Transport signatures of the Mott transition in a 2d organic conductor

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- Patrice Limelette *(Tours)*
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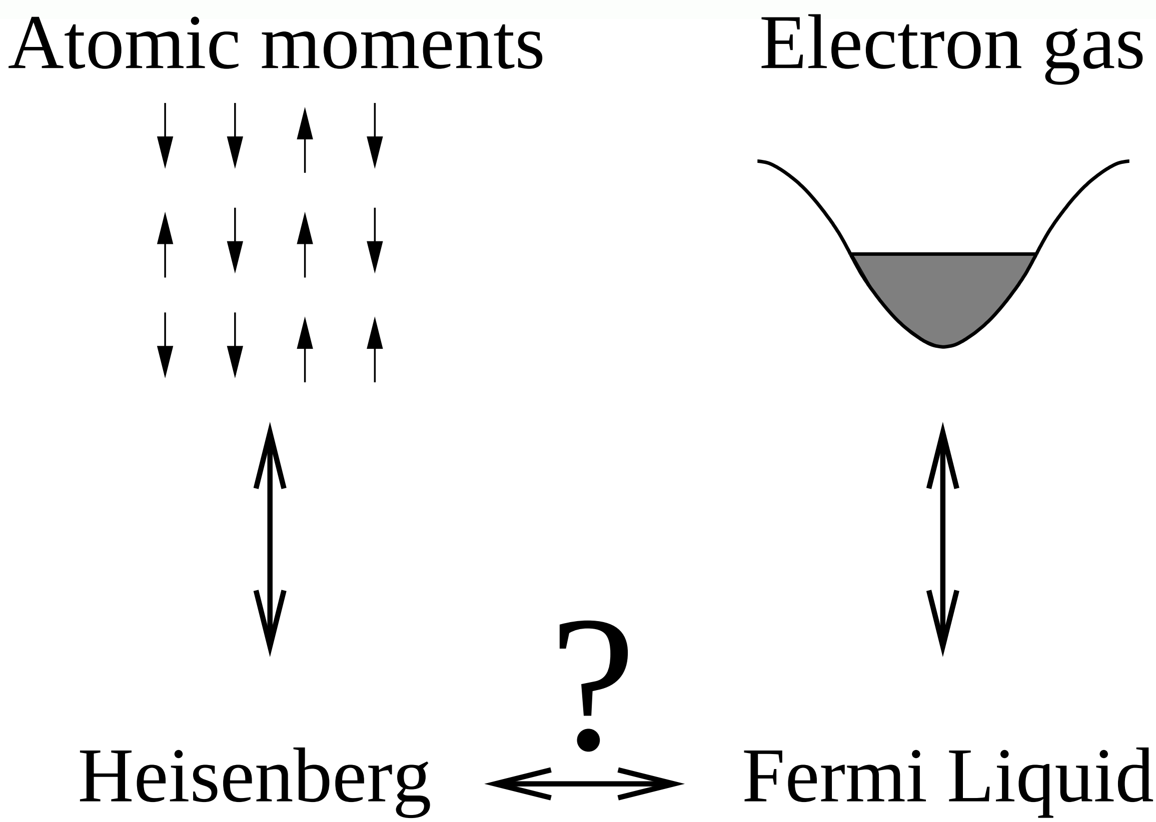
Summary

- Mott transition: an introduction
- Dynamical Mean Field Theory
- Transport in κ-BEDT
- Calculation with DMFT+NRG
- Around the finite-T endpoint: κ-BEDT et V_2O_3
- Zero-T Mott transition?

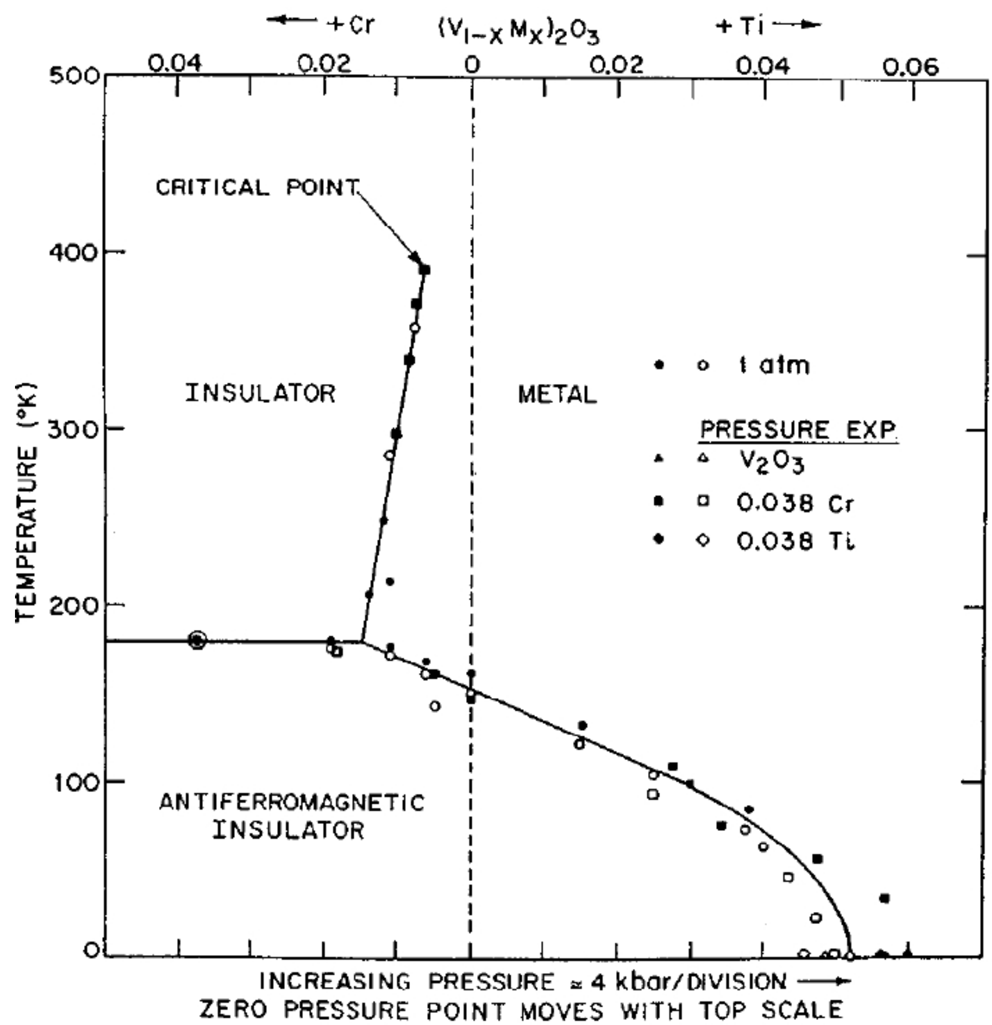
Mott transition: general picture



Control parameters:

- Screened Coulomb interaction U/D
- Doping δ
- Dimensionality
- Frustration
- $\ldots$

Time-honored example: V_2O_3



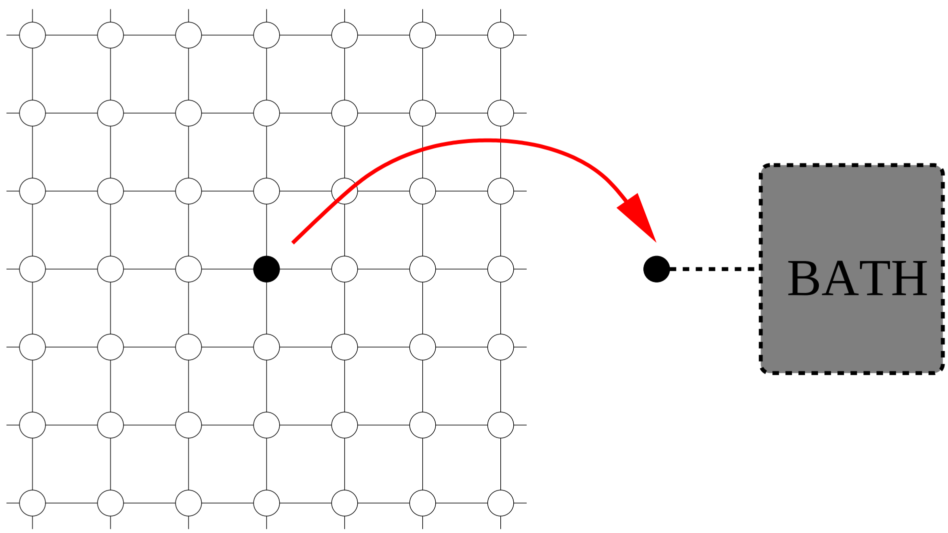
[McWhan et al. PRB 1971]

- Relevance for $T > T_N$
- Paramagnetic phases involved
- 1^{st} order transition
- Electron vs. lattice?

Hubbard model:

$$H = -\sum_{\mathrm{ij}\sigma} t_{ij} d^\dagger_{i\sigma} d_{j\sigma} + U \sum_{\mathrm{i}} n_{i\uparrow} n_{i\downarrow}$$

Cavity:



Self-consistent impurity model:

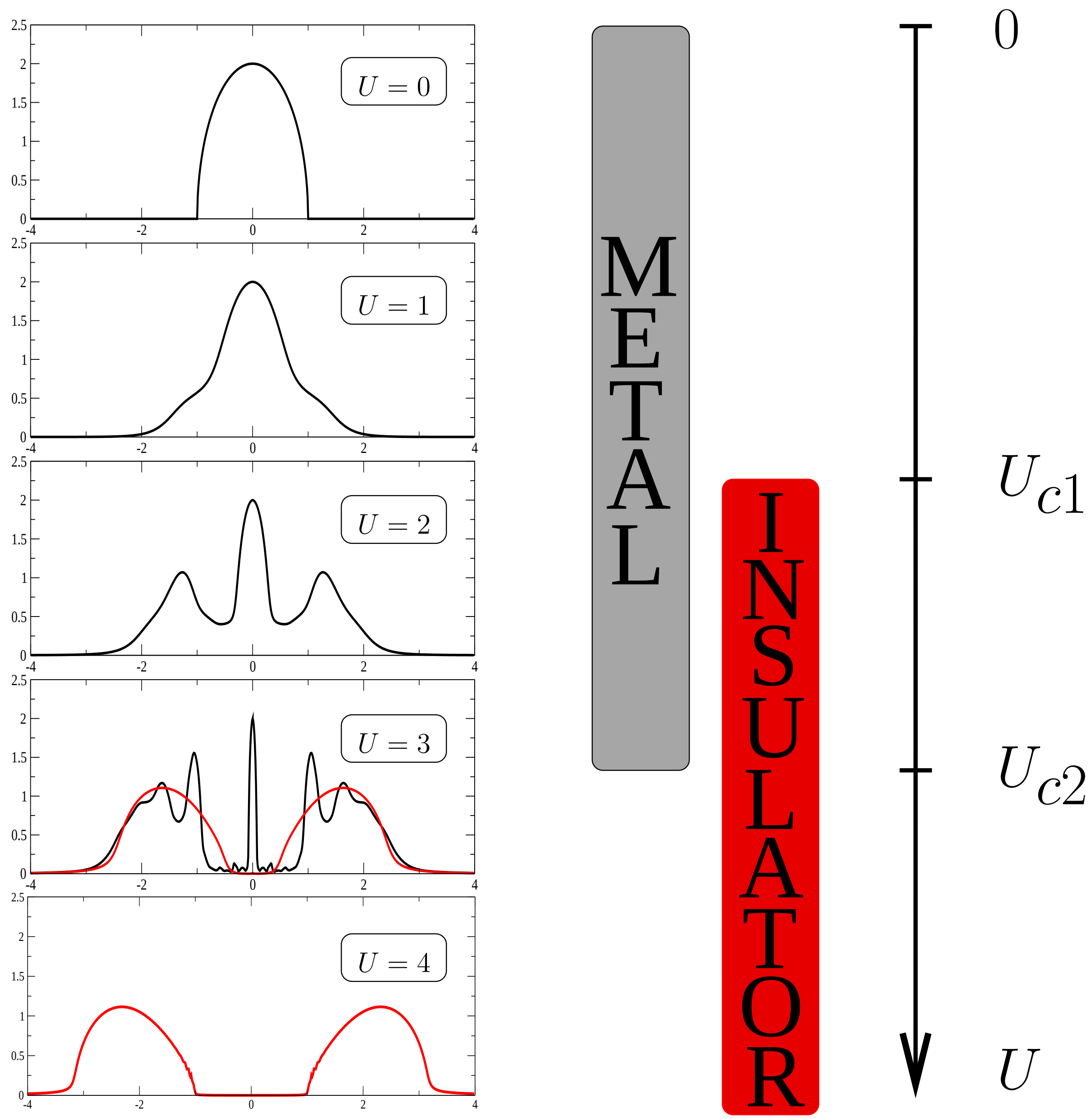
$$S_{\mathrm{eff}} = -\int_0^\beta \mathrm{d}\tau \int_0^\beta \mathrm{d}\tau' \, \mathcal{G}_0^{-1}(\tau - \tau') \sum_\sigma d^\dagger_\sigma(\tau) d_\sigma(\tau') + \int_0^\beta \mathrm{d}\tau \, U n_\uparrow n_\downarrow$$

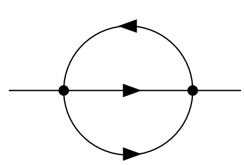
$$\begin{aligned} G_d(i\omega_n) &\equiv \left\langle d^\dagger_\sigma(i\omega_n) d_\sigma(i\omega_n) \right\rangle_{|S_{\mathrm{eff}}} \\ &= \sum_k \frac{1}{i\omega_n - \epsilon_k + G_d^{-1}(i\omega_n) - \mathcal{G}_0^{-1}(i\omega_n)} \end{aligned}$$

Exact for $d \to \infty$ [Metzner&Vollhardt, Georges&Kotliar]

Mott transition in DMFT

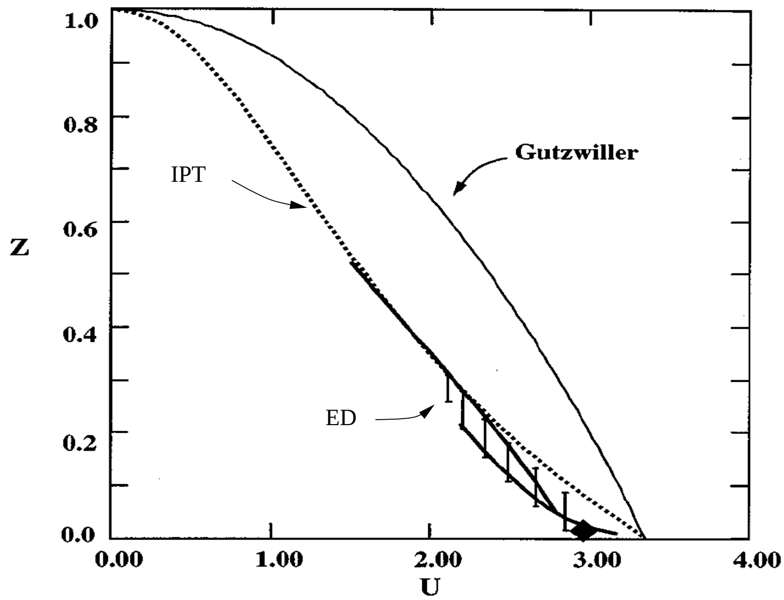
Zero temperature:



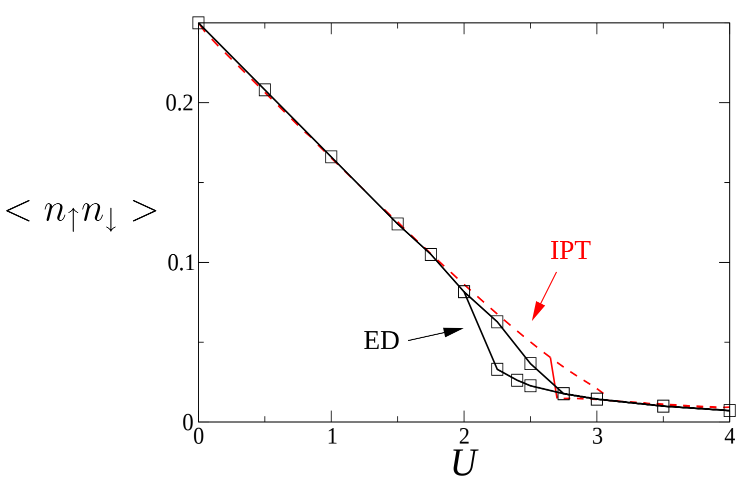
IPT method: $\Sigma(\tau) =$  $= U^2 \mathcal{G}_0(\tau)^3$

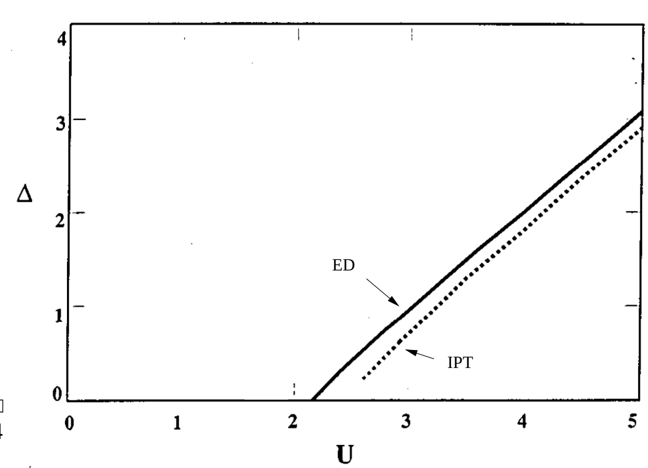
What is the $T = 0$ order parameter?

Quasiparticle weight Z: YES



Double occupancy, Mott gap: NO





Physical properties

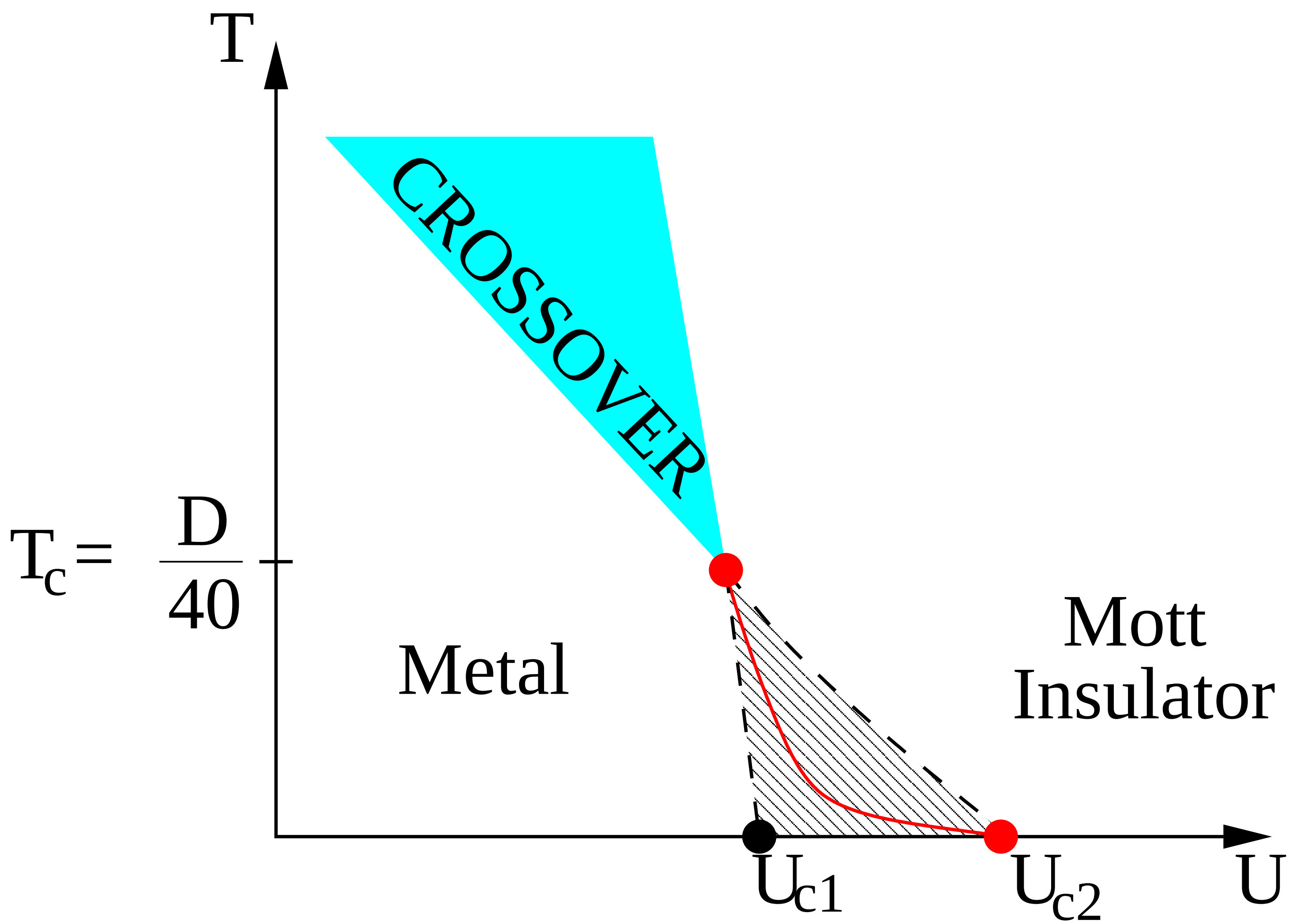
Fermi Liquid:

- Coherence scale $\epsilon_F^* = ZD$
- Quasiparticle weight $Z \sim 1 - U/U_{c2}$
- Effective mass $m^*/m \sim [1 - U/U_{c2}]^{-1}$
- Specific heat coefficient
  $\gamma = C_v/T \propto m^*/m \sim [1 - U/U_{c2}]^{-1}$
- Self-energy $\Sigma''(\omega, T) \sim (\omega^2 + T^2)/Z^2 D$

Mott insulator:

- Paramagnetic state
- Local moments ($\chi_{loc} = \infty$)
- Small non-zero double occupancy

Paramagnetic phase diagram

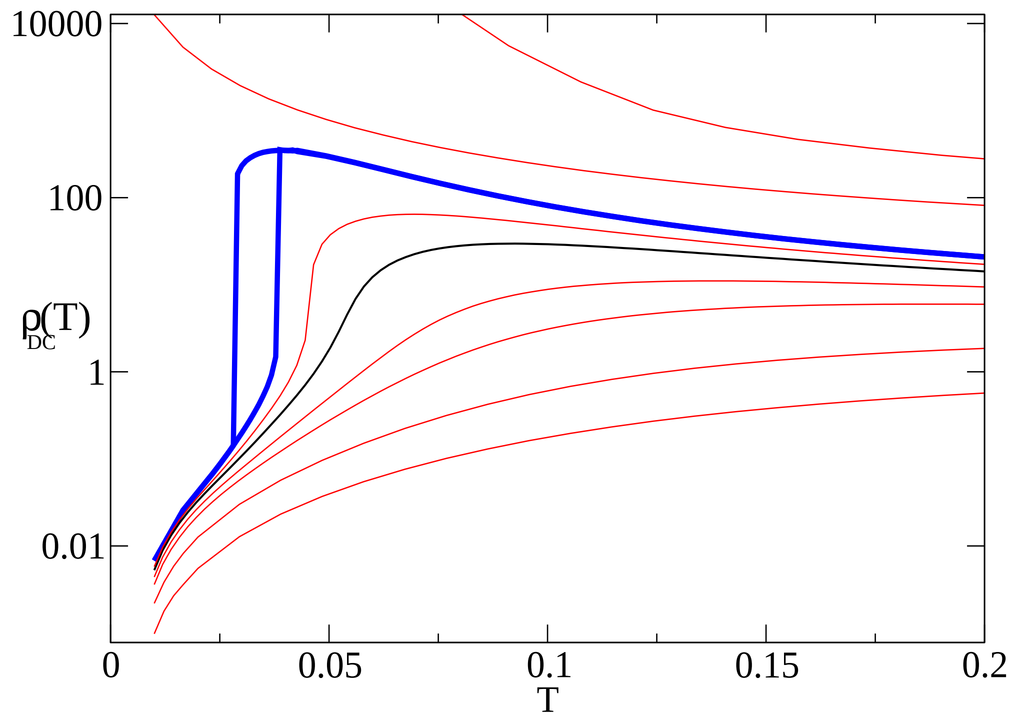


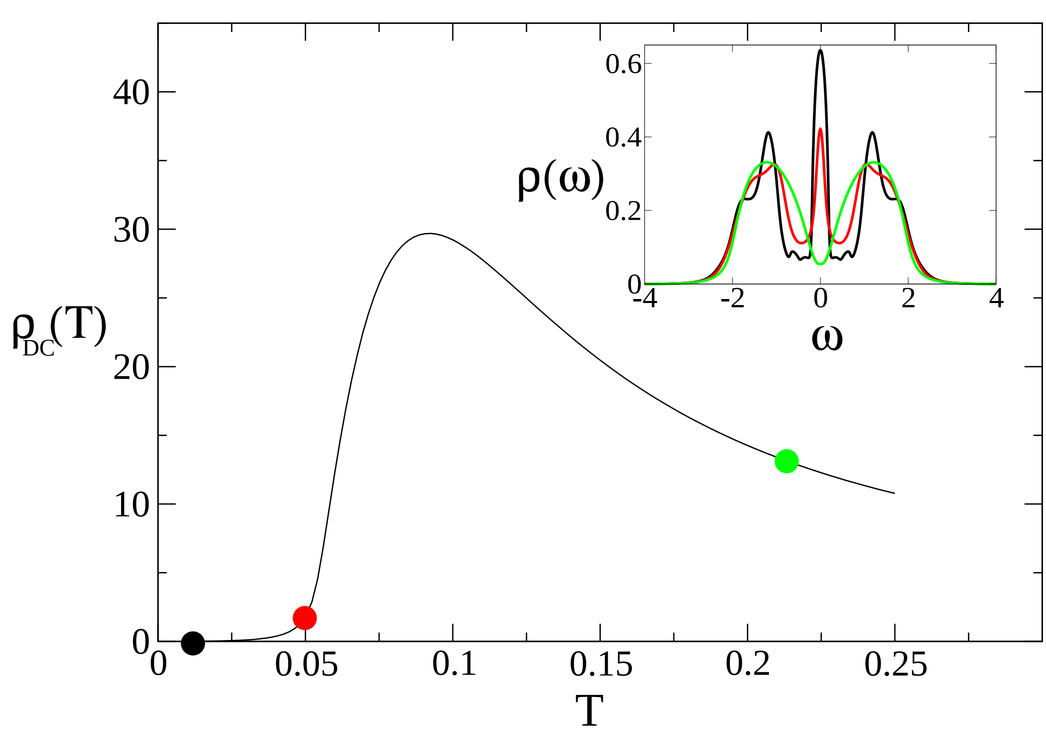
- Purely electronic 1^{st} order transition!
- Entropic effects
- T_c well reproduced

Transport at $T > 0$

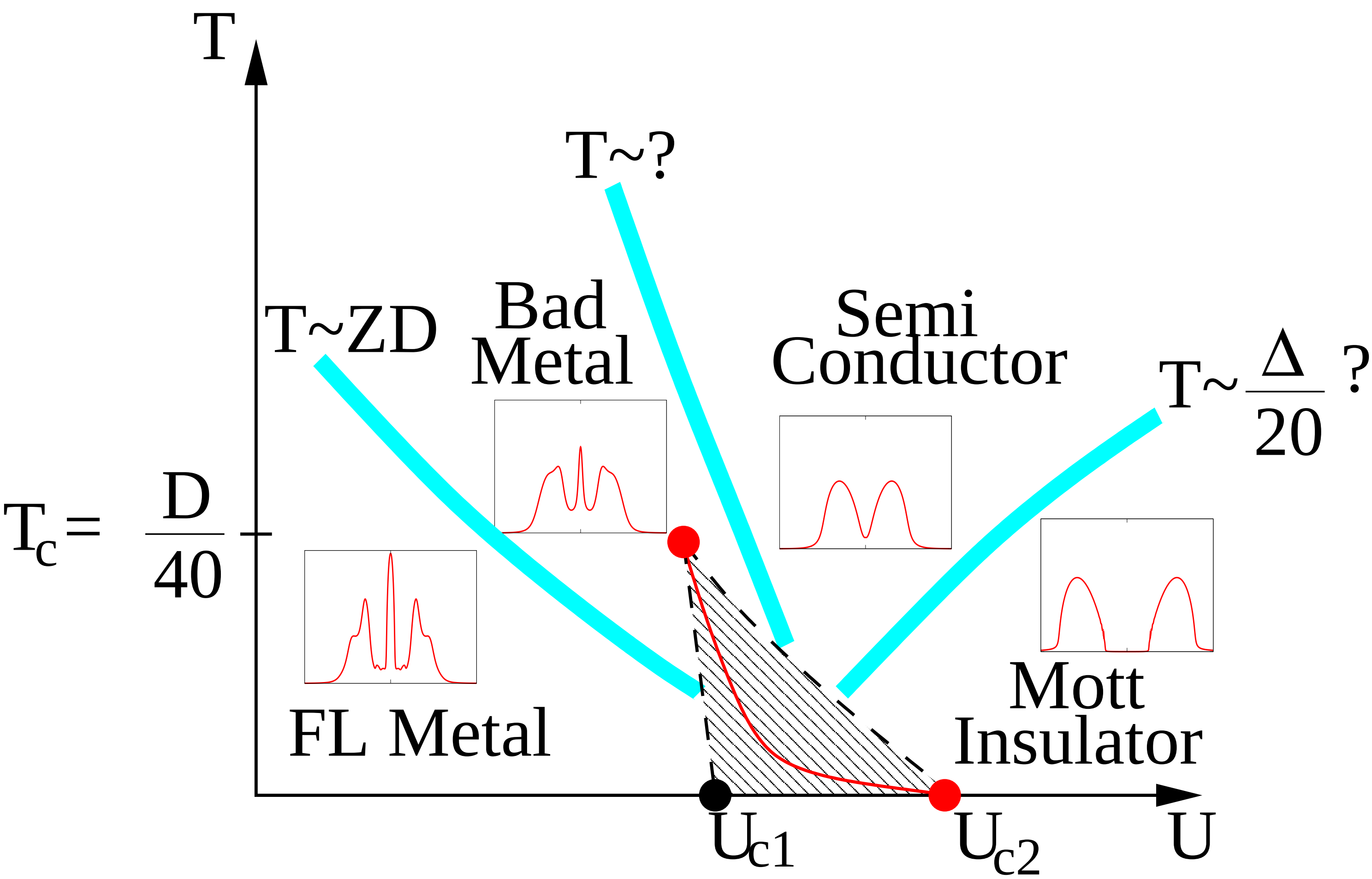
Conductivity: $\sigma_{DC} = 1/\rho_{DC}$

$$\sigma_{DC} = \frac{e^2 D}{\hbar a T} \int d\epsilon \int d\omega \left[\frac{\Sigma''(\omega)}{[\omega - \epsilon - \Sigma'(\omega)]^2 + [\Sigma''(\omega)]^2} \right]^2 \frac{e^{\beta\omega}}{(e^{\beta\omega}+1)^2}$$





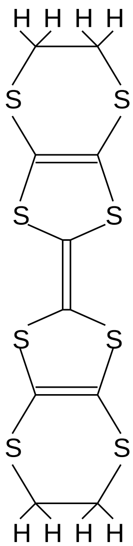
Phases and transport regimes

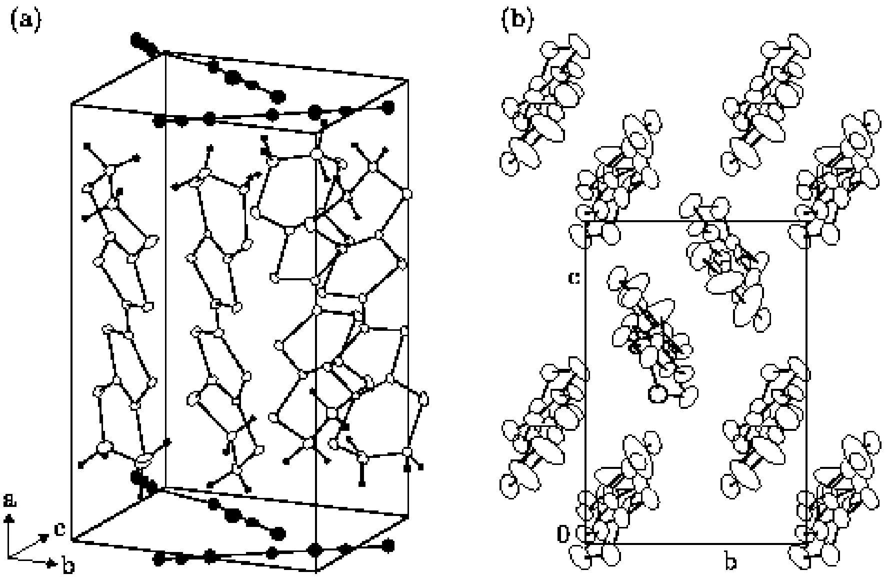


- Complex regimes changes predicted for transport!

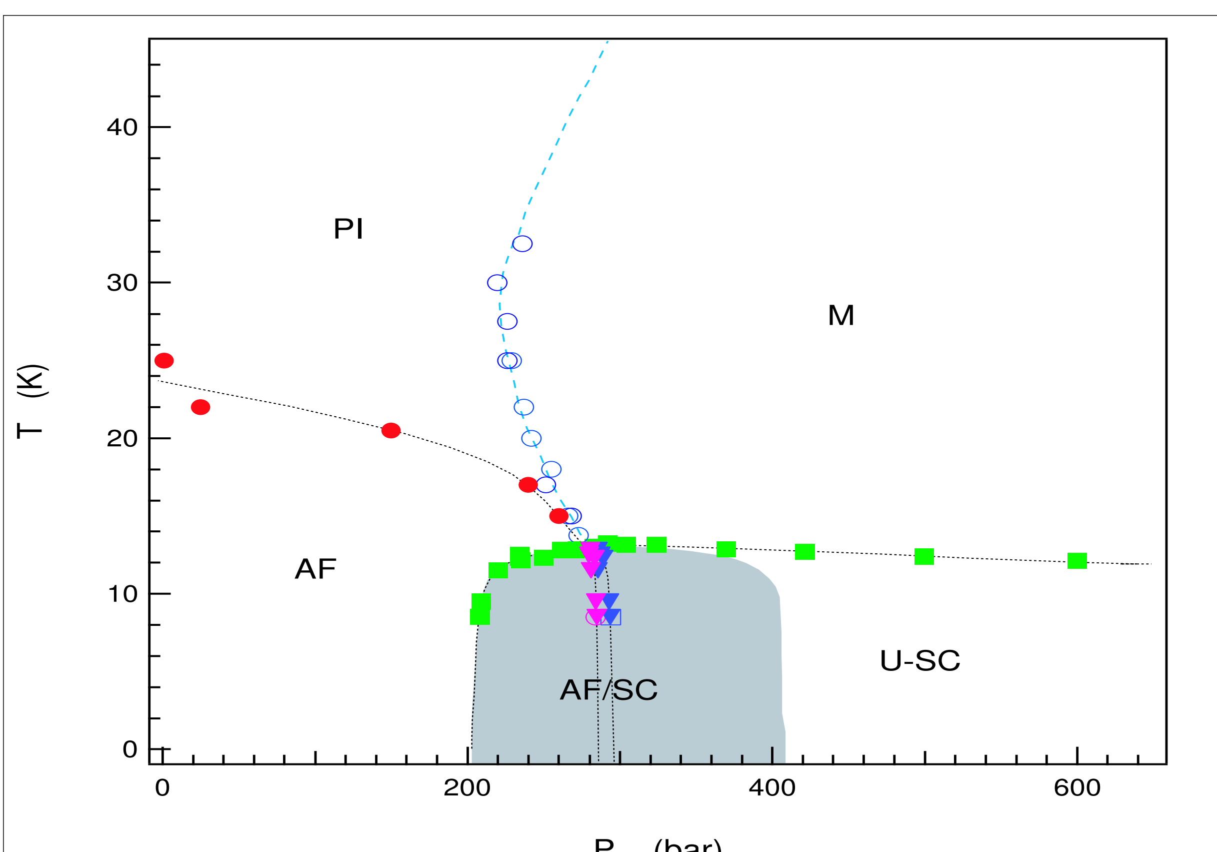
κ-BEDT: an organic metal

κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl:

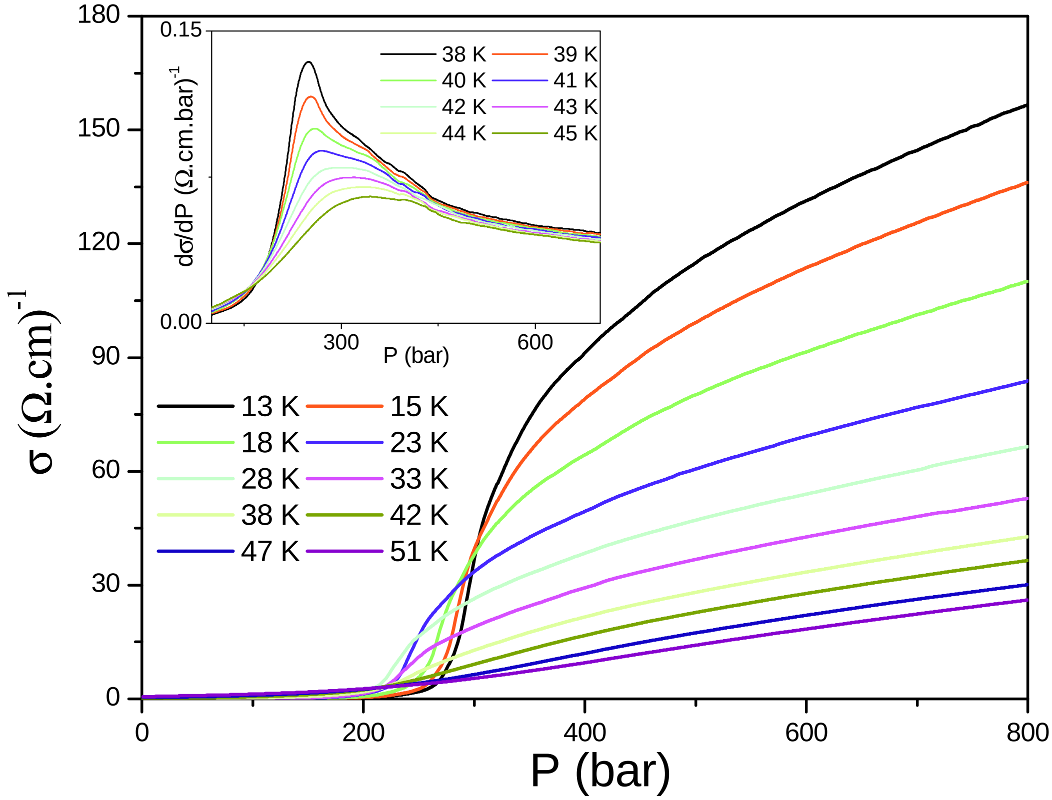




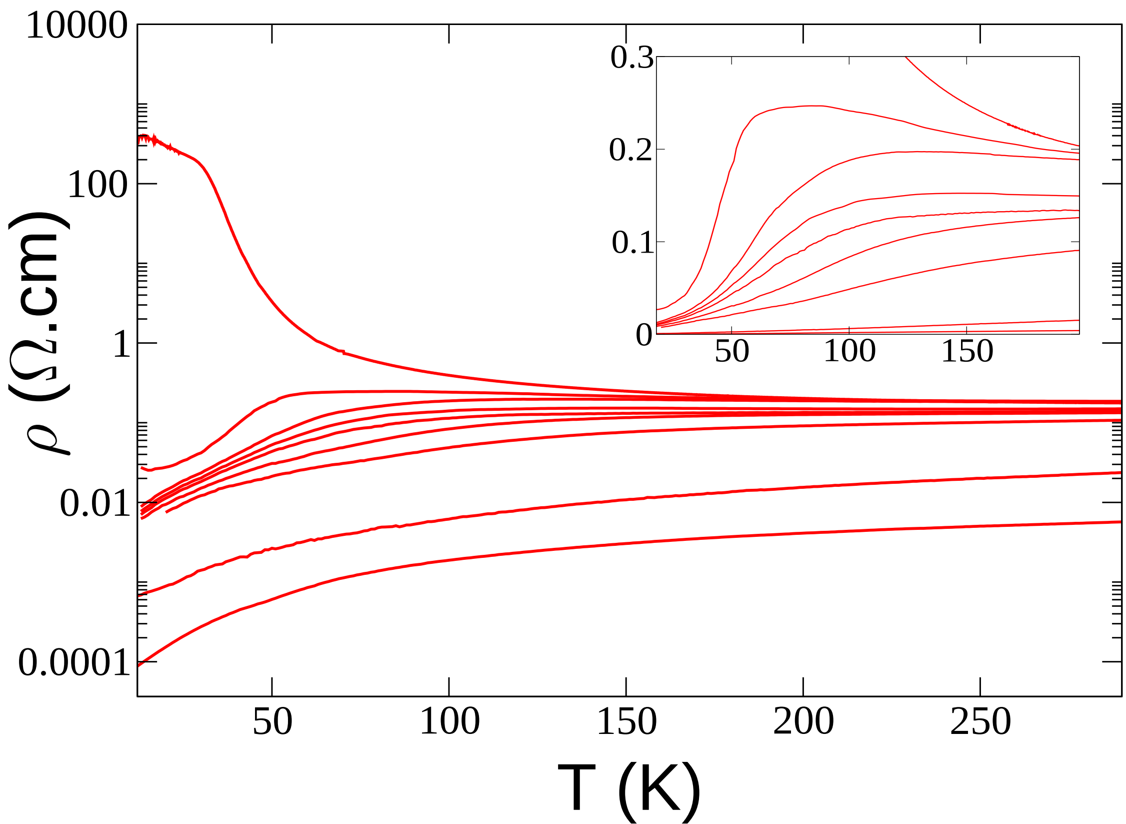
NMR phase diagram: [Lefebvre et al. PRL 2000]



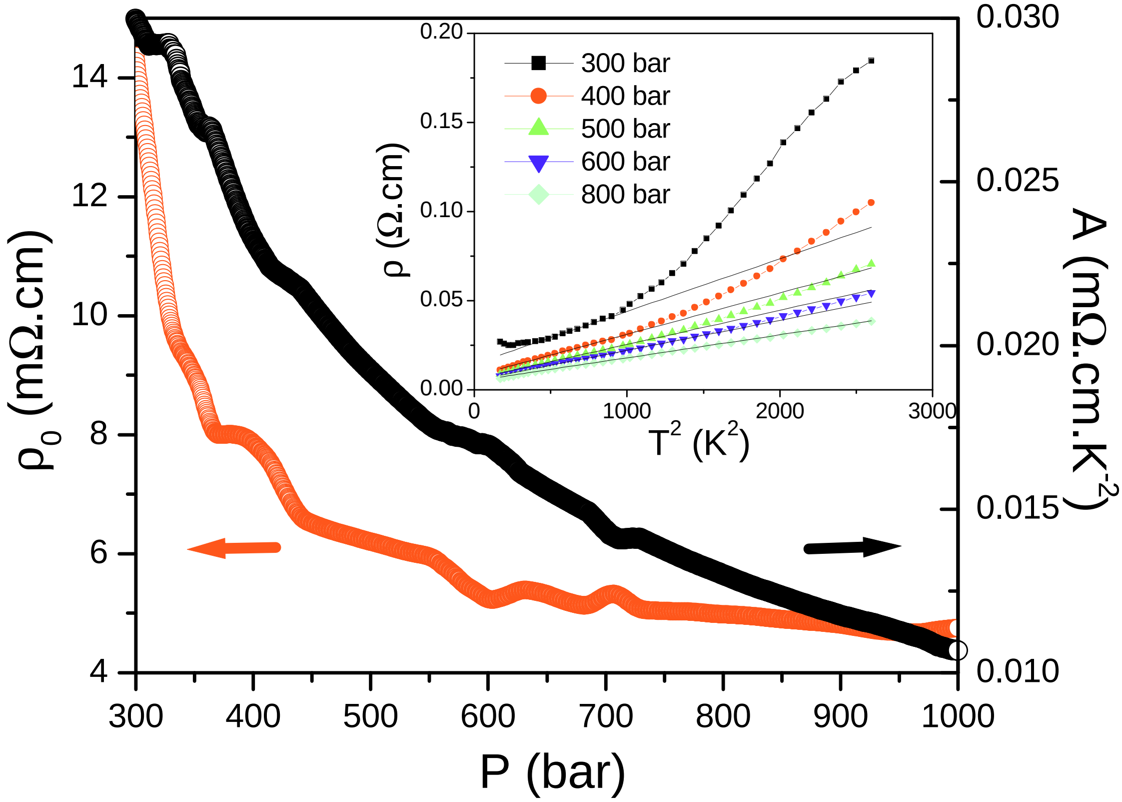
Raw data: [Limelette et al. PRL 2003]



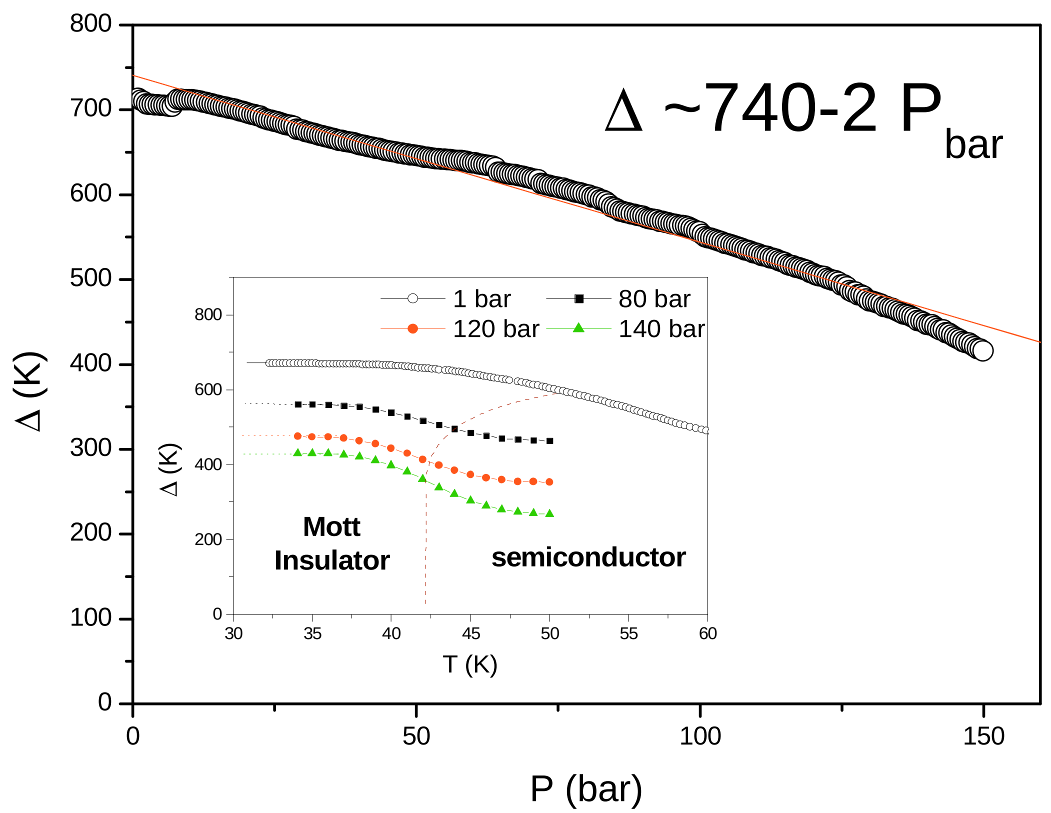
Versus temperature:



Fermi Liquid regime:

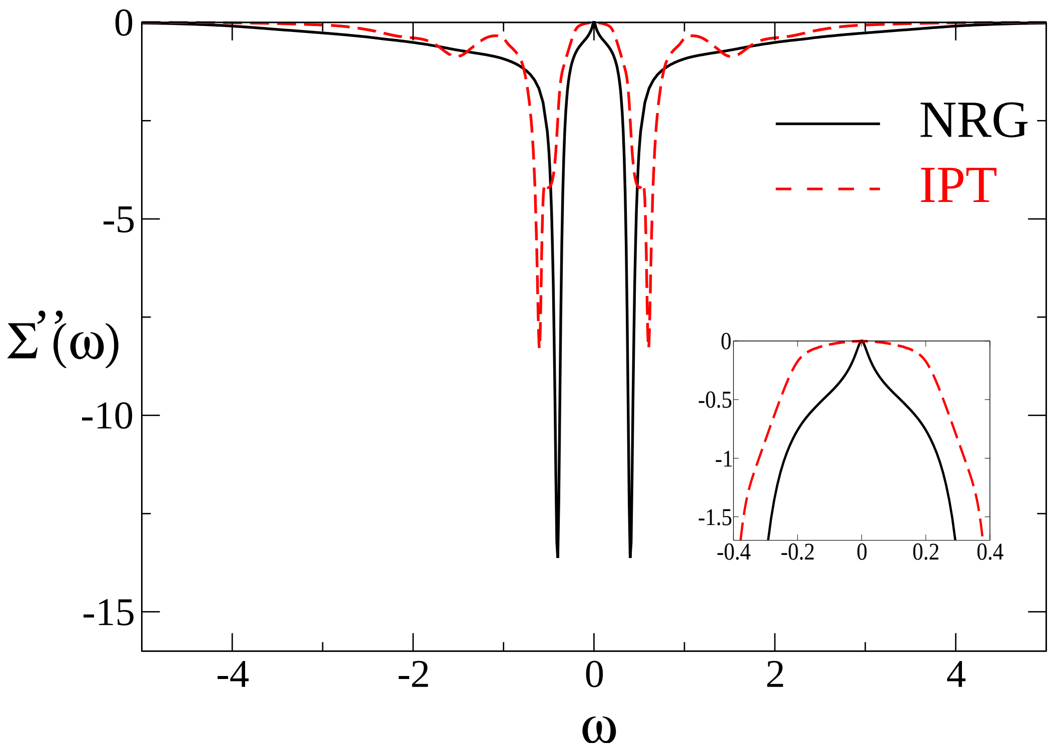


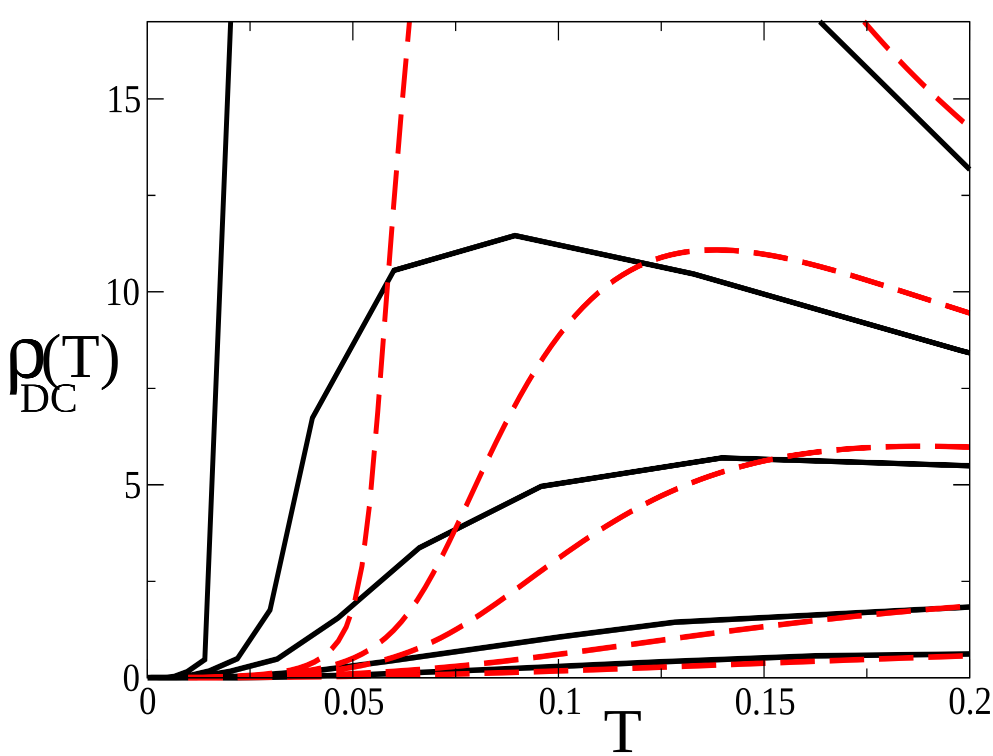
Insulating phase:



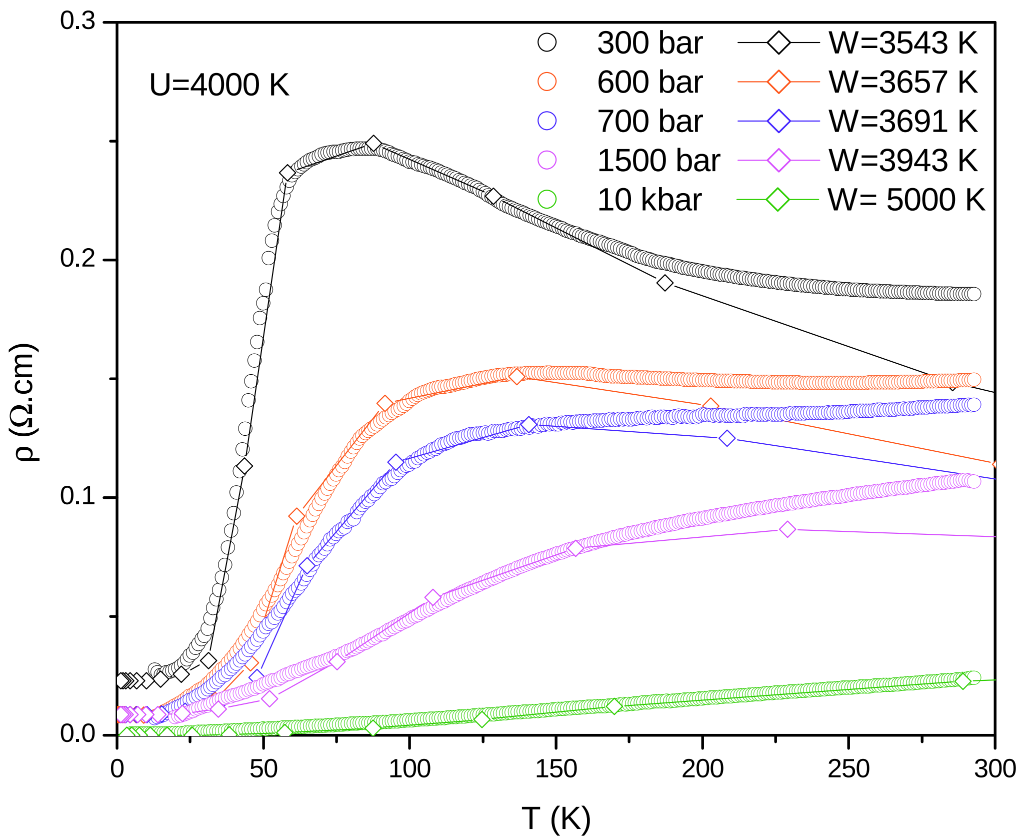
Problem with IPT:

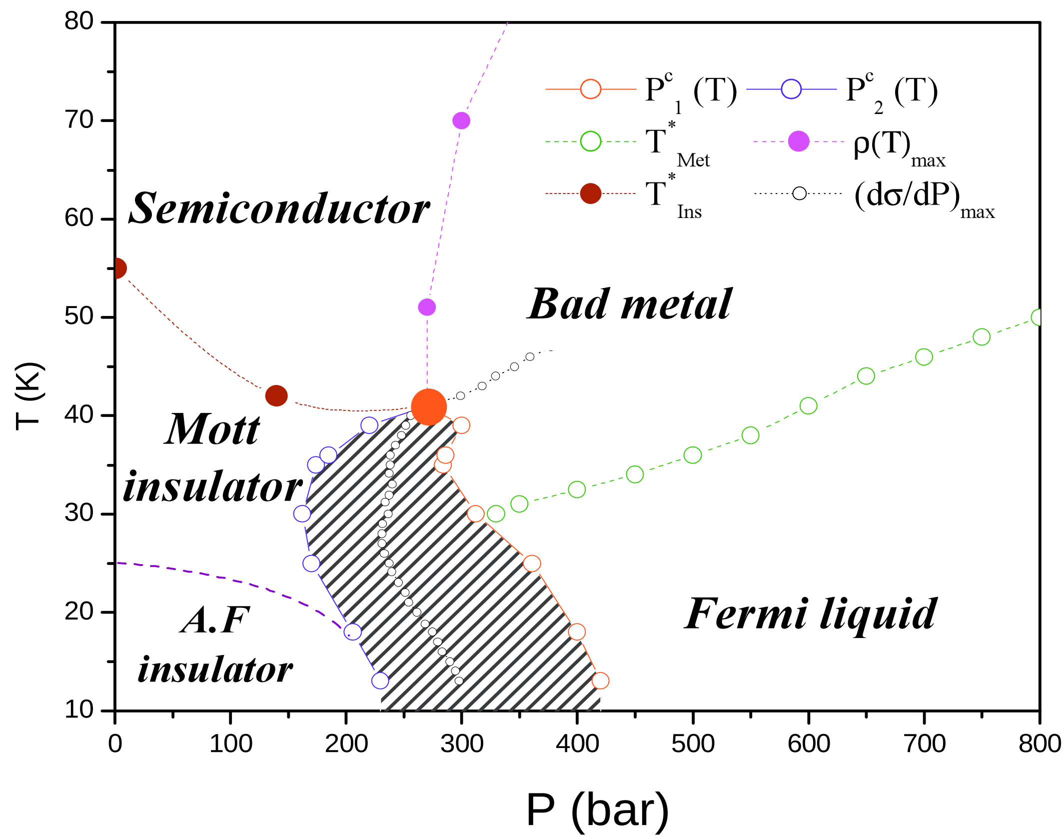
$$|\Sigma''_{\mathrm{IPT}}(\omega)| \propto \frac{U^2}{D^3}\omega^2 \neq |\Sigma''_{\mathrm{exact}}(\omega)| \propto \frac{\omega^2}{Z^2 D}$$





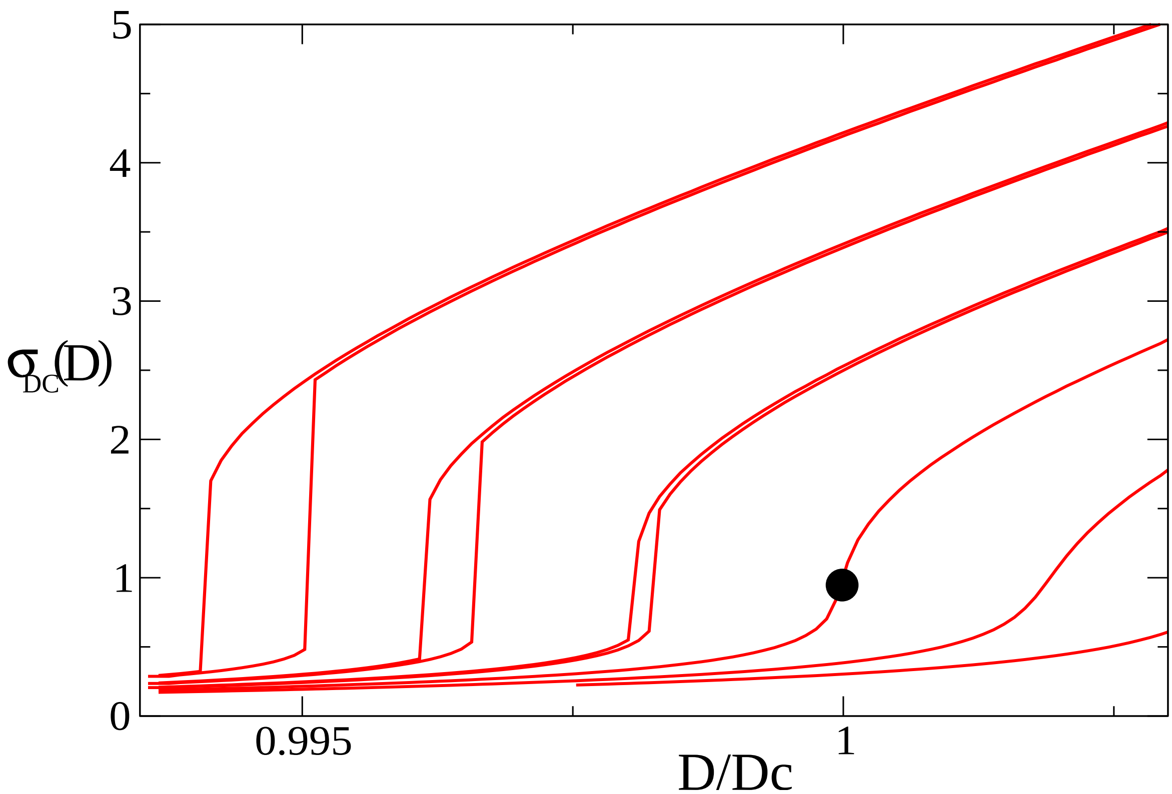
Comparison theory-experiment





Around the finite-T endpoint: theory

DMFT calculation: IPT again



Liquid-Gas analogy:

Hubbard	κ-BEDT	Liquid-Gas	Ising
$D - D_c$	$p - p_c$	$p - p_c$	Field h
$T - T_c$	$T - T_c$	$T - T_c$	Mass r
$\rho_d(\omega = 0)$	$\rho_d(\omega = 0)$	$v_G - v_L$	Order parameter ϕ

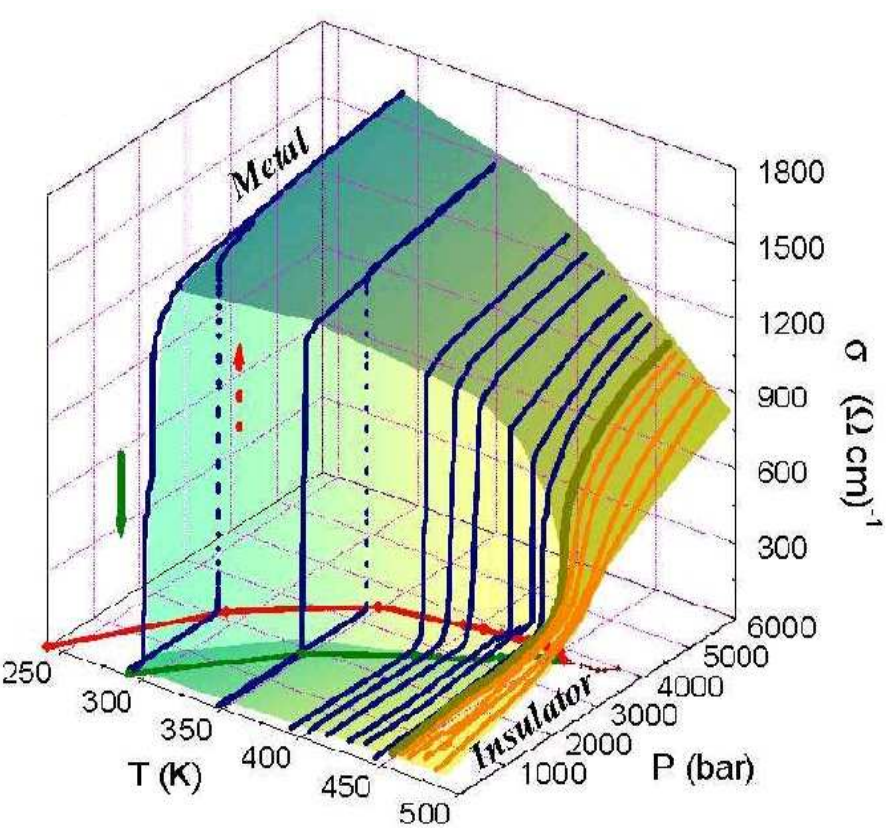
[Castellani et al. PRL 1979, Kotliar et al. PRL 2000]

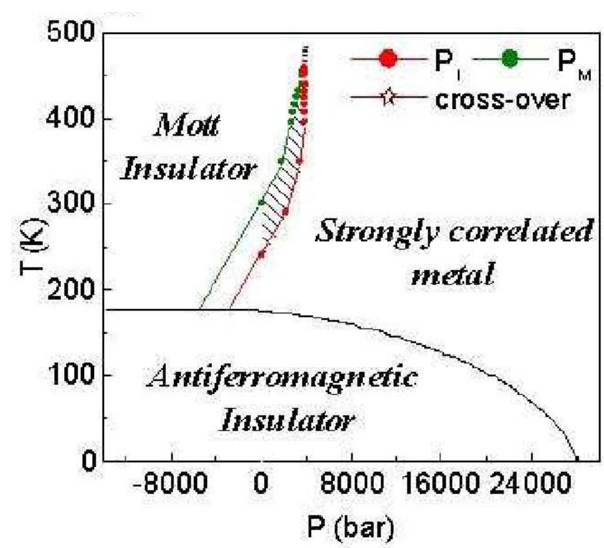
First experimental observation

κ-BEDT:

- $\sigma_{DC}(T)$ curves too soft!
- Bad sample quality?
- See however [Kagawa et al. PRB 2004]

V_2O_3: [Limelette et al. Science 2004]



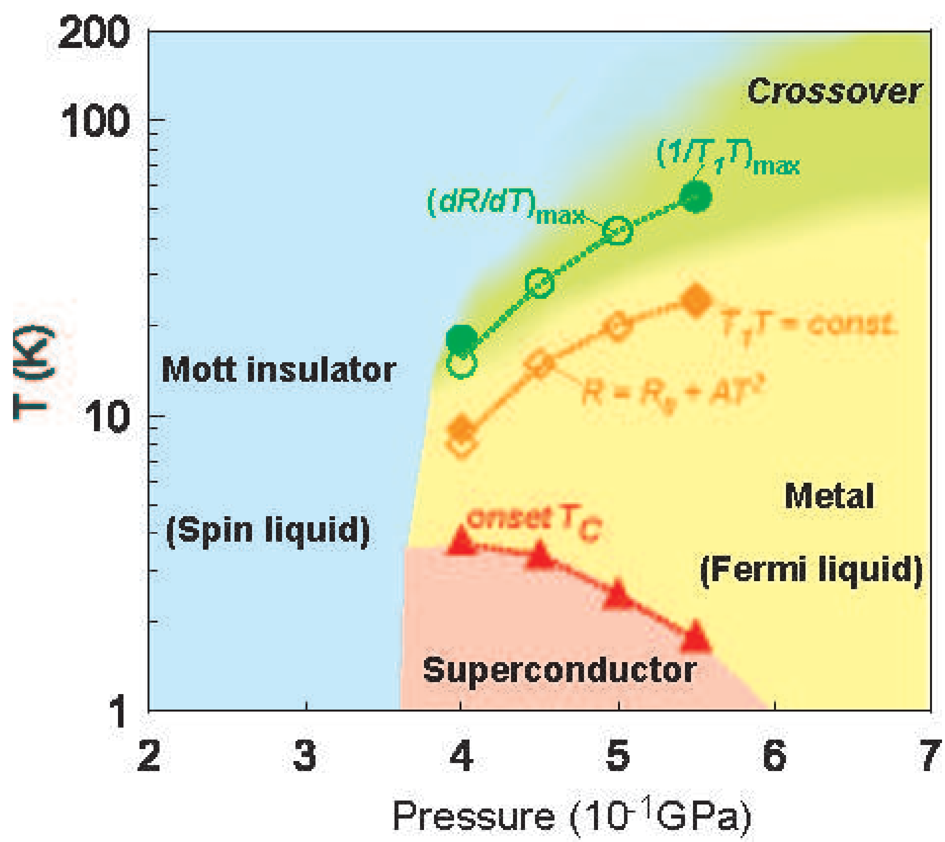


- Liquid-gas transition
- Ising critical exponents

A real T=0 paramagnetic transition!

κ-$BEDTCu_2(CN)_3$: [Kurosaki et al. PRL 2005]

- Higher frustration $t'/t \sim 1$
- Absence of the magnetic insulator



Some theoretical attempts: Open problem!

- Numerics [Imada 2003]
- Spinon MFT [Florens&Georges, Lee&Lee]

Conclusion and prospects

- Rich crossovers for transport in κ-BEDT compound
- Interpretation within the DMFT
- Pressure gas technique important
- NRG calculations crucial for qualitative comparison
- Critical liquid-gas behavior at finite T
- Fundamental question of $T = 0$ Mott transition still open
- Realistic transport calculation difficult
- New experiment: optical conductivity?