Dynamical Mean Field Theory: Introduction

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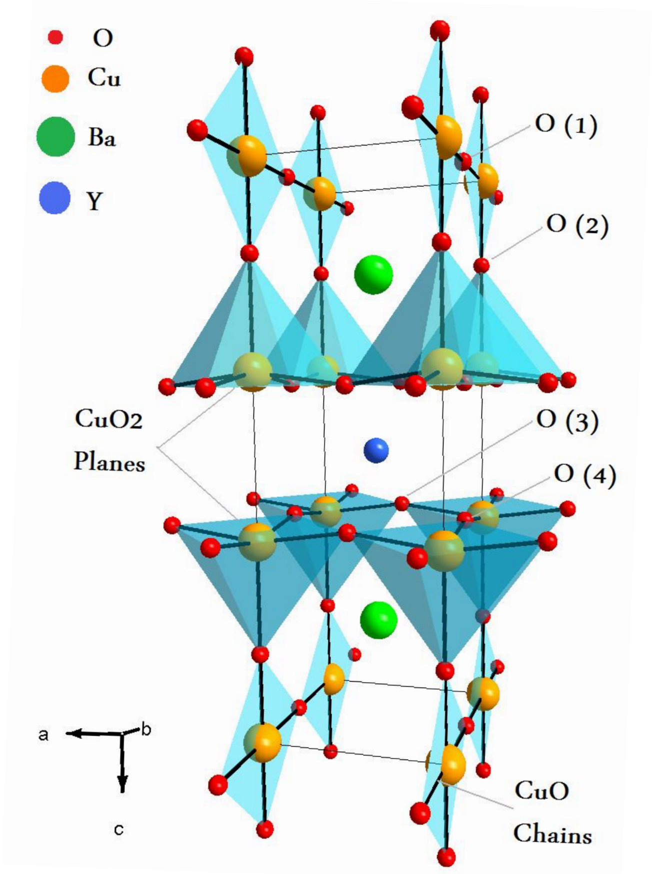
Weak vs Strong Correlations

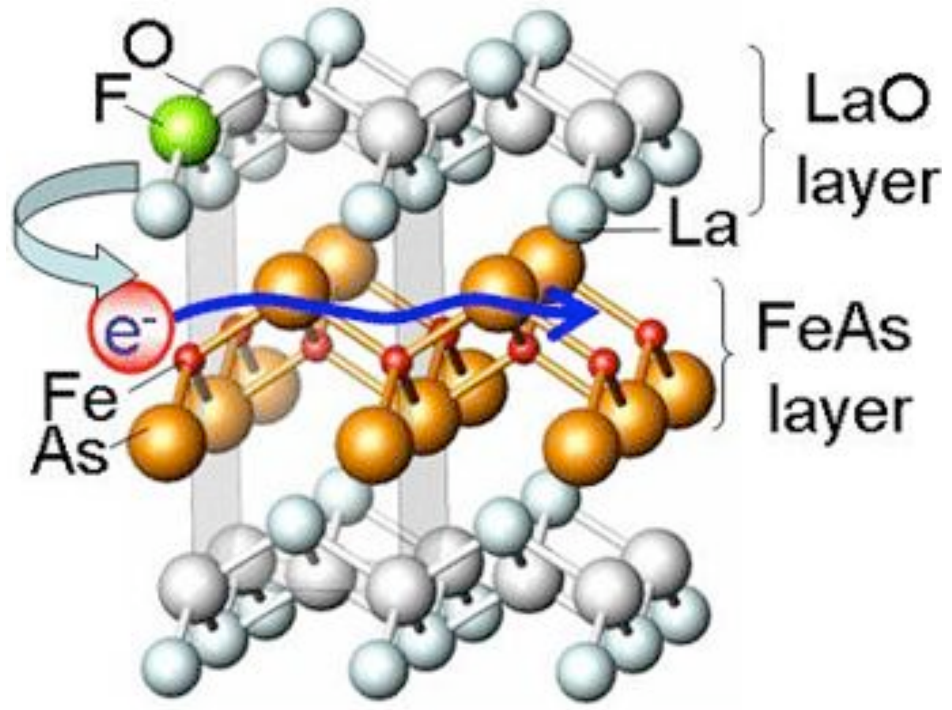
- Weakly correlated systems :
  - The "standard model" : renormalized independent fermions
    - Fermi Liquid Theory *L .Landau 50's*
    - Density Functional Theory (and Local Density Approximation) *Kohn, Sham, Hohenberg*
- Strongly correlated systems :
  - When the "standard model" breaks down.
  - Interaction produces qualitatively new physical effects
  - Many instabilities at low T.

Strongly correlated systems

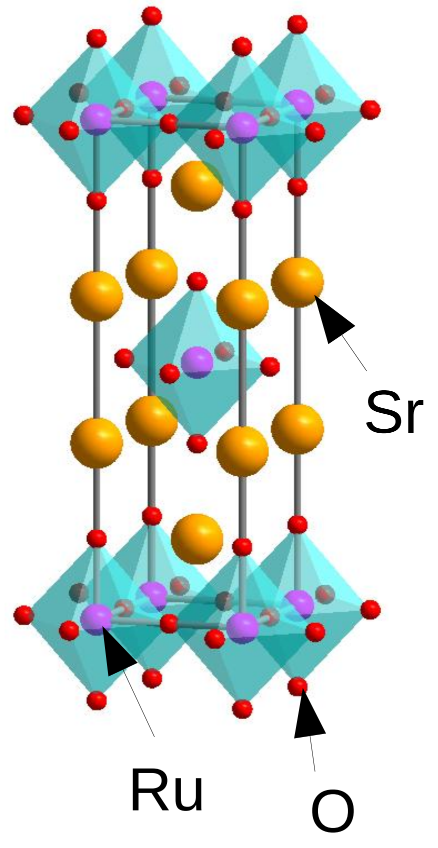
Materials
High Temperature superconductors
Transition metal oxides,



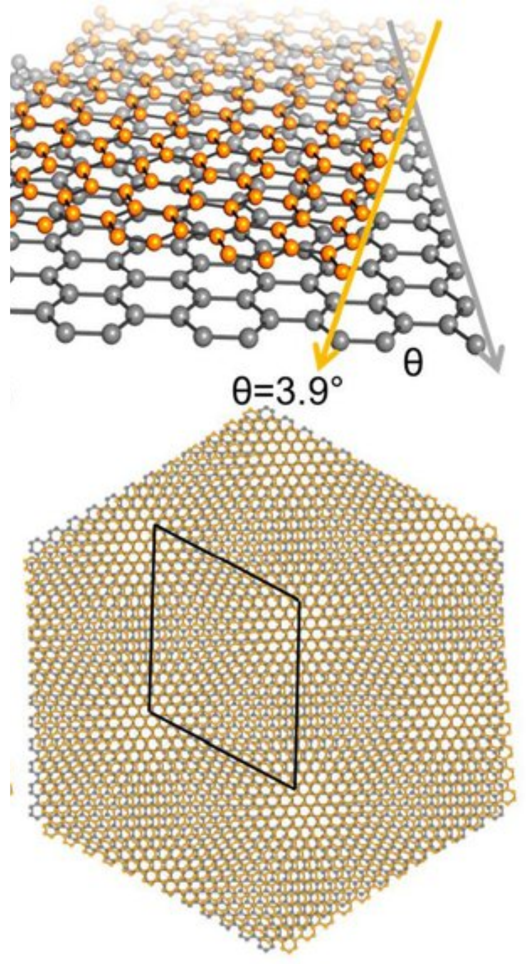
High Temperature superconductors



Fe-Based (2008)

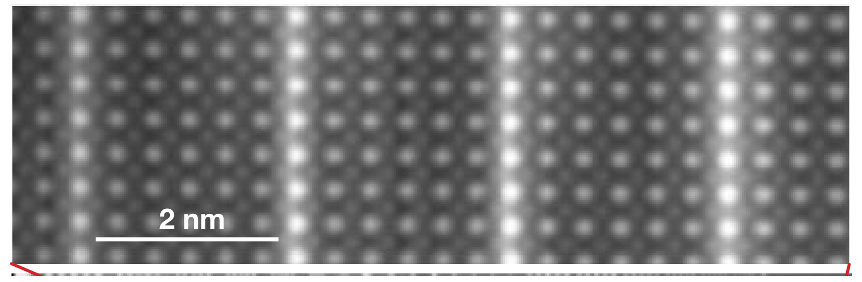


Ruthenates



Twisted bilayer graphene

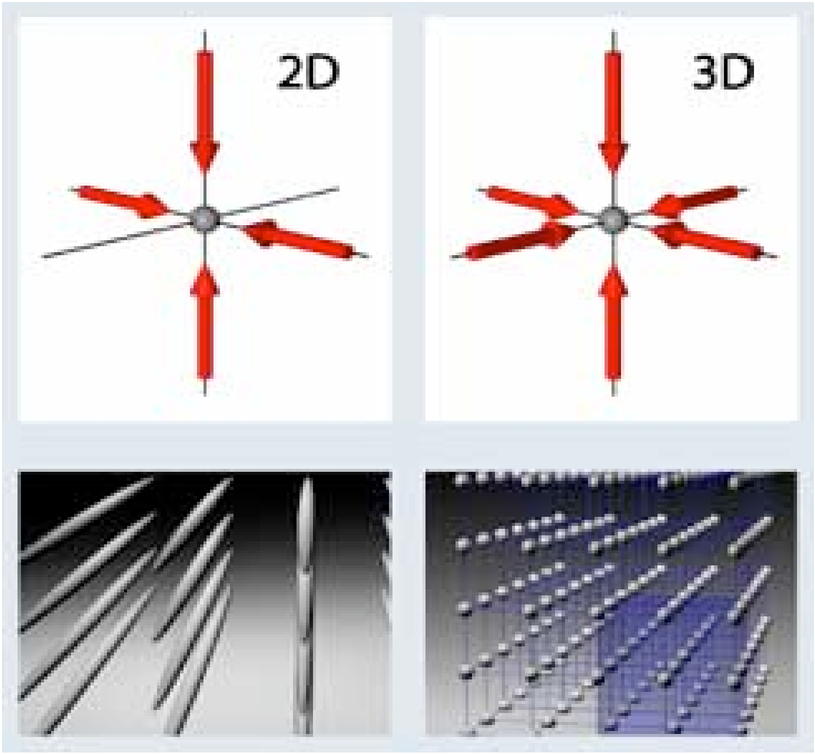
Correlated metal/superconductors at interface of oxides



$SrTiO_3/LaTiO_3$

Ohtomo et al, Nature 2002

Ultra-cold atoms in optical lattices

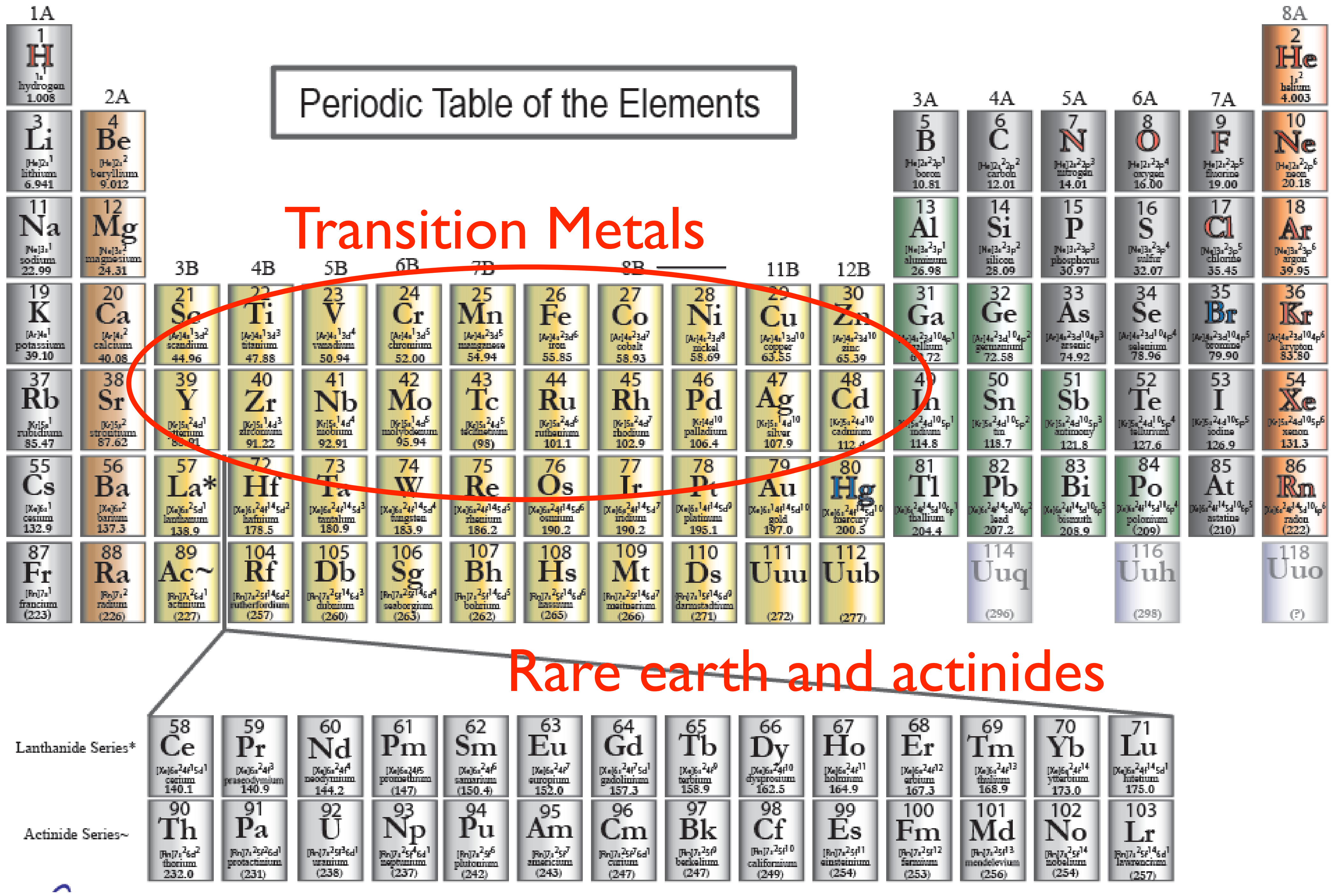


"Artificial solids" of atoms & light

Materials

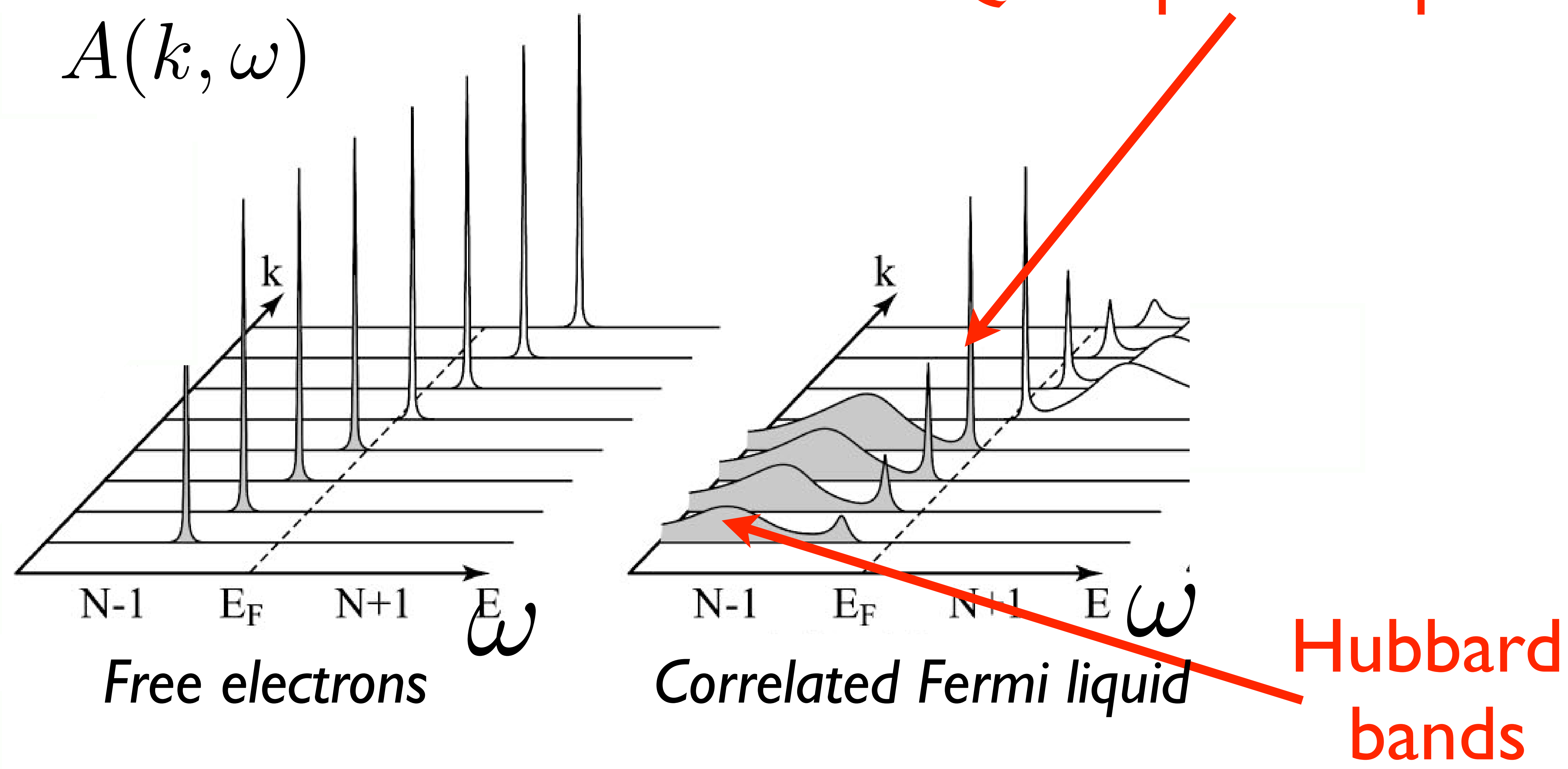
- Usually: Valence (bands) vs core electrons (localized around the atom)
- Some orbitals are only partially localized ($3d$,$4f$ e.g.)
  d, f orbitals are quite close to nuclei
- Electrons “hesitate” between being localized (short time) and delocalized (long time)

Transition-metals and their oxides, rare-earth/actinides, but also some organic materials

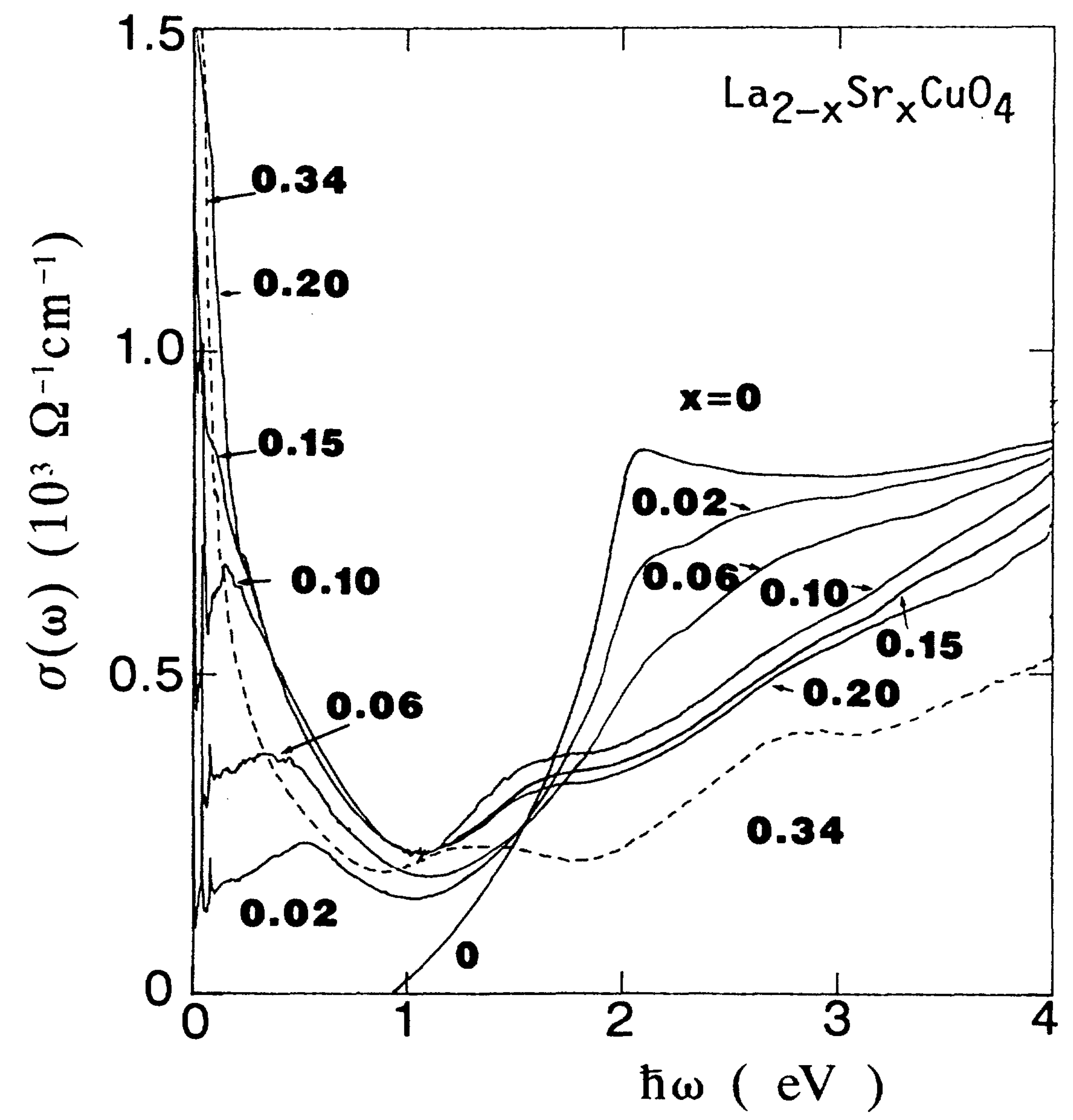


Spectral weight transfer

Spectral function



Optical conductivity



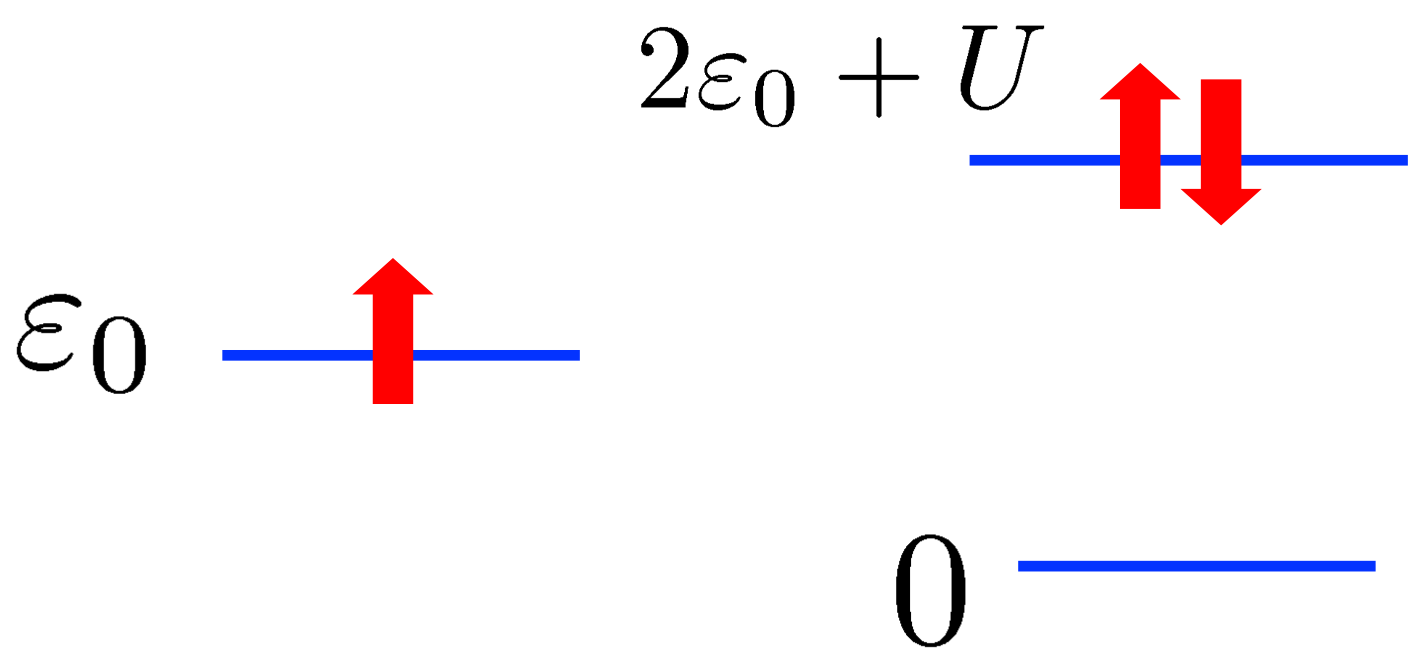
S. Uchida et al, Phys. Rev. B (1991)

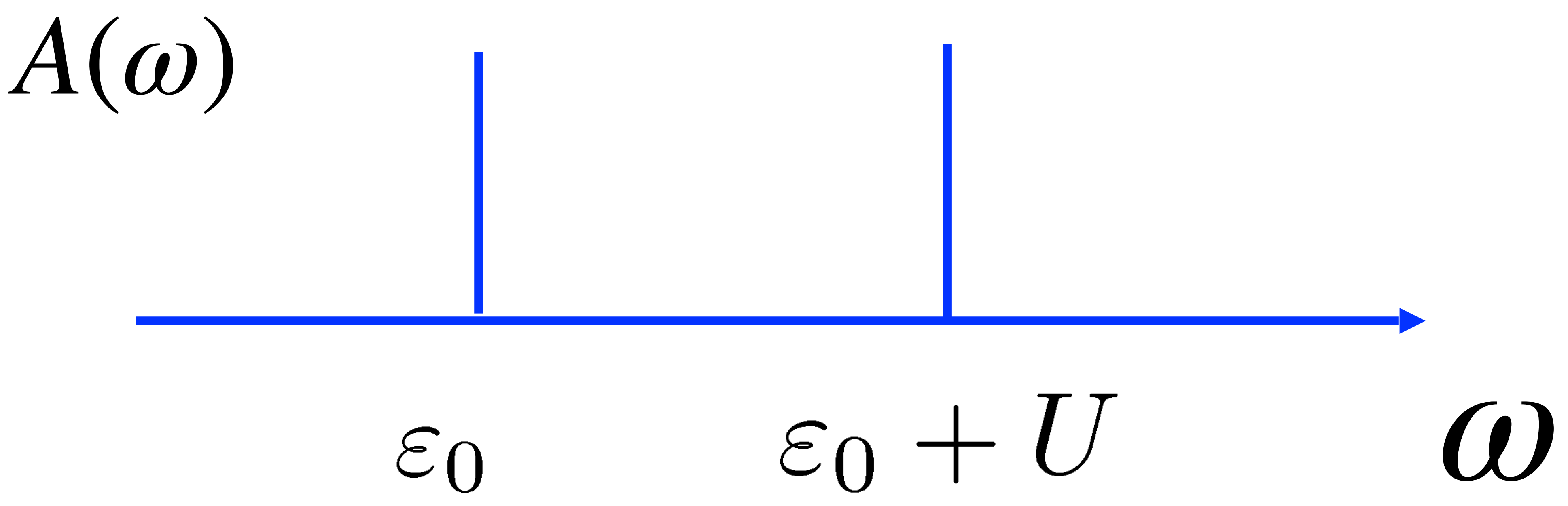
- Spectral weight transfer from low to high energy

Atomic-like localized excitations. Hubbard band
vs
long range, delocalized, quasi-particle peak

Hubbard band = remanent of an atomic transition

- 1 Hubbard atom $H = \epsilon_0(n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow$





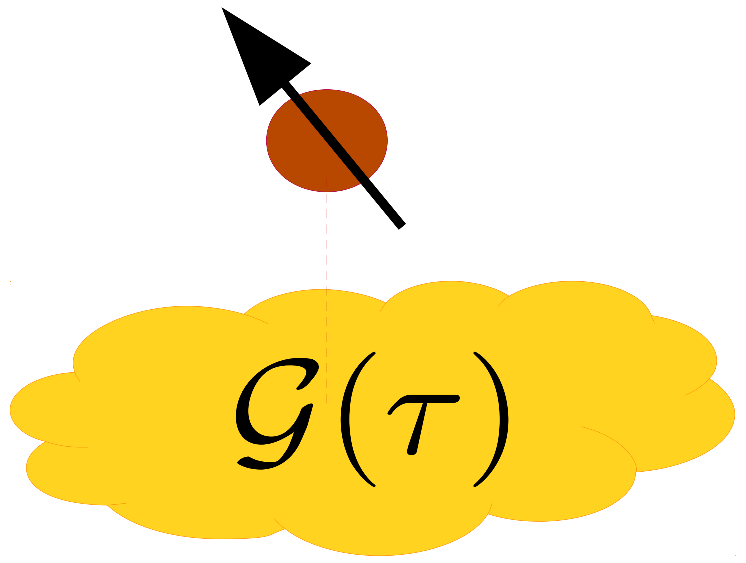
- A ``Hubbard satellite" is an atomic transition broadened by the solid-state environment.
- Understanding the energetics of the Mott gap requires a an accurate description of the many-body eigenstates of single atoms : multiplets, i.e. $U, J_H \ldots$ (cf A. Georges's lecture on Hund's metals).

Dynamical Mean Field Theory
The main idea

- DFT (Density Functional Theory) *[Cf lecture by O. Gingras tomorrow]*
  - Independent electrons in an *effective periodic (Kohn-Sham) potential.*
  - Central object is the electronic density ρ

- DMFT (Dynamical Mean Field Theory)
  - An atom in an effective bath of independent electrons (quantum impurity)
  - Central object is the Green function $G(\omega)$

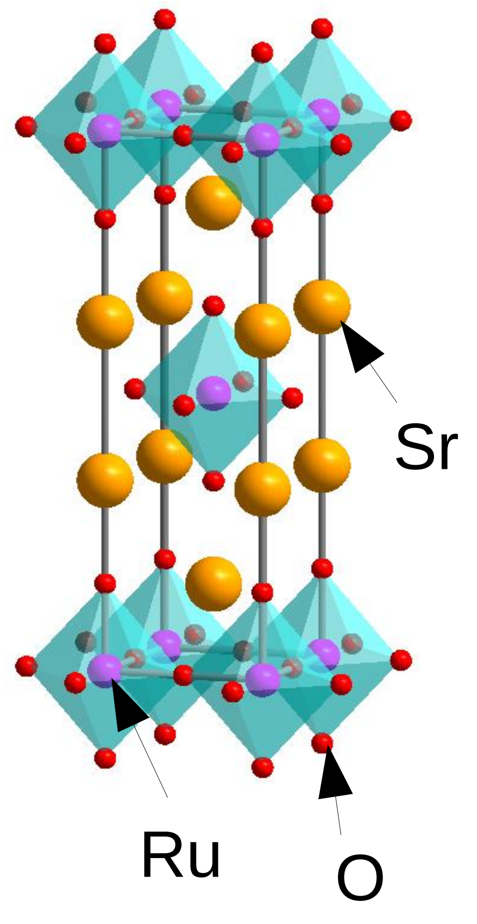
W. Metzner, D.Vollhardt, 1989
A. Georges, G. Kotliar, 1992



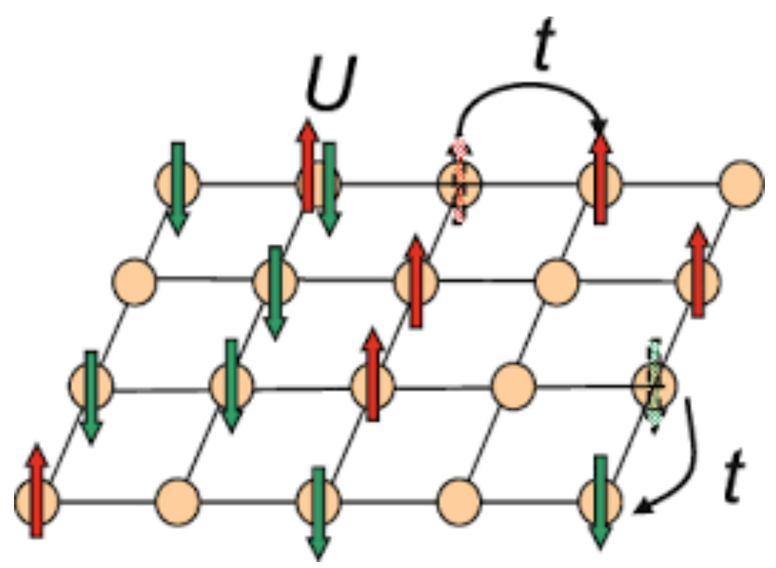
Quantum Embeddings

- A family of methods. DMFT is only the tip of the iceberg.

Correlated material

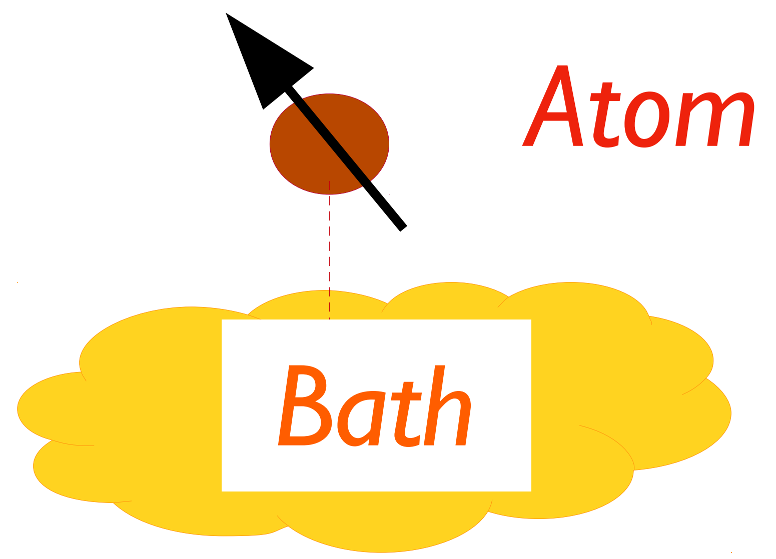


"Toy" model



Select local degree of freedom
atoms, correlated orbitals

Auxiliary model
"Quantum impurity model"



Embedding

Compute physical quantities on the lattice
from the auxiliary model

Good idea when atomic physics plays a major role.

Quantum impurity models

Reminder. Cf lecture 2

Anderson model

$$H = \sum_{k,\sigma=\uparrow,\downarrow} \varepsilon_{k\sigma} \xi^\dagger_{k\sigma} \xi_{k\sigma} + \sum_{\sigma=\uparrow,\downarrow} \varepsilon_d d^\dagger_\sigma d_\sigma + U n_{d\uparrow} n_{d\downarrow} + \sum_{k,\sigma=\uparrow,\downarrow} V_{k\sigma} (\xi^\dagger_{k\sigma} d_\sigma + h.c.)$$

$$\updownarrow$$

$$S = -\int_0^\beta \int_0^\beta d\tau\, d\tau'\, c^\dagger_\sigma(\tau)\, \mathcal{G}^{-1}_{0\sigma}(\tau - \tau')\, c_\sigma(\tau') + \int_0^\beta d\tau\, U\, n_\uparrow(\tau)\, n_\downarrow(\tau)$$

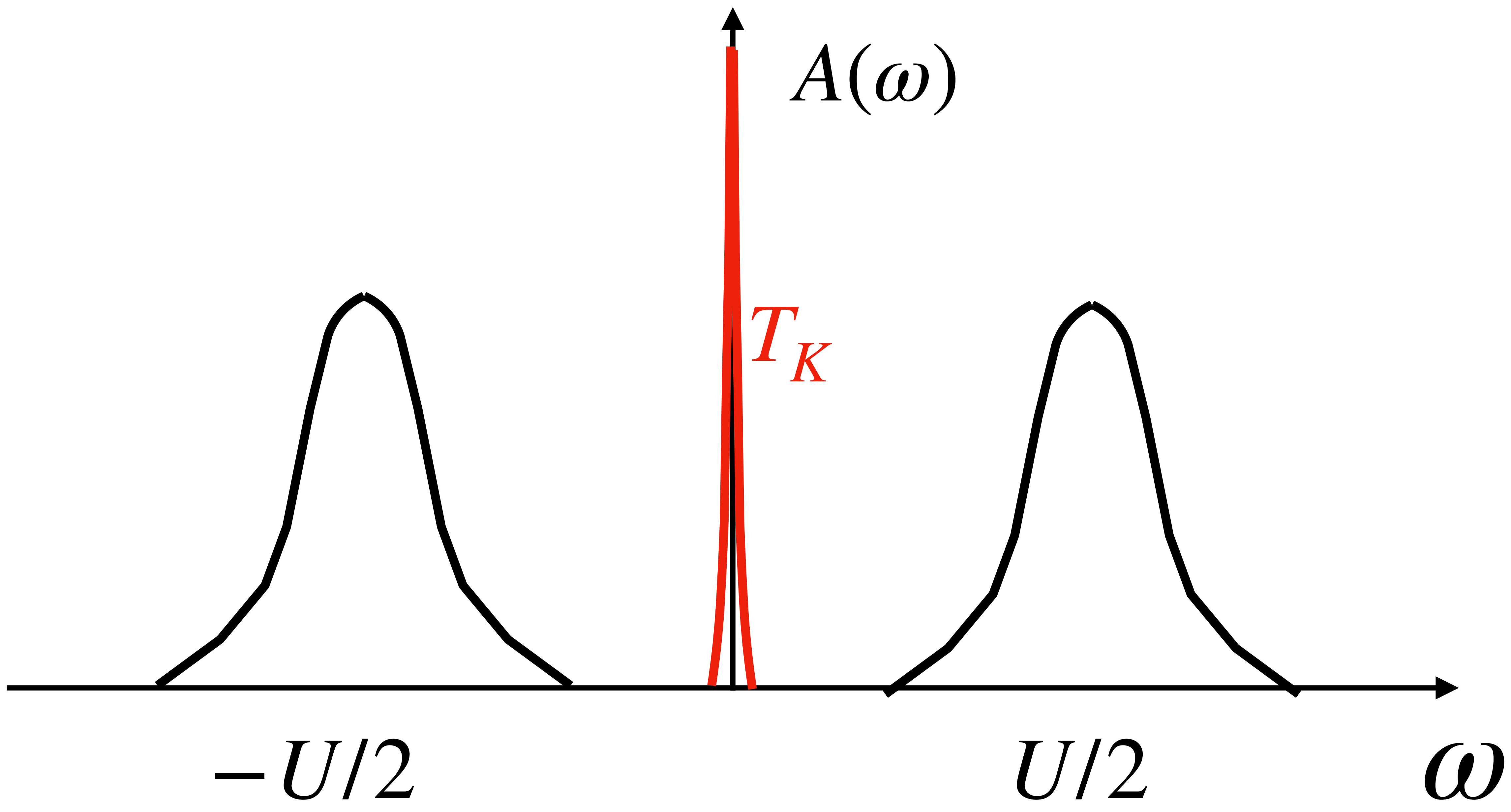
$$\mathcal{G}^{-1}_{0\sigma}(i\omega_n) \equiv i\omega_n - \epsilon_d - \underbrace{\sum_k \frac{|V_{k\sigma}|^2}{i\omega_n - \epsilon_{k\sigma}}}_{\Delta_\sigma(i\omega_n)}$$

Bath

Hybridization function

Spectral function of the d

- Atom + bath, low temperature
  $T \ll T_K$



- Sharp resonance (Kondo-Abrikosov-Suhl) in the spectral function of d of width T_K, at/close to the Fermi level. ***Many-Body effect***

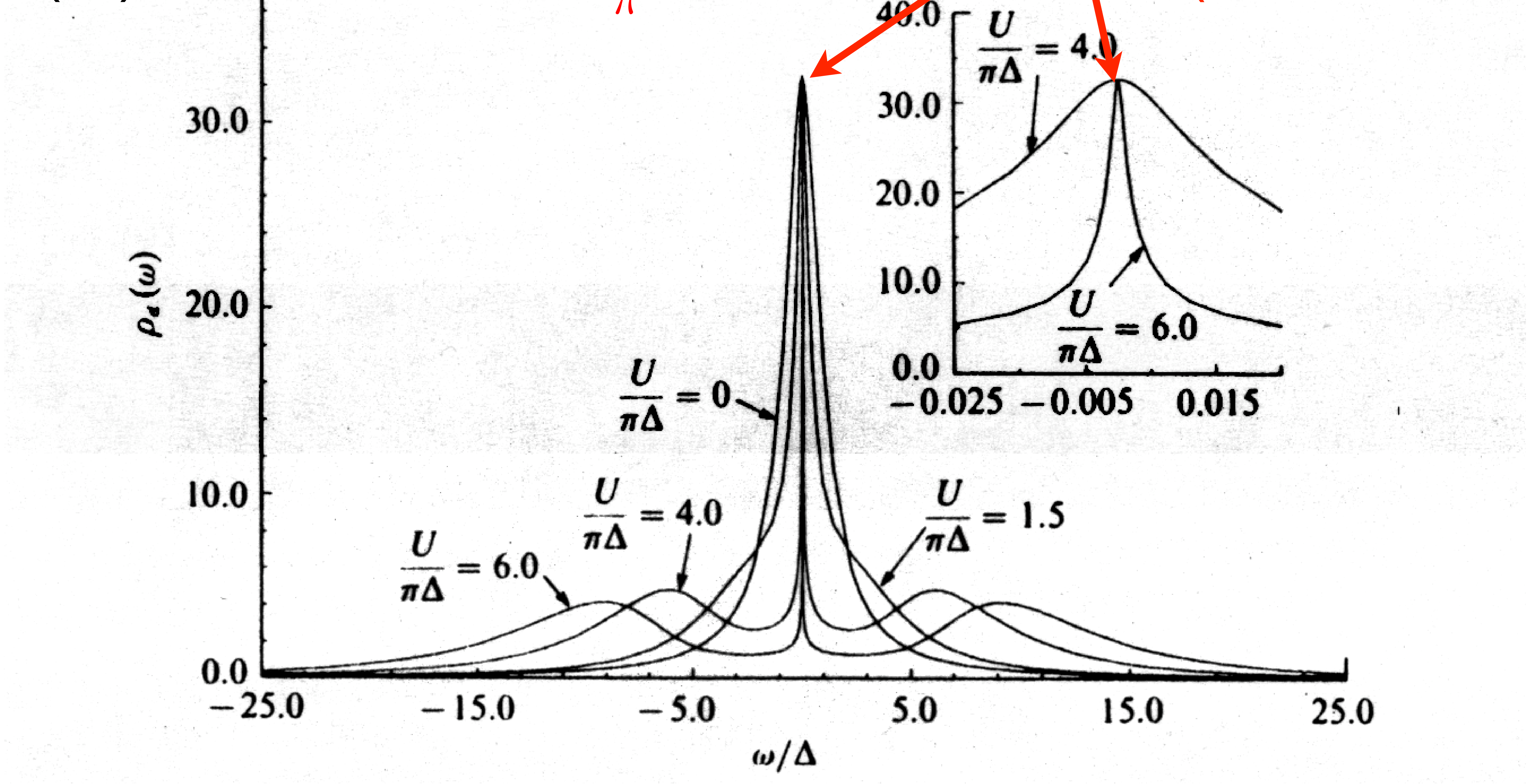
Kondo-Abrikosov-Suhl resonance

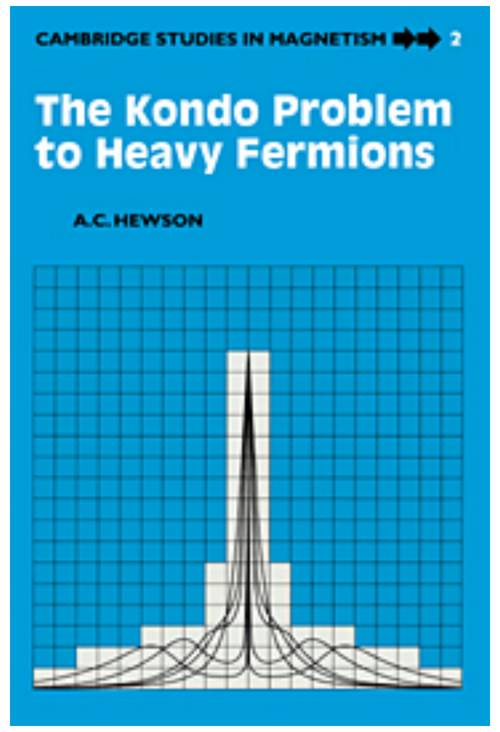
- Evolution from U=0, at T =0
  (using simply perturbation theory in U).
- Spectral weight transfer

$A_d(\omega)$

$$A_d(\omega) = -\frac{1}{\pi} Im G_d^R(\omega)$$

ρ(ω=0) independent of U
(Friedel sum rule)



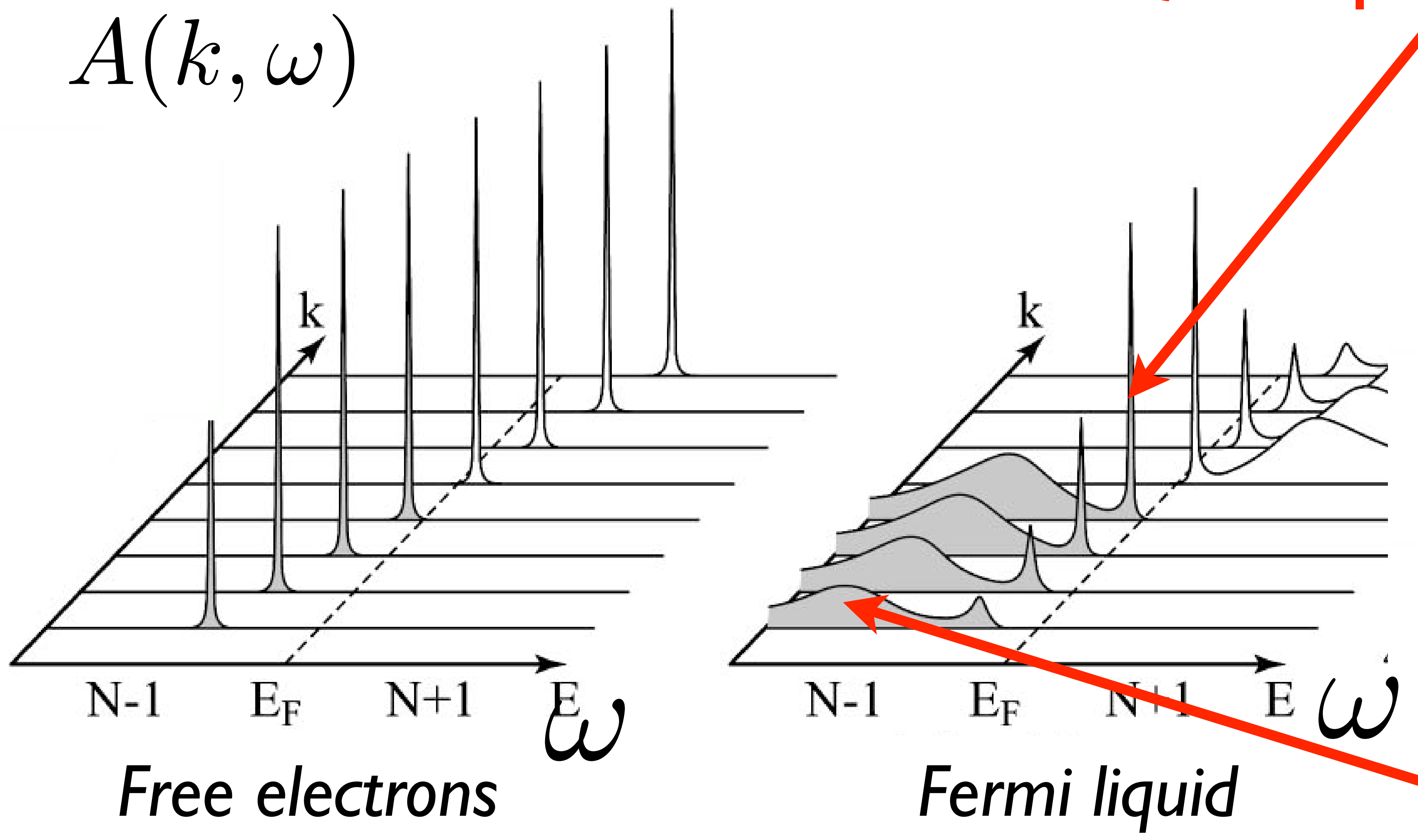


particle-hole symmetric case *(Hewson's book)*

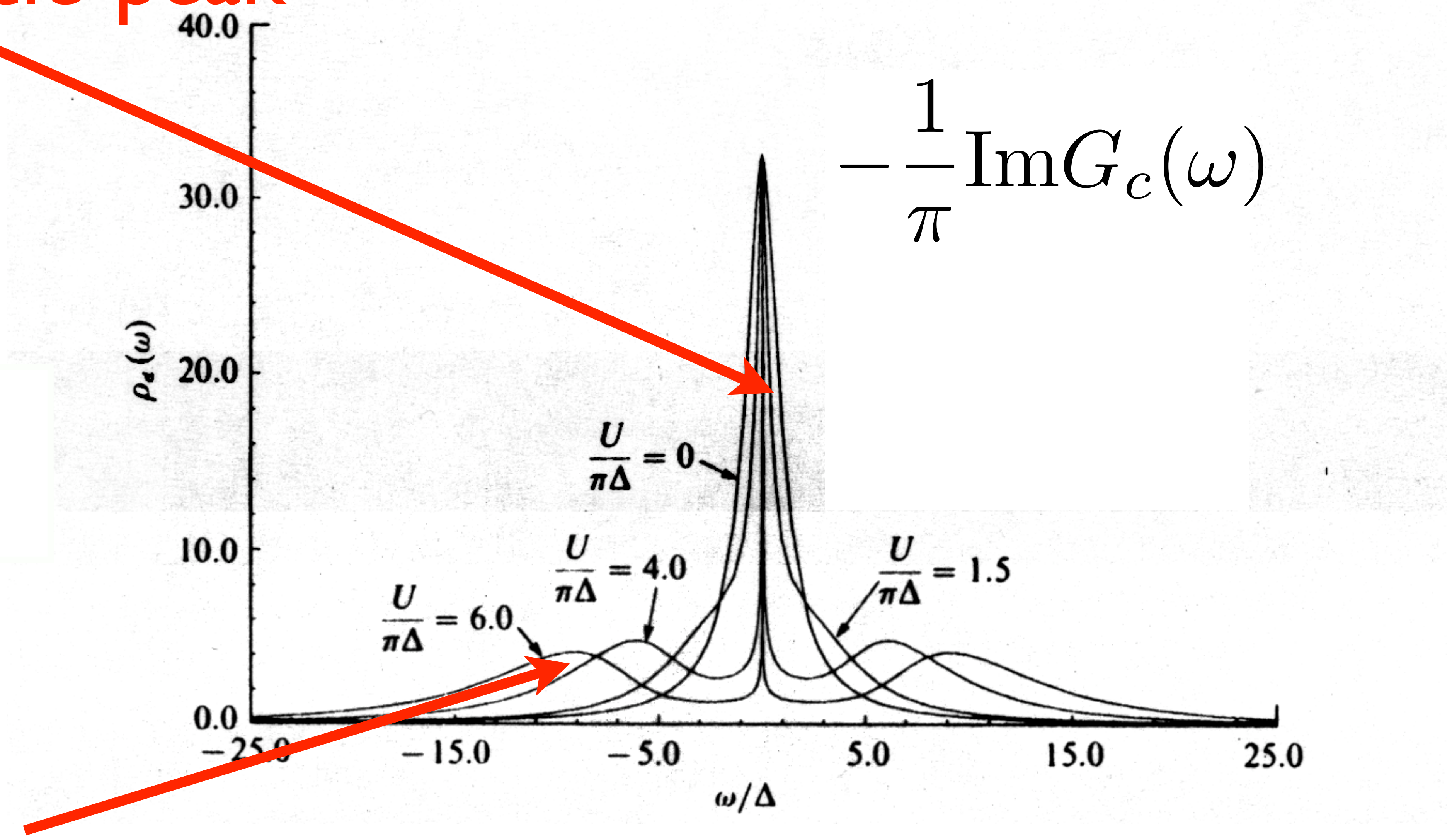
$$\Delta = \Gamma = \pi \rho_0 V^2$$

Lattice vs impurity

Lattice



Anderson impurity



Quasi-particle-peak

Hubbard bands

Mott physics :
Hubbard band (localized)
vs
Q.P. peak (delocalized)

- Abrikosov-Suhl resonance
- Local Fermi liquid with coherence temperature T_K *Nozières, 1974*

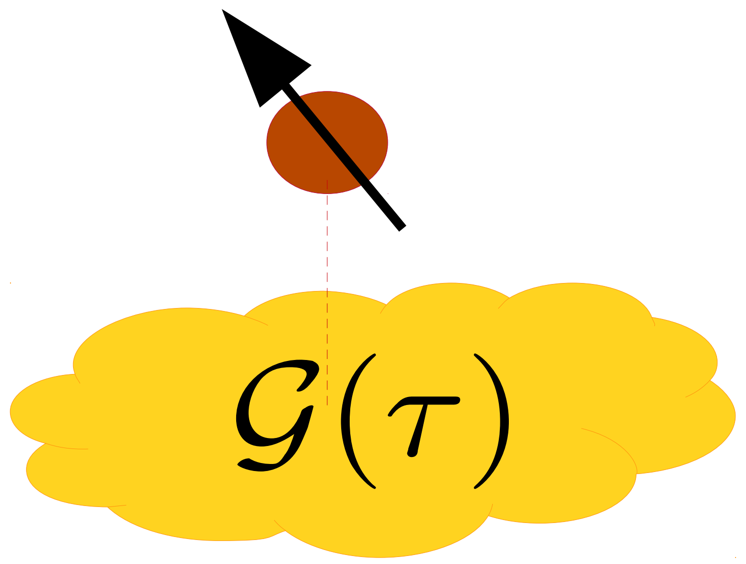
DMFT transform this analogy into a formalism

Dynamical Mean Field Theory
(DMFT)

DMFT : main idea

- DMFT : An atom in a self-consistent bath.

W. Metzner, D.Vollhardt, 1989
A. Georges, G. Kotliar, 1992



DMFT equations (Hubbard model)

- Approximation of the self-energy on the lattice $\Sigma_{latt}(k,\omega)$ by a local self-energy …

$$\boxed{\Sigma_{\sigma\mathrm{latt}}(k, i\omega_n) = \Sigma_{\sigma\mathrm{imp}}(i\omega_n)}$$

- … computed with an auxiliary impurity model …

$$S_{\mathrm{eff}} = -\int_0^\beta\!\!\int_0^\beta d\tau\, d\tau'\; c^\dagger_\sigma(\tau)\, \mathcal{G}^{-1}_{0\sigma}(\tau-\tau')\, c_\sigma(\tau') \;+\; \int_0^\beta d\tau\; U\, n_\uparrow(\tau)\, n_\downarrow(\tau)$$

$$\Sigma_{\sigma\mathrm{imp}}[\mathcal{G}_0](i\omega_n) \;\equiv\; \mathcal{G}^{-1}_{0\sigma}(i\omega_n) \;-\; G^{-1}_{\sigma\mathrm{imp}}[\mathcal{G}_0](i\omega_n) \qquad G_{\sigma\mathrm{imp}}(\tau) \equiv -\langle T c_\sigma(\tau) c^\dagger_\sigma(0)\rangle_{S_{\mathrm{eff}}}$$

- … whose bath is determined by:

$$\boxed{G_{\sigma\mathrm{imp}}[\mathcal{G}_0](i\omega_n) = G_{\sigma loc}(i\omega_n)} \equiv \sum_k \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_{\sigma\mathrm{imp}}[\mathcal{G}_0](i\omega_n)}$$

Two exact limits

- Non interacting limit $U = 0$
  - $\Sigma = 0,$ hence k-independent !

$$H = -\sum_{\langle ij \rangle, \sigma=\uparrow,\downarrow} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U n_{i\uparrow} n_{i\downarrow}, \qquad n_{i\sigma} \equiv c^\dagger_{i\sigma} c_{i\sigma}$$

- Atomic limit ($t_{ij} = 0$)
  - $\Sigma = \Sigma_{atom}$
  - $\Delta = 0$

$$\mathcal{G}^{-1}_{0\sigma}(i\omega_n) \equiv i\omega_n - \epsilon_d - \underbrace{\sum_k \frac{|V_{k\sigma}|^2}{i\omega_n - \epsilon_{k\sigma}}}_{\Delta_\sigma(i\omega_n)}$$

- DMFT interpolates between these limits.

Role of the bath

- Creates the Kondo peak, i.e the quasi-particle peak.

- Contrast with :
  - “Hubbard-1” approximation
    - $\Sigma_{latt} = \Sigma_{atomic}$
    - Fine in an insulator, but not for a metal.

  - DMFT has both atomic character, and quasi-particle peak, due to the Kondo effect /Abrikosov-Suhl resonance with the bath

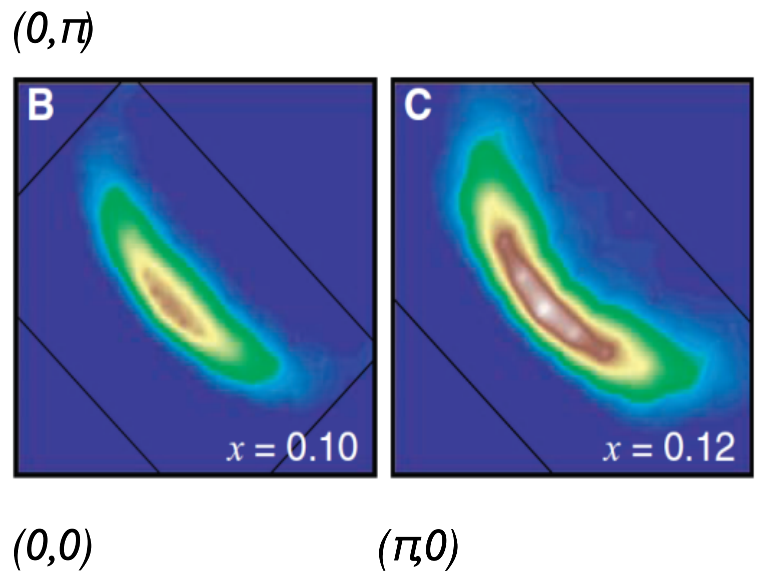
Local approximation for Σ_{latt}

$$G_{\sigma latt}(k, i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_{\sigma \mathrm{imp}}[\mathcal{G}_0](i\omega_n)}$$

Encodes the properties of the quasi-particles in a metals, cf lecture 1-2.

- We can describe a metal:
  - G_{latt} depends on k: Fermi surface in DMFT
  - Z, m^*, coherence energy E_{coh}, finite temperature lifetime Γ
  - Quasi-particle peak on the lattice is "parametrized" by the quasi-particle peak in the Anderson model

- But with some limitations
  - Z, m^*, E_{coh}, Γ are constant along the Fermi surface. (independent of k)
  - Z, m^* are related by $Z = \dfrac{m}{m^*}$



Solving DMFT : iterative method

Impurity solver [hard]

$$S_{\rm eff} = -\int_0^\beta\int_0^\beta d\tau\, d\tau'\; c^\dagger_\sigma(\tau)\, \mathcal{G}^{-1}_{0\sigma}(\tau-\tau')\, c_\sigma(\tau') \;+\; \int_0^\beta d\tau\, U\, n_\uparrow(\tau)\, n_\downarrow(\tau)$$

$$G_{\sigma\rm imp}(\tau) \equiv -\left\langle T c_\sigma(\tau) c^\dagger_\sigma(0)\right\rangle_{S_{\rm eff}}$$

$$\Sigma_{\sigma\rm imp}(i\omega_n) \equiv \mathcal{G}^{-1}_\sigma(i\omega_n) - G^{-1}_{\sigma\rm imp}(i\omega_n)$$

$\mathcal{G}_0$

G imp, Σimp

Self consistency condition [easy]

$$G_{\sigma\rm imp}[\mathcal{G}_0](i\omega_n) = \sum_k \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_{\sigma\rm imp}[\mathcal{G}_0](i\omega_n)}$$

- In practice, the iterative loop is (almost) always convergent.

An ***effective*** impurity model

- Anderson impurity with an effective band determined self-consistently

$$S = -\int_0^\beta\int_0^\beta d\tau\, d\tau'\; c^\dagger_\sigma(\tau)\,\mathcal{G}^{-1}_{0\sigma}(\tau-\tau')\,c_\sigma(\tau') \;+\; \int_0^\beta d\tau\; U\, n_\uparrow(\tau)\, n_\downarrow(\tau)$$

$$\Updownarrow$$

Not Hubbard model

t, ϵ_k

$$H = \underbrace{\sum_{\sigma=\uparrow,\downarrow} \varepsilon_d\, c^\dagger_\sigma c_\sigma + U\, n_\uparrow n_\downarrow}_{\text{Local site}} + \underbrace{\sum_{\lambda,\sigma=\uparrow,\downarrow} V_{\lambda\sigma}\left(\xi^\dagger_{\lambda\sigma} c_\sigma + h.c.\right) + \sum_{\lambda,\sigma=\uparrow,\downarrow} \varepsilon_{\lambda\sigma}\, \xi^\dagger_{\lambda\sigma}\xi_{\lambda\sigma}}_{\text{Effective bath}}$$

DMFT equations depend only on the density of state

- The k dependence is only through ϵ_k for the impurity problem
- Density of states for ϵ_k

$$D(\epsilon) \equiv \sum_k \delta(\epsilon - \epsilon_k)$$

- Self-consistency condition is a Hilbert transform

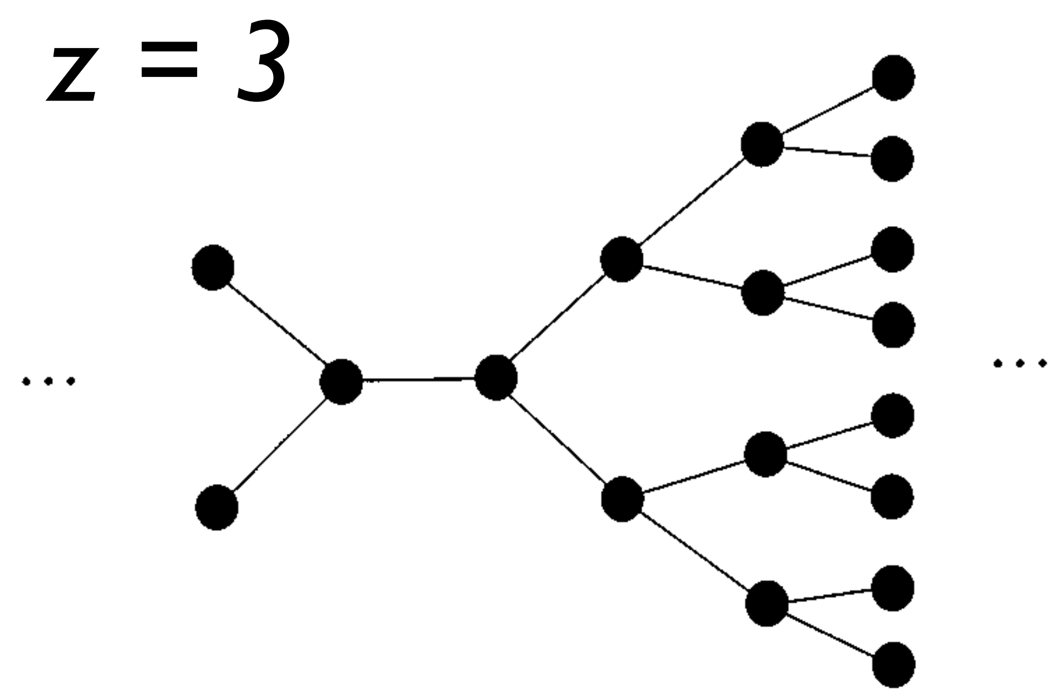
$$\tilde{D}(z) \equiv \int d\epsilon \frac{D(\epsilon)}{z - \epsilon} \qquad \text{for} \quad z \in \mathbb{C}$$

$$\begin{aligned} G_{\sigma\text{imp}}[\mathcal{G}_0](i\omega_n) &= \sum_k \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_{\sigma\text{imp}}[\mathcal{G}_0](i\omega_n)} \\ &= \tilde{D}\big(i\omega_n + \mu - \Sigma_{\sigma\text{imp}}[\mathcal{G}_0](i\omega_n)\big) \end{aligned}$$

The Bethe lattice

The Bethe lattice

- No loop.
- Connectivity z = number of neighbours
- t between nearest neighbours



- Free fermions on the Bethe Lattice for $z \to \infty$

$$\boxed{G^{-1}(i\omega_n) = i\omega_n + \mu - t^2 G(i\omega_n)}$$

- Semi-circular density of states for free fermions.

$$D(\epsilon) = \frac{1}{2\pi t^2}\sqrt{4t^2 - \epsilon^2}, \quad |\epsilon| < 2t.$$

The Bethe lattice

$$D(\epsilon) = \frac{1}{2\pi t^2}\sqrt{4t^2-\epsilon^2}, \quad |\epsilon|<2t.$$

$$\boxed{G^{-1}(i\omega_n) = i\omega_n + \mu - t^2 G(i\omega_n)}$$

- Its Hilbert transform can be done explicitly

$$\tilde{D}(\zeta) \equiv \int_{-\infty}^{\infty} d\epsilon \frac{D(\epsilon)}{\zeta - \epsilon}$$

$$\tilde{D}(\zeta) = (\zeta - s\sqrt{\zeta^2-4t^2})/2t^2 \qquad s = \mathrm{sgn}[\mathrm{Im}(\zeta)]$$

- It is a simple *reciprocal* function R

$$R[\tilde{D}(\zeta)] = \zeta$$

$$\boxed{R(G) = t^2 G + 1/G}$$

- since

$$G(i\omega_n) = \tilde{D}(i\omega_n + \mu) \qquad R[G] = i\omega_n + \mu = t^2 G + G^{-1}$$

The Bethe lattice

- The DMFT self-consistency simplifies

$$\boxed{\mathcal{G}_{0\sigma}^{-1}(i\omega_n) = i\omega_n + \mu - \underbrace{t^2\, G_{\sigma\text{imp}}(i\omega_n)}_{\Delta_\sigma(i\omega_n)}}$$

$$\Delta = t^2 G_{imp}$$

- Proof

$$G_{\sigma\text{imp}}[\mathcal{G}](i\omega_n) = \sum_k \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_{\sigma\text{imp}}[\mathcal{G}](i\omega_n)}$$

$$G_{\sigma\text{imp}}(i\omega_n) = \tilde{D}(i\omega_n + \mu - \Sigma_{\sigma\text{imp}}(i\omega_n))$$

$$R[G_{\sigma\text{imp}}](i\omega_n) = i\omega_n + \mu - \Sigma_{\sigma\text{imp}}(i\omega_n)$$

$$t^2 G_{\sigma\text{imp}}(i\omega_n) + G_{\sigma\text{imp}}^{-1}(i\omega_n) = i\omega_n + \mu - \mathcal{G}_\sigma^{-1}(i\omega_n) + G_{\sigma\text{imp}}^{-1}(i\omega_n)$$

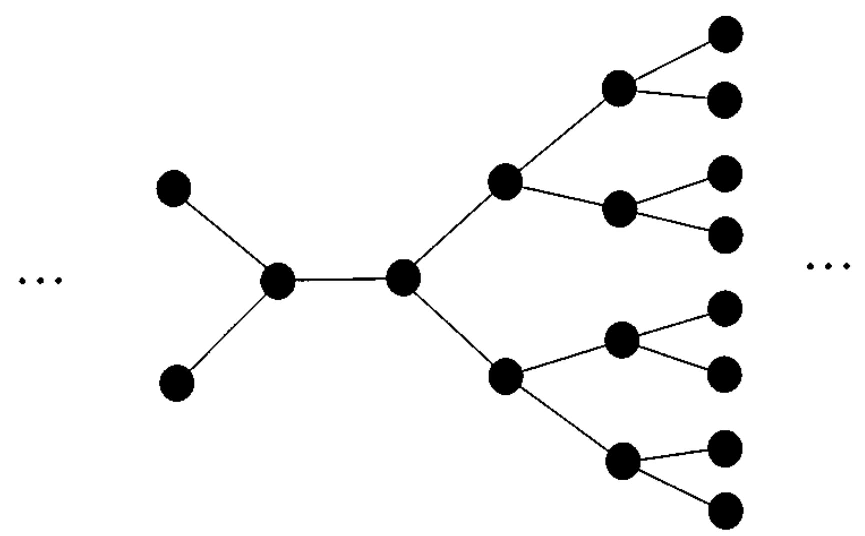
Bethe lattice/semicircular dos : summary of equations

- DMFT on the Bethe lattice

$$S_{\text{eff}} = -\int_0^\beta\!\!\int_0^\beta d\tau\, d\tau'\; c_\sigma^\dagger(\tau)\, \mathcal{G}_{0\sigma}^{-1}(\tau-\tau')\, c_\sigma(\tau') \;+\; \int_0^\beta d\tau\, U\, n_\uparrow(\tau)\, n_\downarrow(\tau)$$

$$G_{\sigma\text{imp}}(\tau) \equiv -\left\langle T c_\sigma(\tau) c_\sigma^\dagger(0)\right\rangle_{S_{\text{eff}}}$$

$$\boxed{\mathcal{G}_{0\sigma}^{-1}(i\omega_n) = i\omega_n + \mu - \underbrace{t^2\, G_{\sigma\text{imp}}(i\omega_n)}_{\Delta_\sigma(i\omega_n)}}$$



- Physically meaning full, since semi-circular dos is a reasonable shape
- The lattice itself is not very physical (issue for transport).

Analogy with Weiss Mean Field Theory for Ising model

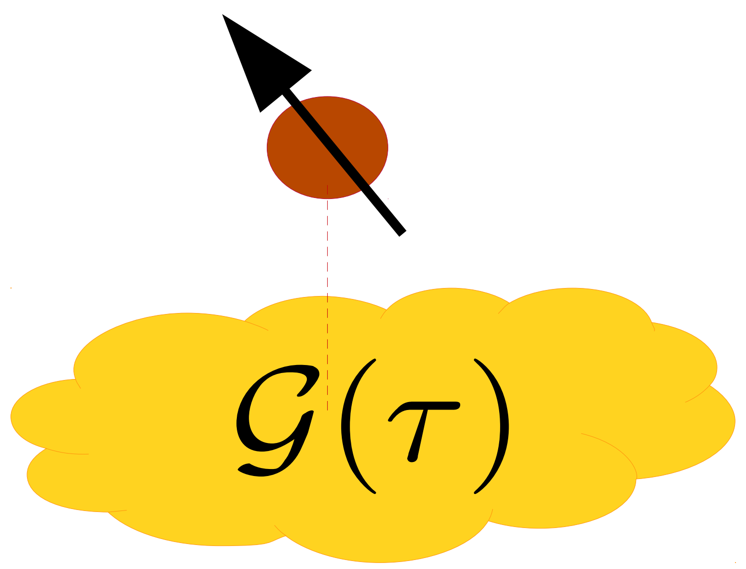
Weiss Mean Field Theory

- *Ising model* (Weiss) : A single spin in an effective field.

$H = -J \sum_{ij} \sigma_i \sigma_j$	Ising model.
$m = \langle \sigma \rangle$	Order parameter.
$H_{\text{eff}} = -J h_{\text{eff}} \sigma$	Effective Hamiltonian
$h_{\text{eff}} = zJm$	Weiss Field
$m = \tanh(\beta h_{\text{eff}})$	Solution of the effective Hamiltonian

- Qualitatively correct (phase diagram, second order transition, but not critical exponents
- Derivation : e.g. large dimension limit on hypercubic lattice

DMFT equations (1 band paramagnetic)



	Ising	*Hubbard*
Lattice model	$H = -J\sum_{\langle ij\rangle}\sigma_i\sigma_j$	$H = -\sum_{\langle ij\rangle} t_{ij} c^\dagger_{i\sigma} c_{i\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow}$
Effective model	$H_{\text{eff}} = -J h_{\text{eff}} \sigma$ $m = \langle \sigma \rangle$	$S_{\text{eff}} = -\int_0^\beta\int_0^\beta d\tau\, d\tau'\, c^\dagger_\sigma(\tau)\, \mathcal{G}^{-1}_{0\sigma}(\tau-\tau')\, c_\sigma(\tau') + \int_0^\beta d\tau\, U\, n_\uparrow(\tau)\, n_\downarrow(\tau)$ $G_{\sigma\text{imp}}(\tau) \equiv -\left\langle T c_\sigma(\tau) c^\dagger_\sigma(0)\right\rangle_{S_{\text{eff}}}$
Self consistency condition	$h_{\text{eff}} = zJm$	$\Sigma_{\sigma\text{imp}}[\mathcal{G}_0](i\omega_n) \equiv \mathcal{G}^{-1}_{0\sigma}(i\omega_n) - G^{-1}_{\sigma\text{imp}}[\mathcal{G}_0](i\omega_n)$ $G_{\sigma\text{imp}}[\mathcal{G}_0](i\omega_n) = \sum_k \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_{\sigma\text{imp}}[\mathcal{G}_0](i\omega_n)}$ *Implicit equation for the bath*

DMFT is an atomic approximation

of the Luttinger-Ward functional $\Phi[G]$

Functionals

- A very general method in statistical physics:
  - Pick up the relevant physical quantity X
  - Build a functional $\Gamma(X)$,
  - Approximate the "complicated" part of $\Gamma(X)$
- Examples:
  - magnetic transition X =m
  - Density functional theory $X = \rho(x)$, electronic density
- DMFT, X = G

Luttinger-Ward functional

- Take action of Hubbard model, with a quadratic source h

$$S = \int d\tau d\tau' \sum_{ij} c^\dagger_{i\sigma}(\tau)\left(g^{-1}_{0ij} + h_{ij}\right)(\tau - \tau')c_{\sigma j}(\tau') + \int d\tau U \sum_i n_{i\uparrow}(\tau)n_{i\downarrow}(\tau)$$

- Free energy is a function of h

$$\Omega[h] = -\log \int \mathcal{D}[c^\dagger c]e^{-S[h]}$$

$$G_{ij}(\tau - \tau') = -\left\langle c_i(\tau)c^\dagger_j(\tau')\right\rangle = \frac{\partial \Omega}{\partial h_{ji}(\tau' - \tau)}$$

- “Grand potential” = Legendre transform to eliminate h for G

$$\Gamma[G] = \Omega[h] - \mathrm{Tr}(hG)$$

$$\Gamma[G] = \underbrace{\mathrm{Tr}\ln G - \mathrm{Tr}(g_0^{-1}G)}_{U=0 \text{ term}} + \Phi[G]$$

$$\frac{\partial \Gamma[G]}{\partial G} = h = 0$$

Self-energy

$$\Gamma[G] = \mathrm{Tr} \ln G - \mathrm{Tr}(g_0^{-1} G) + \Phi[G]$$

Baym, Kadanoff,
De Dominicis, Martin 64

- From the stationarity of Γ[G] at the physical G:

$$\frac{\partial \Gamma[G]}{\partial G} = 0 \qquad G^{-1} = g_0^{-1} - \Sigma[G] \qquad \Sigma_{ij} = \frac{\delta \Phi}{\delta G_{ji}}$$

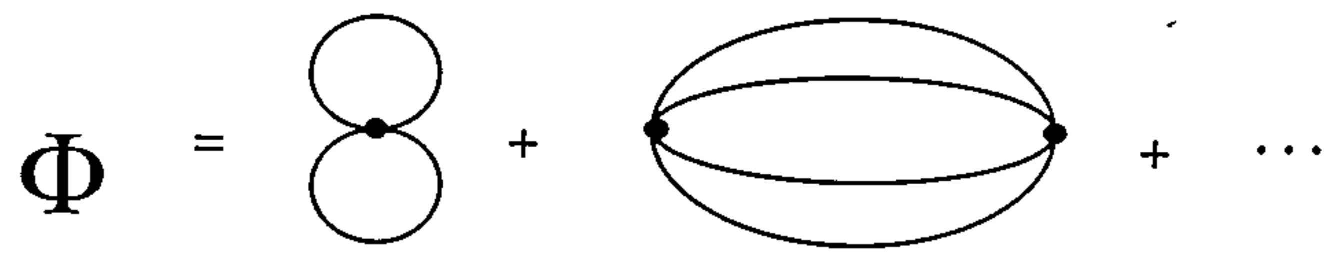
- Dyson as a functional equation for G

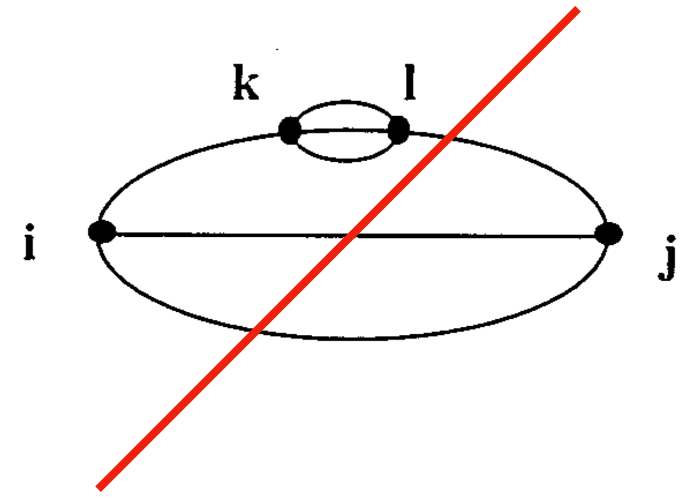
Luttinger-Ward functional

- Diagrammatic interpretation

Baym, Kadanoff, De Dominicis, Martin 64

$\Phi[G]$ is the sum of two-particles irreducible (2PI) diagrams





- Also called "skeleton" diagrams.
- NB : does not depend on the bare propagator.
- A standard object in many-body theory. Conserving approximations
- In strong coupling, Φ is in fact multivalued. $G[g_0]$ is not invertible

E. Kozik, M. Ferrero, A. Georges Phys. Rev. Lett. 114, 156402 (2015)

Definition of DMFT

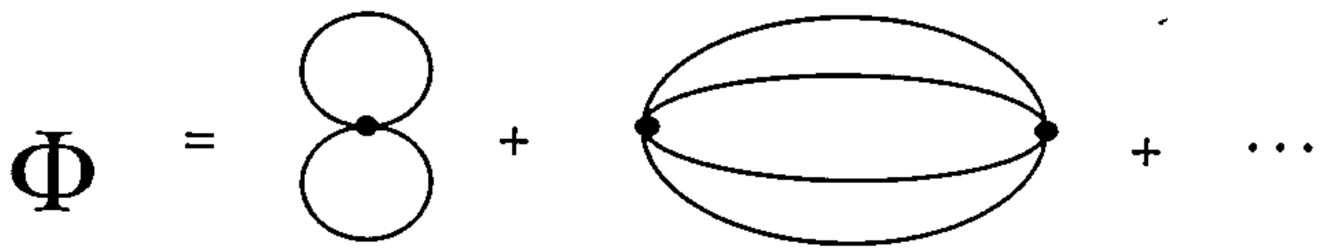
Metzner-Vollhardt '89, Georges-Kotliar '92

- Take a model with local interactions

$$H = -\sum_{\langle ij\rangle,\sigma=\uparrow,\downarrow} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U n_{i\uparrow} n_{i\downarrow}, \qquad n_{i\sigma} \equiv c^\dagger_{i\sigma} c_{i\sigma}$$

- DMFT : only the local diagrams in Φ (in real space, same point on lattice)

$$\boxed{\Phi(G_{ij}) = \sum_i \phi_1(G_{ii})}$$



Where is the bath ?

Impurity = auxiliary local model

$$S_{\mathrm{eff}} = -\int_0^\beta\int_0^\beta d\tau\, d\tau'\, c_\sigma^\dagger(\tau)\, \mathcal{G}_{0\sigma}^{-1}(\tau-\tau')\, c_\sigma(\tau') + \int_0^\beta d\tau\, U\, n_\uparrow(\tau)\, n_\downarrow(\tau)$$

- Φ does not depend on the bare propagator, only on the vertex, so

$$\Phi(G_{ij}) = \sum_i \phi_1(G_{ii})$$

$$\phi_1 = \phi_{\text{Impurity for any } \mathcal{G}} = \phi_{\text{atom}}$$

- The impurity exactly sums in Σ the 2PI local diagrams if we can fix the bath such that the impurity (full) propagator is the lattice local (full) propagator

$$\boxed{G_{\mathrm{imp}} = G_{ii}^{\mathrm{latt}}}$$

$$\Sigma_{ij}^{\mathrm{latt}} = \frac{\partial \Phi}{\partial G_{ji}} = \delta_{ij}\Sigma_{\mathrm{imp}}$$

DMFT self-consistency equations

$$G_{\sigma\mathrm{imp}}[\mathcal{G}_0](i\omega_n) = \sum_k \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_{\sigma\mathrm{imp}}[\mathcal{G}_0](i\omega_n)}$$

Exact limits

$$\boxed{\Phi[G_{ij}] = \sum_i \Phi_{atom}[G_{ii}]}$$

- DMFT is exact:
  - For $U = 0$
  - In the atomic limit ($t_{ij} = 0$).
  - In the $d \to \infty$ limit
    - Consider an hypercubic lattice in dimension d
    - Scale the hopping as : $t/\sqrt{d}$. Then $\Phi(G_{ij}) \underset{d\to\infty}{\to} \sum_i \phi_1(G_{ii})$

Metzner-Vollhardt '89

- Combinatoric proof: *Cf RMP Georges et al. 1996*
  2PI implies at least 3 independent paths between 2 points, hence non local diagrams scale at least like $1\sqrt{d}$

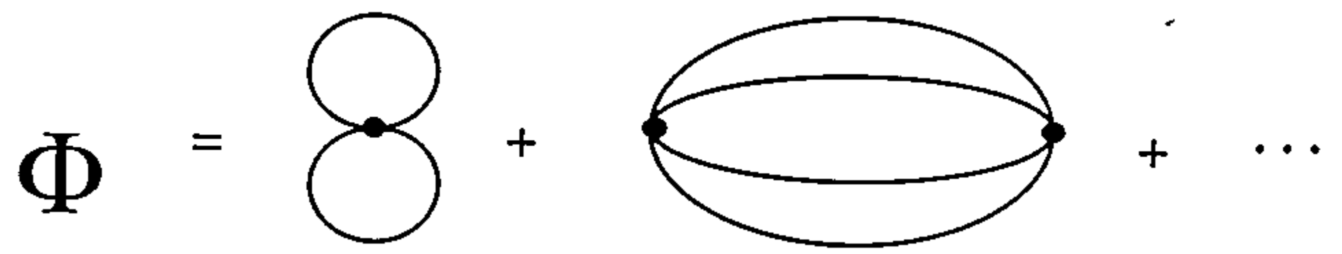
DMFT is an atomic approximation

$$\boxed{\Phi[G_{ij}] = \sum_i \Phi_{atom}[G_{ii}]}$$

- On Φ !
- Not on G, Σ …
- Locality is the control parameter.

DMFT is a diagrammatic method

$$\boxed{\Phi[G_{ij}] = \sum_i \Phi_{atom}[G_{ii}]}$$



- Consequences:
  - Easy to mix with other diagrammatic, e.g. GW + DMFT.
  - Open many ways of generalizations (e.g. clusters, diagrammatic extensions …)
  - ”Straightforward” generalization to non-equilibrium (Schwinger-Keldysh)

Analogy with DFT

For a review, cf G. Kotliar, S.Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, C. Marianetti, Rev. Mod. Phys. 78, 865 (2006)

- Density Functional Theory (DFT)
  - Functional $F[\rho(x)]$.
  - Approximate exchange energy term
  - Effective model : 1 electron in a Kohn-Sham potential
- DMFT
  - Functional $\Gamma[G]$
  - Approximated $\Phi[G]$
  - Effective model : impurity. An atom in a electronic bath

Thermodynamics. Free Energy

- Free energy on the lattice (in DMFT) ≠ Impurity free energy
- On the lattice :

$$\Omega = \Phi + T \sum_{n,\mathbf{k},\sigma} \left[\ln G_\sigma(\mathbf{k}, i\omega_n) - \Sigma_\sigma(i\omega_n) G_\sigma(\mathbf{k}, i\omega_n) \right],$$

- For the impurity :

$$\Omega_{\mathrm{imp}} = \phi[G] + T \sum_{n\sigma} \left[\ln G_\sigma(i\omega_n) - \Sigma_\sigma(i\omega_n) G_\sigma(i\omega_n) \right].$$

- Therefore :

$$\frac{\Omega}{N} = \Omega_{\mathrm{imp}} - T \sum_{n\sigma} \left(\int_{-\infty}^{+\infty} d\epsilon \, D(\epsilon) \right.$$

$$\left. \times \ln[i\omega_n + \mu - \Sigma_\sigma(i\omega_n) - \epsilon] + \ln \, G_\sigma(i\omega_n) \right),$$

A brief introduction to Mott transition

A minimal model for theorists : Hubbard model

Kinetic term

Interaction term (Coulomb) U>0

$$H = -\sum_{\langle ij\rangle,\sigma=\uparrow,\downarrow} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U n_{i\uparrow} n_{i\downarrow}, \qquad n_{i\sigma} \equiv c^\dagger_{i\sigma} c_{i\sigma}$$

Nearest neighbours

Doping (number of charges)

$$\delta = 1 - \langle n_\uparrow + n_\downarrow \rangle$$

- Not realistic for solids, but it is for cold atoms in optical lattices
- Half filling : 1 electron/site in average : $\delta = 0$
- U/t small : Fermi liquid
- t =0 : Insulator. Atomic limit
- What happens at intermediate coupling U/t ?

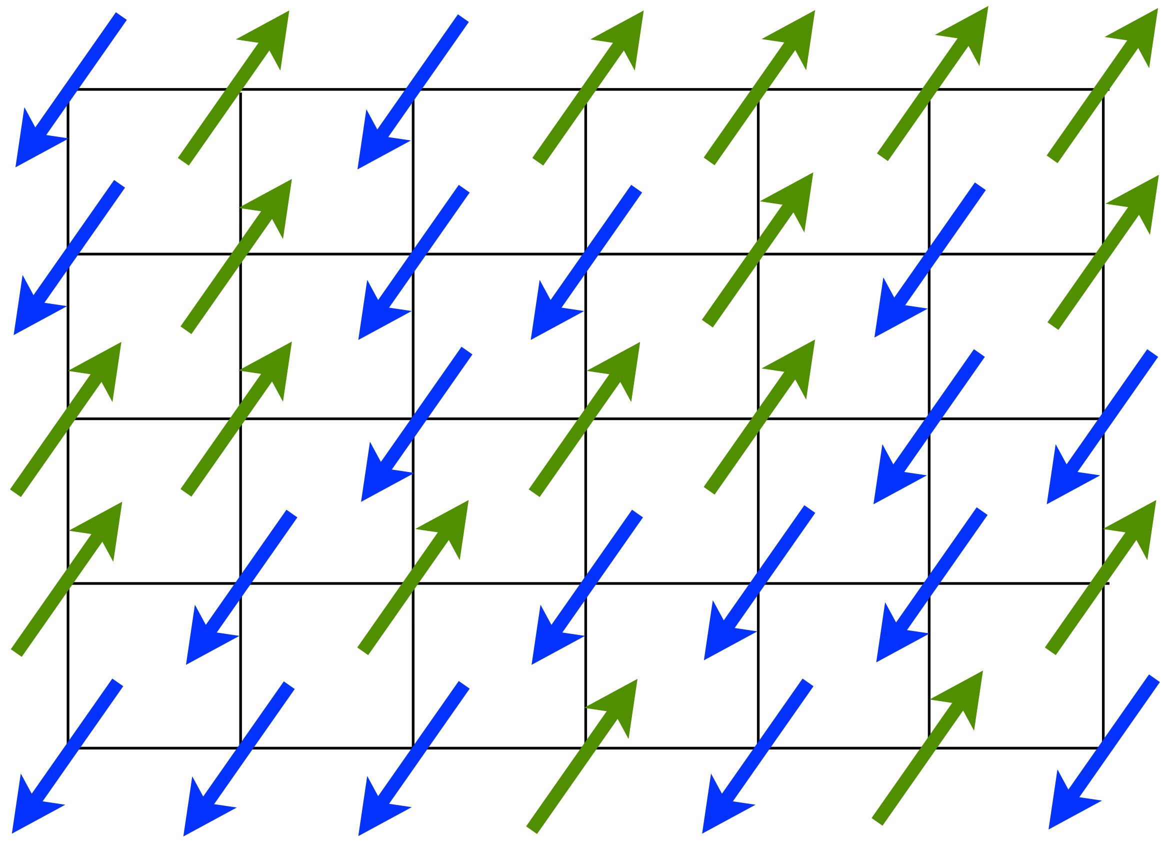
Mott insulator

N. Mott, 50's

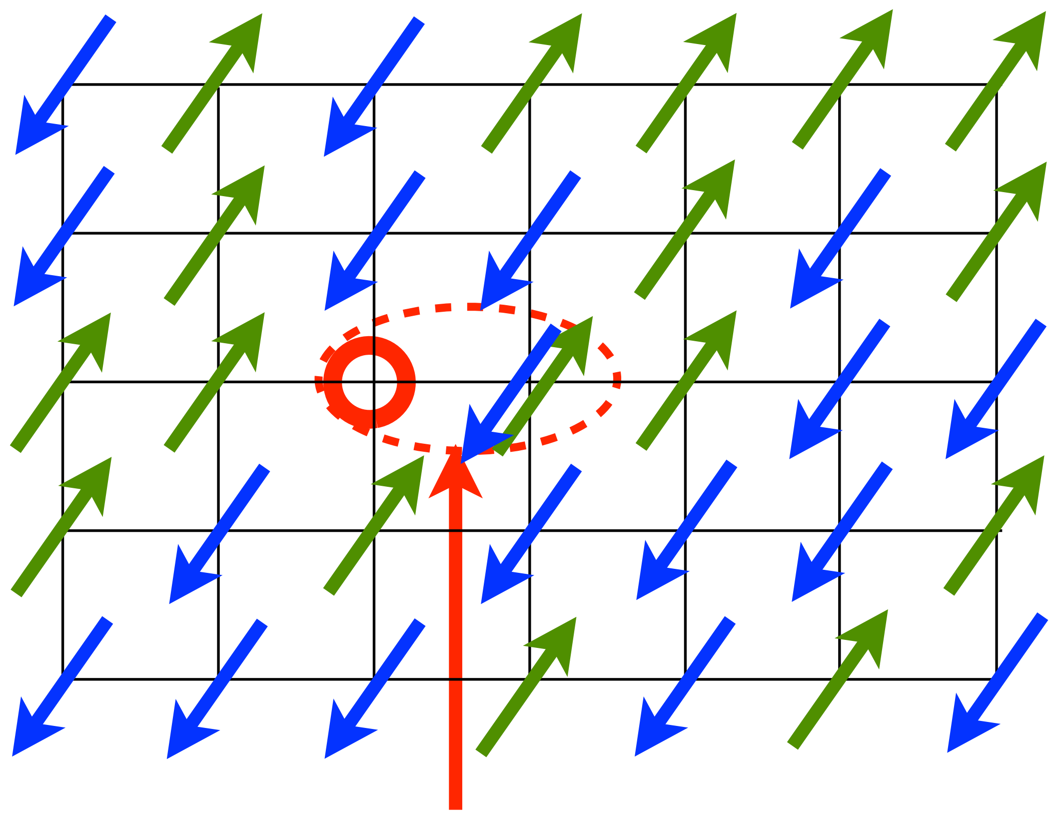
- One electron per site on average (half-filled band).
- At small U, a textbook metal.
- If U is large enough, it is an insulator : charge motion frozen.

$$H = -\sum_{\langle ij\rangle,\sigma=\uparrow,\downarrow} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U n_{i\uparrow} n_{i\downarrow}, \qquad n_{i\sigma} \equiv c^\dagger_{i\sigma} c_{i\sigma}$$

$$\delta = 1 - \langle n_\uparrow + n_\downarrow \rangle$$



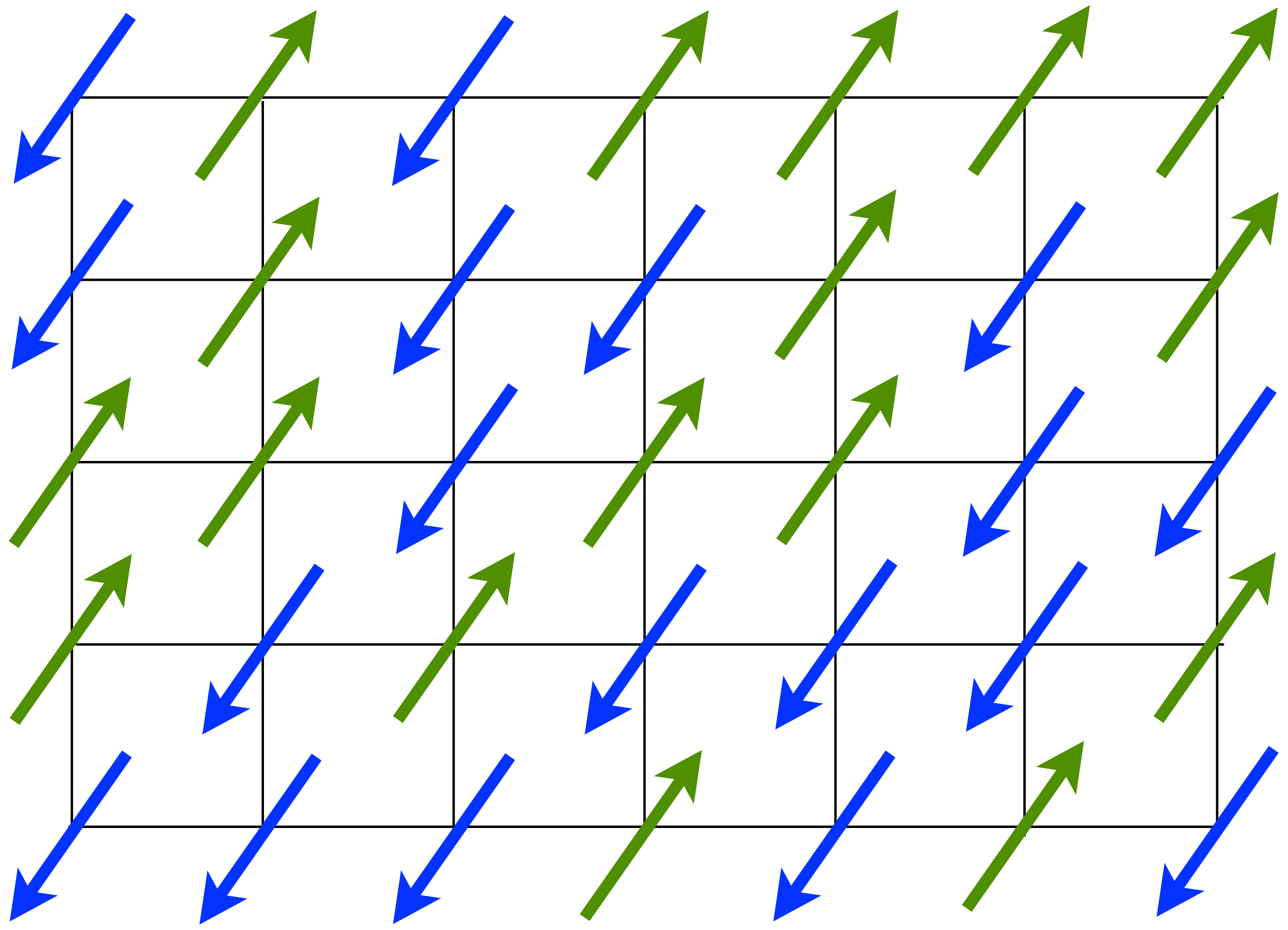
Mott insulator



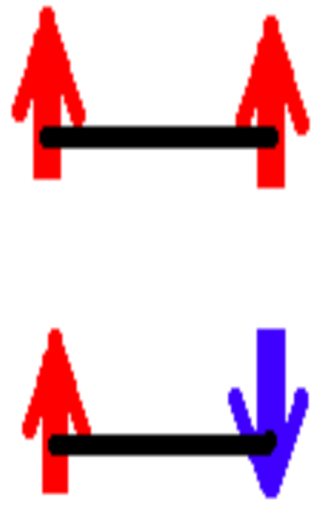
Large Coulomb repulsion U ~ eV ~ 10^4 K

Mott insulators : spins are not frozen !

- Charge motion is frozen, but spin degrees of freedom are not !
- At which physical scale will spin order arise ?



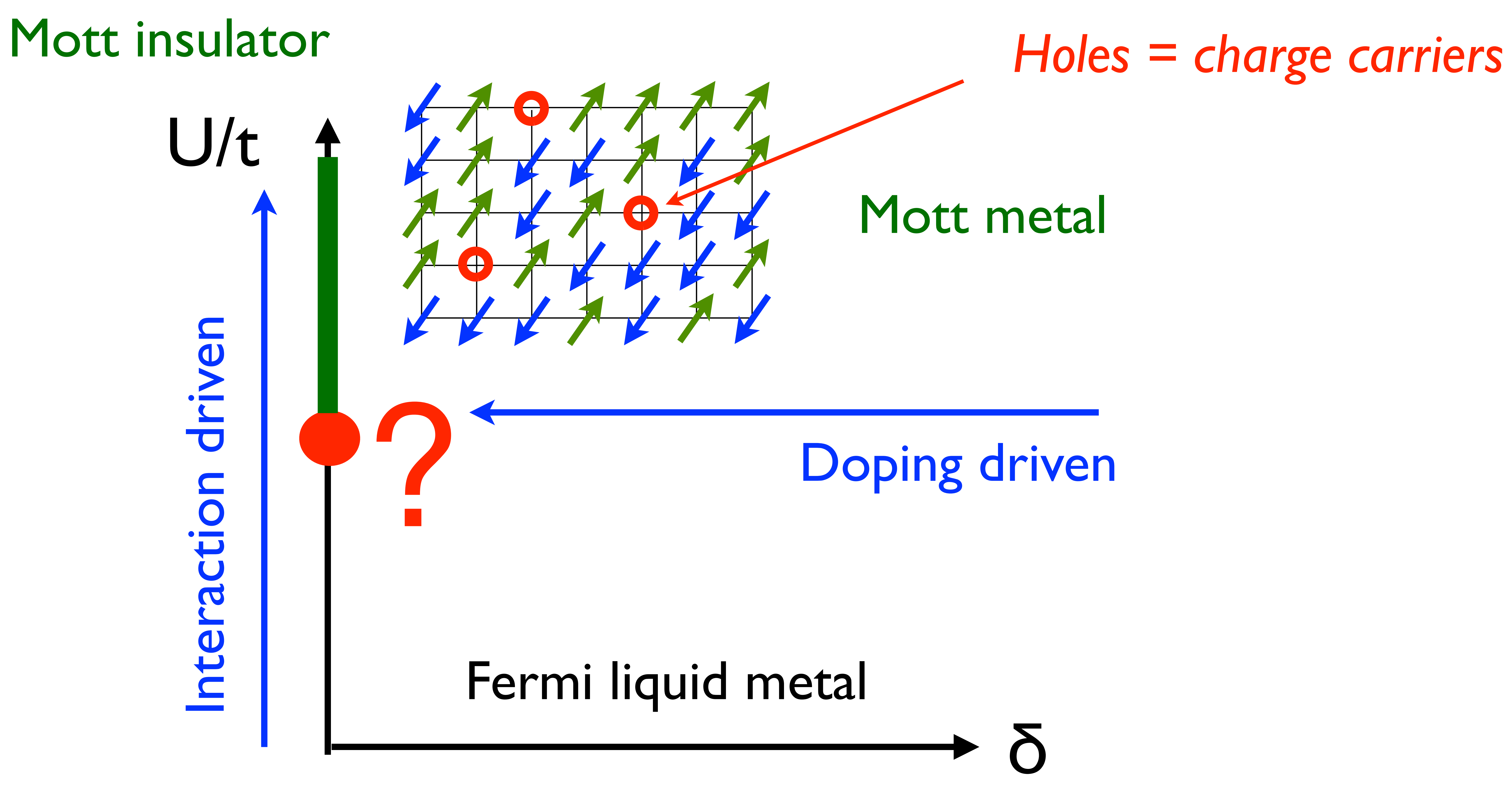
Effective antiferromagnetic interaction between spins



$$J_{AF} = \frac{4t^2}{U}$$

Mott phenomenon at strong coupling not due to magnetism

Doped Mott insulators



- How is a metal destroyed close to a Mott transition ?
  Or a Mott insulator by doping ?

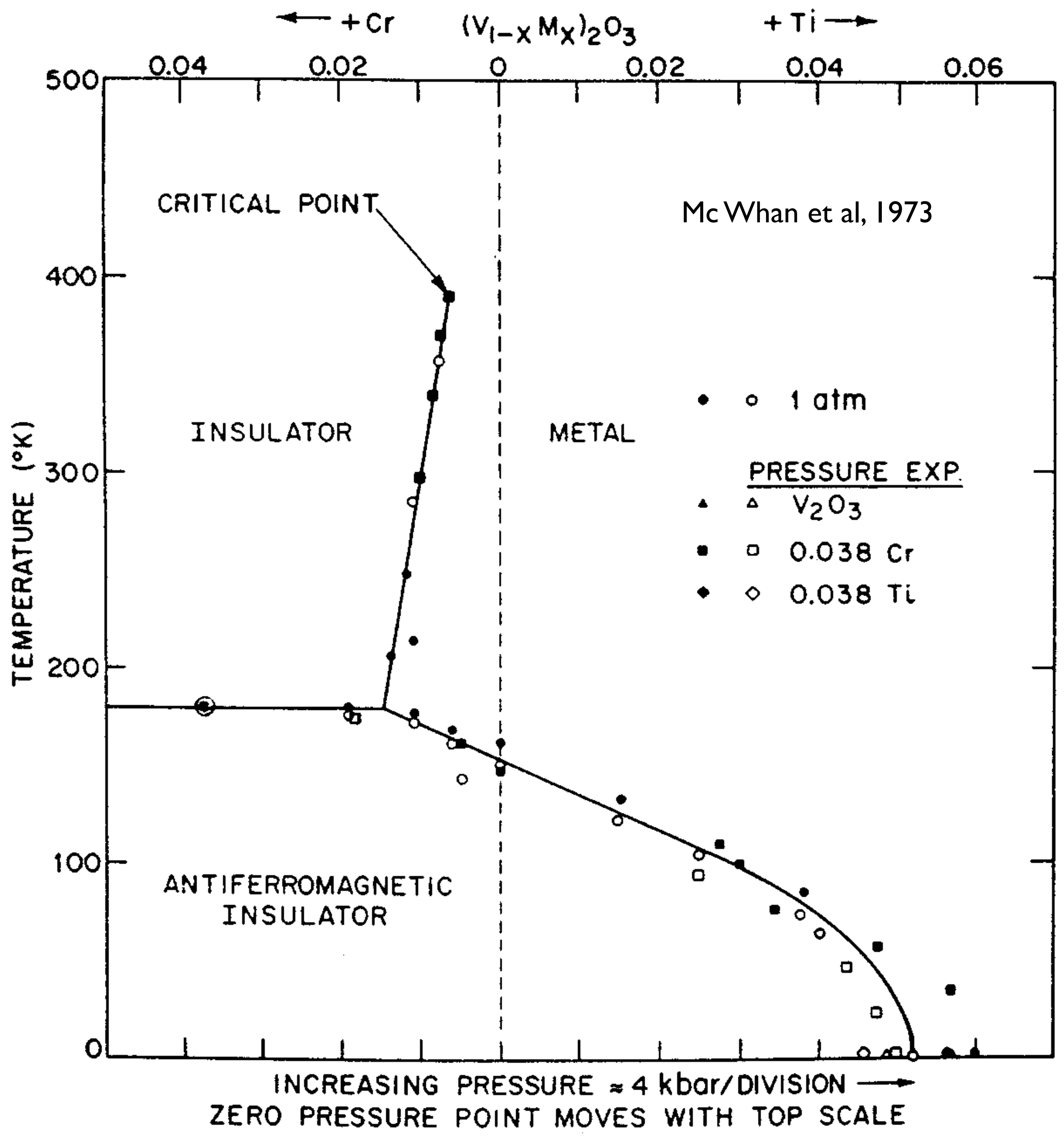
- "Mott metals" are fragile and complex : Many instabilities, rich phase diagrams, large susceptibilities, small coherence energy

In real materials …

Interaction Driven Mott Transition

- Vary pressure P ⇔ 1/U

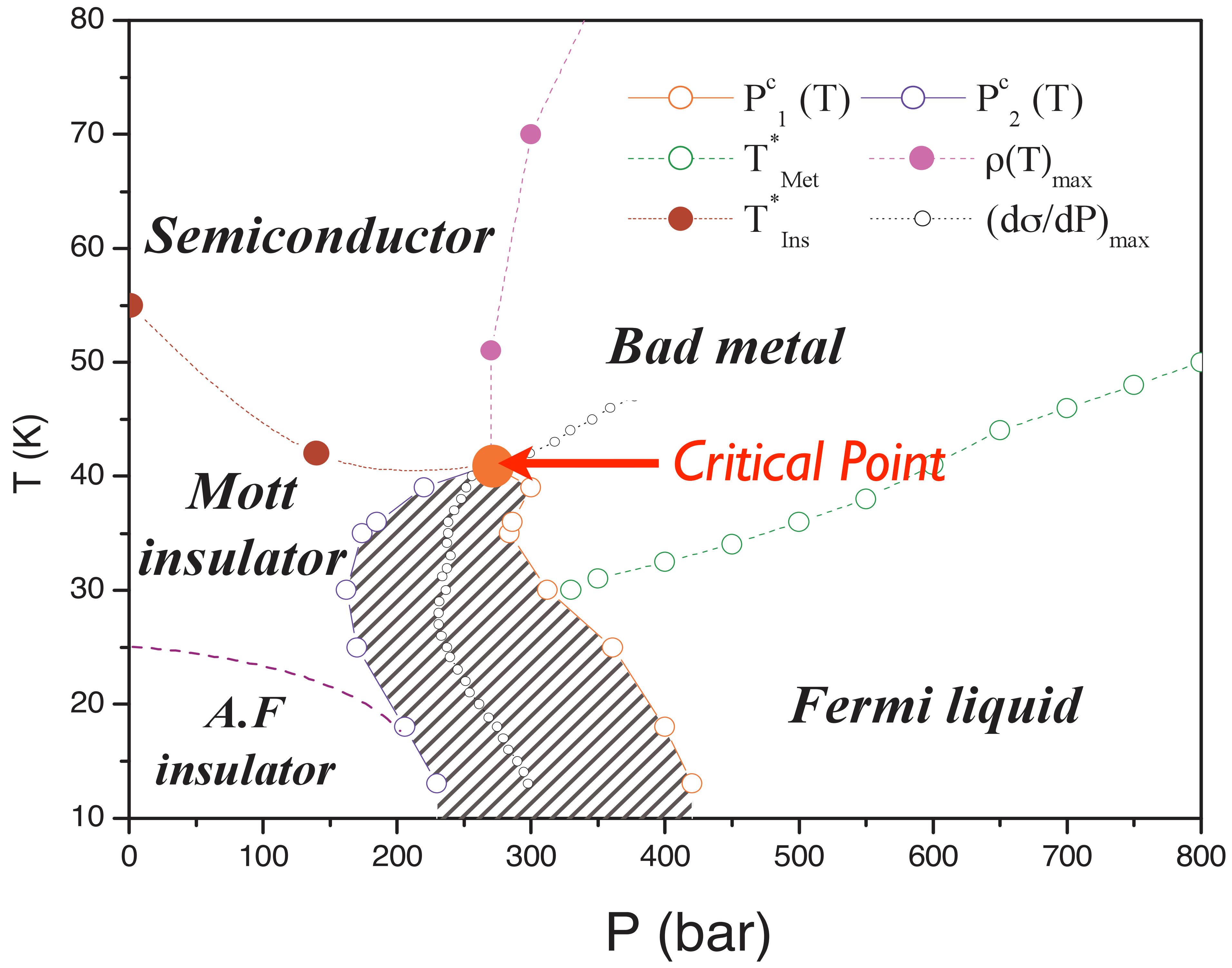
V_2O_3



2-d organics

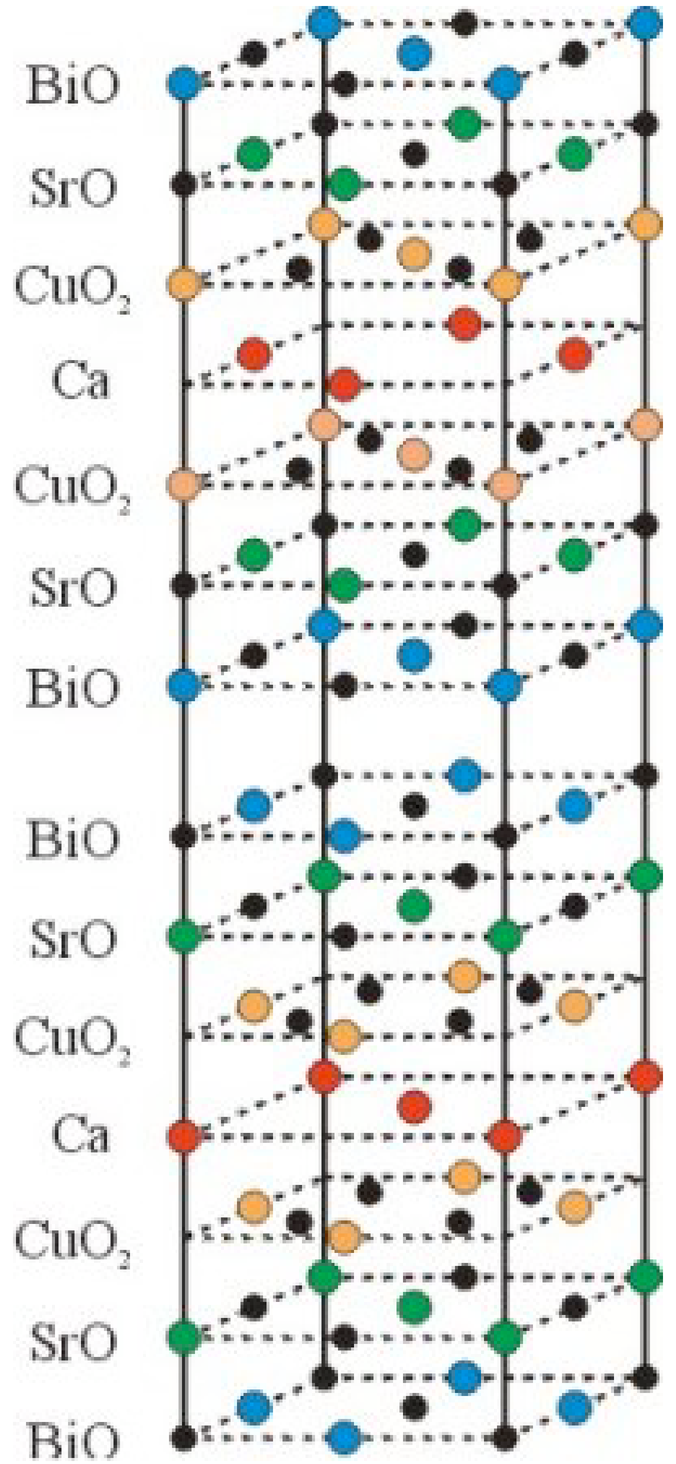
κ-$(BEDT\text{-}TTF)_2Cu[N(CN)_2]Cl$

(but has a simple hubbard modelization)

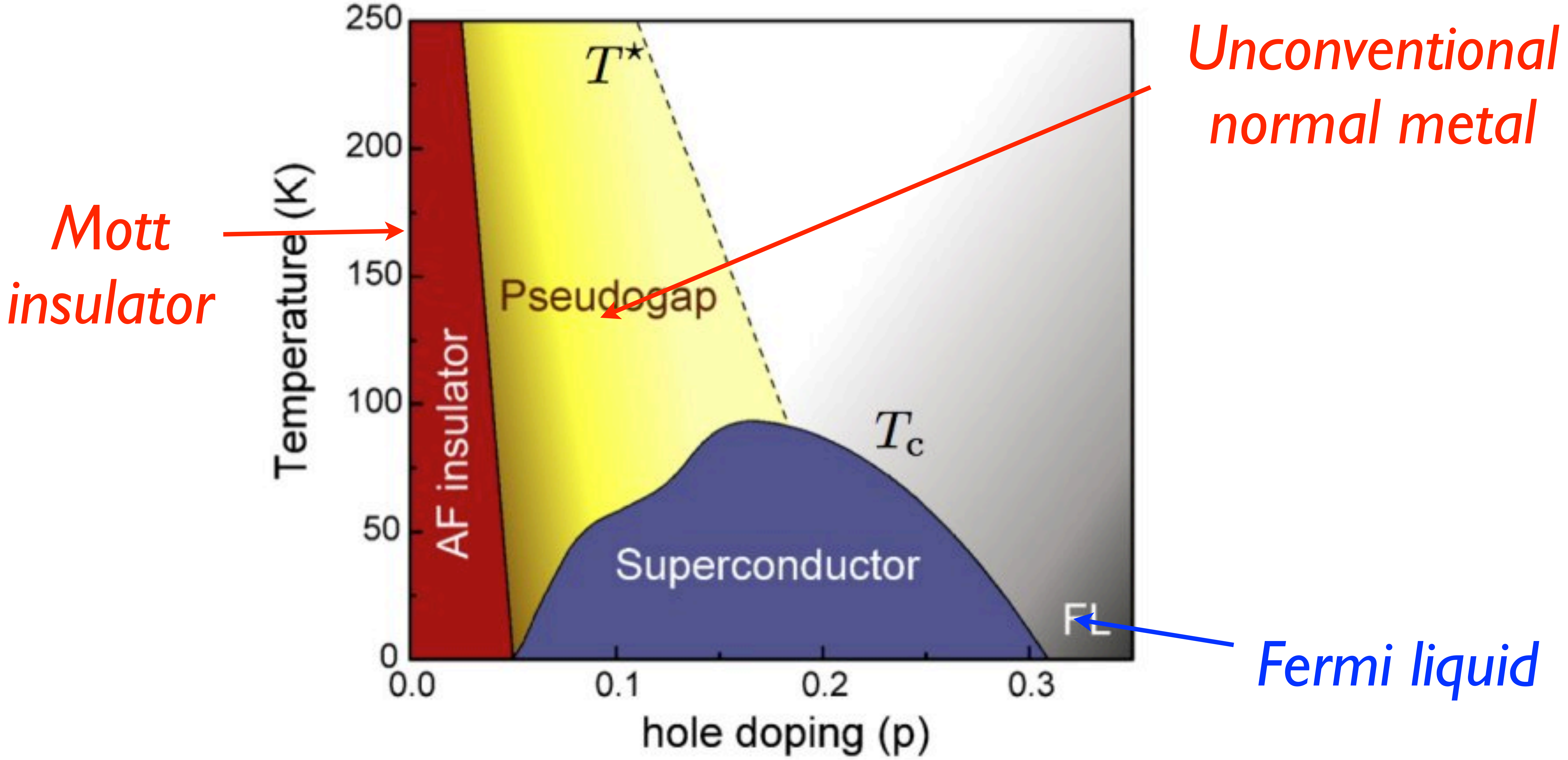


P. Limelette, et al. PRL 91, 016401 (2003)

High-Tc superconductors are doped Mott insulators



High-Tc superconductors
Generic, simplified phase diagram



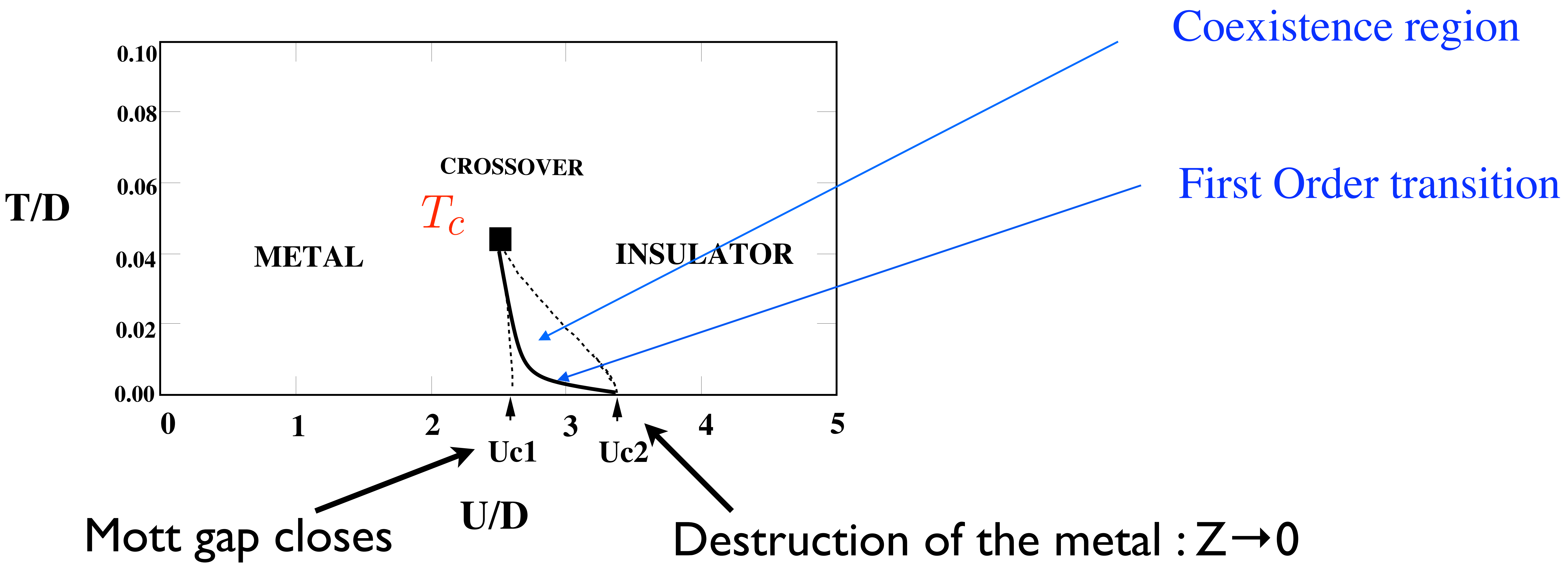
- A family of copper oxides with high critical temperature (90, 100K).
- Physics qualitatively different from conventional superconductors.
- Mechanism of high-Tc superconductivity ?

A DMFT classic

Hubbard model, 1 band, 1/2 filling

Phase diagram

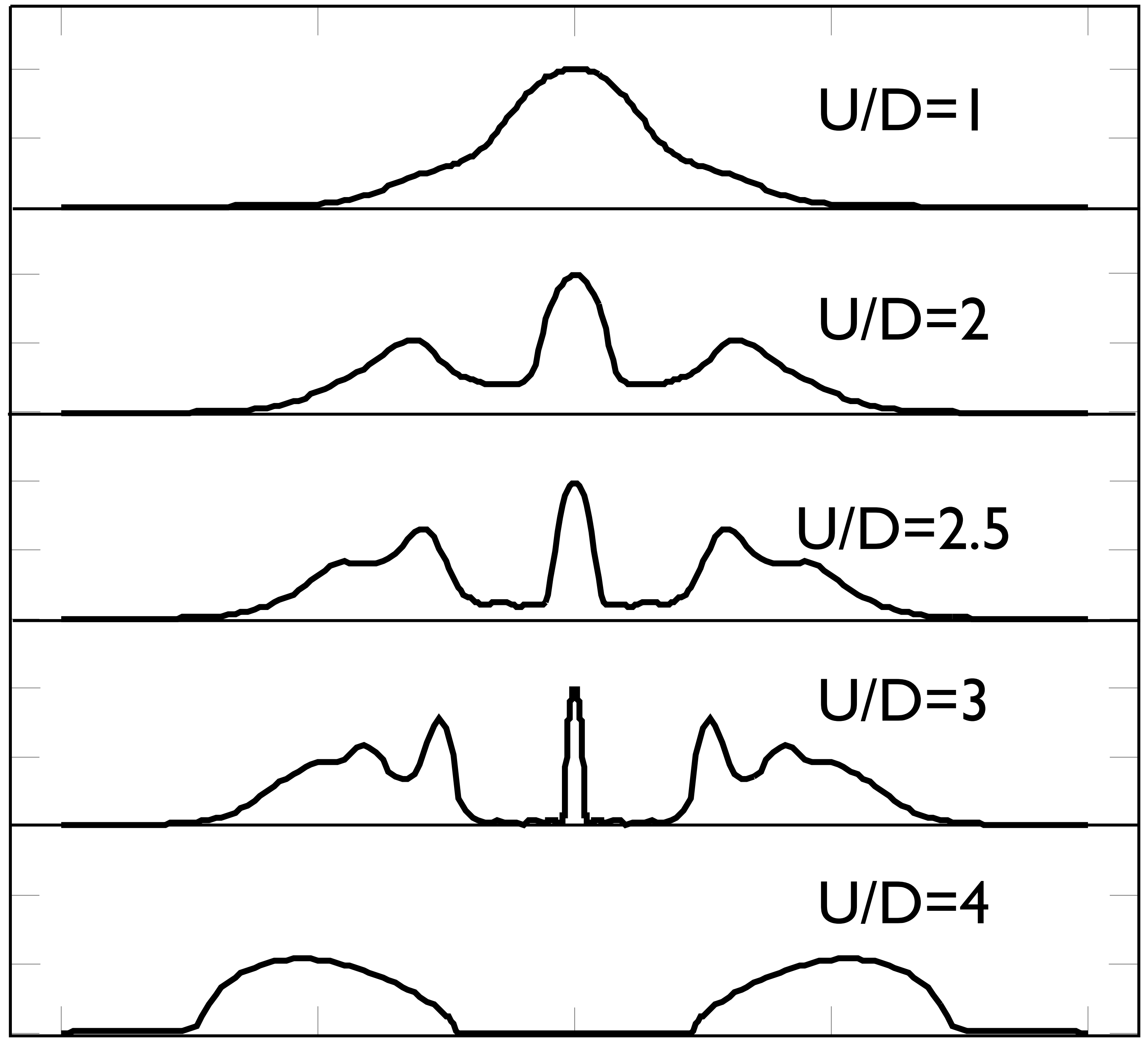
- Hubbard model at half-filling (δ=0). D is half-bandwidth.



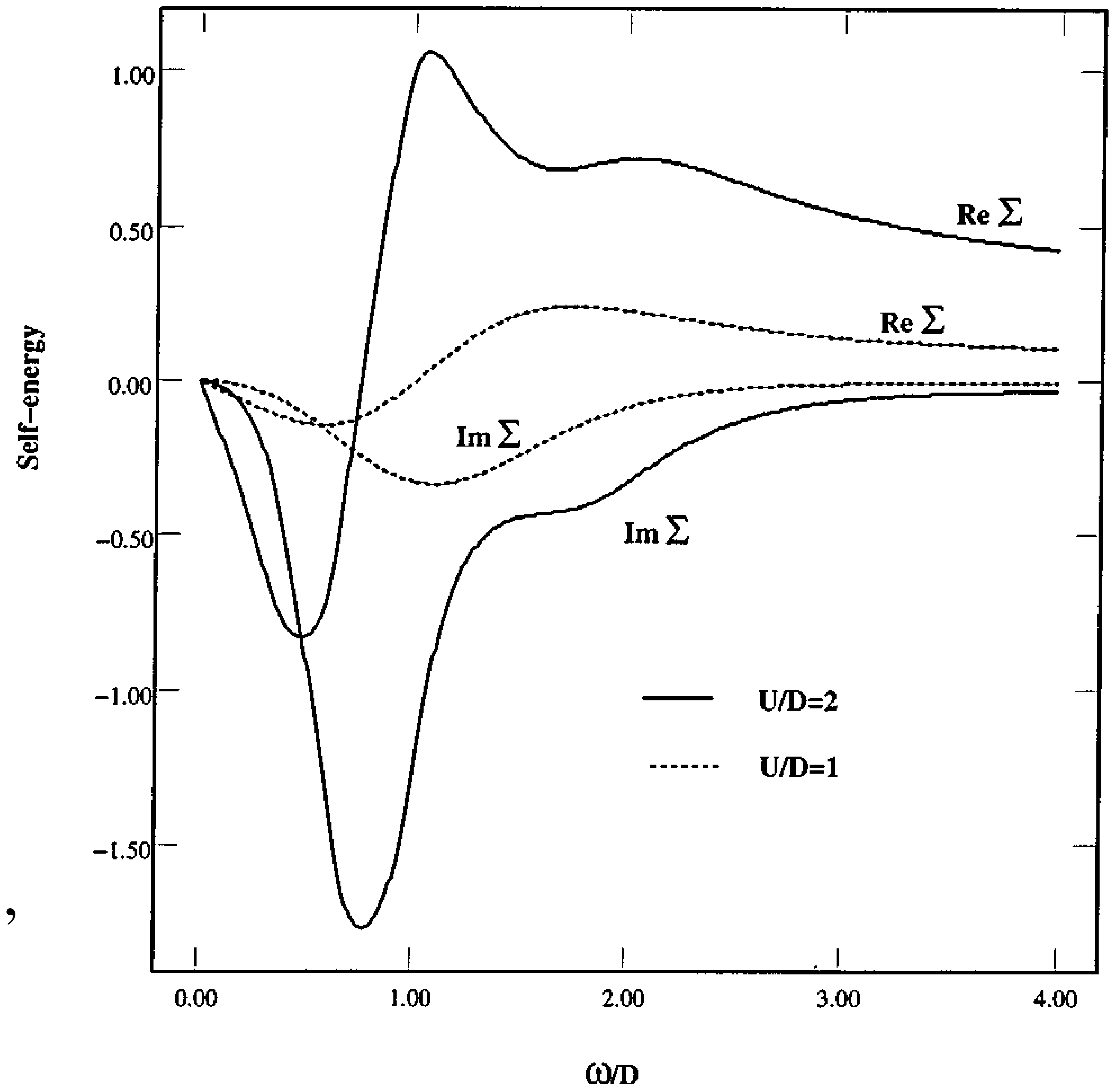
2 solutions

- Metallic solution : $\Delta(0) \neq 0$, Kondo effect

Spectral function



Self-energies in metal



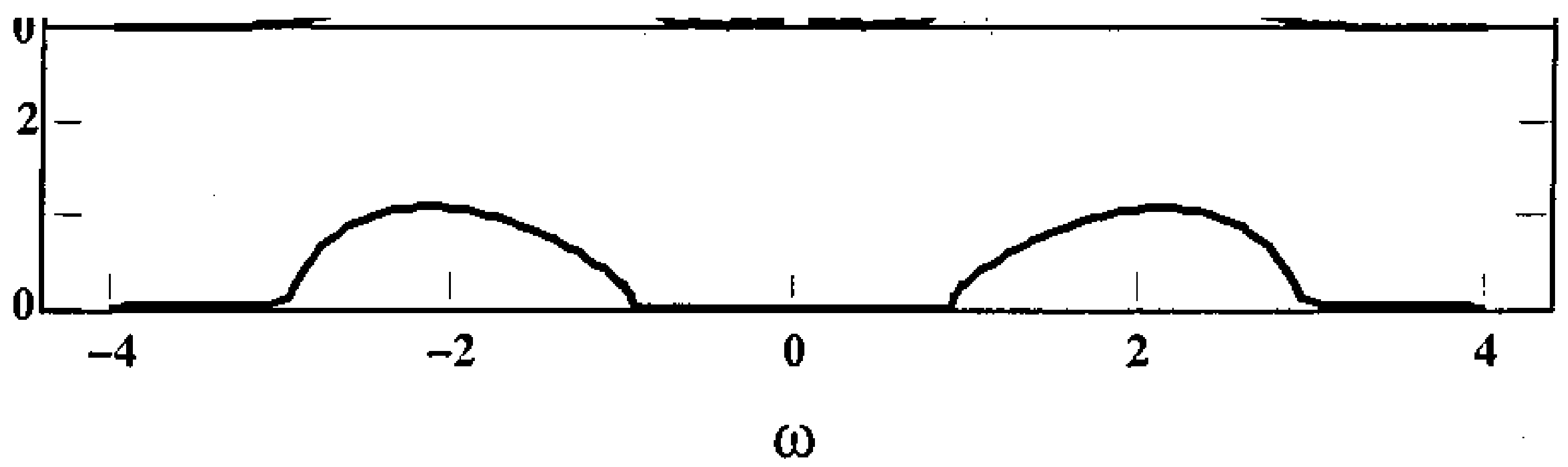
$$\mathrm{Re}\Sigma(\omega+i0^+)=U/2+(1-1/Z)\omega+O(\omega^3),$$

$$\mathrm{Im}\Sigma(\omega+i0^+)=-B\omega^2+O(\omega^4).$$

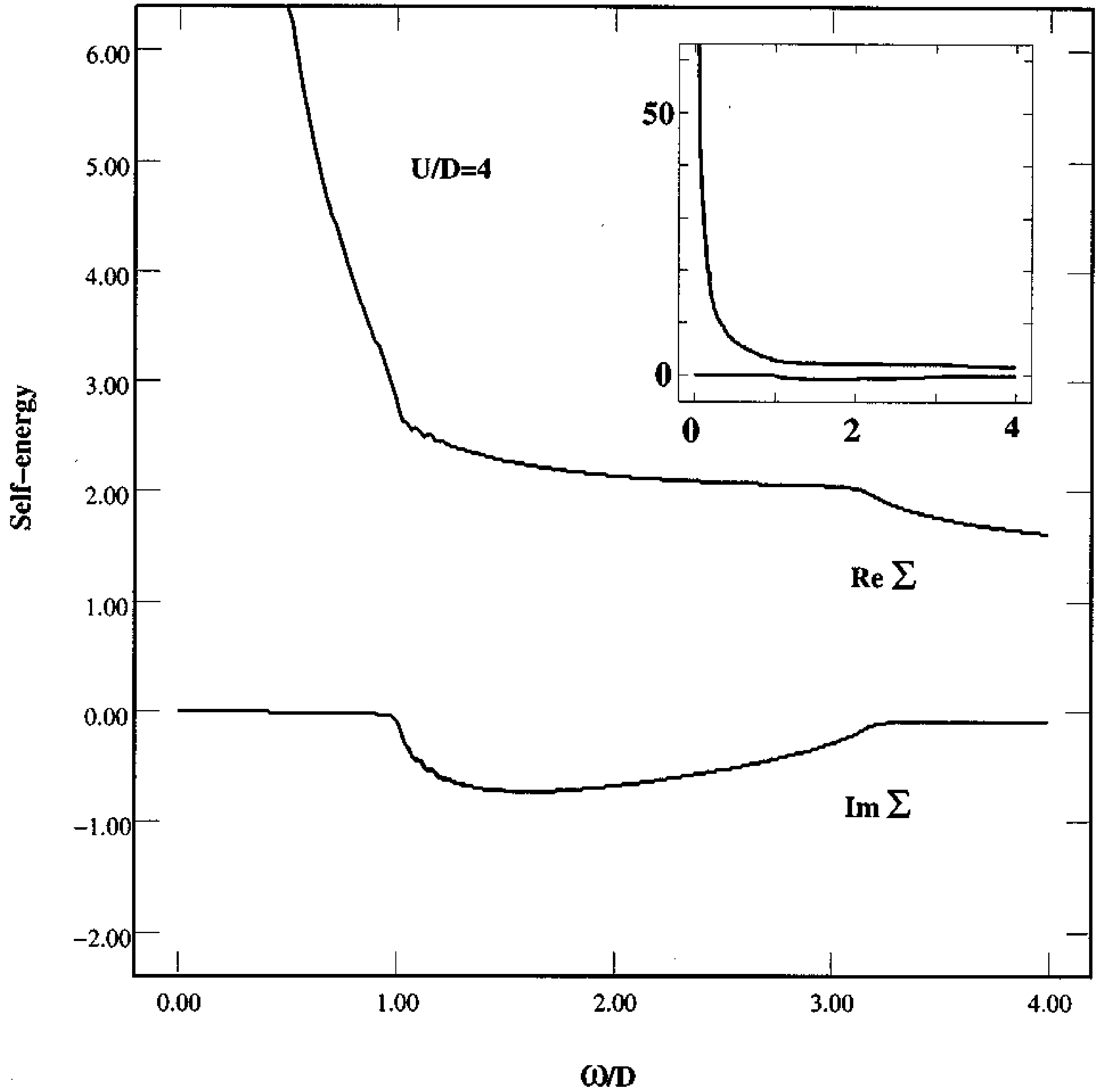
2 solutions

- Insulating solution : Δ(0) = 0 : gapped bath ⇒ no Kondo effect

Spectral function (U/D=4)



Self-energies in insulator



Atomic limit

$$G(i\omega_n) = \frac{1}{2}\left(\frac{1}{i\omega_n + U/2} + \frac{1}{i\omega_n - U/2}\right)$$

$$\Sigma(i\omega_n) = \frac{U^2}{2i\omega_n}$$

A Dynamical Mean Field

- Transfer of spectral weight from low to high ω
- Fermi liquid with low coherence scale $T^* = ZD$
- Hubbard bands
- DMFT valid above T* :
  the QP peak "melts"
- Beyond a low energy static quasi-particle description
  - Given by slave bosons
  - Valid below T*

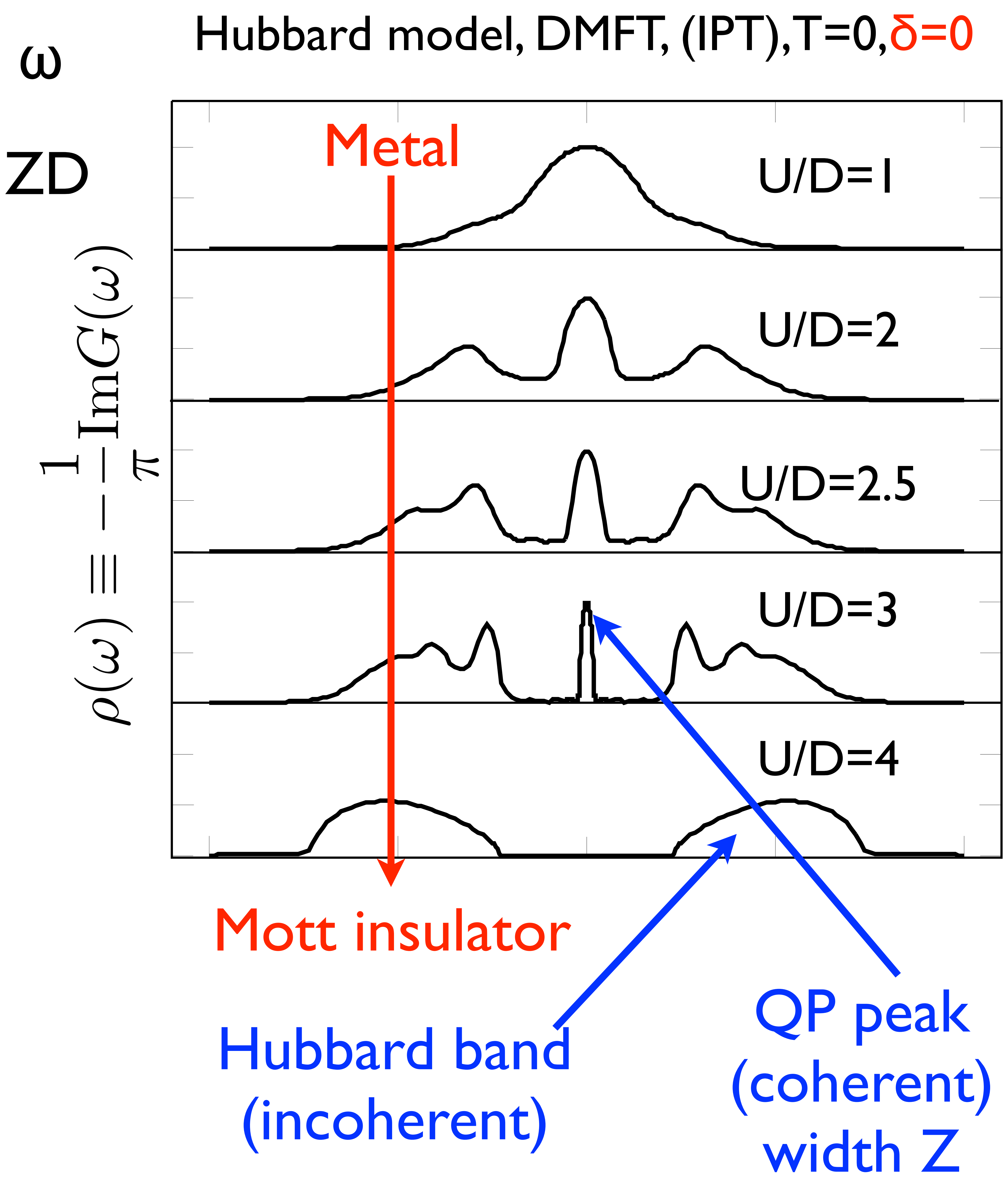
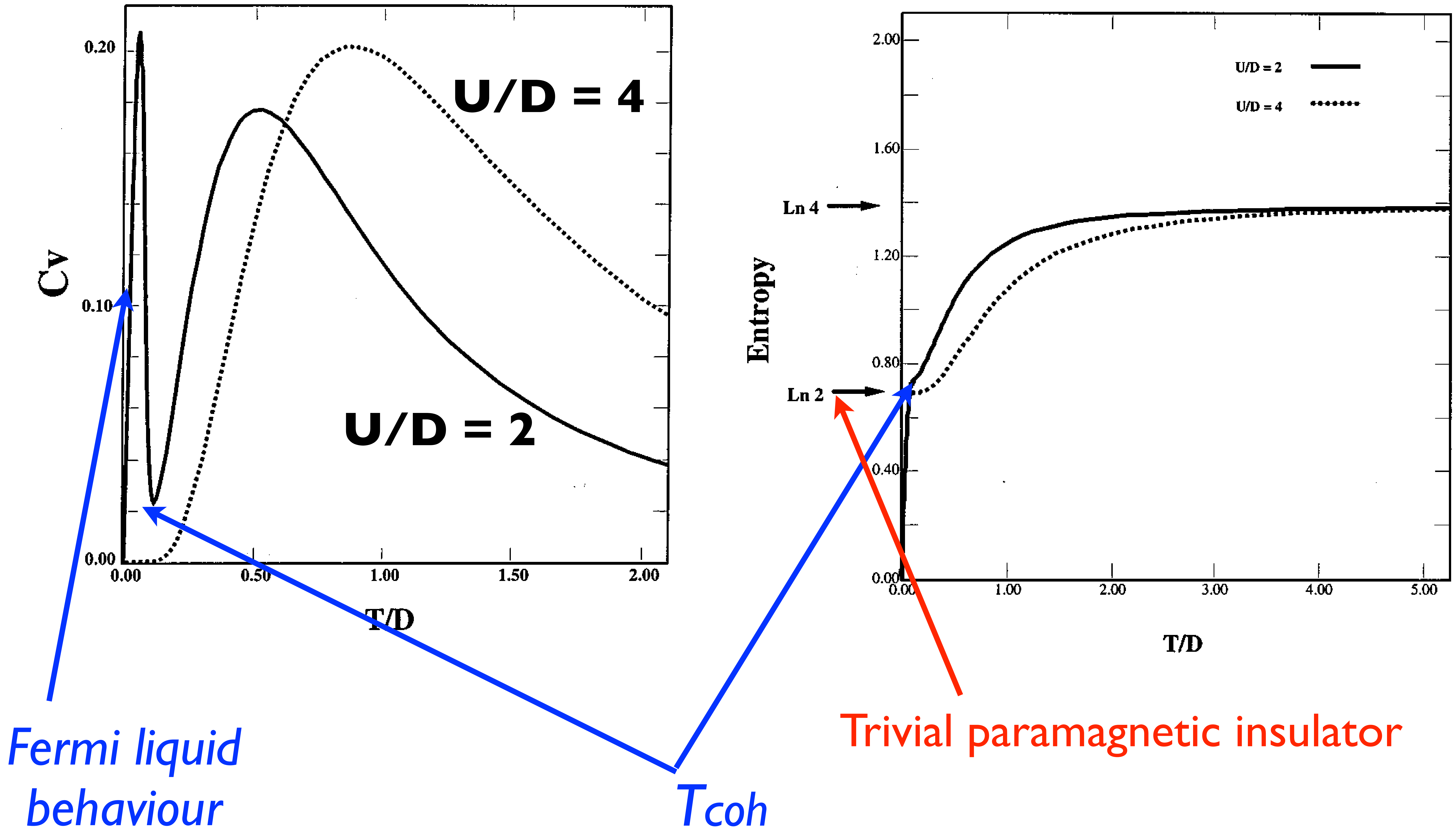
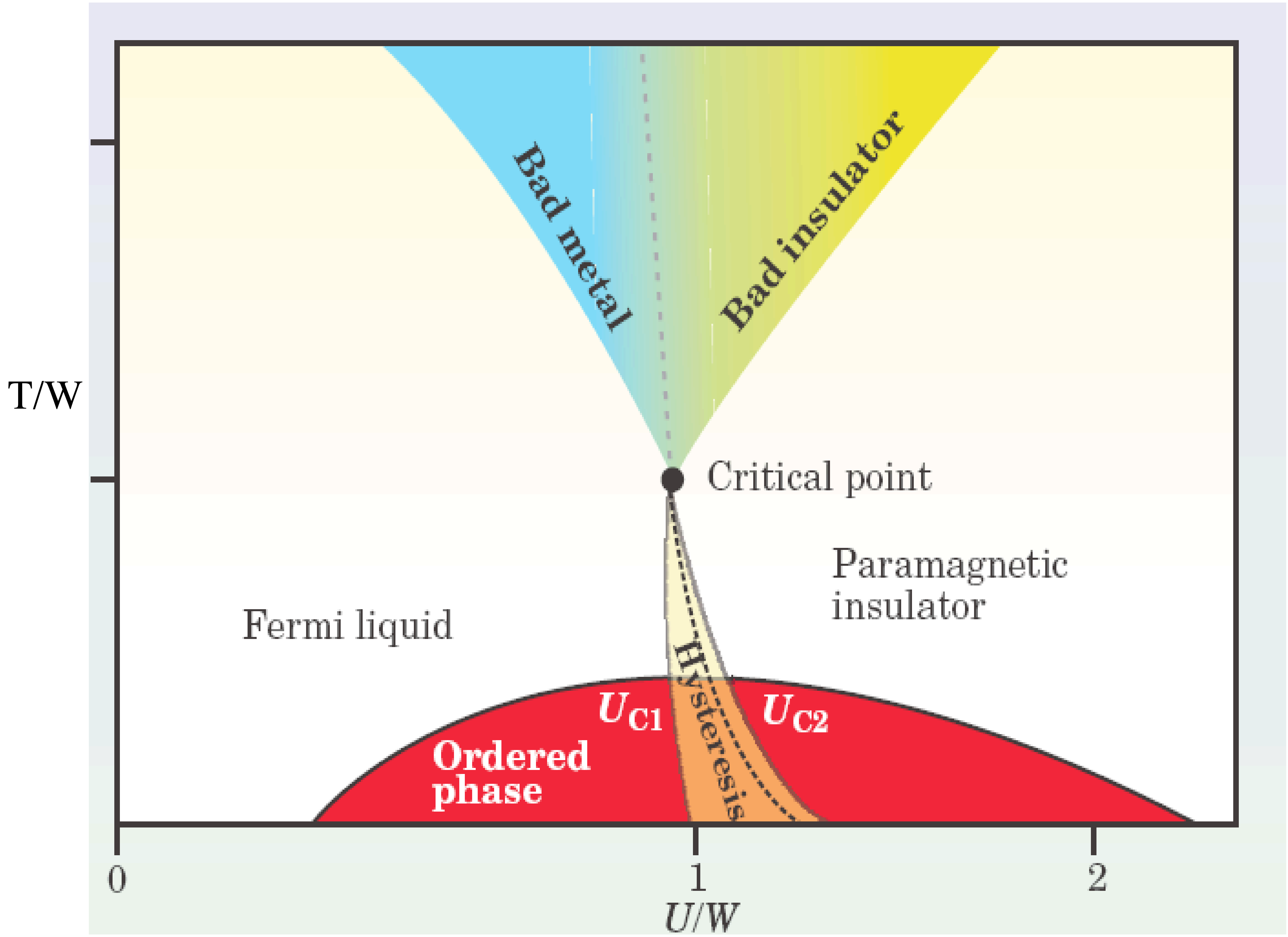


Illustration of the low-coherence temperature

- Thermodynamics quantities

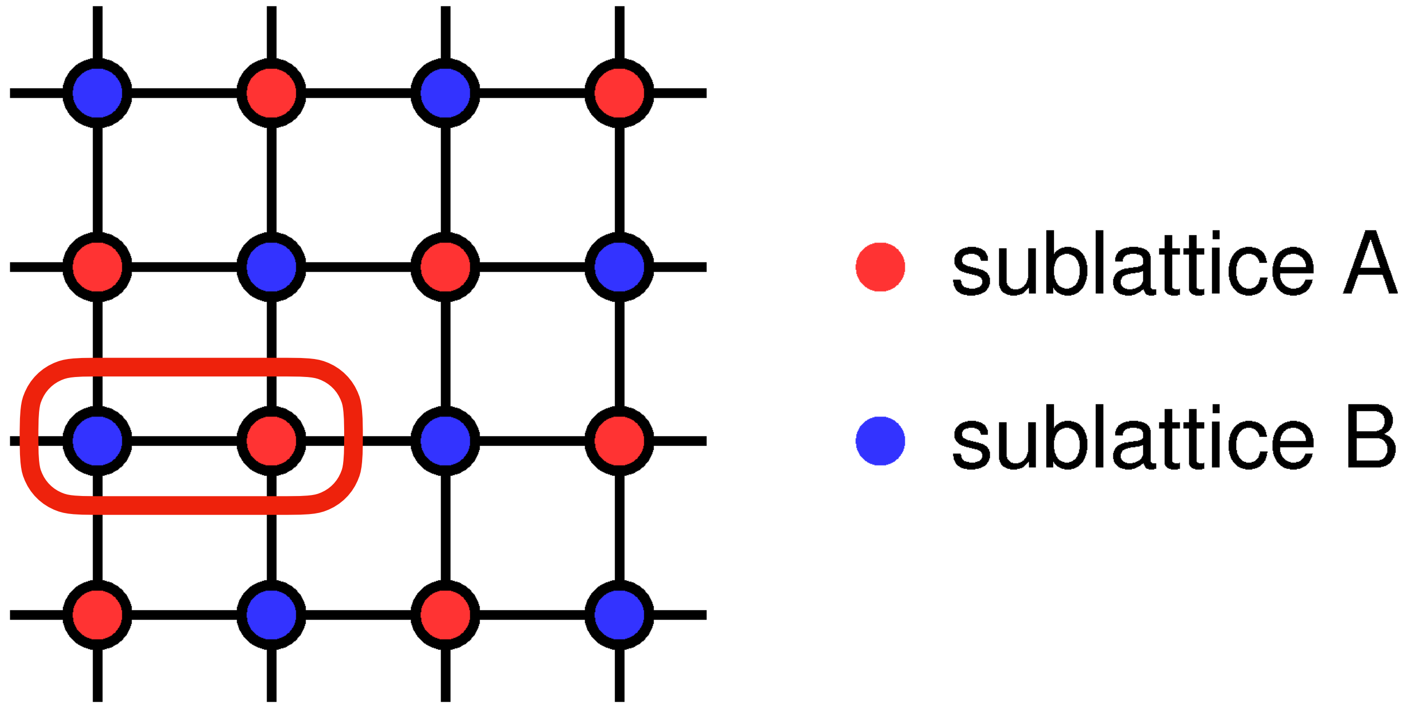


Complete phase diagram



Ordered phase

- DMFT is a mean field. It can be converged in an ordered phase.
- Bath is ordered.
- Example : Antiferromagnetism



$$\Phi[G_{A\sigma}, G_{B\sigma}]$$

$$\Sigma_{A\sigma}(i\omega_n) = \Sigma_{B-\sigma}(i\omega_n)$$

- In the reduced Brillouin zone for cluster (A,B)

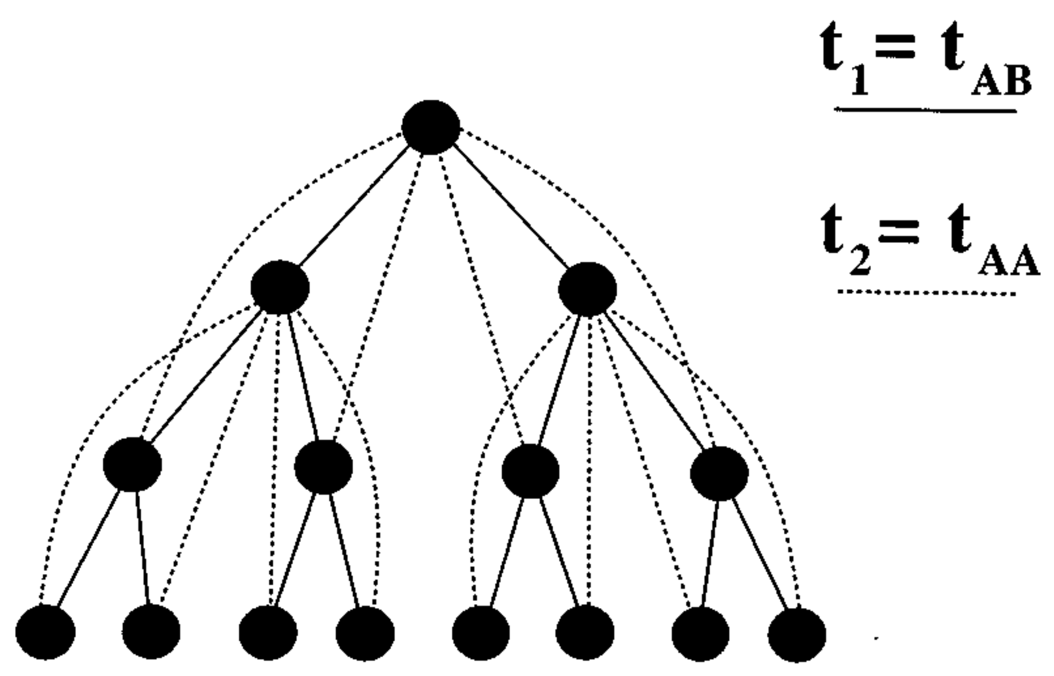
Remark on frustrated systems

- DMFT paramagnetic equations = equations of a frustrated system

$$\mathcal{G}_{0\sigma}^{-1}(i\omega_n) = i\omega_n + \mu - \sigma h_{\mathrm{AF}} - t^2\, G_{-\sigma}^{\mathrm{imp}}(i\omega_n)$$

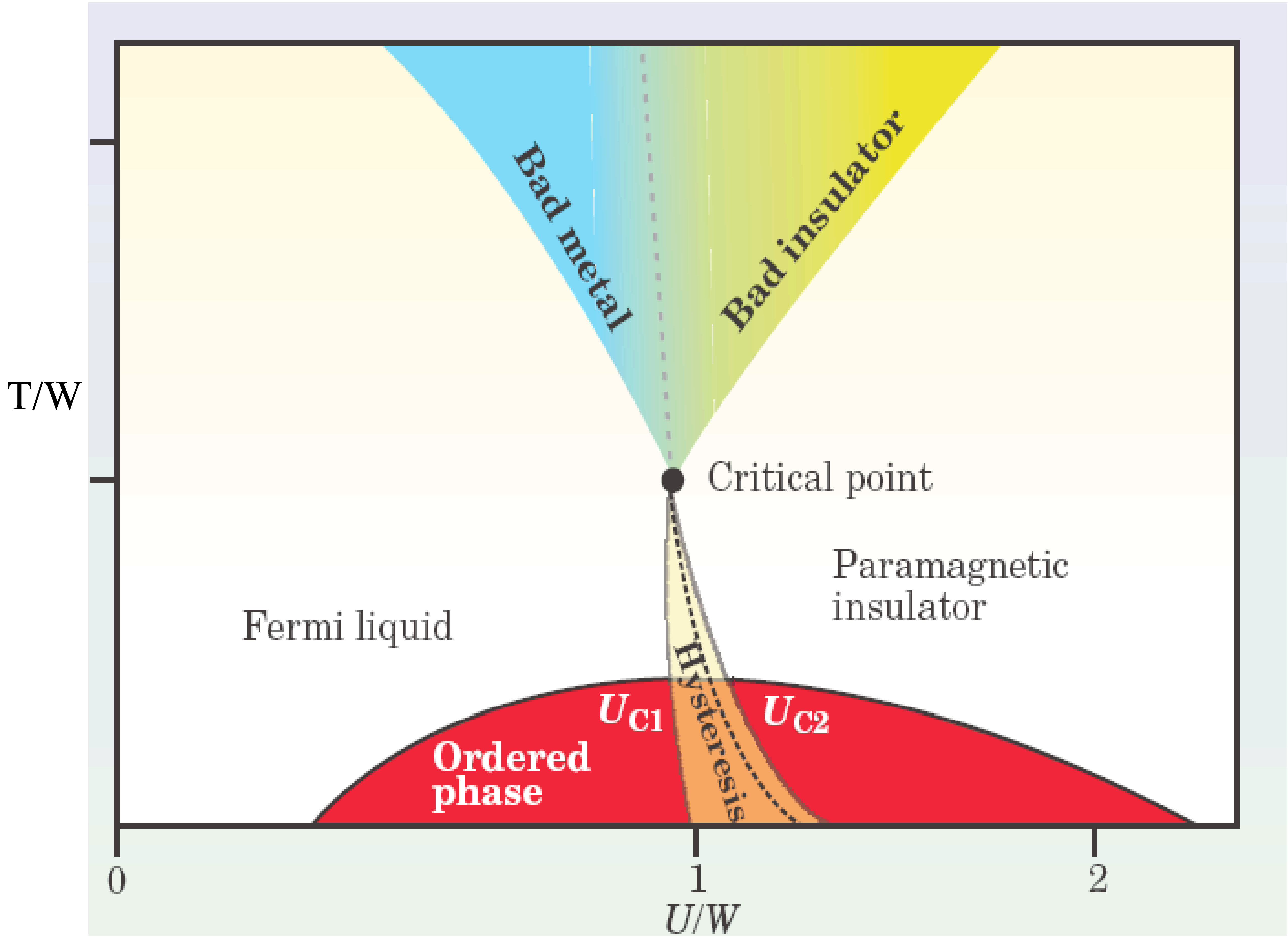
- E.g. a frustrated Bethe lattice (paramagnetic phase).

$$\mathcal{G}_{0\sigma}^{-1}(i\omega_n) = i\omega_n + \mu - \sigma h_{\mathrm{AF}} - (t_1^2 + t_2^2)\, G_{-\sigma}^{\mathrm{imp}}(i\omega_n)$$



Complete phase diagram

- With frustration (or AF would be much higher)

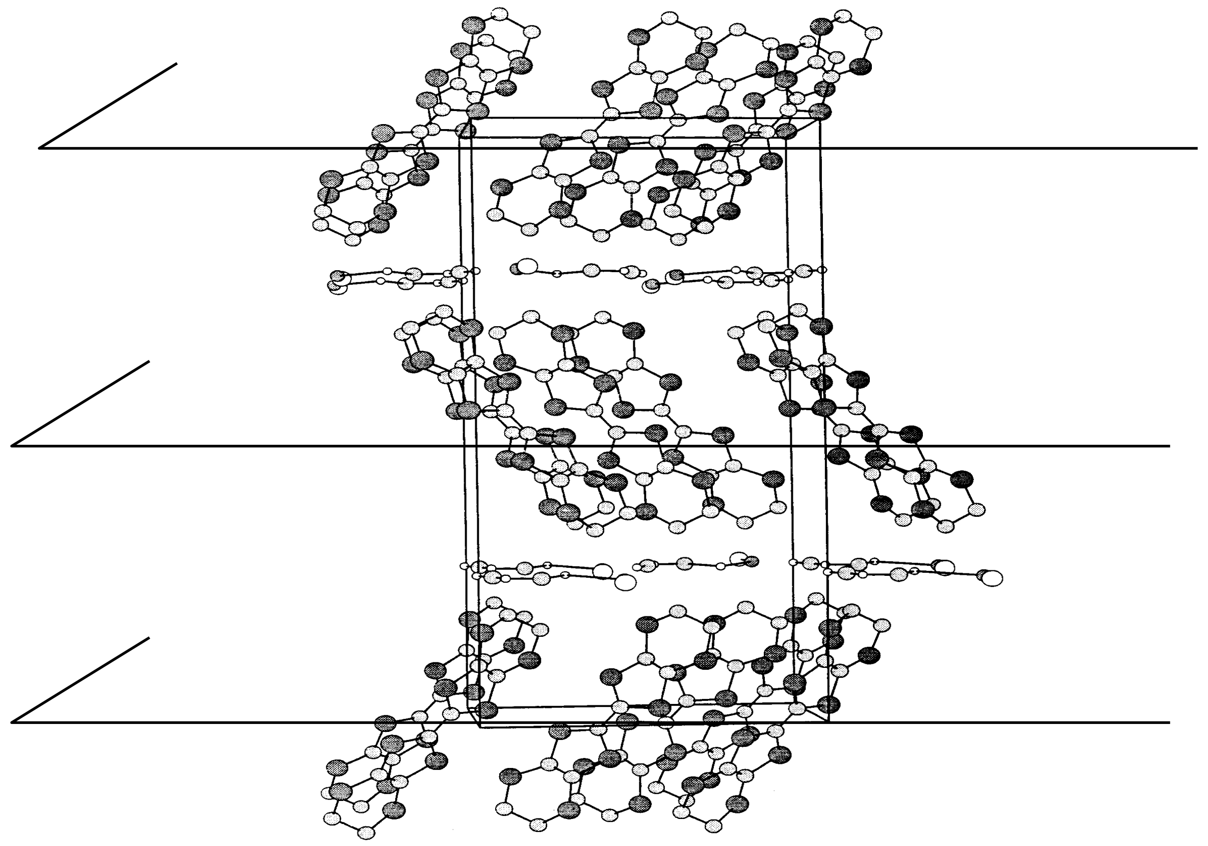


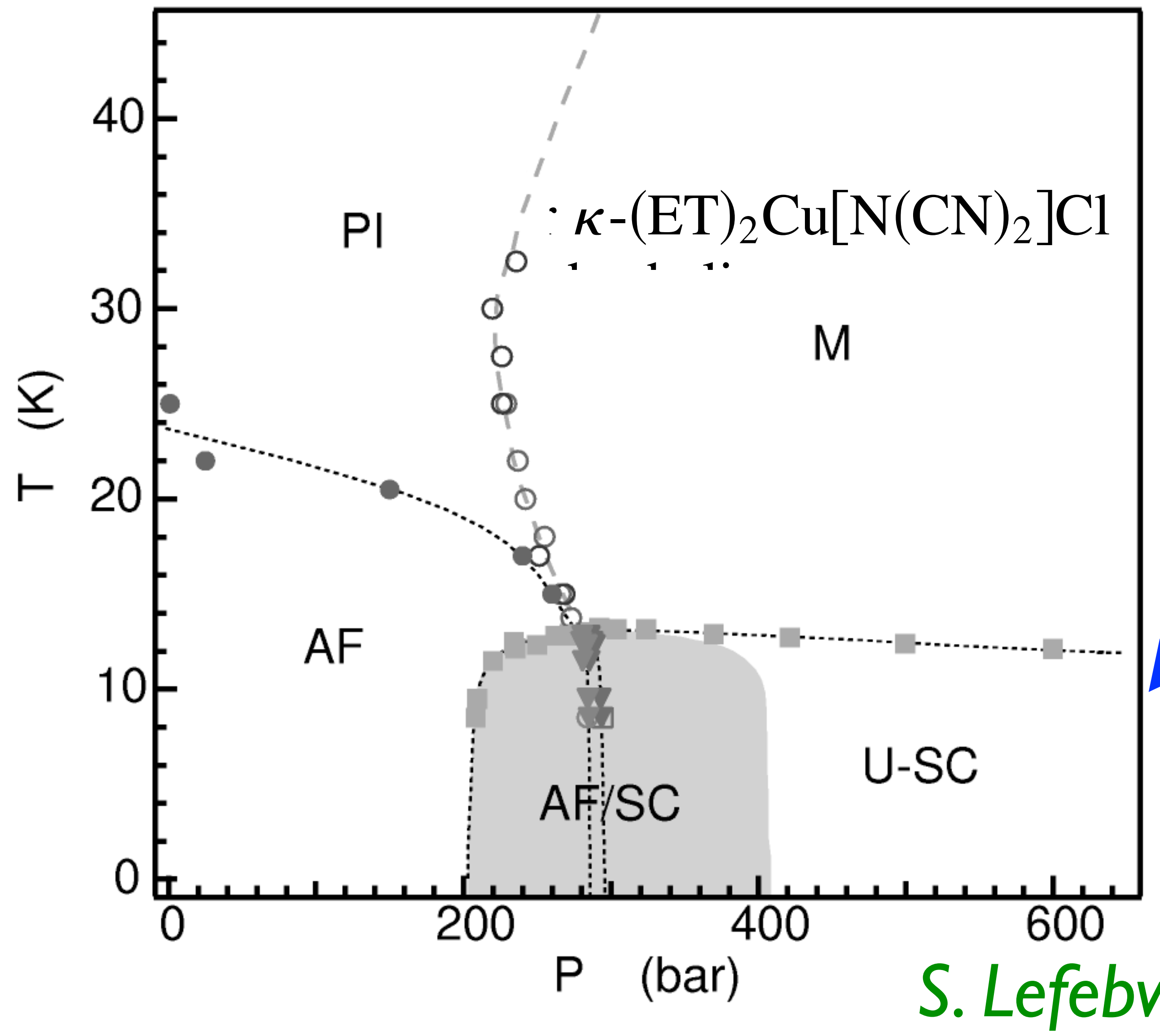
Comparison with some experiments

Organics (resistivity measurements)

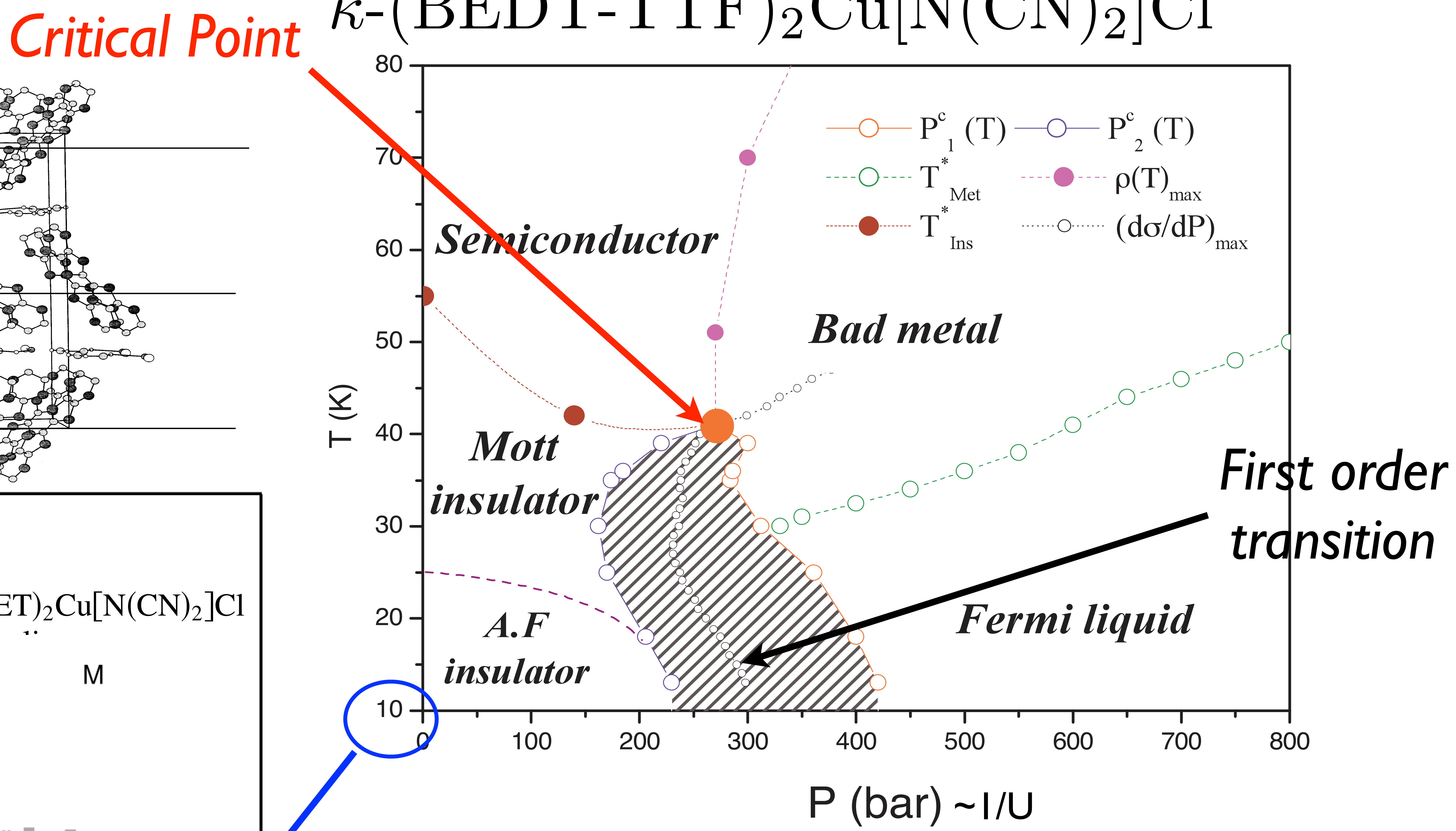
- 2-d organics : resistivity measurement versus T and pressure P.

κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl



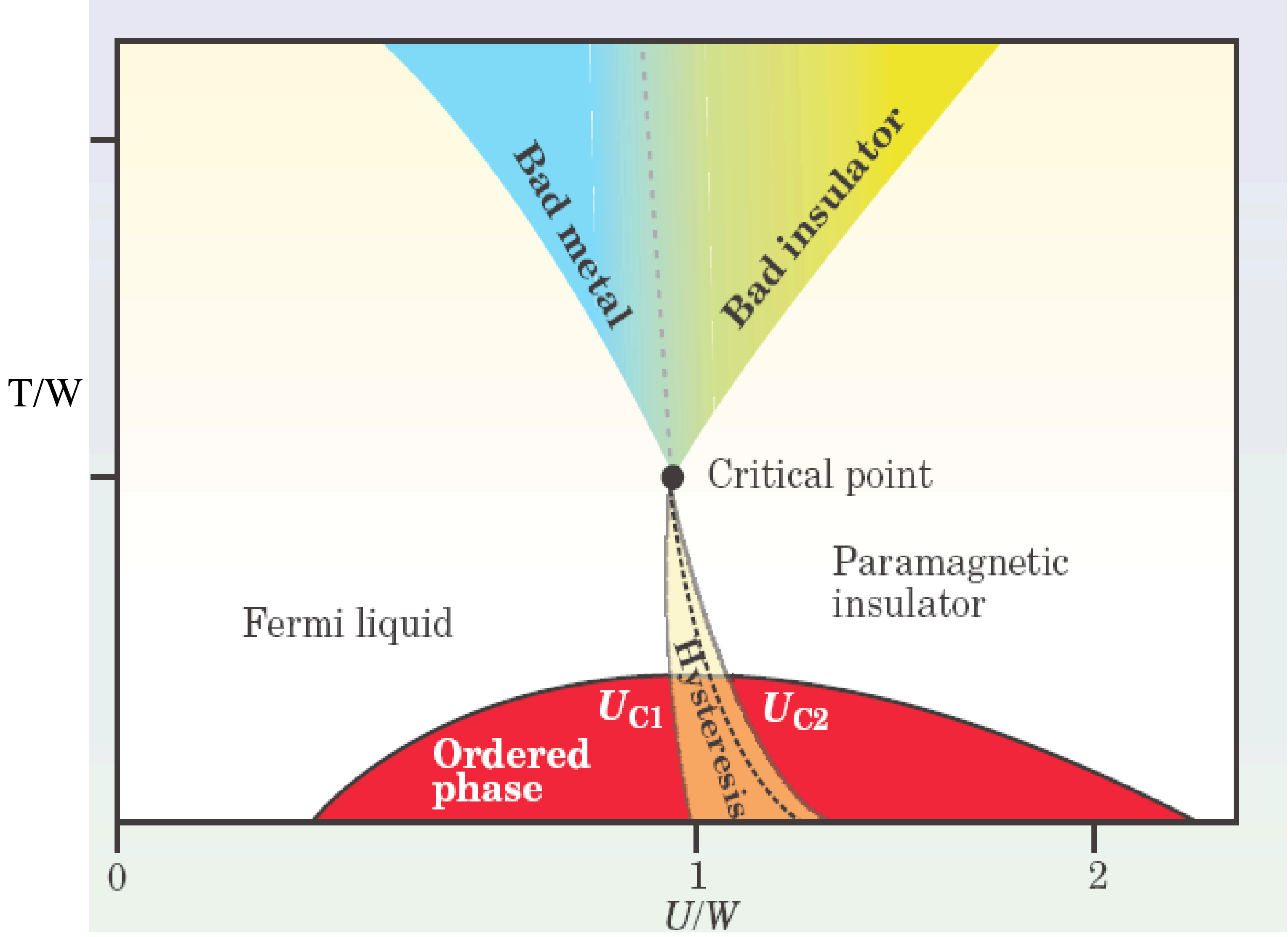


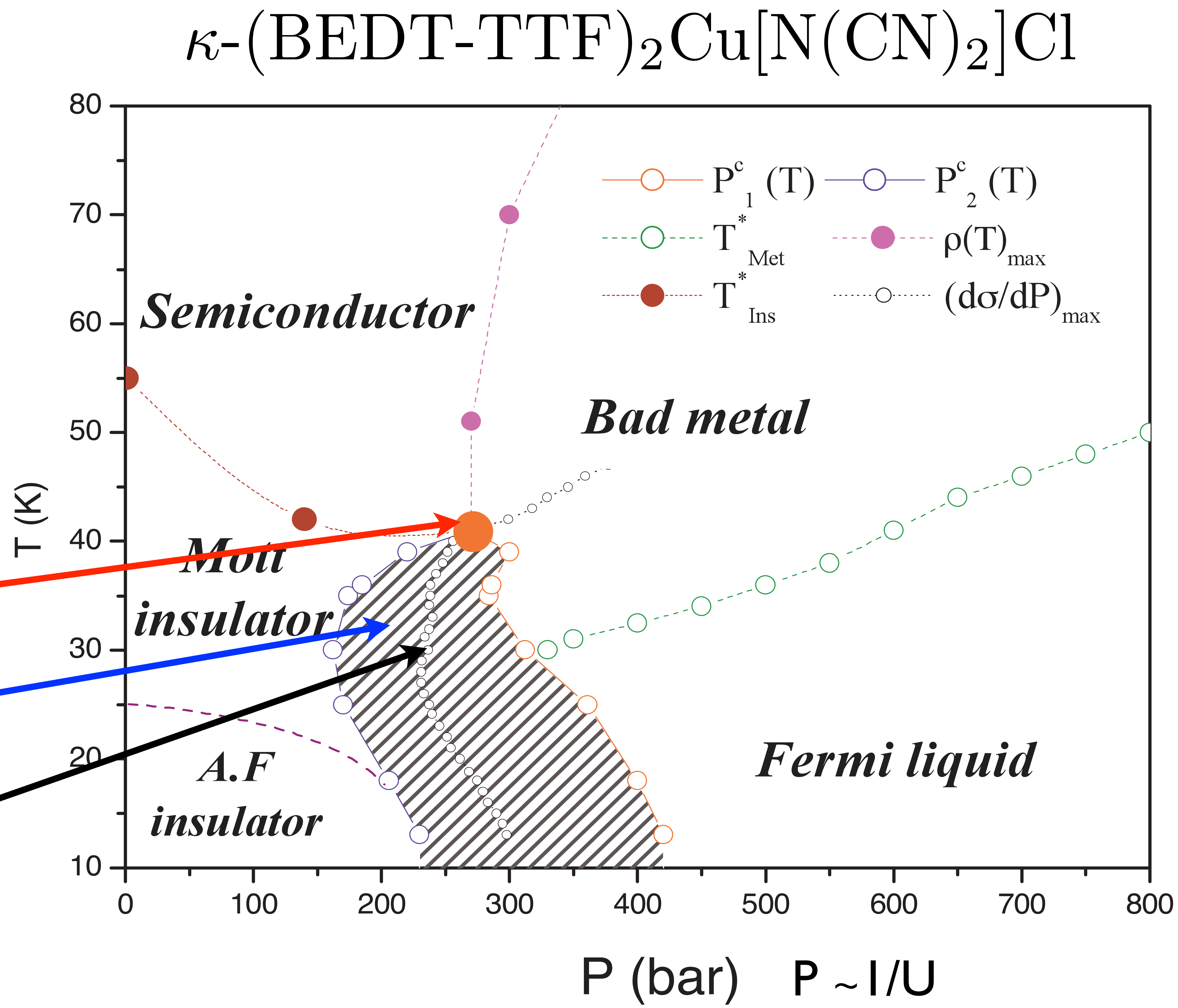
S. Lefebvre et al. PRL 85, 5420 (2000)



P. Limelette, et al. PRL 91, 016401 (2003)

Comparison with organics : phase diagram





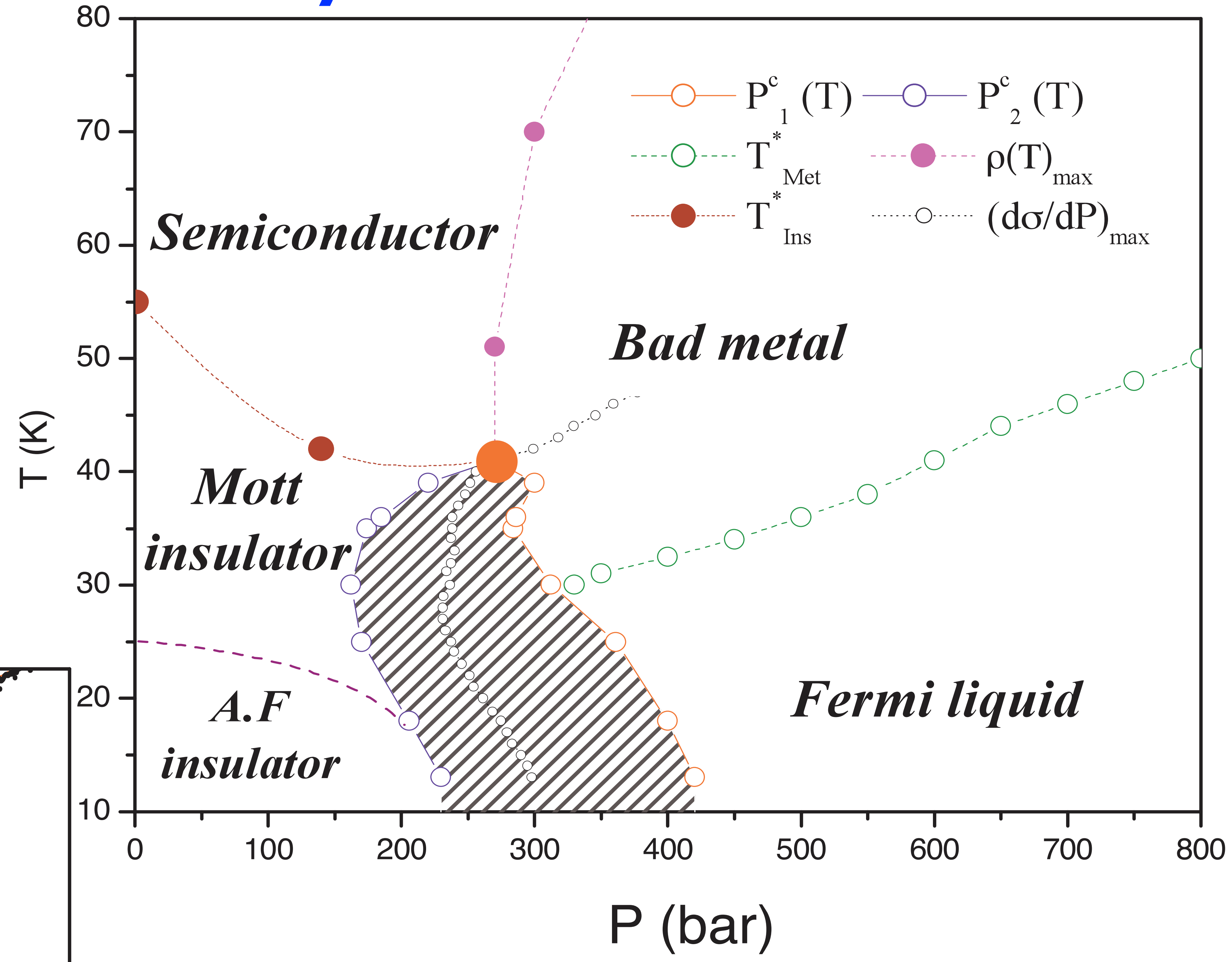
Critical Point

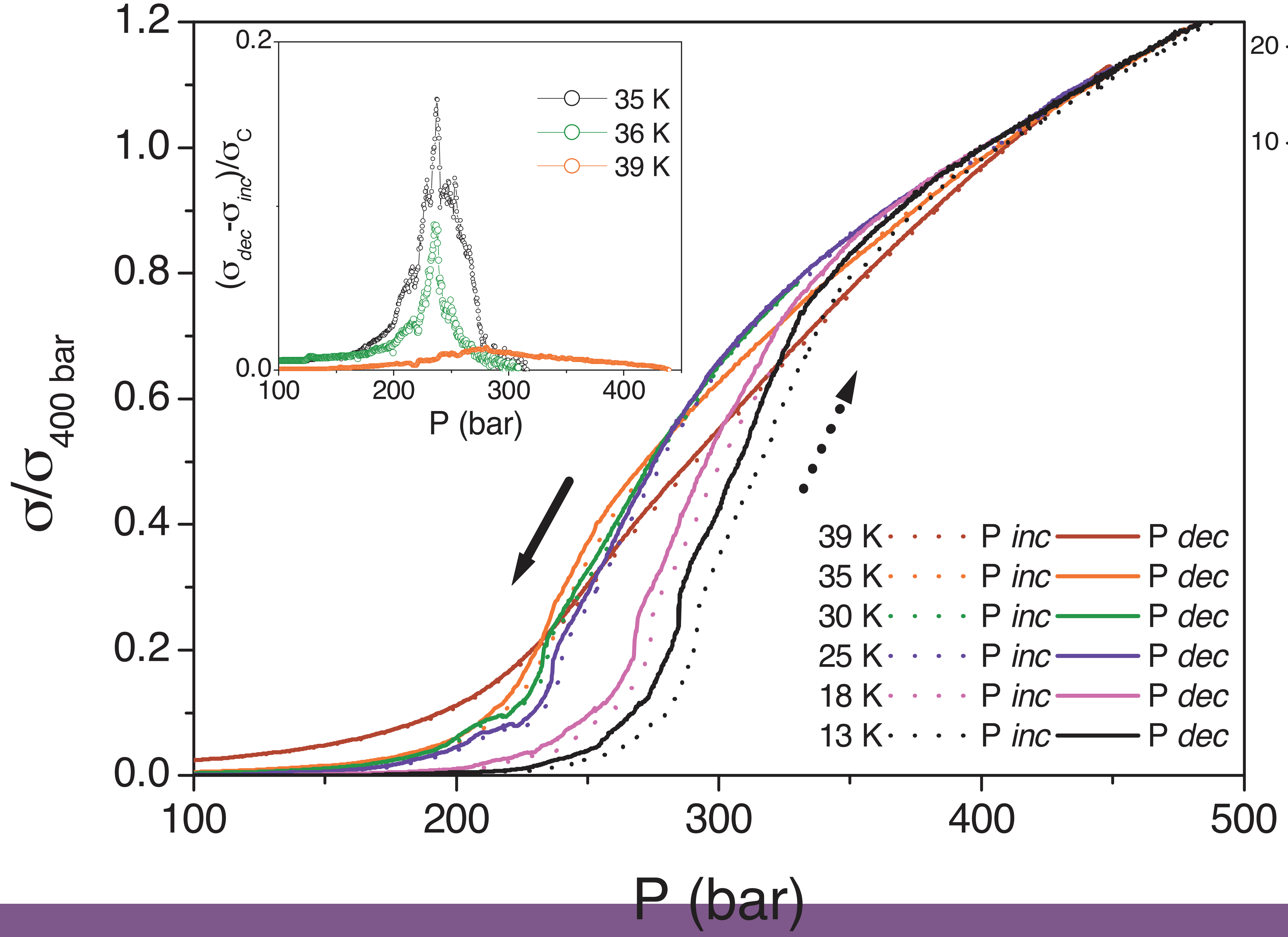
Coexistence region

First order transition

P. Limelette, et al. PRL 91, 016401 (2003)

Experimental evidence for hysteresis





How to solve DMFT equations ?

The toolbox

Solving DMFT : iterative method

Impurity solver

$$S_{\rm eff} = -\int_0^\beta\int_0^\beta d\tau\, d\tau'\; c^\dagger_\sigma(\tau)\,\mathcal{G}^{-1}_{0\sigma}(\tau-\tau')\,c_\sigma(\tau') \;+\; \int_0^\beta d\tau\, U\, n_\uparrow(\tau)\, n_\downarrow(\tau)$$

$$G_{\sigma\rm imp}(\tau) \equiv -\left\langle T c_\sigma(\tau) c^\dagger_\sigma(0)\right\rangle_{S_{\rm eff}}$$

$$\Sigma_{\sigma\rm imp}(i\omega_n) \equiv \mathcal{G}^{-1}_\sigma(i\omega_n) - G^{-1}_{\sigma\rm imp}(i\omega_n)$$

$\mathcal{G}_0$

G imp, Σimp

Self consistency condition

$$G_{\sigma\rm imp}[\mathcal{G}_0](i\omega_n) = \sum_k \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_{\sigma\rm imp}[\mathcal{G}_0](i\omega_n)}$$

- In practice, the iterative loop is (almost) always convergent.

Quantum impurity solvers : the bottleneck !

$$S_{\mathrm{eff}} = -\iint_0^\beta d\tau d\tau' c_a^\dagger(\tau)\mathcal{G}_{ab}^{-1}(\tau-\tau')c_b(\tau') + \int_0^\beta d\tau H_{\mathrm{loc}}(\{c_a^\dagger, c_a\})(\tau)$$

$$\mathcal{G}_{ab}^{-1}(i\omega_n) = (i\omega_n + \mu)\delta_{ab} - \Delta_{ab}(i\omega_n)$$

Bath

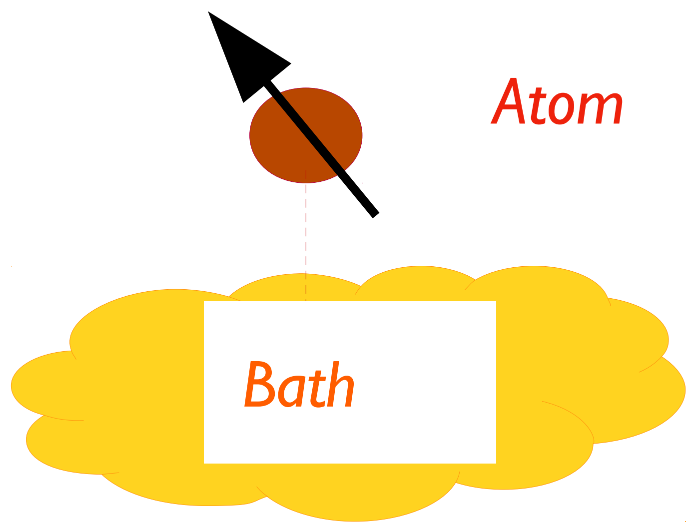
Interaction

a,b = 1,N : degree of freedom (e.g. spin, orbital index, ...)

- Ok for one band systems.
- For realistic systems, many challenges still …

Quantum impurity solvers: challenges

- **Larger,** more complex systems (spin orbit, low symmetry, many orbitals, large clusters)
- *Faster* (explore parameter space, e.g. compute structure).
- High precision (e.g. for transport at low T)
  - Low frequency, temperature.
  - Transport computations (require high precision self-energy at low ω)
- Real time, out of equilibrium.



Algorithm development is crucial here !

The DMFT solver toolbox

- Exact/Controlled algorithms
  - Continuous Time Quantum Monte Carlo (CTQMC). *Cf Lecture by M. Ferrero*
  - Exact diagonalization (ED).
  - Numerical Renormalization group (NRG).
  - Tensor network (DMRG). Many flavors.

- Approximate solvers, e.g.
  - Iterated Perturbation Theory (IPT).
  - NCA family (NCA, OCA, …)
  - Slave bosons / Hartree-Fock / “Hubbard I”

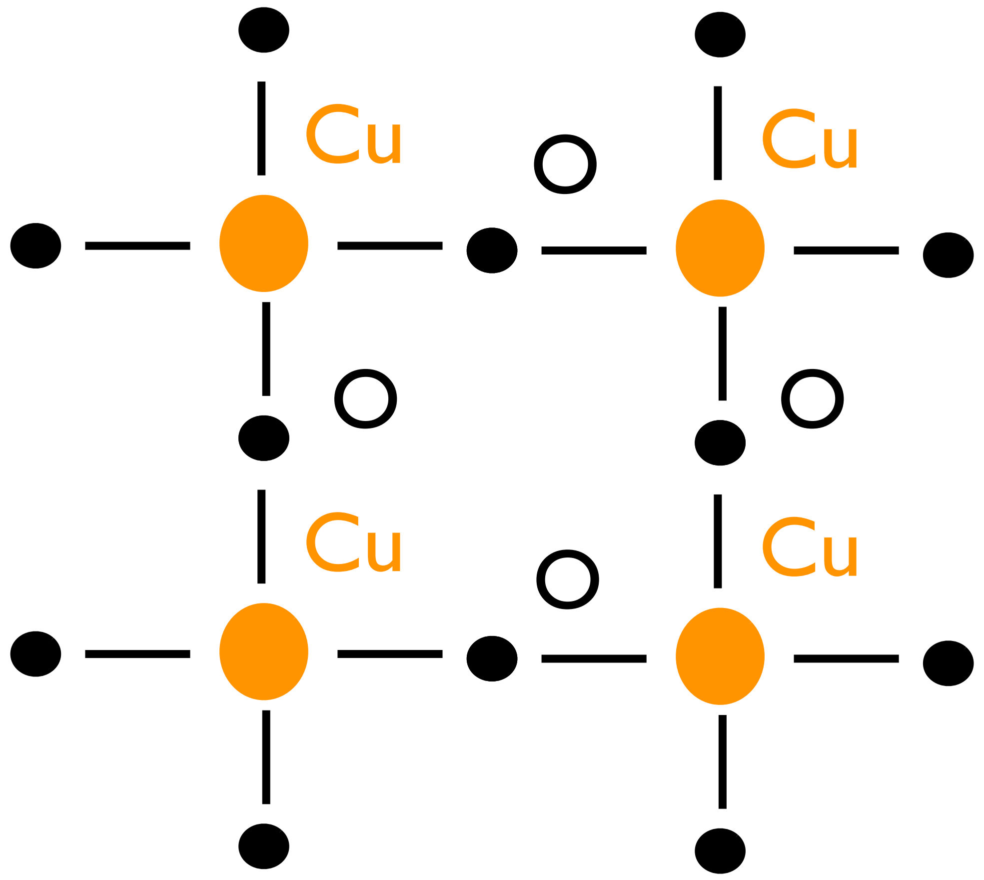
Conclusion:

This is just the beginning …

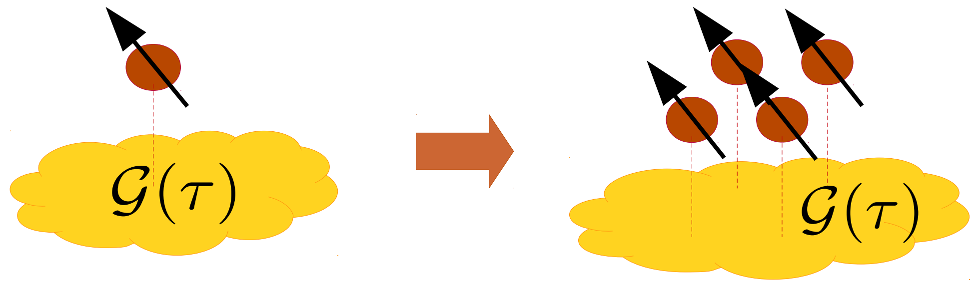
DMFT: a versatile technique

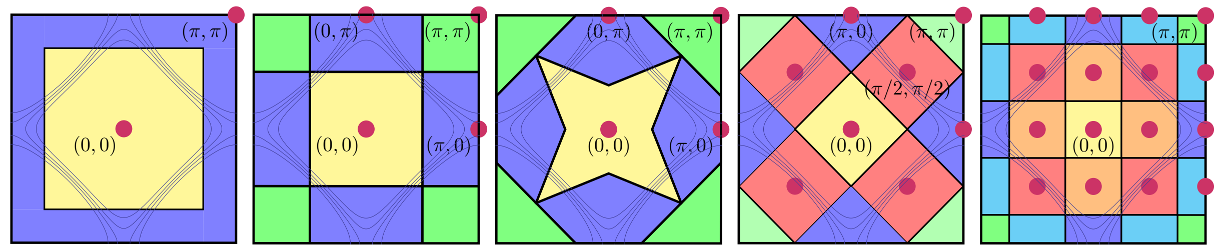
- Choice of correlated orbitals

$$\Sigma(\omega) = \begin{pmatrix} \Sigma^{\mathrm{imp}}(\omega) & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$



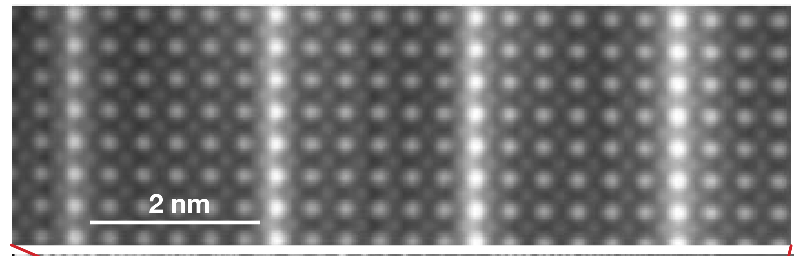
- Clusters (real/reciprocal spaces)





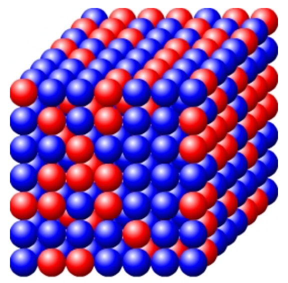
- k-dependence of Σ, ordered phase.

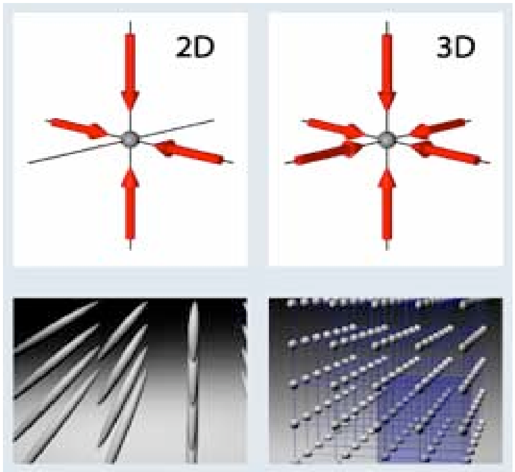
- Non translation invariant systems
  (e.g. correlated interfaces, cold atoms in a trap)



SrTiO3/LaTiO3

Alloy





- Vertex methods (Trilex, DGA, …)

  - Self-consist on two-body
    Green functions instead of self-energy

DMFT : some references

- The classic.
  A. Georges, G. Kotliar, W. Krauth and M. Rozenberg,
  Rev. Mod. Phys. 68, 13, (1996)

- On realistic computations (DFT + DMFT)
  G. Kotliar, S.Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, C. Marianetti,
  Rev. Mod. Phys. 78, 865 (2006)

- On Quantum Monte Carlo (DMFT) Impurity solvers
  E. Gull et al.
  Rev. Mod. Phys. 83, 349 (2011)

- On impurity models
  The beauty of impurities: two revivals of Friedel's virtual bound state
  A.Georges, C.R. Physique 17 430 (2016)

Thank you for your attention