# How bad metals turn good: spectroscopic signatures of resilient quasiparticles

Michel Ferrero
Ecole Polytechnique, CNRS

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# Collaborators

- Xiaoyu Deng (Rutgers)
- Jernej Mravlje (Ljubljana)
- Rok Zitko (Ljubljana)
- Antoine Georges (Ecole Polytechnique)
- Gabriel Kotliar (Rutgers)

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# Transport in strongly-correlated materials

- Strongly-correlated systems often display unconventional behaviors, rich phase diagrams

- This is also true for their transport properties:
  - Bad metallic behavior at high temperatures with resistivity incompatible with Drude description
  - Fermi liquid only at very low temperatures (if at all)

- Resistivity first measured but last understood!

# Mott Ioffe Regel limit

- Quasiparticle description can only make sense if mean free path is longer than the Fermi wavelength
- For a simple quasi 2d geometry with Drude

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

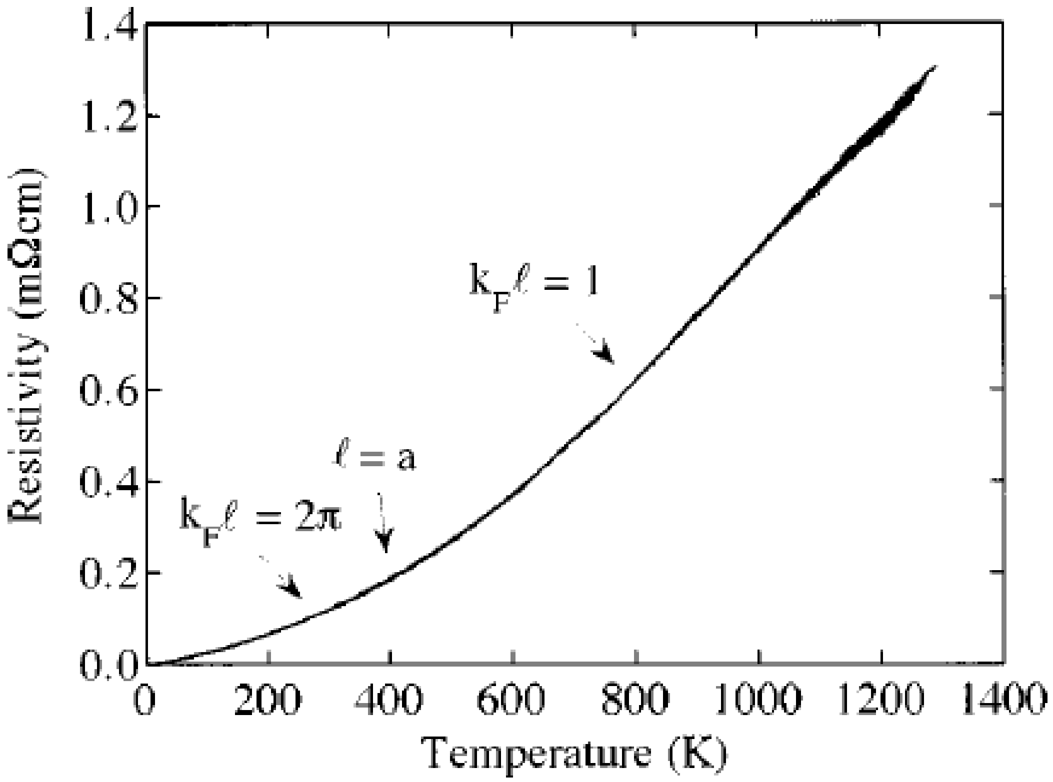
- Setting $k_F l = 1$ we get a maximum Mott-Ioffe-Regel resistivity

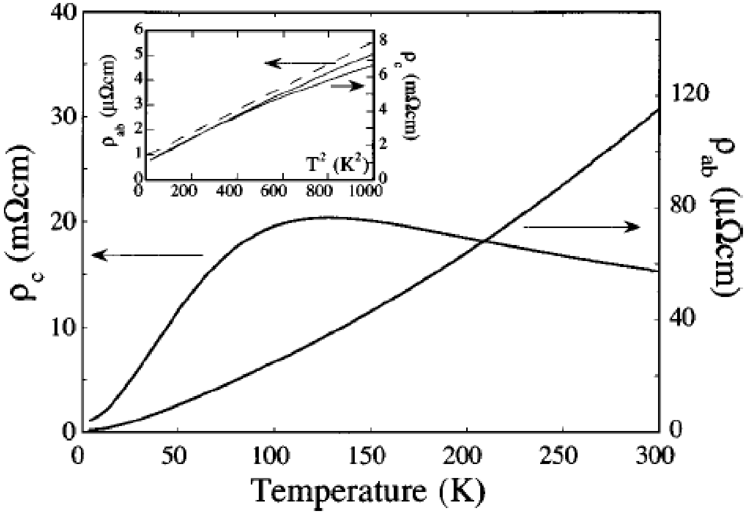
$$\rho_{\mathrm{MIR}} = \frac{h}{e^2} c_0 \sim 0.25 \mathrm{m}\Omega\mathrm{cm} \times c_0 [\mathrm{nm}]$$

Gunnarsson, Calandra and Han, RMP (2003)
Hussey, Takenaka and Takagi, Phil. Mag. (2004)

# A prototypical bad metal: $Sr_2RuO_4$

- High-T resistivity exceeds MIR limit (~ 800K)
- However, the low-T state is a well-defined Fermi liquid when T < 20K
- Other examples:
  - $LiV_2O_4$<br>
    $T_{FL} = 2K$<br>
    $T_{MIR}$ = few 100K
  - Cuprates<br>
    low-T state?





Tyler, Mackenzie, Nishizaki and Maeno, PRB (1998); Hussey et al., PRB (1998)

# The key questions

- How to describe transport in strongly-correlated metals?
- What is $T_{FL}$? Are there still quasiparticles above $T_{FL}$?
- What happens for $T_{FL} < T < T_{MIR}$? Is a Drude description still possible even without Landau quasiparticles?
- What happens at $T_{MIR}$? Is there any signal of disappearing quasiparticles?
- Why are these questions interesting?

# The simplest model

- Hole-doped single-band Hubbard model within DMFT
- U = 4D, D = half-bandwidth (typically D ~ 1eV)
- Computing transport is very delicate!
  - Numerical Renormalization Group
    Ljubljana code, `http://nrgljubljana.ijs.si`
  - Continuous-time quantum Monte Carlo both hybridization and interaction expansion versions + Pade approximants
    TRIQS, `http://ipht.cea.fr/triqs`, Gull et. al, RMP (2011)
- Allow to study the full range of temperatures and to cross-check results

Palsson et al., PRL (1998); Merino and McKenzie, PRB (2000); Limelette et al., PRL and Science (2003); Grete et al., PRB (2010), ...

# Conductivity within DMFT

- The dynamical mean-field theory (DMFT) maps the original lattice model on a self-consistent quantum impurity problem
- Self-energy has no momentum dependence

$$A(k,\omega) = -\frac{1}{\pi}\mathrm{Im}\frac{1}{\omega+\mu-\epsilon_k-\Sigma(\omega)}$$

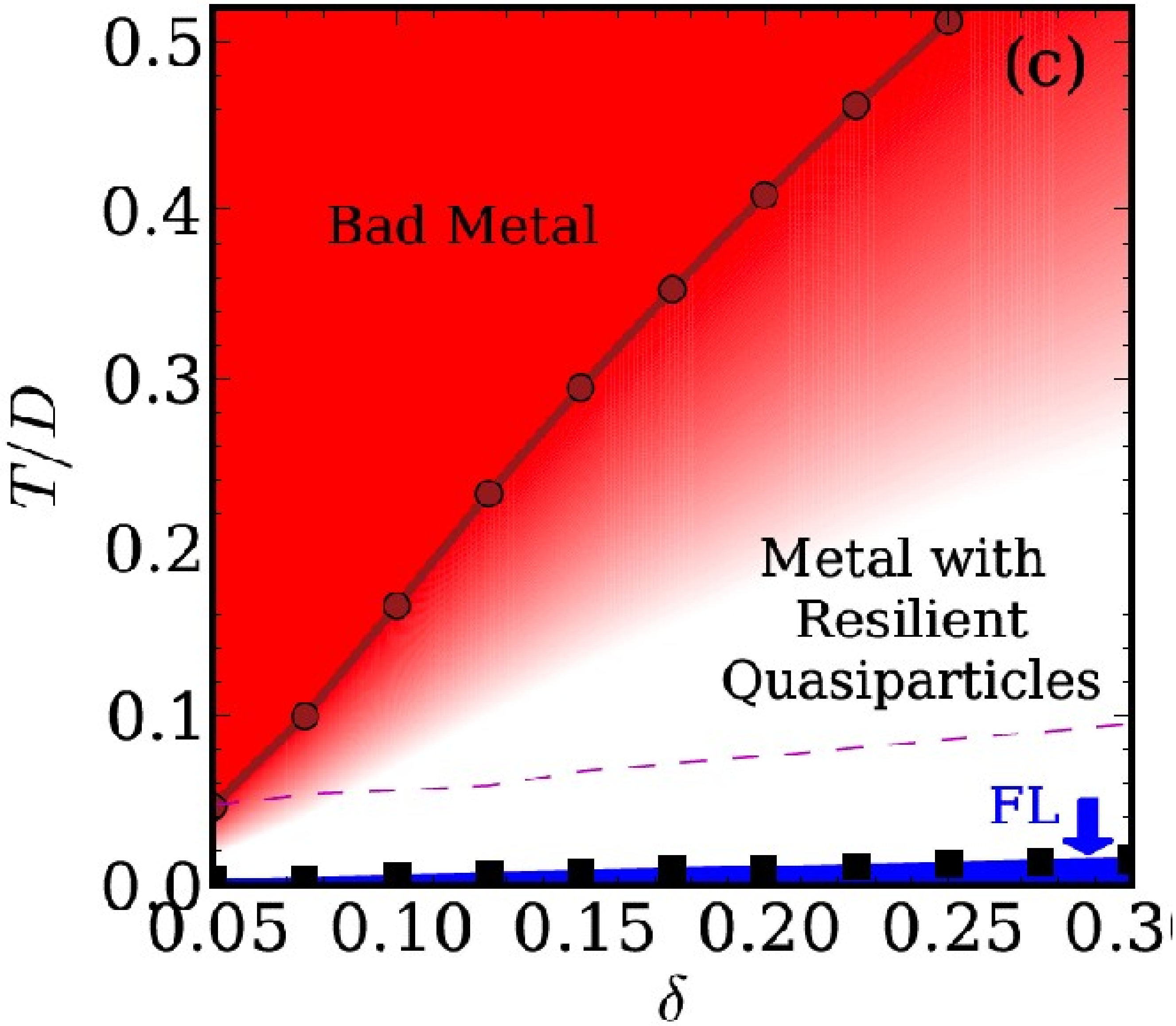
- Vertex corrections vanish

$$\sigma = \frac{2\pi e^2}{\hbar}\int d\omega\Big(-\frac{\partial f(\omega)}{\partial\omega}\Big)\sum_k v_k A(k,\omega) v_k A(k,\omega)$$

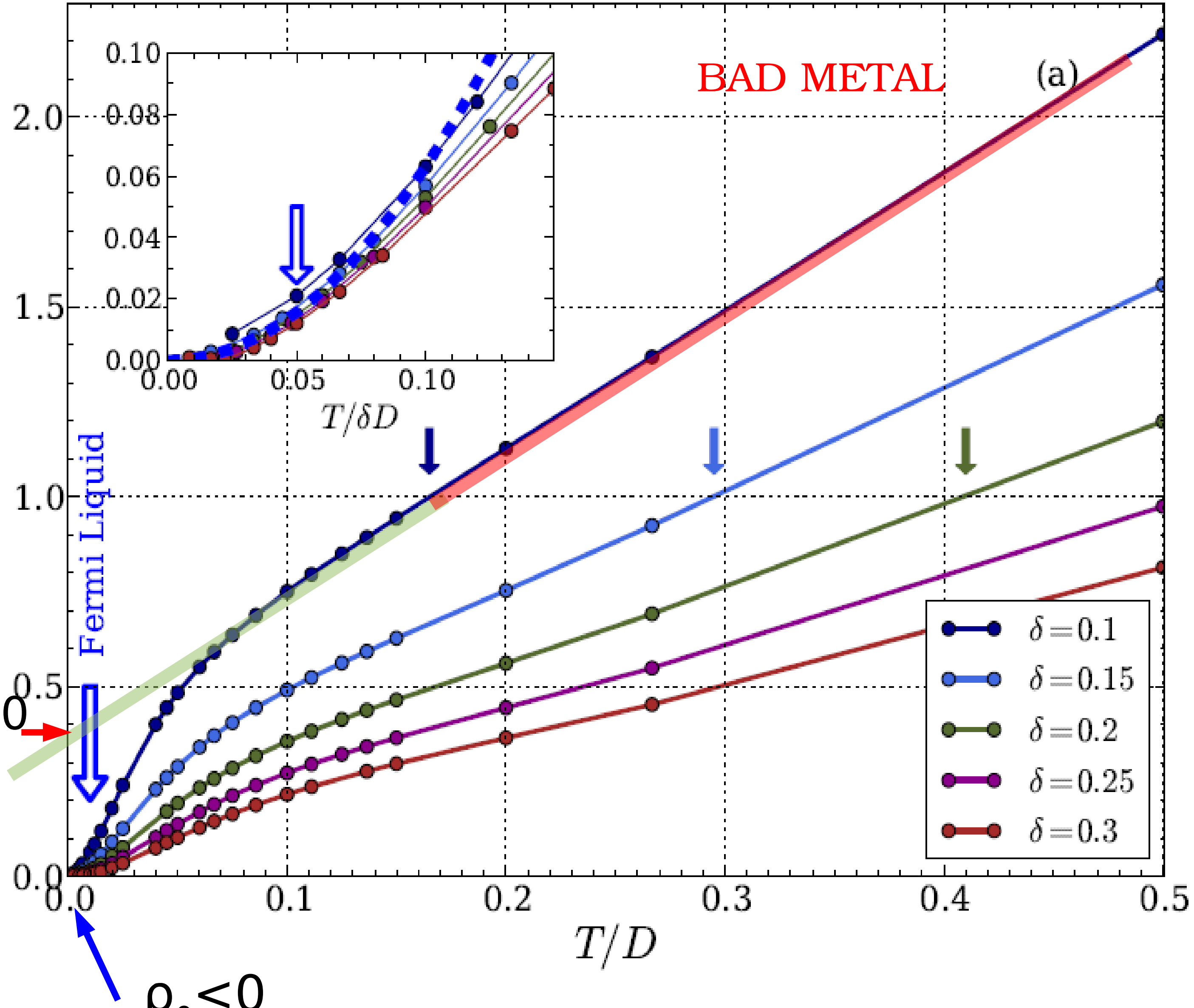
$$v_k = \partial\epsilon_k/\partial k_x$$

# Three transport regimes

- No quasiparticles above $T_{MIR}$
- FL below $T_{FL}$
- Big region with “resilient” quasiparticles that are not Fermi-liquid



# Resistivity versus temperature



$\rho_0 > 0$

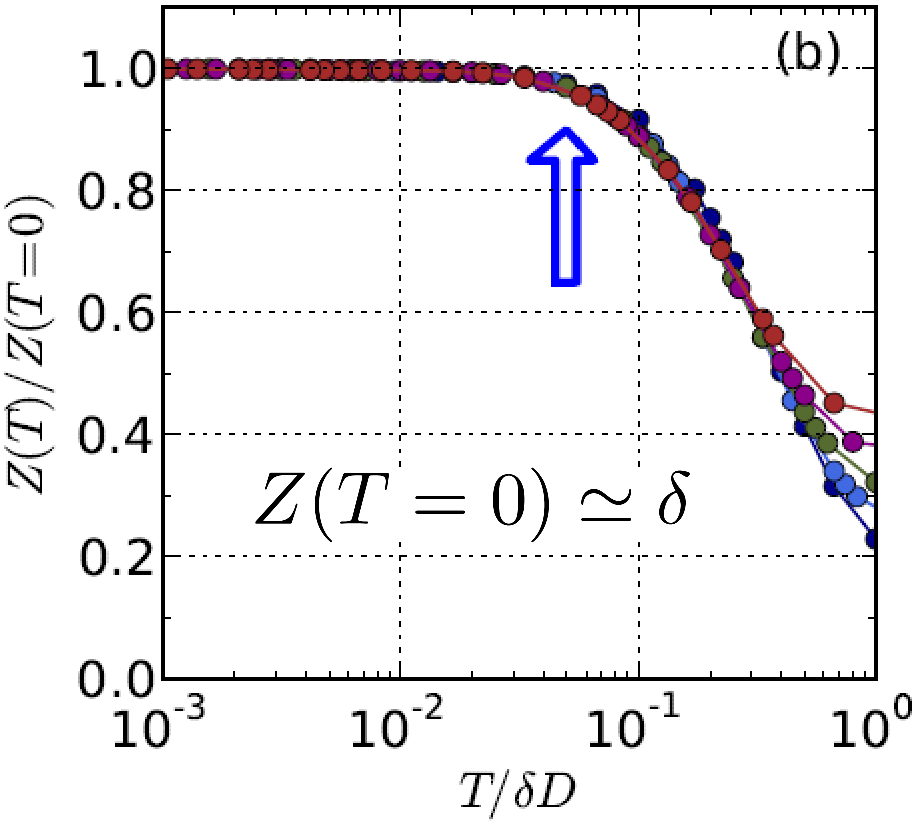
$\rho_0 < 0$

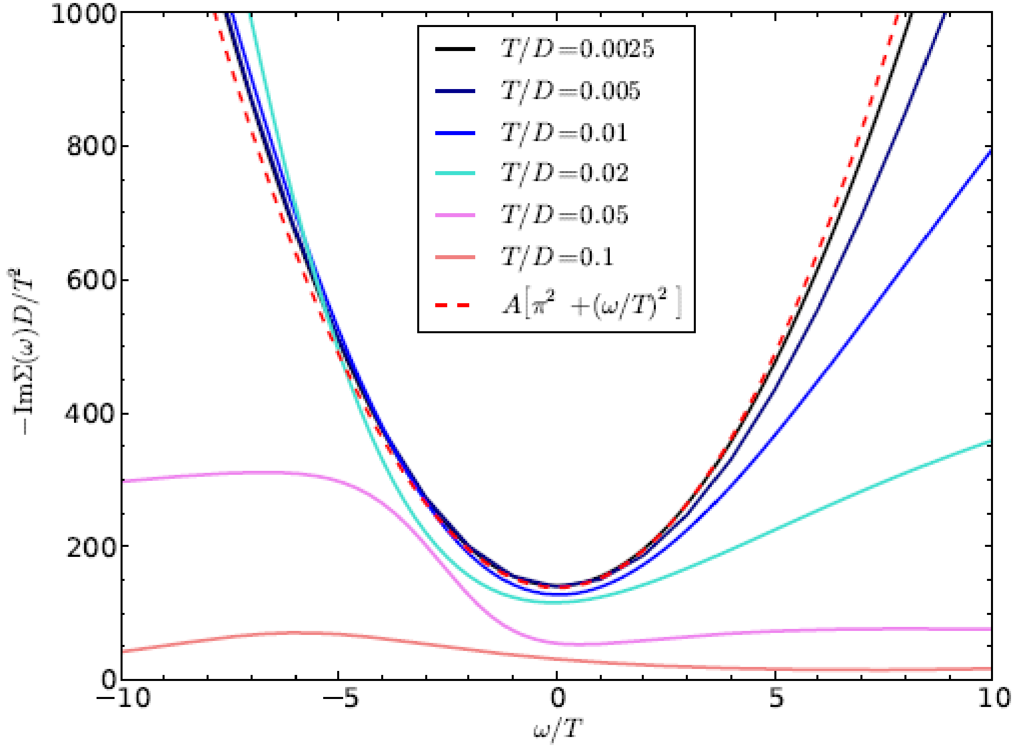
# Fermi liquid regime

- $T_{FL}$ = 0.05 δD (a very small scale)
- Proportional to Brinkman-Rice scale δD but with a small prefactor
- Much smaller than $T_{MIR}$

$$\Sigma' = \Sigma_0 + (1 - Z^{-1})\omega + \ldots$$

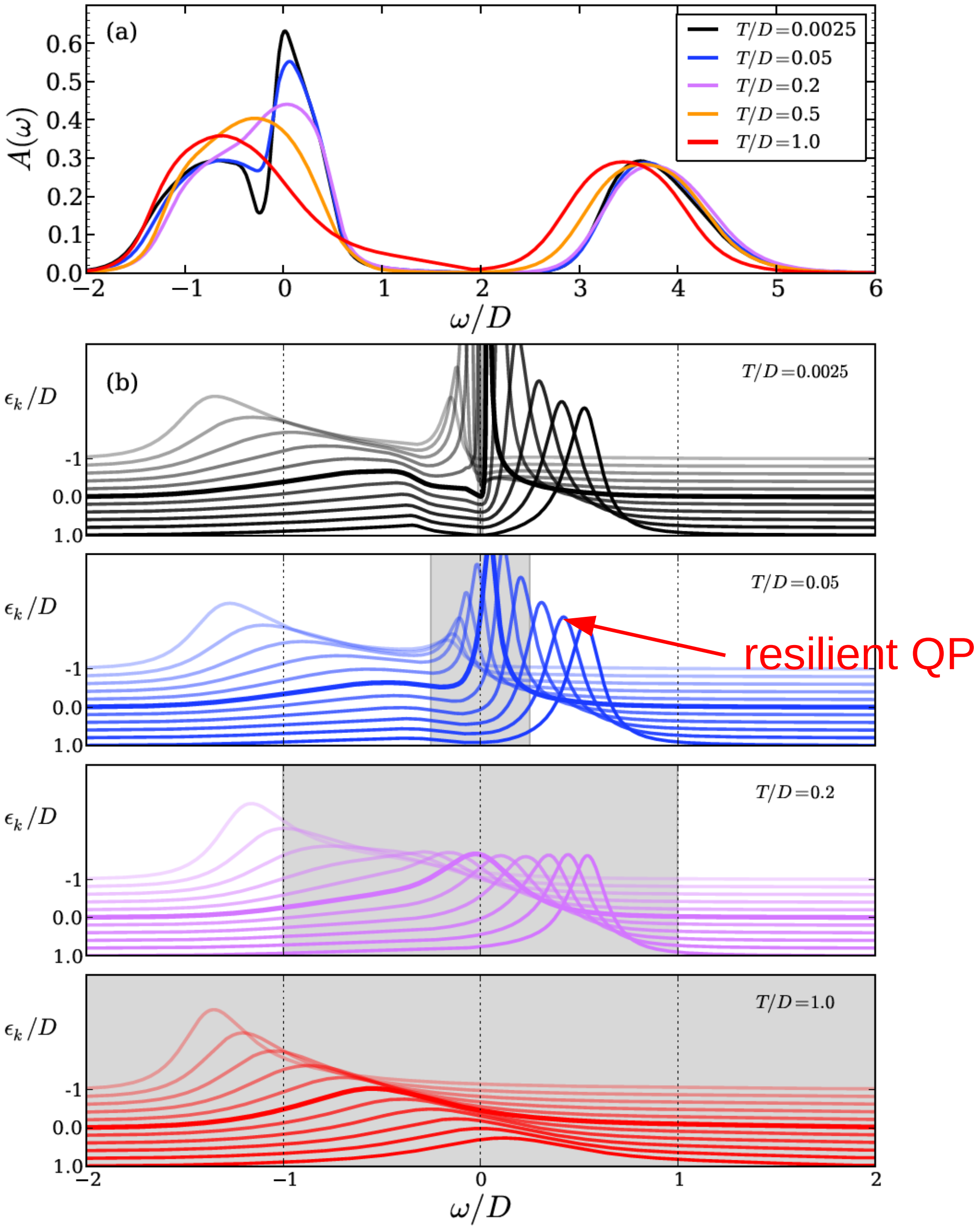
$$\Sigma''(\omega) \sim \omega^2 + \pi T^2$$

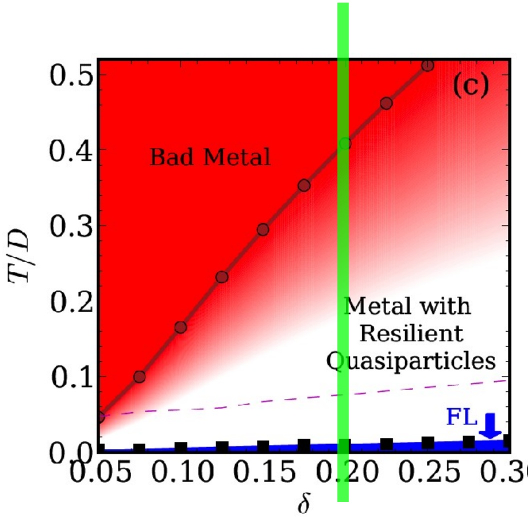




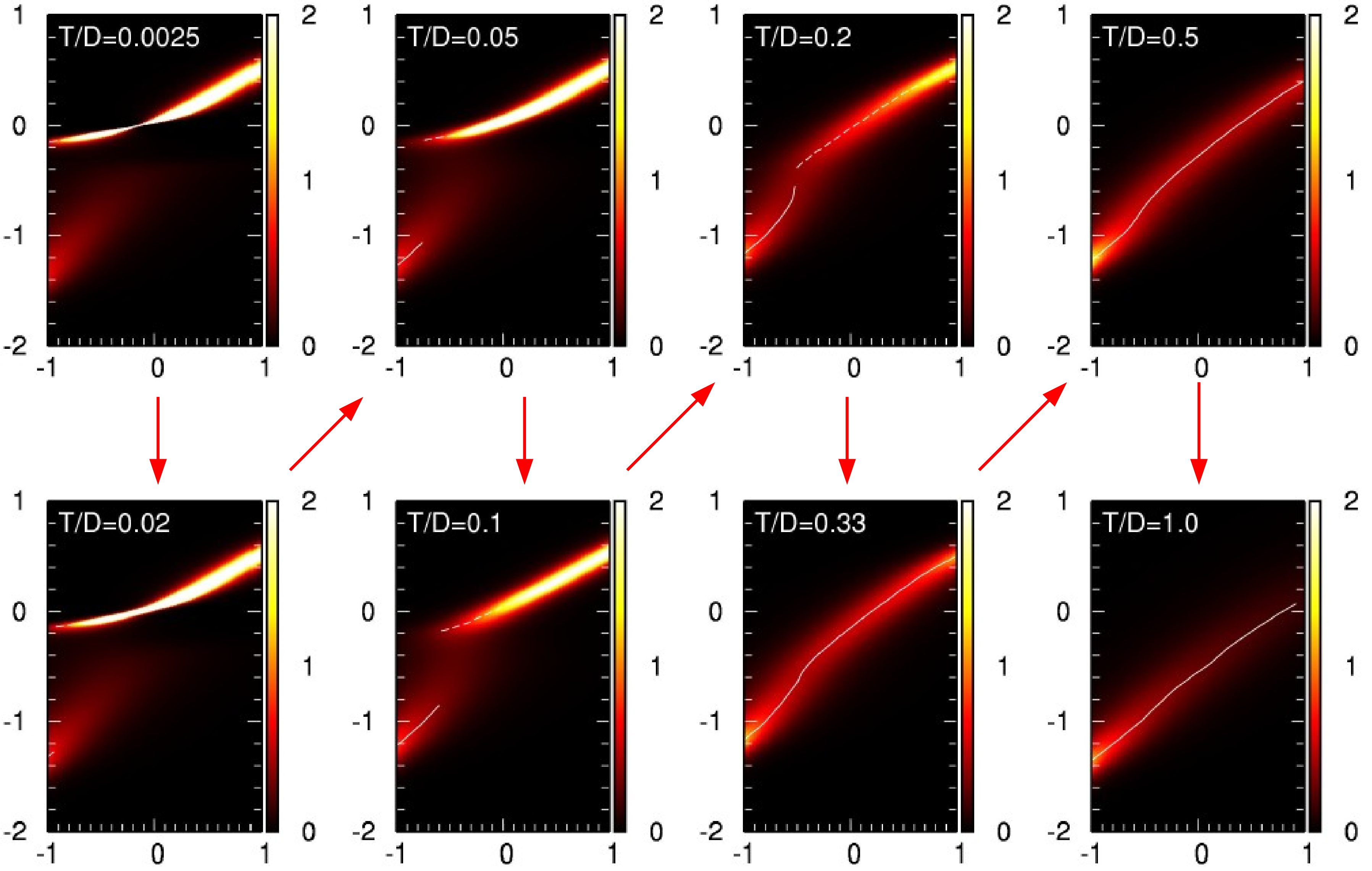
# Resilient quasiparticle regime

- Clear signature of quasiparticles up to $T_{MIR}$
- From 3-peak to 2-peak structure
- The QP band eventually merges in the LHB





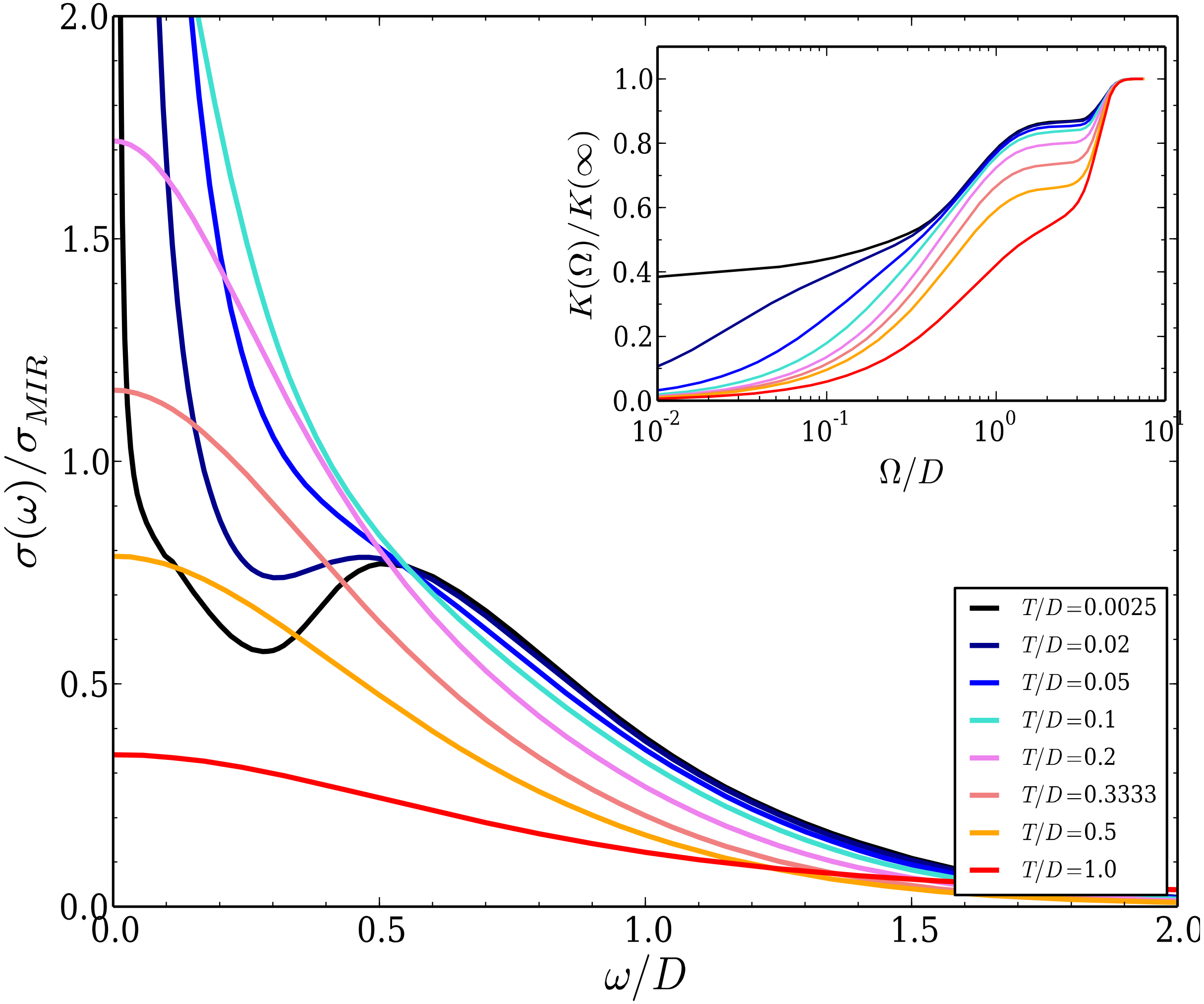
# Spectral function intensity maps



It would be very useful to see the dark side of the Fermi surface!

# Signatures in optical conductivity

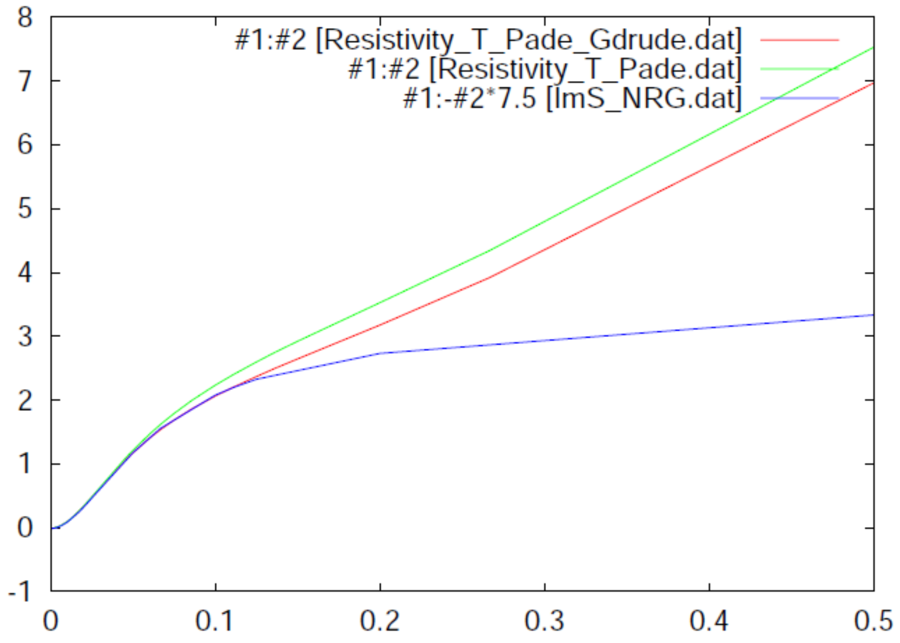
- Merging of Drude peak and mid-infrared peak at $T_{FL}$
- Redistribution of spectral weight over wide range at $T_{MIR}$
- Only involving up to mid-infrared below $T_{MIR}$

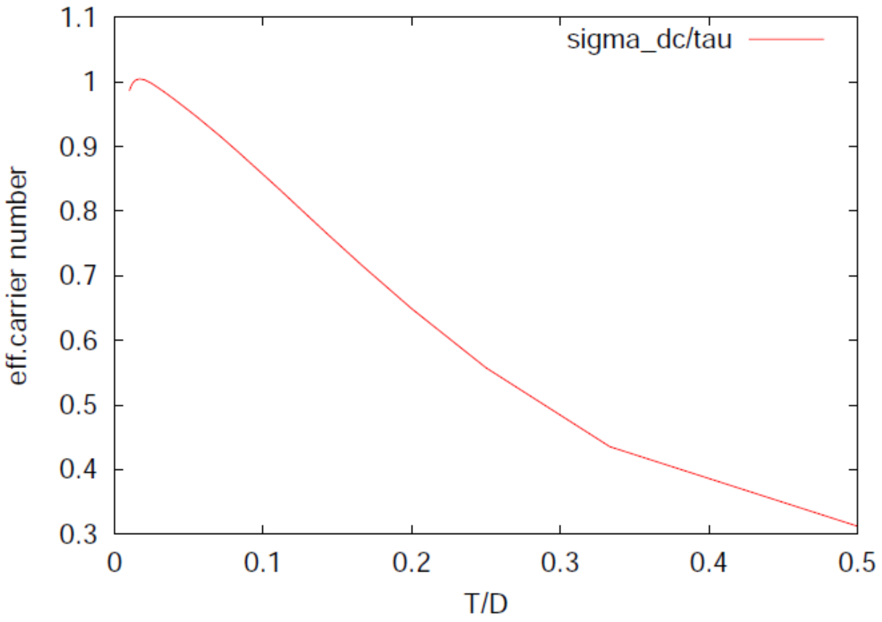


Hussey, Takenaka and Takagi, Phil Mag (2004)

# Description of transport

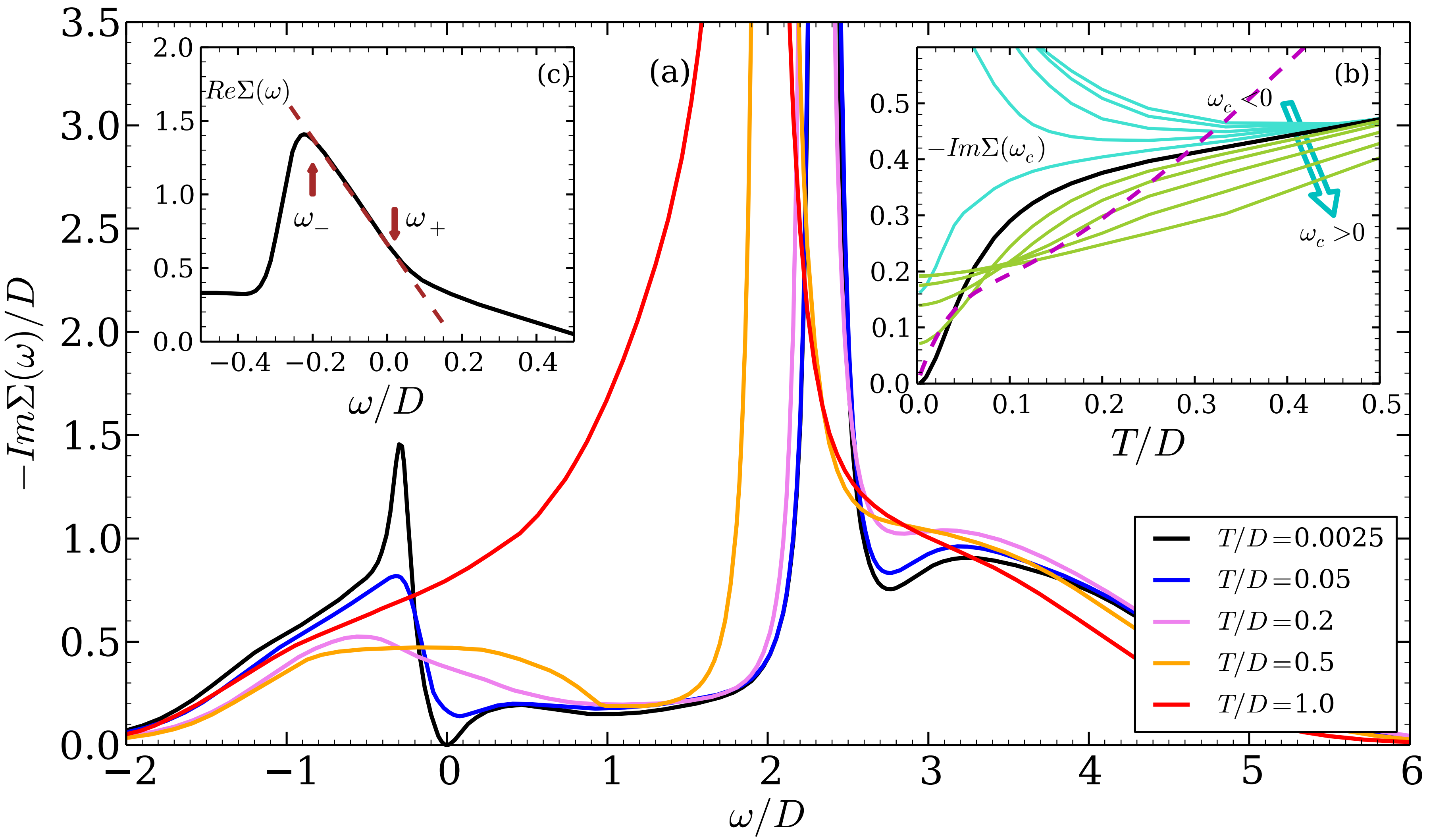
- Up to intermediate temperature, transport is controlled by the temperature dependence of the scattering rate
- At higher temperatures, the scattering rate saturates and it is rather the effective carrier number that matters
- Eventually we reach an incoherent regime. Think of it as carriers in rigid Hubbard bands





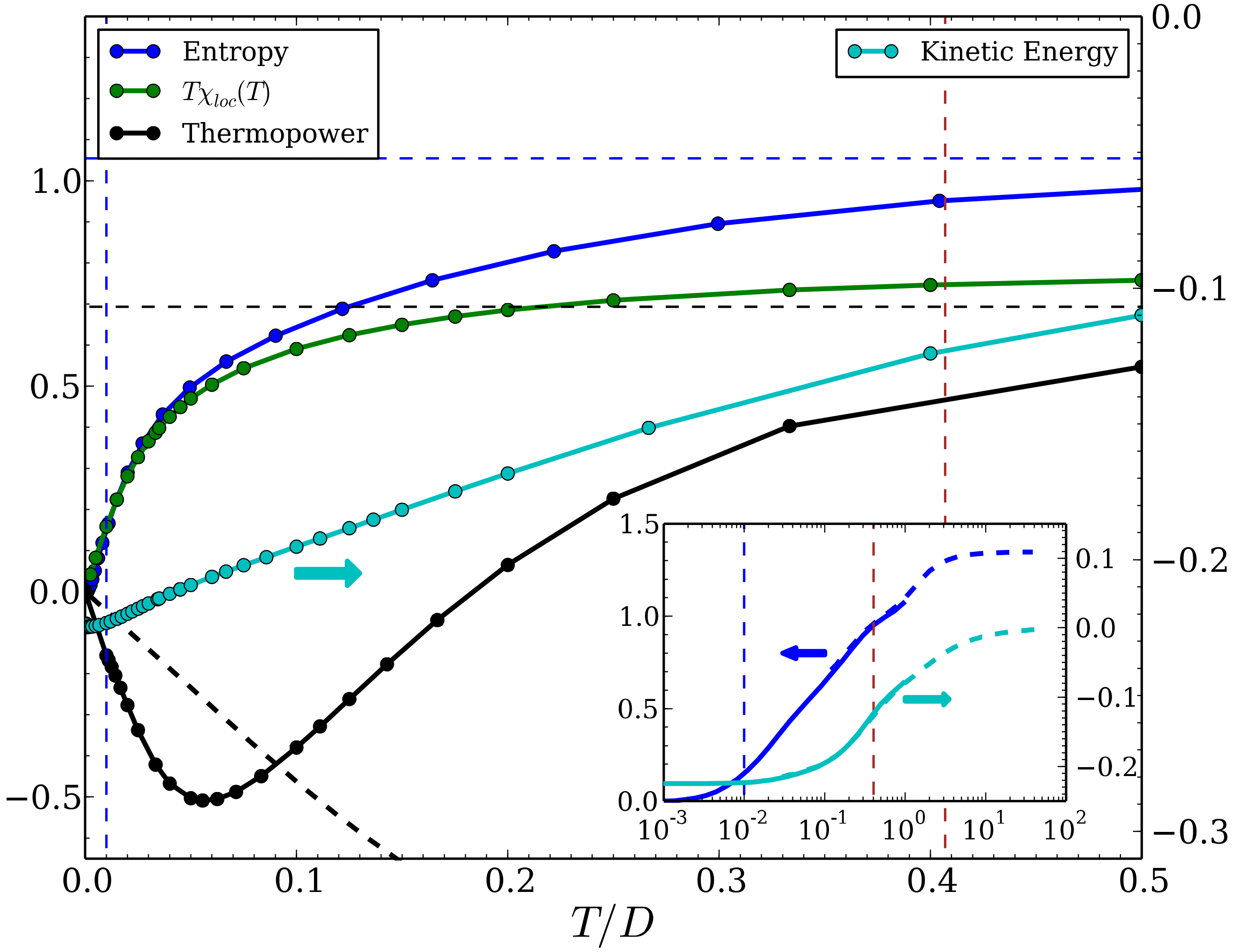
# Particle-hole asymmetry

- Longer lifetimes for electron-like excitations



# Consequence for thermopower

- Seebeck coefficient in the resilient QP regime has a minimum dominated by electron-like quasiparticles



# Summary

- Well-defined QP exist above $T_{FL}$ all the way up to $T_{MIR}$ with a resistivity much smaller than the MIR value
- In the bad metallic regime above $T_{MIR}$, QP have disappeared. The system is not really metallic, it looks more like a doped semiconductor
- Spectroscopic signatures (a lot of action on the dark side of the Fermi surface)
- Hole-doped: electron-like excitations are longer-lived
- Motivation for the quest of low-T quasiparticles (maybe relevant for cuprates?)