Quantum Embeddings, Dynamical Mean Field Theory: an introduction. Part I

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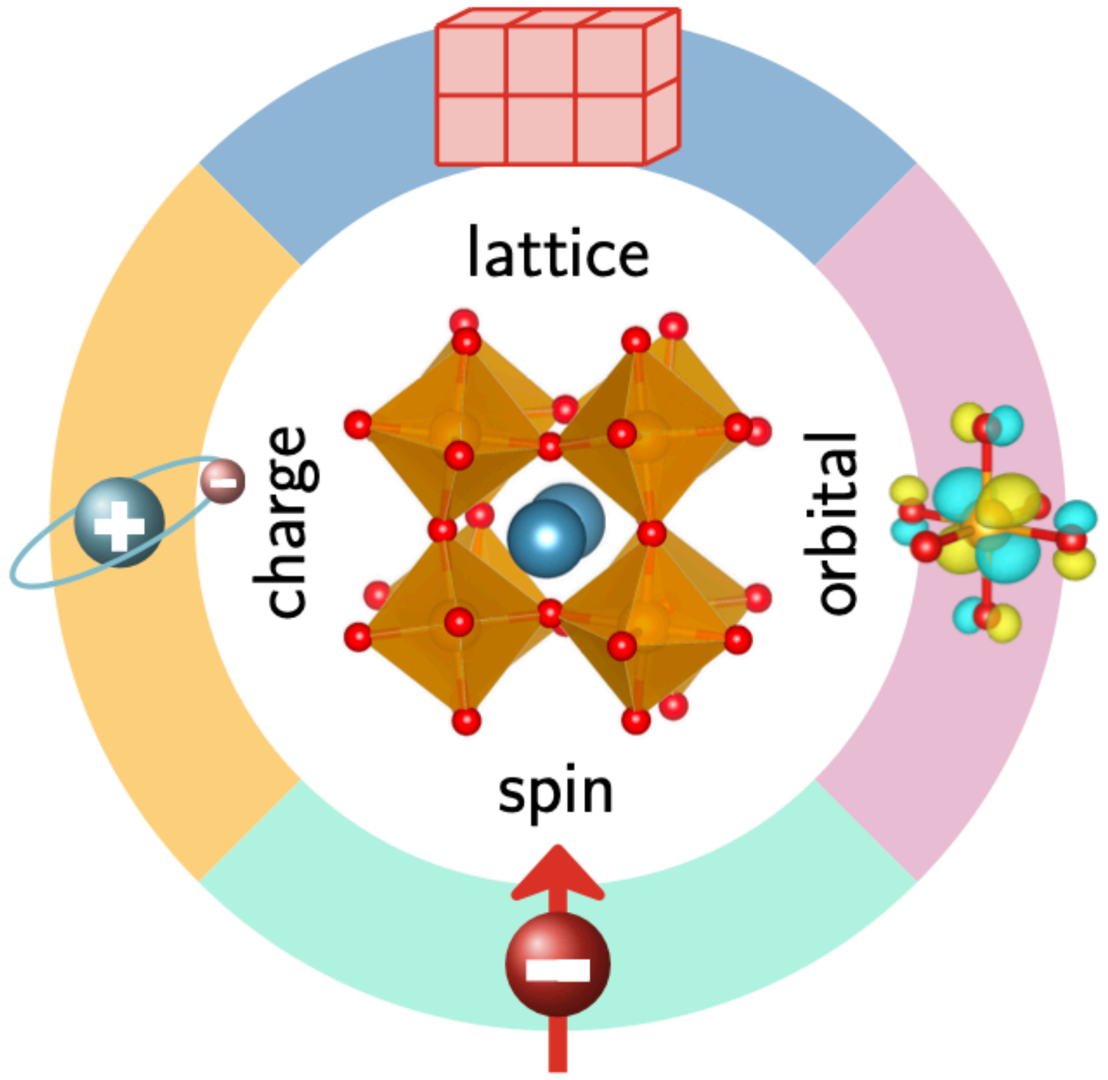
Outline (part I & II)

- Introduction
- Mott transition
- Quantum impurity models
- DMFT: basic formalism
- The Mott transition in DMFT.
- Towards realism: Hund's metal
- Cluster extensions of DMFT.
- Two particle quantities: susceptibilities, transport.
- Quantum impurity solvers: an overview.
- Outlook

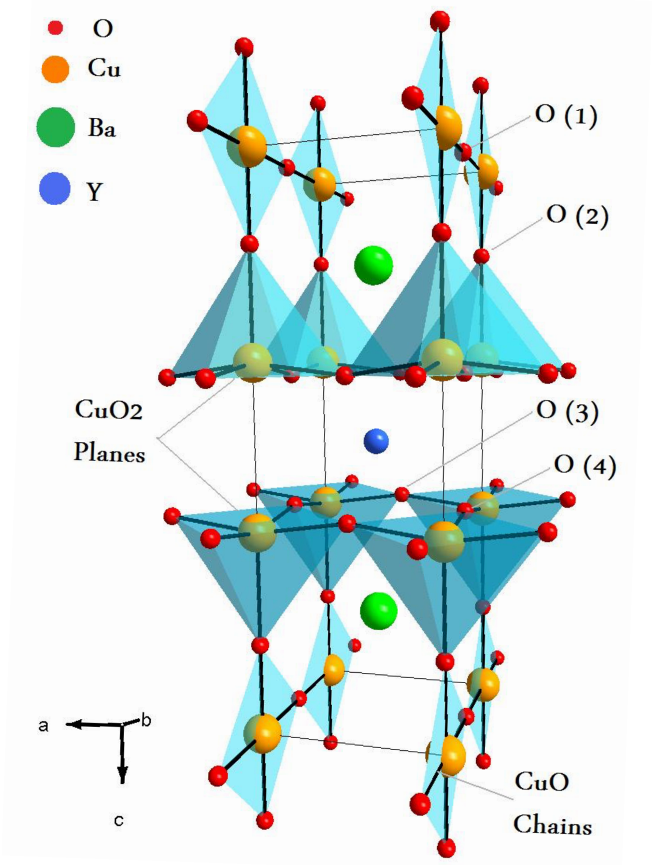
Weak vs Strong Correlations

- 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.

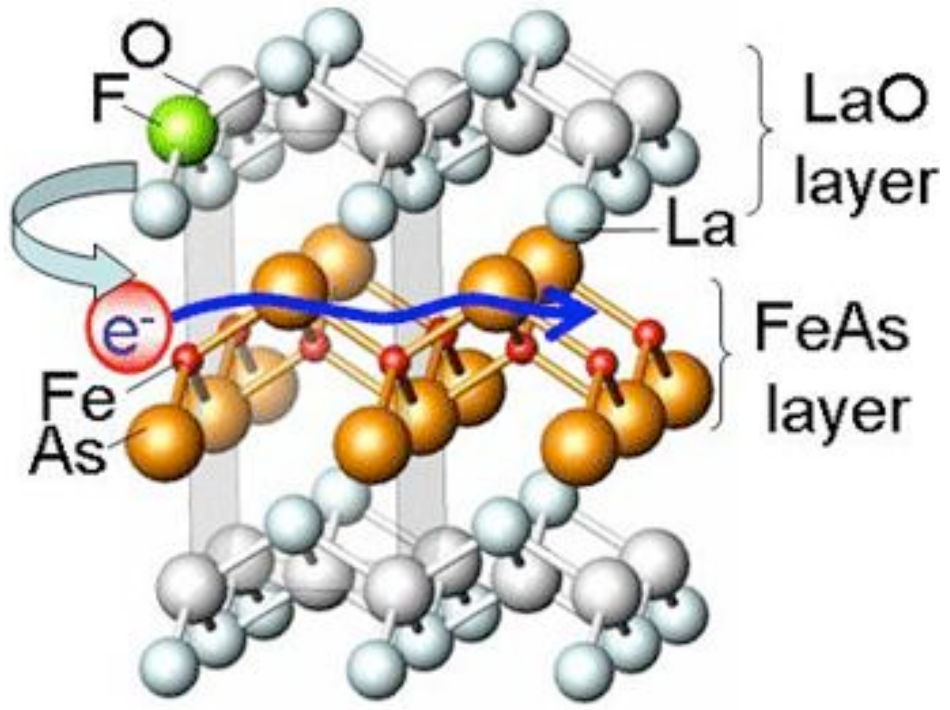


Strongly correlated systems

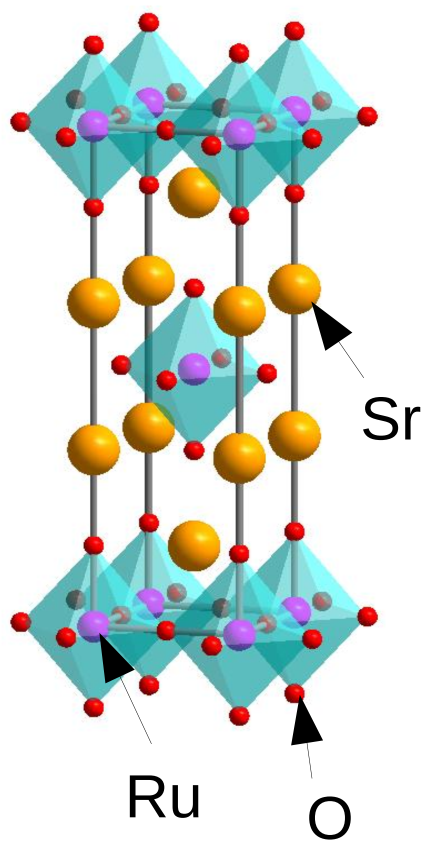
Materials
High Temperature superconductors
Transition metal oxides,



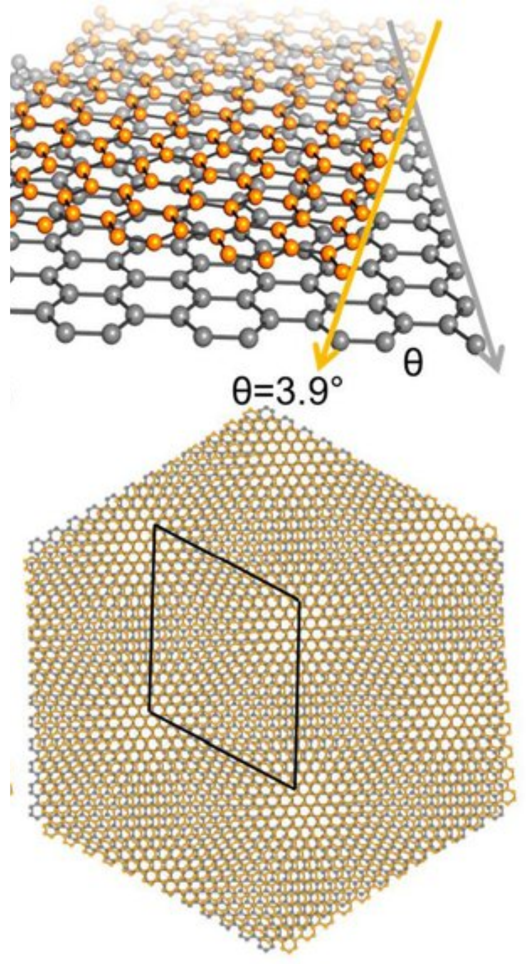
High Temperature superconductors



Fe-Based (2008)

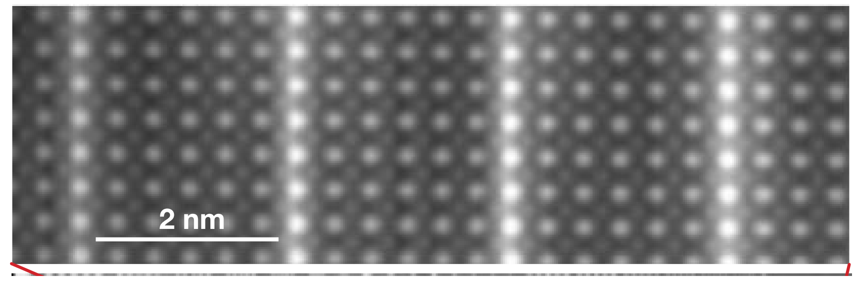


Ruthenates



Twisted bilayer graphene

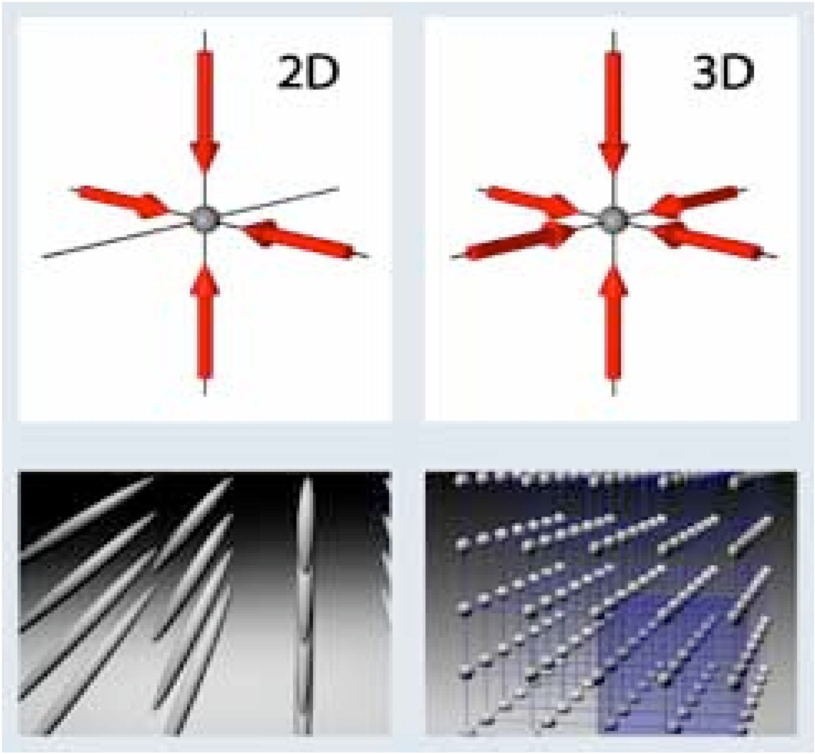
Correlated metal/superconductors at interface of oxides



$SrTiO_3/LaTiO_3$

Ohtomo et al, Nature 2002

Ultra-cold atoms in optical lattices

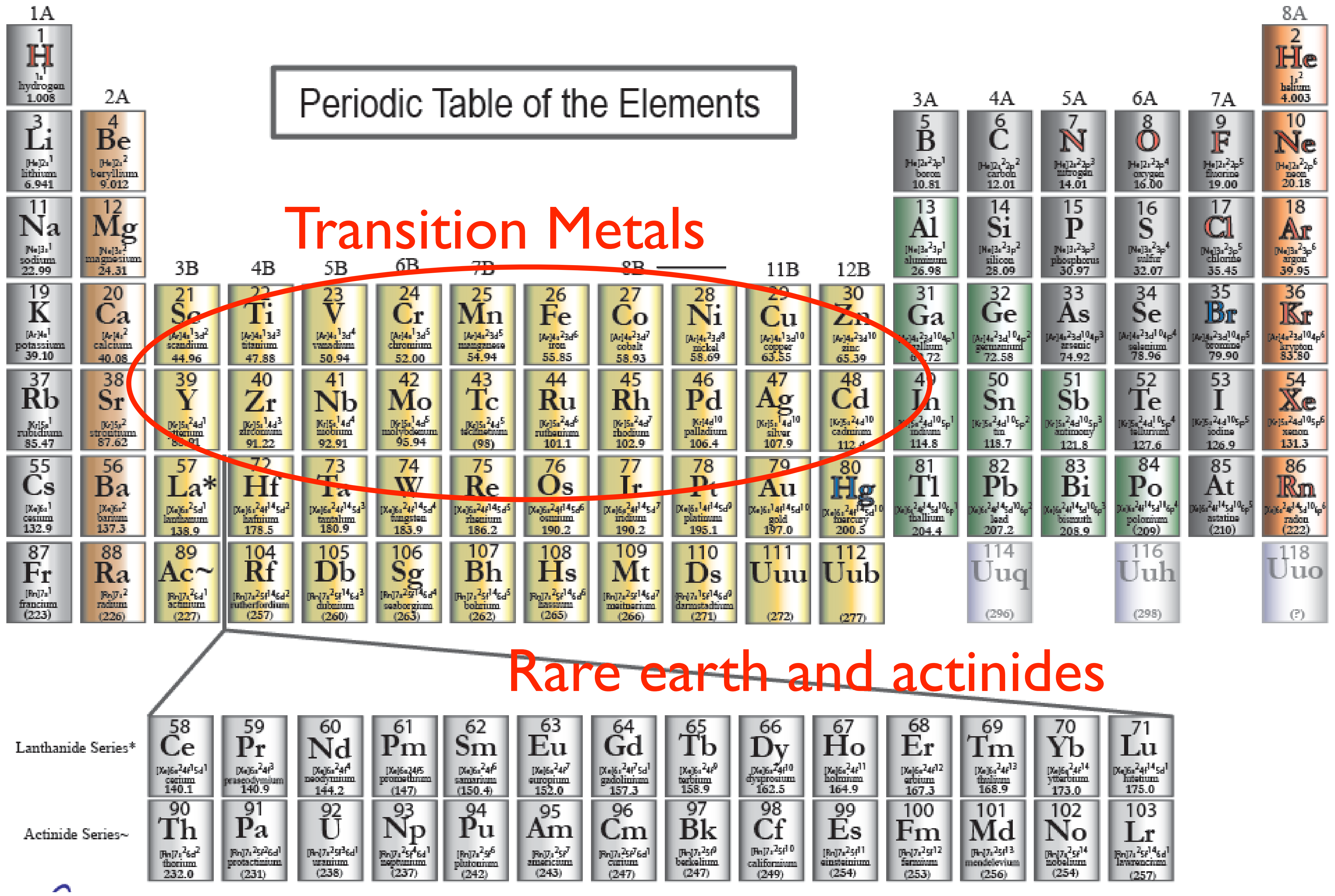


"Artificial solids" of atoms & light

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

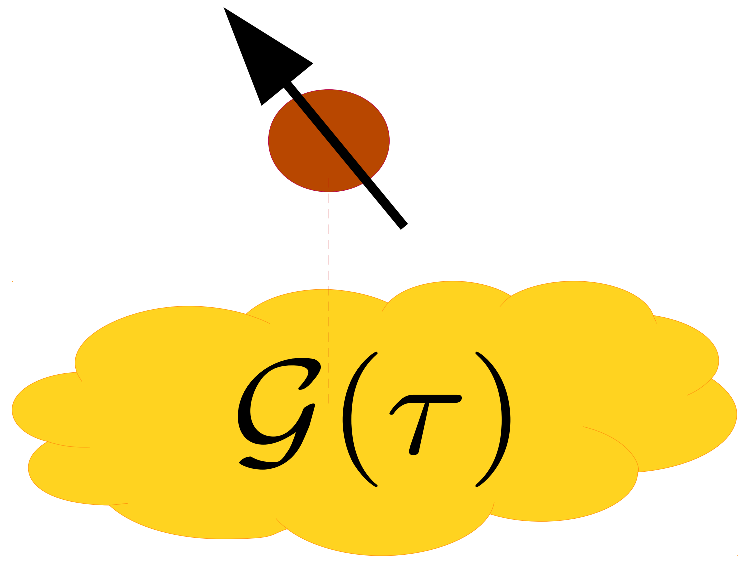


Dynamical Mean Field Theory
The main idea

- DFT (Density Functional Theory)
  - Independent electrons in an *effective periodic (Kohn-Sham) potential.*
  - Central object is the electronic density ρ

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

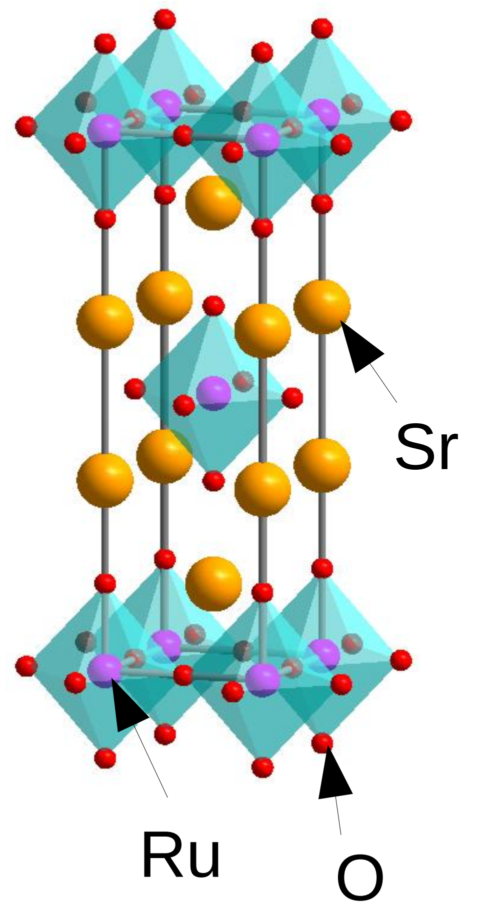
W. Metzner, D.Vollhardt, 1989
A. Georges, G. Kotliar, 1992



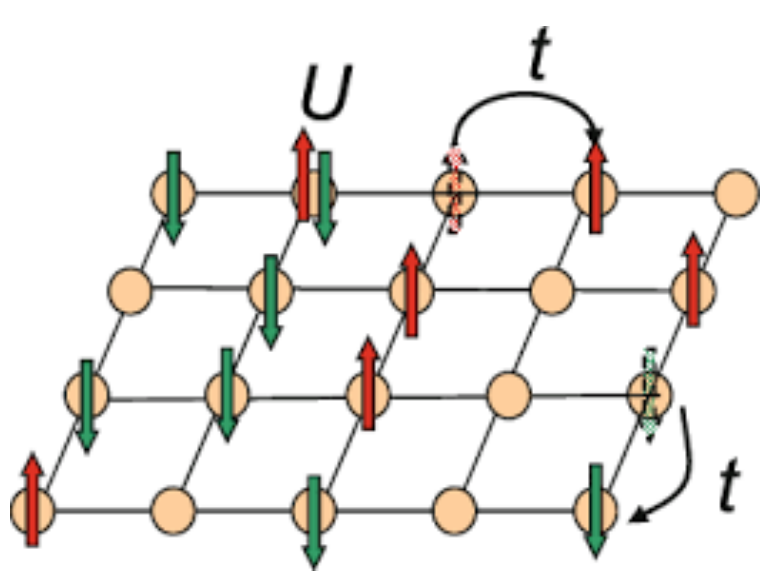
Quantum Embeddings

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

Correlated material

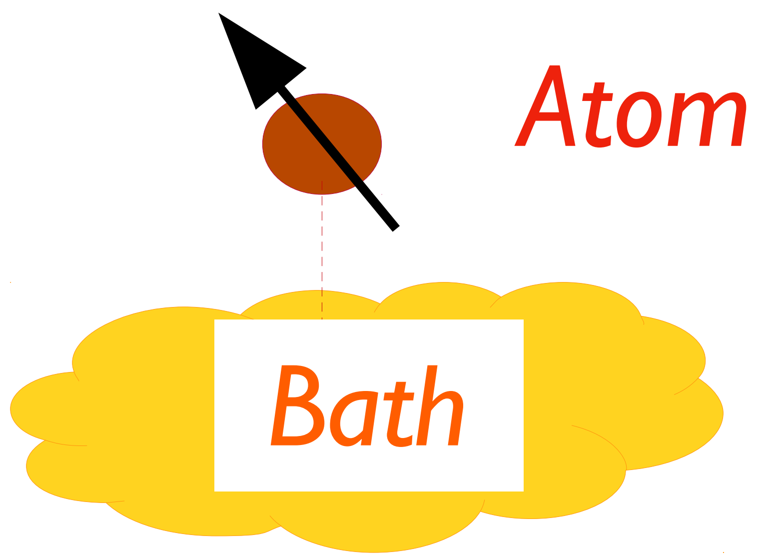


"Toy" model



Select local degree of freedom
atoms, correlated orbitals

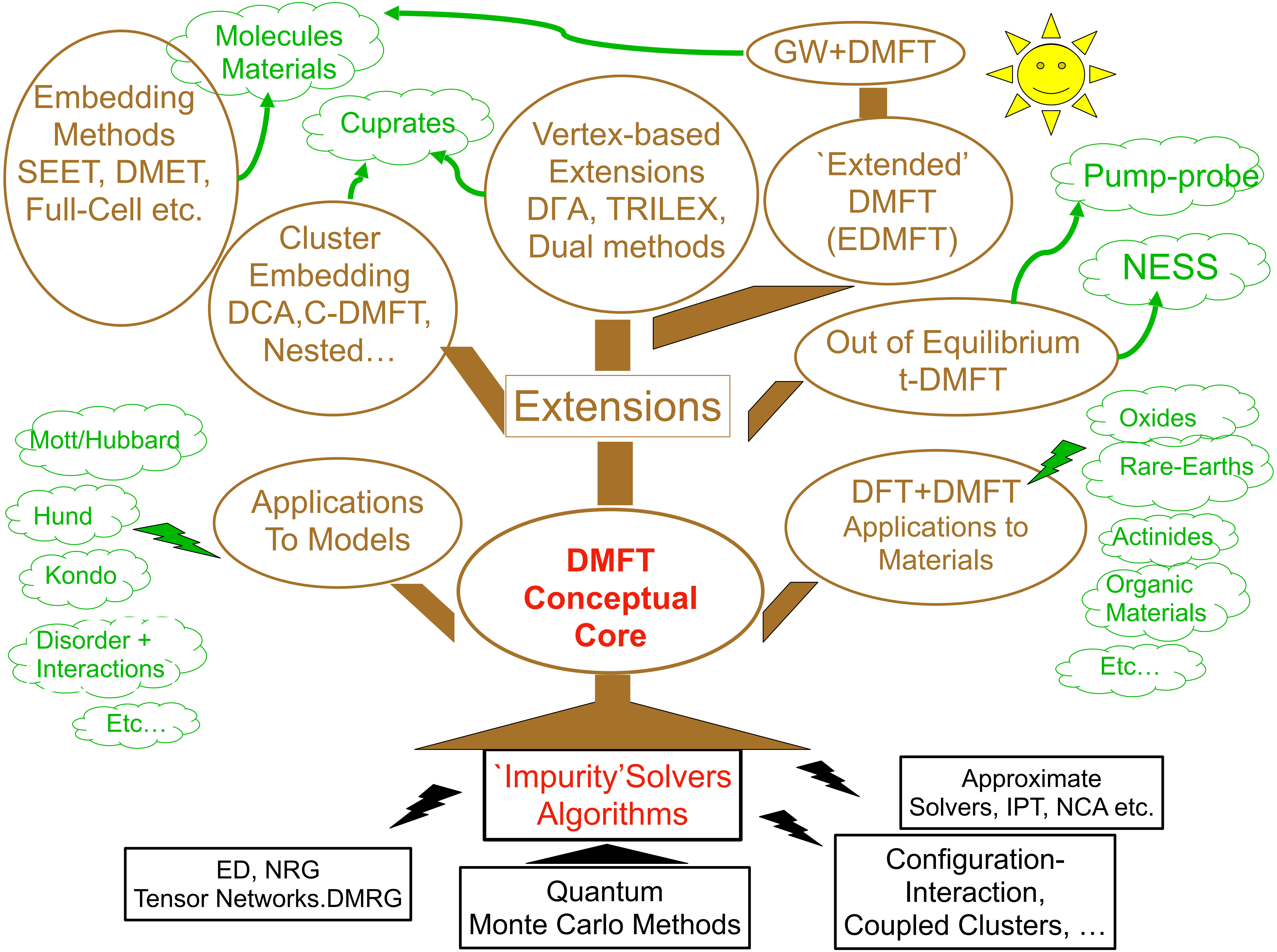
Auxiliary model
"Quantum impurity model"



Embedding

Compute physical quantities on the lattice
from the auxiliary model

Good idea when atomic physics plays a major role.


Molecules
Materials
GW+DMFT
Embedding
Methods
SEET, DMET,
Full-Cell etc.
Cuprates
Vertex-based
Extensions
DΓA, TRILEX,
Dual methods
`Extended'
DMFT
(EDMFT)
Pump-probe
NESS
Cluster
Embedding
DCA,C-DMFT,
Nested…
Out of Equilibrium
t-DMFT
Extensions
Oxides
Rare-Earths
Mott/Hubbard
Hund
Kondo
Disorder +
Interactions
Etc…
Applications
To Models
DMFT
Conceptual
Core
DFT+DMFT
Applications to
Materials
Actinides
Organic
Materials
Etc…
`Impurity'Solvers
Algorithms
Approximate
Solvers, IPT, NCA etc.
ED, NRG
Tensor Networks.DMRG
Quantum
Monte Carlo Methods
Configuration-
Interaction,
Coupled Clusters, …

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

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

Doping (number of charges)

- 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 ?

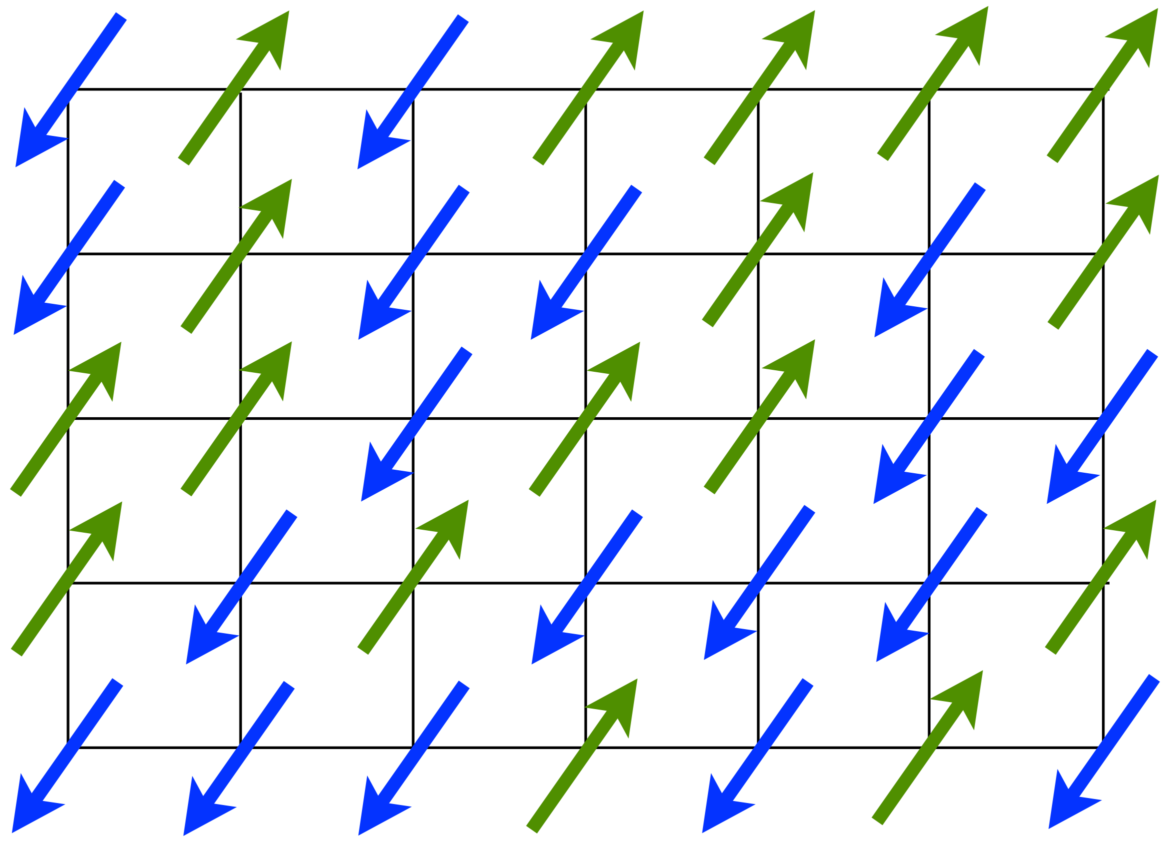
Mott insulator

N. Mott, 50's

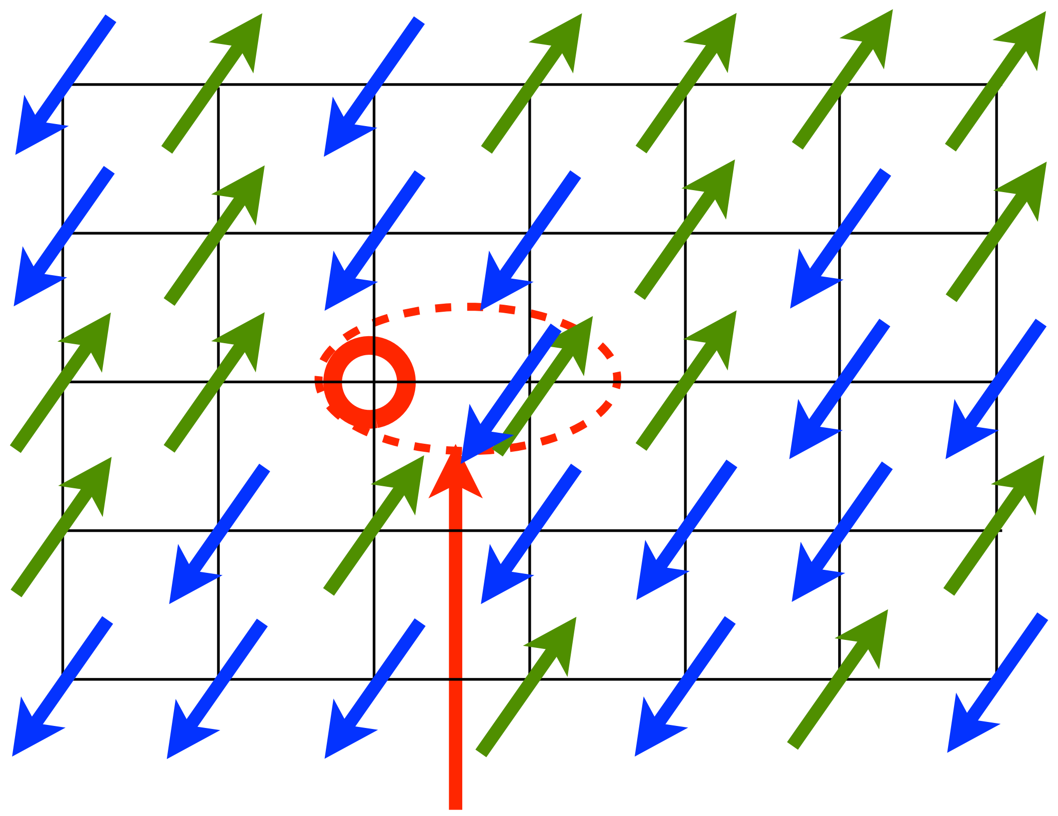
- One electron per site on average (half-filled band).
- At small U, a textbook metal.
- If U is large enough, it is an insulator : charge motion frozen.

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

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



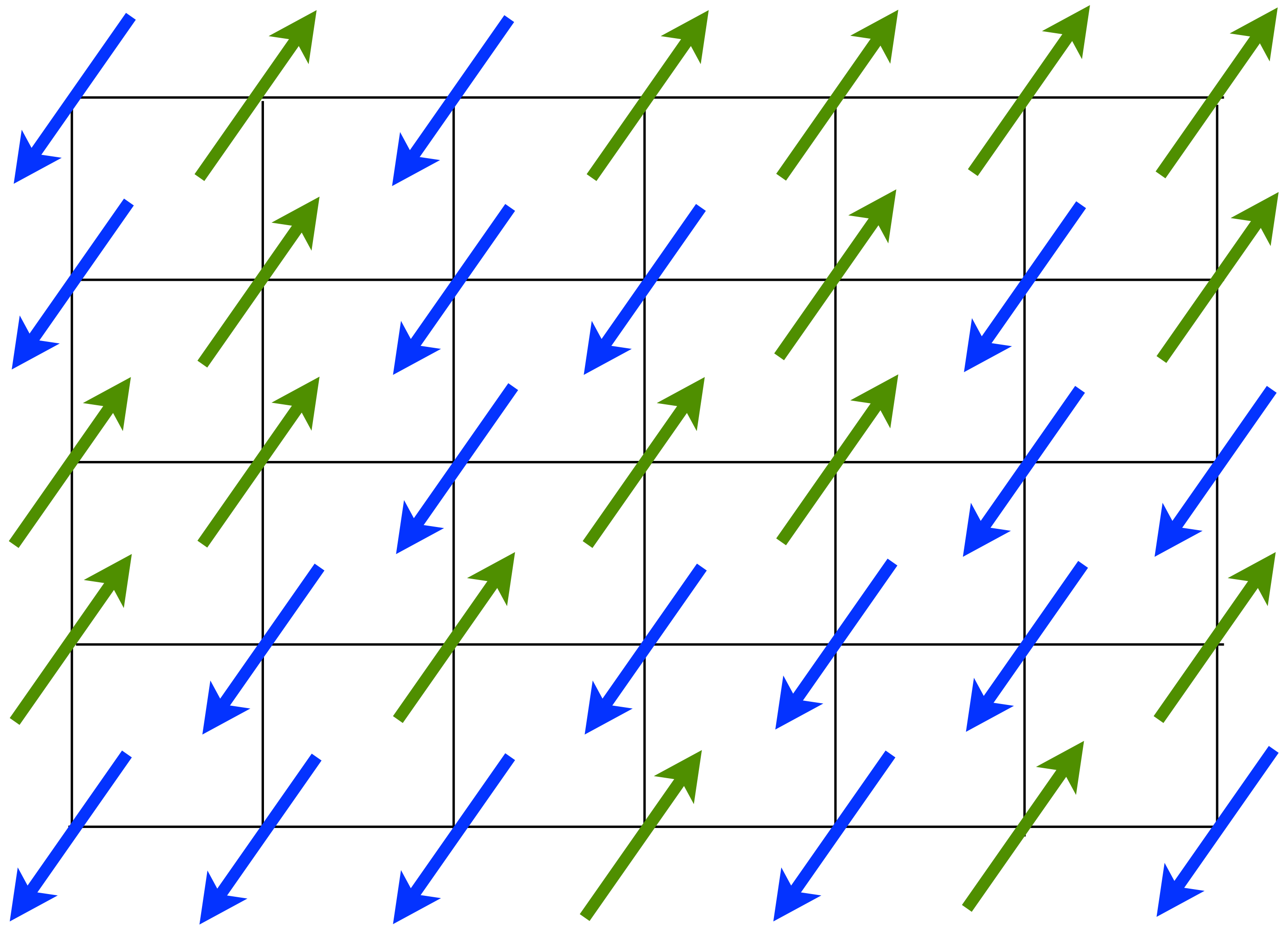
Mott insulator



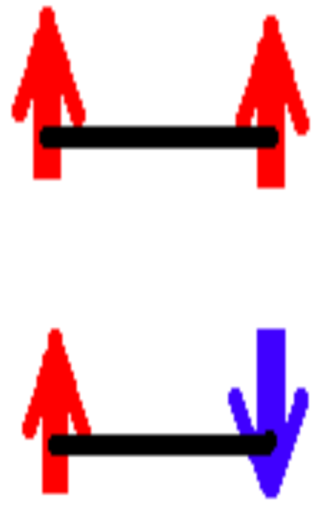
Large Coulomb repulsion U ~ eV ~10^4 K

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

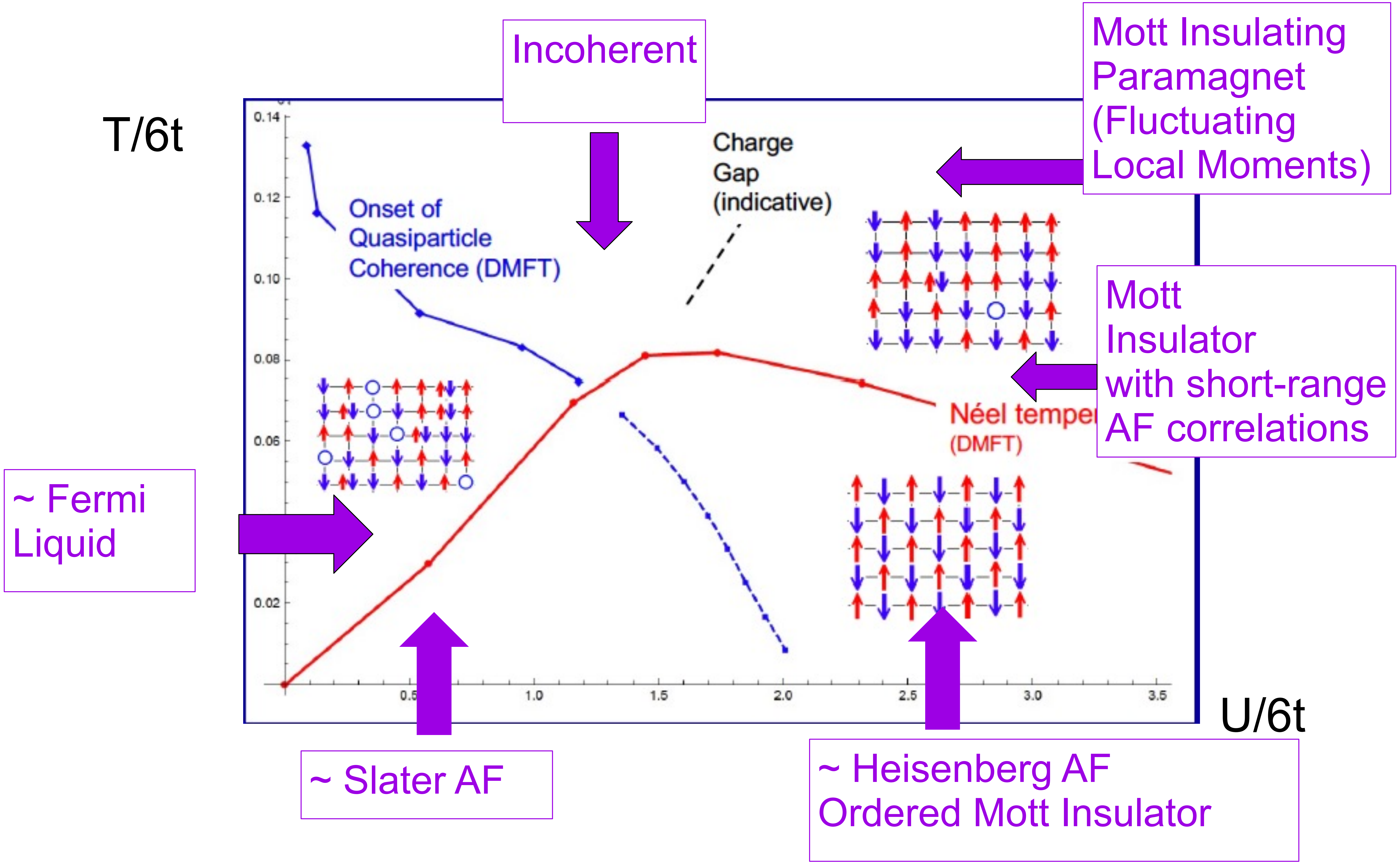


$$J_{AF} = \frac{4t^2}{U}$$

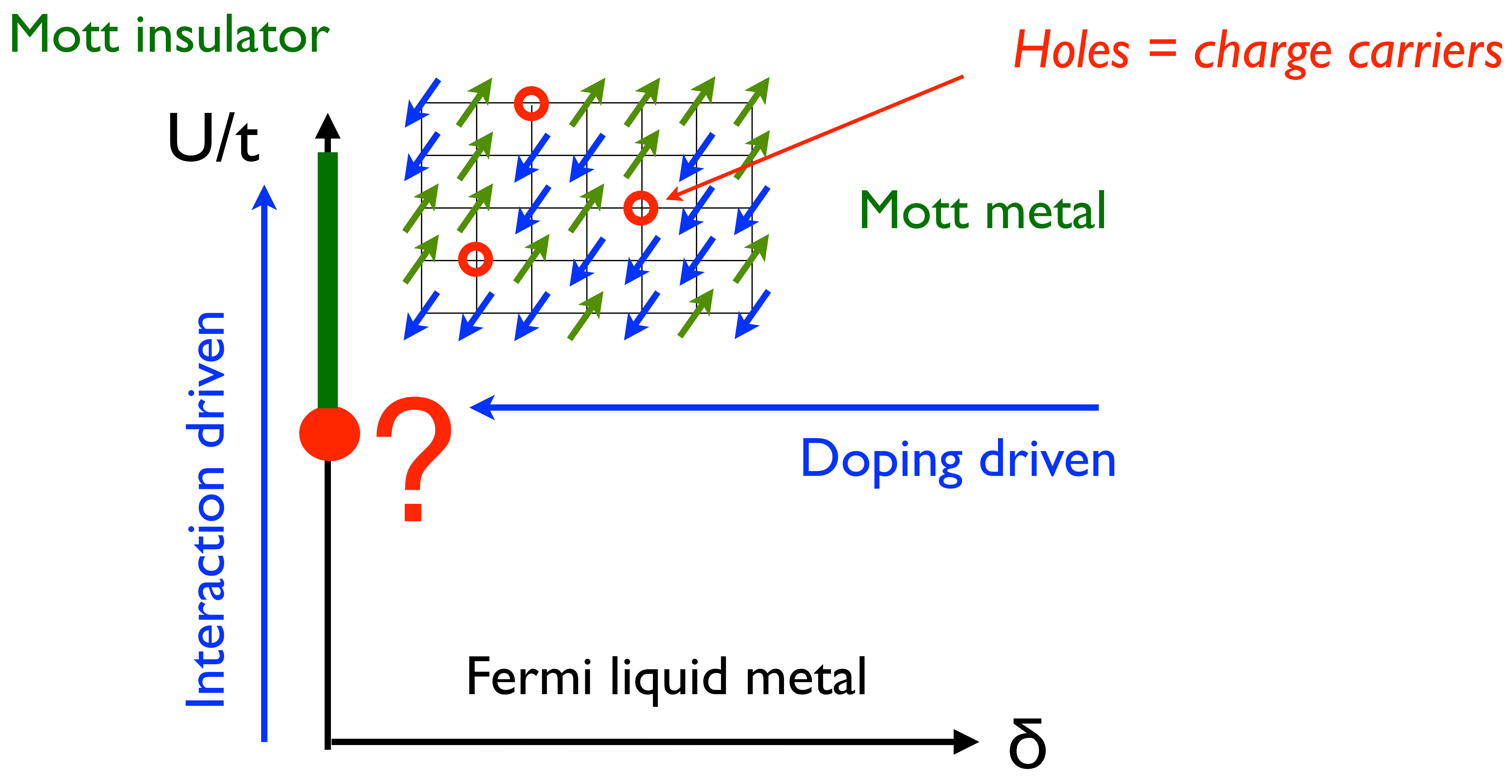
Mott phenomenon at strong coupling has nothing to do with magnetism

Various regimes in Hubbard model at half filling

$\delta = 0$



Doped Mott insulators



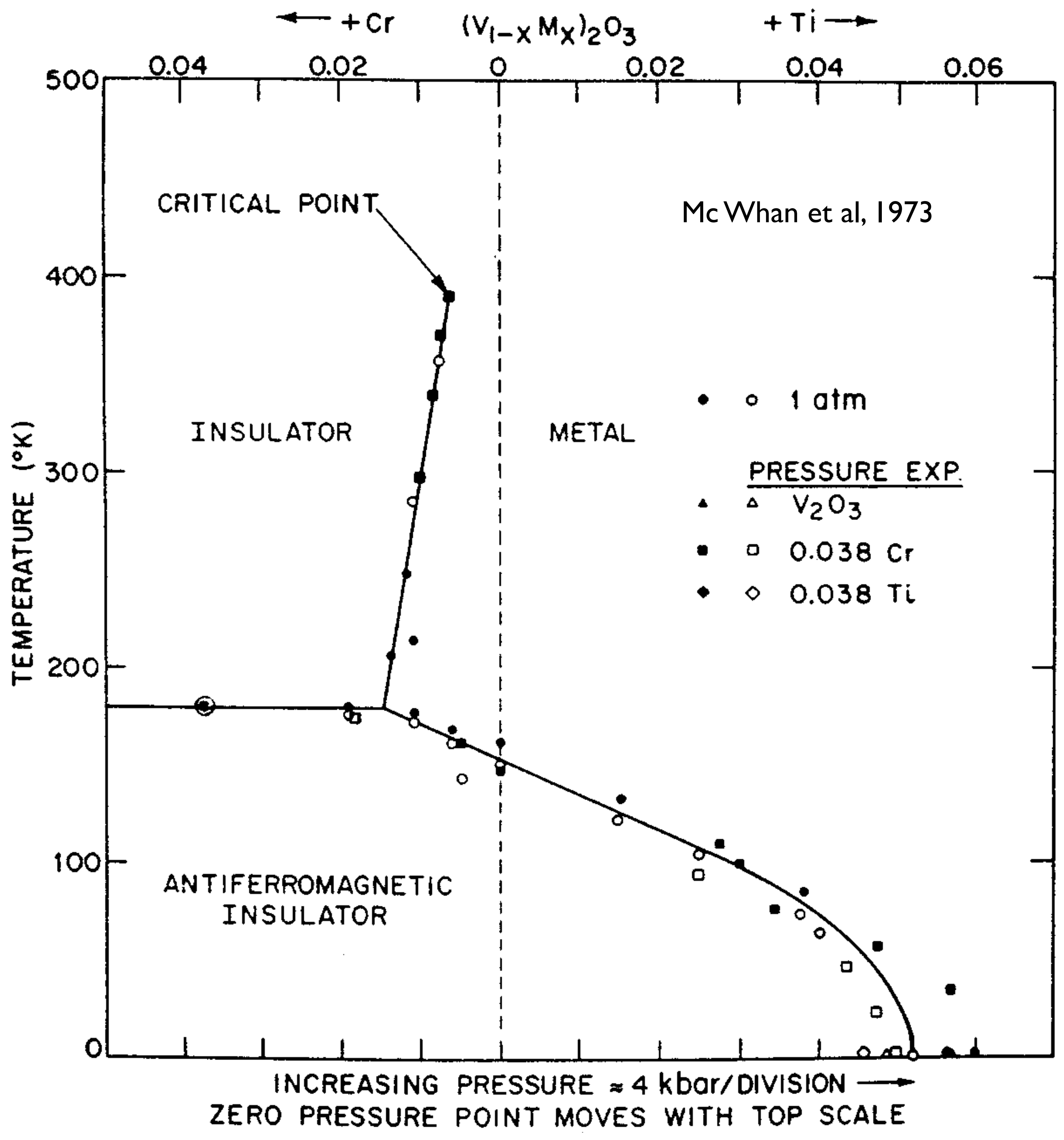
- How is a metal destroyed close to a Mott transition ?
  Or a Mott insulator by doping ?
- "Mott metals" are fragile and complex : Many instabilities, rich phase diagrams, large susceptibilities, small coherence energy

In real materials …

Interaction Driven Mott Transition

- Vary pressure P ⇔ 1/U

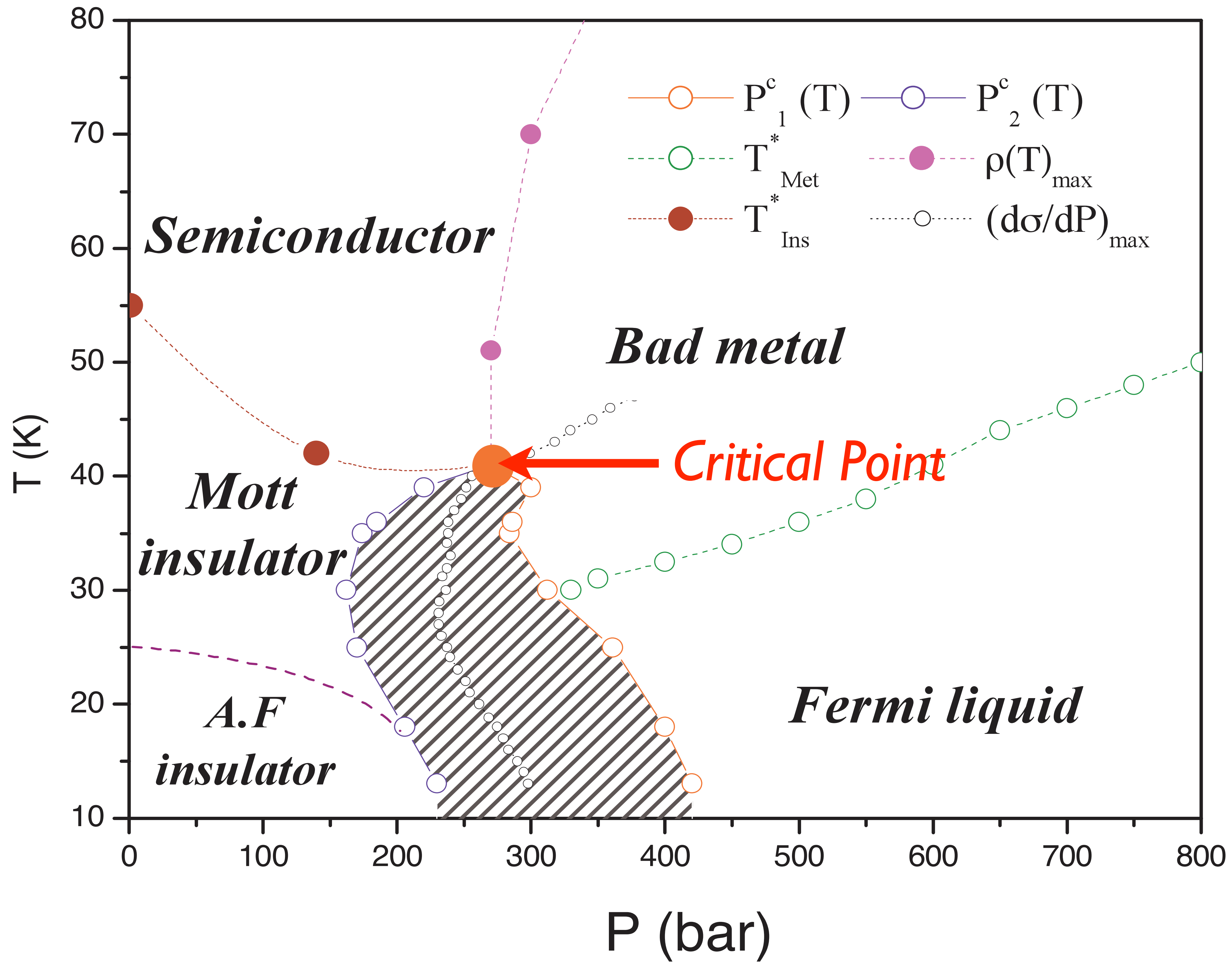
V_2O_3



2-d organics

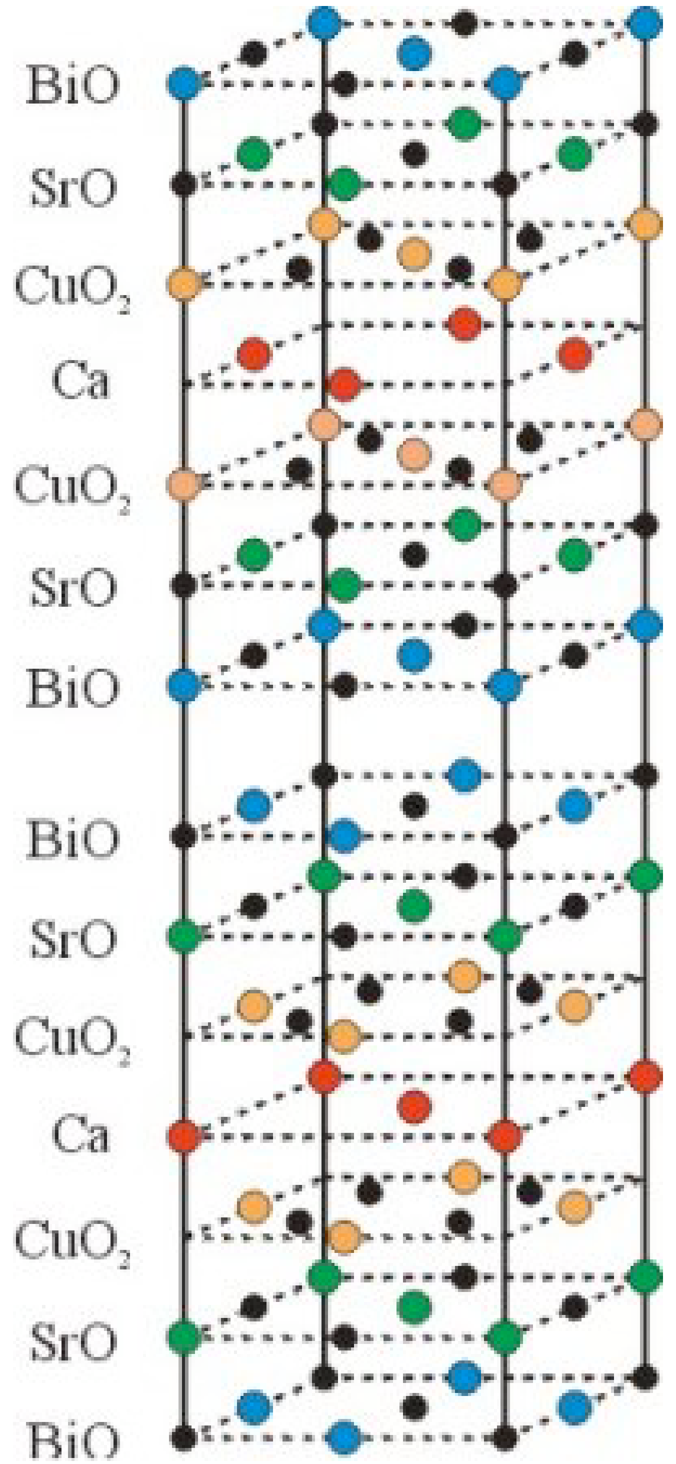
κ-$(\mathrm{BEDT\text{-}TTF})_2\mathrm{Cu}[\mathrm{N}(\mathrm{CN})_2]\mathrm{Cl}$

(but has a simple hubbard modelization)

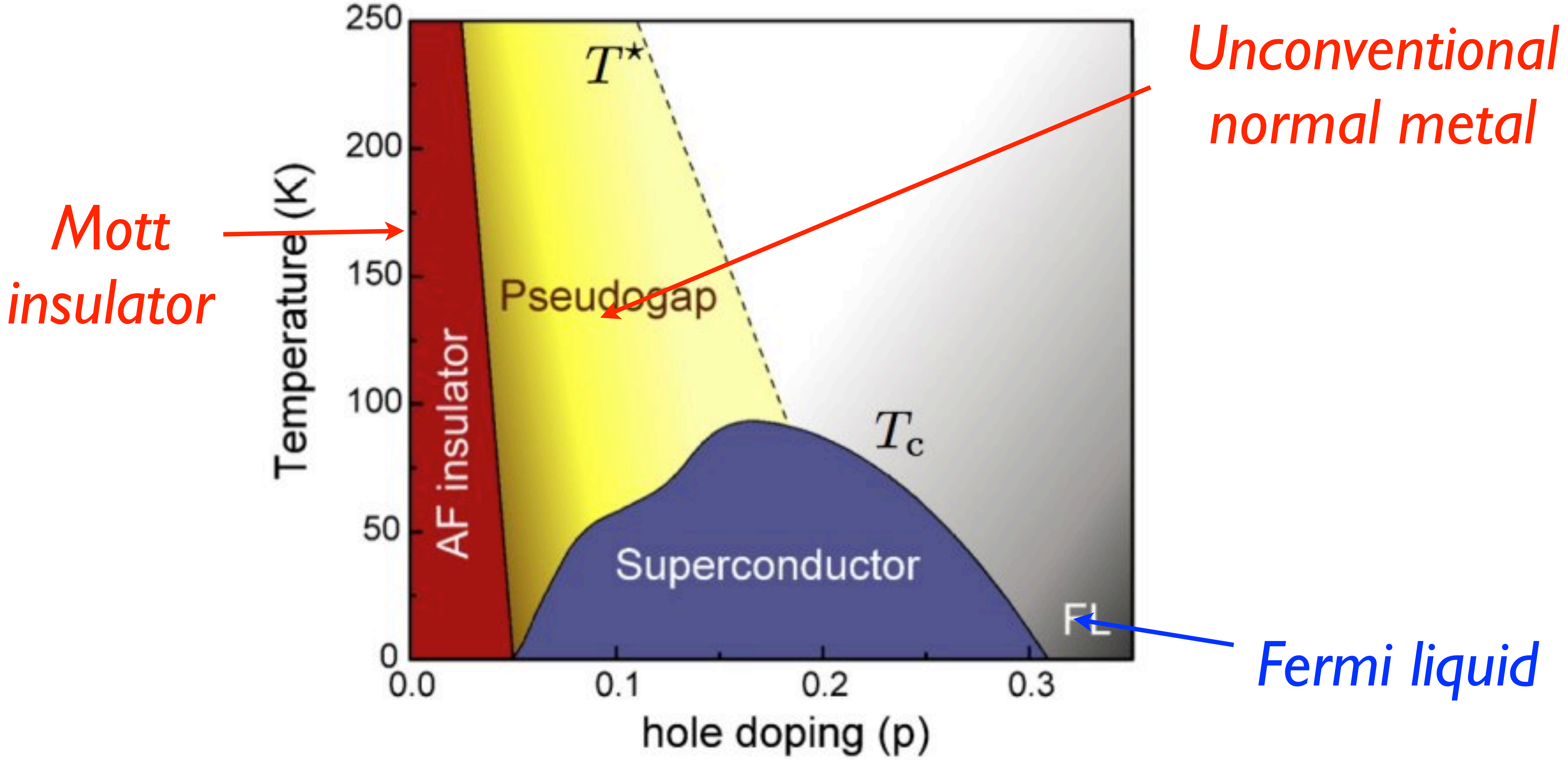


P. Limelette, et al. PRL 91, 016401 (2003)

High-Tc superconductors are doped Mott insulators



High-Tc superconductors
Generic, simplified phase diagram

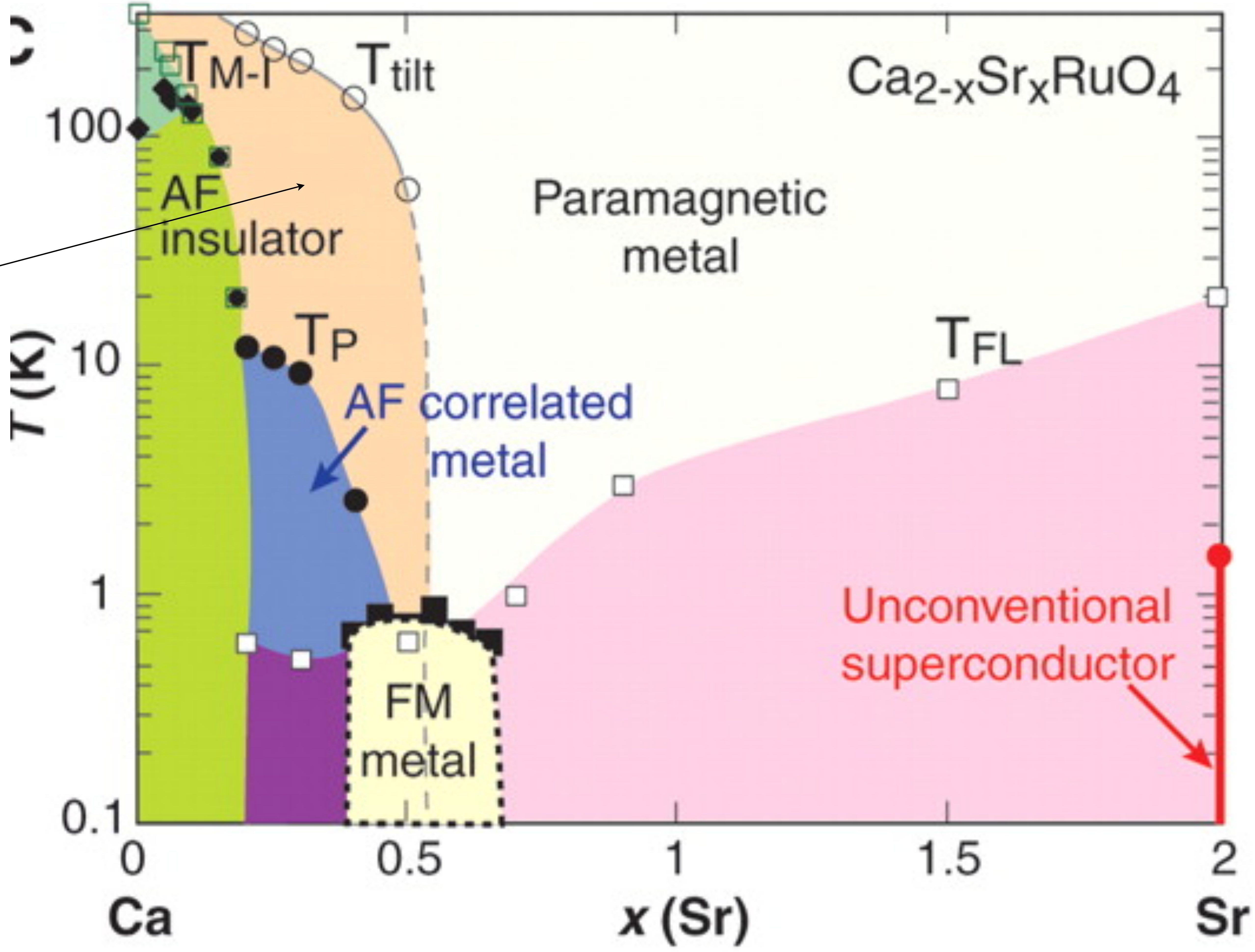


- A family of copper oxides with high critical temperature (90, 100K).
- Physics qualitatively different from conventional superconductors.
- Mechanism of high-Tc superconductivity ?

$Ca_{2-x}Sr_xRuO_4$

- A correlated material, with a complex phase diagram.

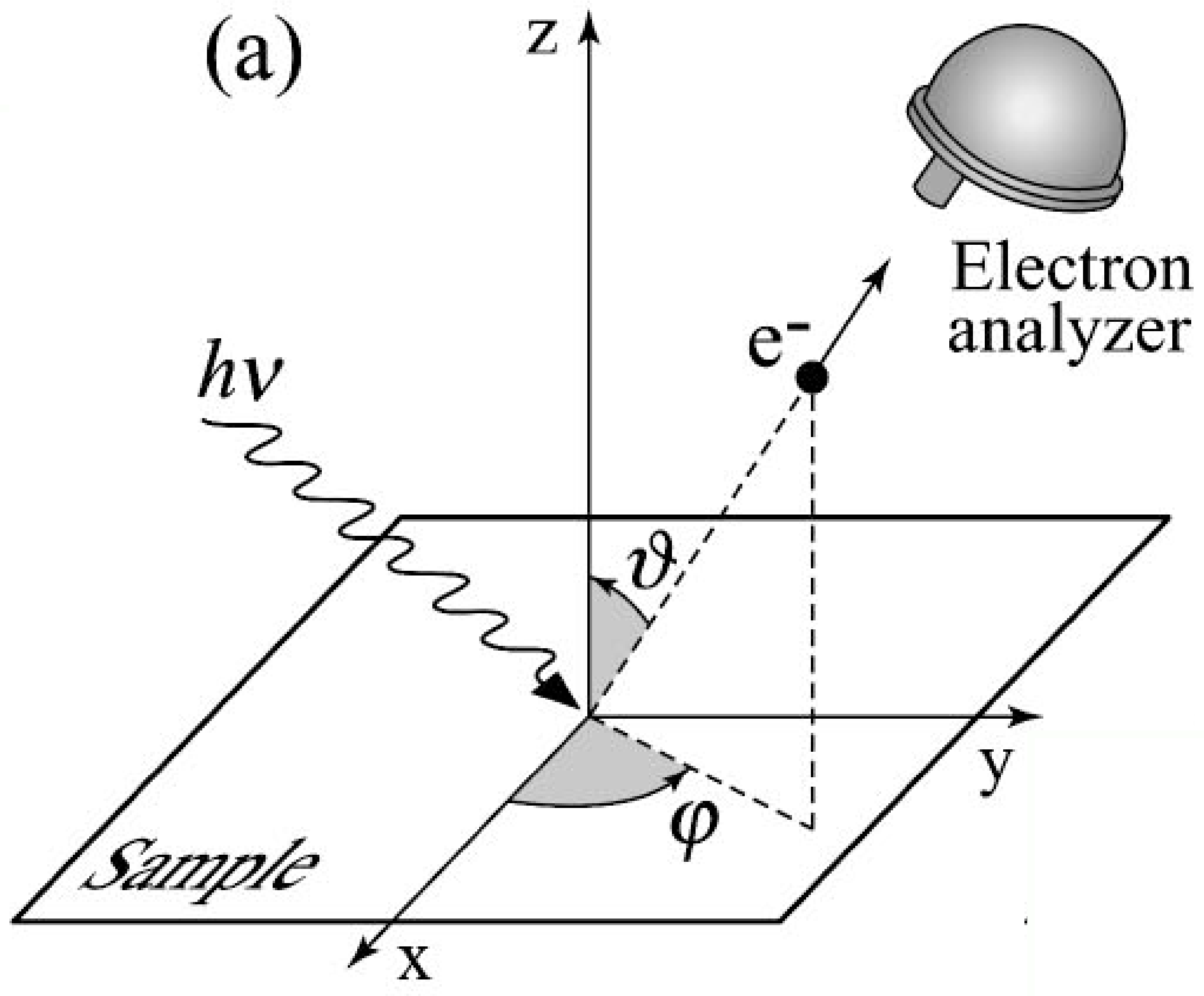
Paramagnetic Mott insulator



Reminder : spectral function

$$A(k,\omega) = \frac{1}{\pi}\mathrm{Im}\int dxdt e^{i(kx-\omega t)} i\theta(t)\langle[c(x,t),c^\dagger(0,0)]\rangle$$

- (Theorist's view of) photoemission experiments (ARPES)



Photoemission geometry

A. Damascelli et al, Rev. Mod. Phys. 75, 473 (2003)

- ARPES: hole excitations

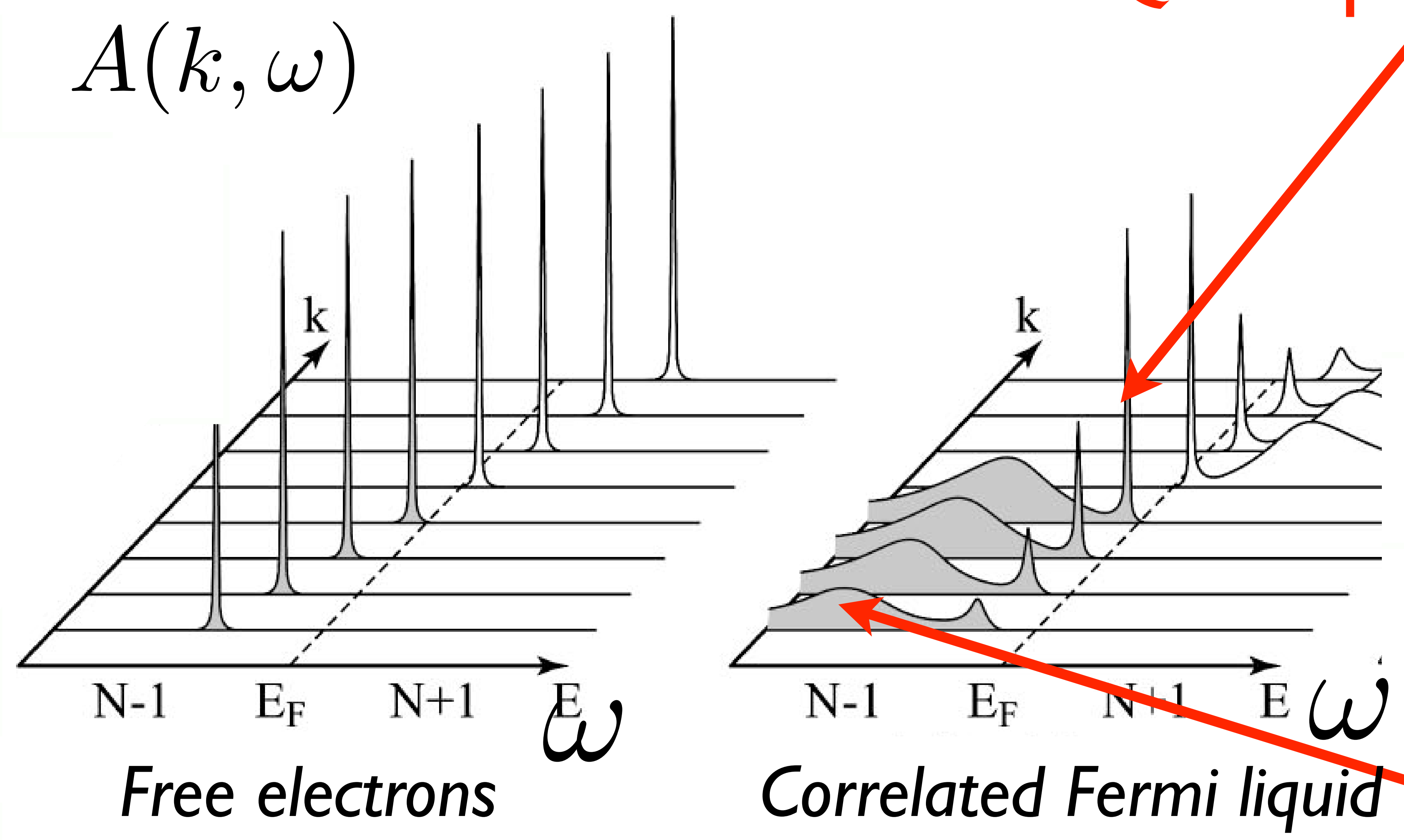
$$A(k,\omega)n_F(\omega)$$

Fermi function

Spectral weight transfer

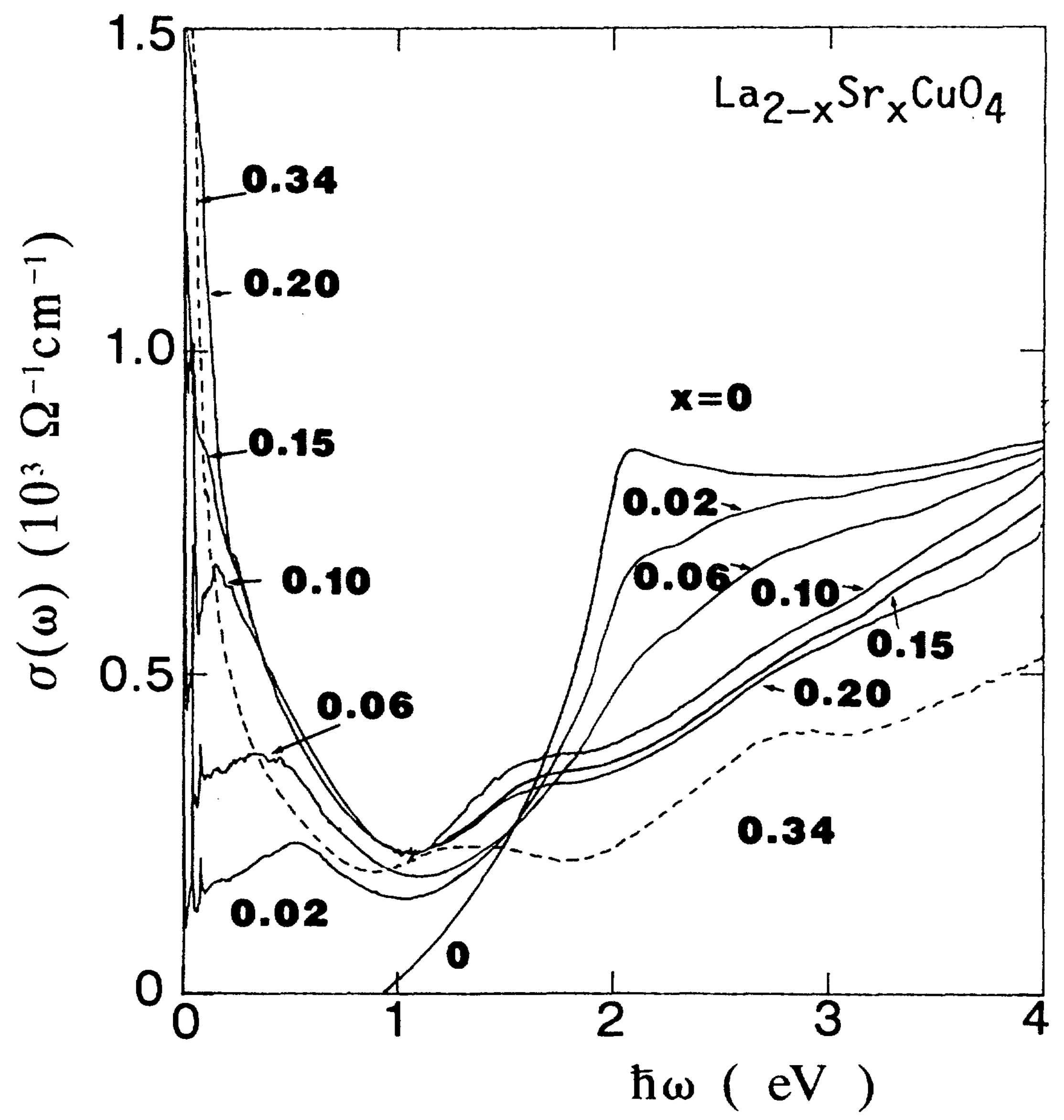
Spectral function

Quasi-particle-peak



Hubbard bands

Optical conductivity



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

- Spectral weight transfer from low to high energy

Mott physics

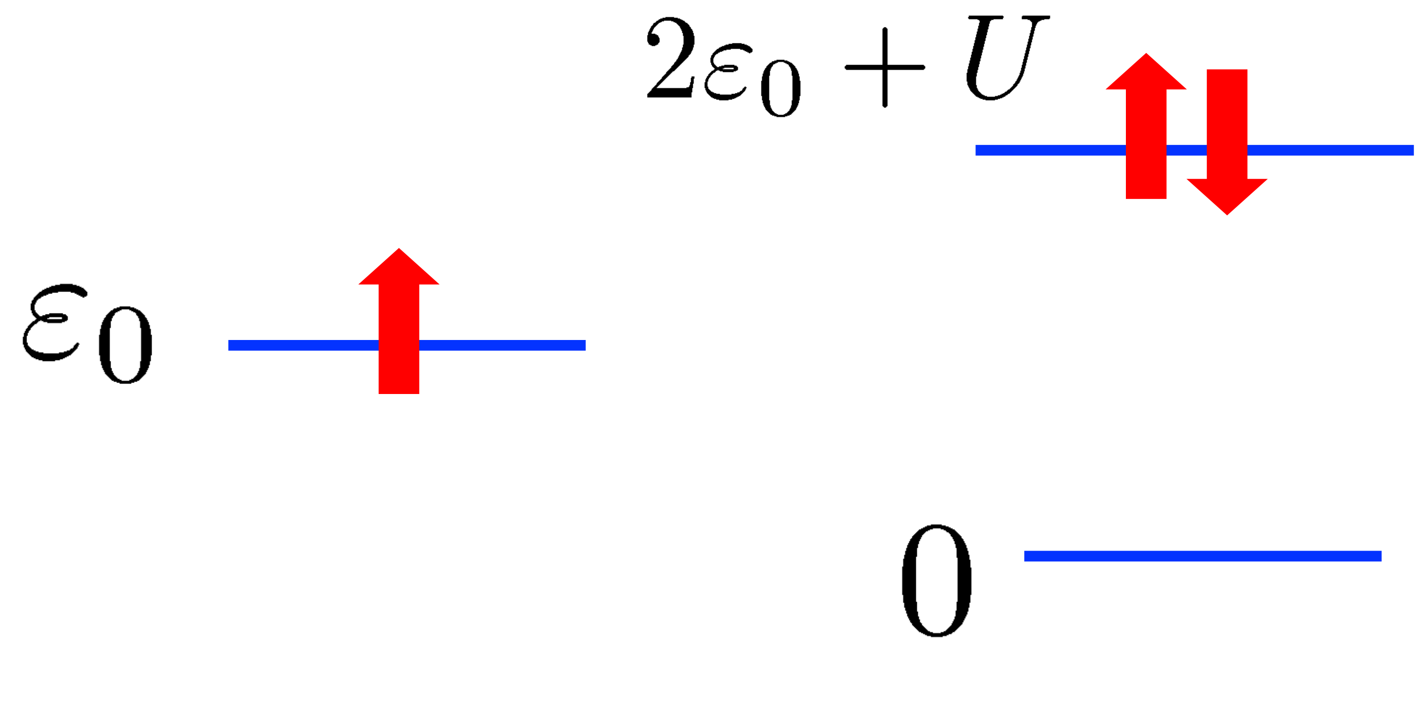
Atomic-like localized excitations. Hubbard band

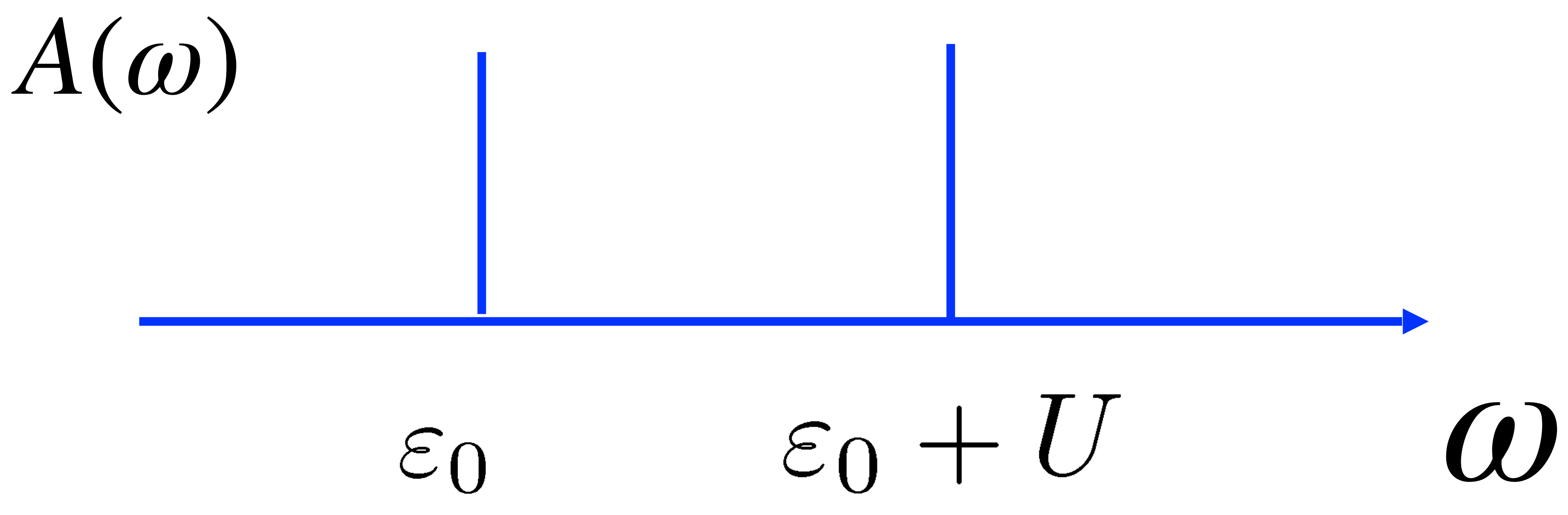
vs

long range, delocalized, quasi-particle peak

Hubbard band = remanent of an atomic transition

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

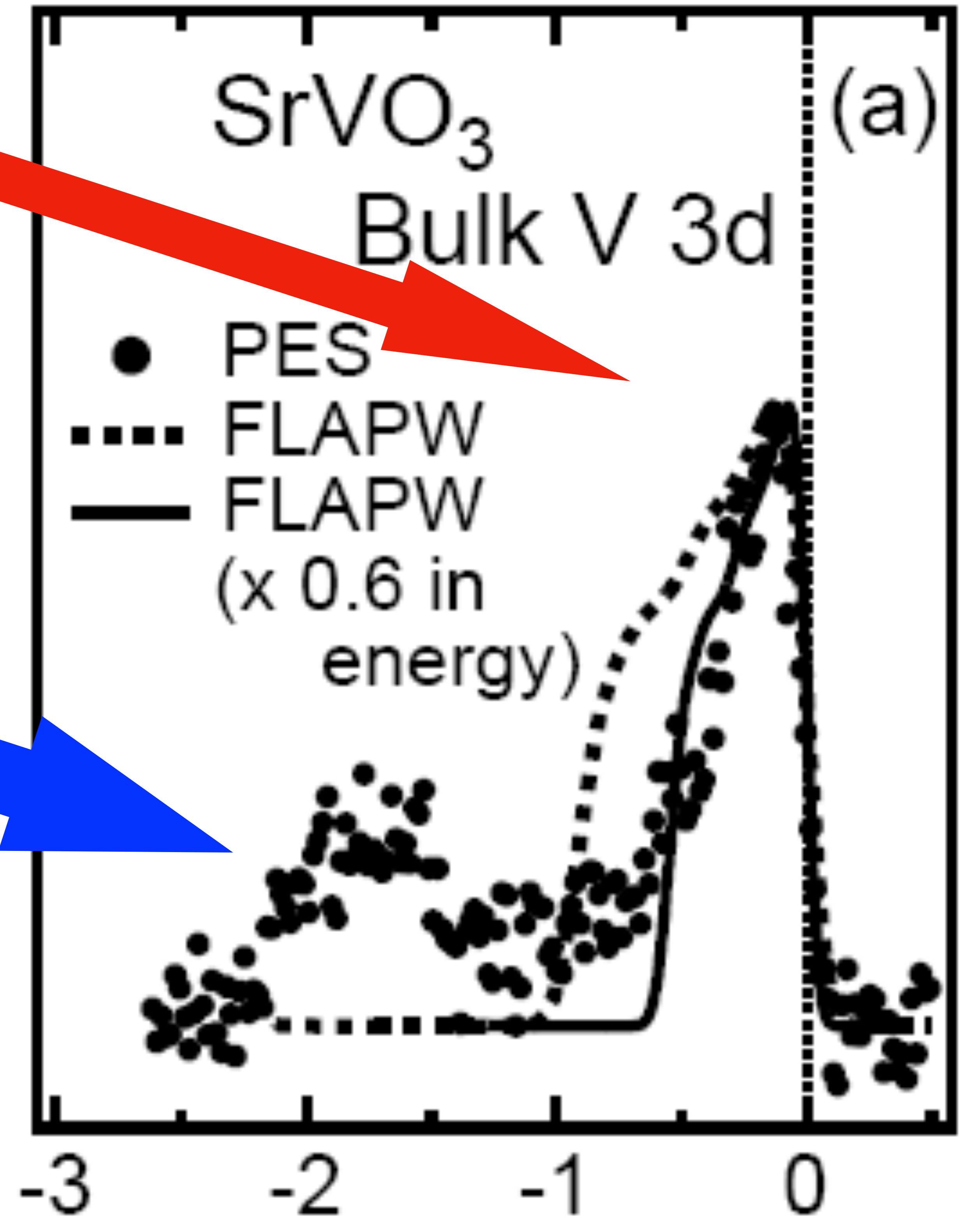




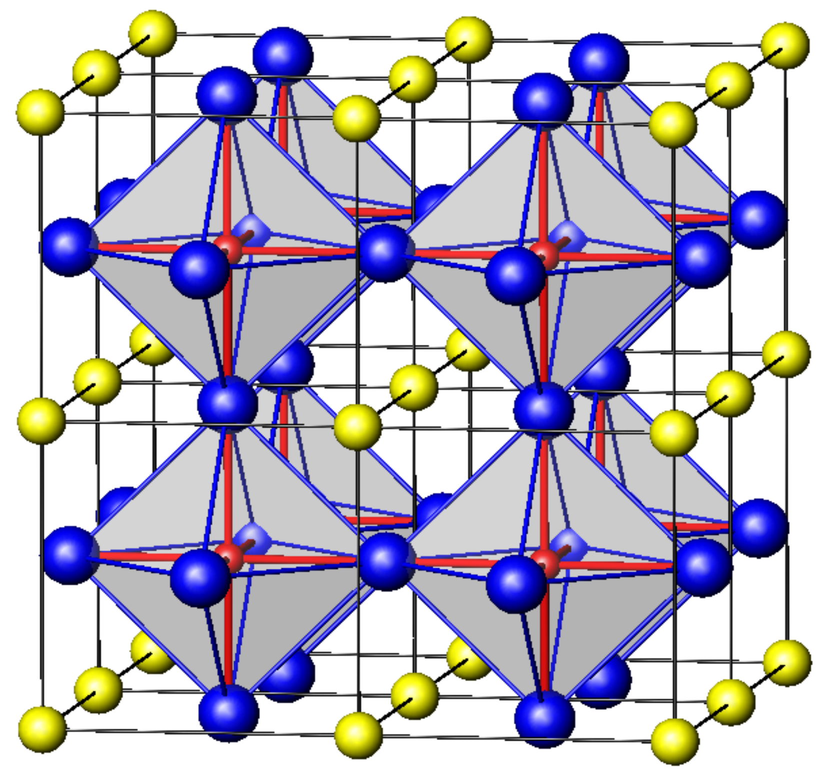
- A ``Hubbard satellite" is just an atomic transition broadened by the solid-state environment.
- Understanding the energetics of the Mott gap requires a an accurate description of the many-body eigenstates of single atoms : multiplets, i.e. $U, J_H \ldots$ (cf later on Hund's metals).

Correlated metals : spectroscopy

- Narrowing of quasiparticle bands due to correlations (the Brinkman-Rice phenomenon)
- Hubbard satellites (i.e extension to the solid of atomic-like transitions)



$$\sum_{\mathbf{k}} A(\mathbf{k},\omega)$$



$SrVO_3$

Dashed line:
Spectrum obtained from
band-structure methods (DFT-LDA)

Sekiyama et al., PRL 2004

Mott insulator

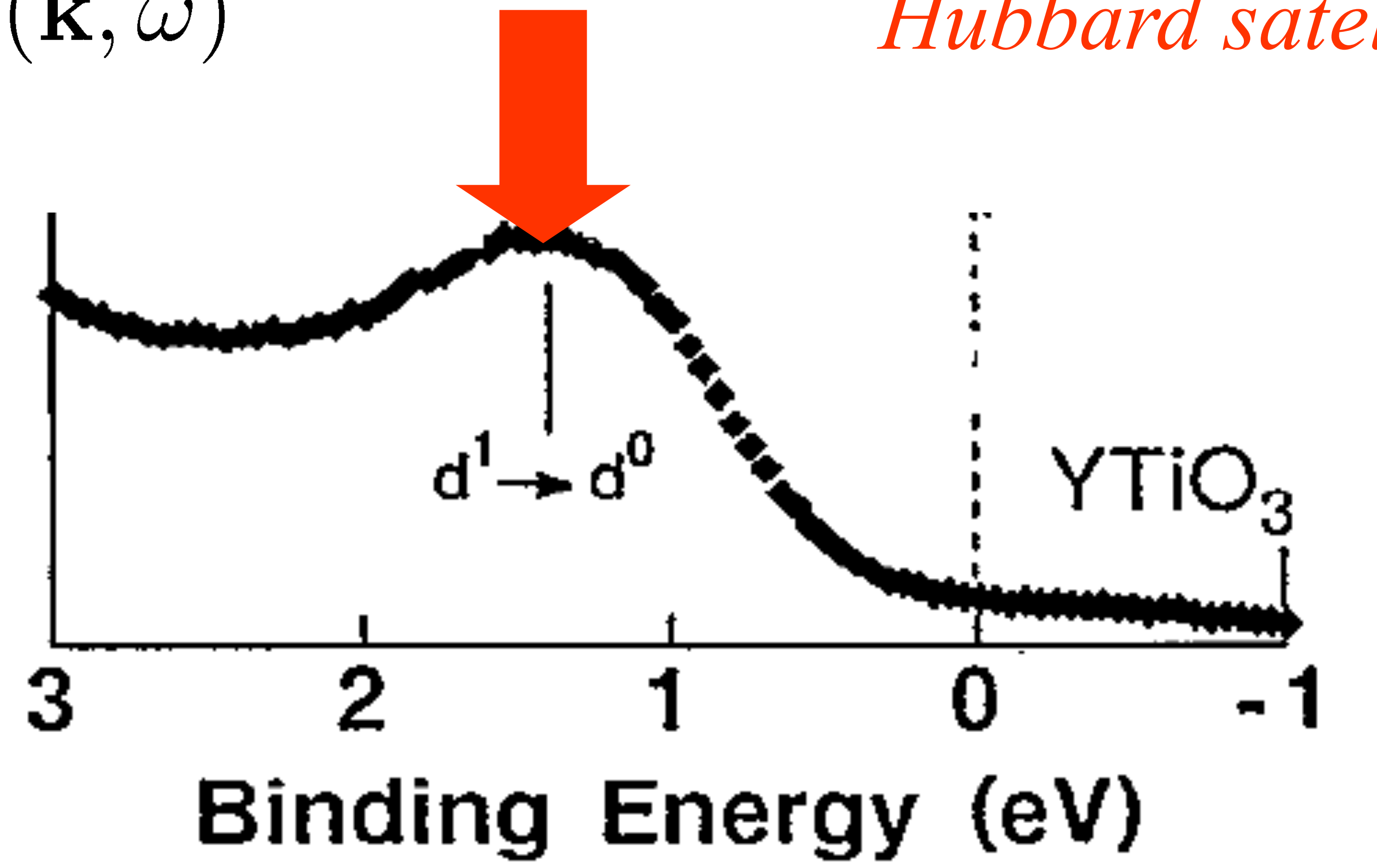
- Even harder for conventional DFT methods

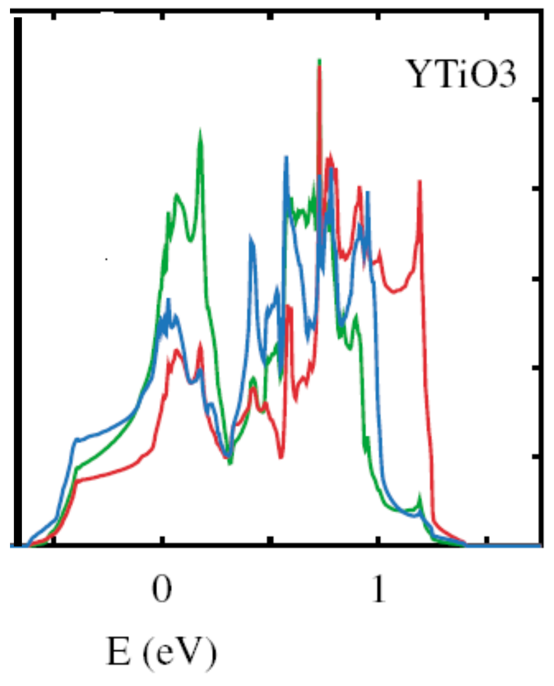
Puzzle: Why is $SrVO_3$ a metal and $LaTiO_3$, $YTiO_3$ Mott insulators ?

$YTiO_3$

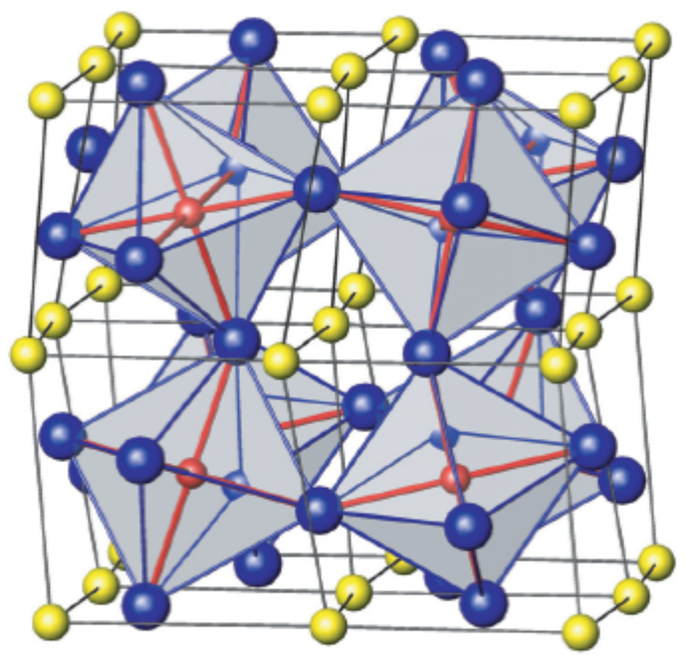
$$\sum_{\mathbf{k}} A(\mathbf{k},\omega)$$

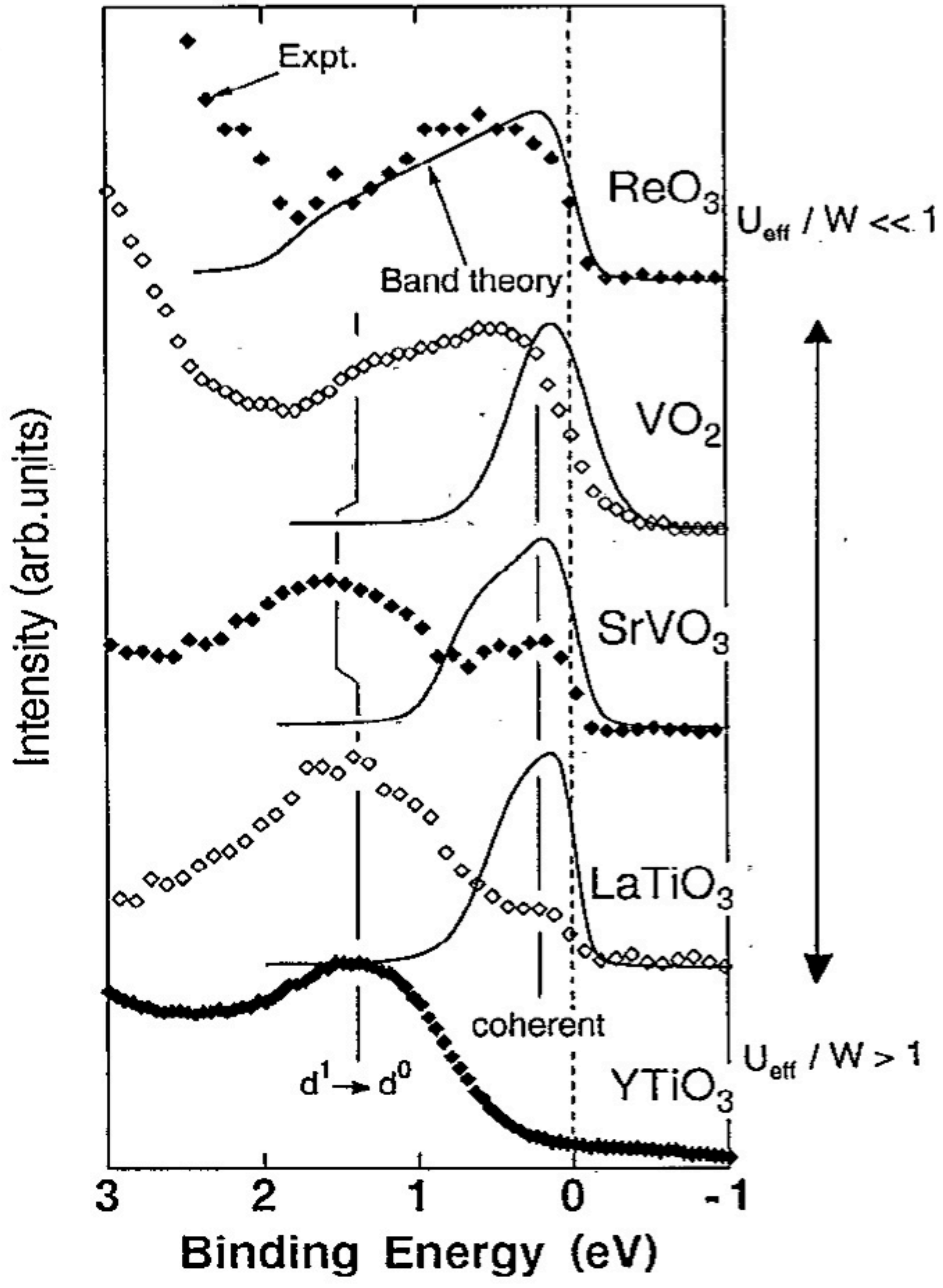
Hubbard satellite





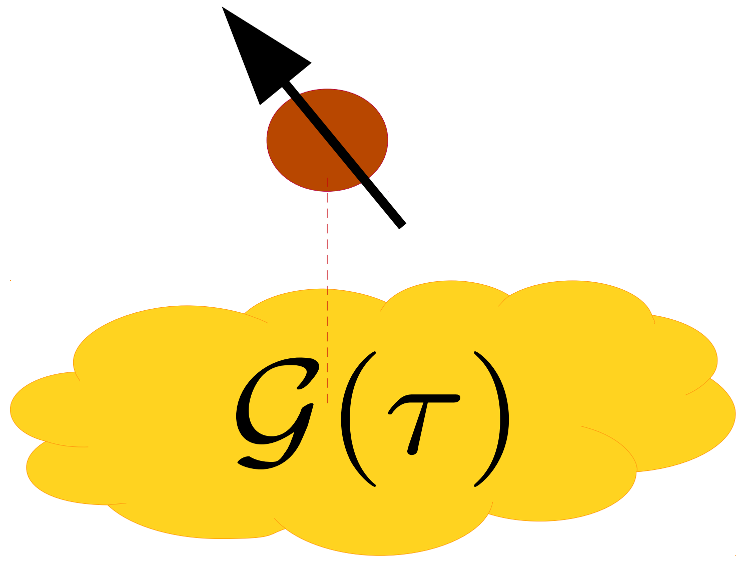
Metallic LDA (KS) spectrum !





Why DMFT ?

- Theoretical framework
  - Describes **both**
    - atomic multiplets & low energy Fermi liquid
    - low and high energy features (and spectral weight transfer)
    - Mott insulator & metal



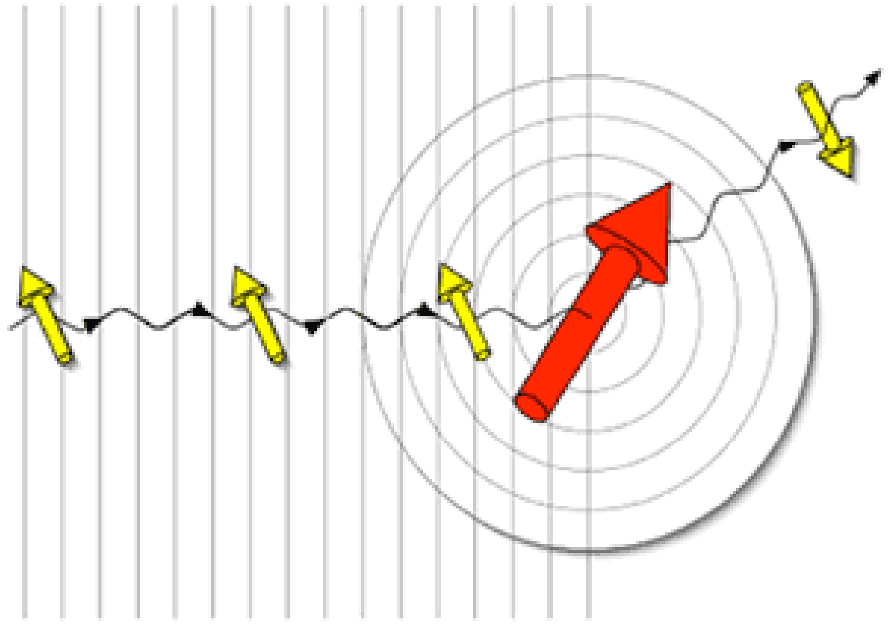
- Computational method
  - Control : cluster, vertex extension (in principle and sometimes in practice)
  - Cooperates well with electronic structure method.
    Partition between "correlated" and "non correlated orbitals"
    DFT + DMFT, GW + DMFT *Cf lecture III*

A brief introduction to quantum impurity models

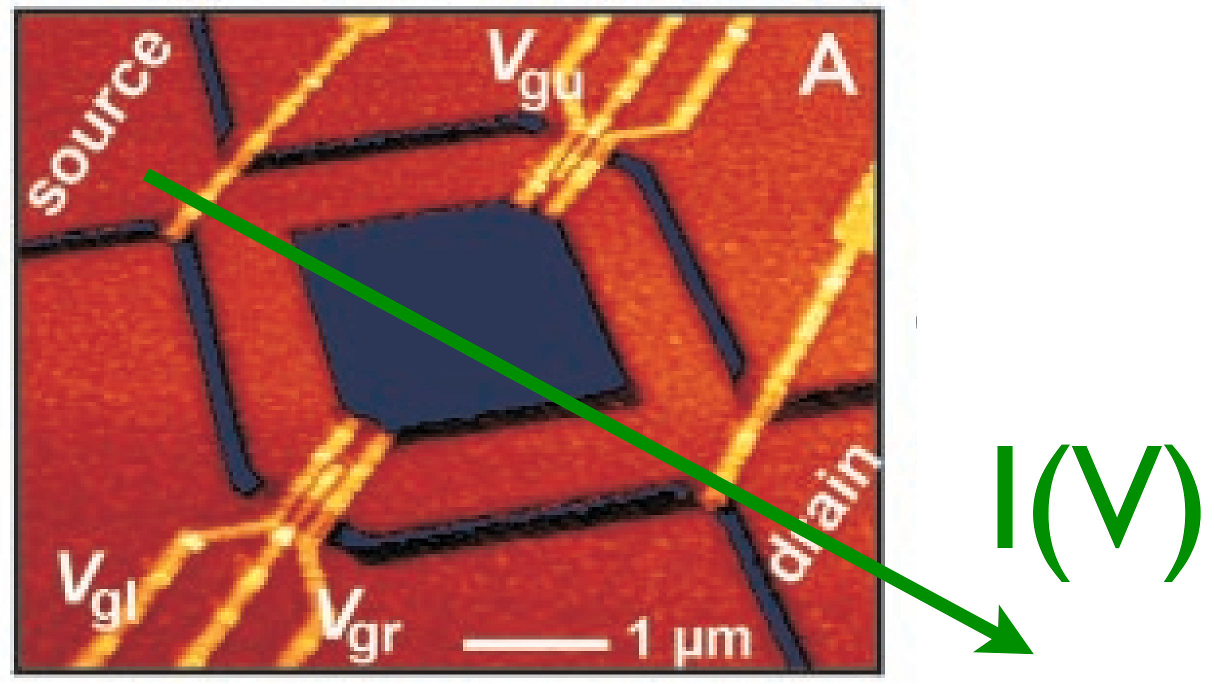
Quantum impurity models

Magnetic impurity

- In a metallic host
- Thermodynamics : C, χ, transport : ρ ?



Nanostructures/Quantum dots



- Quantum dots. Non-equilibrium
- Current : I(V), conductance, noise ?

DMFT

- This lecture …

Quantum impurity models: definition

- Scalar impurity : not a many body problem

$$H = \sum_{k\sigma\alpha} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{\substack{kk'\\ \sigma}} V_{k,k'} c^\dagger_{k\sigma} c_{k'\sigma}$$

- Anderson model
  - Impurity with a local, quantum degree of freedom.

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

  - One site of Hubbard model (c instead of d) and a bath

Action versus Hamiltonian form

- An equivalent formulation obtained by integrating the fermions

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

$$\updownarrow$$

$$S = -\iint_0^\beta d\tau d\tau' d^\dagger_\sigma(\tau)\mathcal{G}^{-1}_\sigma(\tau-\tau')d_\sigma(\tau') + \int_0^\beta d\tau\; U n_{d\uparrow}(\tau) n_{d\downarrow}(\tau)$$

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

Bath

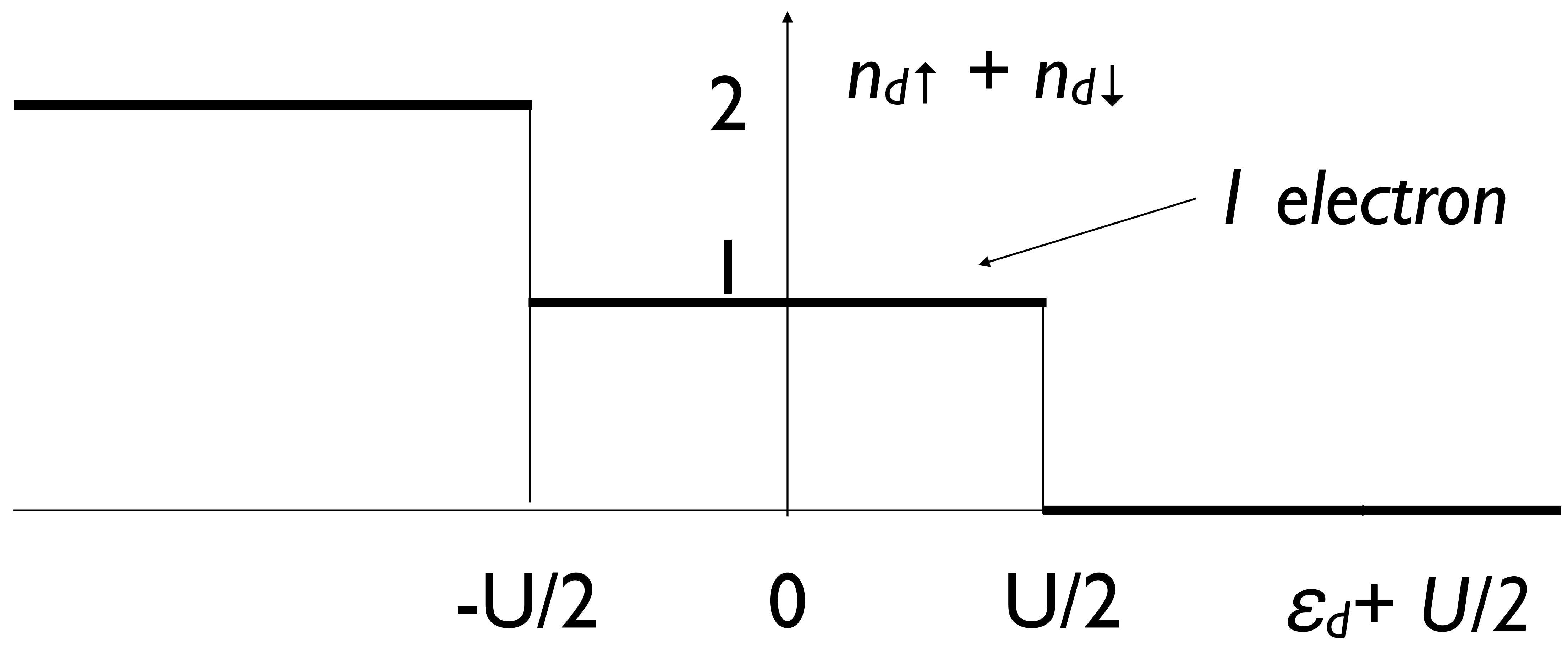
Hybridization function

Kondo model

- Anderson model

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

  - Atomic limit = without the bath



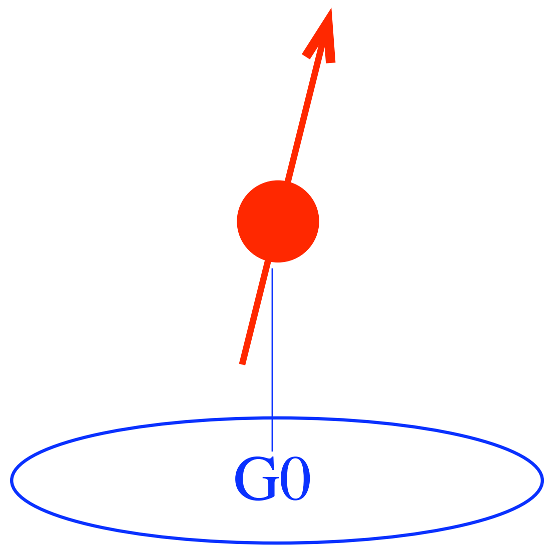
<u>Schrieffer-Wolf Phys.Rev. 66</u>

$$-\epsilon_d, U \to +\infty$$

$$J_K \propto \frac{V^2}{U}$$

- Kondo model

$$H = \sum_{k\sigma} \varepsilon_k \xi^\dagger_{k\sigma} \xi_{k\sigma} + J_K \vec{S} \cdot \sum_{\substack{kk' \\ \sigma\sigma'}} \xi^\dagger_{k\sigma} \vec{\sigma}_{\sigma\sigma'} \xi_{k'\sigma'}$$



A single spin 1/2 + a free fermion

A non-trivial problem

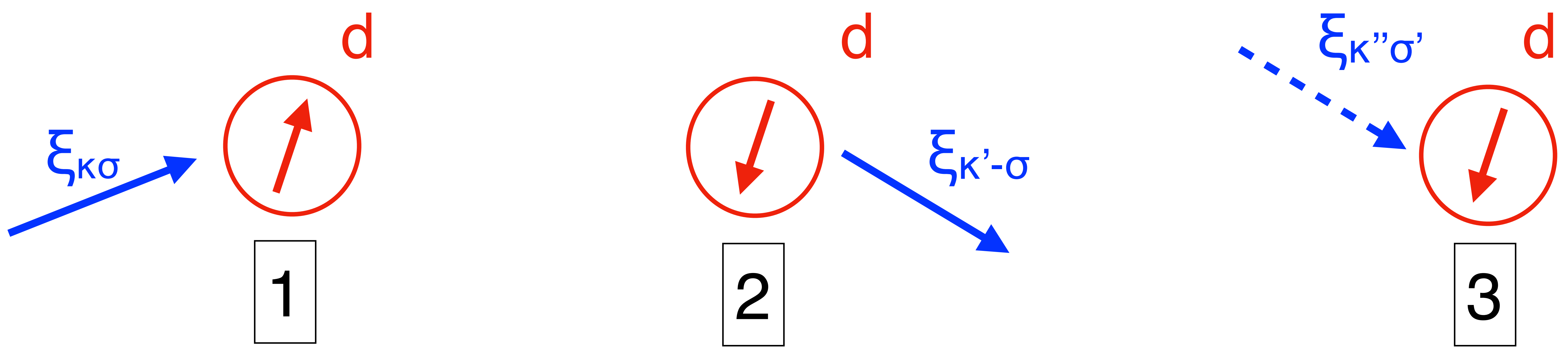
Impurity models are correlated systems

- Local but correlated problems

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

$$H = \sum_{k\sigma} \varepsilon_k \xi^\dagger_{k\sigma} \xi_{k\sigma} + J_K \overrightarrow{S} \cdot \sum_{\substack{kk' \\ \sigma\sigma'}} \xi^\dagger_{k\sigma} \vec{\sigma}_{\sigma\sigma'} \xi_{k'\sigma'}$$

- A second electron sees a local degree of freedom (e.g. spin) flipped by the first.
- Sufficient to create strong correlation effects. Solving impurity models will not be easy !

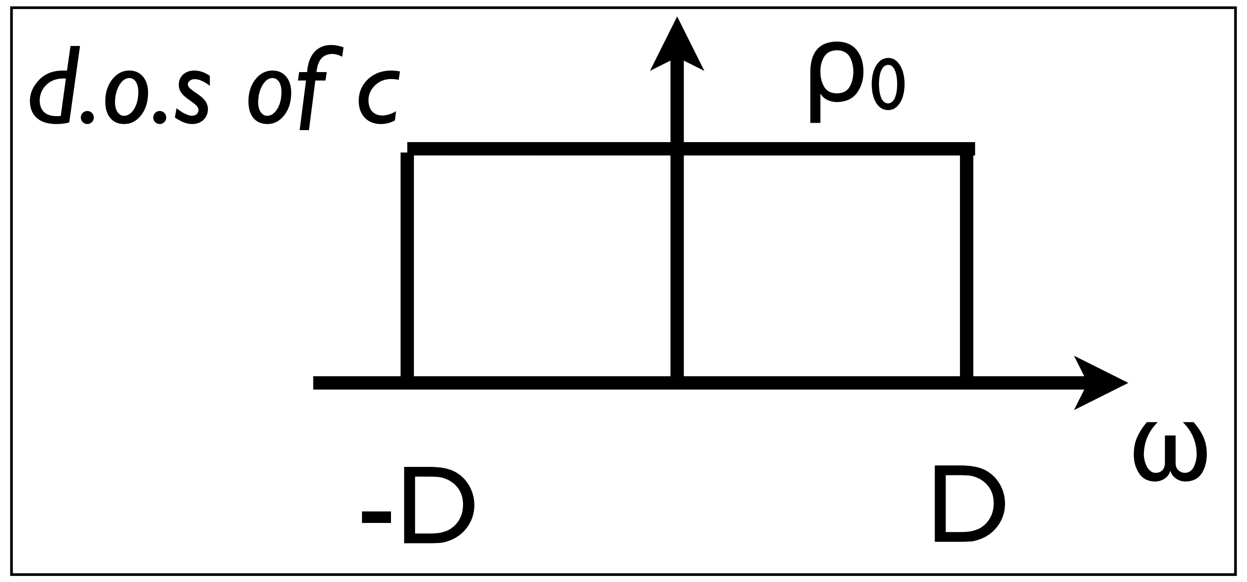


Kondo Temperature

- Perturbation theory at second order in J_K

Kondo 64

- Impurity quantities, e.g.
  $\chi_{imp} = \chi - \chi_{Pauli}$



$$\chi_{\rm imp} = \chi_0 \left(1 - 2J_K\rho_0\left(1 + 2J_K\rho_0 \ln\frac{D}{T}\right)\right) + \dots$$

$$C_{\rm imp} = 8S(S+1)(J_K\rho_0)^4\left(1 + 2J_K\rho_0 \ln\frac{D}{T}\right)^4 + \dots$$

$$R_{\rm imp} = R_0(J_K\rho_0)^2\left(1 + 2J_K\rho_0 \ln\frac{D}{T}\right)^2 + \dots$$

- Low T, large D divergences :
  absorbed in a coupling constant renormalization. $J \rightarrow J_{eff}$

$$J_{\rm eff} \equiv J_K\rho_0\left(1 + 2J_K\rho_0 \ln\frac{D}{T}\right)$$

- $J_{eff} \sim 1$: breakdown of perturbation theory at the Kondo temperature

$$T \approx T_K \equiv De^{-\frac{1}{2J_K\rho_0}}$$

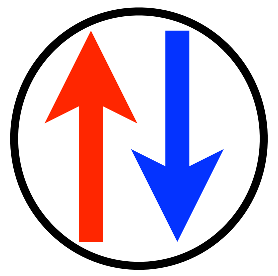
Kondo effect

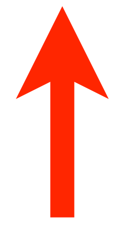
- Screening of the Kondo impurity by the metallic bath

Kondo temperature $T_K \sim De^{-1/J\rho_0}$ *d.o.s of the bath at the Fermi level*

0 — T

$T \ll T_K$ $\qquad$ $T \gg T_K$





$$\chi_{imp}(T) \sim \frac{1}{T_K}$$

$$\chi_{imp}(T) \sim \frac{1}{T}$$

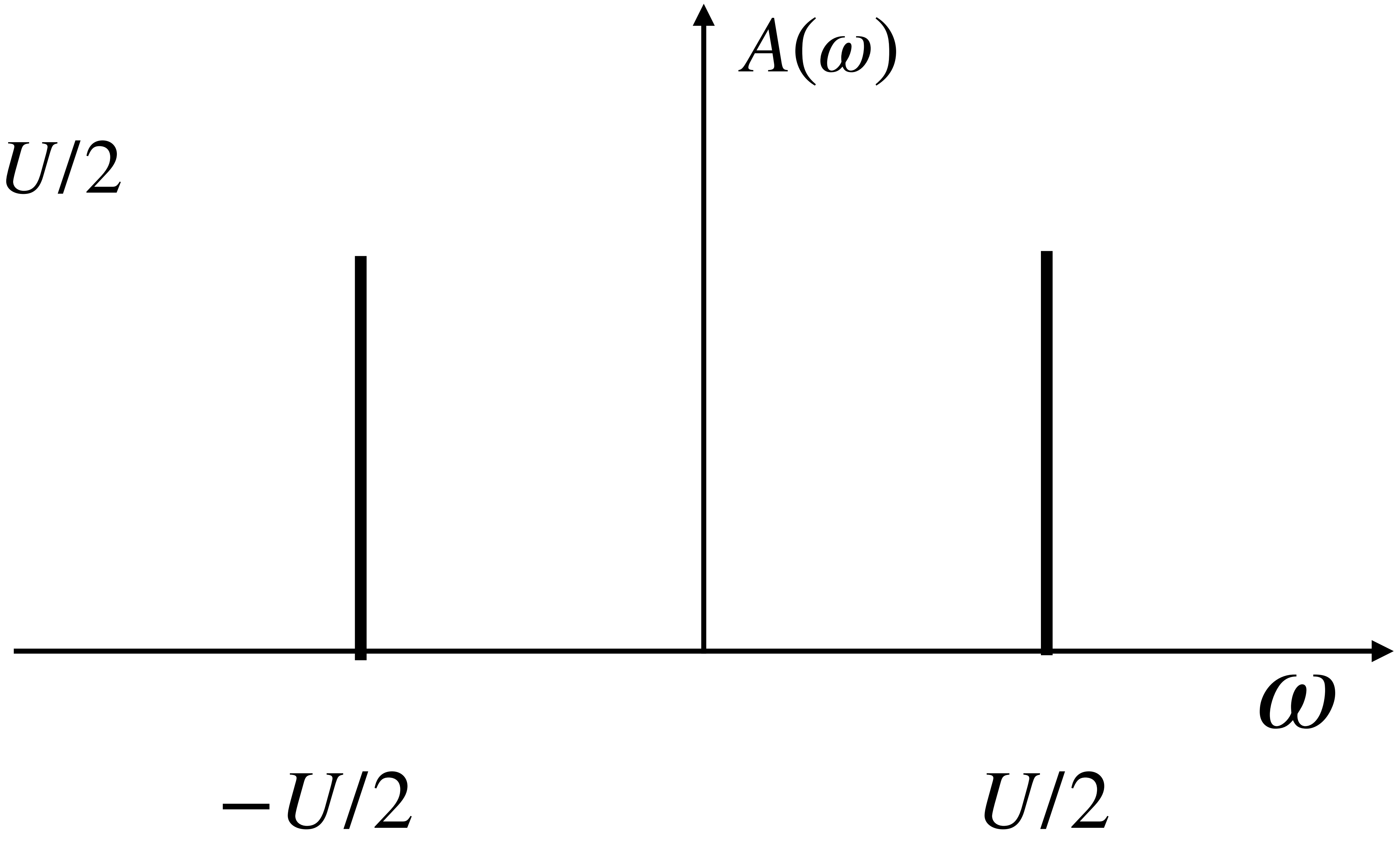
- Local Fermi liquid (*P. Nozières, '74*)
- Strong coupling picture : single "Confinement" of the spin.
- Free spin (Curie law)
- 1+1 Field Theory with asymptotic freedom (similar to QCD)

Spectral function of the d

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

$$A_d(\omega)=-\frac{1}{\pi}ImG^R_d(\omega)$$

- Atomic limit, $\epsilon_d = -U/2$

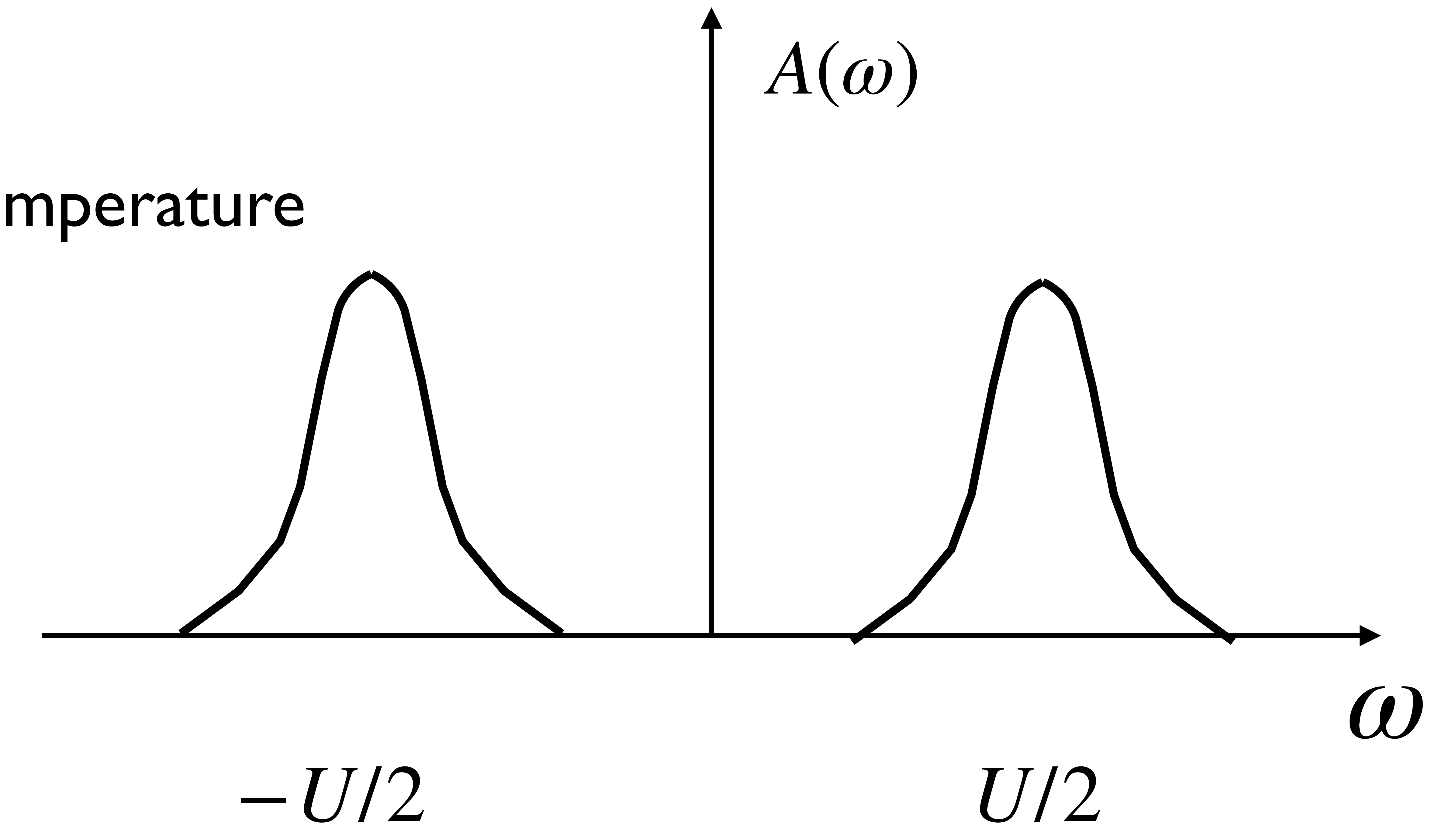


Spectral function of the d

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

$$A_d(\omega) = -\frac{1}{\pi} Im G^R_d(\omega)$$

- Atom + bath, high temperature
  $T \gg T_K$

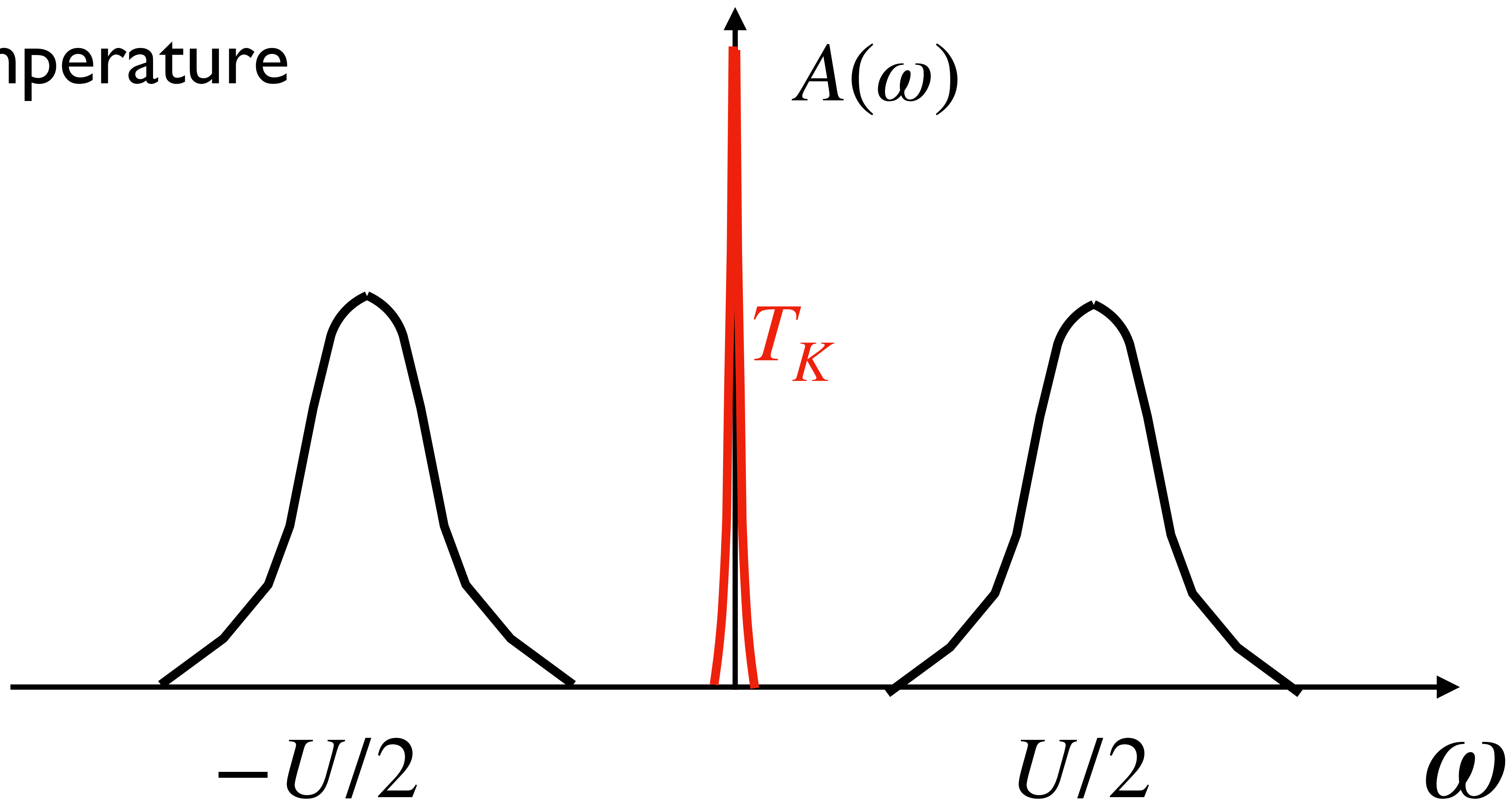


Spectral function of the d

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

$$A_d(\omega) = -\frac{1}{\pi} Im G^R_d(\omega)$$

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



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

Kondo-Abrikosov-Suhl resonance

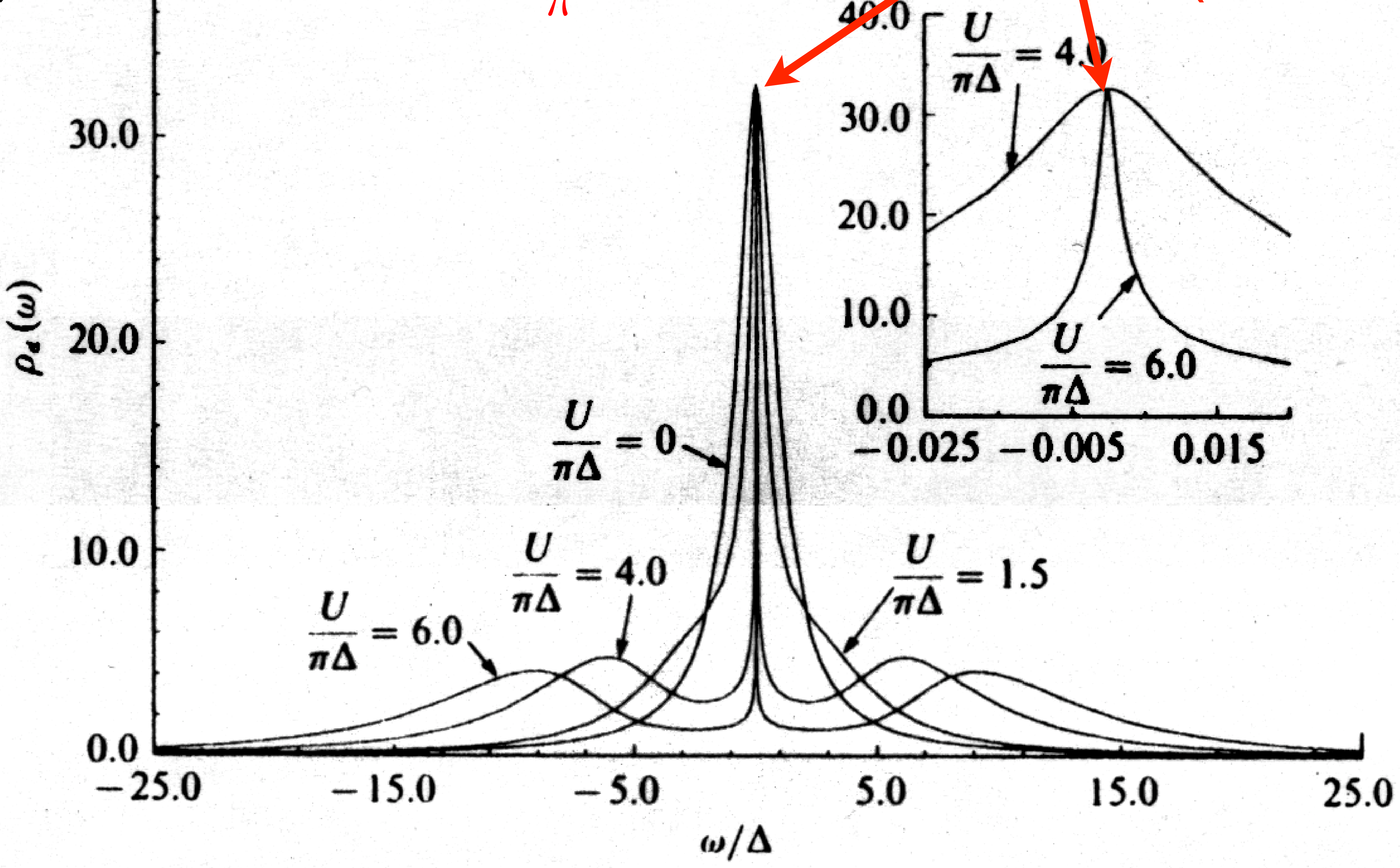
$$H = \sum_{k,\sigma=\uparrow,\downarrow} \varepsilon_{k\sigma} \xi^\dagger_{k\sigma} \xi_{k\sigma} + \sum_{\sigma=\uparrow,\downarrow} \varepsilon_d d^\dagger_\sigma d_\sigma + U n_{d\uparrow} n_{d\downarrow} + \sum_{k,\sigma=\uparrow,\downarrow} V_{k\sigma}(\xi^\dagger_{k\sigma} d_\sigma + h.c.)$$

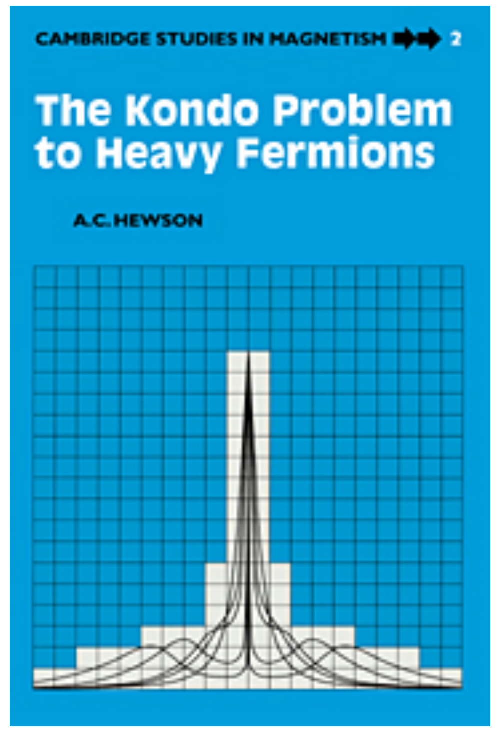
- Evolution from U=0, at T =0 (using simply perturbation theory in U).
- Spectral weight transfer

$A_d(\omega)$

$$A_d(\omega) = -\frac{1}{\pi} Im G^R_d(\omega)$$

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





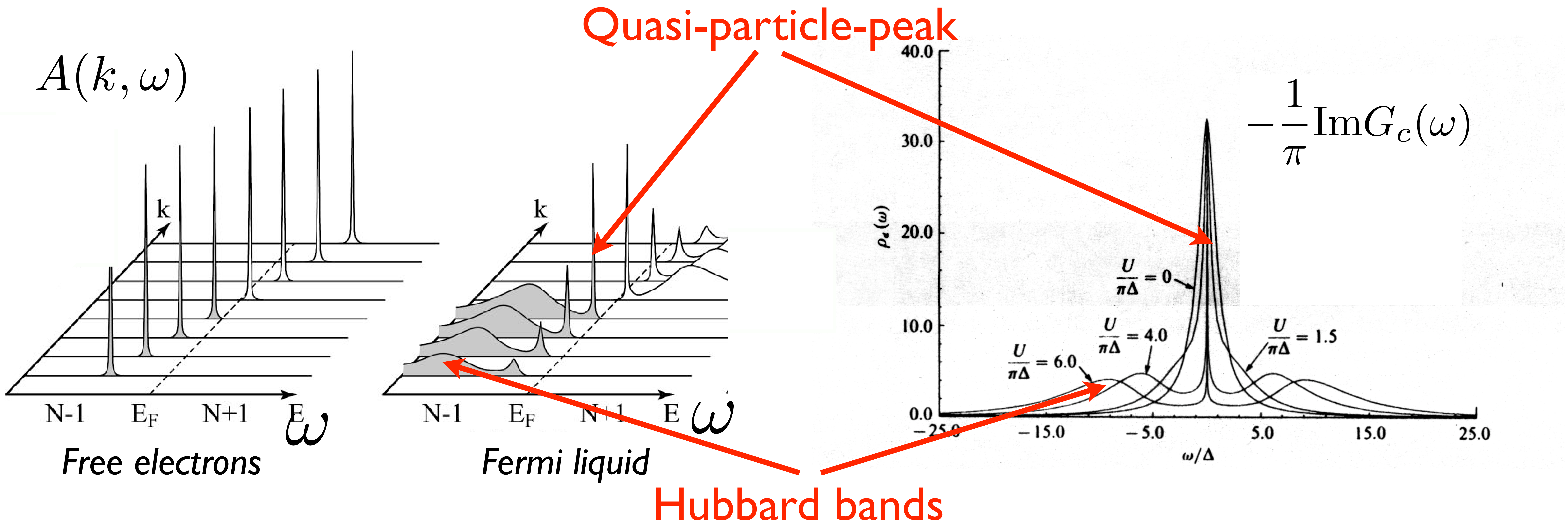
particle-hole symmetric case *(Hewson's book)*

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

Analogy with Mott problem

Lattice

Anderson impurity



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

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

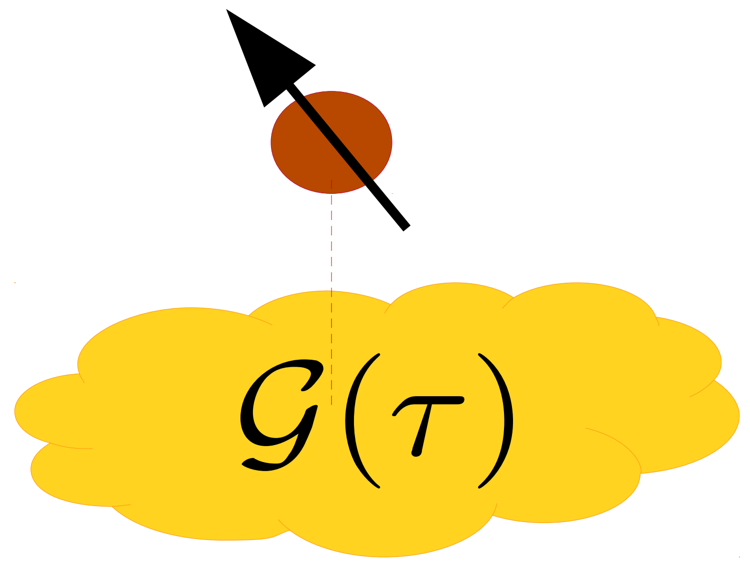
DMFT transform this analogy into a formalism

Dynamical Mean Field Theory
(DMFT)

DMFT : main idea

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

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



- First a reminder of the simple 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
$h_{\text{eff}} = z J m$	Weiss Field
$m = \tanh(\beta h_{\text{eff}})$	Solution of the effective Hamiltonian

- Qualitatively correct (phase diagram, second order transition) even if critical exponents are wrong (R.G., Field theory....,)
- Derivation : e.g. large dimension limit on hypercubic lattice

Generalisation for quantum models, electrons ?

Dynamical Mean Field Theory

Ising model

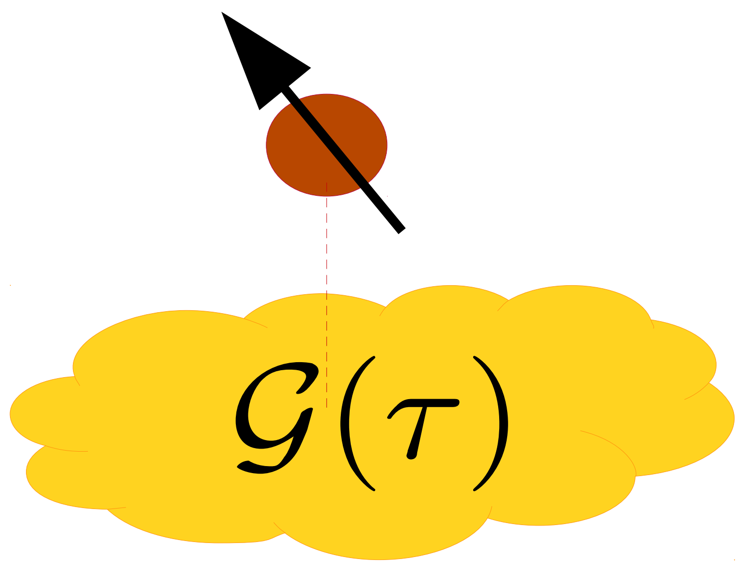
$$H = -J \sum_{ij} \sigma_i \sigma_j$$

$$m = \langle \sigma \rangle$$

$$H_{\text{eff}} = -J h_{\text{eff}} \sigma$$

$$h_{\text{eff}} = zJm$$

$$m = \tanh(\beta h_{\text{eff}})$$



?

Dynamical Mean Field Theory

- Anderson impurity with an effective band determined self-consistently

$$H = \underbrace{\sum_{\sigma=\uparrow,\downarrow} \varepsilon_d c^\dagger_\sigma c_\sigma + U n_\uparrow n_\downarrow}_{\text{Local site}} + \underbrace{\sum_{k,\sigma=\uparrow,\downarrow} V_{k\sigma}(\xi^\dagger_{k\sigma} c_\sigma + h.c.) + \sum_{k,\sigma=\uparrow,\downarrow} \varepsilon_{k\sigma} \xi^\dagger_{k\sigma} \xi_{k\sigma}}_{\text{Coupled to an effective electronic bath}}$$

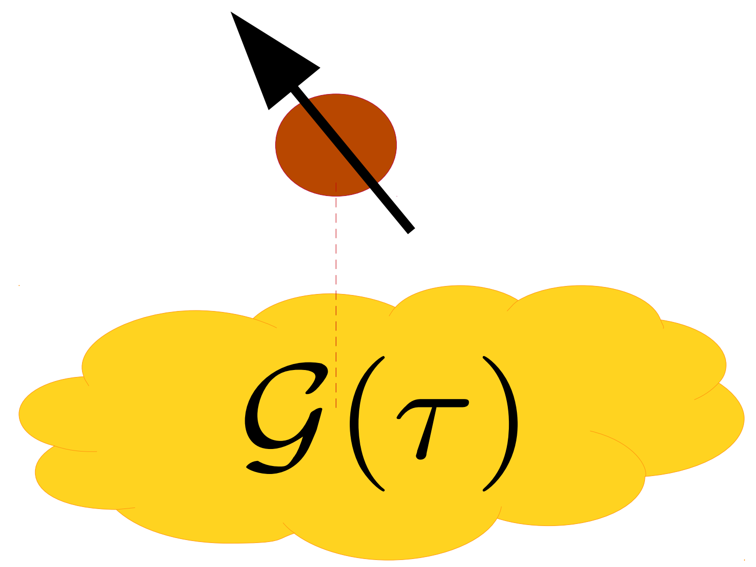
- Action form

$$S = -\iint_0^\beta d\tau d\tau' c^\dagger_\sigma(\tau) \mathcal{G}^{-1}_\sigma(\tau - \tau') c_\sigma(\tau') + \int_0^\beta d\tau \; U n_\uparrow(\tau) n_\downarrow(\tau)$$

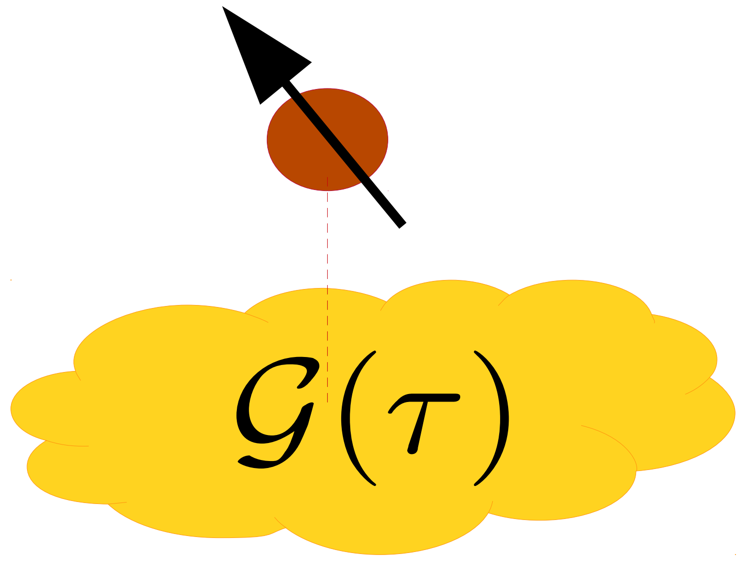
$$\mathcal{G}^{-1}_\sigma(i\omega_n) \equiv i\omega_n + \epsilon_0 - \underbrace{\sum_k \frac{|V_{k\sigma}|^2}{i\omega_n - \epsilon_{k\sigma}}}_{\Delta_\sigma(i\omega_n)}$$

Bath
"Weiss field"

Hybridization function



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	$H_{\text{eff}} = -J h_{\text{eff}} \sigma$ $m = \langle \sigma \rangle$	$S_{\text{eff}} = -\iint_0^\beta d\tau d\tau' c^\dagger_\sigma(\tau) \mathcal{G}_\sigma^{-1}(\tau - \tau') c_\sigma(\tau') + \int_0^\beta d\tau \, U n_\uparrow(\tau) n_\downarrow(\tau)$ $G_{\sigma \text{imp}}(\tau) \equiv -\left\langle T c_\sigma(\tau) c^\dagger_\sigma(0) \right\rangle_{S_{\text{eff}}}$
Self consistency condition	$h_{\text{eff}} = zJm$	$\Sigma_{\sigma \text{imp}}[\mathcal{G}](i\omega_n) \equiv \mathcal{G}_\sigma^{-1}(i\omega_n) - G^{-1}_{\sigma \text{imp}}[\mathcal{G}](i\omega_n)$ $G_{\sigma \text{imp}}[\mathcal{G}](i\omega_n) = \sum_k \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_{\sigma \text{imp}}[\mathcal{G}](i\omega_n)}$ *Implicit equation for the bath*

Lattice quantities vs impurity quantities

- Dyson equation on the lattice

$$G_{\sigma \mathrm{latt}}(k, i\omega_n) \equiv \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_{\sigma \mathrm{latt}}(k, i\omega_n)}$$

- DMFT : the self-energy on the lattice is local :

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

$$G_{\sigma \mathrm{loc}}(i\omega_n) \equiv \sum_k G_{\sigma \mathrm{latt}}(k, i\omega_n) = G_{\sigma \mathrm{imp}}(i\omega_n)$$

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

- G_{latt} depends on k: Fermi surface in metals.
- Z, m^*, coherence temperature, finite temperature lifetime of metals are constant along the Fermi surface.
- Effective mass and Z are related :

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

Depends only the d.o.s of free electrons

- 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

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

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

Semi circular d.o.s

- A simpler case, when the d.o.s is a semi-circular

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

- Its Hilbert transform can be done explicitly

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

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

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

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

Semi circular d.o.s

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

$$R(G) = t^2G + 1/G$$

- Its Hilbert transform can be done explicitly

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

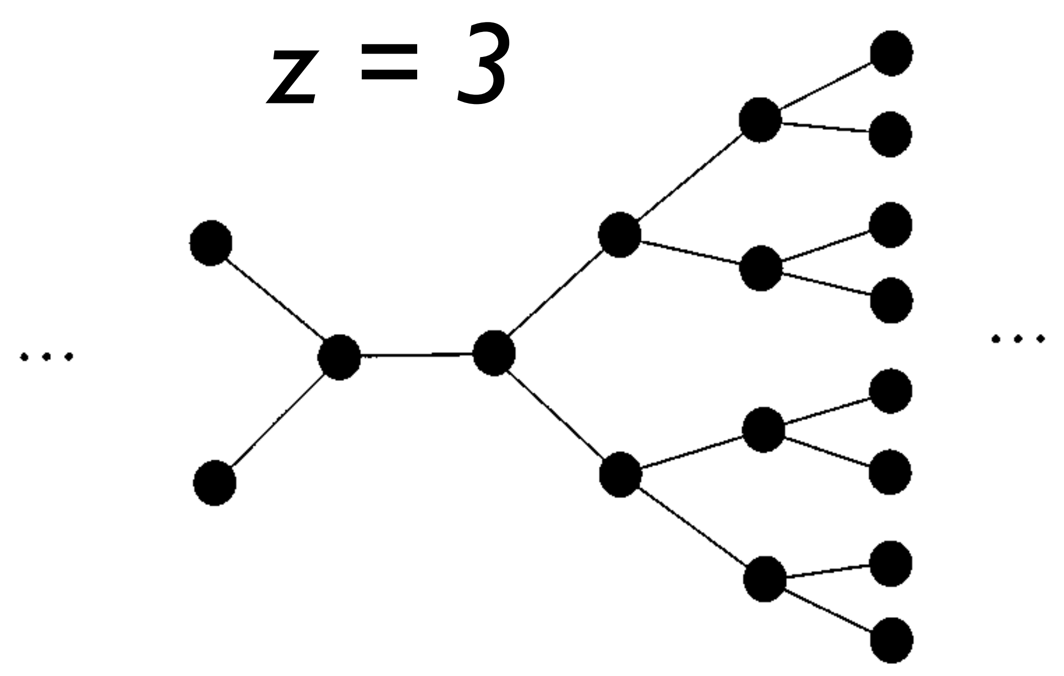
$$\begin{aligned}
G_{\sigma\text{imp}}(i\omega_n) &= \tilde{D}(i\omega_n + \mu - \Sigma_{\sigma\text{imp}}(i\omega_n)) \\
R[G_{\sigma\text{imp}}](i\omega_n) &= i\omega_n + \mu - \Sigma_{\sigma\text{imp}}(i\omega_n) \\
t^2 G_{\sigma\text{imp}}(i\omega_n) + G^{-1}_{\sigma\text{imp}}(i\omega_n) &= i\omega_n + \mu - \mathcal{G}^{-1}_\sigma(i\omega_n) + G^{-1}_{\sigma\text{imp}}(i\omega_n)
\end{aligned}$$

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

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

The Bethe lattice

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



- Free fermions on the Bethe Lattice for $z \to \infty$ have a semi circular dos.

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

$$G(i\omega_n) = \tilde{D}(i\omega_n + \mu)$$

$$i\omega_n + \mu = R[G] = t^2 G + G^{-1}$$

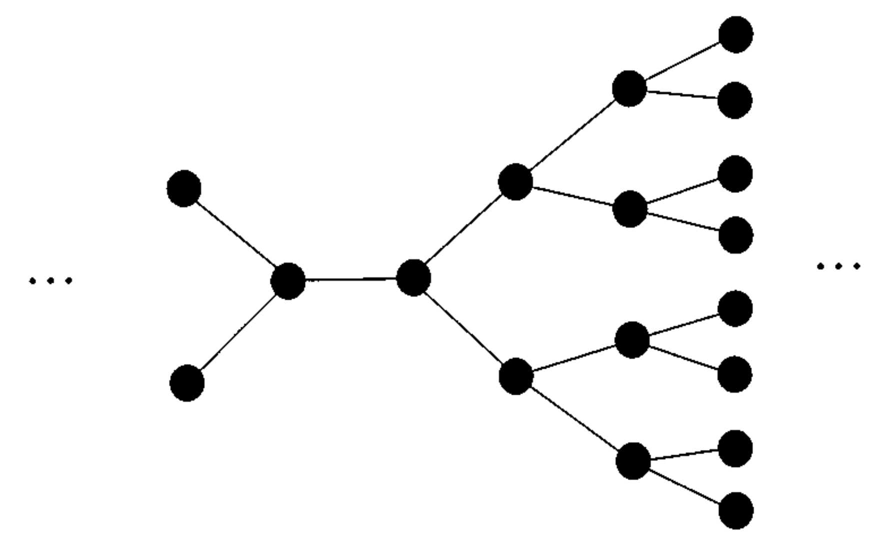
Bethe lattice/semicircular dos : summary of equations

- DMFT on the Bethe lattice

$$S_{\text{eff}} = -\iint_0^\beta d\tau d\tau' c_\sigma^\dagger(\tau)\mathcal{G}_\sigma^{-1}(\tau-\tau')c_\sigma(\tau') + \int_0^\beta d\tau\, U n_\uparrow(\tau) n_\downarrow(\tau)$$

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

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



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

Exact limits for DMFT

- Non interacting limit $U = 0$
  - $\Sigma = 0,$ hence k-independent!
- Isolated atom $\Delta = 0$
  - $\Sigma = \Sigma_{atom}$
- Hence DMFT interpolates between weak and strong coupling.
- In the formal limit of infinite dimensionality $d \to \infty$ *Metzner and Vollhardt, PRL 62 (1989) 324*

More relevant to physics:
it is a good approximation
when spatial correlations are not too long-range

Derivation of the DMFT equations

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:

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

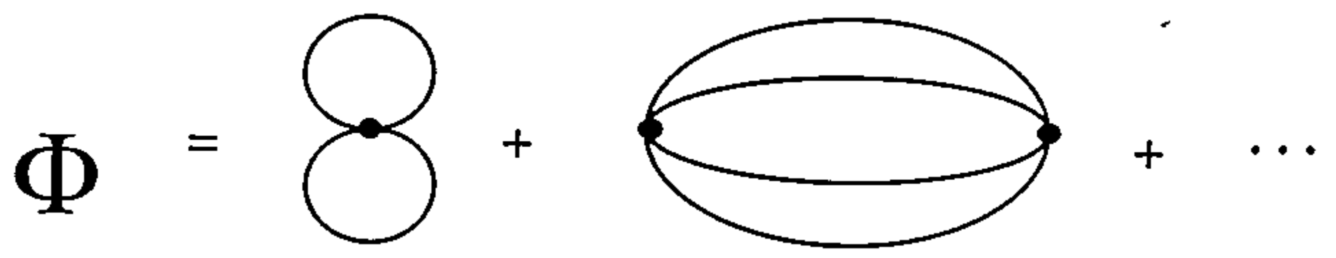
- Dyson as a functional equation for G

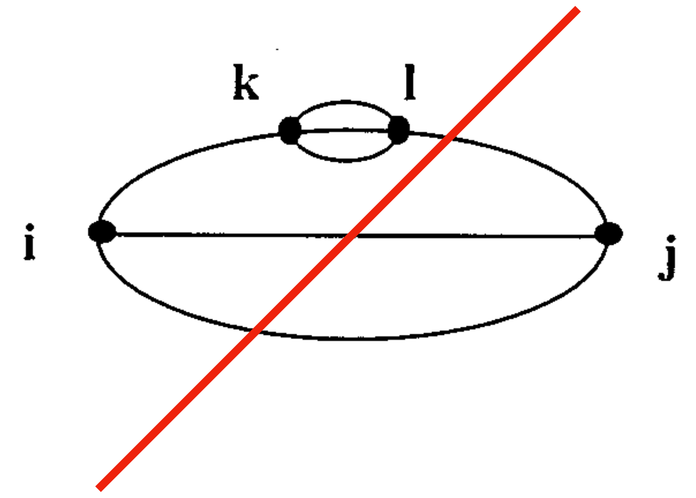
Luttinger-Ward functional

- 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

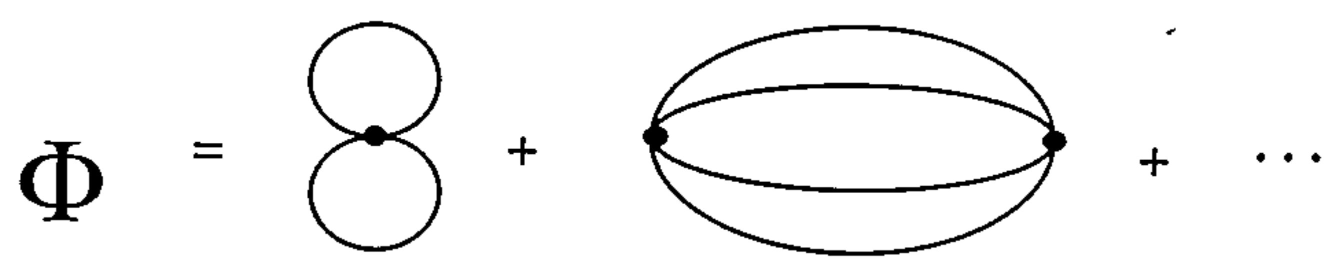
Metzner-Vollhardt '89, Georges-Kotliar '92

- 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)

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



Wait … where is the bath ?

Impurity = auxiliary local model

$$S_{\text{imp}} = -\iint_0^\beta d\tau d\tau' \sum_\sigma \bar{c}_{\sigma\tau} \mathcal{G}^{-1}(\tau - \tau') c_{\sigma\tau'} + \int_0^\beta d\tau U n_\uparrow(\tau) n_\downarrow(\tau)$$

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

$$\Phi(G_{ij}) = \sum_i \phi_1(G_{ii}) \qquad \phi_1 = \phi_{\text{Impurity for any } \mathcal{G}} = \phi_{\text{atom}}$$

- 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

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

DMFT self-consistency equations

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

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

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/√d.

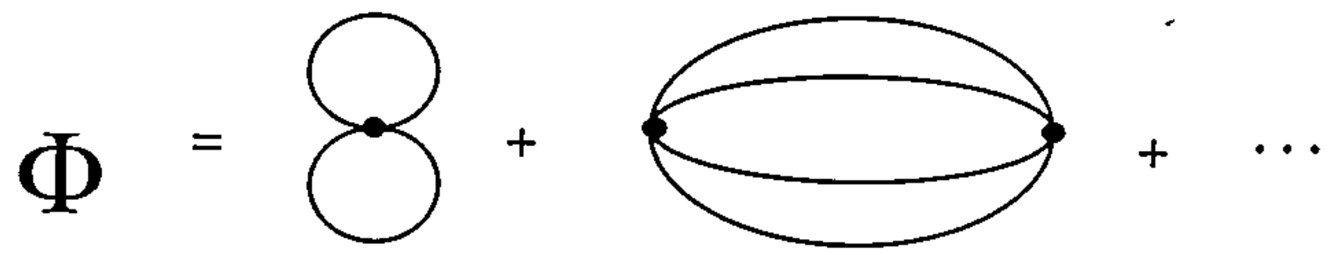
DMFT is an atomic approximation

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

- 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 …)
    Cf lectures by D. Sénéchal, A. Toschi
  - Straightforward generalization to non equilibrium (Schwinger-Keldysh)
    Cf lectures by P. Werner, M. Eckstein

Analogy with DFT

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 :

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

- For the impurity :

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

- Therefore :

$$\frac{\Omega}{N} = \Omega_{\text{imp}} - T \sum_{n\sigma} \left(\int_{-\infty}^{+\infty} d\epsilon \, D(\epsilon) \times \ln[i\omega_n + \mu - \Sigma_\sigma(i\omega_n) - \epsilon] + \ln G_\sigma(i\omega_n) \right),$$

How to solve DMFT equations ?

The toolbox

Solving DMFT : iterative method

Impurity solver

$$S_{\text{eff}} = -\iint_0^\beta d\tau d\tau' c_\sigma^\dagger(\tau)\mathcal{G}_\sigma^{-1}(\tau-\tau')c_\sigma(\tau') + \int_0^\beta d\tau\, U n_\uparrow(\tau)n_\downarrow(\tau)$$

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

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

$\mathcal{G}$

$G_{\text{imp}}, \Sigma_{\text{imp}}$

Self consistency condition

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

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

The DMFT solver toolbox

- Exact/Controlled algorithms
  - Continuous Time Quantum Monte Carlo (CTQMC). *Cf Lecture by M. Ferrero tomorrow*
  - Exact diagonalization (ED). *Cf lecture by D. Sénéchal on Monday*
  - Numerical Renormalization group (NRG). *Cf Lecture by F. Kugler on Tuesday*
  - Tensor network (DMRG). *Cf Lecture DMFT Part 2*

- Approximate solvers
  - Iterated Perturbation Theory (IPT).
  - NCA family (NCA, OCA, …)
  - Slave bosons / Hartree-Fock / "Hubbard I" (= atomic self-energy)

Iterated Perturbation Theory (IPT)

- Anderson model : perturbation in U is regular *(Yosida,Yamada, 70's.)*.
- Use first non-trivial order *(Kotliar-Georges, 1992)*.
- **Bare** perturbation theory (don't use bold diagrams !)

$$\Sigma(i\omega_n) \simeq \frac{U}{2} + U^2 \int_0^\beta d\tau \, e^{i\omega_n \tau} \hat{\mathscr{G}}_0(\tau)^3$$

- Exact for $U = 0$ and $U = \infty$.
- Qualitatively good for Mott transition in DMFT.

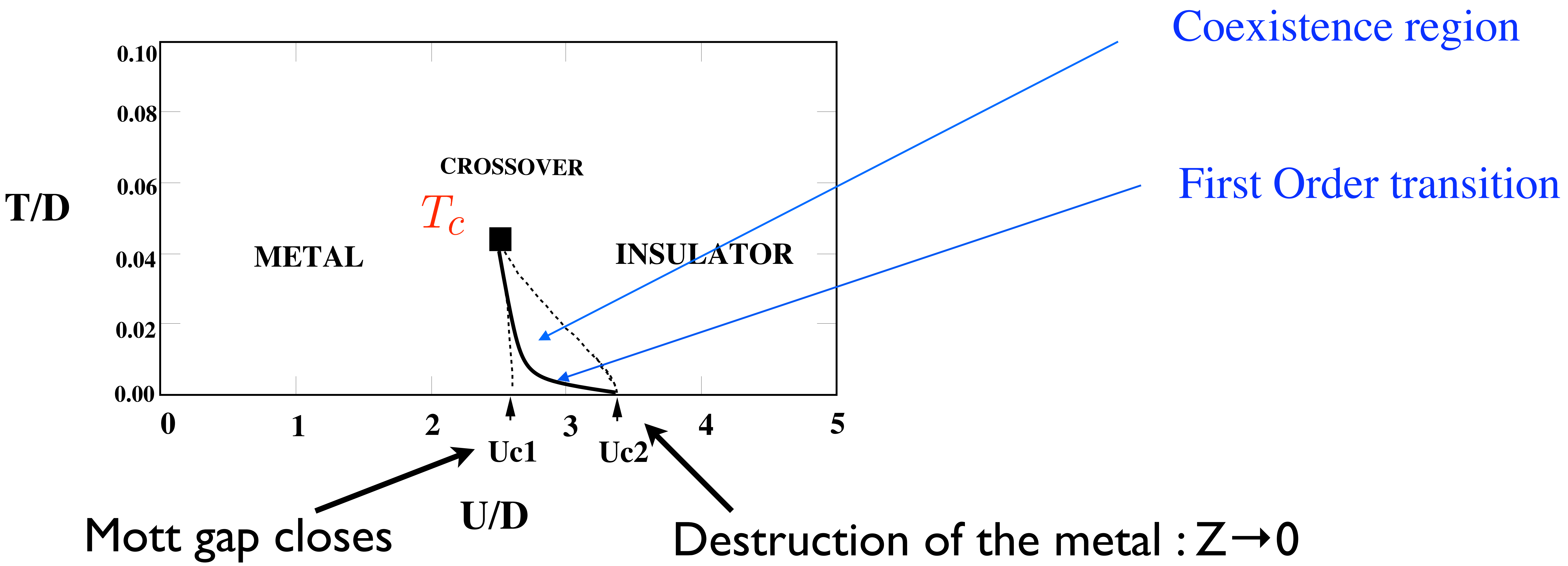
- *Cf TRIQS tutorial*

A DMFT classic

Hubbard model, 1 band, 1/2 filling

Phase diagram

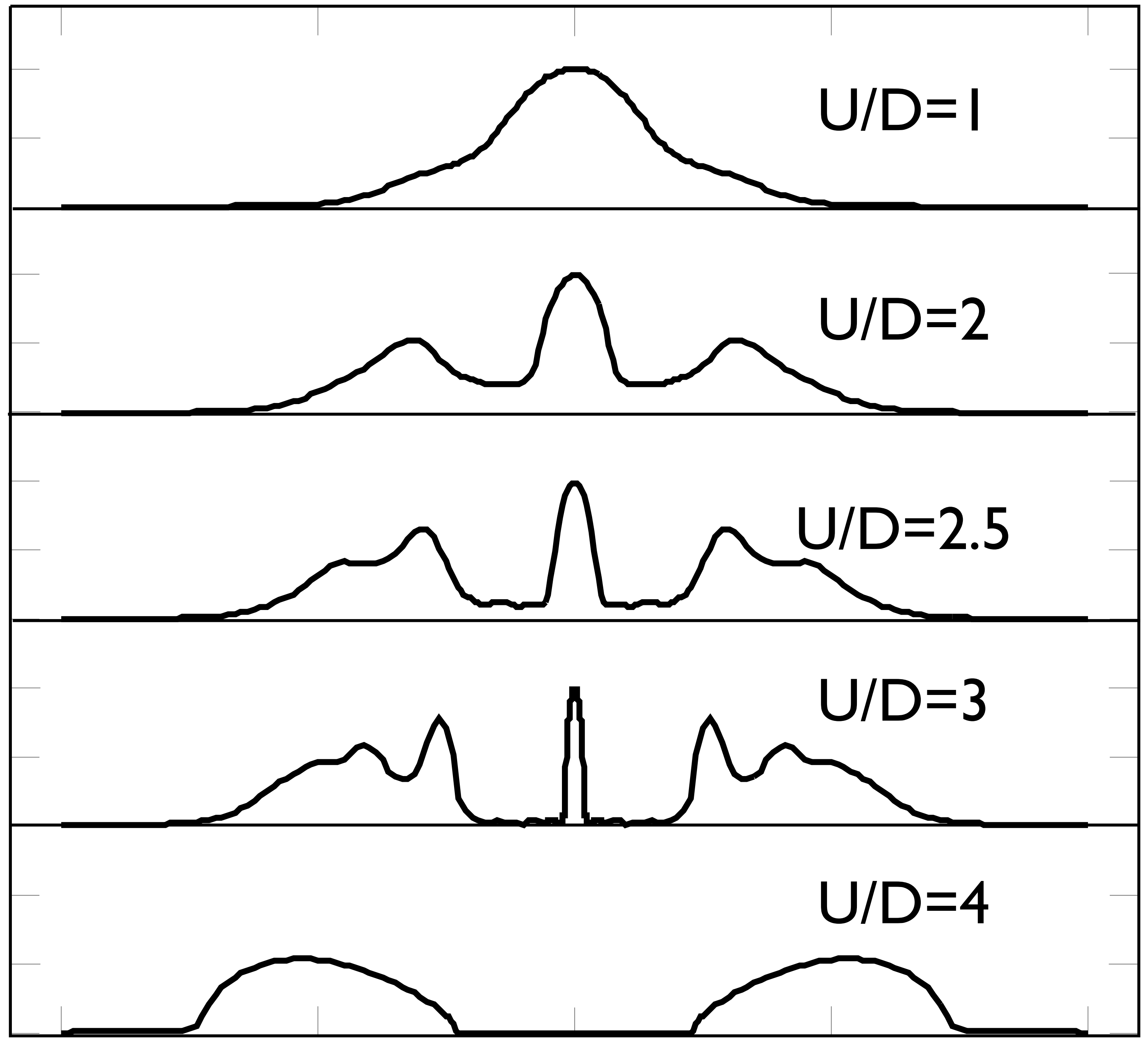
- Hubbard model at half-filling (δ=0). D is half-bandwidth.



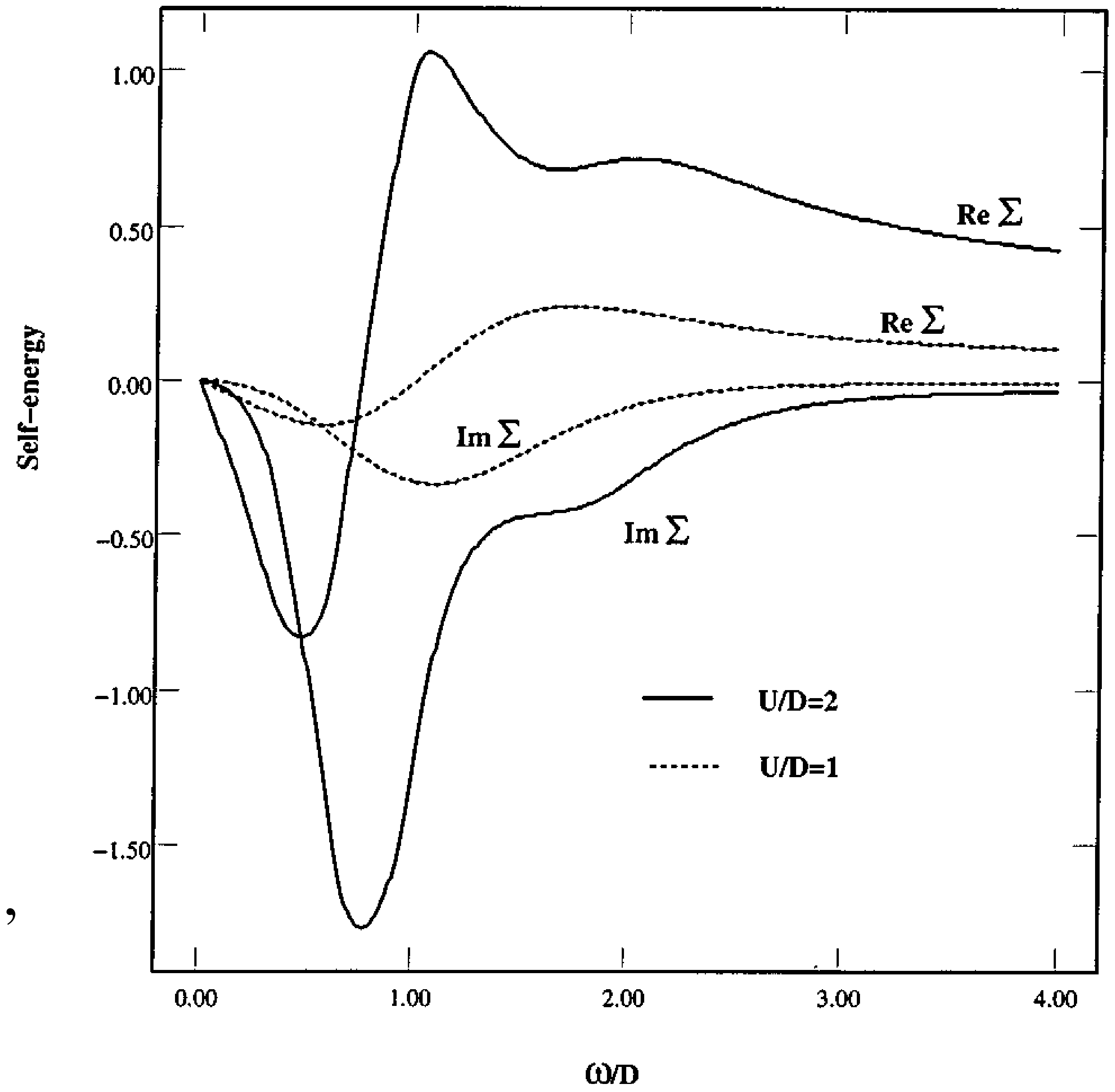
2 solutions

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

Spectral function



Self-energies in metal



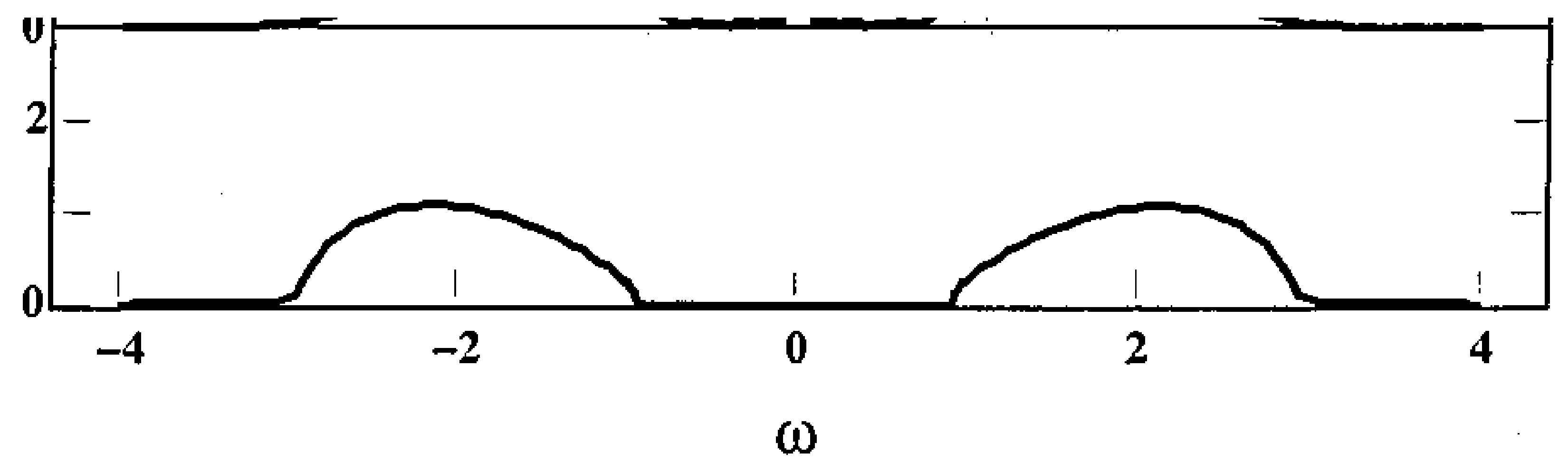
$$\mathrm{Re}\Sigma(\omega+i0^+) = U/2 + (1-1/Z)\omega + O(\omega^3),$$

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

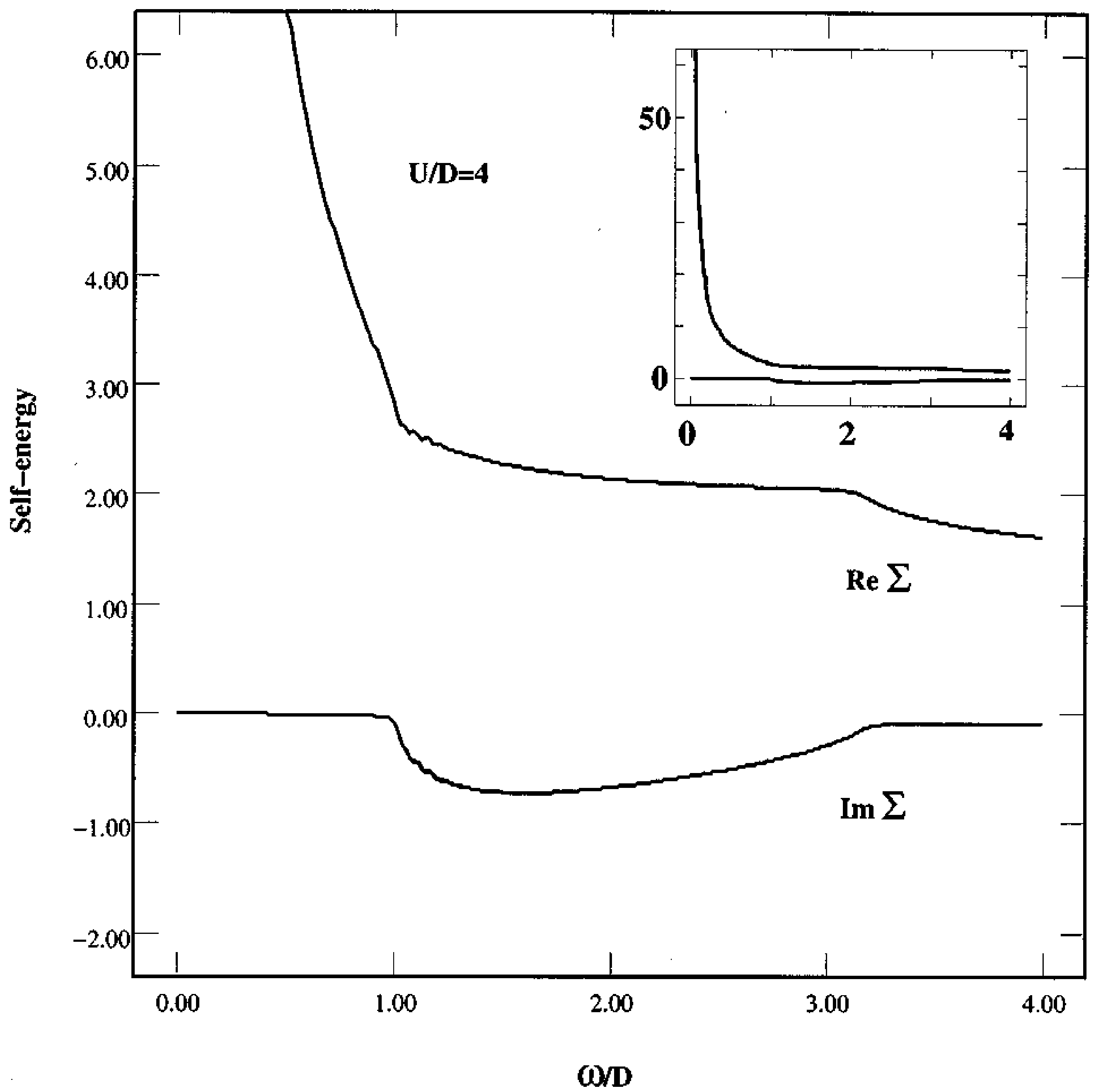
2 solutions

- 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*

Hubbard model, DMFT, (IPT),T=0,δ=0

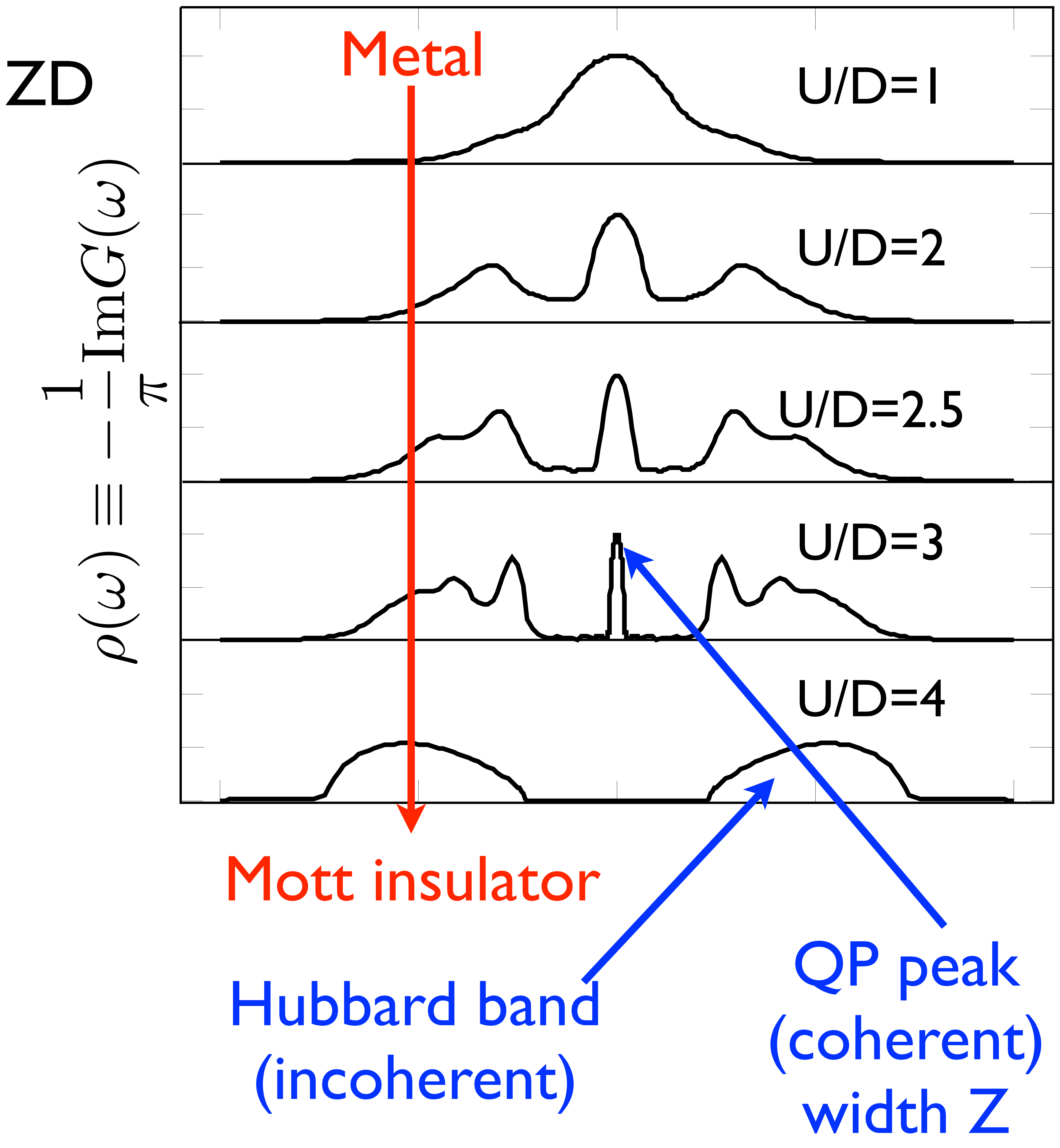
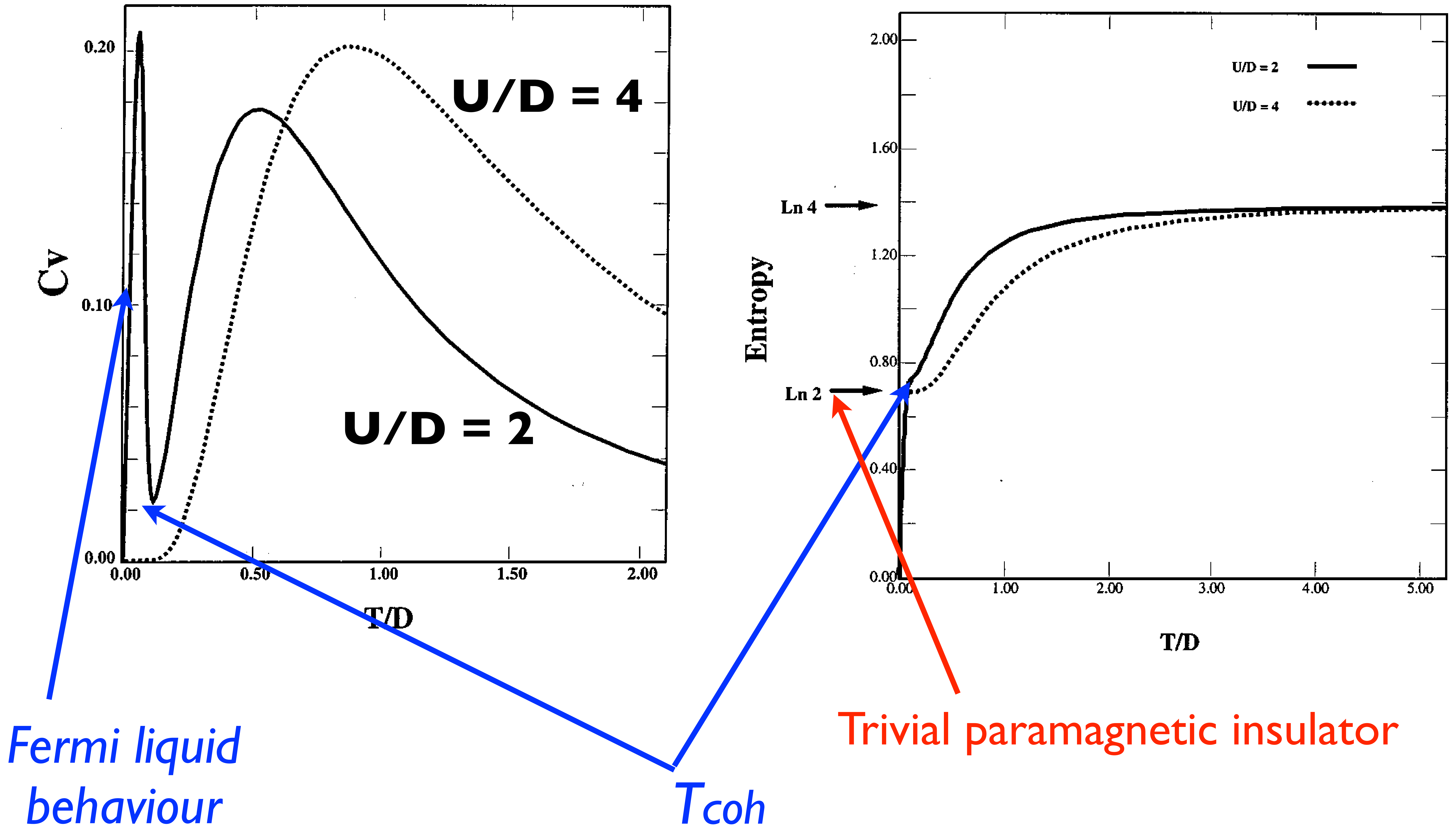
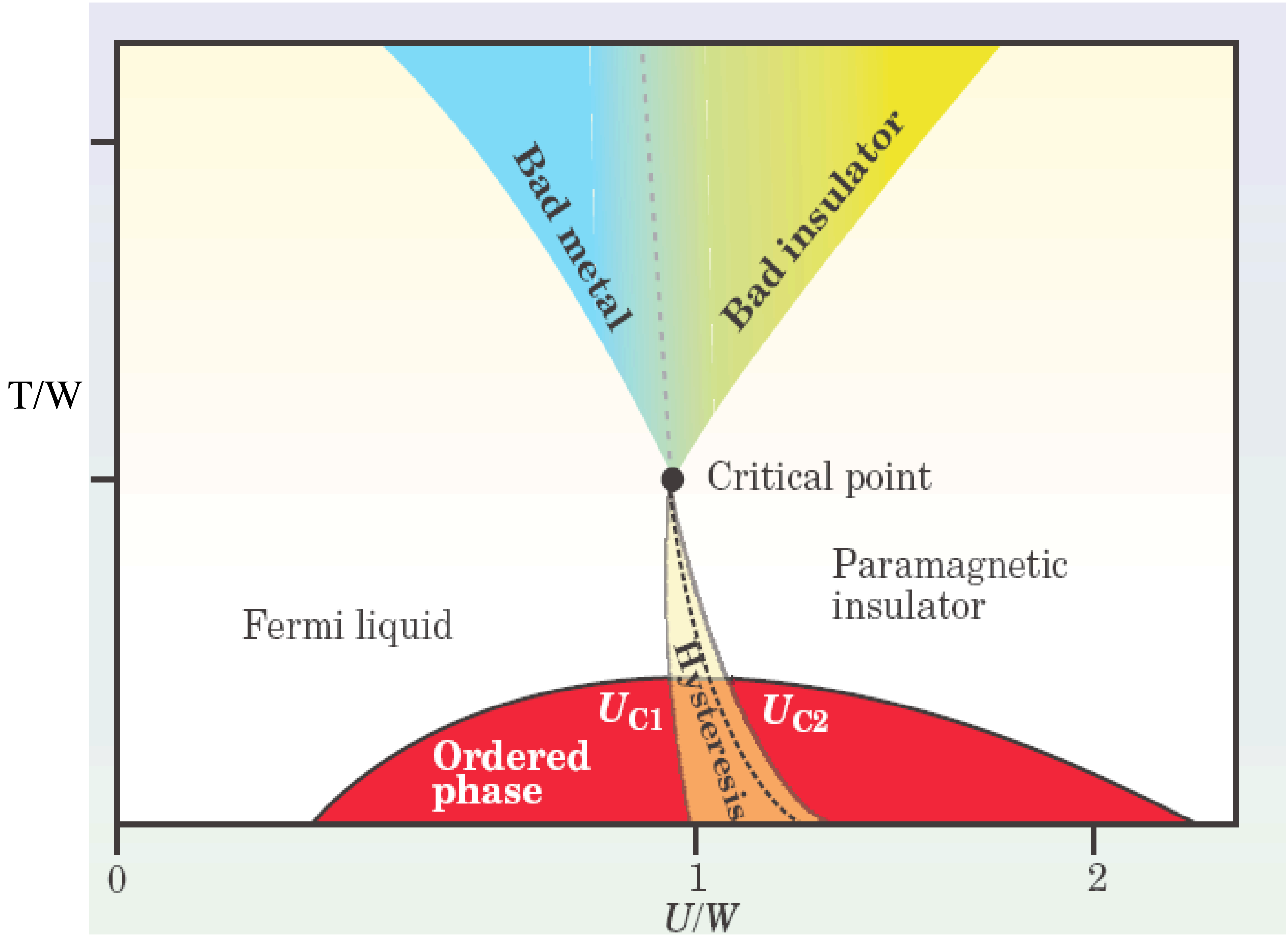


Illustration of the low-coherence temperature

- Thermodynamics quantities

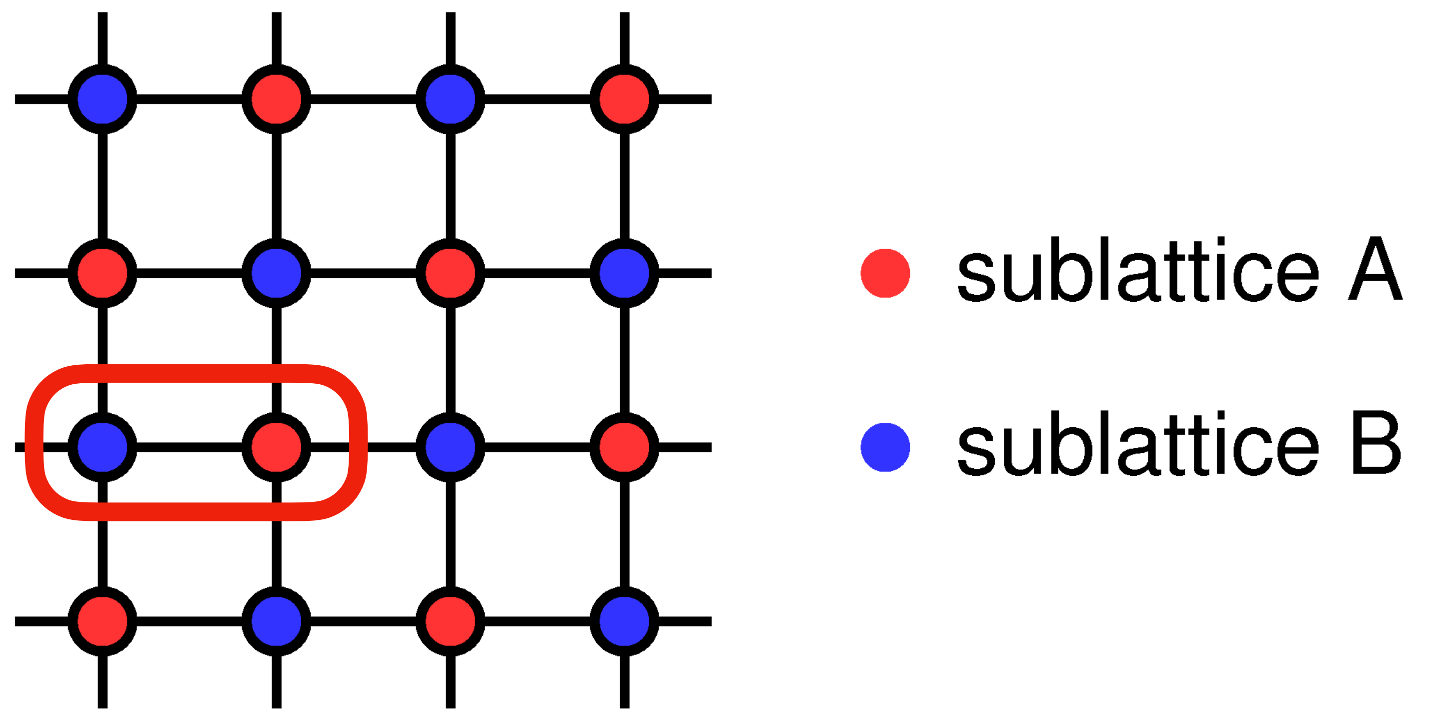


Complete phase diagram



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)

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

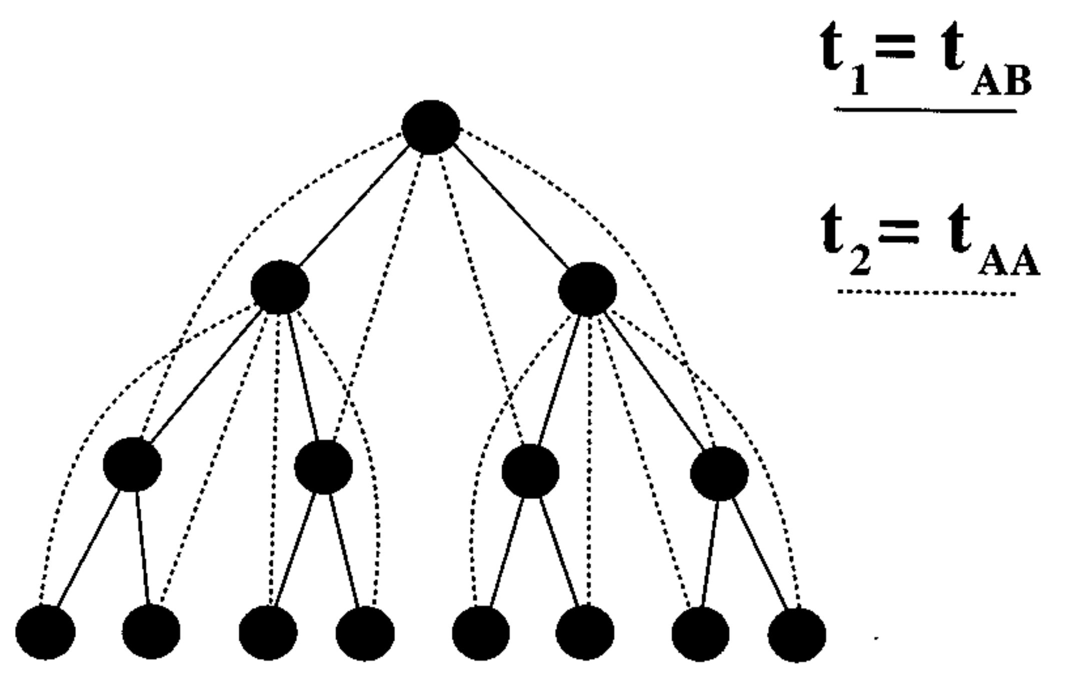
Remark on frustrated systems

- DMFT paramagnetic equations = equations of a frustrated system

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

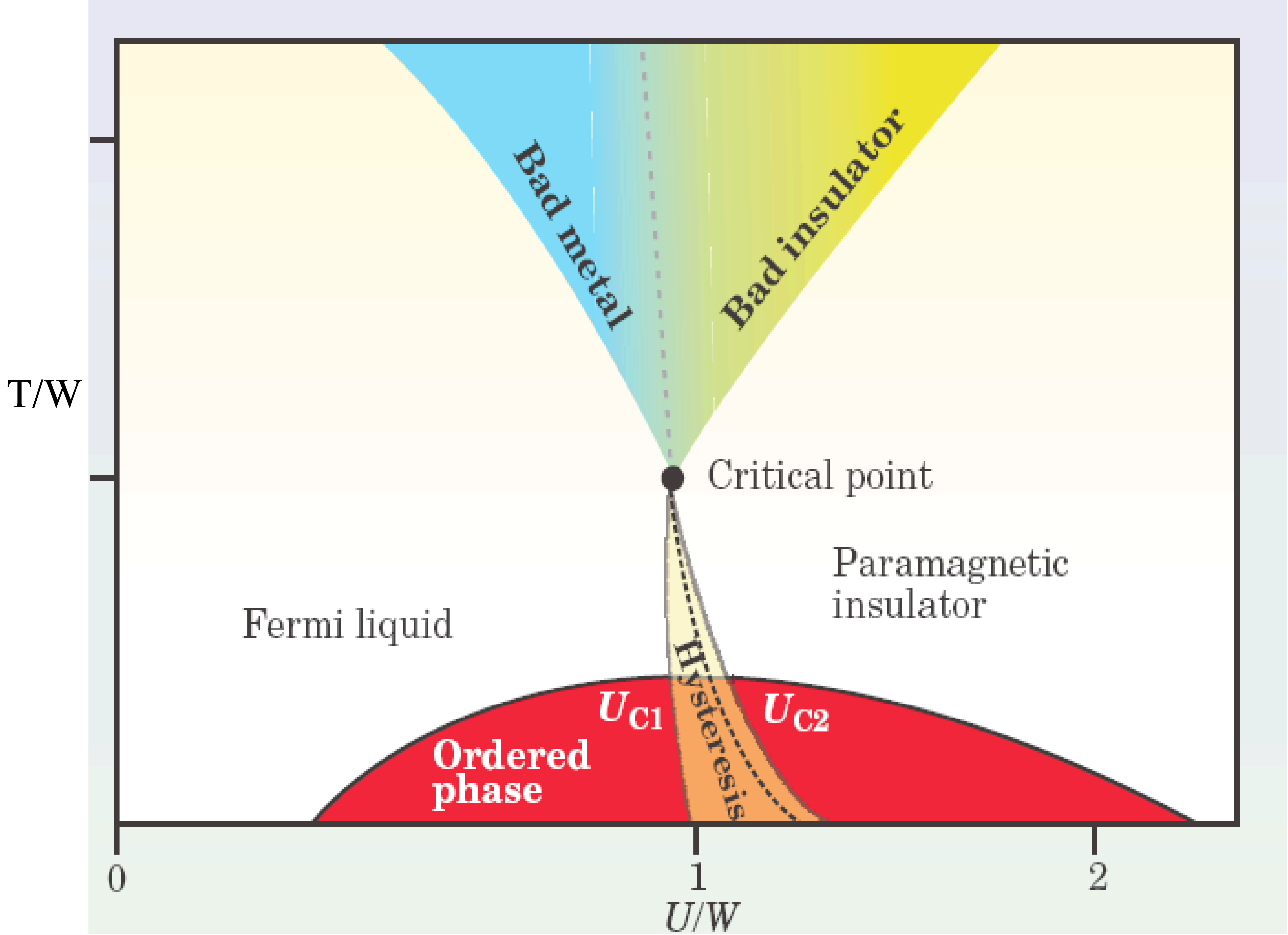
- E.g. a frustrated Bethe lattice (paramagnetic phase).

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



Complete phase diagram

- With frustration (or AF would be much higher)



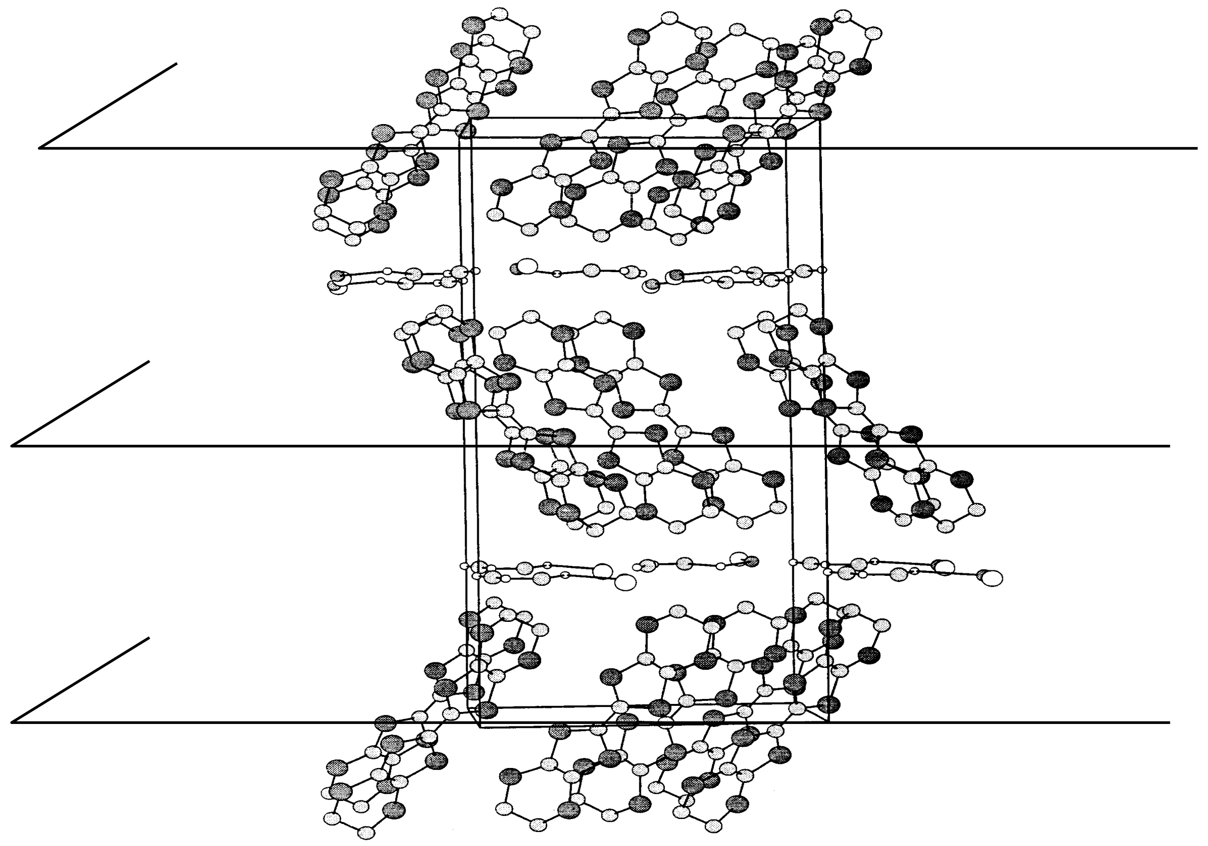
Comparison with some experiments

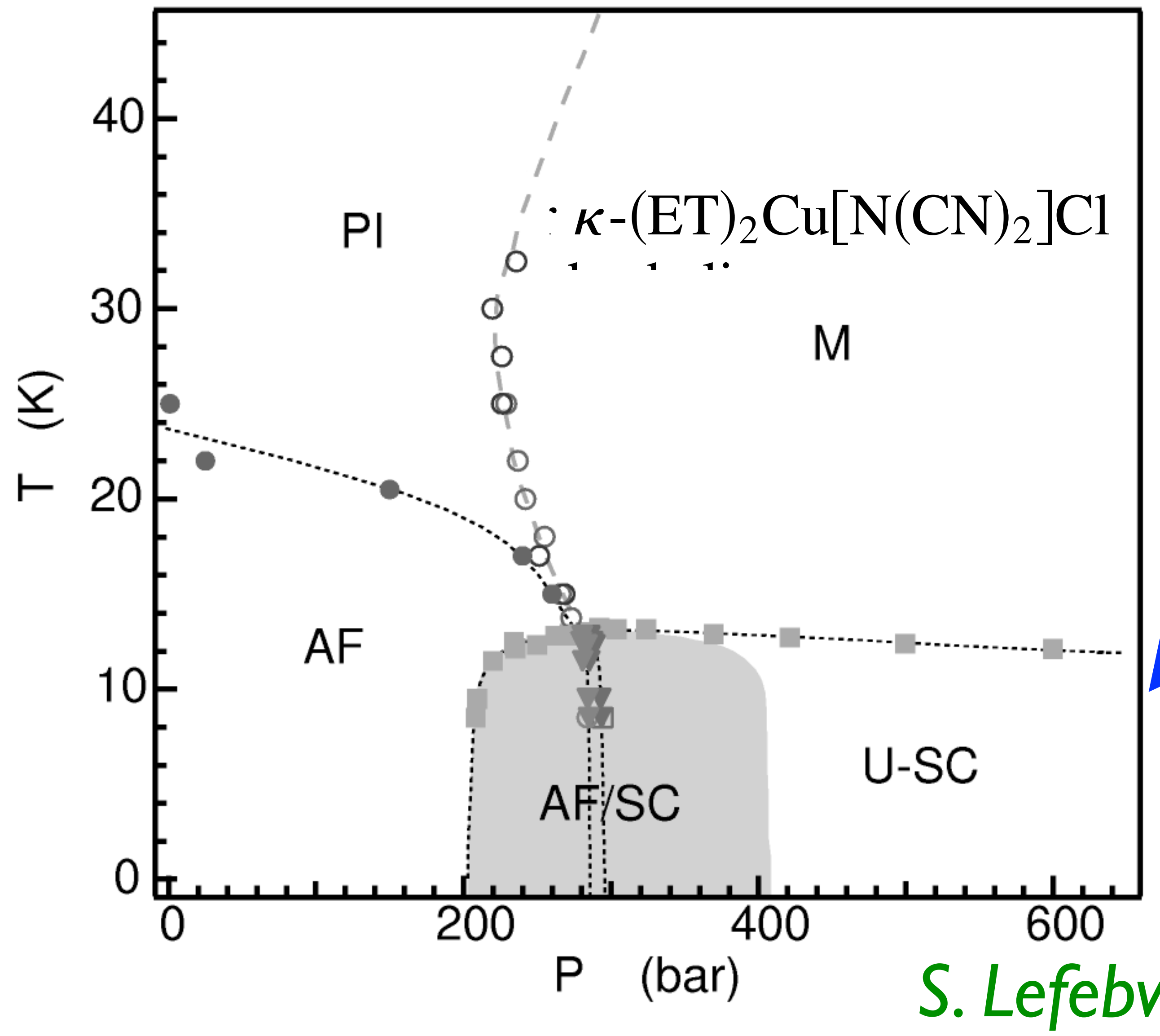
Organics (resistivity measurements)

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

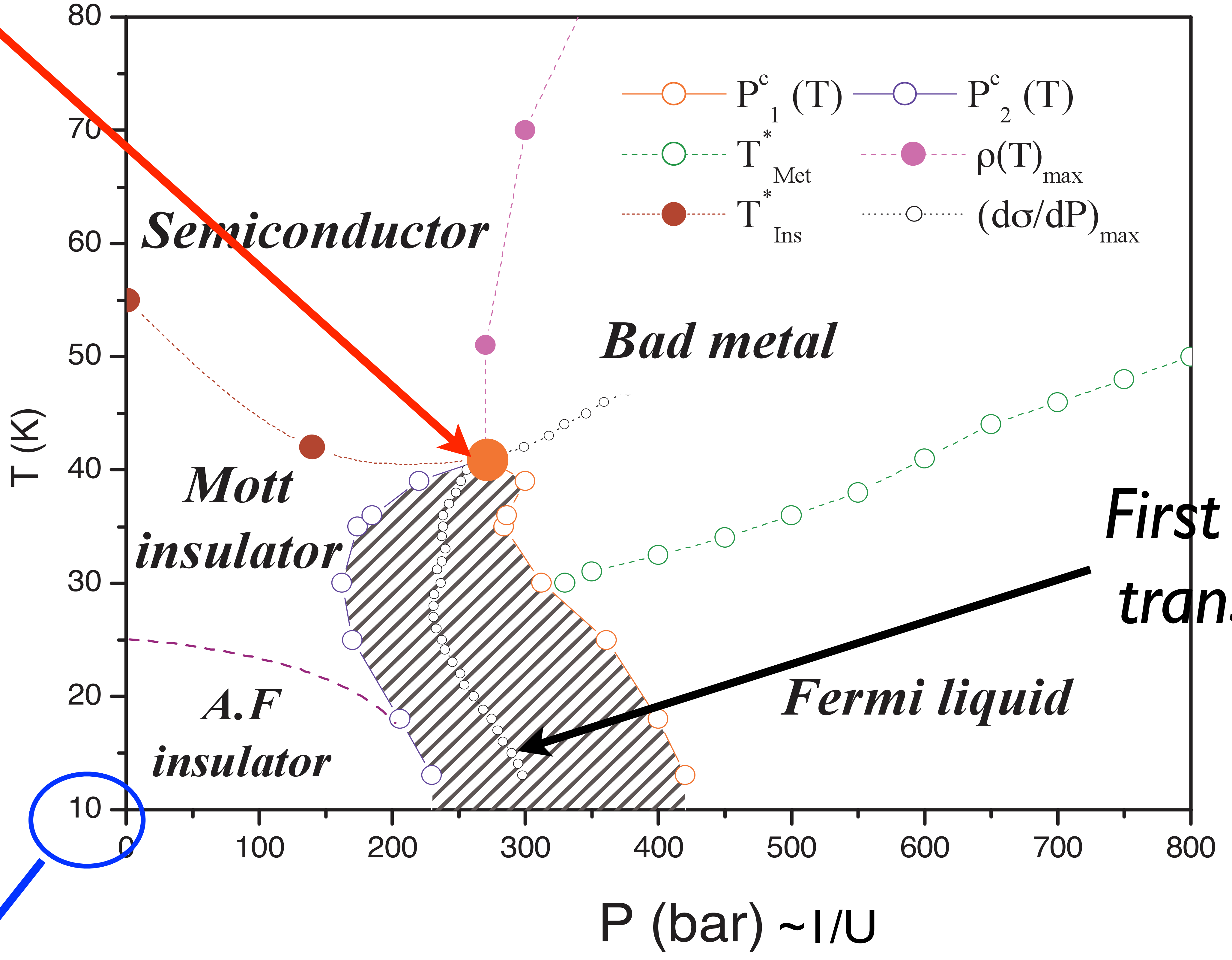
κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl

Critical Point





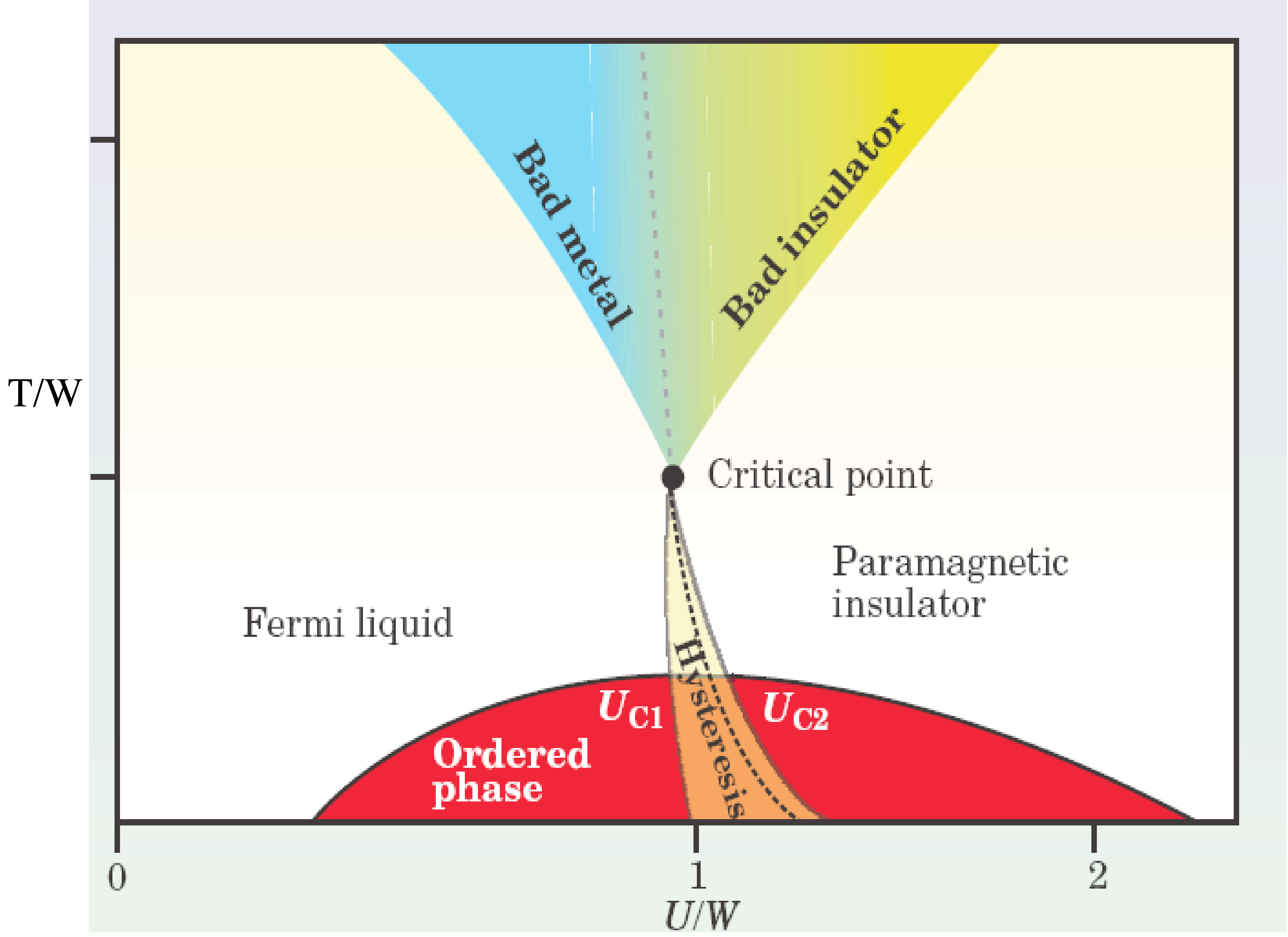
S. Lefebvre et al. PRL 85, 5420 (2000)



First order transition

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

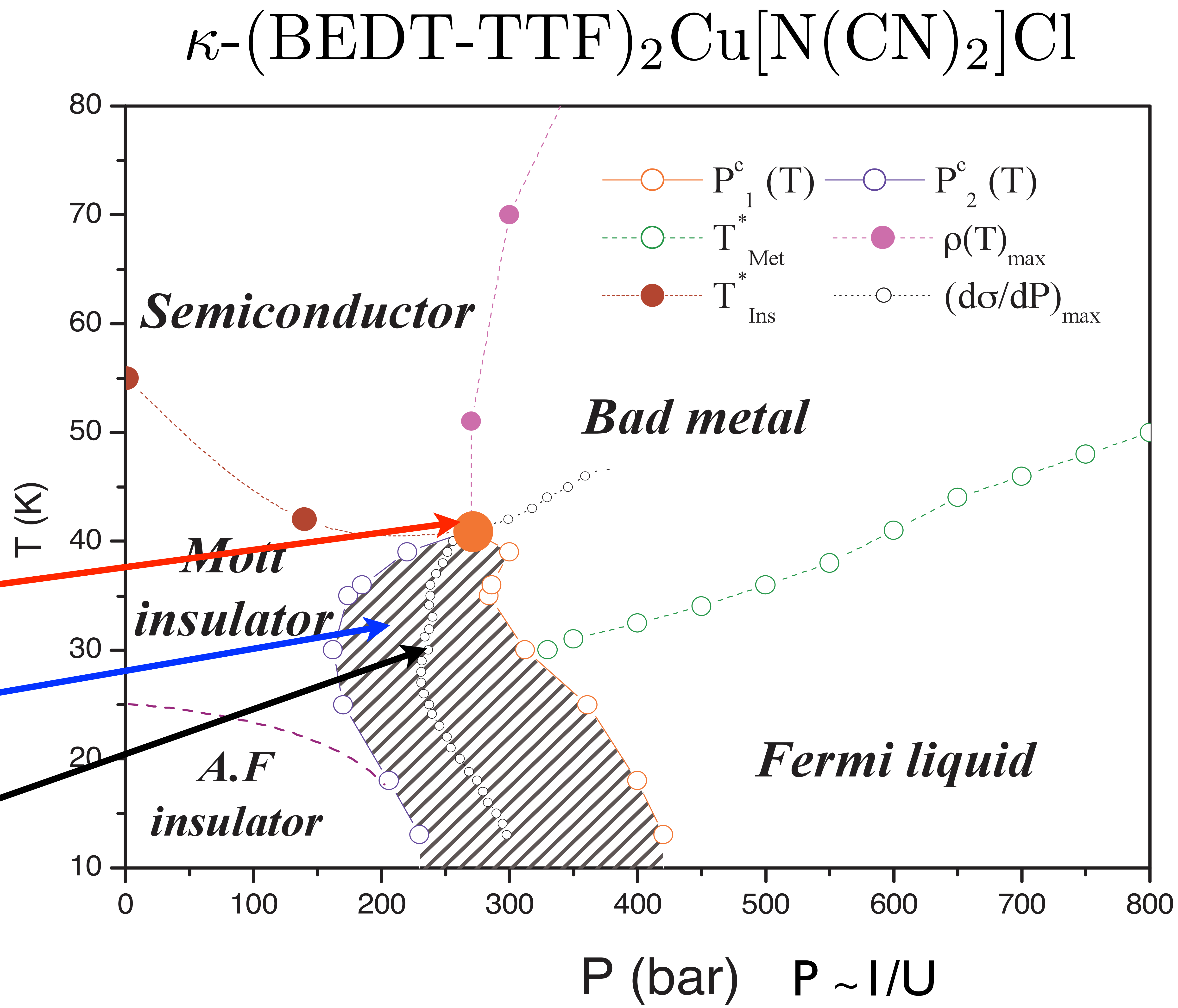
Comparison with organics : phase diagram



Critical Point

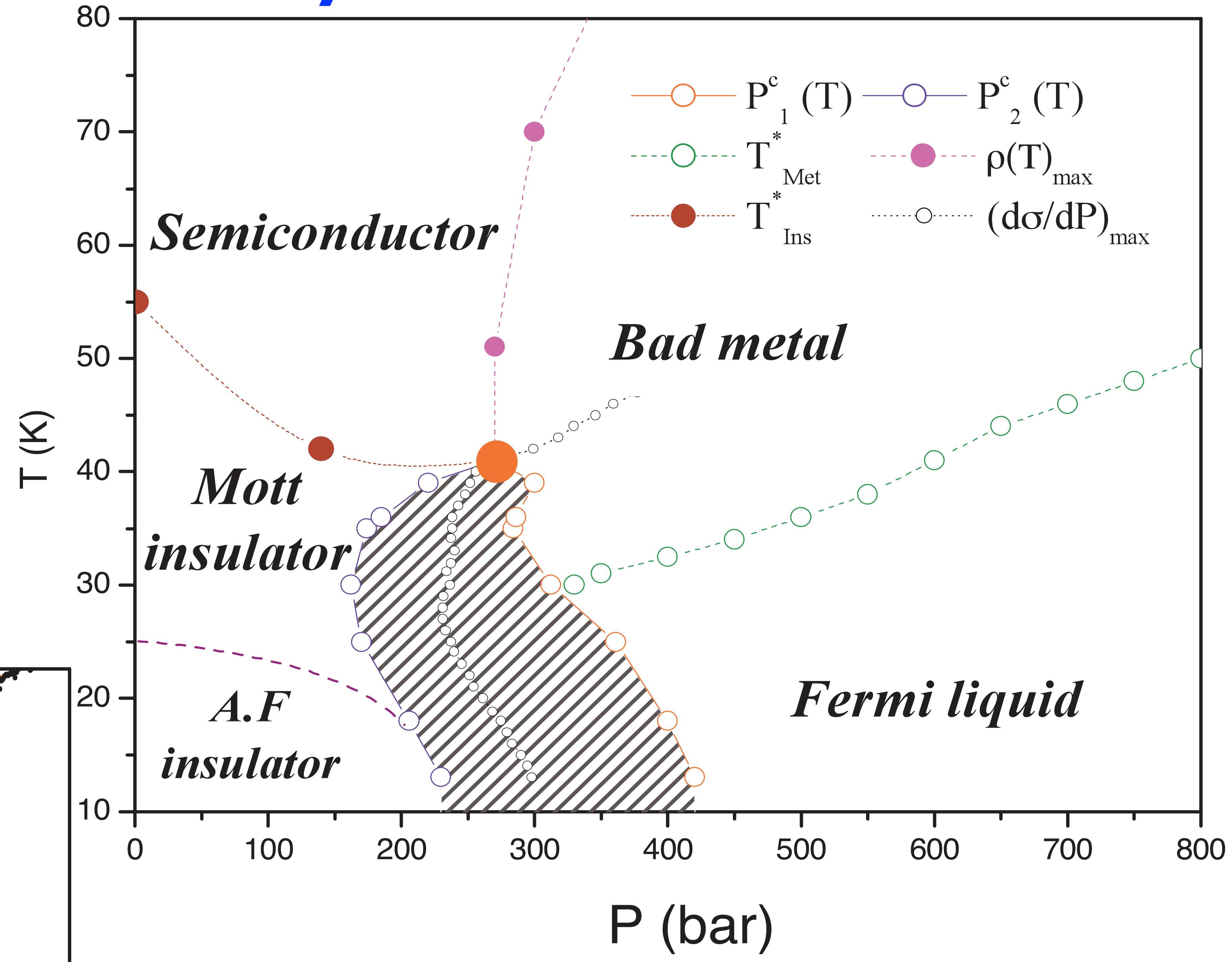
Coexistence region

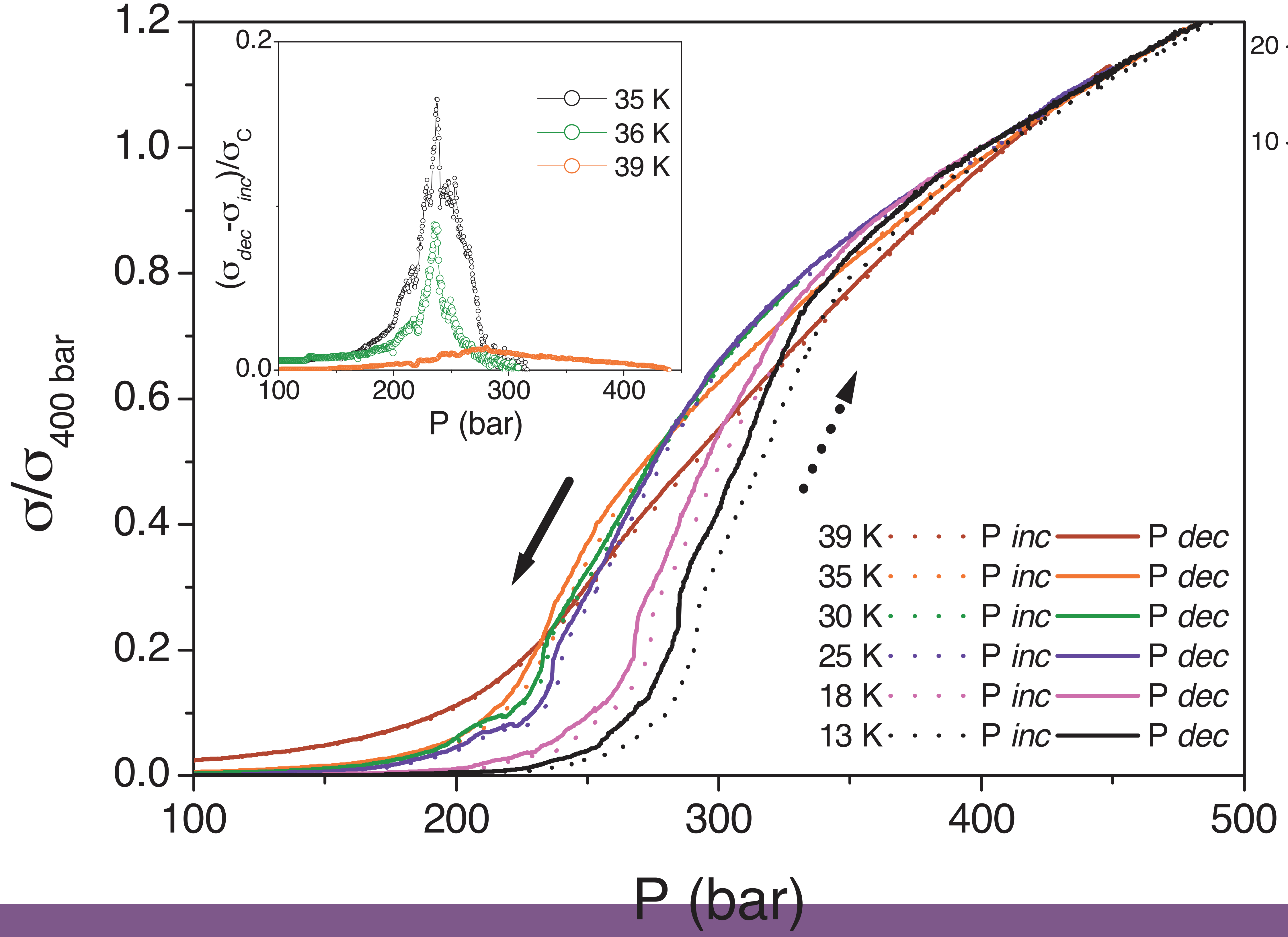
First order transition



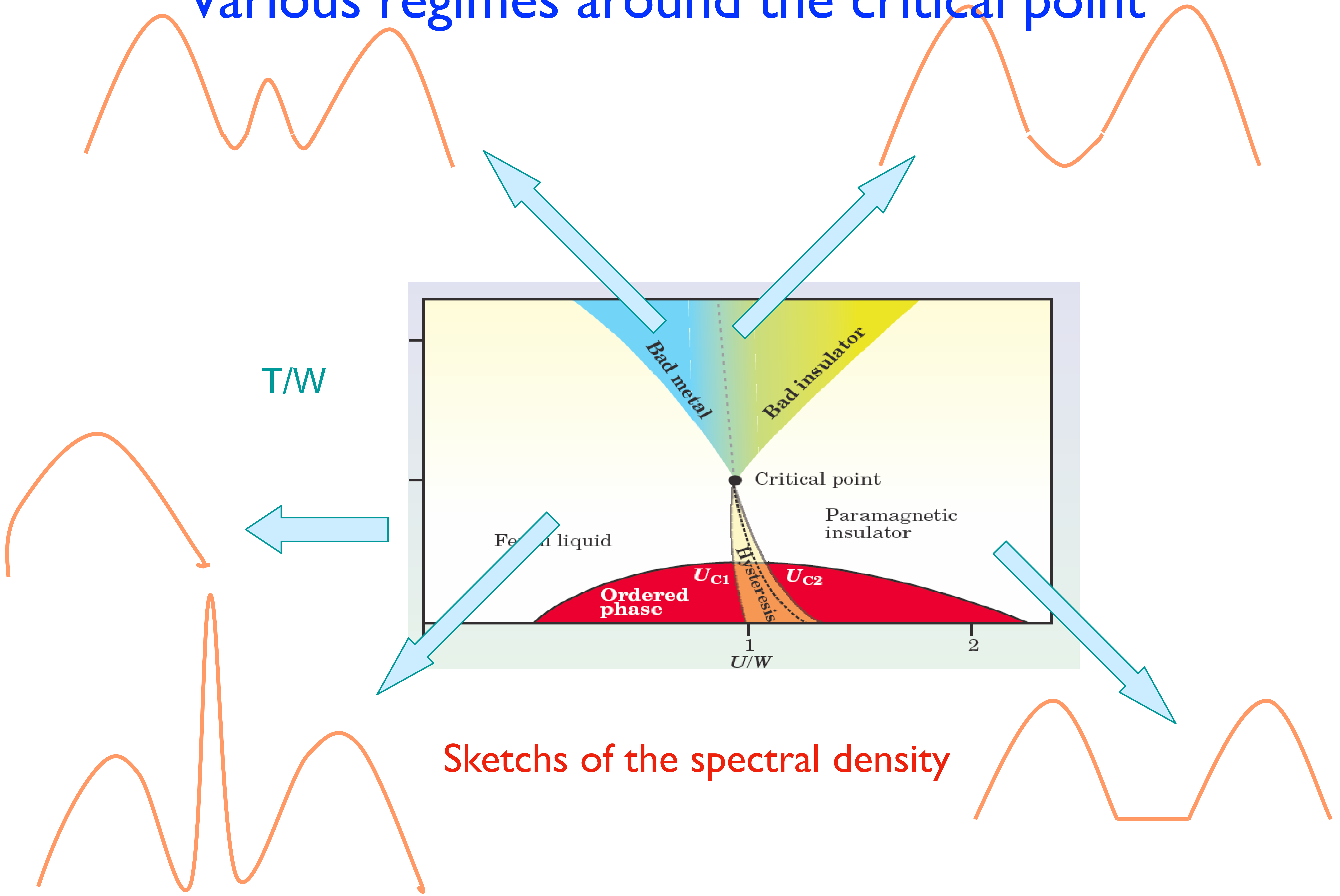
P. Limelette, et al. PRL 91, 016401 (2003)

Experimental evidence for hysteresis





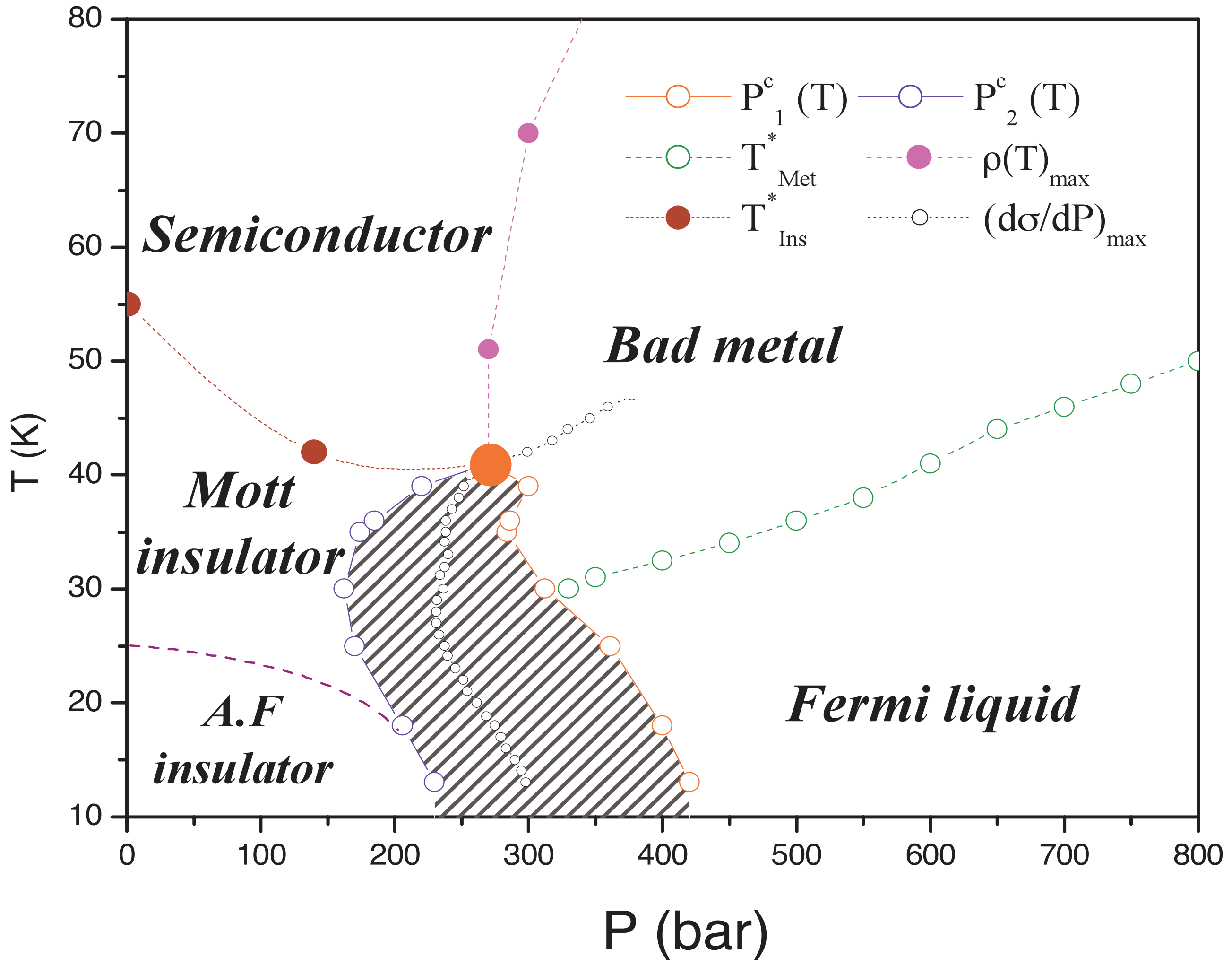
Various regimes around the critical point

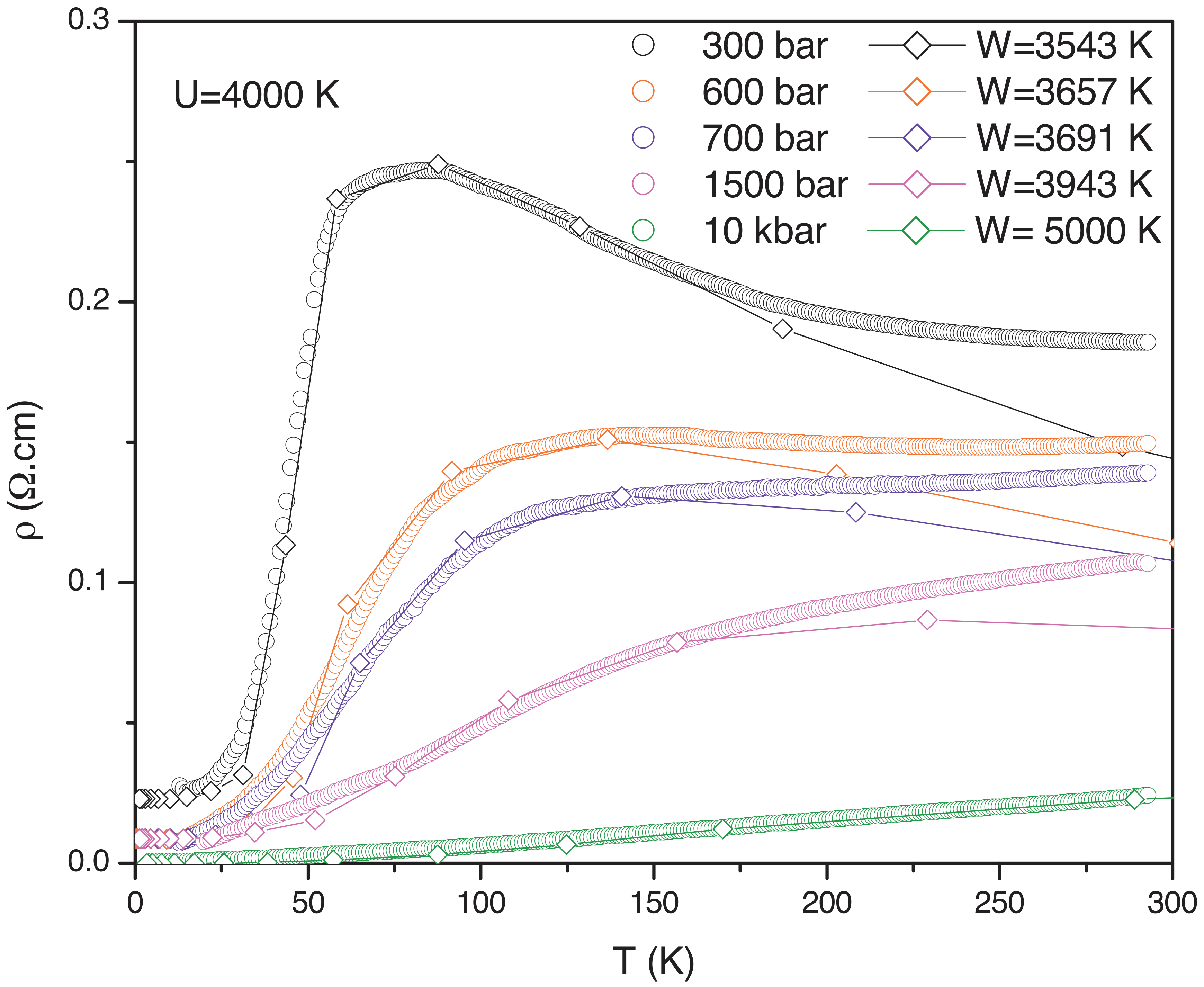


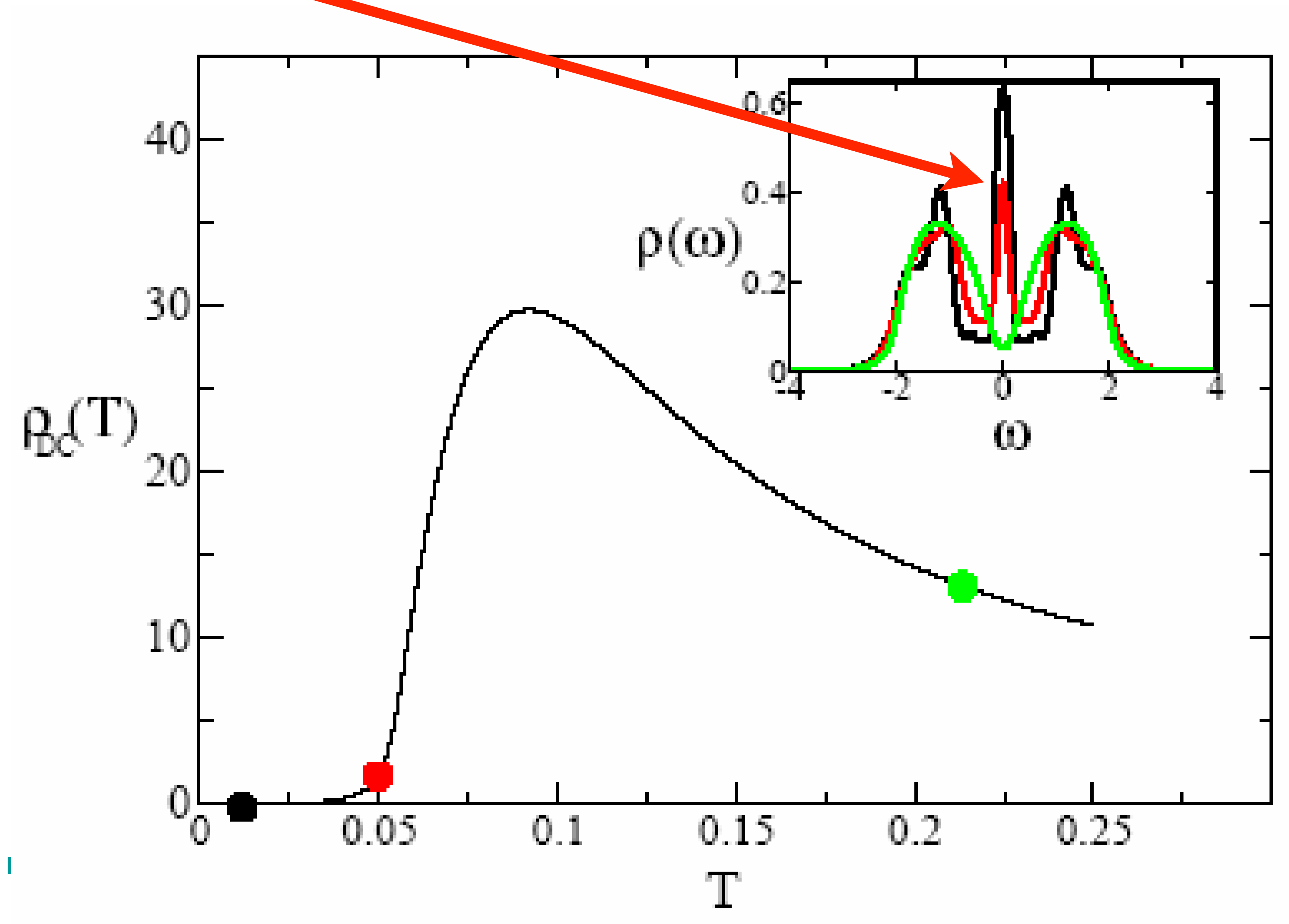
Sketchs of the spectral density

Bad metal regime. Comparison with DMFT

- DMFT. Bethe lattice, NRG solver
- Adjusted parameters :
  D, ρ(T=0), global scale and U.
- Melting of quasi-particles

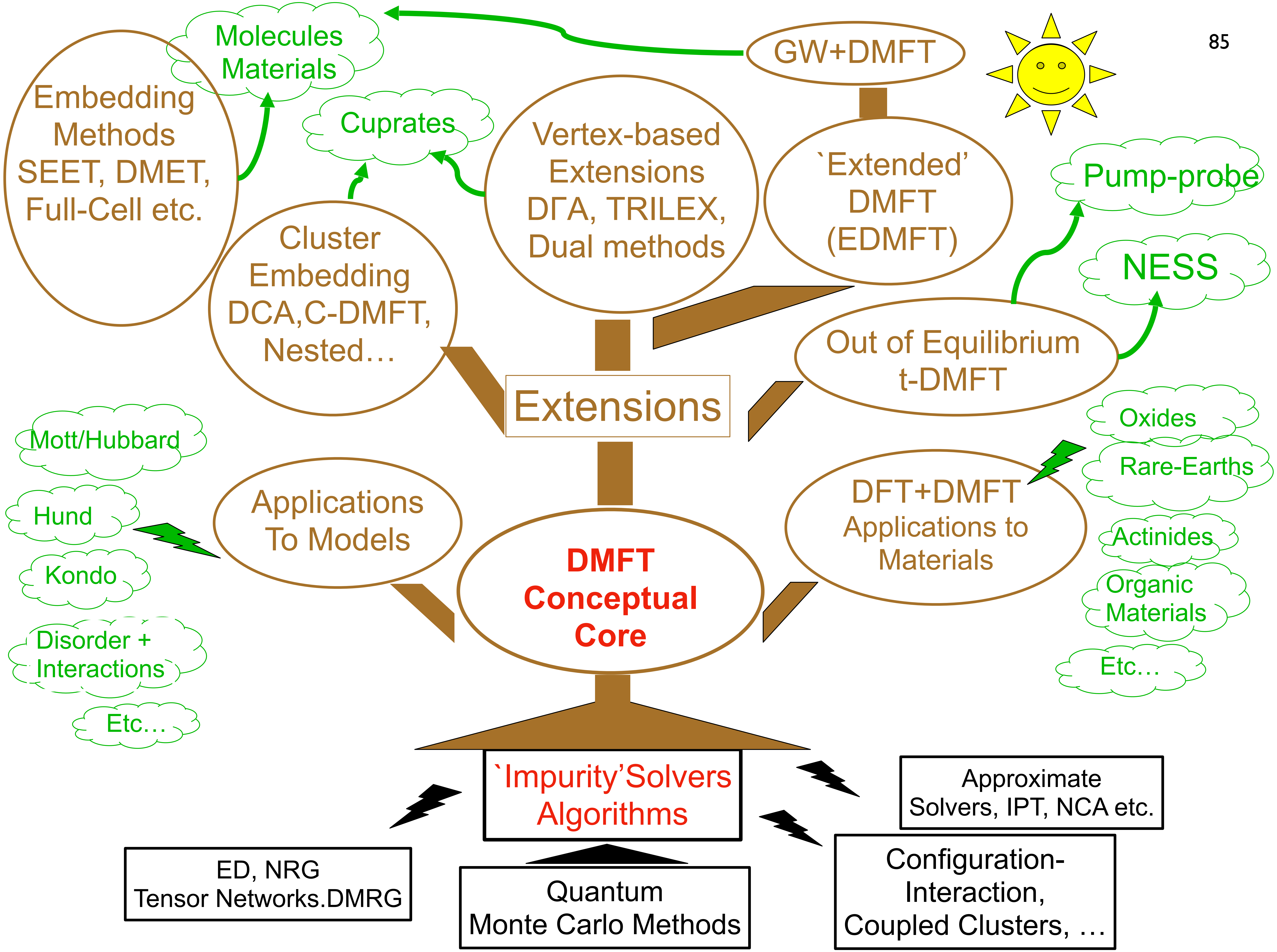






Conclusion:

This is just the beginning …


Molecules
Materials
GW+DMFT
Embedding Methods SEET, DMET, Full-Cell etc.
Cuprates
Vertex-based Extensions DΓA, TRILEX, Dual methods
`Extended' DMFT (EDMFT)
Pump-probe
NESS
Cluster Embedding DCA,C-DMFT, Nested…
Out of Equilibrium t-DMFT
Extensions
Oxides
Rare-Earths
Mott/Hubbard
Hund
Kondo
Disorder + Interactions
Etc…
Applications To Models
DMFT Conceptual Core
DFT+DMFT Applications to Materials
Actinides
Organic Materials
Etc…
`Impurity'Solvers Algorithms
Approximate Solvers, IPT, NCA etc.
ED, NRG Tensor Networks.DMRG
Quantum Monte Carlo Methods
Configuration-Interaction, Coupled Clusters, …

Outline: lecture 2

- Multiorbital models: a step toward realism
- Cluster extensions of DMFT: how to get control and restore some k dependence of Σ
- A quick review of quantum impurity solvers : pros and cons…
- Two particle quantities, transport.

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 Cluster DMFT methods
  T. Maier et al.
  Rev. Mod. Phys. 77, 1027 (2005)

- On Vertex and DMFT extensions
  G. Rohringer et al. Rev. Mod. Phys. 90, 025003 (2018)

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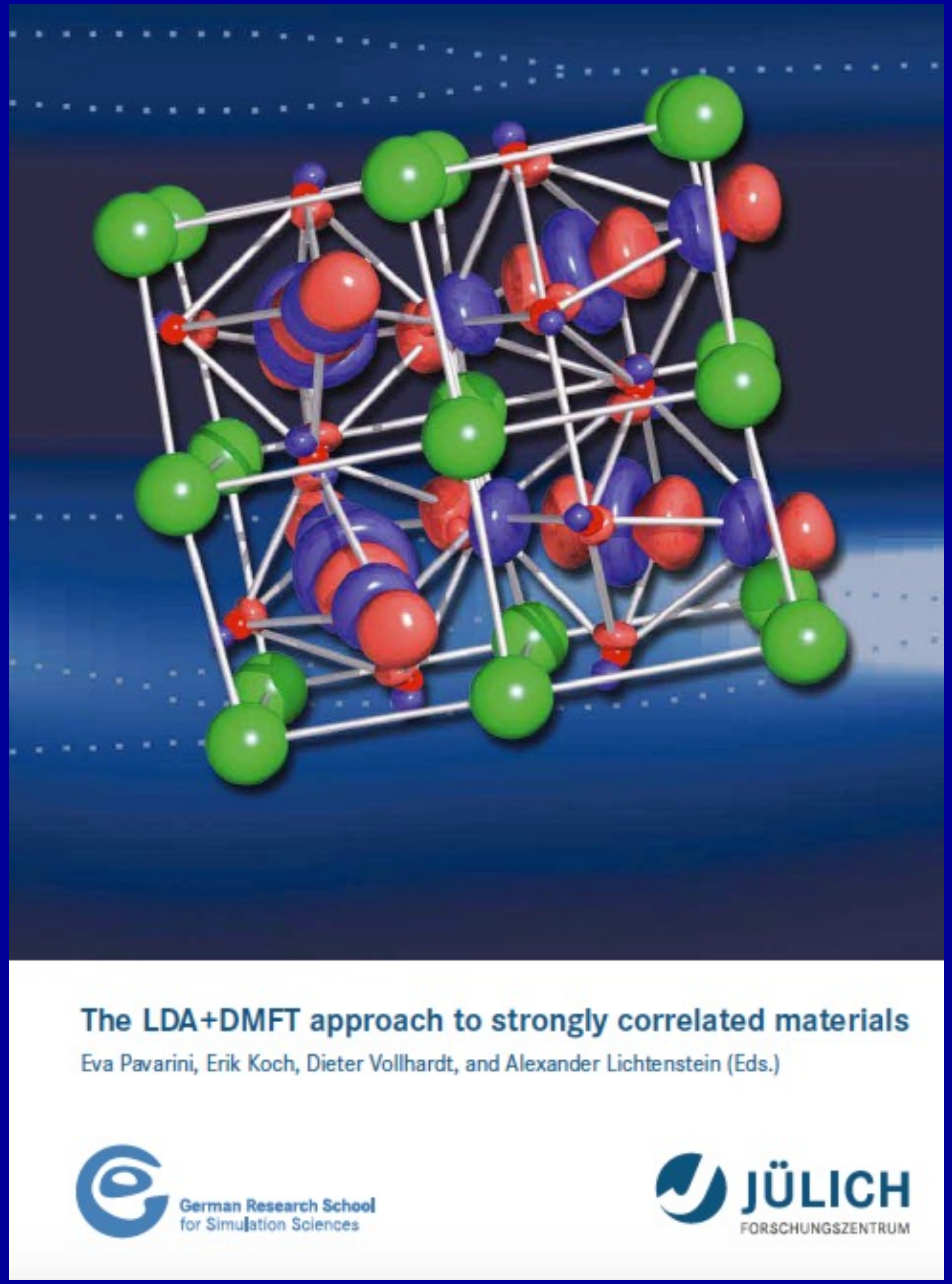

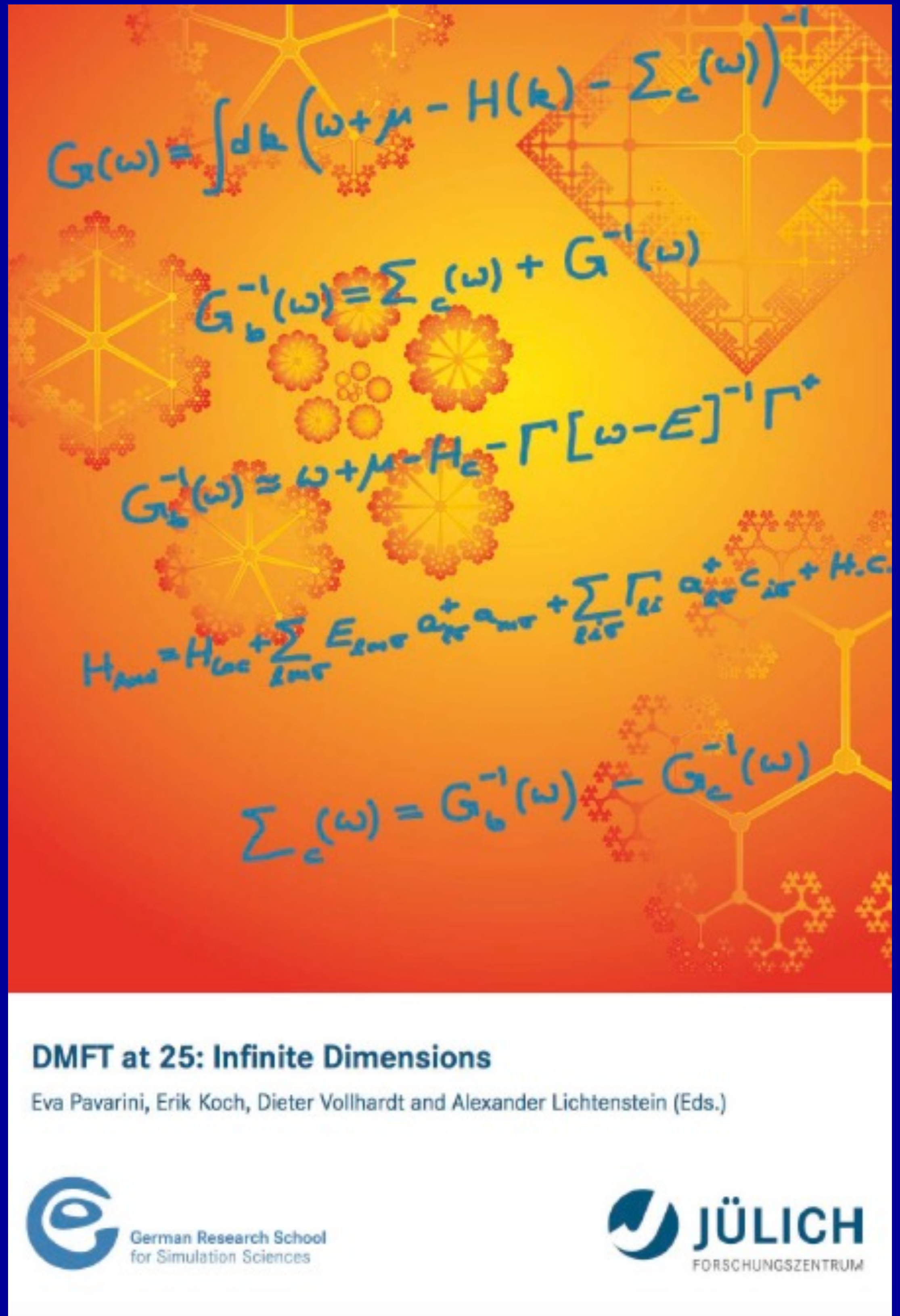

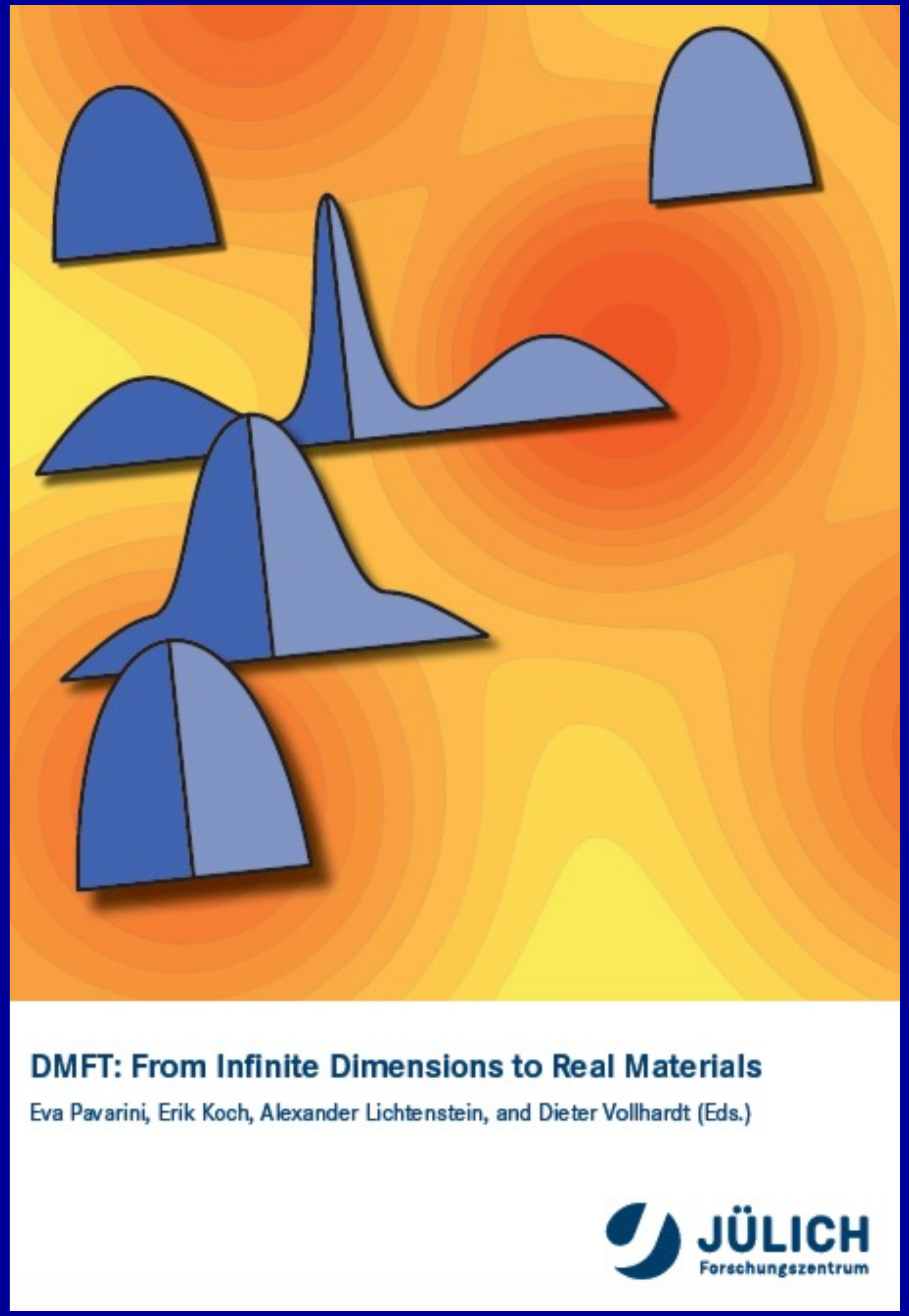

https://www.cond-mat.de/events/correl.html

Also: recent book by V.Turkowski (Springer)

Thank you for your attention