DMFT insights to incoherent transport in strongly correlated metals

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Paris Edge, Oct 18 2017

PRL **110,** 086401 (2013) PHYSICAL REVIEW LETTERS week ending 22 FEBRUARY 2013

How Bad Metals Turn Good: Spectroscopic Signatures of Resilient Quasiparticles

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PHYSICAL REVIEW B **94**, 235115 (2016)

Transport and optical conductivity in the Hubbard model: A high-temperature expansion perspective

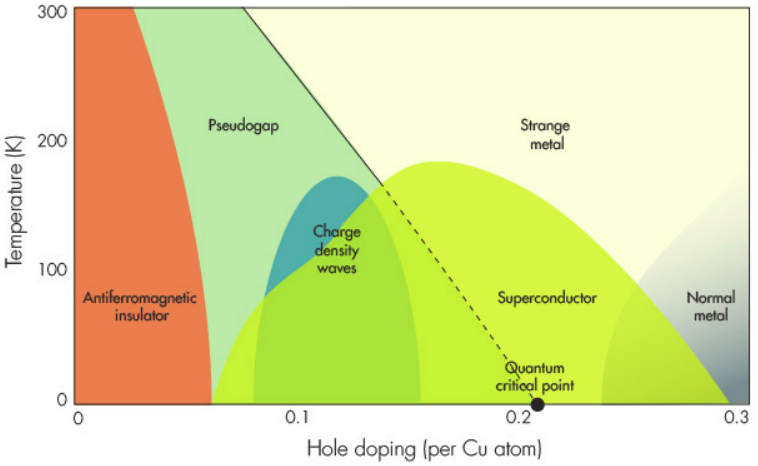
Edward Perepelitsky,[1,2] Andrew Galatas,[3] Jernej Mravlje,[4] Rok Žitko,[4] Ehsan Khatami,[5] B. Sriram Shastry,[3] and Antoine Georges[1,2,6]

Ana Vranic, Jure Kokalj, Rok Zitko, Jan Skolimowski, Jaksa Vucicevic, Olivier Parcollet, Darko Tanaskovic, Jernej Mravlje, in preparation

- Bad metals (intro)
- (i) DMFT picture of a bad-metal: low T FL, high T bad-metal
- (ii) high-T regime for doped U=infinity Hubbard model (from DMFT and high-temperature expansion techniques)
- lattice theories vs. continuum theories
- (iii) beyond DMFT

What happens at T above the strange metal

?



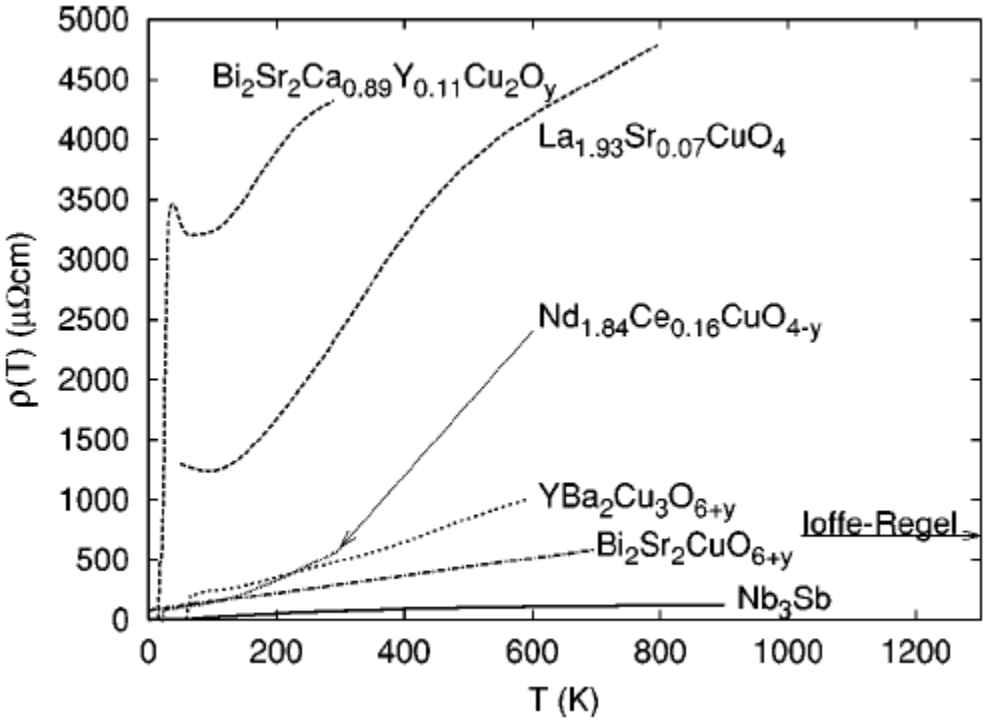
- Question of transport related also to DOS. How does the DOS for a Hubbard model look like at infinite-T?

Bad metal

- 1990s: “Bad metals”, ?=? no quasiparticles

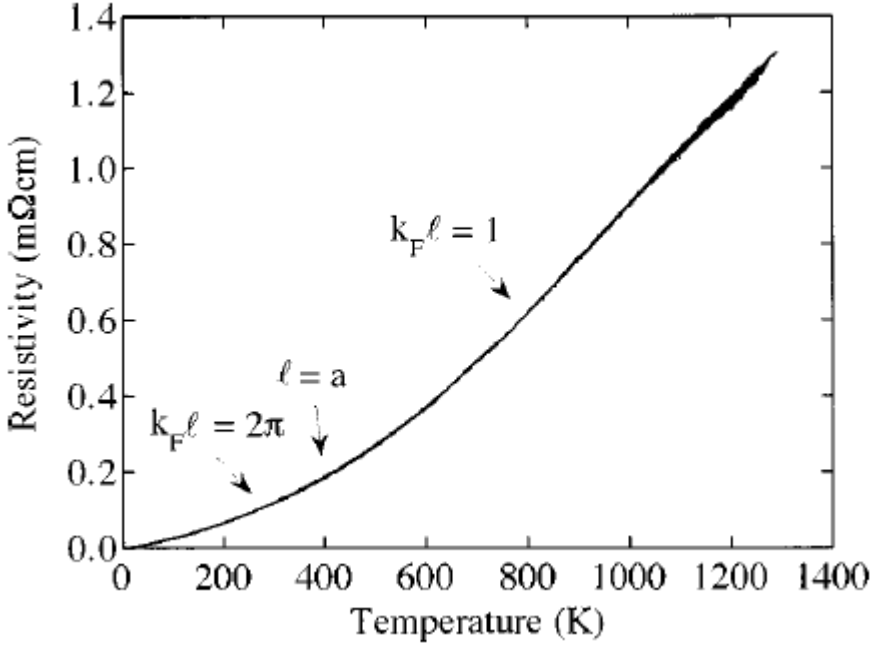
Emery & Kivelson, PRL (1995)

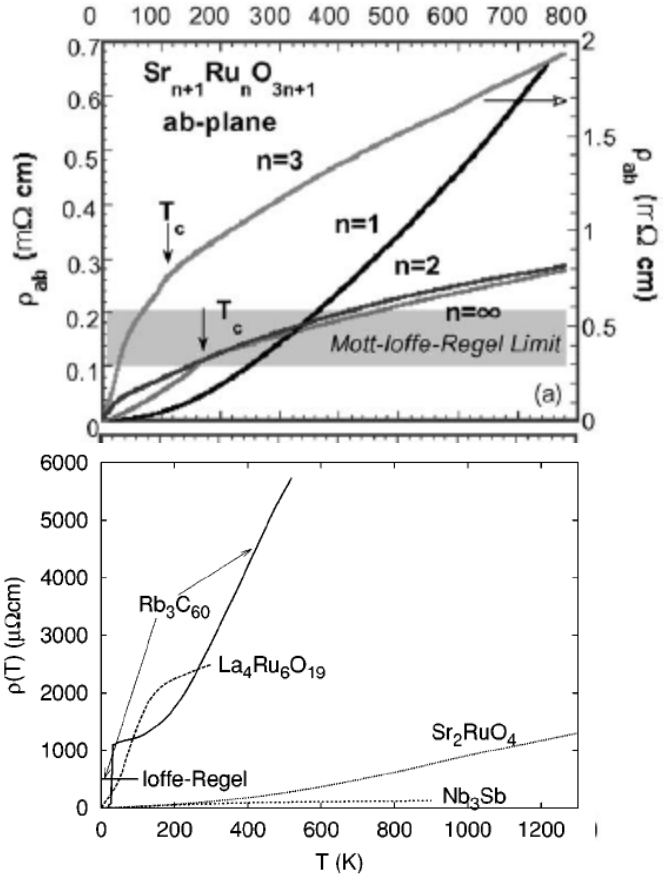
The failure of bad metals to exhibit resistivity saturation strongly suggests that any theory based on conventional quasiparticles with more or less well-defined crystal momenta suffering occasional scattering events does not apply. *Since there is no crossover in the temperature dependence of the resistivity 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].



Other bad metals

- Ruthenates, cuprates, organics (el-el driven)
- Alkali doped fullerides (el-ph driven)

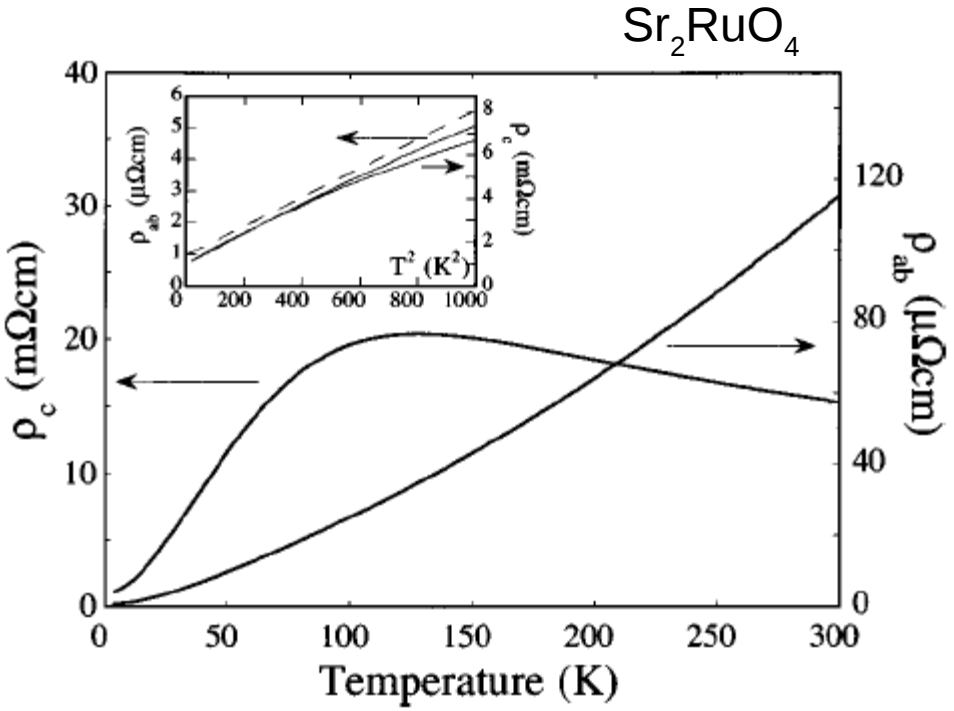




Tyler et al, Phys. Rev. B (1998)
Cao et al. Solid State Comm (2004)
Gunnarsson, Calandra & Han, Rev. Mod. Phys. (2003)
Hussey, Takenaka & Takagi, Phil. Mag. (2004)

Bad metals turn good at low T

- Many (all?) “bad metals”, however do show crossover and are at low T Fermi liquids



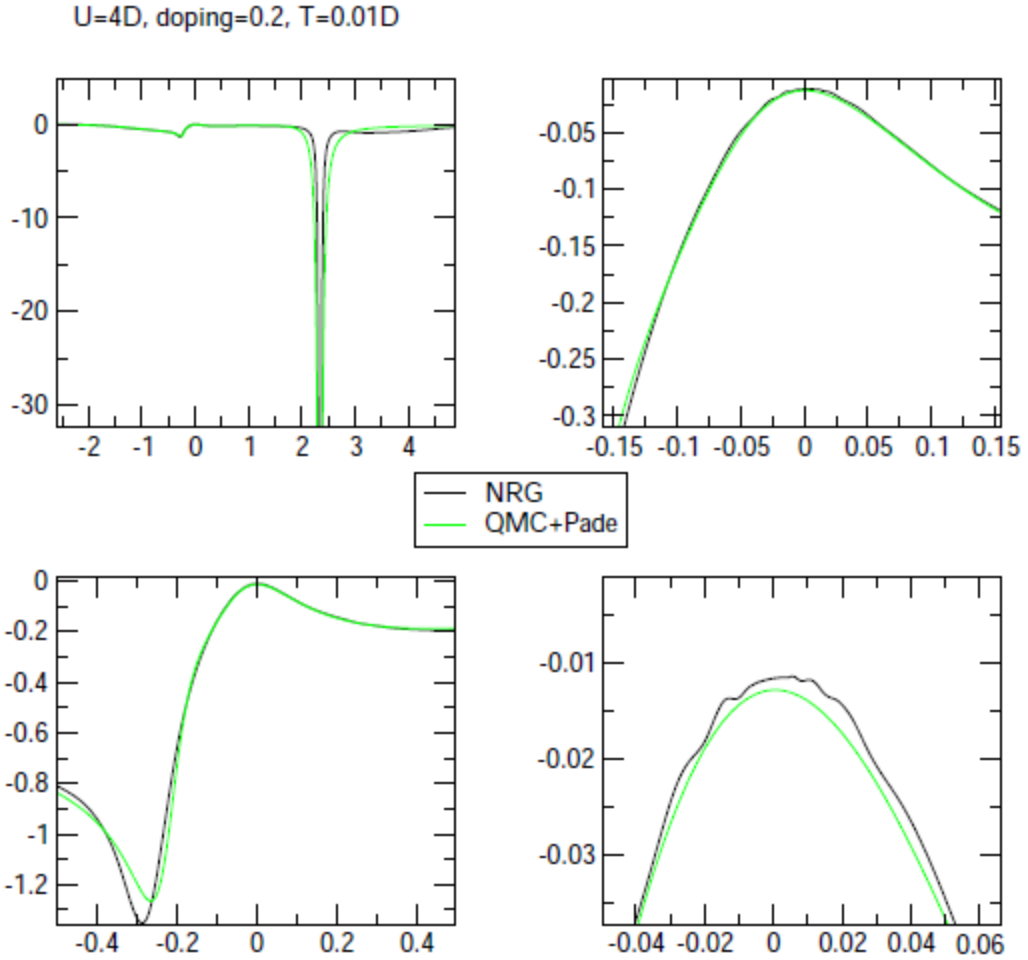
Hussey et al, Phys. Rev. B (1998)

Questions

- Does a MIR criterion have a meaning for strongly correlated 'bad' metals?
- Are there quasiparticles and at what temperature do they disappear (close to T_{FL}, or close to much larger T_{MIR})?

Case study and tools

- Single band Hubbard model, semicircular DOS
- U=4 in units of D. To compare with a typical material, think of D=1eV=11600K.
- DMFT equations solved with accurate impurity solvers:
  - continuous-time Monte Carlo (TRIQS : O. Parcollet & M. Ferrero: `ipht.cea.fr/triqs`)+Pade analytical continuation
  - NRG (NRG Ljubljana : Rok Zitko, `nrgljubljana.ijs.si`)
- Converged & compatible results using both techniques


U=4D, doping=0.2, T=0.01D
0
-10
-20
-30
-2 -1 0 1 2 3 4
-0.05
-0.1
-0.15
-0.2
-0.25
-0.3
-0.15 -0.1 -0.05 0 0.05 0.1 0.15
NRG
QMC+Pade
0
-0.2
-0.4
-0.6
-0.8
-1
-1.2
-0.4 -0.2 0 0.2 0.4
-0.01
-0.02
-0.03
-0.04 -0.02 0 0.02 0.04 0.06

Transport in DMFT

- Vertex correction vanish, from Kubo formula one has

$$\sigma = \frac{2\pi e^2}{\hbar} \int d\omega \left(-\frac{\partial f}{\partial \omega} \right) \frac{1}{V} \sum_k v_k A_{\mathbf{k}}(\omega) v_k A_{\mathbf{k}}(\omega)$$

$$v_k = \partial \varepsilon_{\mathbf{k}} / \partial \mathbf{k}_x \ ; \ A_{\mathbf{k}}(\omega) = -(1/\pi) \mathrm{Im}[\omega + \mu - \varepsilon_{\mathbf{k}} - \Sigma(\omega)]^{-1}$$

- Velocity distribution function (units $[x]^{2\text{-}d}$ $[\omega]$)

$$\Phi(\varepsilon) = (1/V) \sum_{\mathbf{k}} (\partial \varepsilon_{\mathbf{k}} / \partial \mathbf{k}_x)^2 \delta(\varepsilon - \varepsilon_{\mathbf{k}})$$

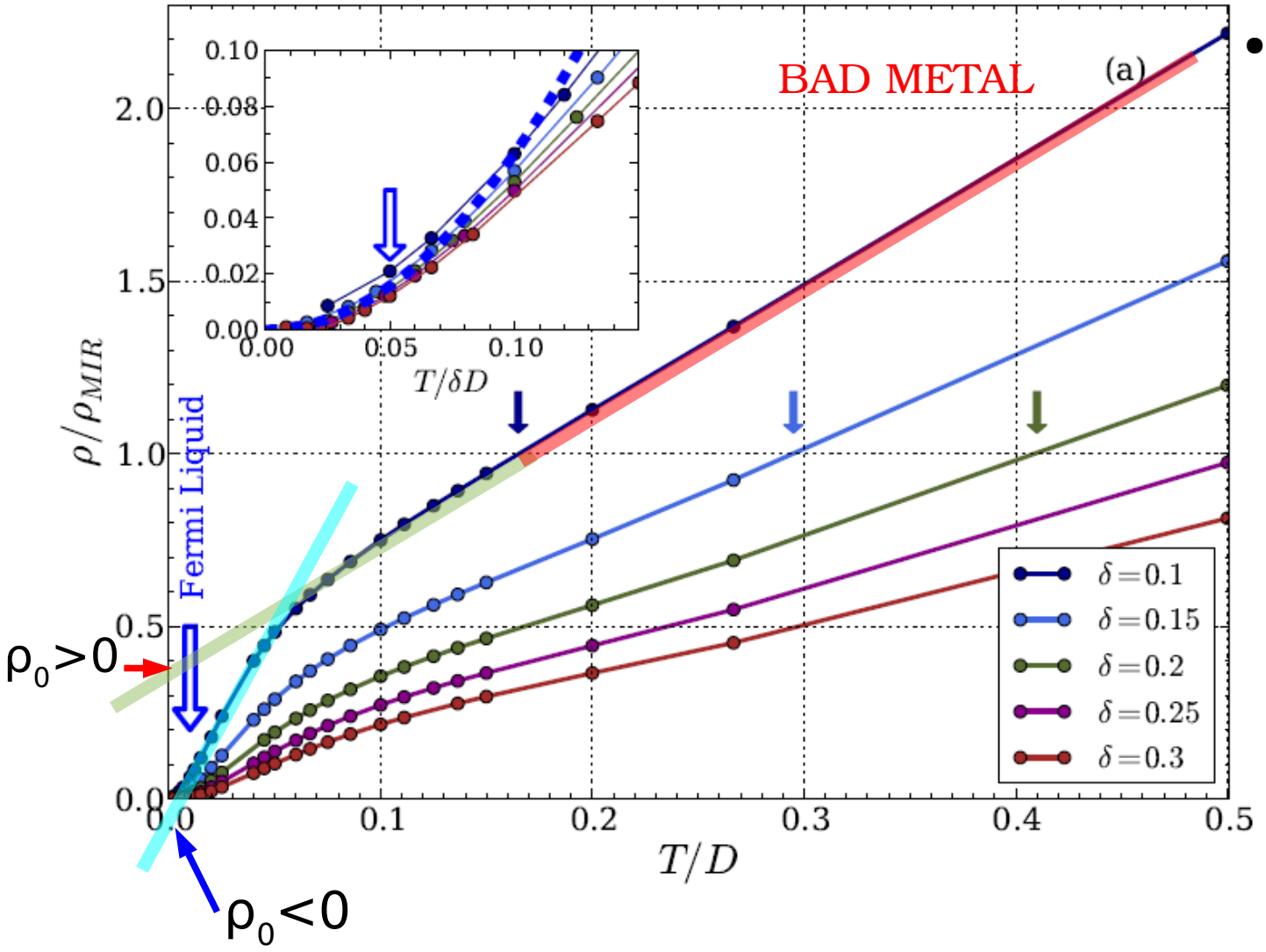
$$\sigma = \frac{2\pi e^2}{\hbar} \int d\omega \left(-\frac{\partial f}{\partial \omega} \right) \int d\epsilon \Phi(\epsilon) A_\epsilon(\omega) A_\epsilon(\omega)$$

- For semicircular DOS:

$$\Phi(\epsilon) \ = \ \Phi(0) \left[1 - (\epsilon/D)^2 \right]^{3/2}$$

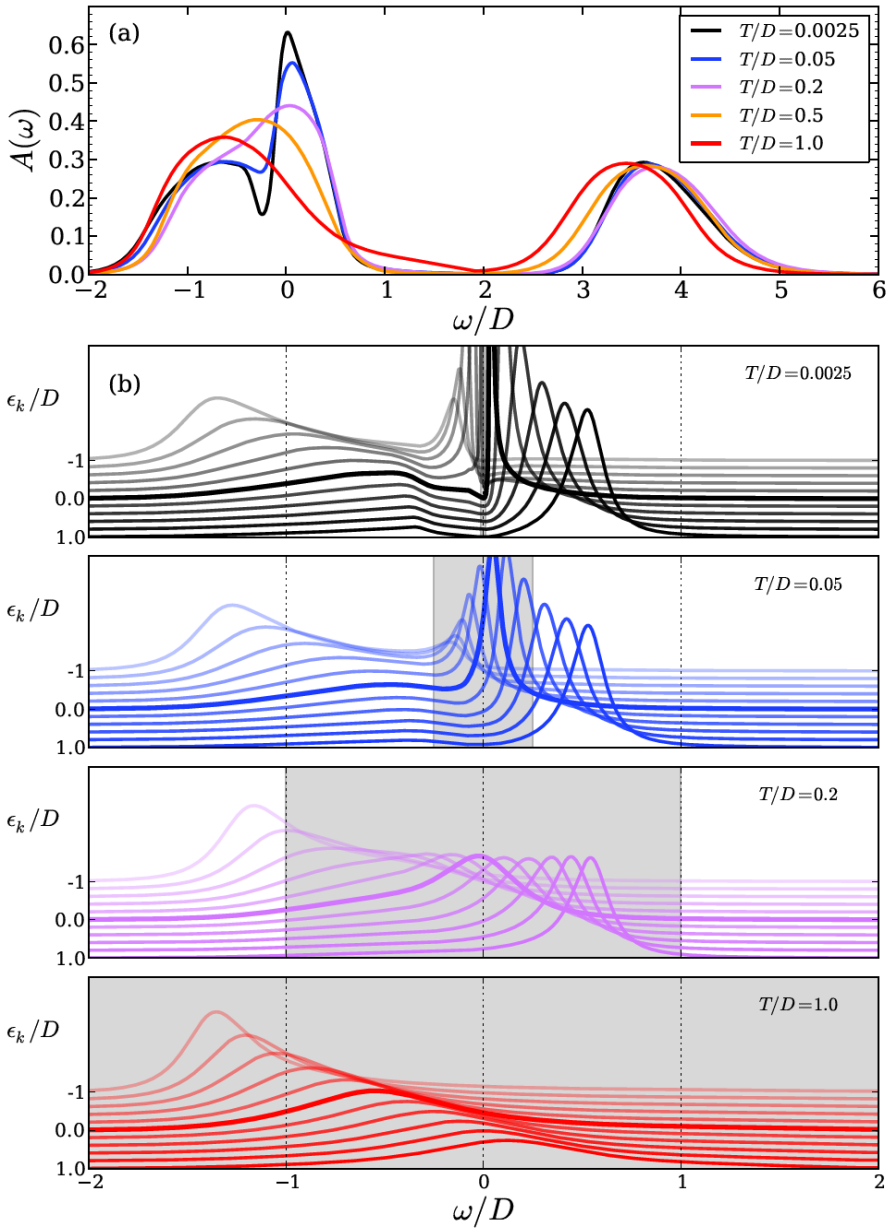
$$1/\rho_{\mathrm{MIR}} \equiv e^2 \Phi(0) / \hbar D$$

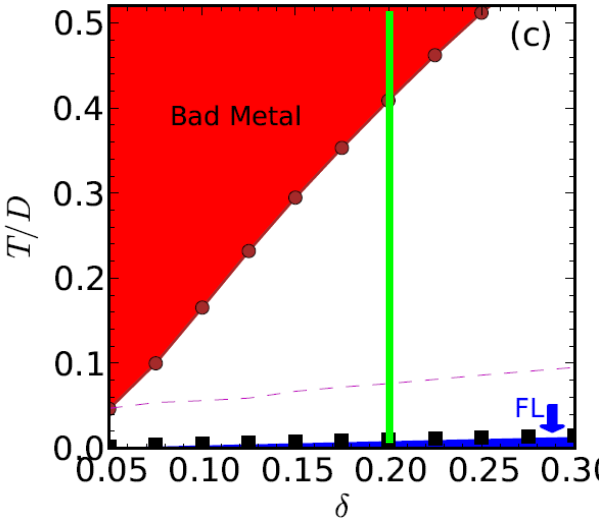
DMFT results: resistivity



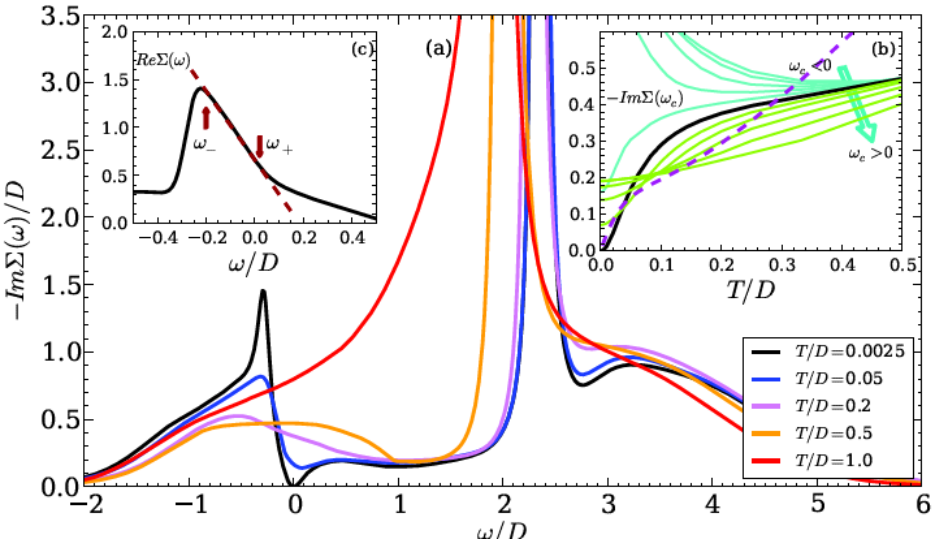
- Several regimes
  - FL : $\rho \sim T^2$; $T < T_{FL}$
  - $\rho \sim T$ with $\rho_0 < 0$; $T_{FL} < T < T_*$
  - $\rho \sim T$ with $\rho_0 < 0$; $T_* < T$
  - Bad metal $T > T_{MIR}$

Calculated photoemission

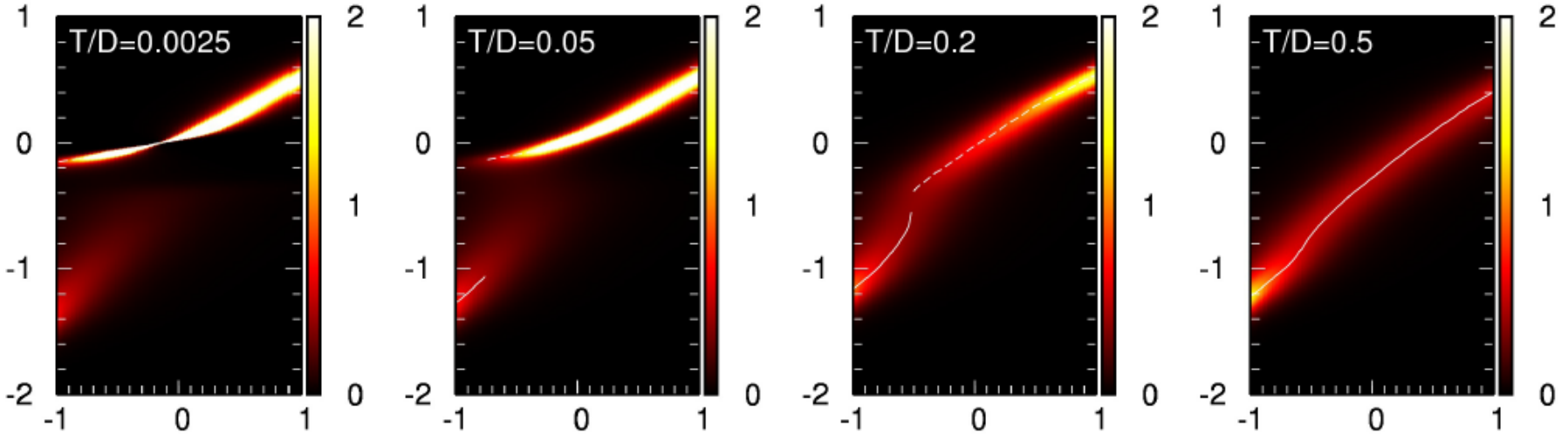




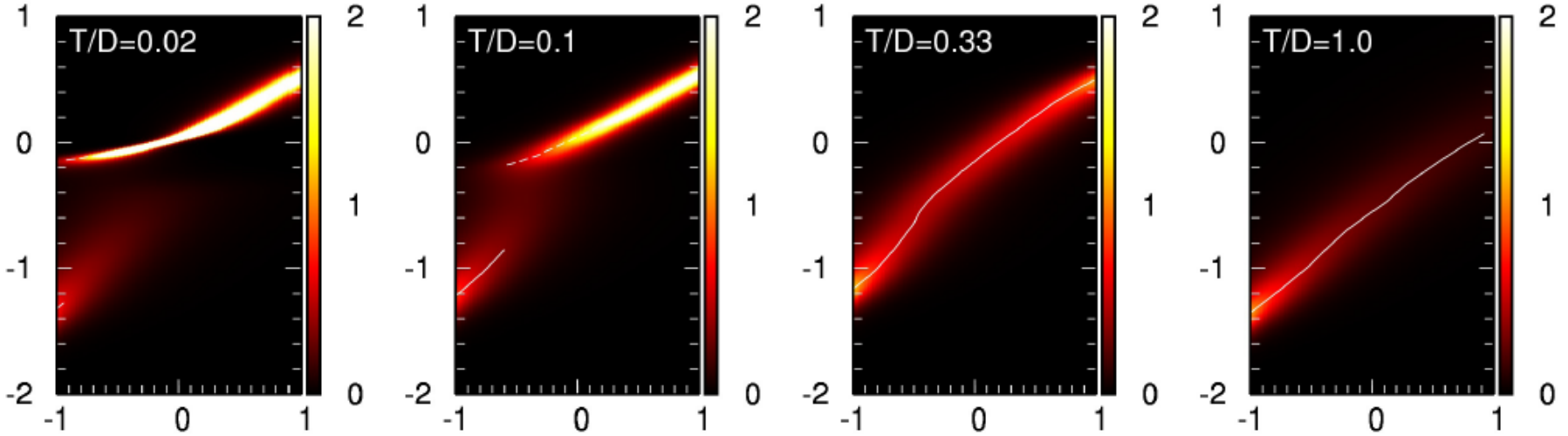
- δ=0.2



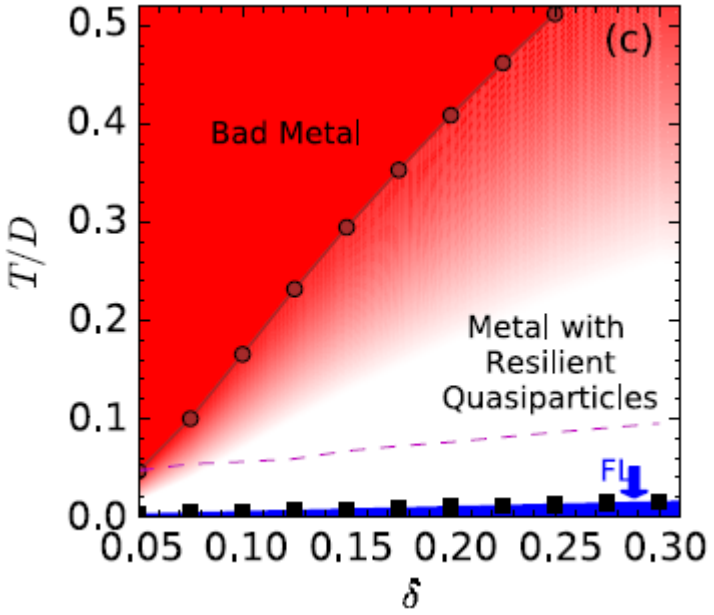
Calculated photoemission (ii) resillient quasiparticles



Quasiparticle excitations persist up to temperature δD ~T
Their width Γ>T, yet smaller than D, so they are well discernible.



- quasiparticles in spectroscopy disappear (only) on approaching ρ_{MIR}



Drude-like formula

Peaked spectral functions enable rewriting of transport eqs. to Drude (Boltzmann) form

$$\sigma = \frac{2\pi e^2}{\hbar} \int d\omega \left(-\frac{\partial f}{\partial \omega}\right) \int d\epsilon \Phi(\epsilon) A_\epsilon(\omega) A_\epsilon(\omega)$$

$$\Phi(\varepsilon) = (1/V) \sum_{\mathbf{k}} (\partial \varepsilon_{\mathbf{k}} / \partial \mathbf{k}_x)^2 \delta(\varepsilon - \varepsilon_{\mathbf{k}}) \qquad A(\epsilon, \omega) = -\frac{1}{\pi} ImG(\epsilon, \omega) = -\frac{1}{\pi} \frac{\Sigma''}{(\omega + \mu - \Sigma' - \epsilon)^2 + \Sigma''^2}$$

so

$$\Gamma(\omega) = -\Sigma'', \; \epsilon^*(\omega) = \omega + u - \Sigma'(\omega)$$

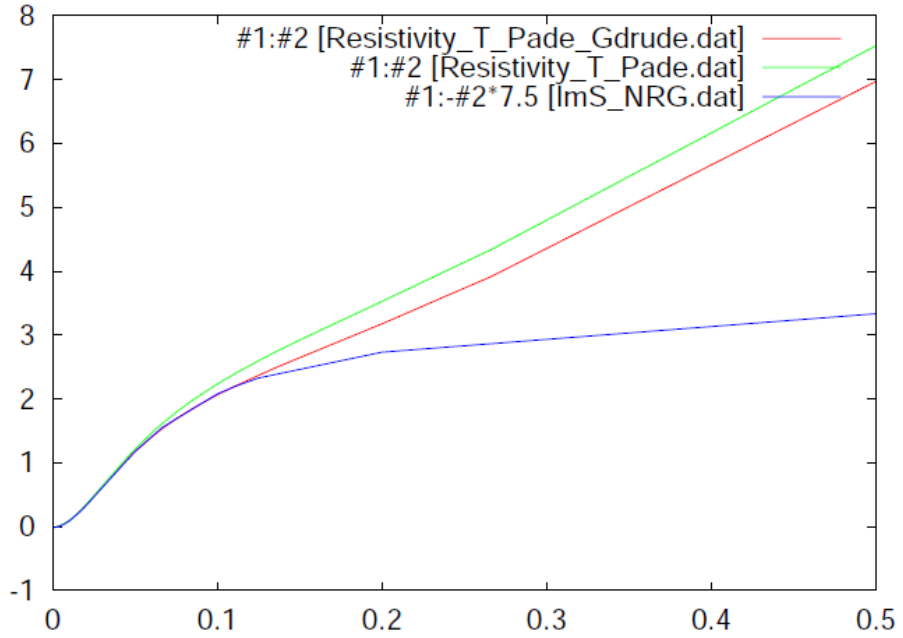
$$\begin{aligned}
&= A \frac{1}{\pi^2} \int_{-\infty}^{\infty} d\omega (-\frac{\partial f}{\partial \omega}) \Phi(\epsilon^*(\omega)) \int d\epsilon [\frac{\Gamma(\omega)}{(\epsilon^*(\omega) - \epsilon)^2 + \Gamma^2(\omega)}]^2 \\
&= A \frac{1}{\pi^2} \int_{-\infty}^{\infty} d\omega (-\frac{\partial f}{\partial \omega}) \Phi(\epsilon^*(\omega)) \frac{1}{\Gamma(\omega)} \int dy [\frac{1}{y^2 + 1}]^2 \\
&= A \int_{-\infty}^{\infty} d\omega (-\frac{\partial f}{\partial \omega}) \frac{\Phi(\epsilon^*(\omega))}{2\pi \Gamma(\omega)}
\end{aligned}$$

compare with el.-ph. coupling analysis of Prange, Kadanoff Phys Rev '64

$$\sigma = \int -\left(\frac{\partial f}{\partial \omega}\right) \tilde{\Phi}(\omega) \tau(\omega) d\omega \approx n_{\text{eff}} e^2/m \int d\omega \tau(\omega)$$

Generalized Drude

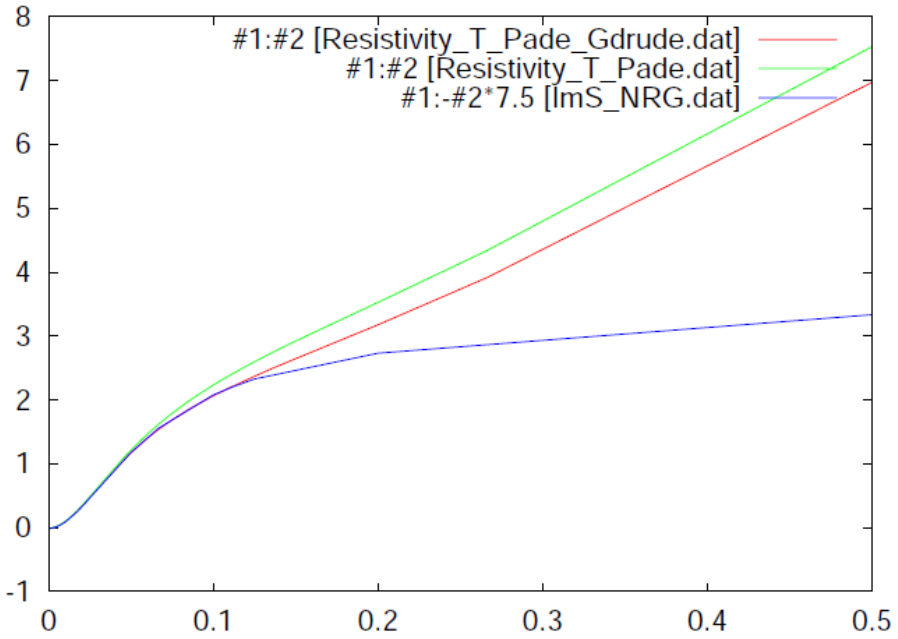
- Works remarkably well at all T.

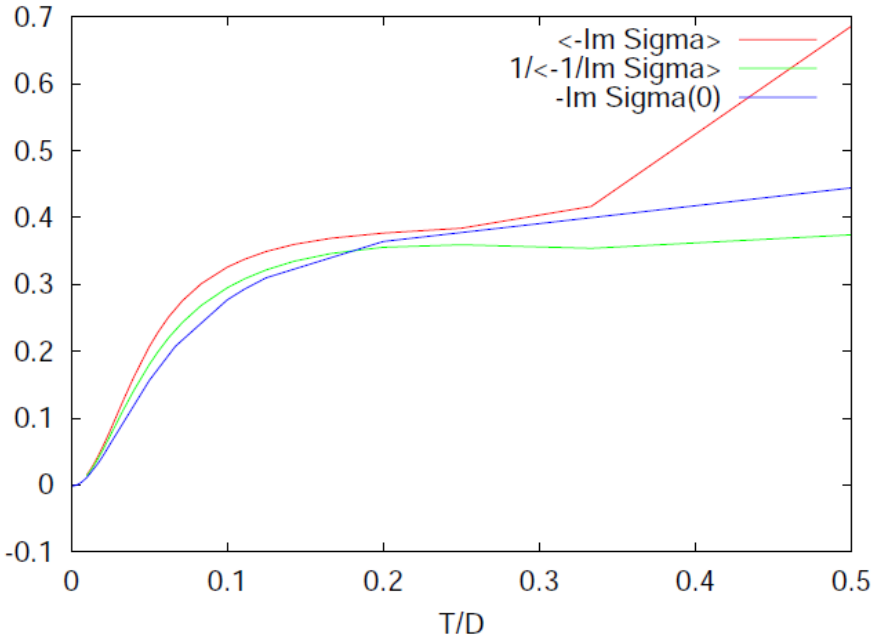


About resistivity saturation & generalized Drude

- Scattering rate saturates, resistivity not

$$\sigma = \int -\left(\frac{\partial f}{\partial \omega}\right) \tilde{\Phi}(\omega)\tau(\omega)d\omega \approx n_{\text{eff}} e^2/m \int d\omega \tau(\omega)$$



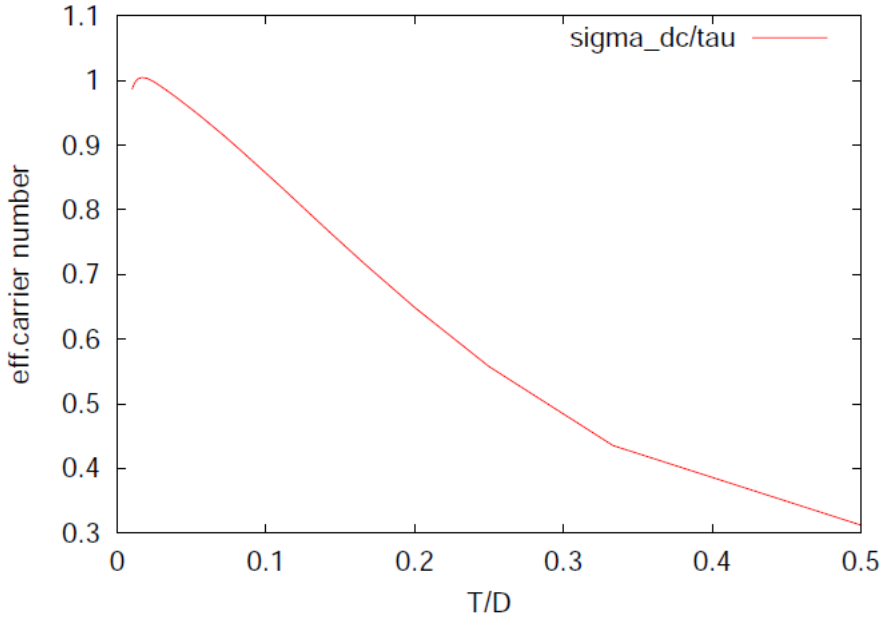


Carrier number

- Within Drude description, at high temperature τ saturates, plasma frequency (effective carrier number) keeps dropping

$$\sigma = \frac{ne^2}{m}\tau = \omega_p^2\tau$$

- Bad metal regime is like doped semiconductor, controlled by T-dependence of carrier # not their scattering



- $$\sigma = \int -\left(\frac{\partial f}{\partial \omega}\right) \tilde{\Phi}(\omega)\tau(\omega)d\omega \approx n_{\text{eff}} e^2/m \int d\omega\tau(\omega)$$

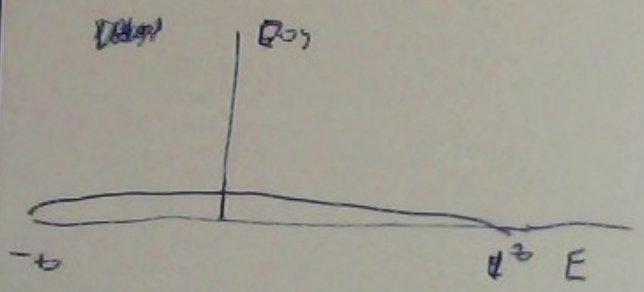
- Tau = 1/Im Sigma(omega) = T independent
- Is this the asymptotic high-T regime?/ What happens at higher temperature still?

- Take hole doped case, U-> Infinity
- How does the DOS look like?

SCENARIO 1

$T \to 0$

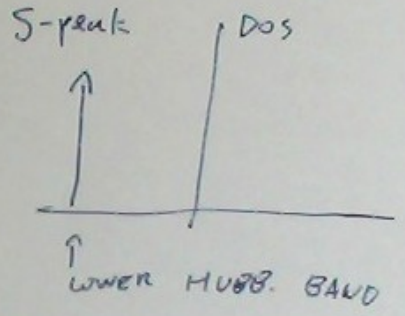
NO CHARACT. SCALE



SCENARIO 2

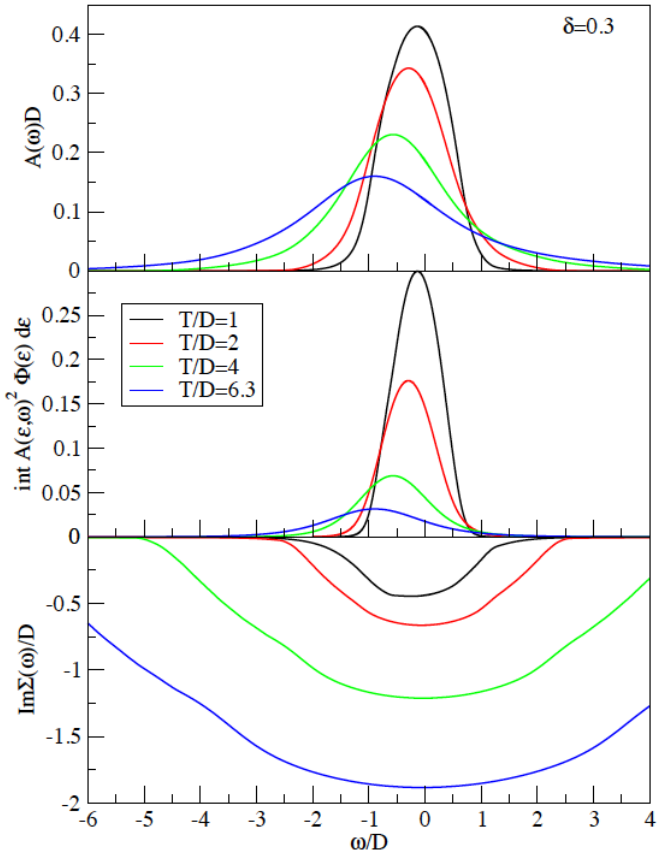
$T \to \infty$

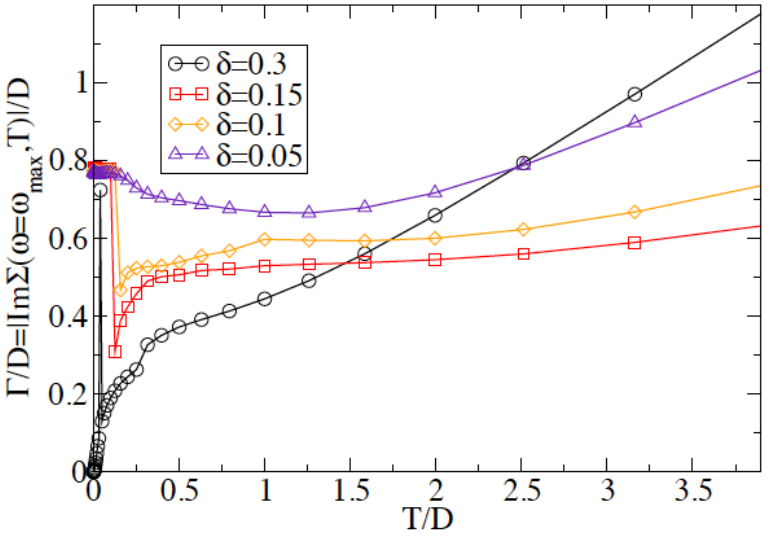
PHYSICS ATOMIC LIKE

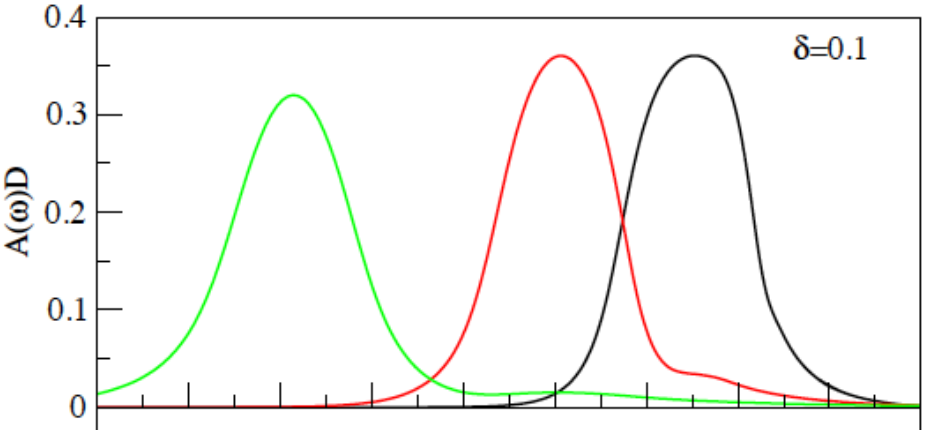


Preliminary results from 2013 support scenario 1 (wrong!)

- Technically difficult







A tiny bit on the high-T expansion

$$\rho_G(\vec{k}, -\mu + \delta\omega) = \frac{1}{t} \sum_{i=0}^{\infty} \left(\frac{t}{T}\right)^i g^{(i)}\left(\vec{k}, \frac{\delta\omega}{t}\right)$$

$$\rho_\Sigma(\vec{k}, -\mu + \delta\omega) = t \sum_{i=0}^{\infty} \left(\frac{t}{T}\right)^i h^{(i)}\left(\vec{k}, \frac{\delta\omega}{t}\right)$$

$$\frac{\sigma(\omega)}{\sigma_0} = (1-n)\frac{t}{T}\sigma^{(1)}\left(\frac{\omega}{t}\right) + (1-n)\frac{t^3}{T^3}\sigma^{(3)}\left(\frac{\omega}{t}\right) + \cdots .$$

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Transport and optical conductivity in the Hubbard model: A high-temperature expansion perspective

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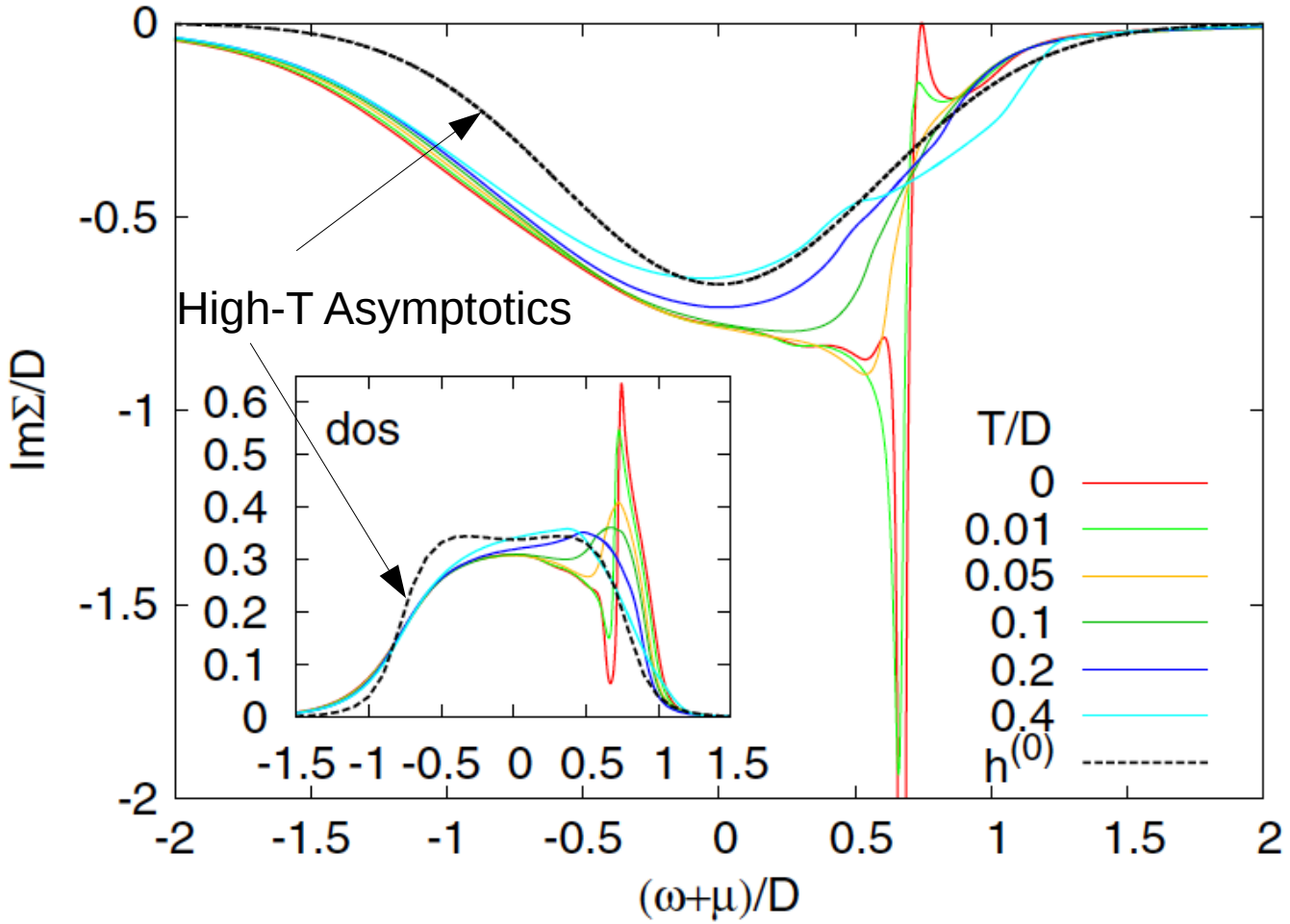
TABLE I. The moments calculated in the present work for various models and quantities.

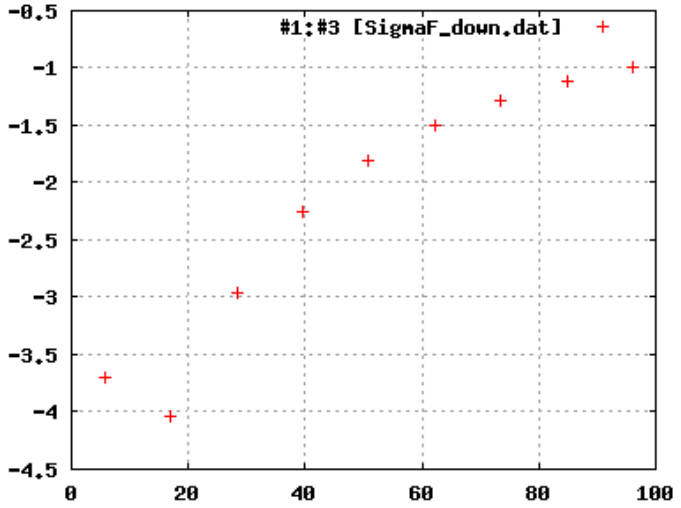
Quantity	Lattice	dimension	U	highest moment
$\rho_G(\vec{k},\omega)$	hypercubic	d	infinite	4
$\rho_G(\vec{k},\omega)$	hypercubic	infinite	infinite	9
$\rho_G(\vec{k},\omega)$	Bethe	infinite	infinite	9
$\rho_G(\vec{k},\omega)$	hypercubic	d	finite	2
$\rho_\Sigma(\vec{k},\omega)$	hypercubic	d	infinite	2
$\rho_\Sigma(\omega)$	hypercubic	infinite	infinite	7
$\rho_\Sigma(\omega)$	Bethe	infinite	infinite	7
$\sigma(\omega)$	hypercubic	d	infinite	2
$\sigma(\omega)$	hypercubic	d	finite	0
$\sigma(\omega)$	hypercubic	infinite	infinite	8

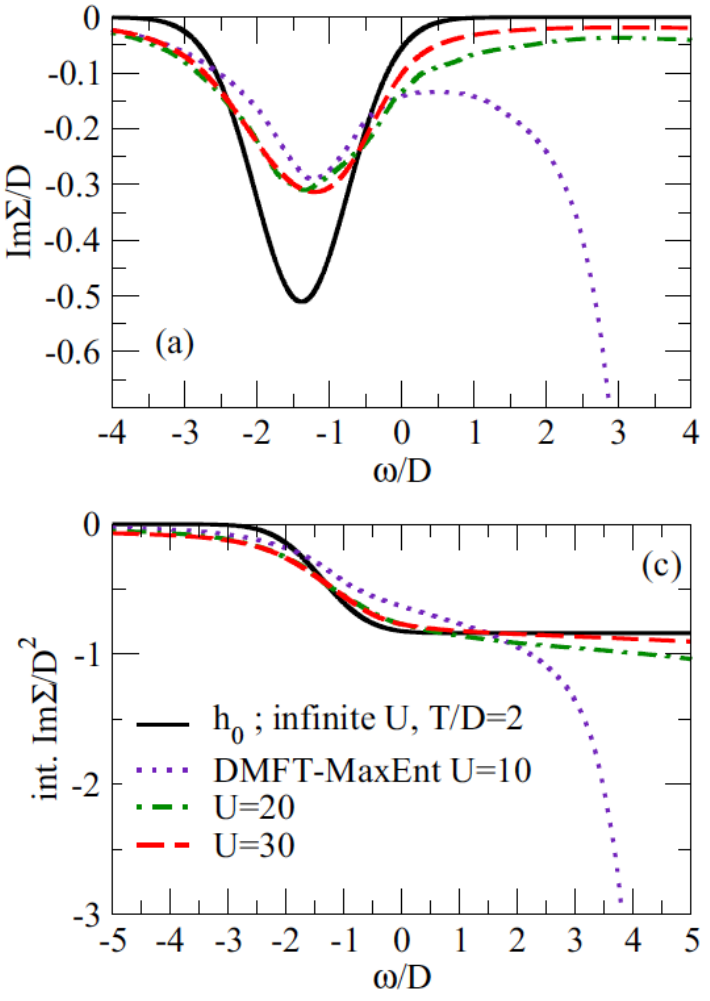
DMFT vs high-T expansion: Self energy

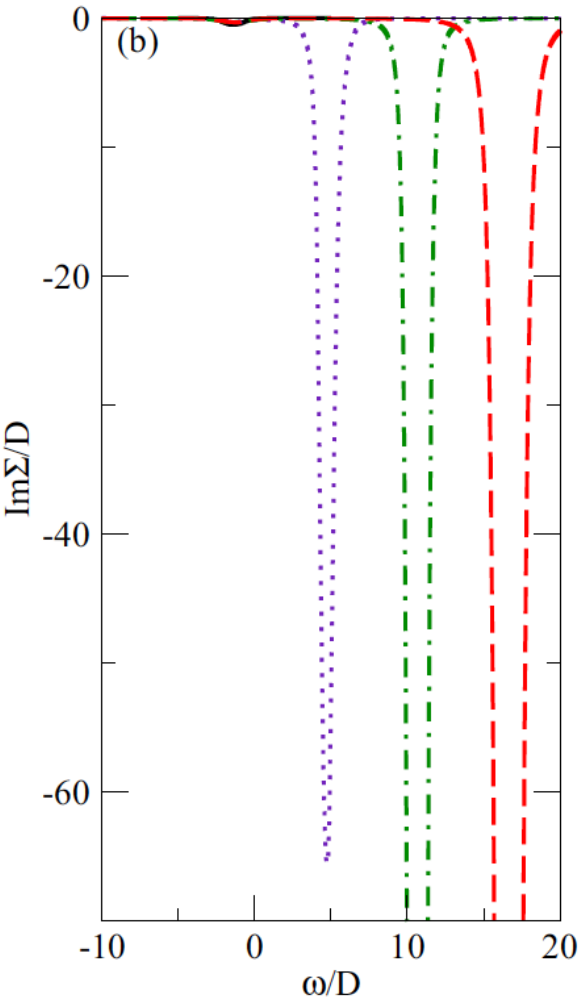
- high-T expansion predicts saturated self
- more careful NRG (better broadening kernel) consistent with that



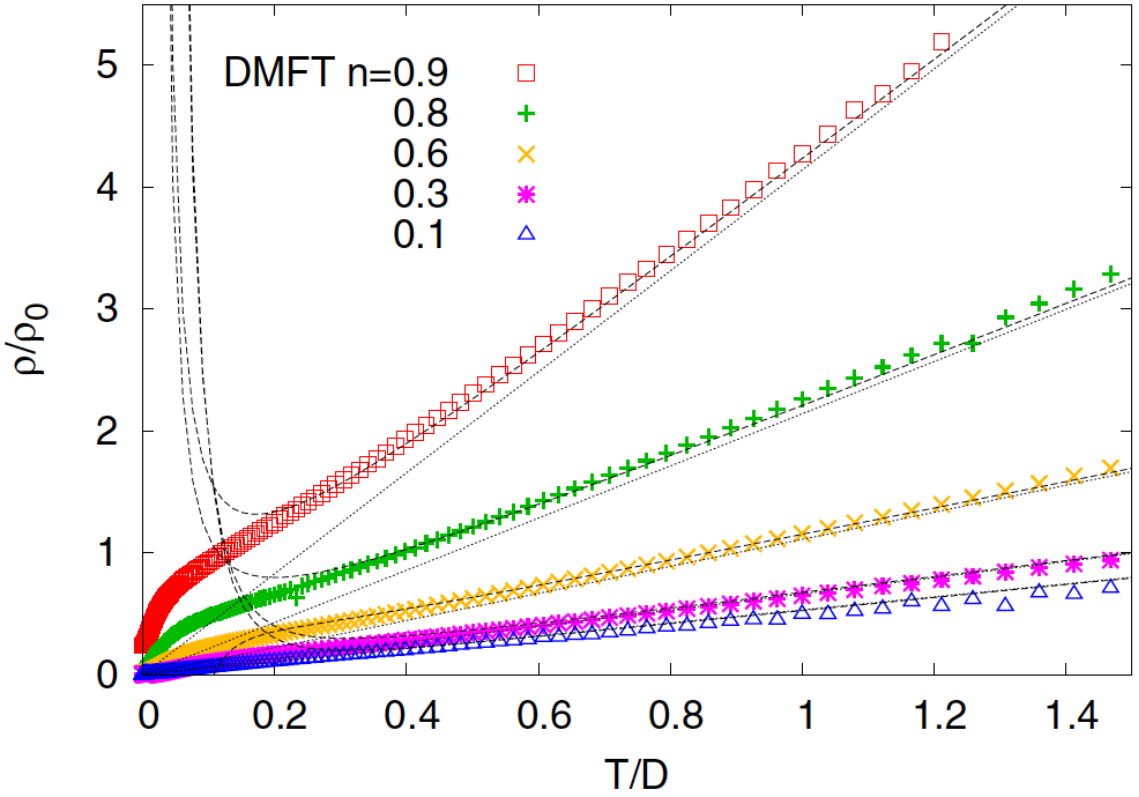
Interaction expansion QMC results

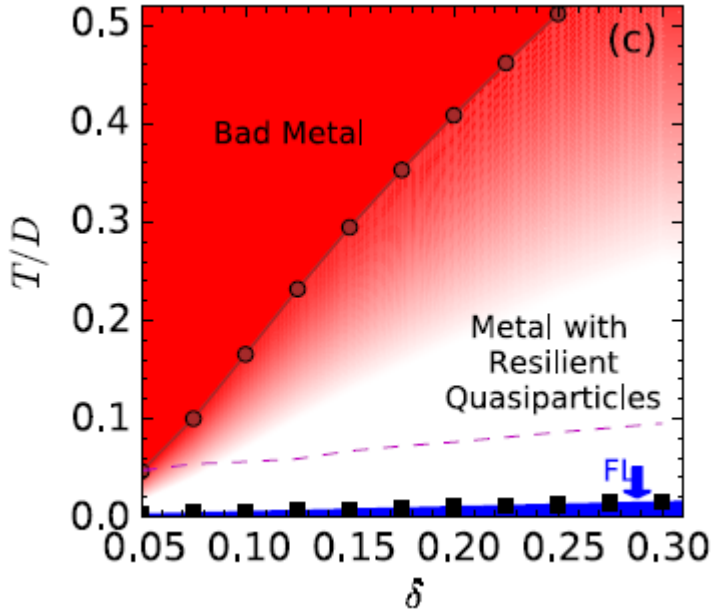






DMFT vs. high-T expansion





$$\frac{\sigma(\omega)}{\sigma_0} = (1-n)\frac{t}{T}\sigma^{(1)}\left(\frac{\omega}{t}\right) + (1-n)\frac{t^3}{T^3}\sigma^{(3)}\left(\frac{\omega}{t}\right) + \cdots .$$

- dominant term agrees with DMFT at large T
- T^3 correction explains describes quantitatively DMFT down to ρ_{MIR} (fails to describe RQP reg)

Einstein relation

$$\sigma = e^2 \kappa \mathcal{D}, \quad \kappa \equiv \frac{\partial n}{\partial \mu},$$

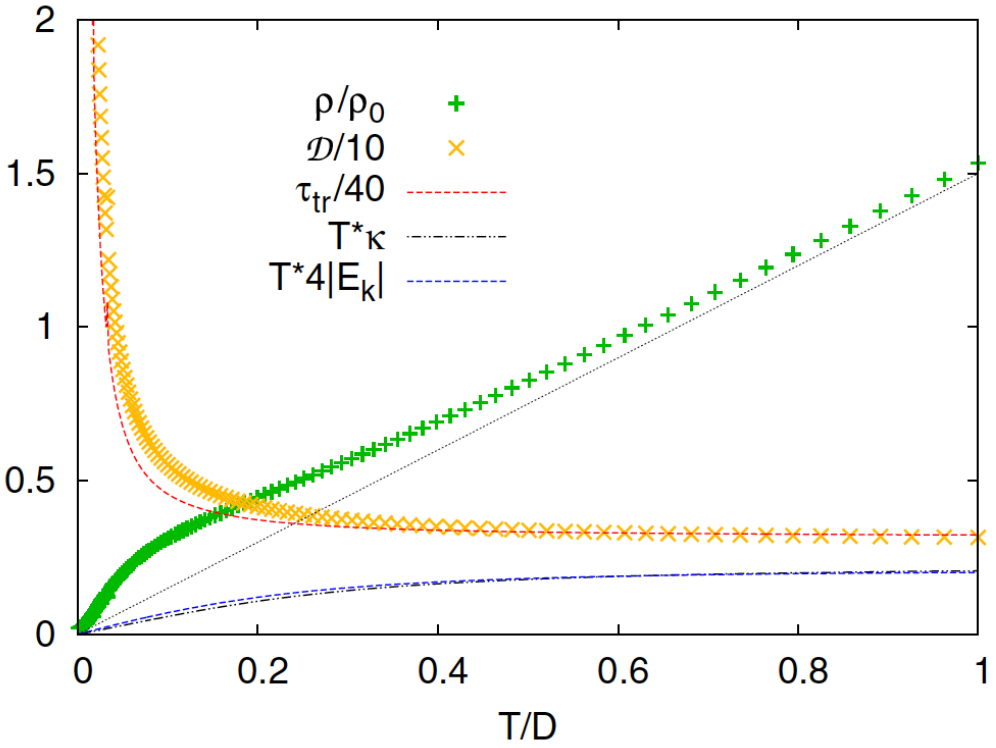
Drude formula

$$\sigma = \frac{\omega_p^2}{4\pi} \tau_{\mathrm{tr}} \qquad \omega_p^2 = 4 \int_{-\infty}^{\infty} \sigma(\omega) d\omega = 4\pi \frac{\sigma_0}{d} \frac{(-E_K)}{\hbar}$$

- kinetic energy and charge compressibility drop as 1/T

See also, Calandra, Gunnarsson, EPL 61 88 (2003)

Saturation of diffusion constant



Note also direction of the effect: charge susceptibility deviates more strongly from 1/T behavior than diffusion constant from a constant, hence upturn with respect to T-linear!

For more on the charge sucs. see
J. Kokalj, PRB 95 041110R (2017)

Distinct from continuum theories

ARTICLES
PUBLISHED ONLINE: 23 DECEMBER 2014 | DOI: 10.1038/NPHYS3174
nature physics

Theory of universal incoherent metallic transport

Sean A. Hartnoll

$$\frac{\eta}{s} \geq C \frac{\hbar}{k_B}$$

$$\frac{D_\pm}{v_F^2} \gtrsim \frac{\hbar}{k_B T}$$

10. Kovtun, P., Son, D. T. & Starinets, A. O. Viscosity in strongly interacting quantum field theories from black hole physics. *Phys. Rev. Lett.* **94,** 111601 (2005).
11. Son, D. T. & Starinets, A. O. Viscosity, black holes, and quantum field theory. *Annu. Rev. Nucl. Part. Sci.* **57,** 95–118 (2007).
12. Cremonini, S. The shear viscosity to entropy ratio: A status report. *Mod. Phys. Lett. B* **25,** 1867–1888 (2011).
13. Adams, A., Carr, L. D., Schäfer, T., Steinberg, P. & Thomas, J. E. Strongly correlated quantum fluids: Ultracold quantum gases, quantum chromodynamic plasmas, and holographic duality. *New J. Phys.* **14,** 115009 (2012).

Two key differences between continuum theory and lattice models

- In lattice, the kinetic energy (charge compressibility drops as 1/T
- In continuum, this is not the case.
- In lattice, there is a minimal diff. constant

  D=a^2 /time =a^2* t. There is no such thing in continuum.

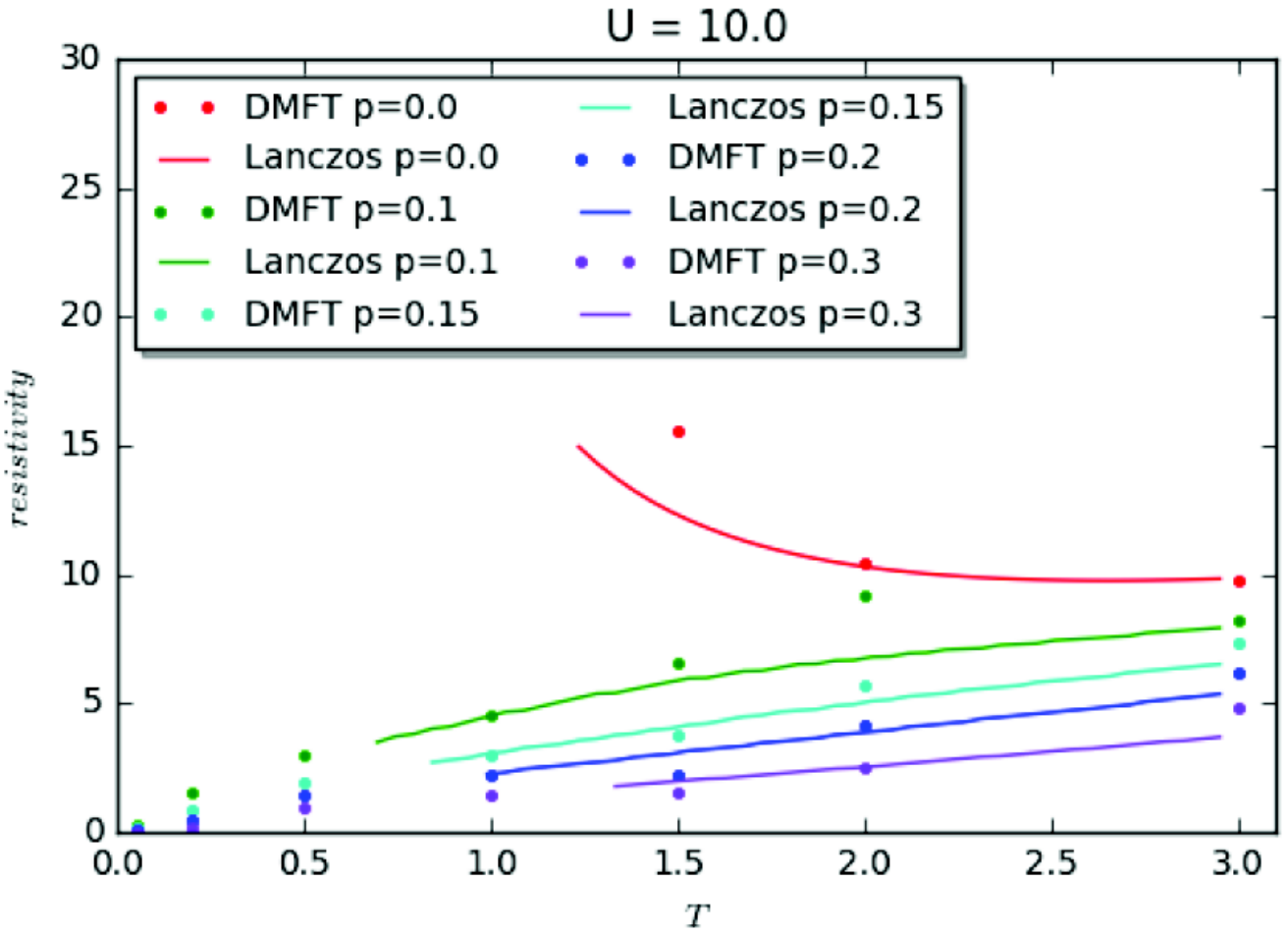
- These two work in opposite direction

Summary so far

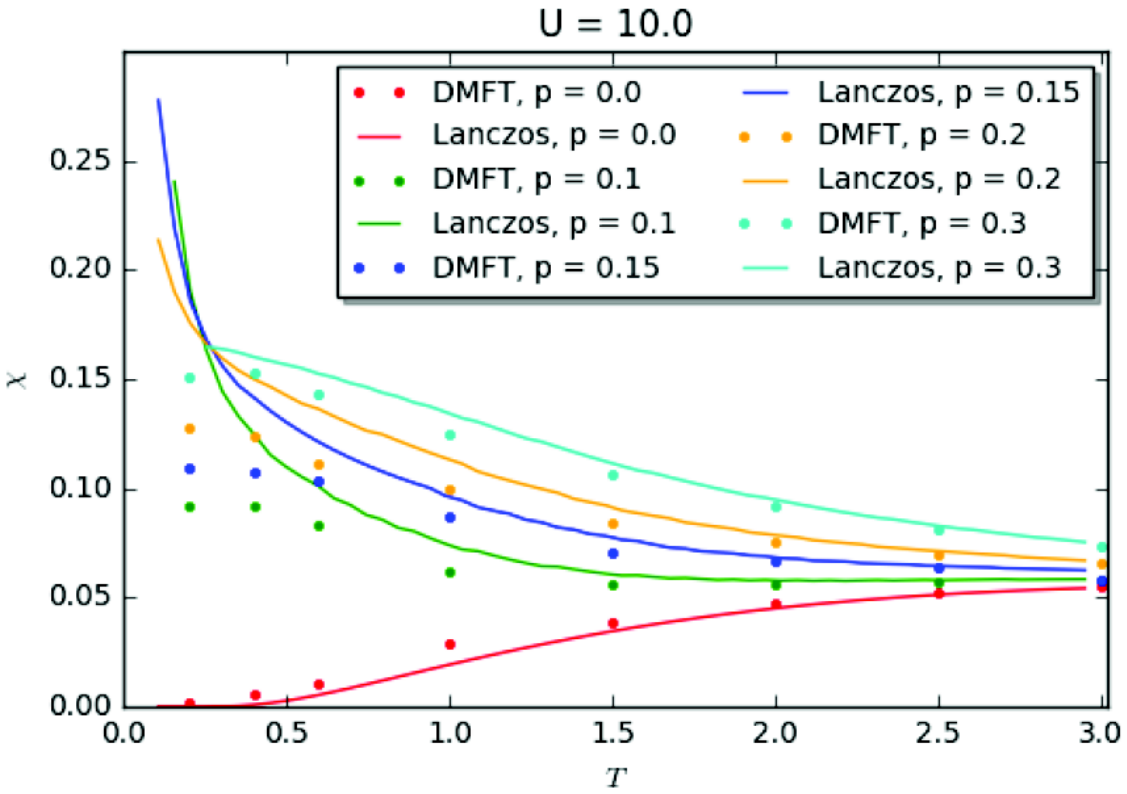
- In a single band situation, at high-T
  - DOS, Σ become T-independent (up to a shift)
  - Resistivity ~ T
  - Kinetic energy, charge compressibility ~ 1/T
  - Diffusion constant , scattering rate saturate
- In materials, all this somewhat academic, at high T one has multiple bands, but perhaps cold atoms could realize this high-T regime.
- I was mostly discussing DMFT, but turns that DMFT in high-T representative of the true behavior

Mazurenko et al., Nature 545 462(2017), down to T=0.25t

square lattice in 2d solved by Lanczos vs. DMFT



Ana Vranic, Jure Kokalj, et al. in preparation


U = 10.0
DMFT, p = 0.0
Lanczos, p = 0.0
DMFT, p = 0.1
Lanczos, p = 0.1
DMFT, p = 0.15
Lanczos, p = 0.15
DMFT, p = 0.2
Lanczos, p = 0.2
DMFT, p = 0.3
Lanczos, p = 0.3
0.25
0.20
0.15
0.10
0.05
0.00
χ
0.0
0.5
1.0
1.5
2.0
2.5
3.0
T

THANK YOU !

From good old days – to the present

1: Good (nonsaturating) metals

Prior to 1960s: Bloch-Grueneisen describes it all

- Resistivity due to el-ph interaction

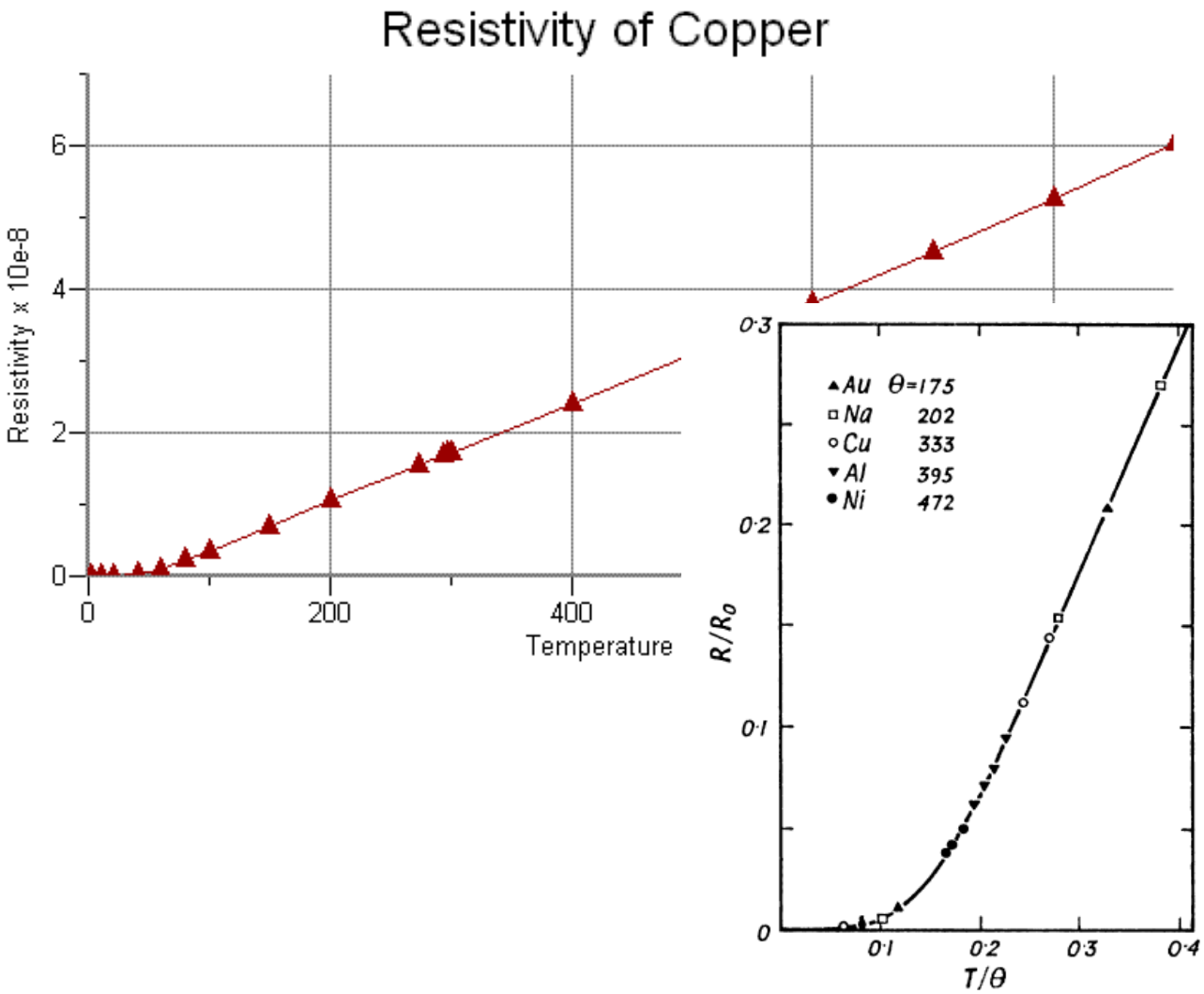
$$\rho_L = 4\left(\frac{T}{\Theta}\right)^5 \mathcal{J}_5\left(\frac{\Theta}{T}\right)\cdot\rho_\Theta,$$

Ziman,1960

- At high T, ρ~T

$$\int_0^{\Theta/T} z^3\,dz = \frac{1}{4}\left(\frac{\Theta}{T}\right)^4;$$

$$\rho_L \sim \frac{T}{\Theta}\rho_\Theta \quad (T \gg \Theta).$$



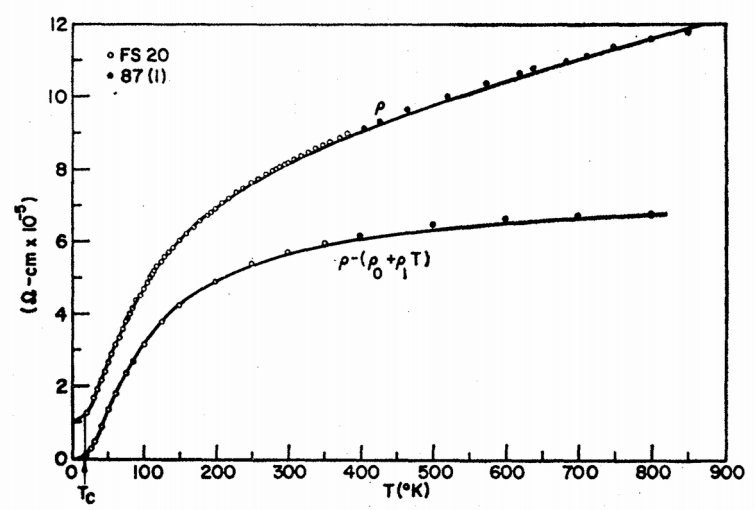
2.Metals with saturated resistivity at high T

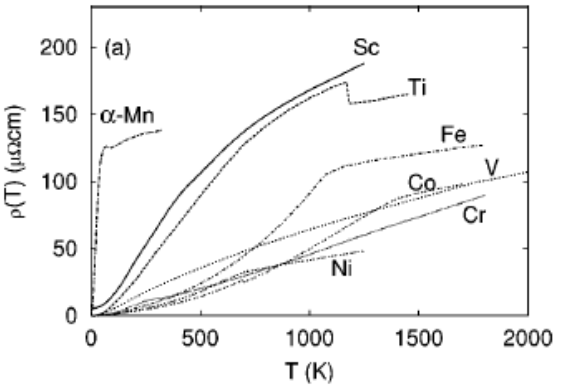
Saturating metals

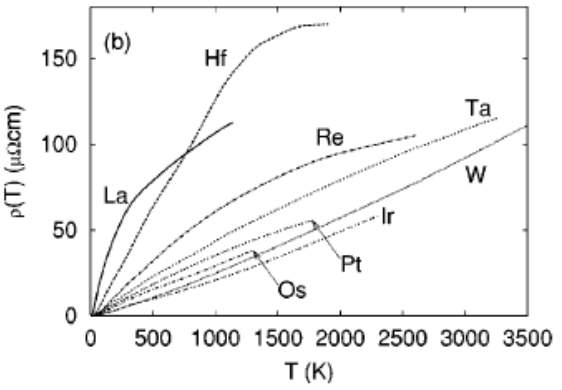
PHYSICAL REVIEW VOLUME 136, NUMBER 1A 5 OCTOBER 1964

Anomalous Resistivity of Nb_3Sn†

D. W. WOODARD AND G. D. CODY
RCA Laboratories, Princeton, New Jersey
(Received 3 April 1964)

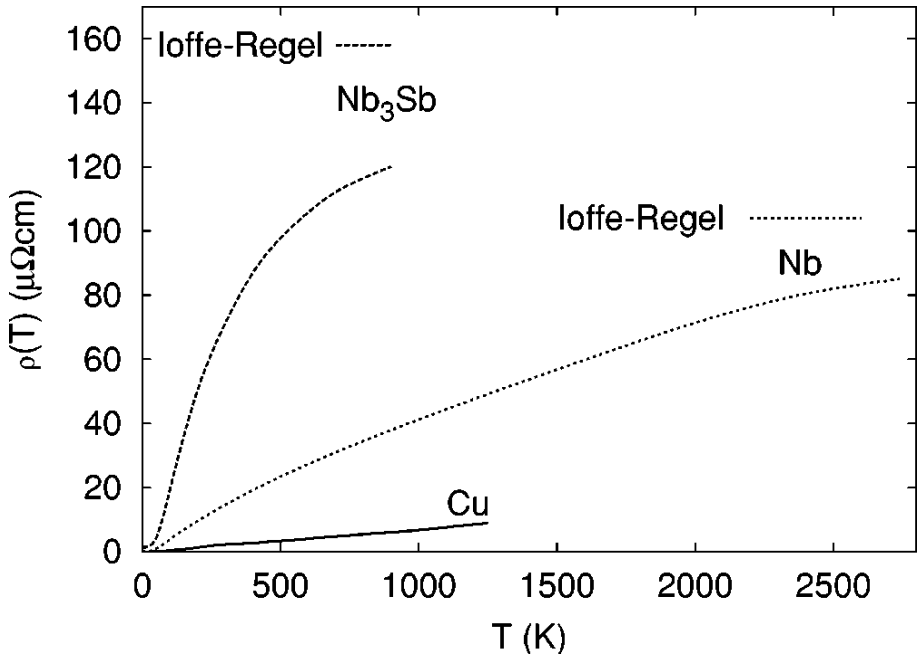






Saturating metals, MIR

In 1970s: Omnipresent saturation, Mott-Ioffe-Regel



Compound	ρ_{sat} (μΩcm)	ℓ_{min} (*a*)
Elements		
La	175	~ 1
Ti	200	~ 1
A15 compounds		
Nb_3Sn	135 -150	~ 1
Nb_3Ge	135	~ 1
Nb_3Pt	105	~ 1
V_3Si	135	~ 1
Mo_3Ge	120	~ 1
Alloys and Intermetallics		
$Ti_{1-x}Al_x$	190 – 330	1 – 1.5
In_5B_3	140	1 – 1.5
$Fe_{80-x}Ni_xCr_{20}$	180 – 250	1 – 1.5

- Minimal metalic conductivity corresponding to $k_F l=1$ or $l \sim a$

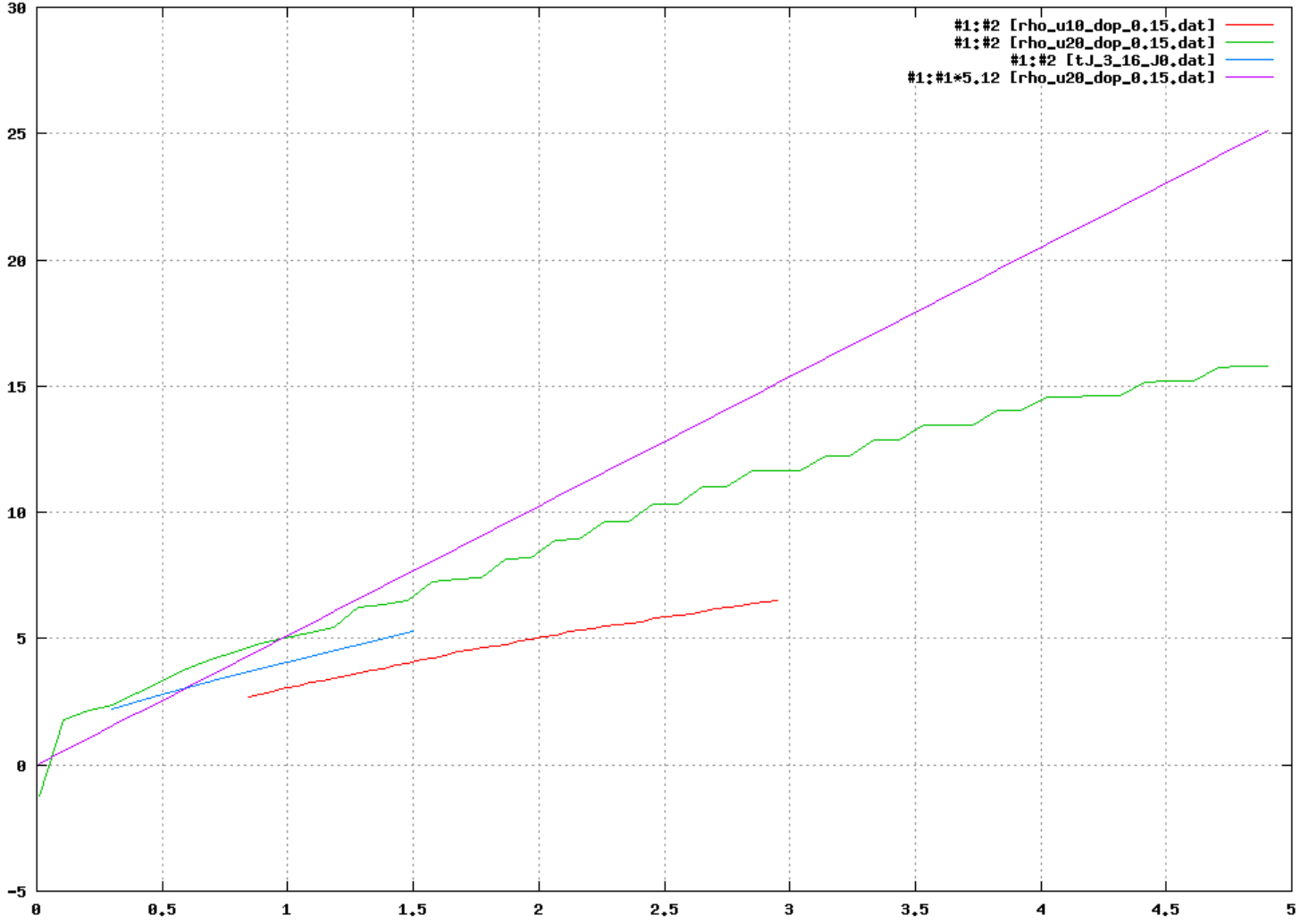
Gurvitch, PRB'81

PB Allen, “Superconductivity in d- and f-band metals” (1980); N. Mott (Nobel Lecture 1977)
Gunnarsson, Calandra & Han, Rev. Mod. Phys. (2003)
Hussey, Takenaka & Takagi, Phil. Mag. (2004)

3. Metals with unsaturated $\rho > \rho_{MIR}$

=

“Bad metals”


#1:#2 [rho_u10_dop_0.15.dat]
#1:#2 [rho_u20_dop_0.15.dat]
#1:#2 [tJ_3_16_J0.dat]
#1:#1*5.12 [rho_u20_dop_0.15.dat]
30
25
20
15
10
5
0
-5
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5

Transport in DMFT (ii)

- Velocity distribution function (units $[x]^{2-d}$ $[\omega]$)

$$\Phi(\varepsilon) = (1/V)\sum_{\mathbf{k}} (\partial\varepsilon_{\mathbf{k}}/\partial\mathbf{k}_x)^2 \delta(\varepsilon - \varepsilon_{\mathbf{k}})$$

$$\sigma = \frac{2\pi e^2}{\hbar}\int d\omega \left(-\frac{\partial f}{\partial\omega}\right)\int d\epsilon \Phi(\epsilon) A_\epsilon(\omega) A_\epsilon(\omega)$$

- At low T, only $\omega \sim 0$, $k \sim k_F$ states contribute.

$1/\rho_{\mathrm{MIR}} \equiv e^2\Phi(0)/\hbar D$ a natural unit for conductivity, used henceforth

- If evaluated for a 2d electron gas, one gets

$$\sigma = (k_F l)\, e^2\Phi(\varepsilon_F)/\hbar\varepsilon_F = (k_F l)e^2/h$$

$k_F l$ times the conductivity quantum, thus this choice corresponds to ρ_{MIR} for criterion $k_F l = 1$

MIR for a 2d electron gas

$$\sigma = \frac{ne^2\tau}{m} = \frac{ne^2 l}{mv_F} = \frac{ne^2 l}{k_F}$$

- In 2d, $n \sim k_F^2$, sheet conductivity is $G_0 k_F l$

$$\sigma = \frac{1}{2\pi}\frac{N_s e^2}{2\hbar}\frac{1}{c}k_F l = \frac{1}{2\pi}\frac{e^2}{\hbar}\frac{1}{c}\cdot k_F l$$

- Taking $k_F l = 2\pi$, c=0.3nm one gets

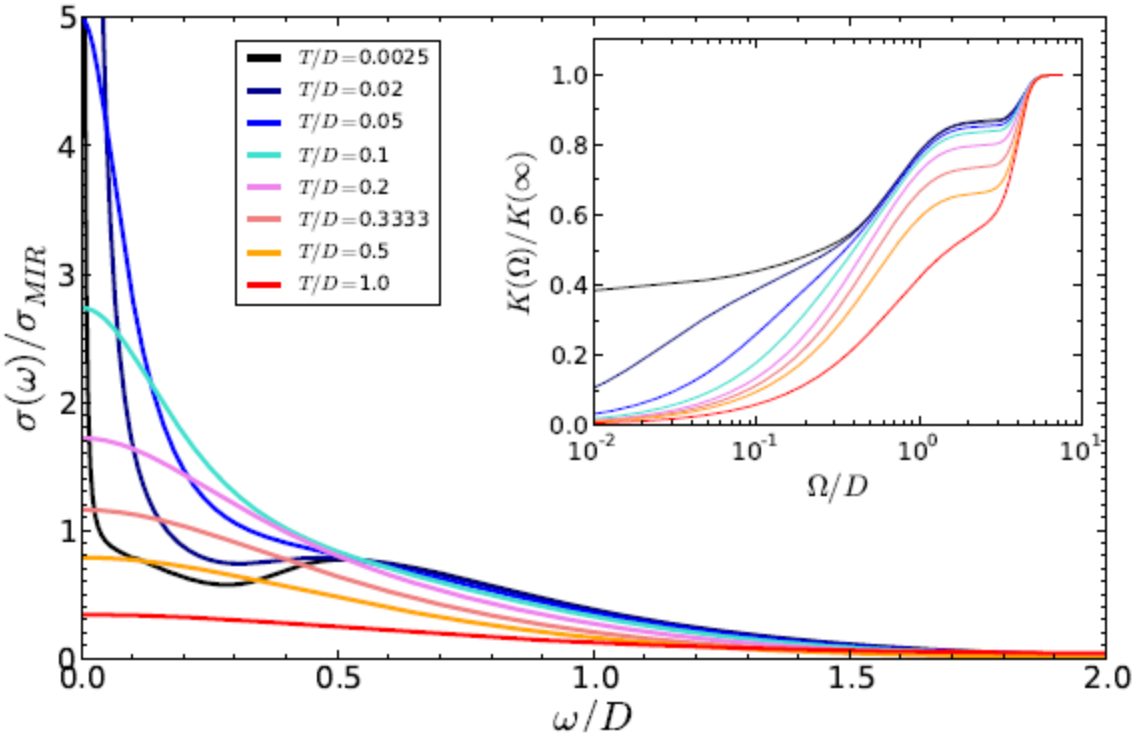
  130 μΩcm
- 2d → 3d; $2\pi/c \rightarrow 4/3\ k_F$; taking further $k_F = \pi/a$, one gets 200 μΩcm
- Several criterions: most to least restrictive
- $l = 2\pi/k_F$, a, $1/k_F$

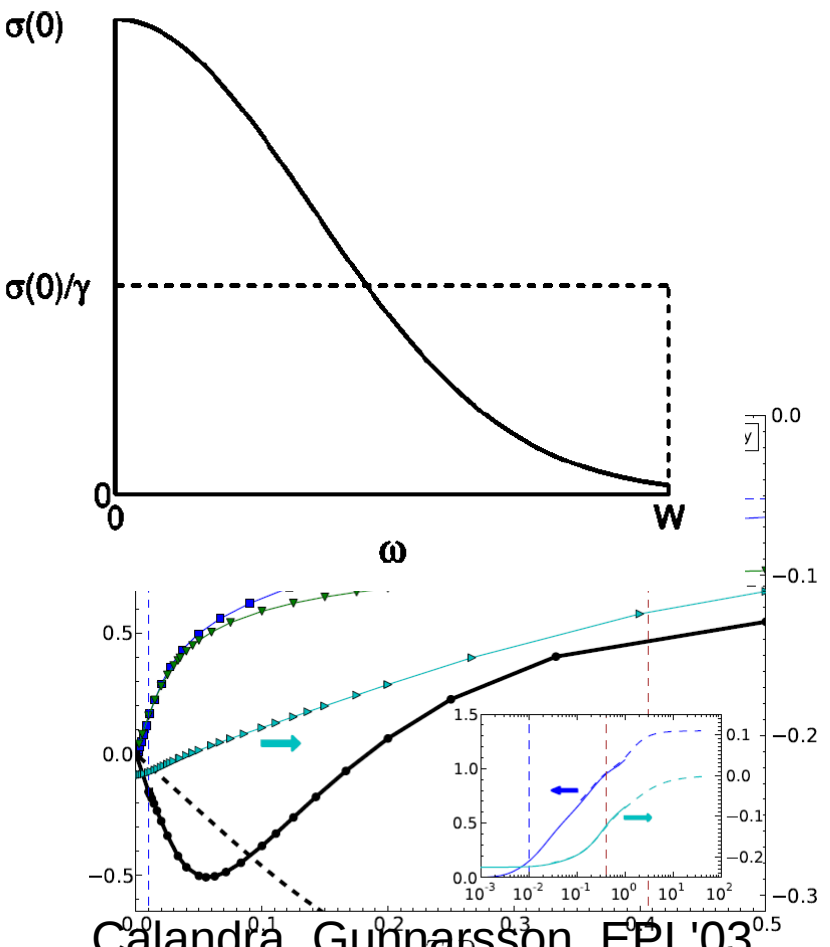
- Asymptotic high-T Hubbard model has T-lin resistivity and saturated scattering rate
- Saturated diffusion constant, scattering rate
- “carrier density”, kinetic energy ~ 1/T
- (in distictinction with continuum)

Optical conductivity

- Integrates to kinetic energy,
- Size of kinetic energy diminishes frequency, hence conductivity)
- At MIR isosbestic point is lost

$$\int_0^{D^*} \sigma(\omega) d\omega = W_K = \sigma(0) D^* \rightarrow \sigma(0) = W_K / D^*$$

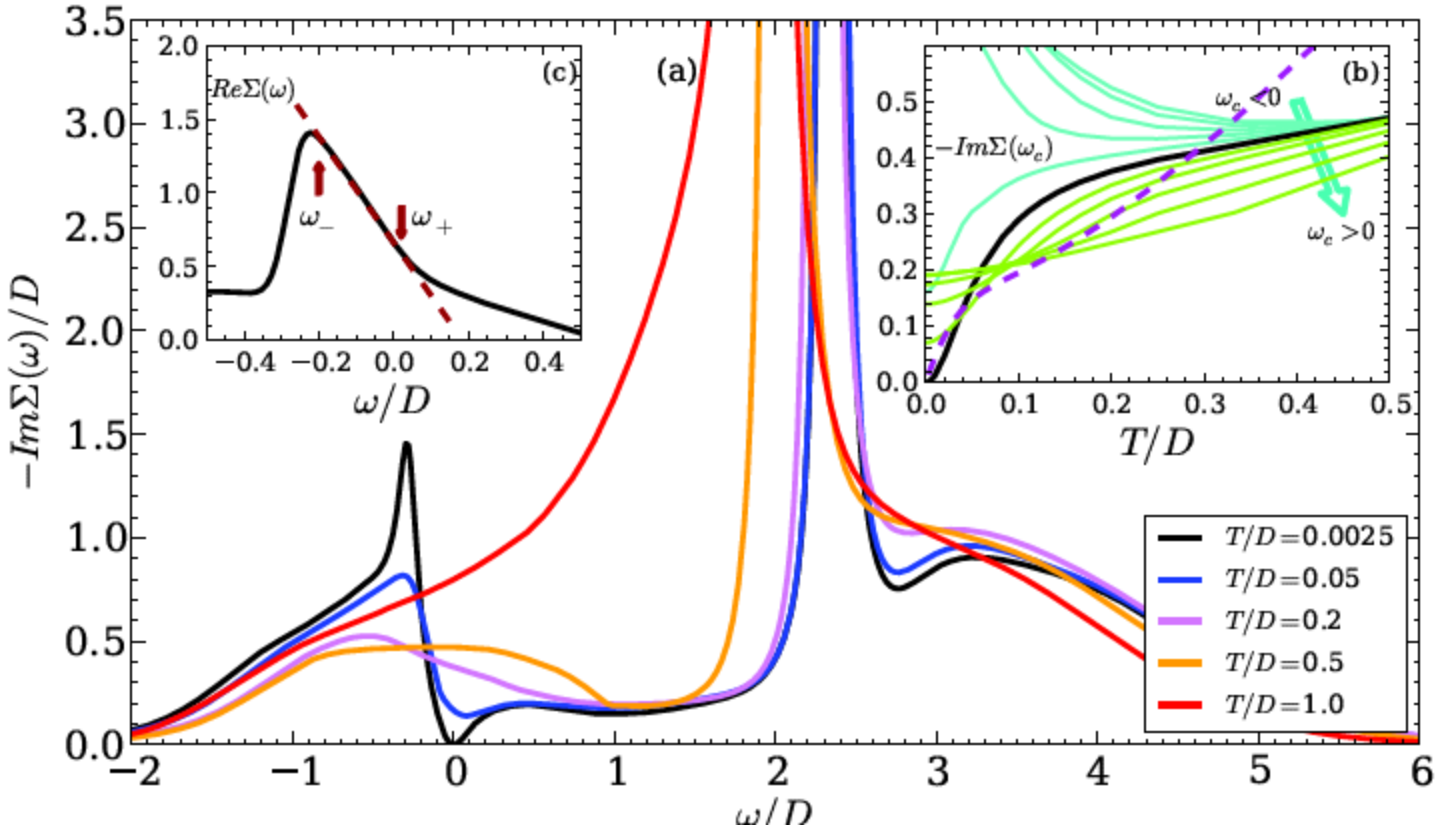




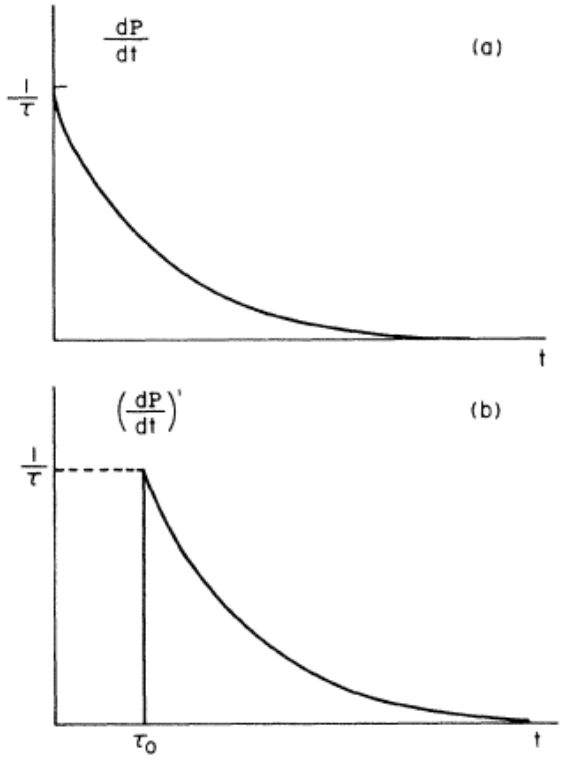
Calandra, Gunnarsson, EPL'03

Self energies &particle-hole asymmetry

- -imag part of self energy



Parallel resistor formula



The drift velocity in a field E will be found as

$$V_D = \int V(t)dP = \frac{eE}{m\tau}\int_0^\infty te^{-t/\tau}dt = \frac{eE}{m}\tau,$$

the current $j = enV_D = \sigma E$ and $\sigma = \sigma_{\text{ideal}} = e^2 n\tau/m$.

However, if we use the new distribution (5), we get

$$V_D' = \int V(t)dP' = \frac{eE}{m\tau}\int_{\tau_0}^\infty te^{-(t-\tau_0)/\tau}dt$$

$$= \frac{eE}{m}(\tau+\tau_0)$$

and

$$\sigma' = \frac{e^2 n\tau}{m} + \frac{e^2 n\tau_0}{m} = \sigma_{\text{ideal}} + \sigma_{\text{sat}}$$

which is the parallel-resistor formula.

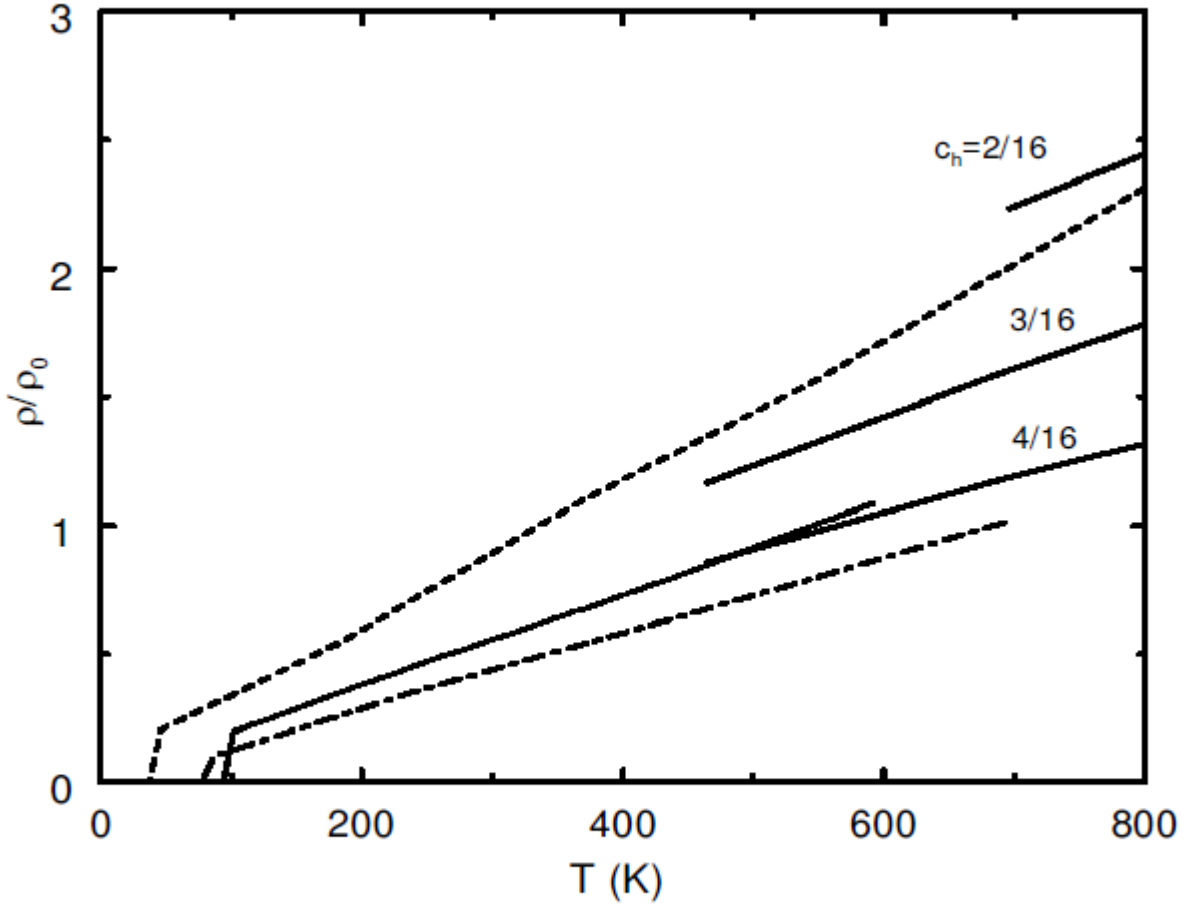


Figure 24. Sheet resistivities $\rho(T)$ for various dopings (full lines) in comparison with measurements in LSCO with $x = 0.15$ (dotted), BSCCO (dashed), and YBCO (dash-dotted).

Jaklic Prelovsek, Adv. Phys.'00