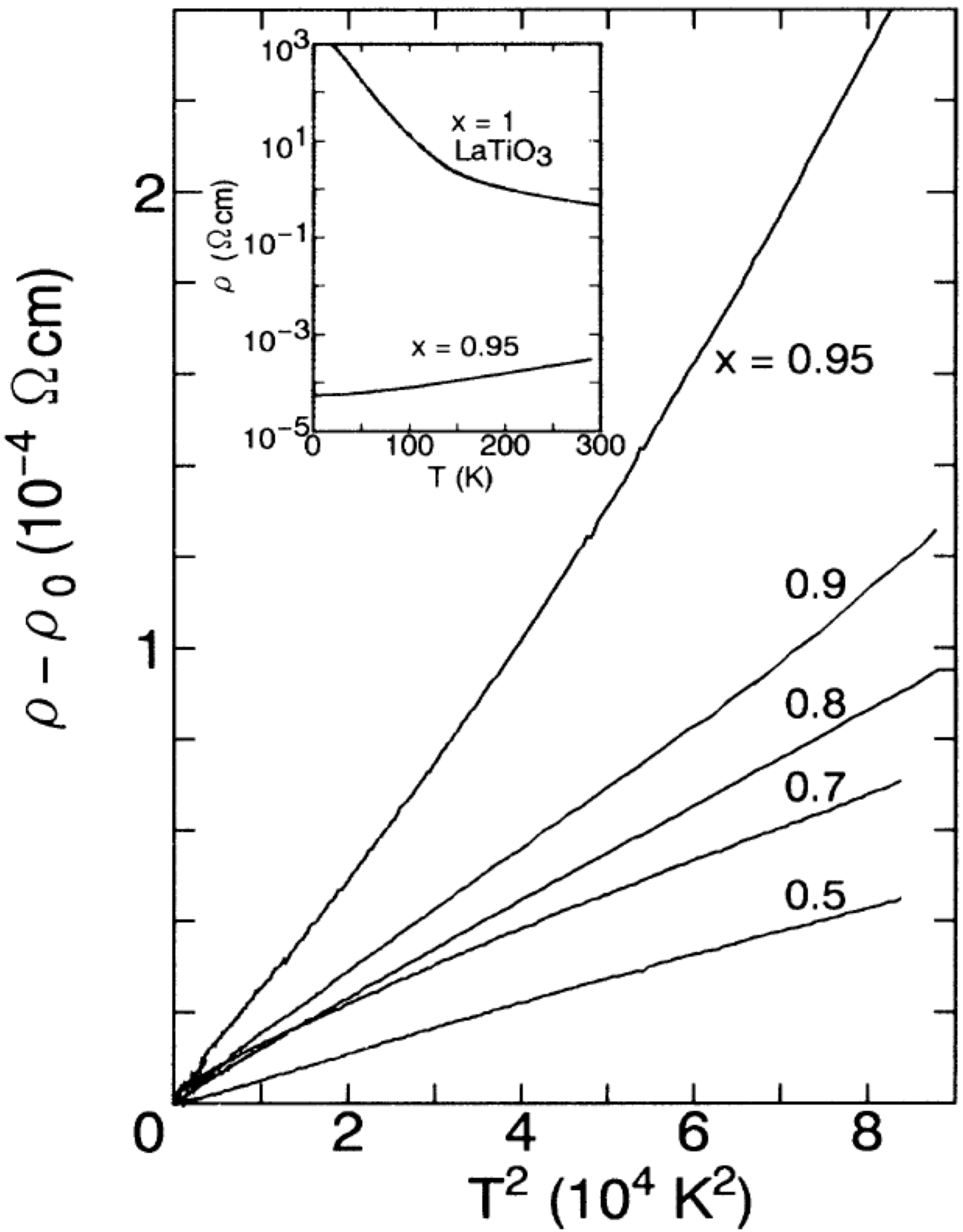
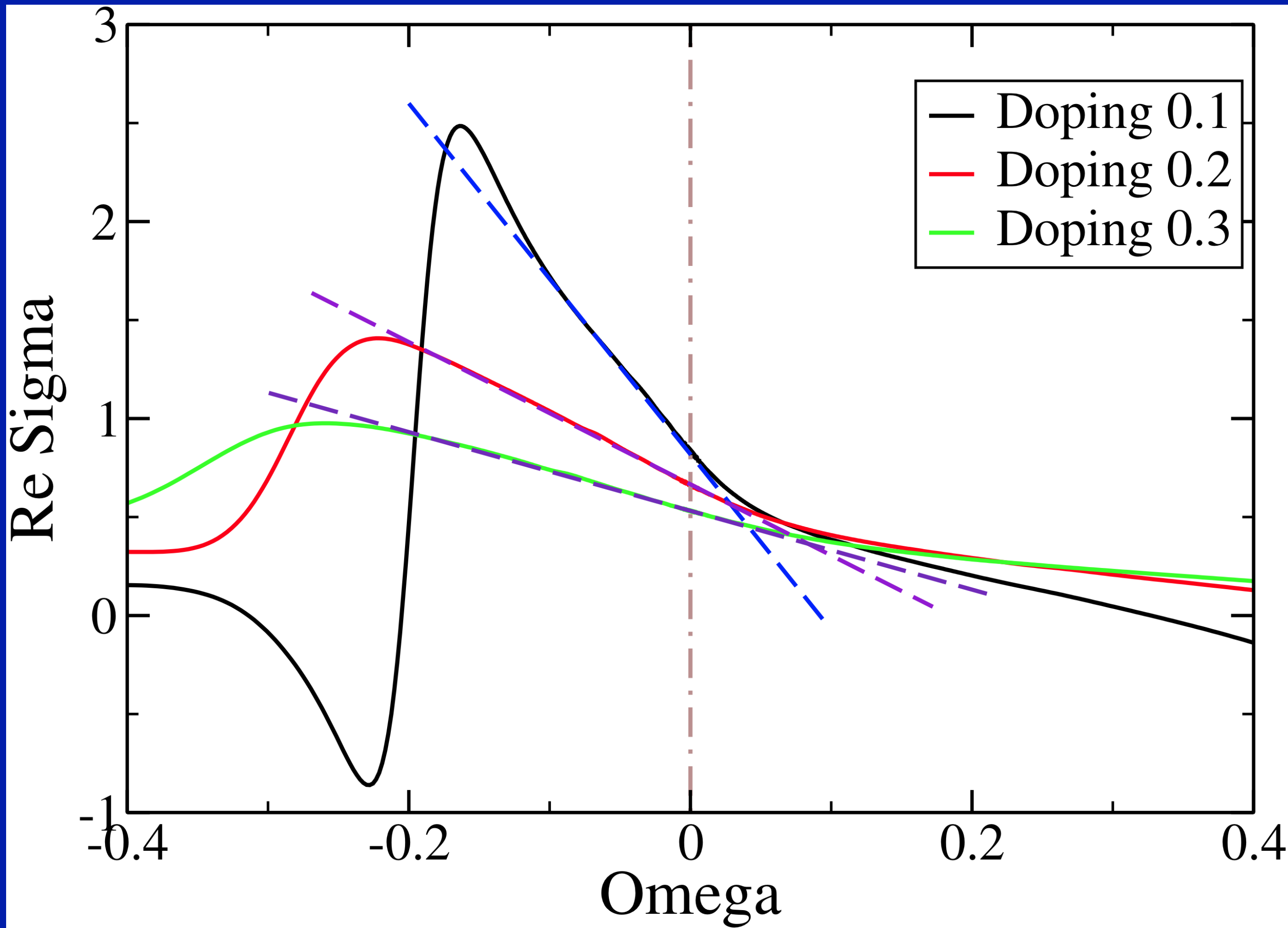


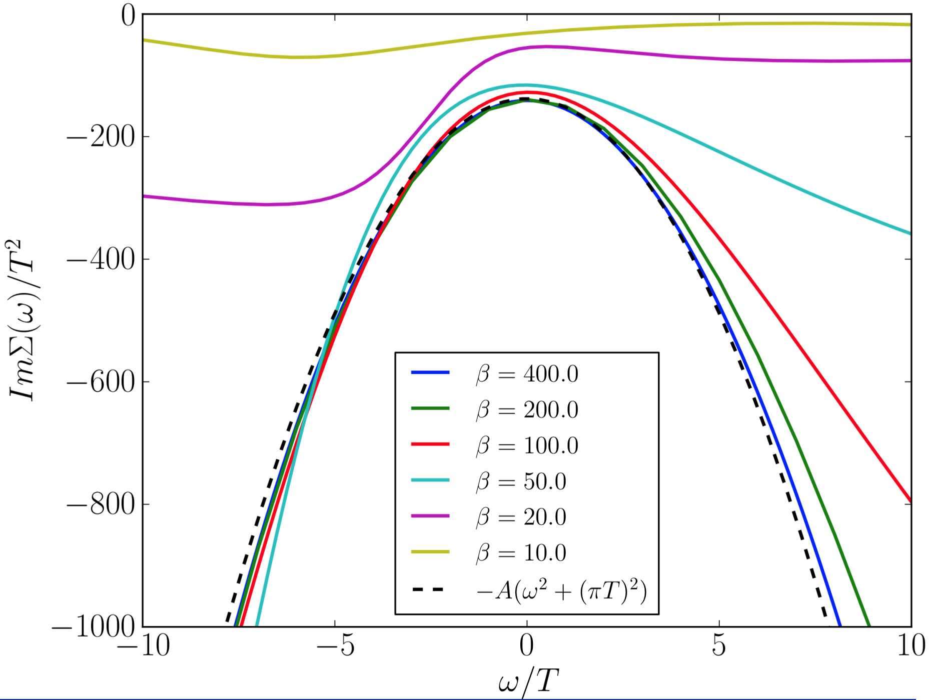
FIG. 2. The filling (x) dependence of the inverse of Hall coefficient (R_H^{-1}) in $Sr_{1-x}La_xTiO_3$. Open and closed circles represent the values measured at 80 K and 173 K, respectively. A solid line indicates the calculated one based on the assumption that each substitution of a Sr^{2+} site with La^{3+} supplies the compound with one electron-type carrier per Ti site.



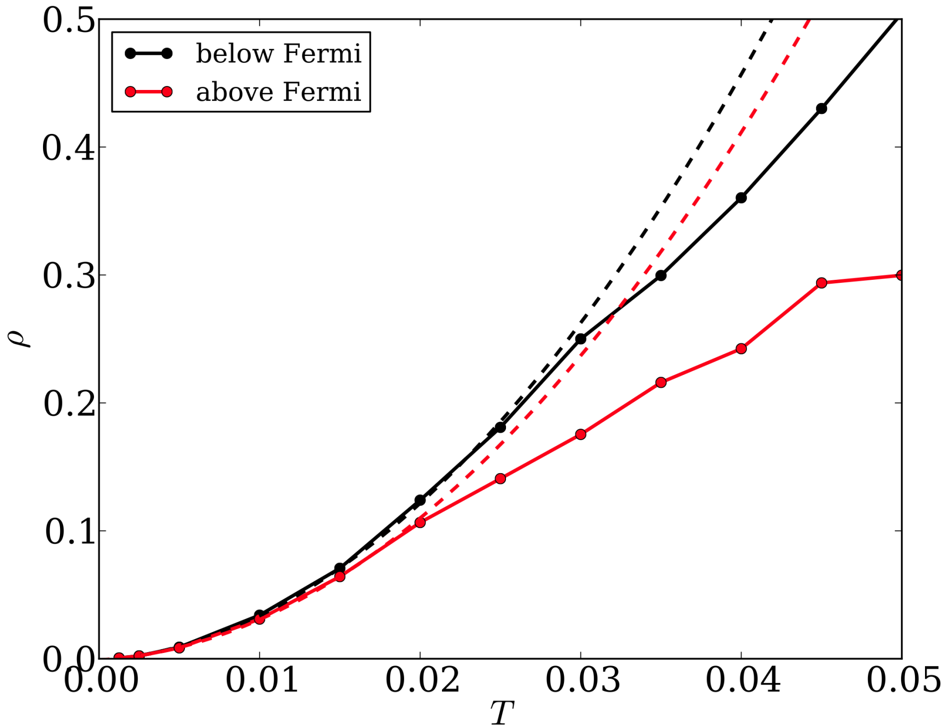
Hole- and electron- like `kinks' and the FL coherence scale



Strong particle-hole asymmetry of the scattering rate in the FL regime



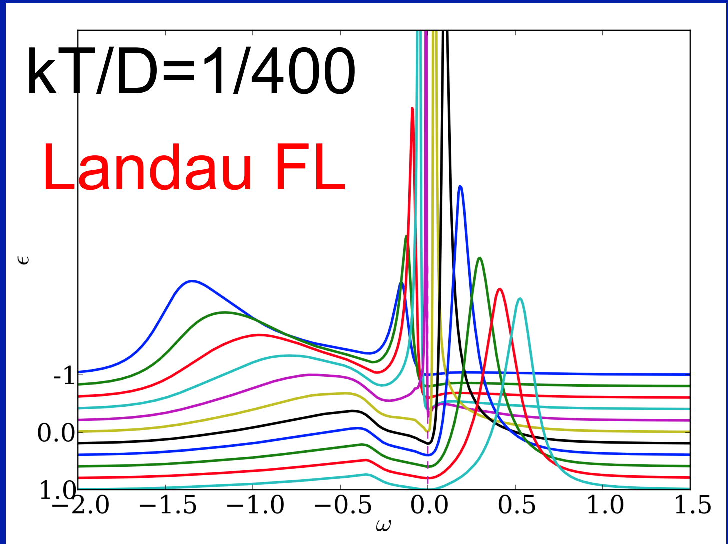
Positive ω and negative ω contributions to Kubo-Drude formula:

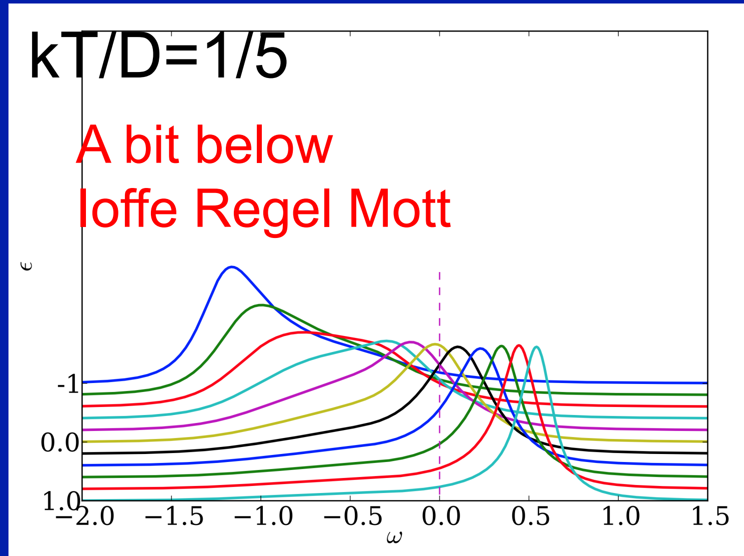


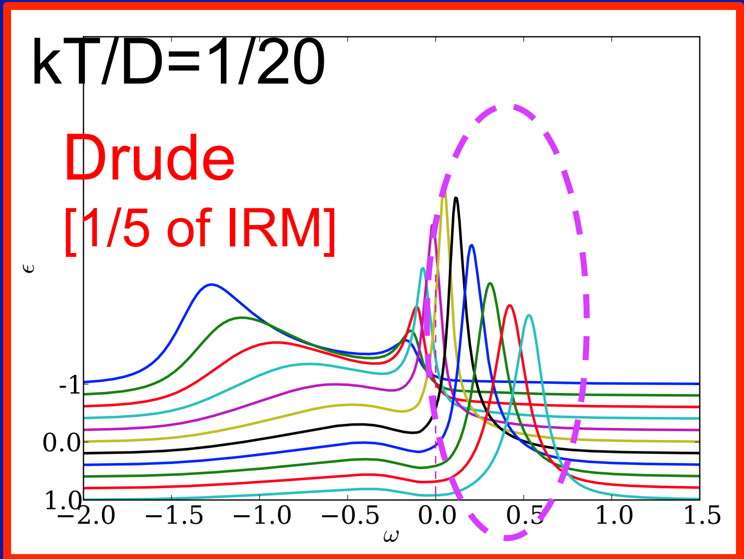
2. The `Drude' regime for $T>T_{FL}$ $(T<T_{IRM})$

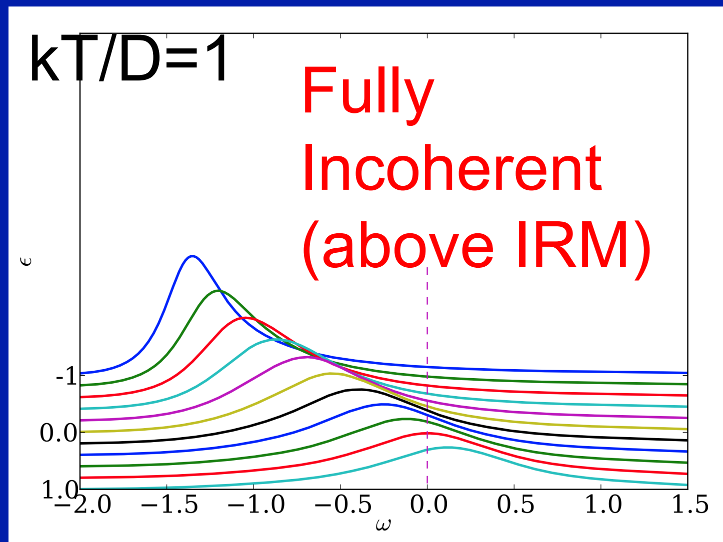
Quasiparticles SURVIVE but they no longer obey Landau's theory

The 'dark side' of the Fermi surface

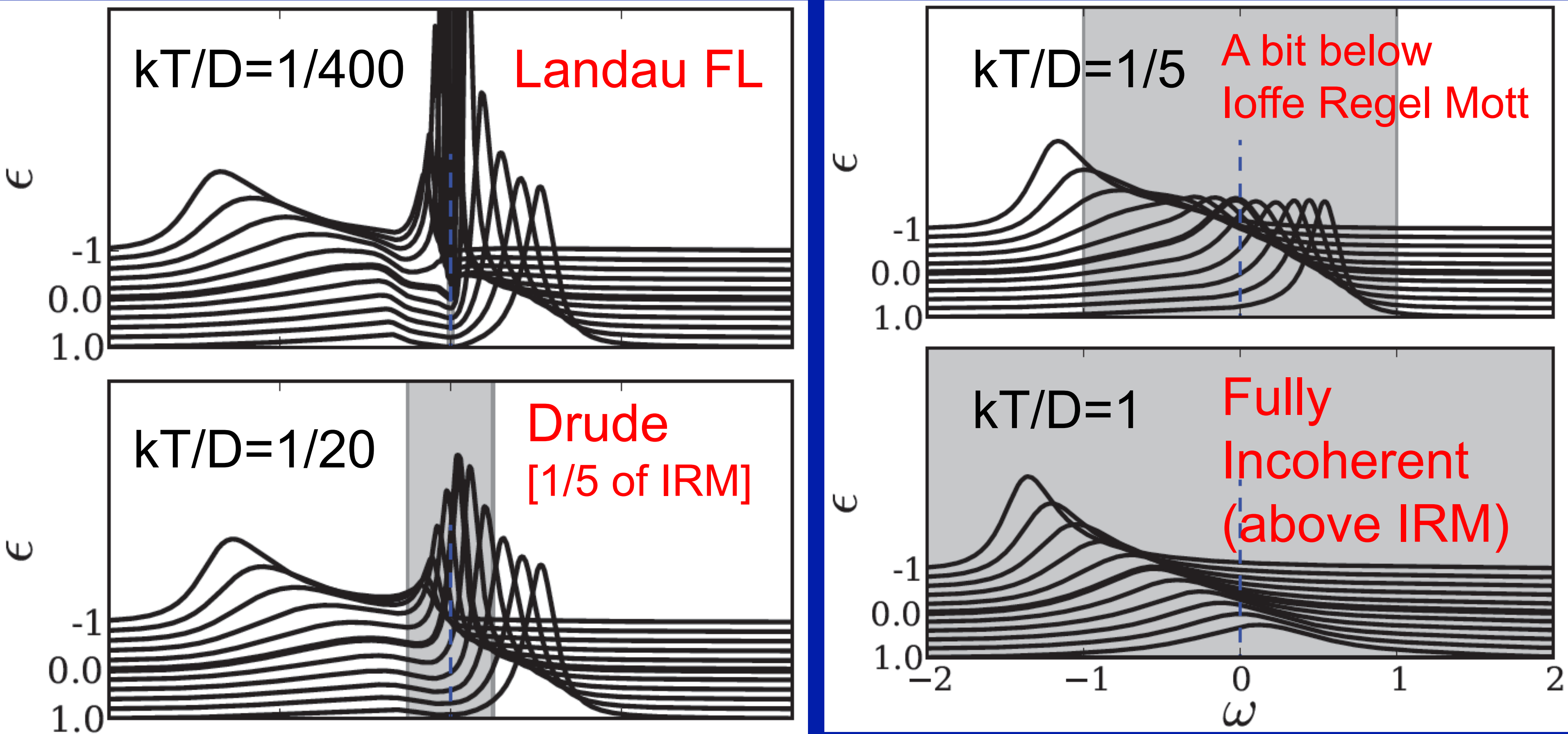




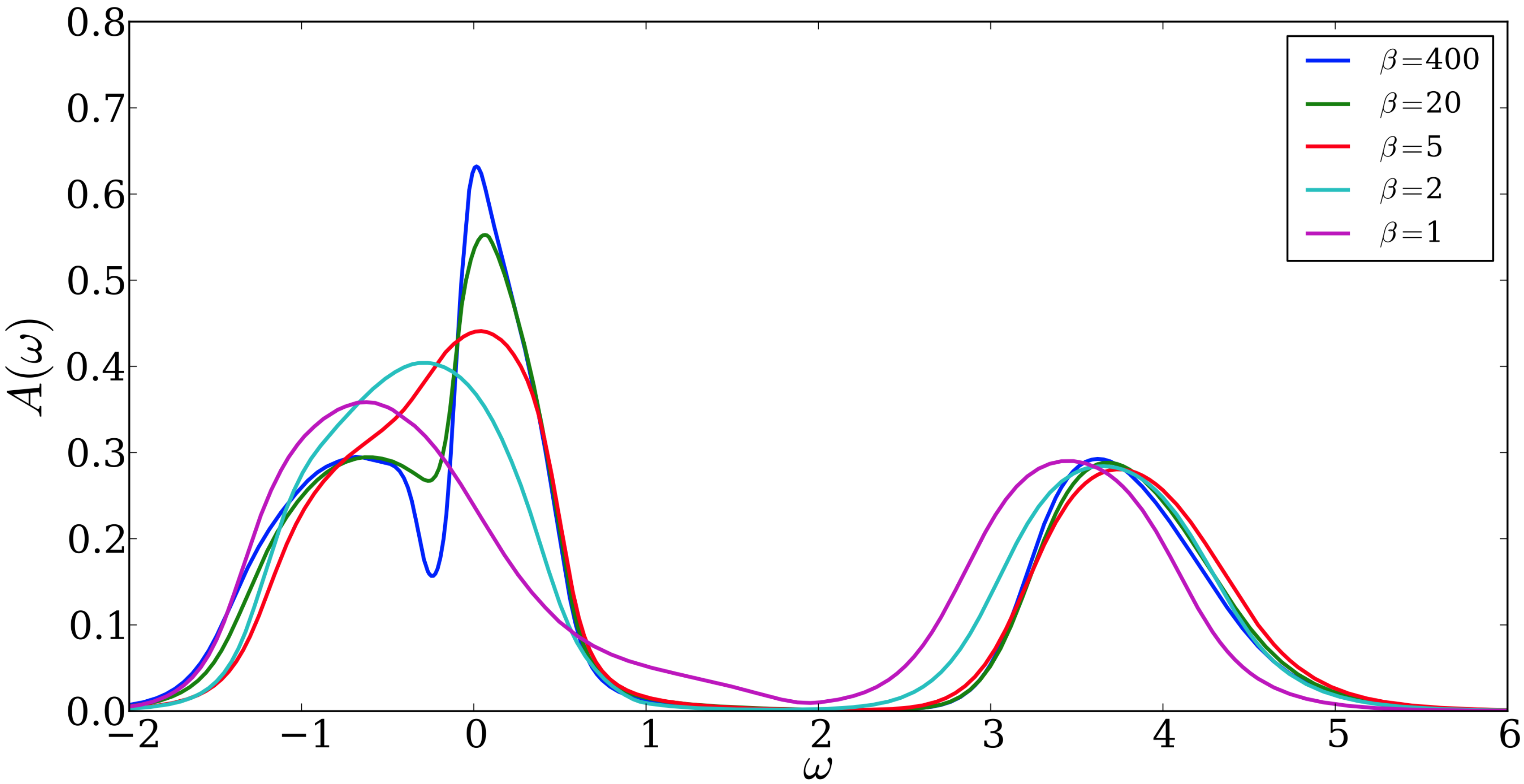




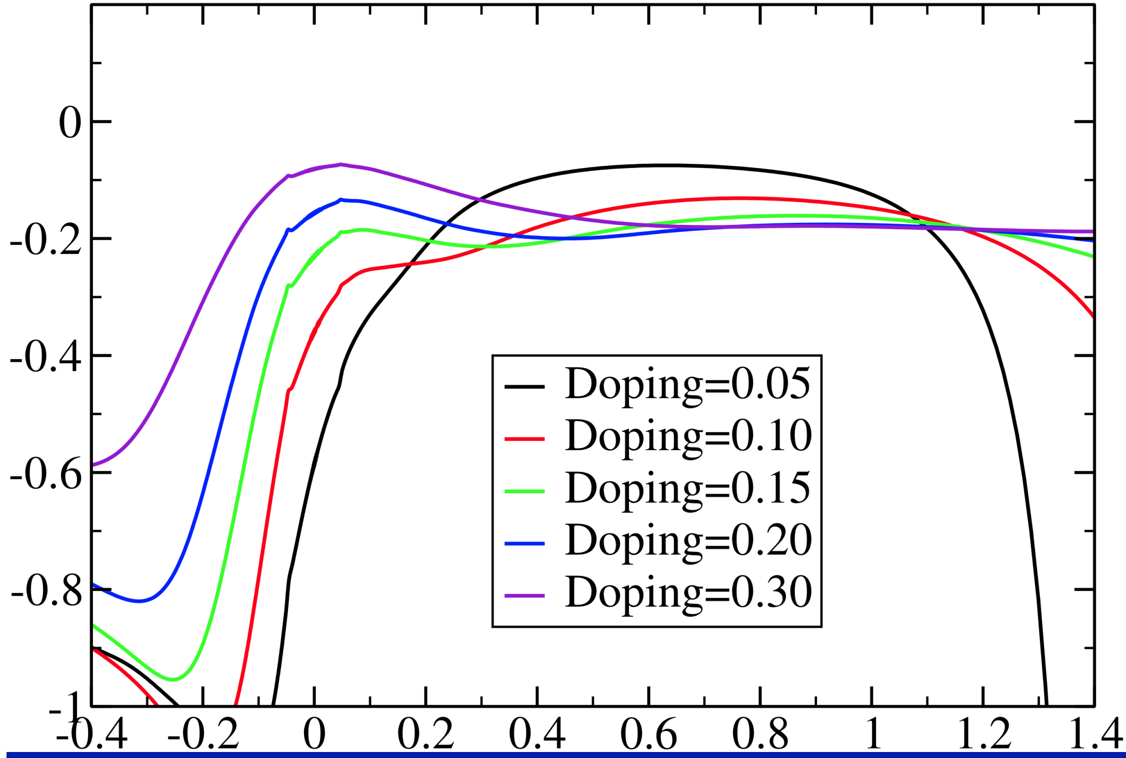
Which excitations contribute to dc transport ?



Total DOS



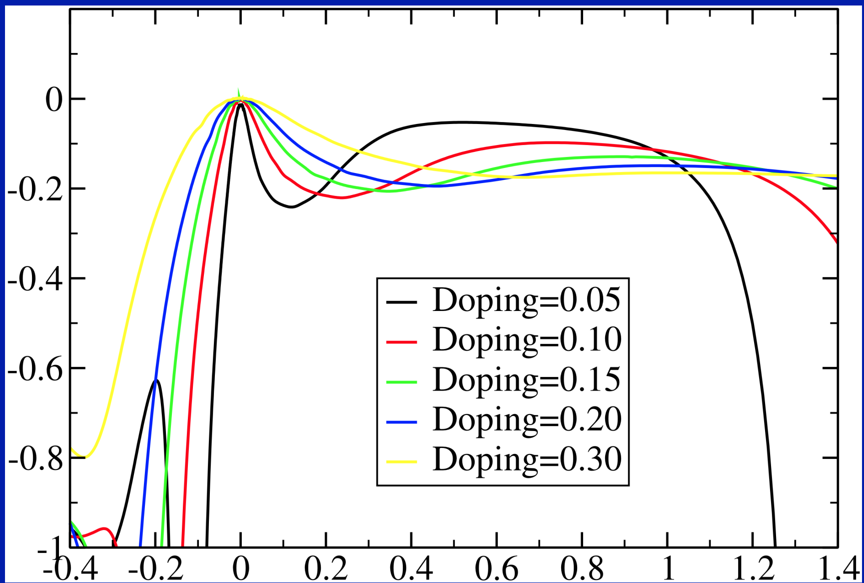
Clear 3-peak structure way above T_{FL}

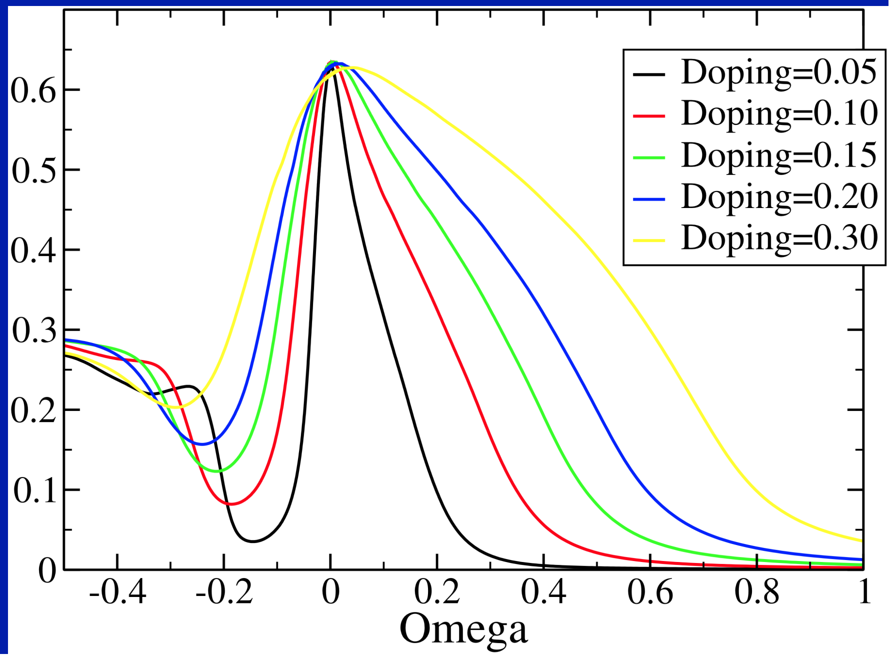


`Drude' quasiparticles:

Scattering rate >> kT
but << D

Weakly-temperature and energy-dependent (`plateau')
over some range





Claims about destruction of quasiparticles as seen in ARPES: to be reconsidered

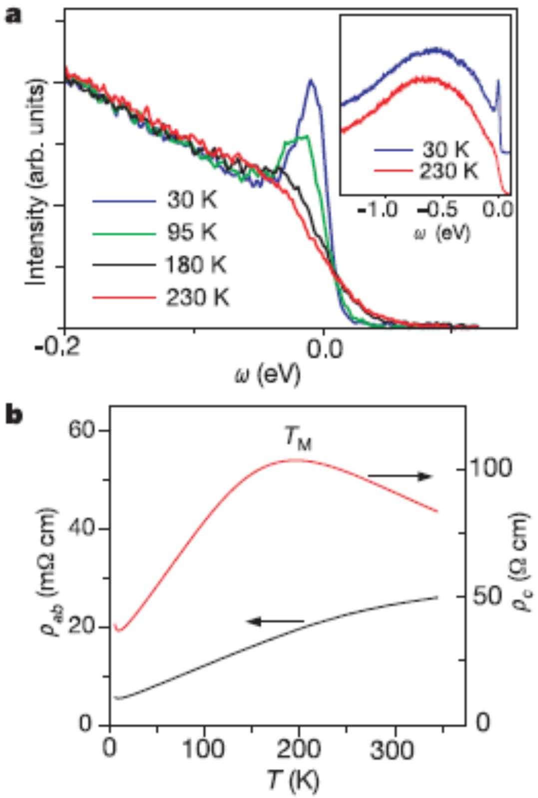


Figure 2 Correlation between the ARPES and transport in $(Bi_{0.5}Pb_{0.5})_2Ba_3Co_2O_y$. **a**, The changes in energy distribution curves (vertical cross-sections of the ARPES data shown in Fig. 1) (for $k = k_F$) with temperature. The inset shows the wide-range energy distribution curves. **b**, Transport data. The in-plane and the out-of-plane resistivities are measured on a sample from the same batch with a conventional four-probe technique.

T.Valla et al. Nature 417 (2002) 628

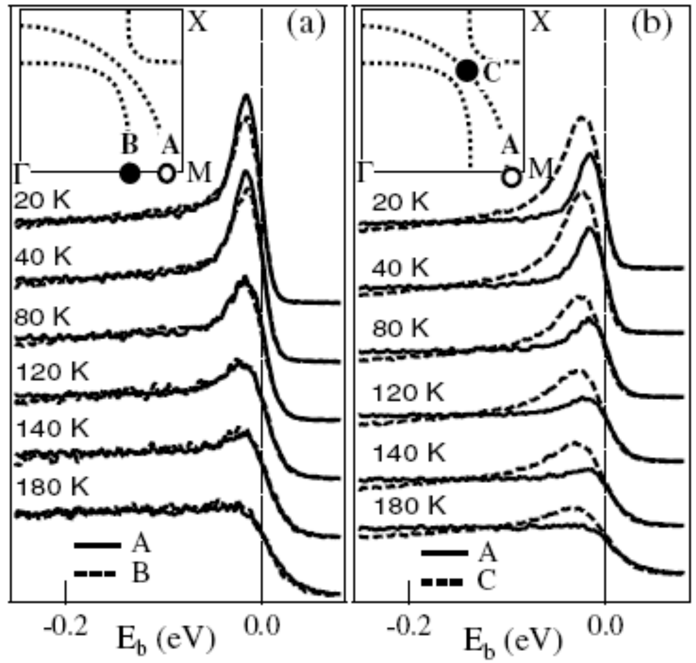
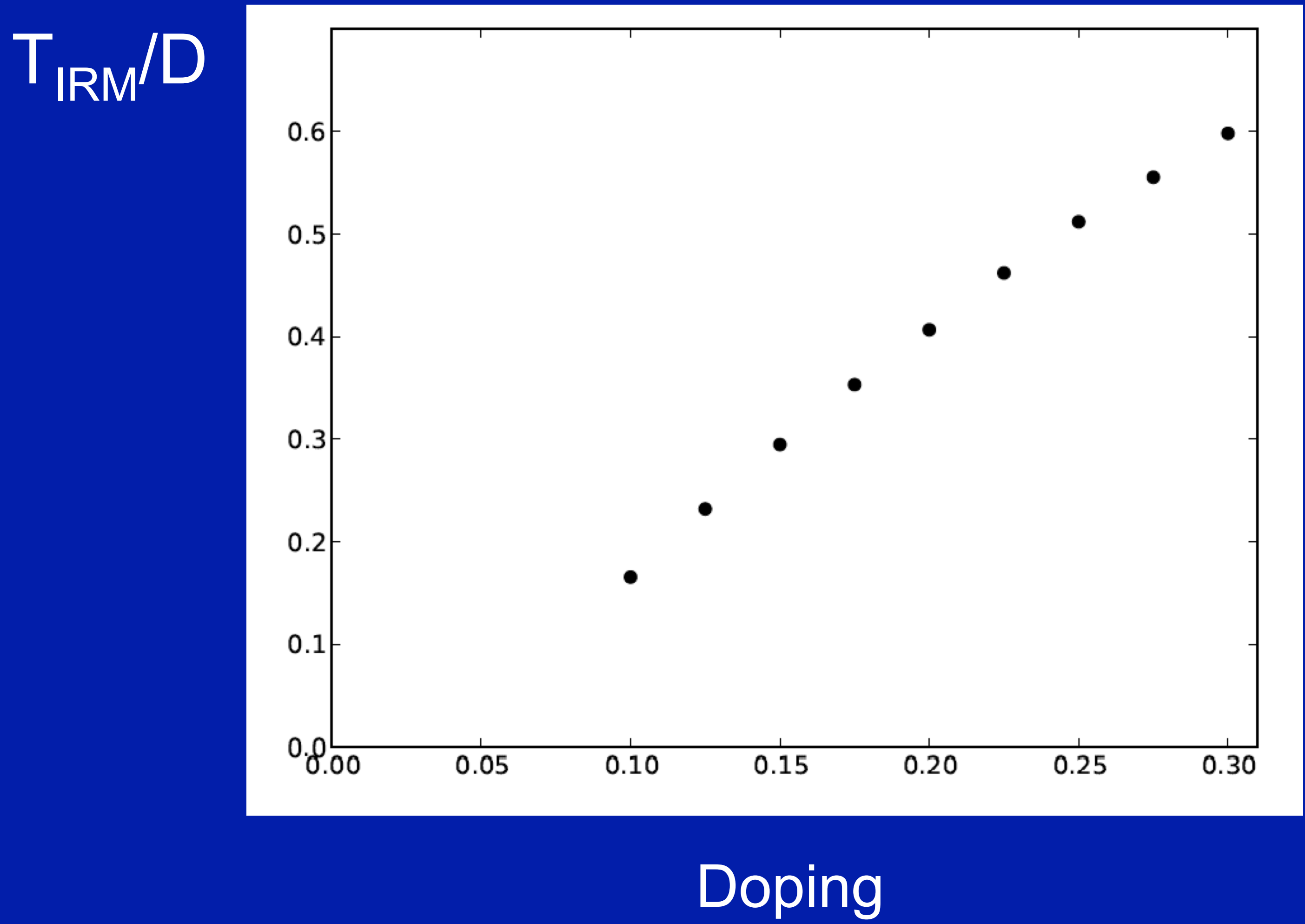


FIG. 2. Temperature dependence of spectra at the three FSCPs: A, B, and C (see the insets). (a) Comparison of spectra between A and B. (b) Comparison of spectra between A and C. The insets show measurement locations in the Brillouin zone.

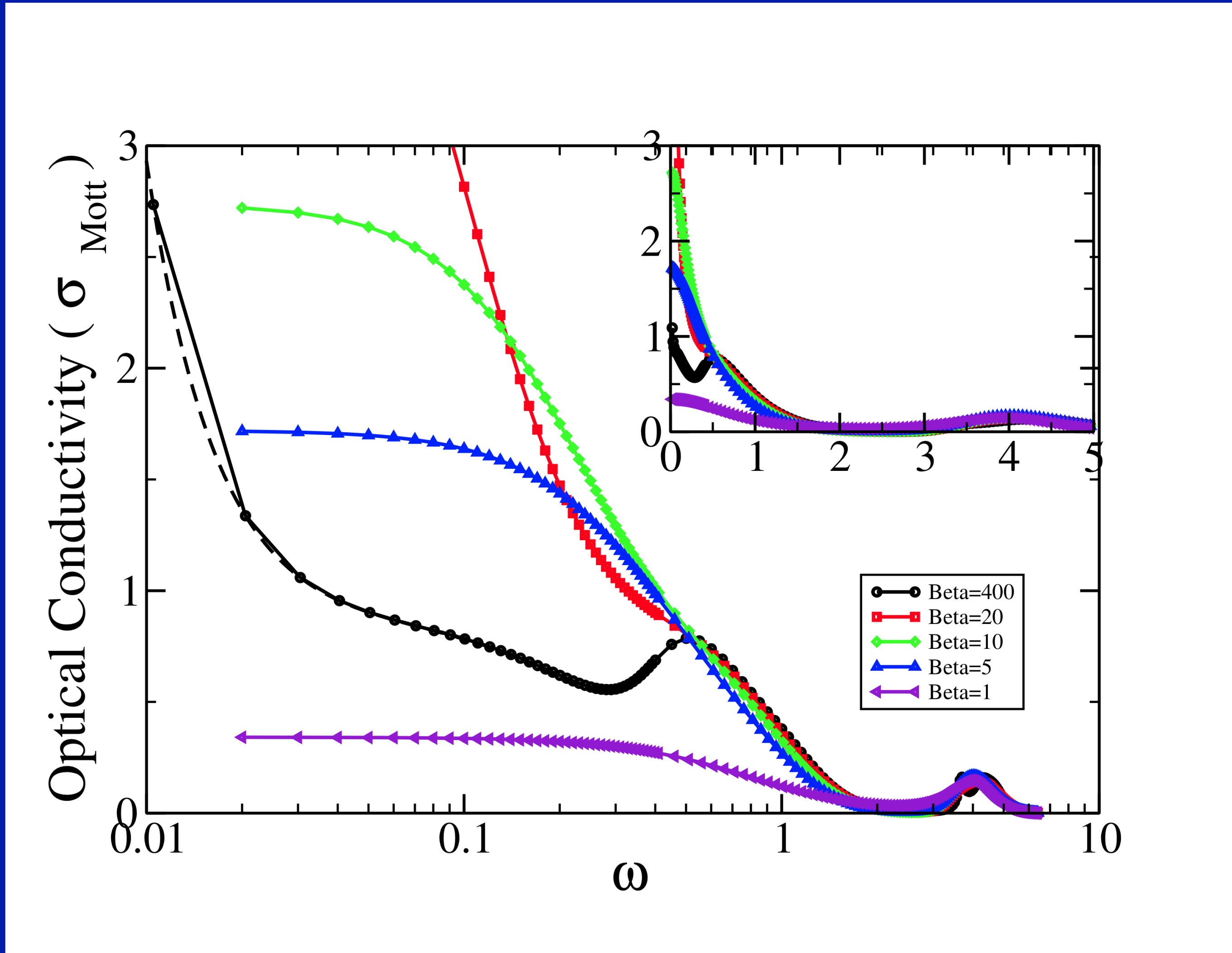
Wang et al PRL 92 (2004) 137002

When is the IRM 'limit' reached ?

The true meaning of the Brinkman-Rice scale ~ δD

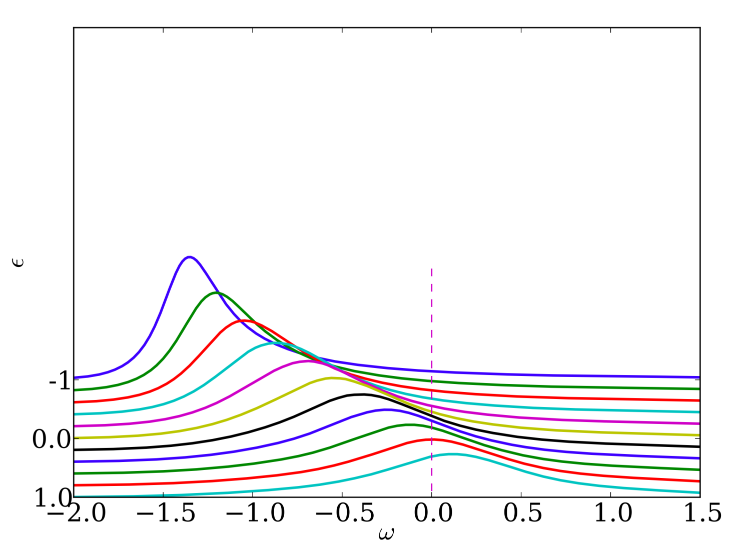


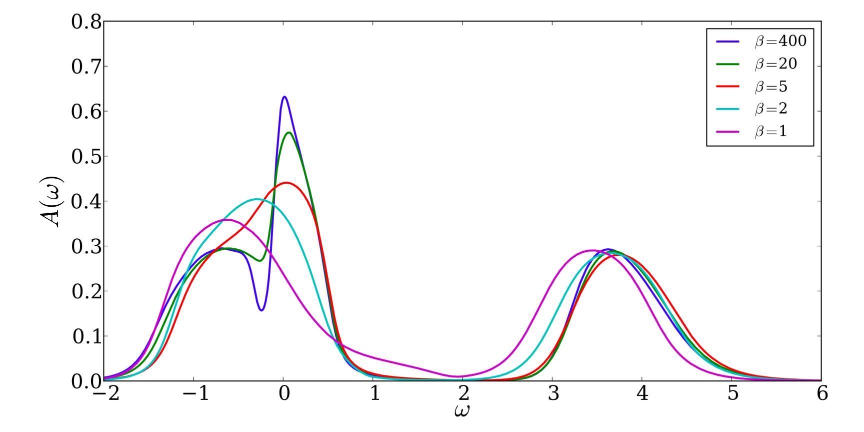
Signatures of IRM in optics:
``IRM limit = changes in MIR range''

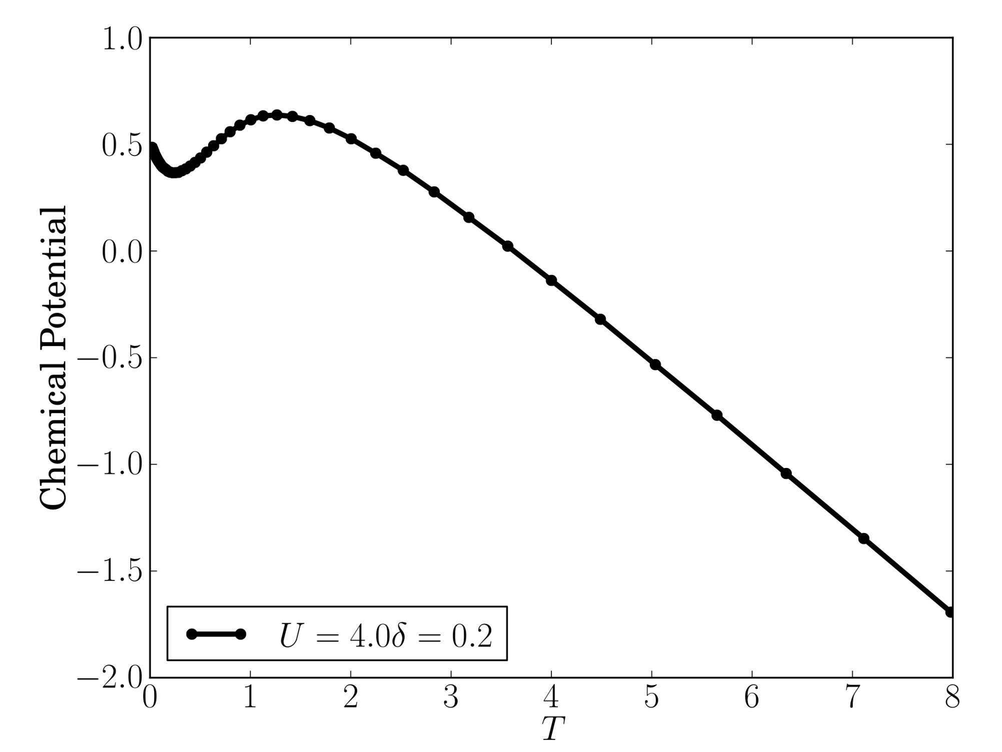


cf. N.Hussey, Takenaka, Takagi review in Phil Mag, 2004.

3. High temperatures: T>T_{IRM} and beyond…
Incoherent regime – Hubbard band physics
~ classical carriers in a rigid band







Chemical potential is linear in T at very hi-T

$$\tilde{\rho}(\omega,\epsilon) = \rho(\omega-\mu,\epsilon).$$

Hence the coefficients A_n from §3.4 become[4]:

$$A_n = \frac{\pi N}{4}\int d\omega \frac{(\beta\omega-\alpha)^n}{\cosh^2(\frac{\beta\omega-\alpha}{2})}\int d\epsilon\tilde{\rho}^2(\omega,\epsilon)\Phi(\epsilon).$$

We now expand the hyperbolic cosine in Taylor series around $\beta = 0$.

$$\frac{1}{\cosh^2(\frac{\beta\omega-\alpha}{2})} = \frac{1}{\cosh^2(\frac{\alpha}{2})}\left(1+\beta\omega\tanh(\frac{\alpha}{2}) + \frac{\omega^2\beta^2}{4}\left[3\tanh(\frac{\alpha}{2})-1\right]\right).$$

Before we go any further we also define

$$\gamma_n = \int d\epsilon d\omega\omega^n\tilde{\rho}^2(\omega,\epsilon)\Phi(\epsilon) \quad \text{and let} \quad \tau = \tanh(\frac{\alpha}{2}) \quad \text{and} \quad \zeta = \frac{1}{4\cosh^2(\frac{\alpha}{2})}.$$

T-linear above IRM $\rho(T) \sim \dfrac{T}{\gamma_0\zeta}$ From G.Palsson's PhD