Dynamical Mean Field Theory and beyond

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Outline

- Lecture 1 : Introduction to DMFT
  - Why DMFT ?
    - Introduction to Mott transition.
    - Introduction to Quantum Impurity models.
  - DMFT equations.
  - A classic : solution of DMFT for 1 band 1/2 filling Hubbard model
- Lecture 2 : Beyond DMFT. Clusters.
- Lecture 3 : Impurity solvers
- Lecture 4 : Introduction to TRIQS & Hands-on

DMFT : some references

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

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

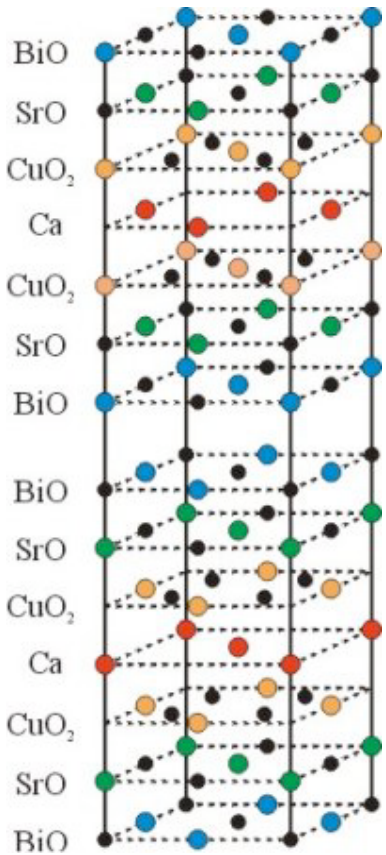
- On Quantum Monte Carlo (DMFT) Impurity solvers
  E. Gull et al.
  Rev. Mod. Phys. 83, 349 (2011)

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

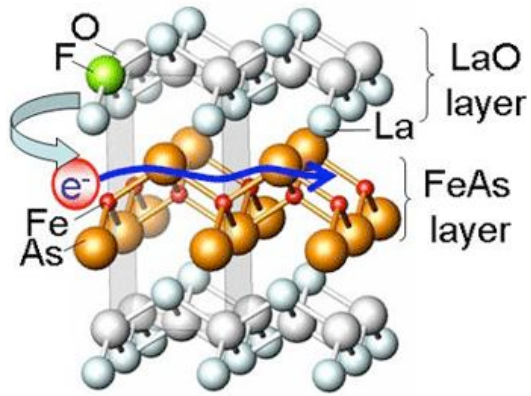
Strongly correlated systems

Quantum many-body systems, fermions (or bosons),
with interactions, at low temperature

Materials
High Temperature superconductors
Transition metal oxides,

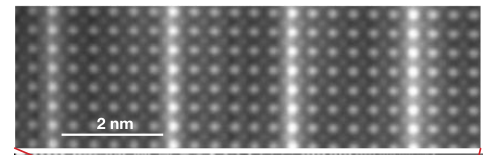


Cuprate (1986)



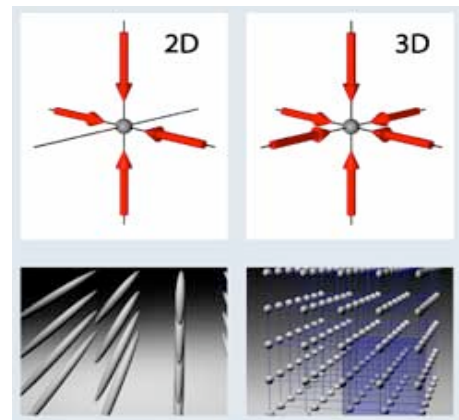
Fe-Based (2008)

Correlated metal/superconductors
at interface of oxides



SrTiO3/LaTiO3
Ohtomo et al, Nature 2002

Ultra-cold atoms in optical lattices



"Artificial solids"
of atoms & light

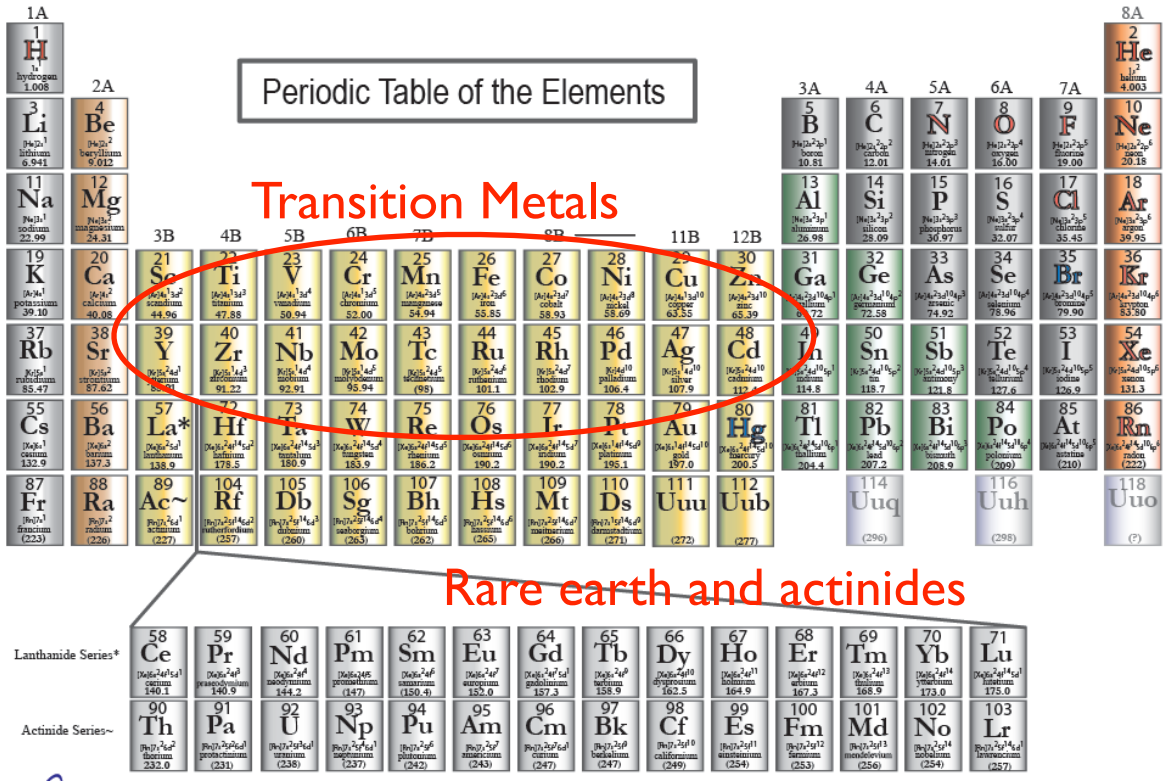
Weak vs Strong Correlations

- The problem : Interaction between electrons (Coulomb) is not small U ~ a few eV ~ Bandwidth.
- 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
  - Not simply reducible to an effective one-body problem

Two components in electronic fluid

- 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

- Not regular band-forming orbitals, nor core states. Some atomic-like aspects
- Materials: transition-metals and their oxides, rare-earth/ actinides, but also some organic materials

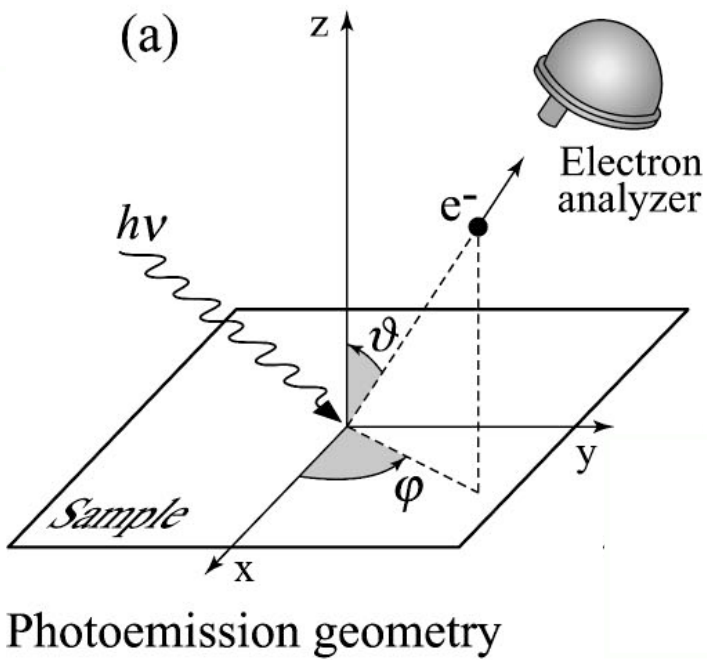


Reminder : spectral function

- Definition : spectral function.

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

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



Photoemission geometry

- ARPES : only hole excitations

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

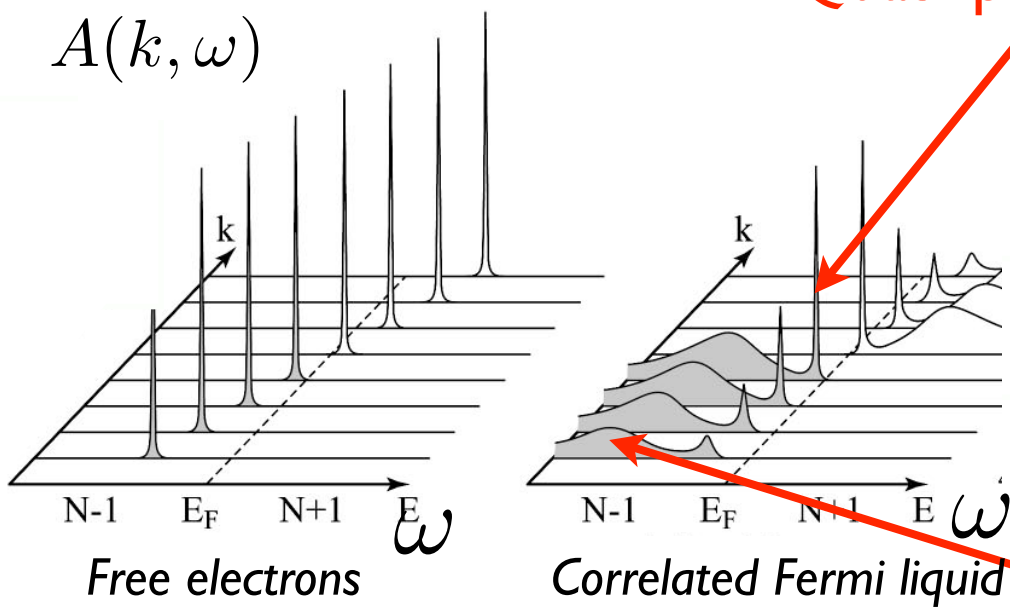
Fermi function

- Theorist's view (surface probe, requires some modelling "sudden approximation")

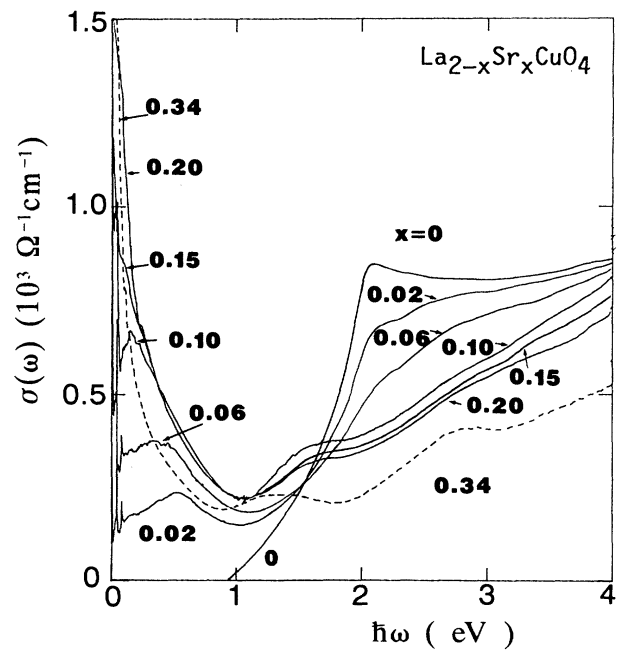
A. Damascelli et al, Rev. Mod. Phys. 75, 473 (2003)

Spectral weight transfer

Spectral function



Optical conductivity



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

Mott physics

Atomic-like localized excitations. Hubbard band

vs

long range, delocalized, quasi-particle peak

- Spectral weight transfer from low to high energy

A brief introduction to Mott transition

A minimal model for theorists : Hubbard model

Kinetic term

Interaction term (Coulomb) U>0

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

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

Doping (number of charges)

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

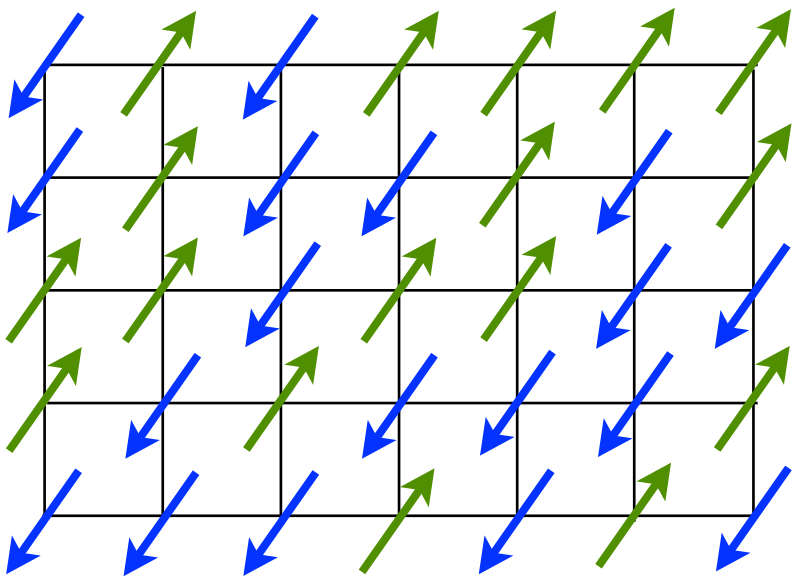
Mott insulator

N. Mott, 50's

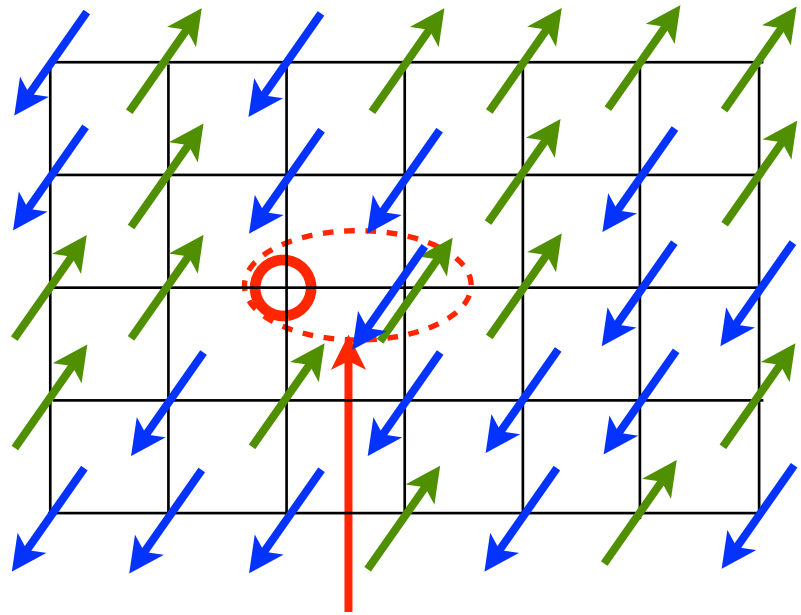
- One electron per site on average (half-filled band).
- Should be a textbook metal.
- If U is large enough, it is an insulator : charge motion frozen.

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

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



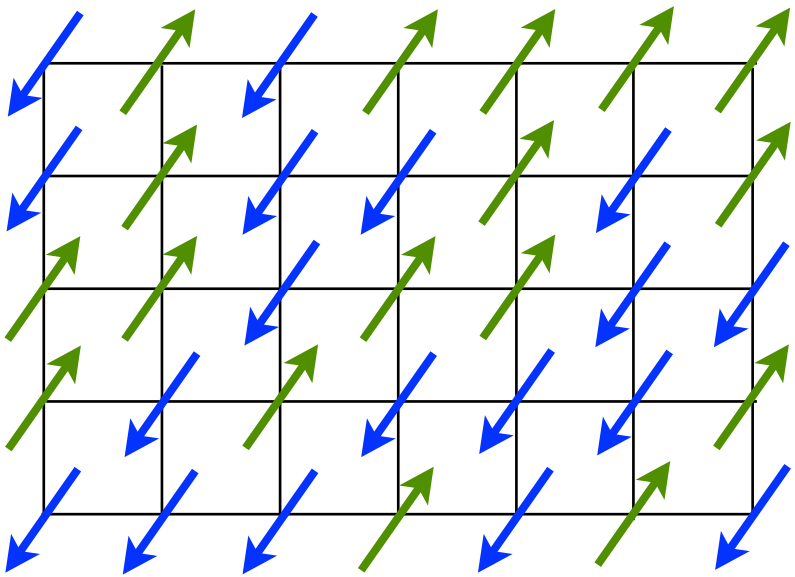
Mott insulator



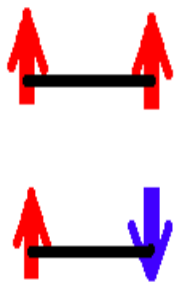
Large Coulomb repulsion U ~ eV ~ 10^4 K

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 ?

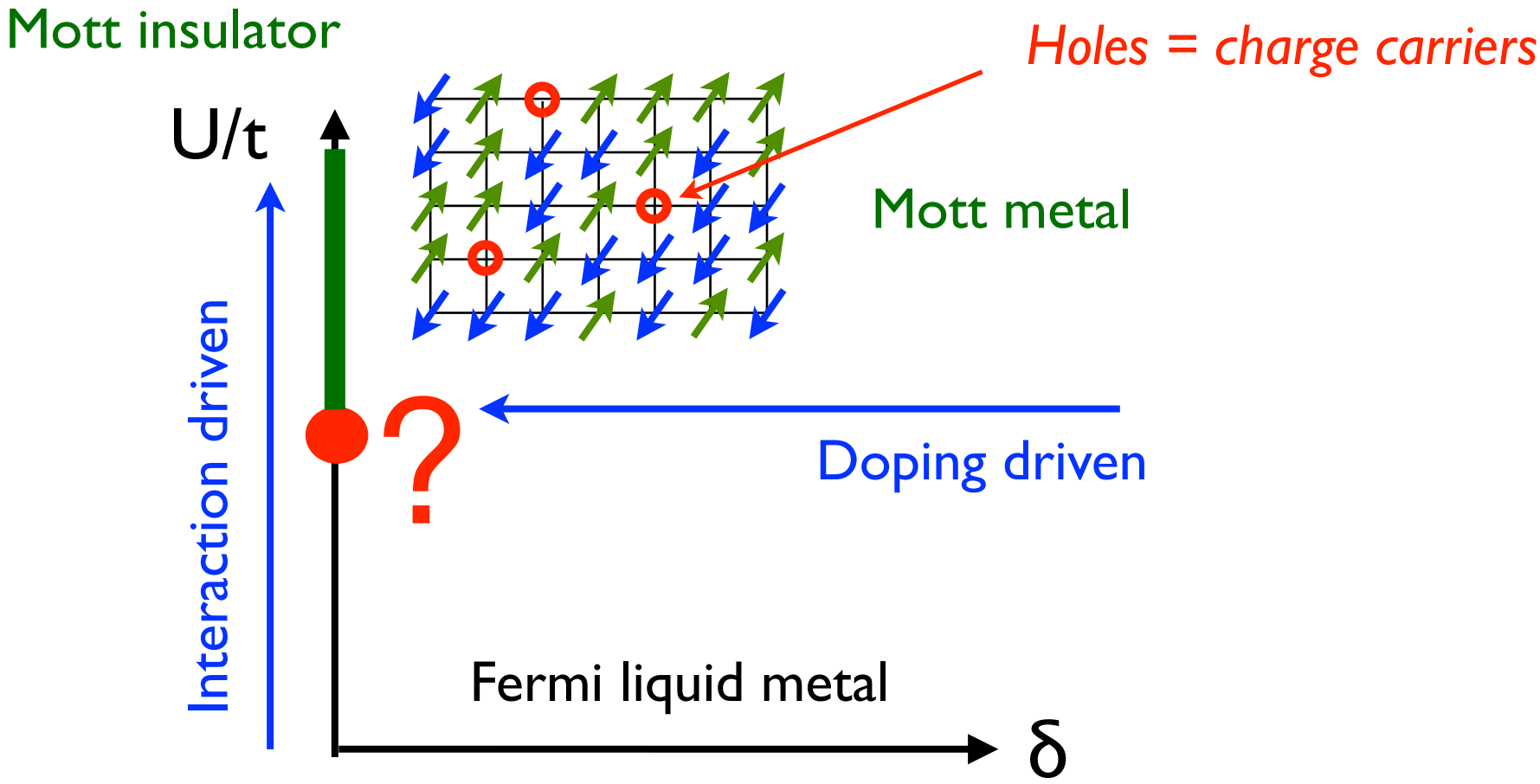


Effective antiferromagnetic interaction between spins



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

Doped Mott insulators



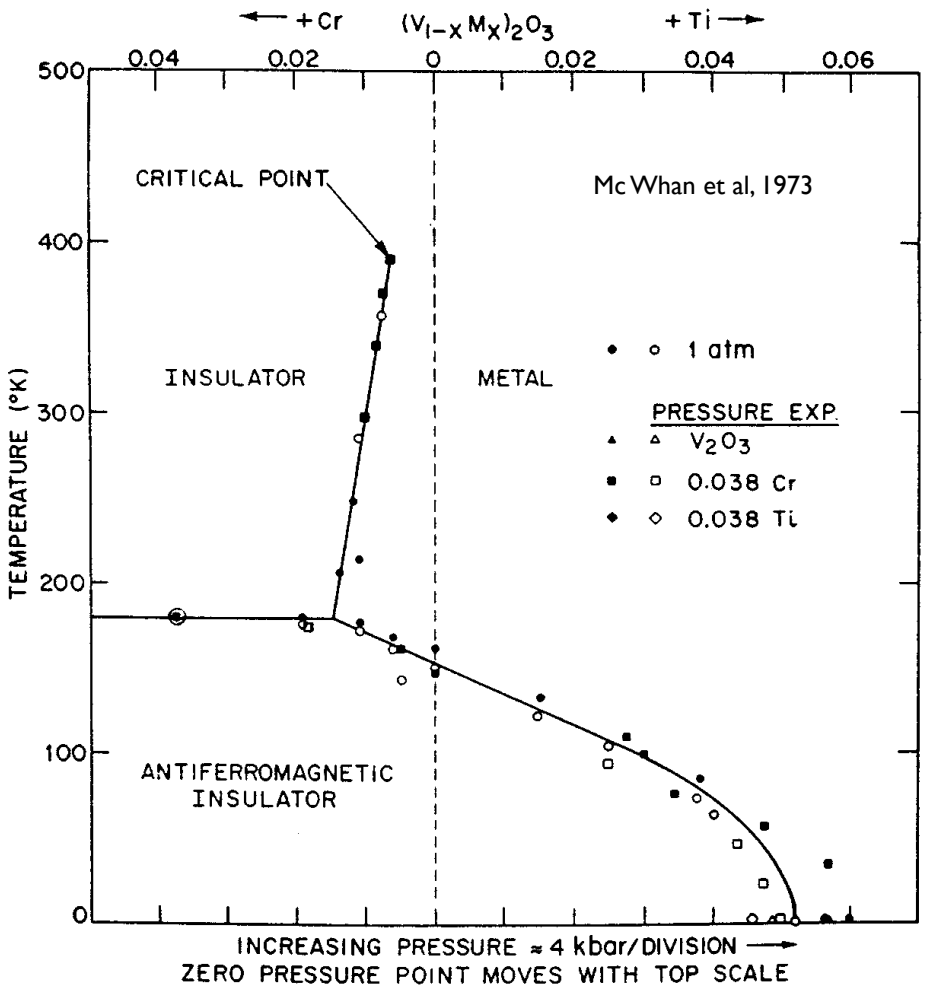
- How is a metal destroyed close to a Mott transition ?
  Or a Mott insulator by doping ?
- "Mott metals" are fragile and complex : Many instabilities, rich phase diagrams, large susceptibilities, small coherence energy

In real materials ?

Interaction Driven Mott Transition

- Vary pressure P ⇔ 1/U

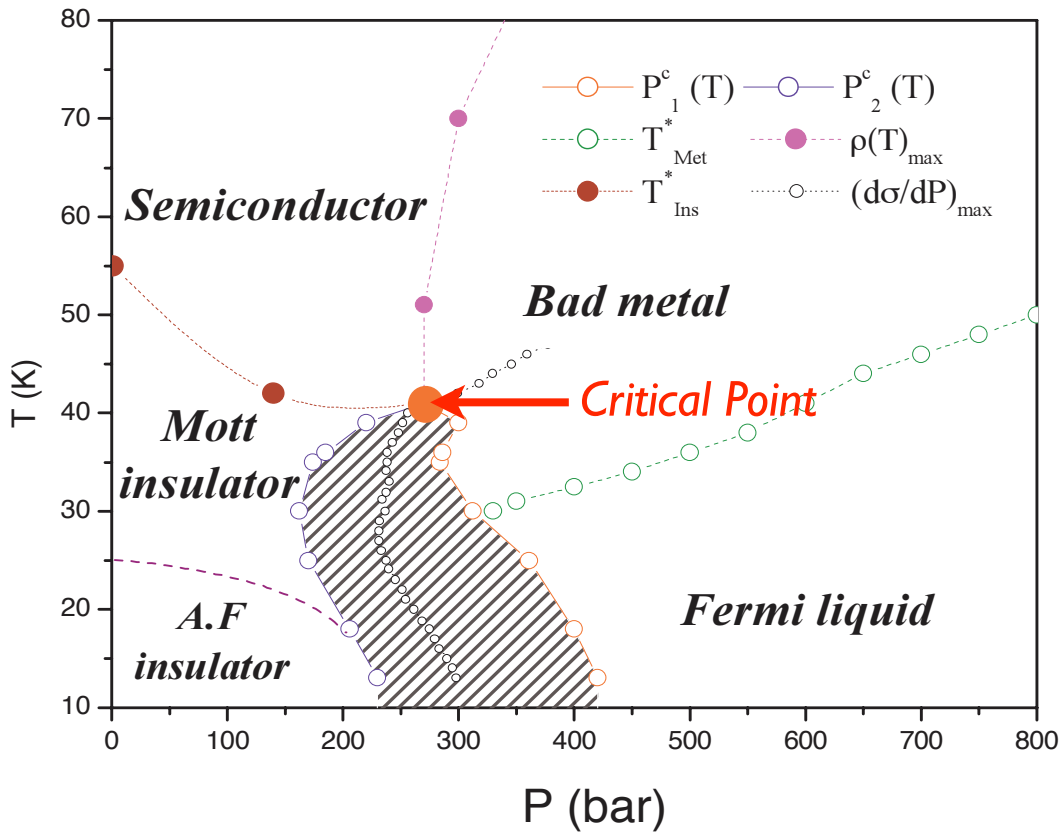
V_2O_3



2-d organics

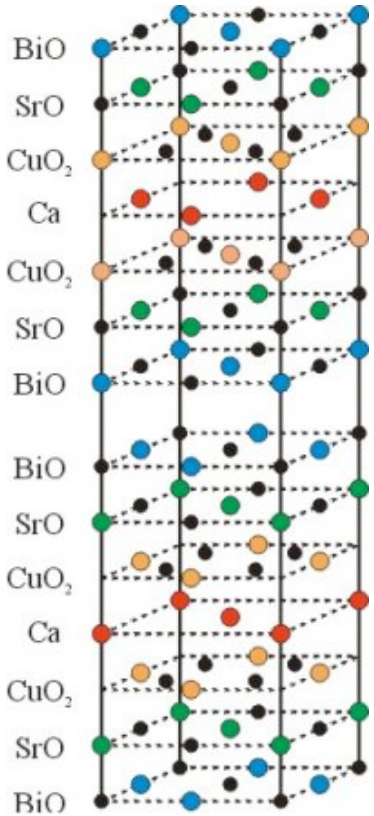
κ-$(BEDT\text{-}TTF)_2Cu[N(CN)_2]Cl$

(but has a simple hubbard modelization)

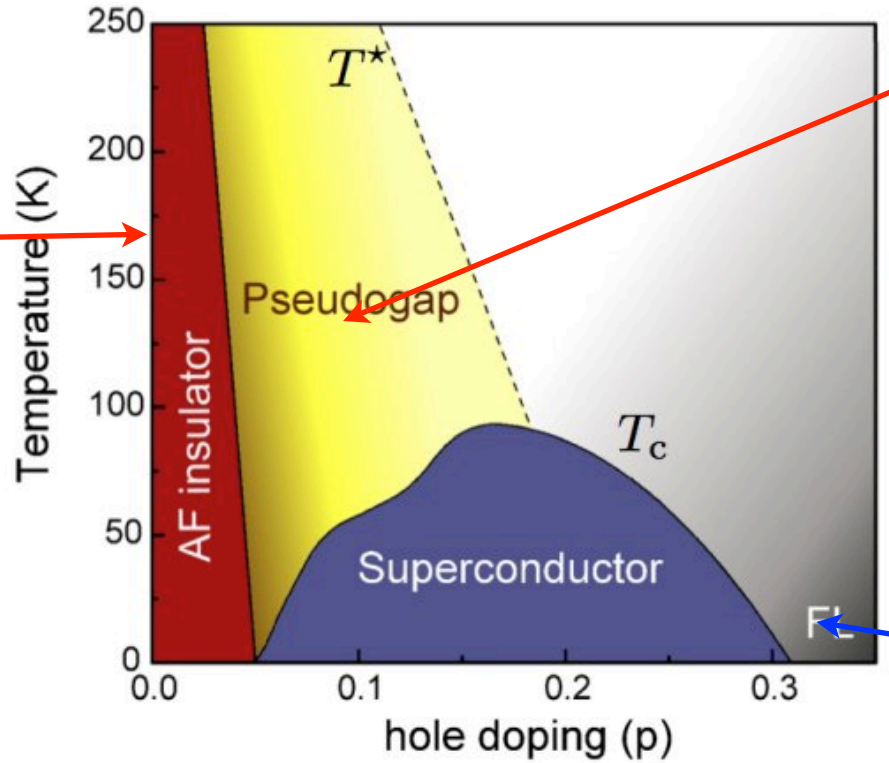


P. Limelette, et al. PRL 91, 016401 (2003)

High-Tc superconductors are doped Mott insulators



High-Tc superconductors
Generic, simplified phase diagram



Mott insulator

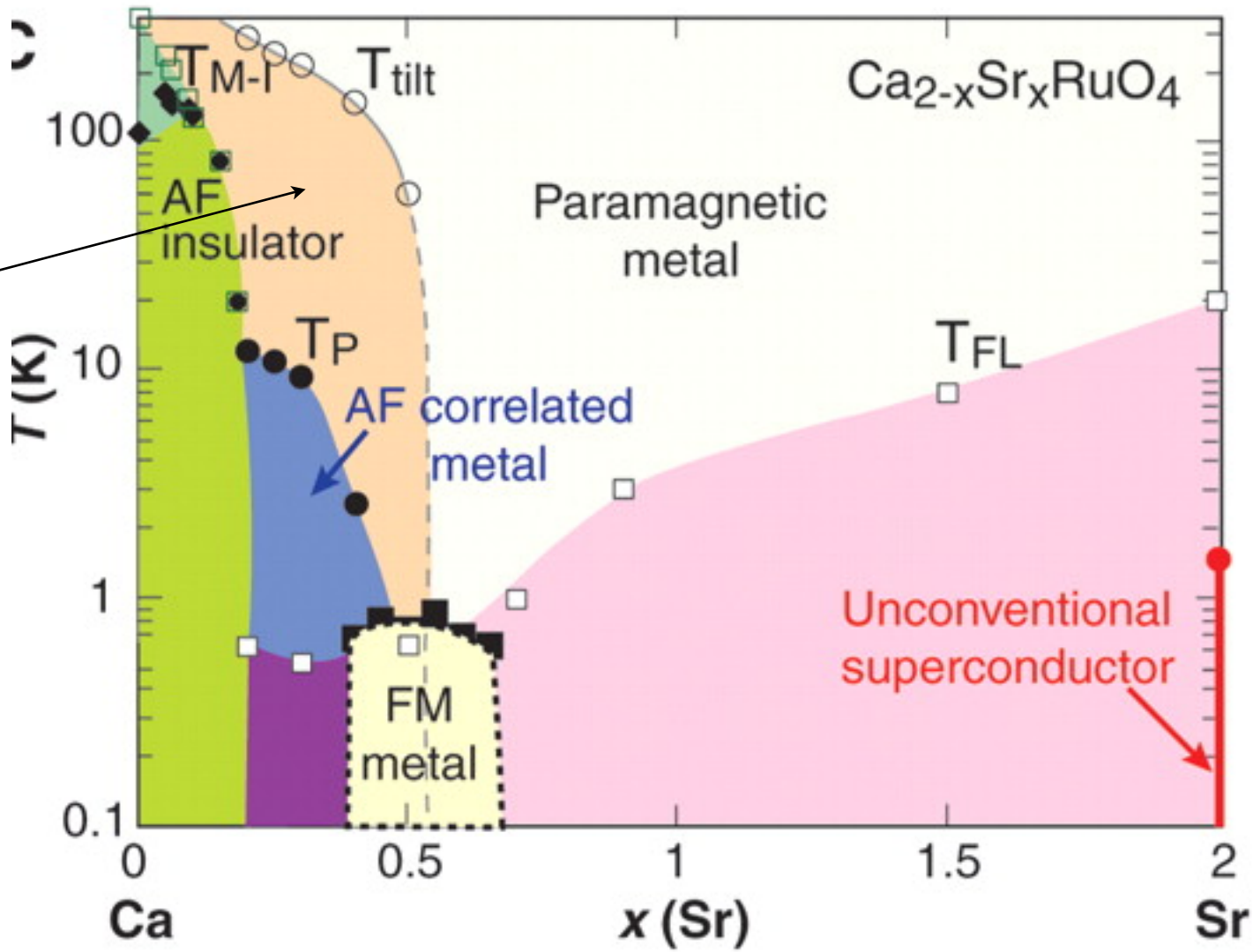
Unconventional normal metal

Fermi liquid

$Ca_{2-x}Sr_xRuO_4$

- A correlated material, with a complex phase diagram.

Paramagnetic Mott insulator



Wishlist for a theoretical method

- Describes atomic multiplets and Fermi liquid
- Real and reciprocal space (Mott insulator vs metal)
- Treat both low and high energy features of electronic fluid. Describe spectral weight transfer
- Can be controlled systematically
- Works not only for models, but also for realistic computation (with DFT/LDA/GW).

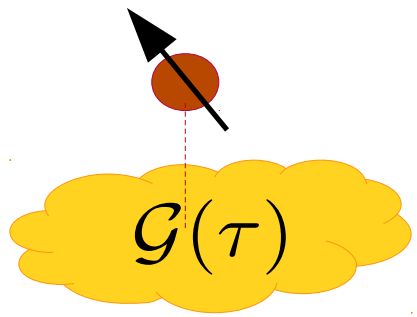
→ The DMFT family.

DMFT : main idea

- DFT (Density Functional Theory)
  Independent electrons in an *effective periodic potential.*
  Interaction taken into account "in average" (Kohn-Sham potential).

- DMFT : change of "paradigm"
  An atom in a self-consistent bath.

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



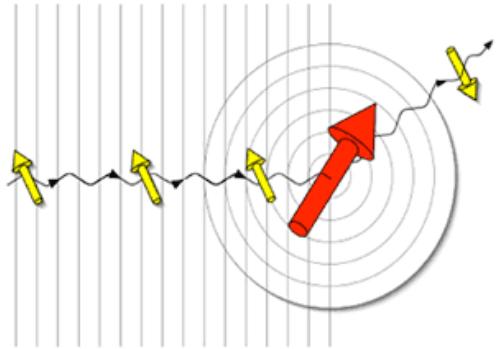
- Atom + bath = quantum impurity model …

A brief introduction to quantum impurity models

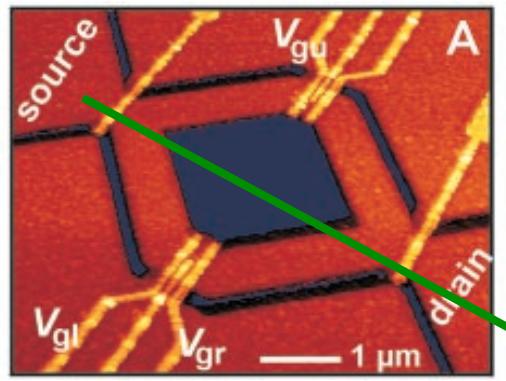
Quantum impurity models

Magnetic impurity

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



Nanostructures



I(V)

- 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

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

$$\Updownarrow$$

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

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

Bath

Hybridization function

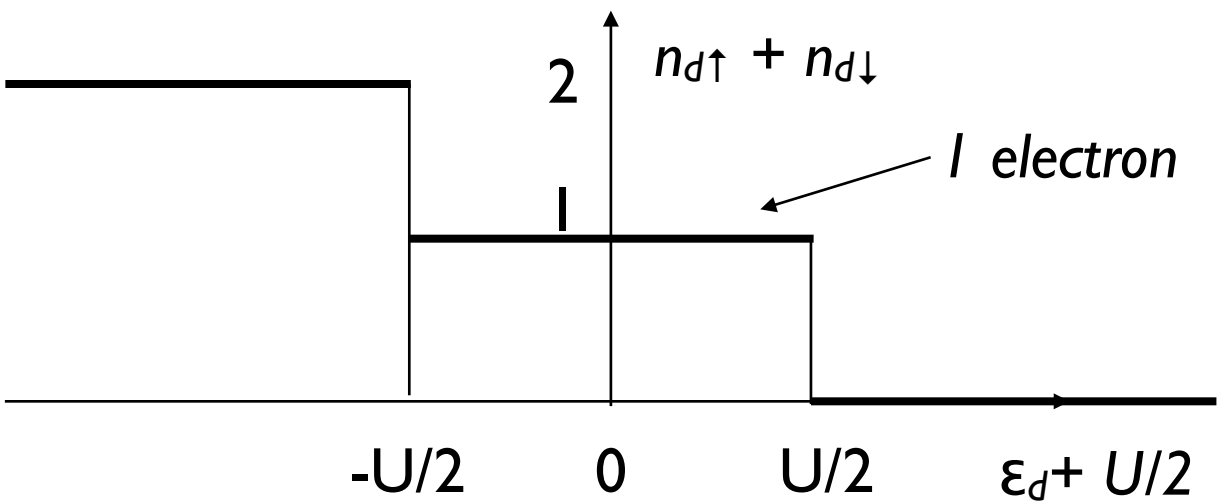
- The only important quantity for the ξ-electrons is the hybridisation.

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



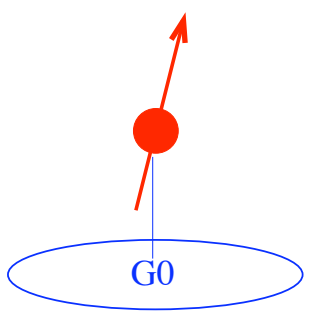
Schrieffer-Wolf Phys.Rev. 66

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

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

- Kondo model

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



Both are local correlated many-body problems.

A single spin 1/2 + a free fermion

A non-trivial problem

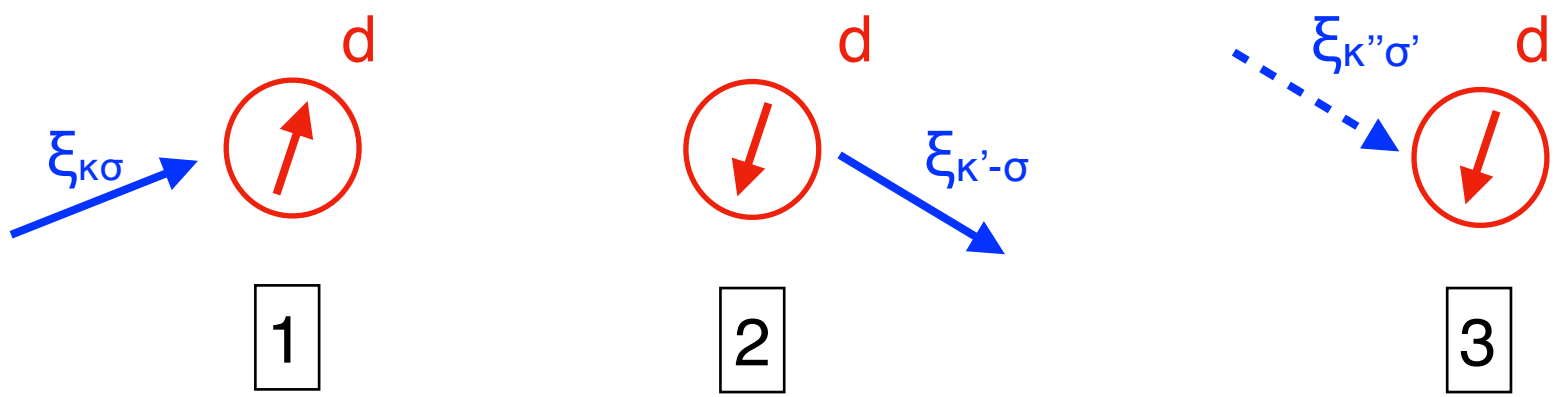
Impurity models are correlated systems

- Local but correlated problems

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

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

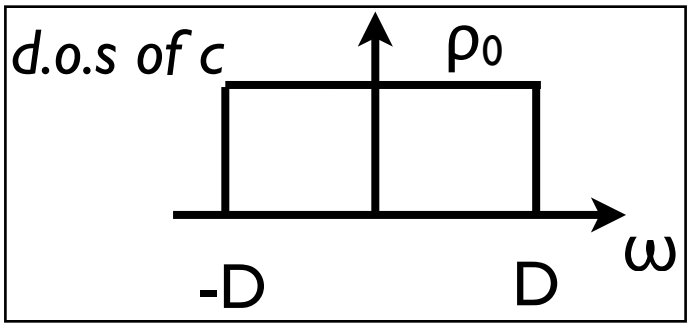
- A second electron sees a local degree of freedom (e.g. spin) flipped by the first.
- Sufficient to create strong correlation effects.



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 → 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

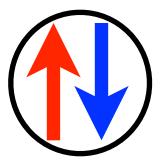
- Screening of the Kondo impurity by the metallic bath

Kondo temperature

$$T_K \sim De^{-1/J\rho_0}$$

d.o.s of the bath at the Fermi level

$T \ll T_K$



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

- Local Fermi liquid (*P. Nozières, '74*)
- Strong coupling picture : singlet "Confinement" of the spin.

$T \gg T_K$

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

- Free spin (Curie law)

- 1+1 Field Theory with asymptotic freedom (similar to QCD)

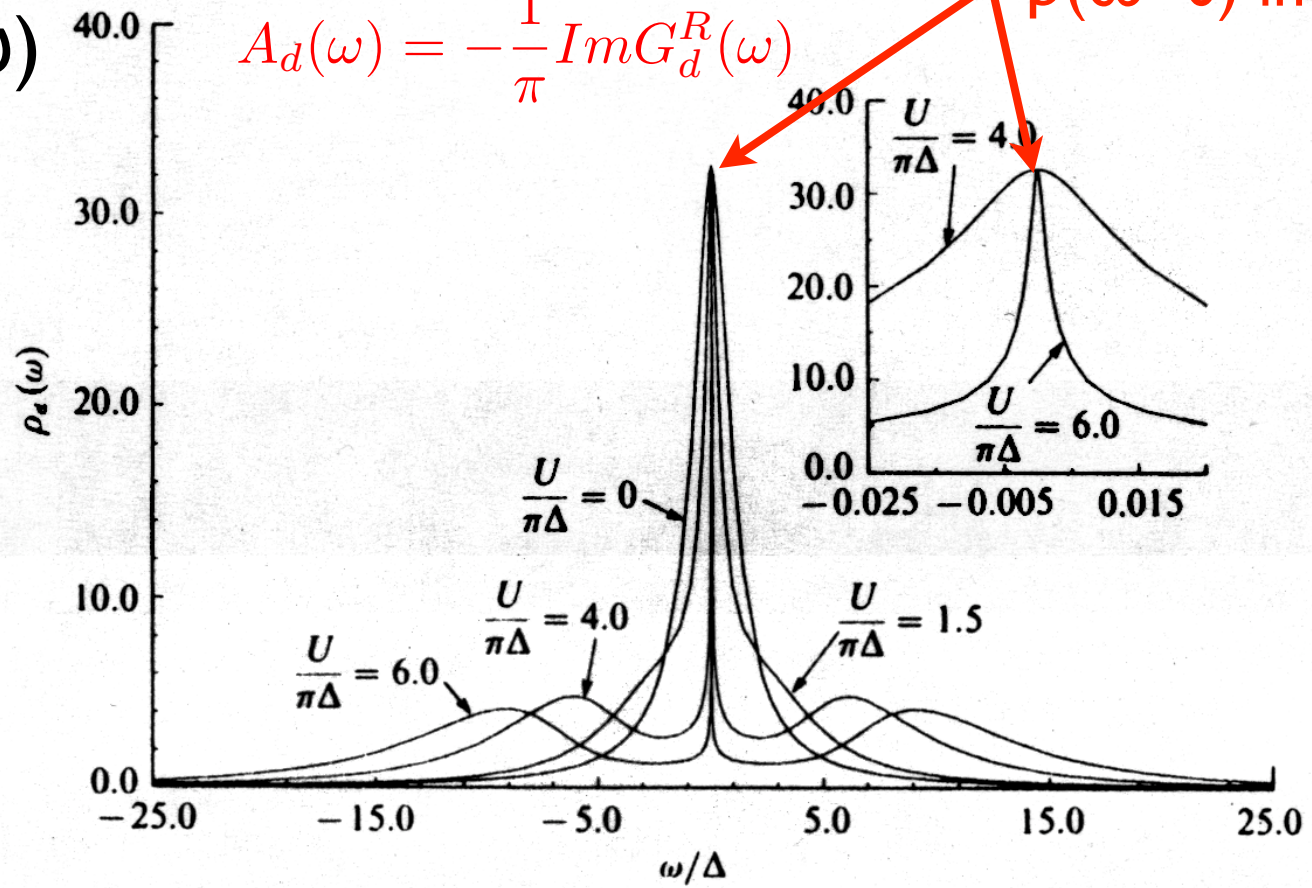
Kondo-Abrikosov-Suhl resonance

- Sharp resonance in the spectral function of *d* at the Fermi level, of width T_K , for $T << T_K$
- "Melts" for $T >> T_K$

$A_d(\omega)$

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

ρ(ω=0) independent of U



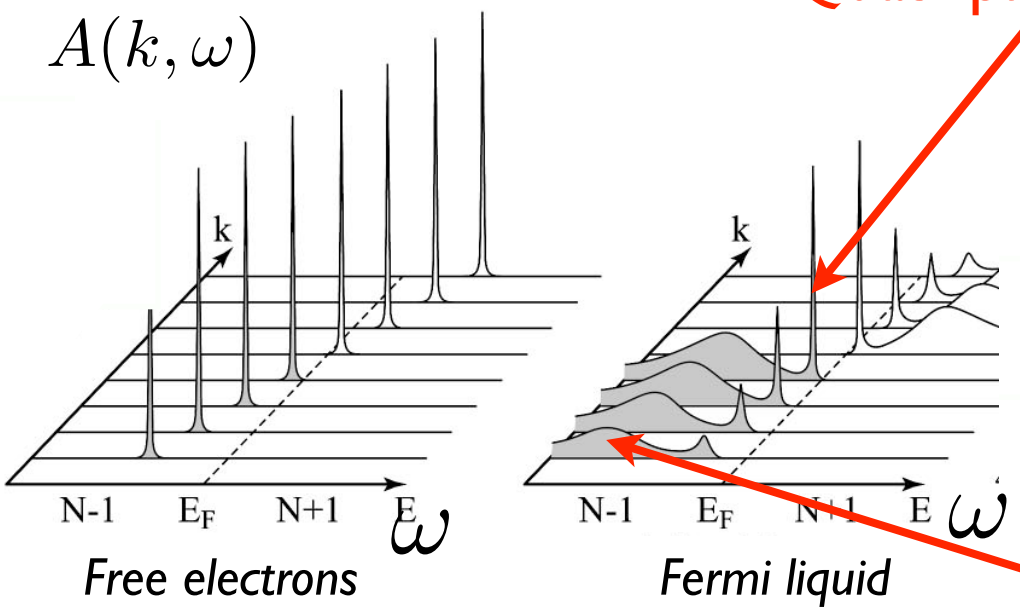
particle-hole symmetric case *(Hewson's book)* $\Delta = \Gamma = \pi\rho_0 V^2$

Analogy with Mott problem

Lattice

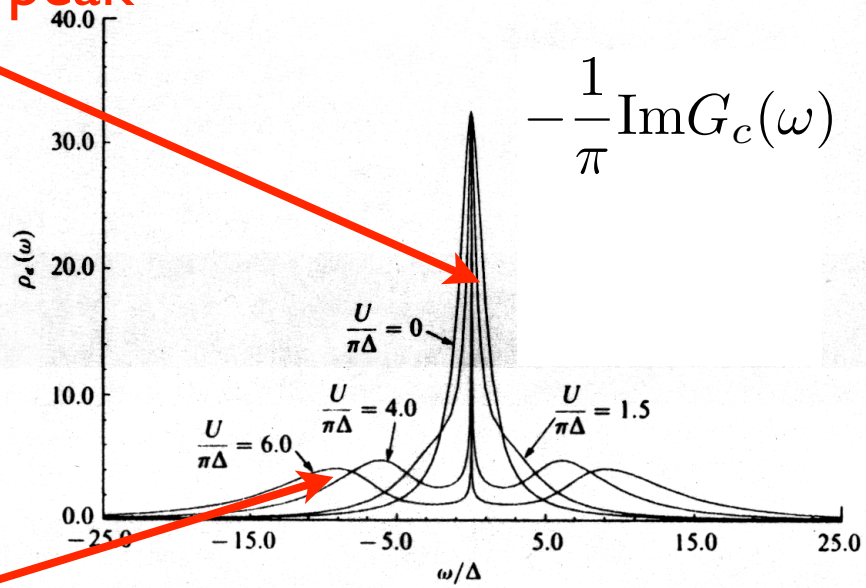
Anderson impurity

Quasi-particle-peak



Free electrons

Fermi liquid



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

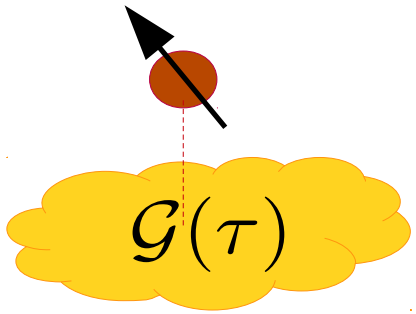
DMFT : transform this analogy into a formalism

Dynamical Mean Field Theory (DMFT)

DMFT : main idea

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

Dynamical Mean Field Theory

Ising model

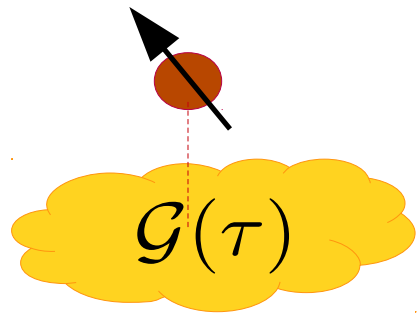
$$H = -J \sum_{ij} \sigma_i \sigma_j$$

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

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

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

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



?

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

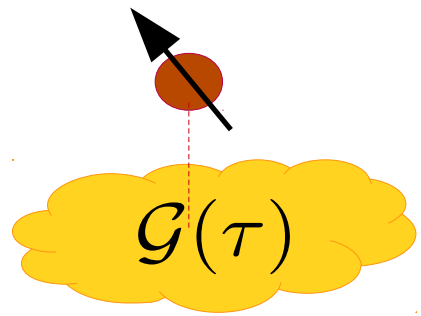
$$\Updownarrow$$

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

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

Bath
"Weiss field"

Hybridization function



DMFT equations (1 band paramagnetic)

Lattice model

Ising

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

Hubbard

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

Effective model

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

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

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

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

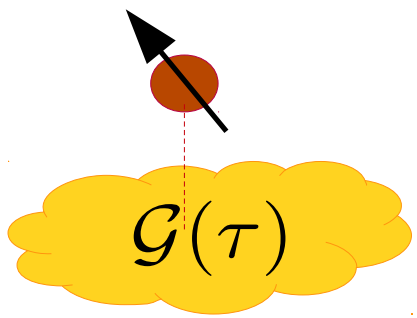
Self consistency condition

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

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

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

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 :

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

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

- G_{latt} depends on k. There is a Fermi surface in metallic regimes.
- Within DMFT, 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

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

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

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

$$\tilde{D}(\zeta)\equiv\int_{-\infty}^{+\infty}d\epsilon\,\frac{D(\epsilon)}{\zeta-\epsilon},\quad R[\tilde{D}(\zeta)]=\zeta.$$

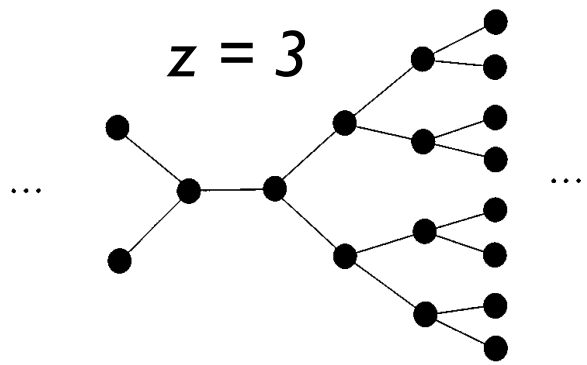
$$\tilde{D}(\zeta)=(\zeta-s\sqrt{\zeta^2-4t^2})/2t^2,\quad R(G)=t^2G+1/G\qquad s=\mathrm{sgn}[\mathrm{Im}(\zeta)]$$

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

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

The Bethe lattice

- A lattice with no loop.
- Hopping t between nearest neighbours
- Connectivity z = number of neighbours
- In the limit of infinite number of neighbours : $z \to \infty$



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

$$R(G) = t^2 G + G^{-1}$$

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

$$\left.\begin{aligned} G^{-1}(i\omega_n) &= i\omega_n + \mu - t^2 G(i\omega_n) \\ G(i\omega_n) &= \tilde{D}(i\omega_n + \mu) \end{aligned}\right| \Longrightarrow i\omega_n + \mu = R[G] = t^2 G + G^{-1}$$

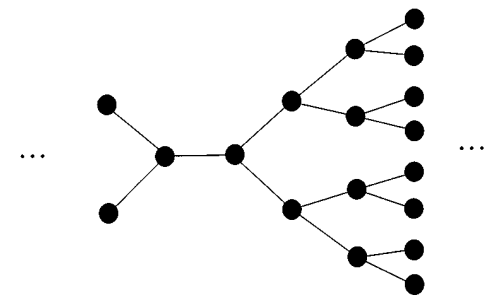
Bethe lattice : summary of equations

- DMFT on the Bethe lattice at $z \to \infty$

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

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

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



- Bethe lattice = semi-circular dos
- Physically meaning full, since semi-circular dos is a reasonable shape

How to solve DMFT equations ?

Notion of "Impurity Solver"

- Any method/algorithm that compute G from $\mathcal{G}$

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

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

- The most challenging part of a DMFT computation.
- Cf Lecture 3.
  In Lecture 1 & 2, I simply assume that I have an impurity solver.

Solving DMFT : iterative method

Impurity solver

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

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

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

$\mathcal{G}$

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

Self consistency condition

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

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

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

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

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

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

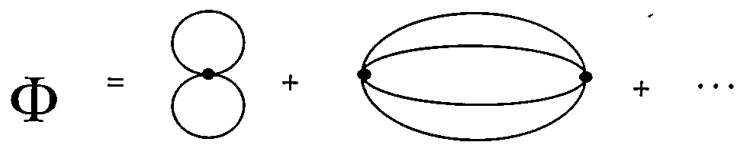
Luttinger-Ward functional : properties

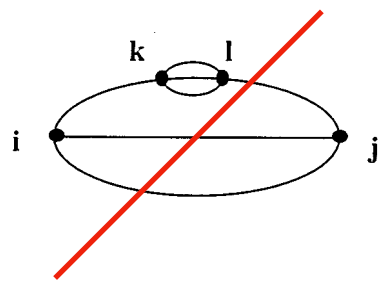
- From the stationarity of Γ[G] at the physical G:

Baym, Kadanoff,
De Dominicis, Martin 64

$$\frac{\partial \Gamma[G]}{\partial G} = 0 \quad \Longrightarrow \quad \Sigma_{ij} = \frac{\delta \Phi}{\delta G_{ji}}$$

- Diagrammatics:
  Φ[G] is the sum of two-particles irreducible (2PI) diagrams





- Dyson as a functional equation for G

$$G^{-1} = g_0^{-1} - \Sigma[G]$$

- A standard object in many-body theory. Conserving approximations

In strong coupling, **Φ** is in fact multivalued. G[g_0] is not inversible

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

Definition of DMFT

Metzner-Vollhardt '89, Georges-Kotliar '92

- Hubbard model

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

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

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

- DMFT is exact for U=0 and in the atomic limit (t_{ij}=0).
- *Exercise : Show it from the previous equations*

Why is it the same as before ? Where is the bath ?

Impurity = auxiliary local model

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

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

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

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

- The impurity exactly sums in Σ the 2PI local diagrams if we fix the bath such that :

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

- Moreover

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

DMFT self-consistency equations

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

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

Large dimension : d → ∞

Metzner-Vollhardt '89

- Consider an hypercubic lattice in dimension d
- Scale the hopping as :

$$\frac{t}{\sqrt{d}}$$

- Then

$$\Phi(G_{ij}) \underset{d\to\infty}{\to} \sum_i \phi_1(G_{ii})$$

- 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 $1/\sqrt{d}$.

Open various routes for generalisation

- Control
  - Successive approximation of Φ. Cluster, Cf lecture 2

$$\Phi_{\text{Hubbard}}[G_{ij}] = \underbrace{\sum_i \phi_1(G_{ii})}_{\textbf{Local = DMFT}} + \underbrace{\sum_{\langle i,j\rangle} \phi_2(G_{i,j}) + \sum_{\langle i,j,k\rangle} \phi_3(G_{i,j}, G_{i,k}, G_{j,k}) + \dots}_{\textbf{Non local = clusters}}$$

- Unification DFT + DMFT
  - Take a functional of G and ρ ! *Cf Ref 2, Kotliar et al. RMP 2007*

- Higher order functional (more Legendre transform).
  - The central object is not G, but a higher order correlator/vertex. Cf lecture 2. Trilex, DΓA

Other physical quantities than G ?

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 :

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

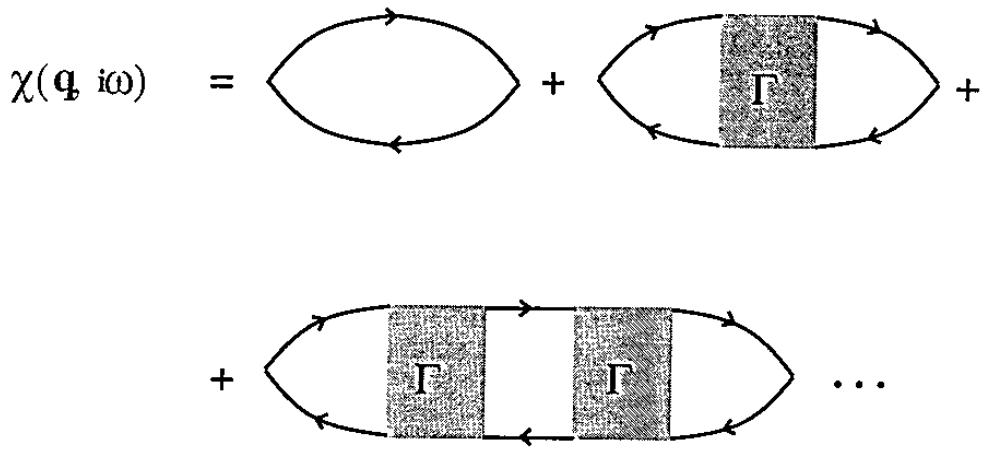
- Therefore :

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

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

Response functions

- Susceptibilities are given by the Bethe-Salpeter equation



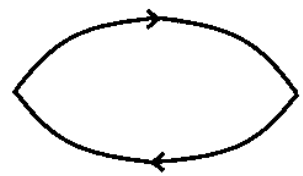
- DMFT approximation :

$$\Gamma^{\mathrm{latt}}(k, k', q, i\nu, i\nu', i\Omega) \approx \Gamma_{\mathrm{imp}}(i\nu, i\nu', i\Omega)$$

- X, Γ do <u>not</u> enter the self-consistency DMFT equation directly.
- Hence collective modes do not directly affect the electron gas. Cf methods beyond DMFT, like Trilex, DΓA

Resistivity, optical conductivity

- Neglect vertex correction (exact in d $\to\infty$)
  Particle-hole current-current bubble (with full propagators).



$$\sigma(i\omega)=\frac{1}{\omega}\frac{1}{\beta}\sum_{\nu_n}\int_{-\infty}^{+\infty}d\epsilon\, D(\epsilon)G(\epsilon,i\nu_n)G(\epsilon,i\nu_n+i\omega).$$

$$\mathrm{Re}\ \sigma(\omega+i0^+)=\pi\frac{e^2}{\hbar a d}\int_{-\infty}^{+\infty}d\epsilon\int_{-\infty}^{+\infty}d\nu\, D(\epsilon)\rho(\epsilon,\nu)$$

$$\times\rho(\epsilon,\nu'+\omega)\,\frac{f(\nu)-f(\nu+\omega)}{\omega}.$$

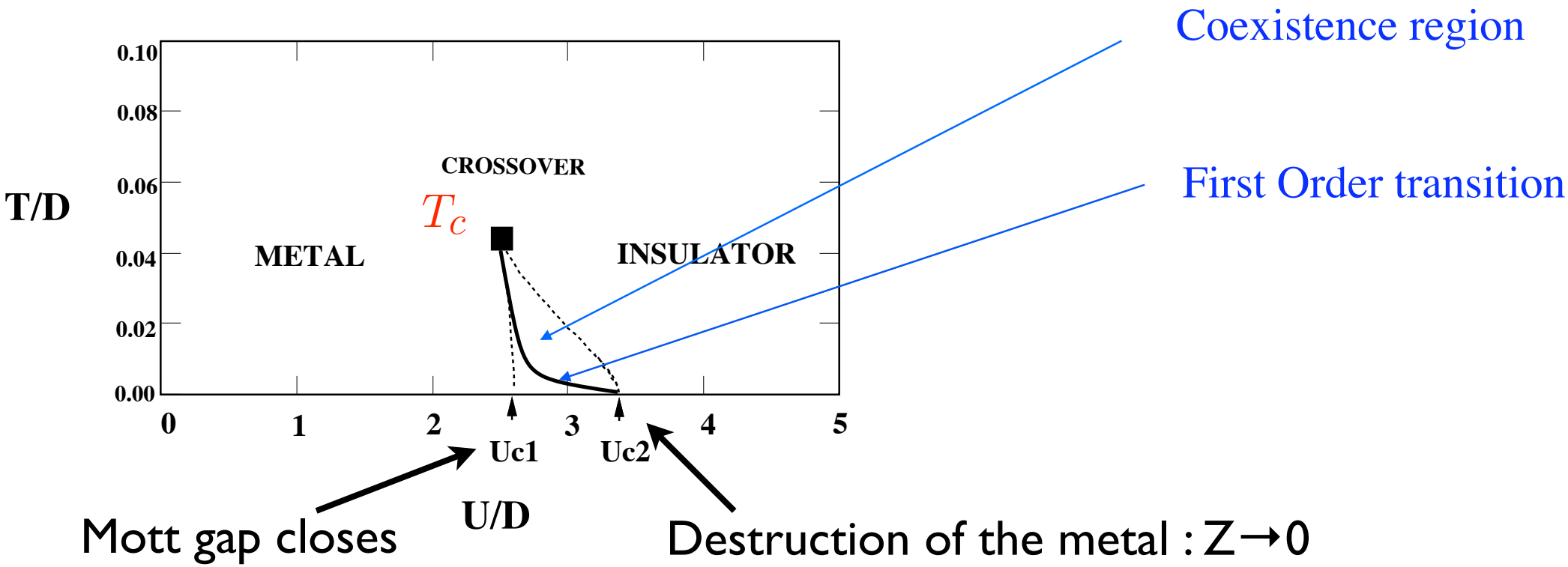
- Need a computation of $\Sigma(\omega)$ at real frequencies.
  Very sensitive to quality of low frequencies computation.

A DMFT classic

Hubbard model, 1 band, 1/2 filling

Phase diagram

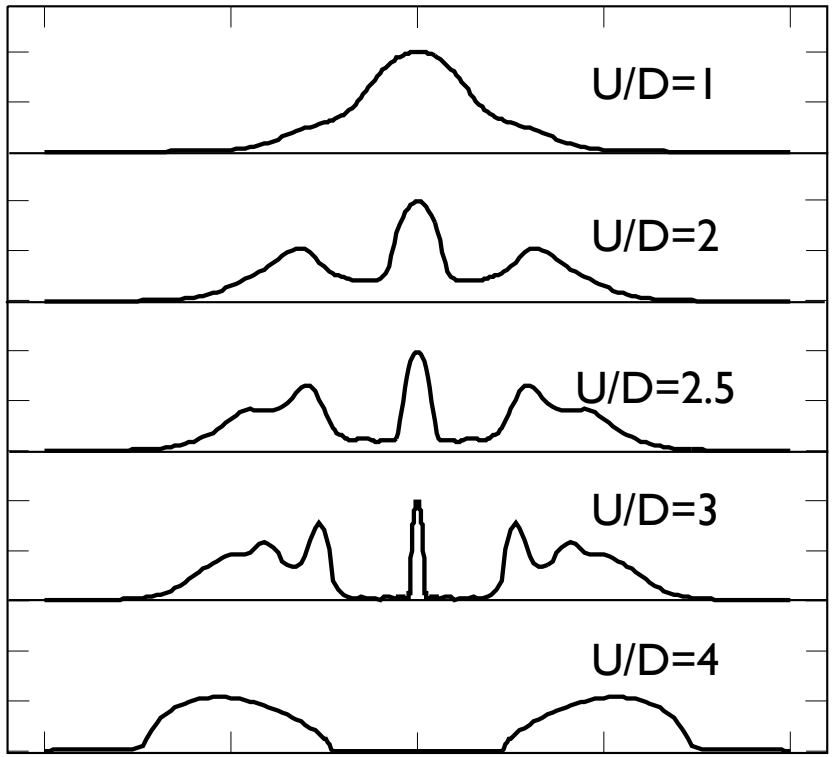
- Hubbard model at half-filling (δ=0). D is half-bandwidth.



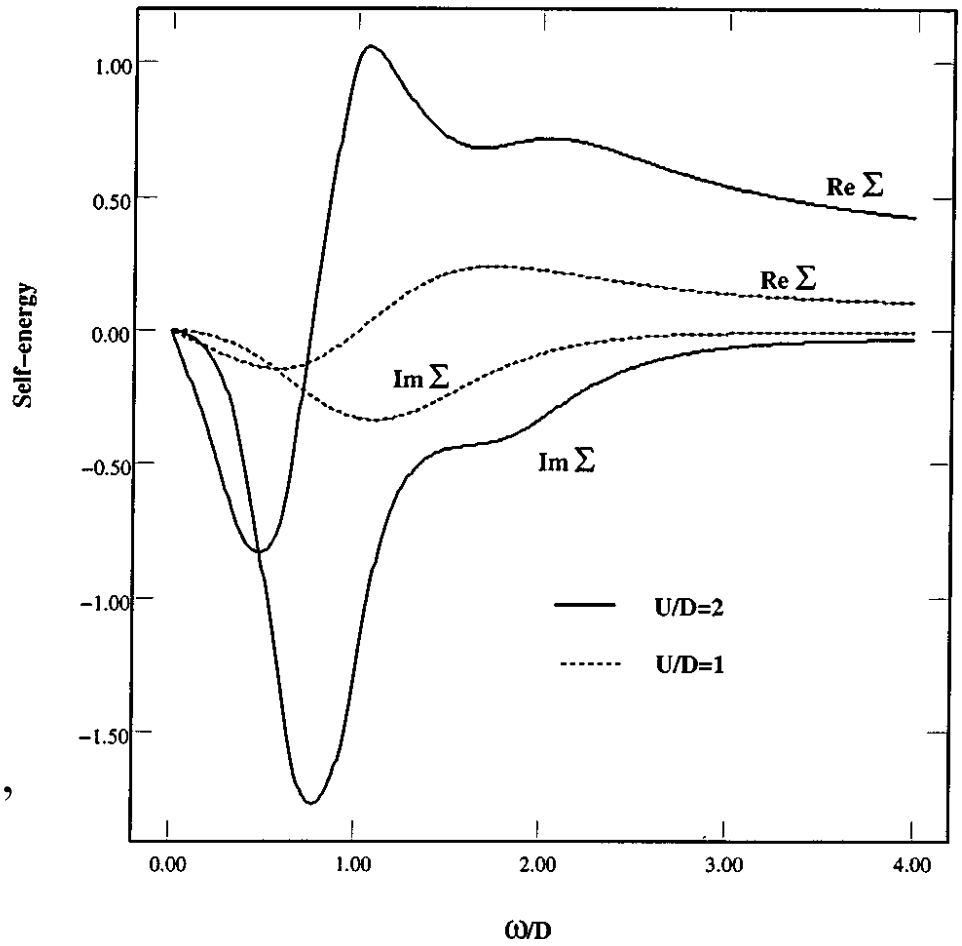
2 solutions

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

Spectral function



Self-energies in metal



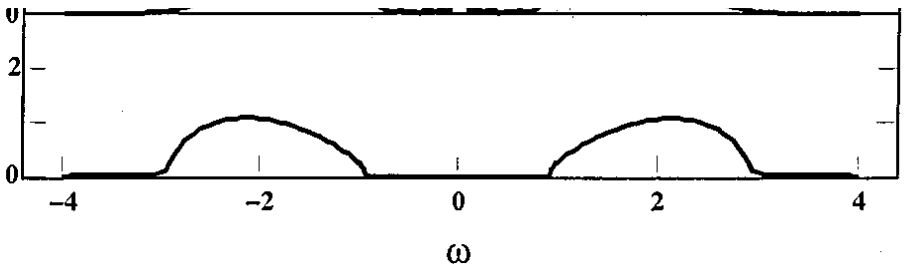
$$\mathrm{Re}\Sigma(\omega+i0^+) = U/2 + (1-1/Z)\omega + O(\omega^3),$$

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

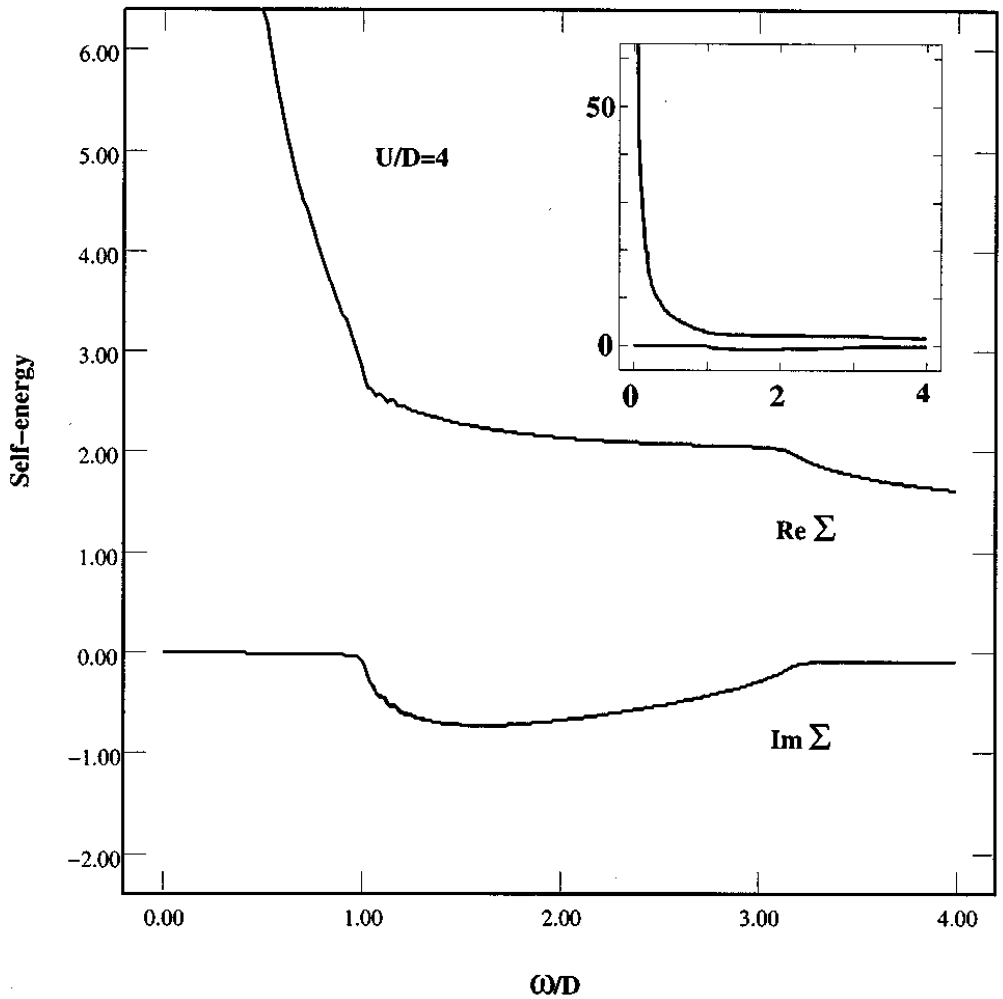
2 solutions

- Insulating solution : $\Delta(0) = 0$: gapped bath $\Rightarrow$ 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*

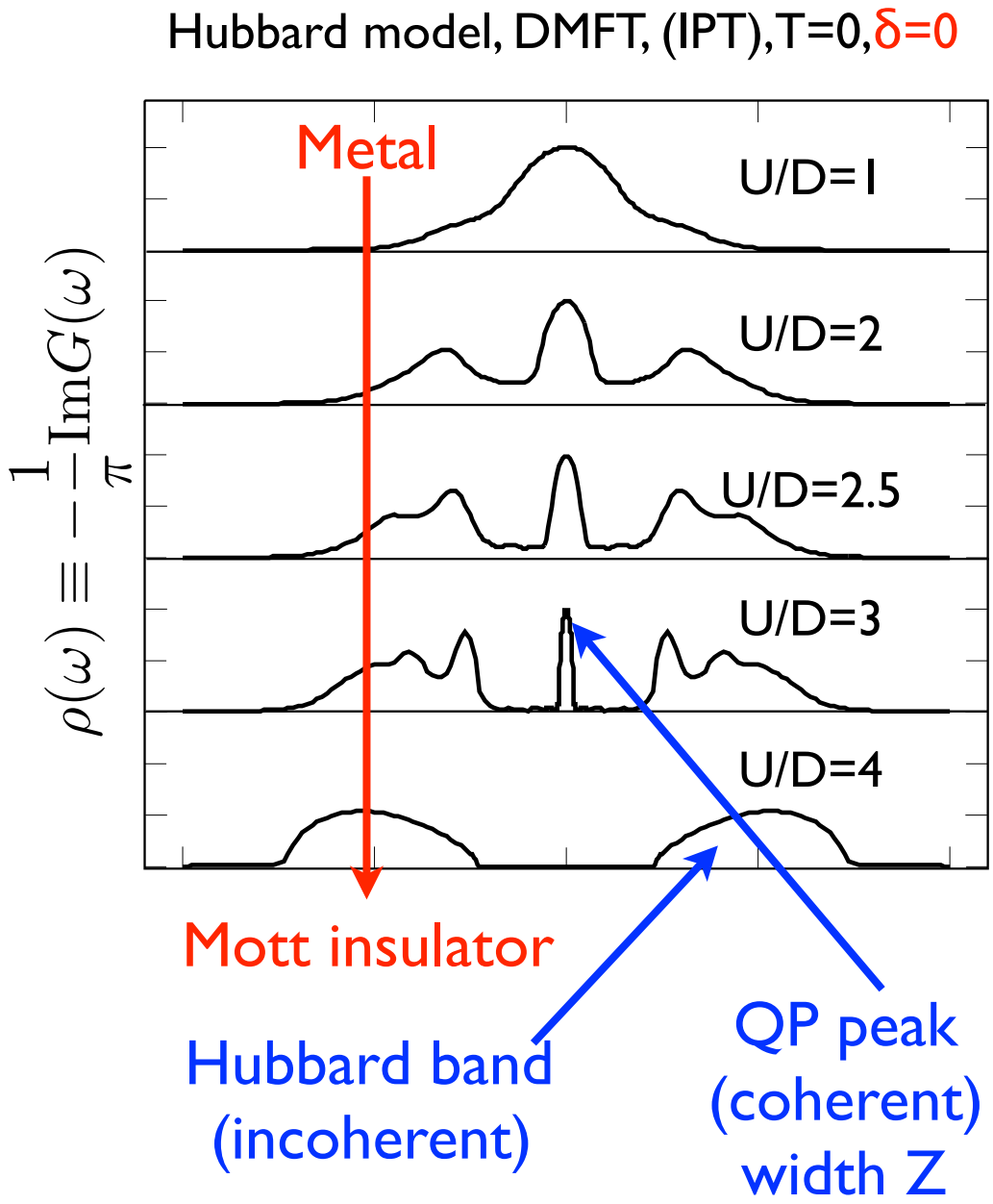
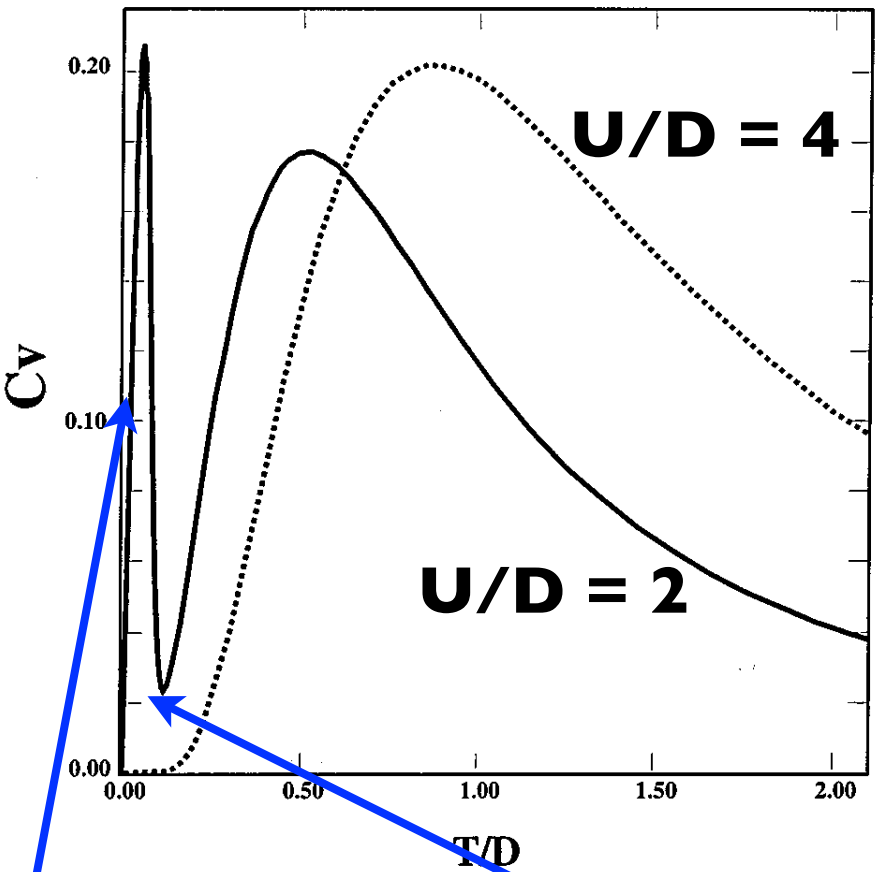
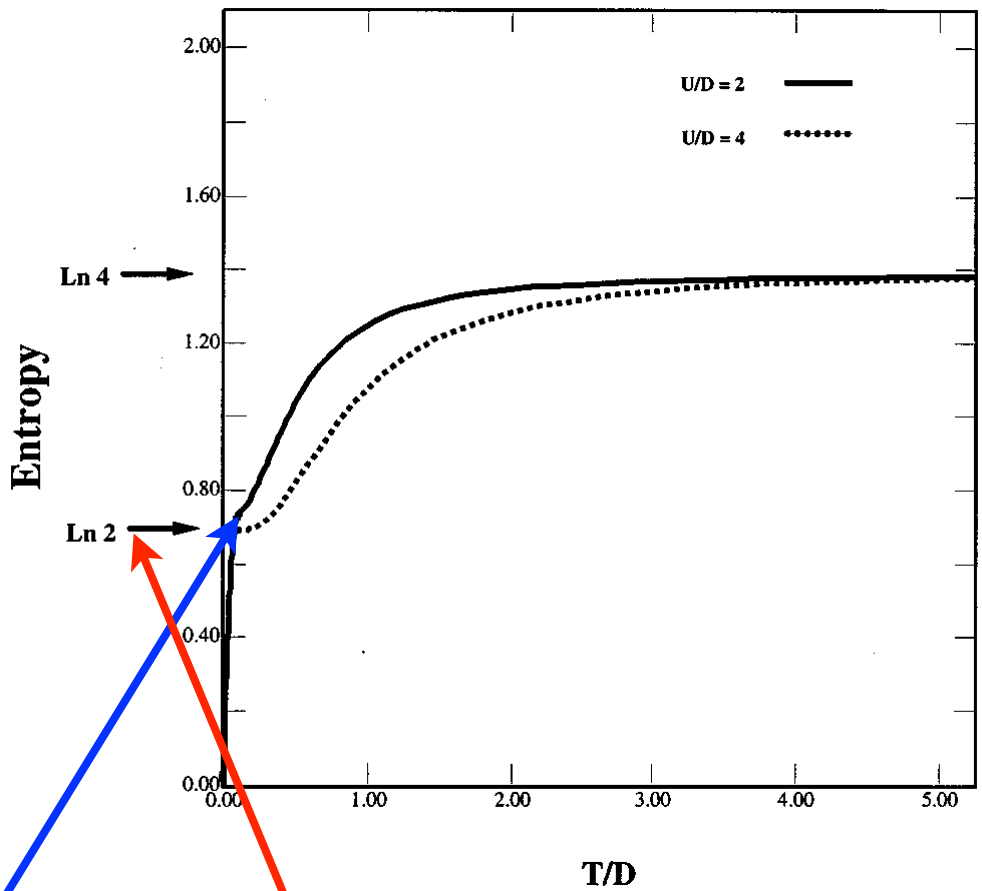


Illustration of the low-coherence temperature

- Thermodynamics quantities



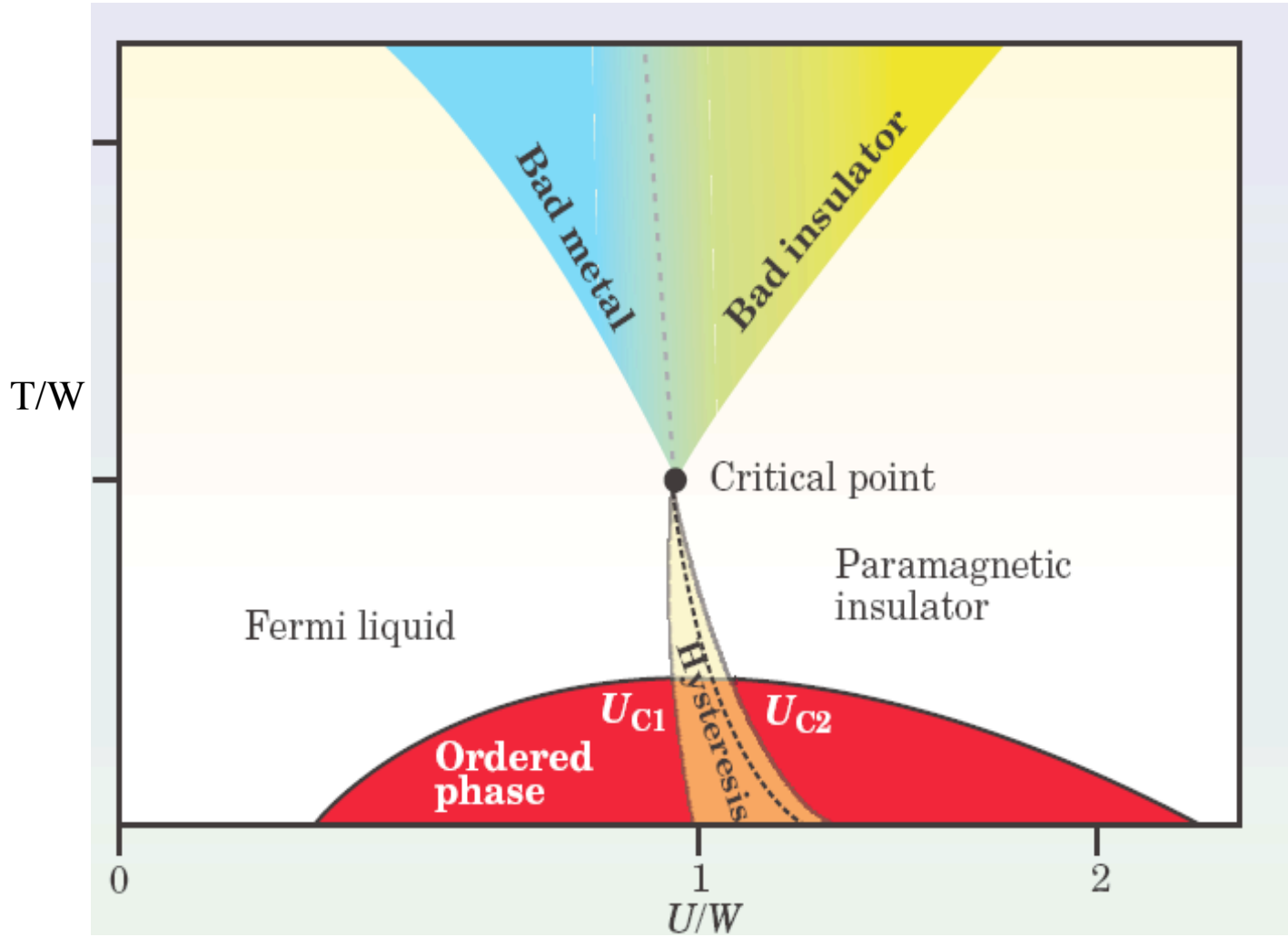


Fermi liquid behaviour

T_{coh}

Trivial paramagnetic insulator

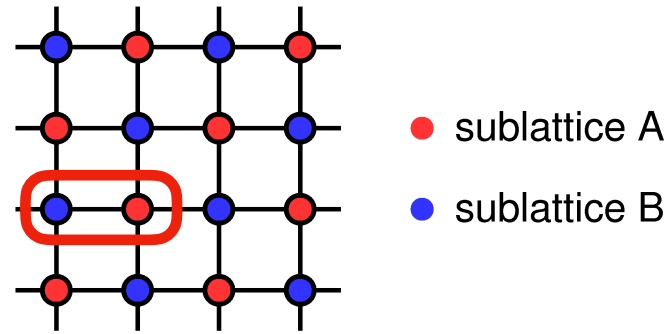
Complete phase diagram



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)

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

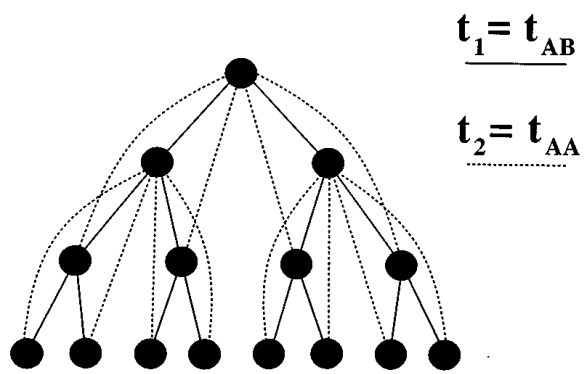
Remark on frustrated systems

- DMFT paramagnetic equations = equations of a frustrated system

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

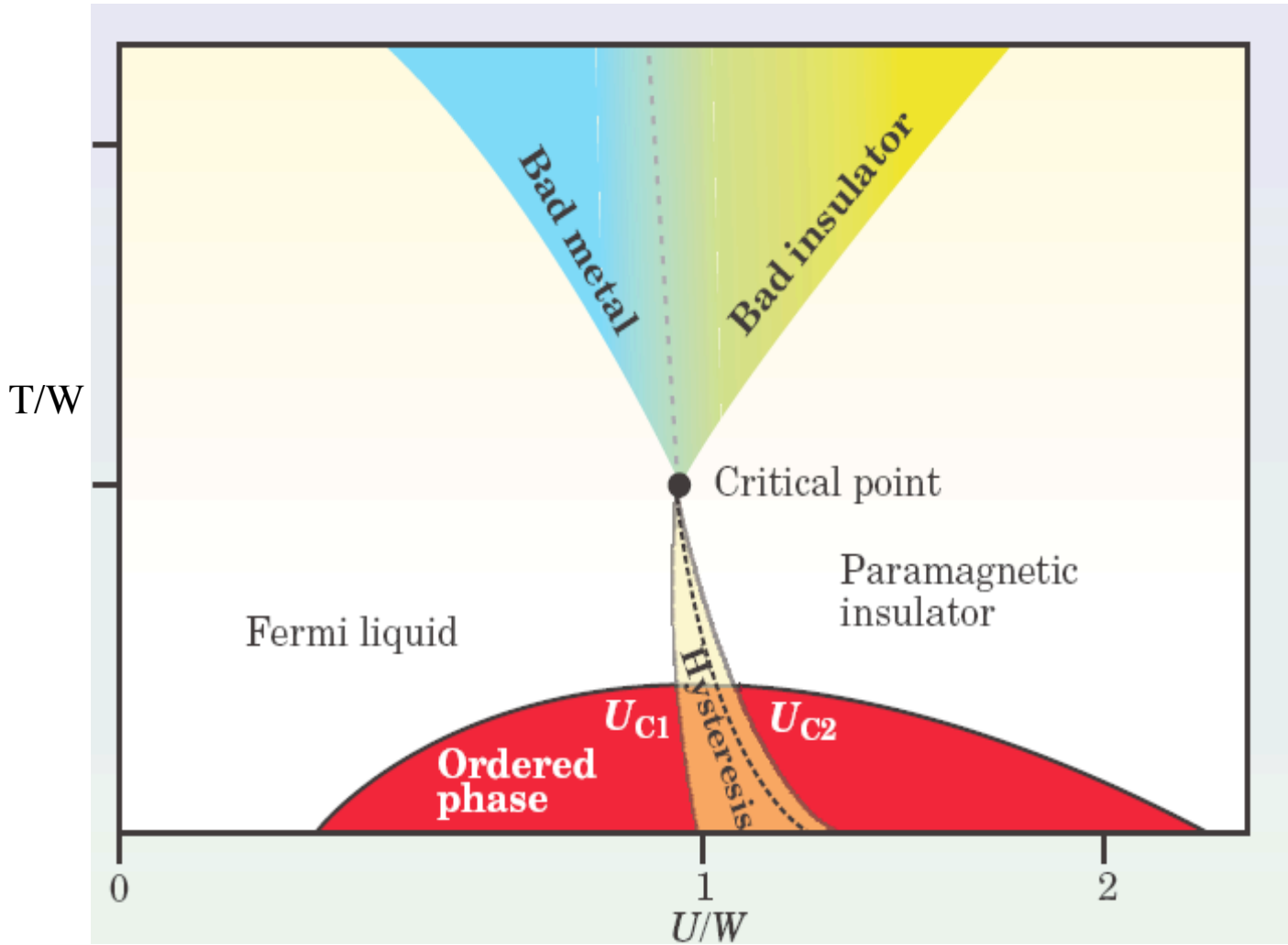
- E.g. a frustrated Bethe lattice (paramagnetic phase).

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



Complete phase diagram

- With frustration (or AF would be much higher)



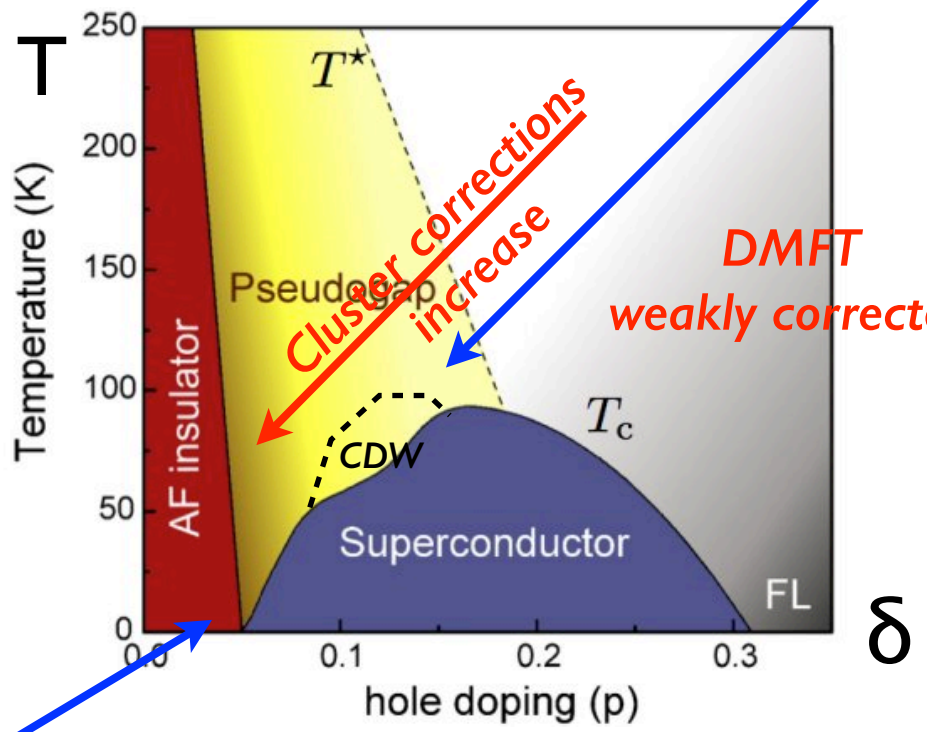
DMFT is high temperature method

"Top to Bottom"

Start from high T/doping

R.G.

Diagrammatic methods



"Bottom to Top"

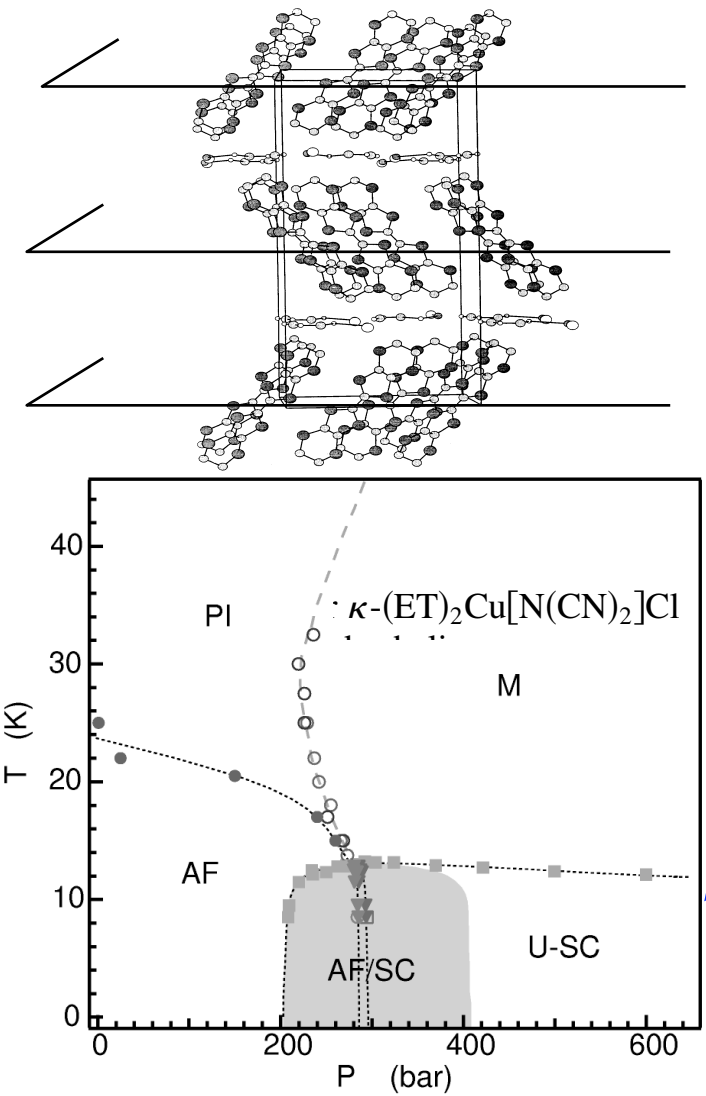
Study the many-body ground state

DMRG, PEPS, MERA

Comparison with some experiments

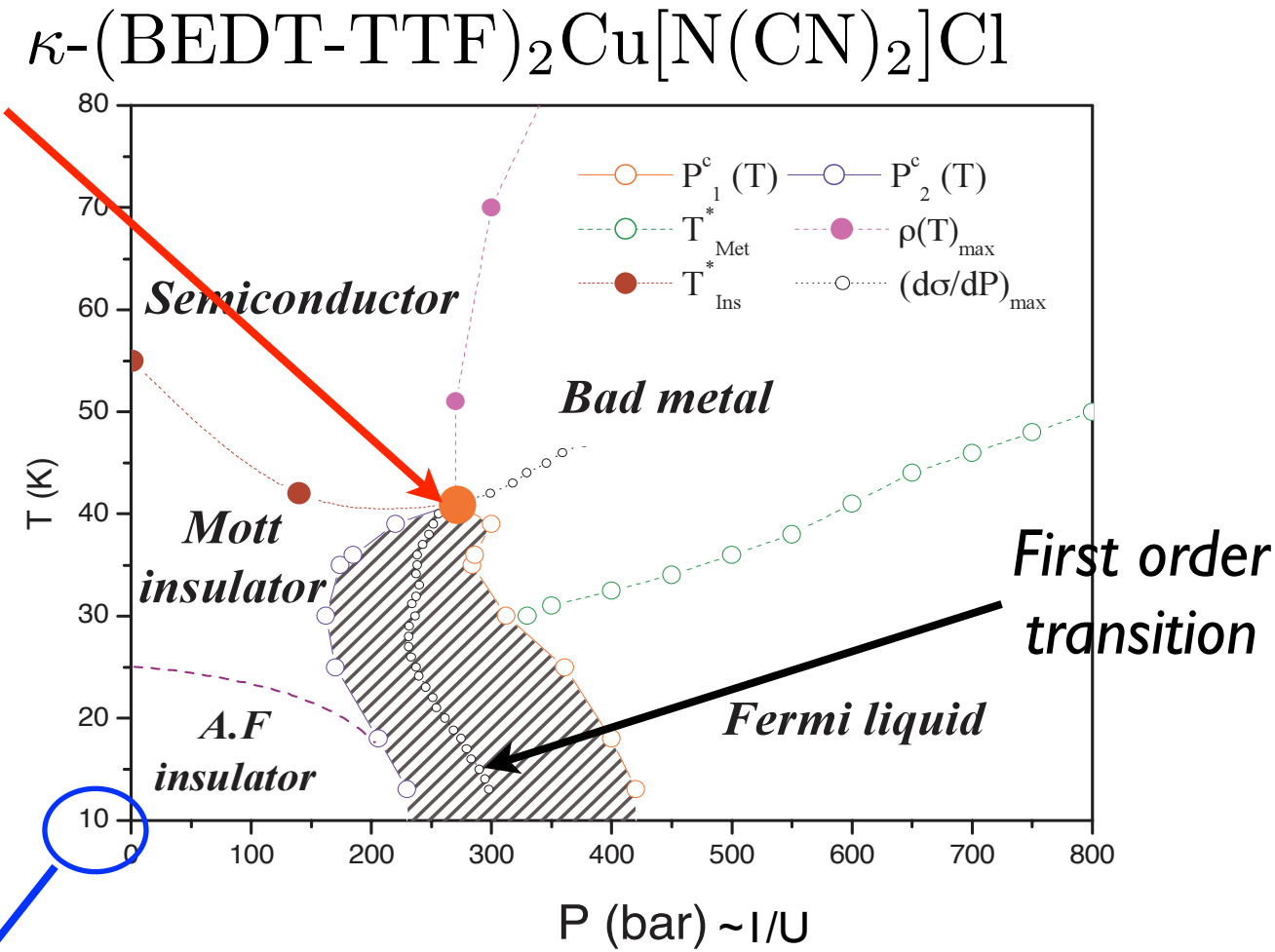
Organics (resistivity measurements)

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



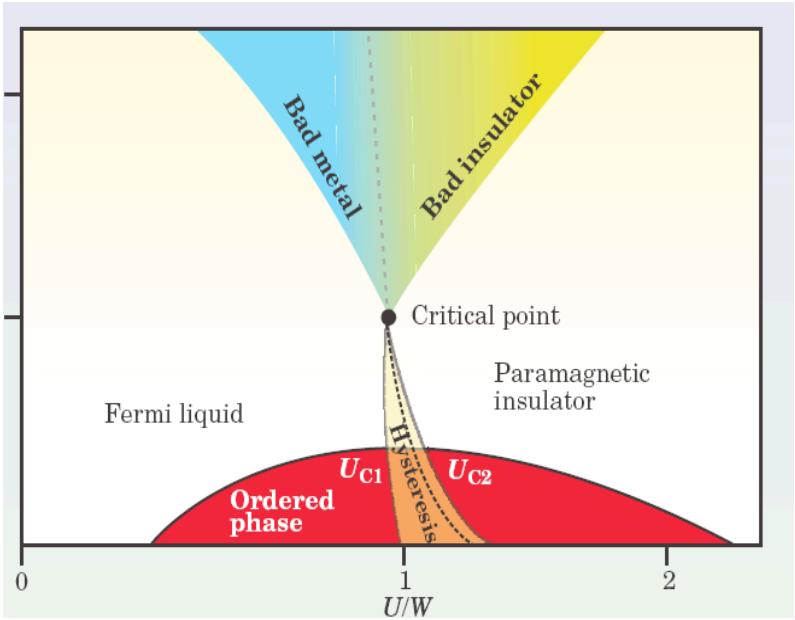
S. Lefebvre et al. PRL 85, 5420 (2000)

Critical Point



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

Comparison with organics : phase diagram

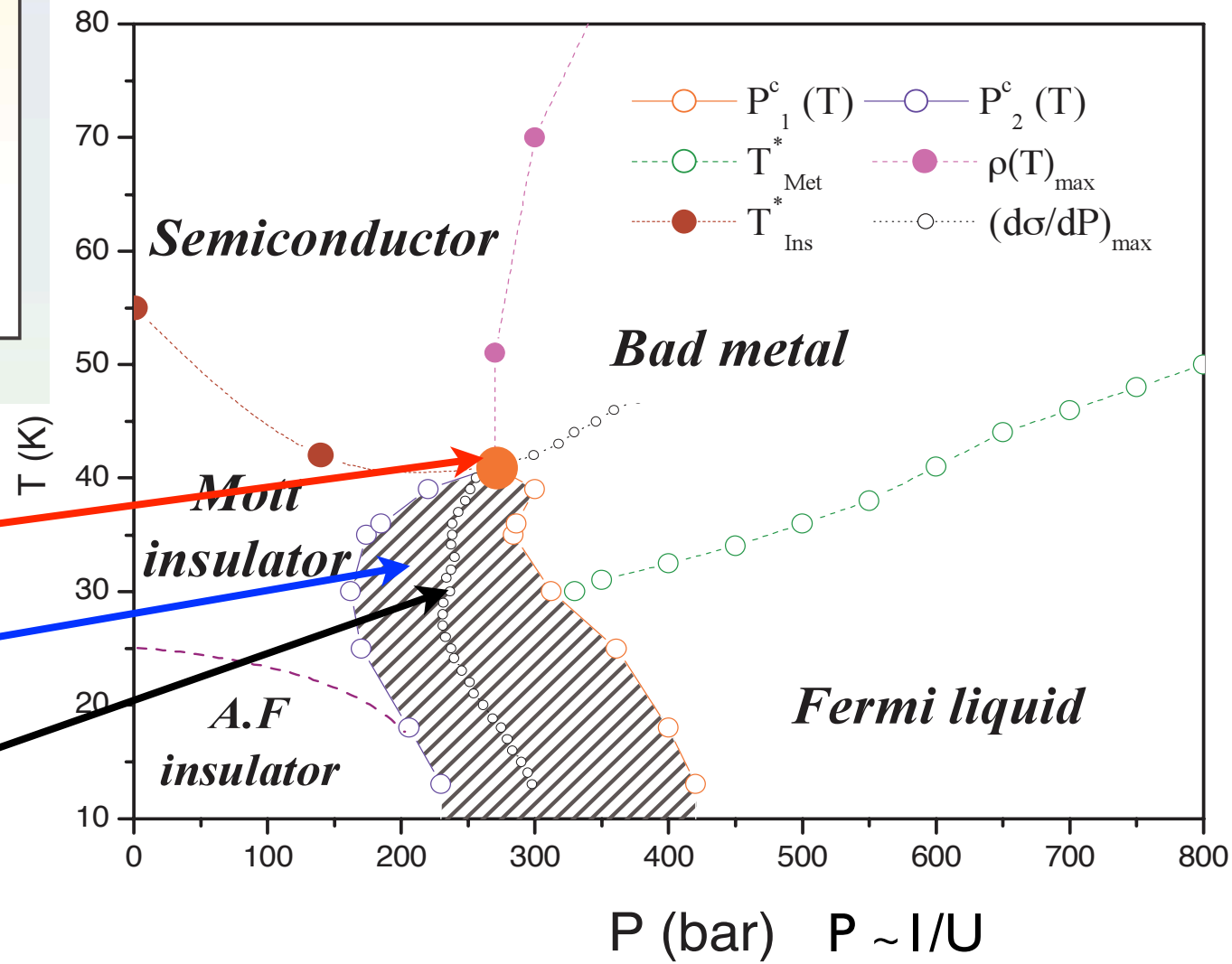


κ-$(BEDT\text{-}TTF)_2Cu[N(CN)_2]Cl$

Critical Point

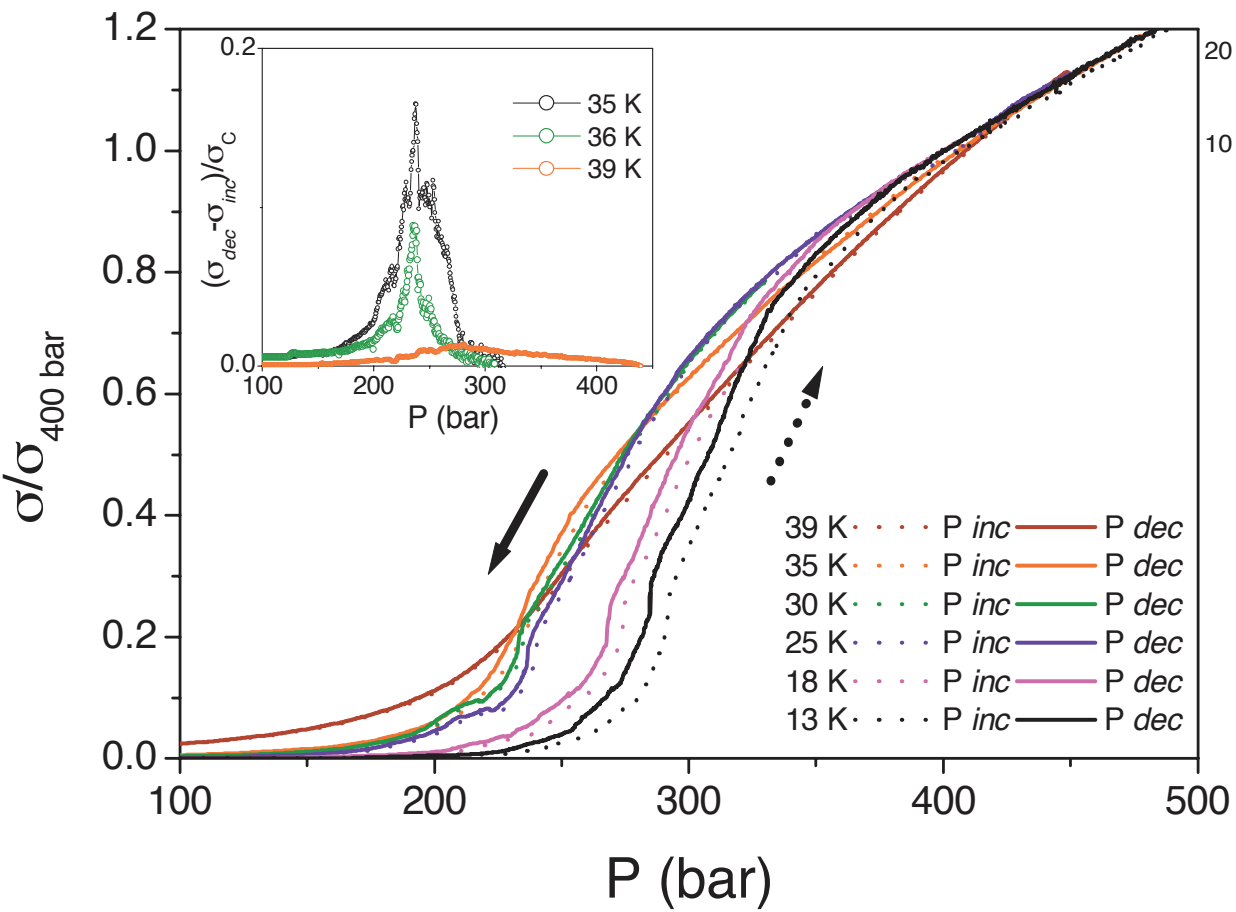
Coexistence region

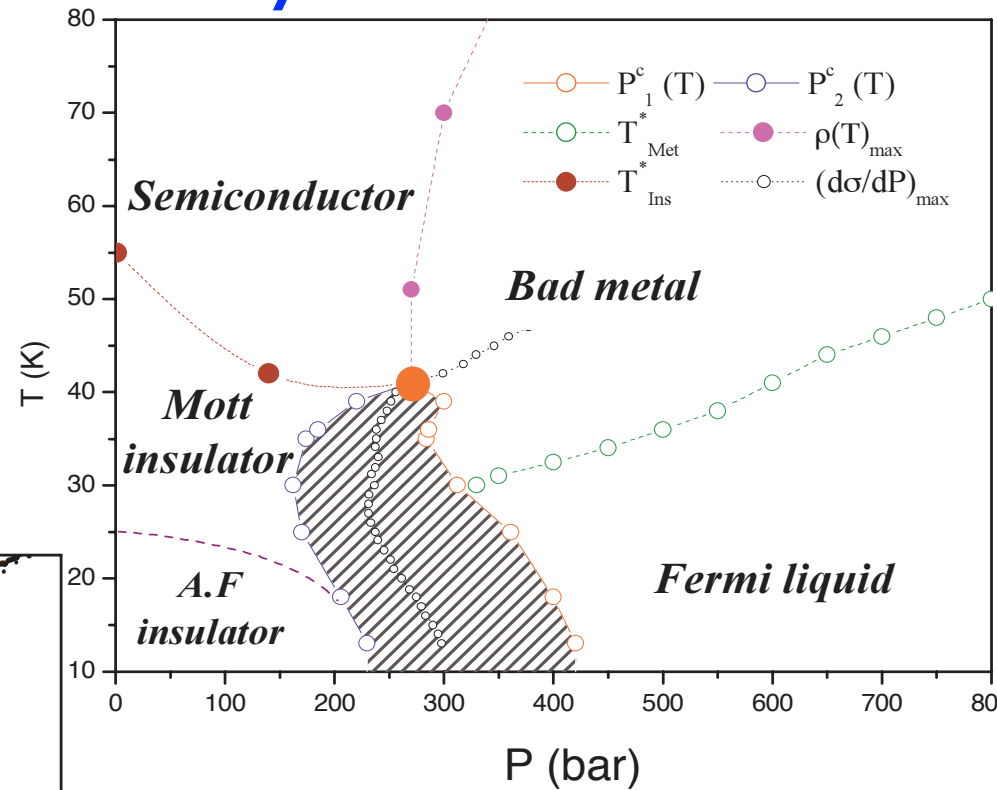
First order transition



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

Experimental evidence for hysteresis



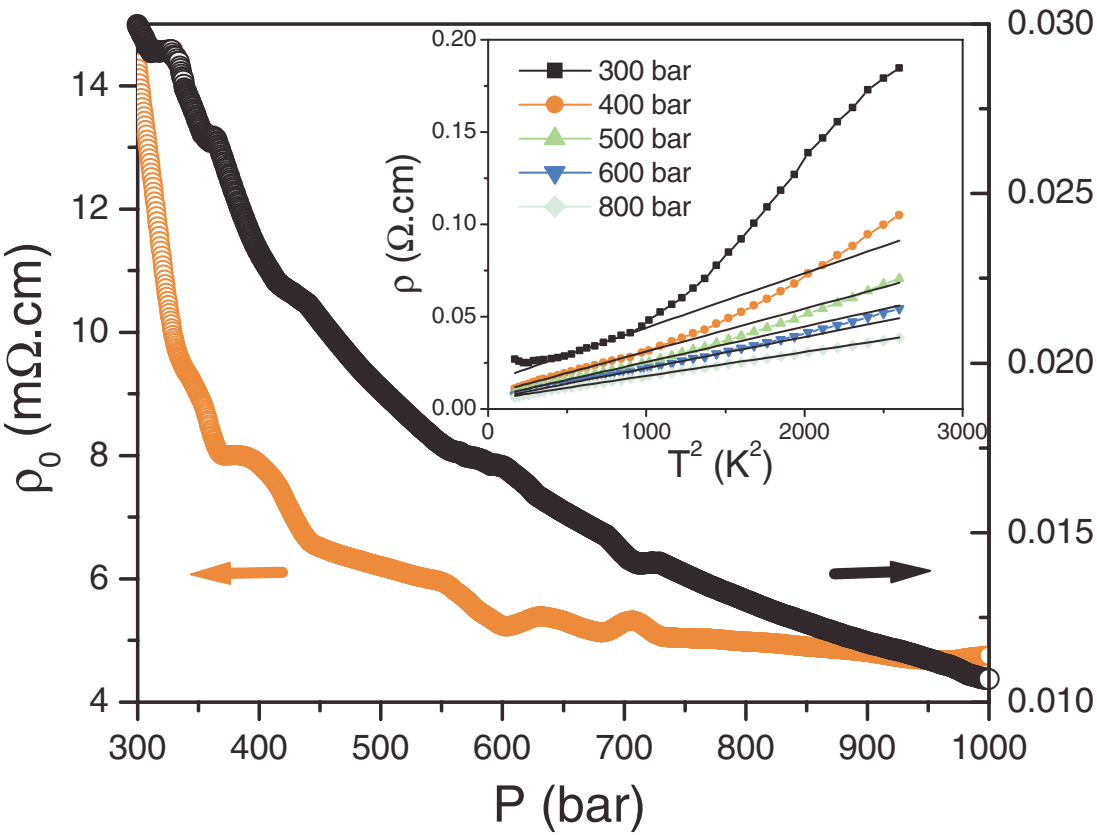


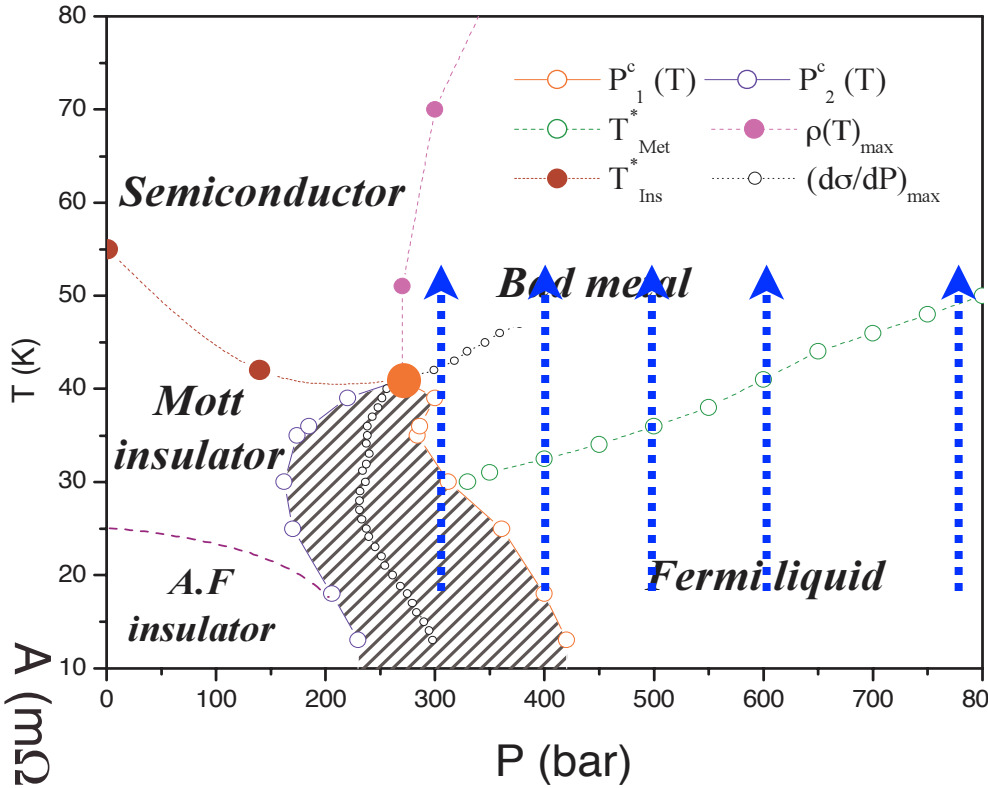
Metallic regime

- At low temperature, Fermi liquid

$$\rho \approx \rho_0 + A(P)T^2$$

$$A(P)T_{coh}^2 \approx const$$





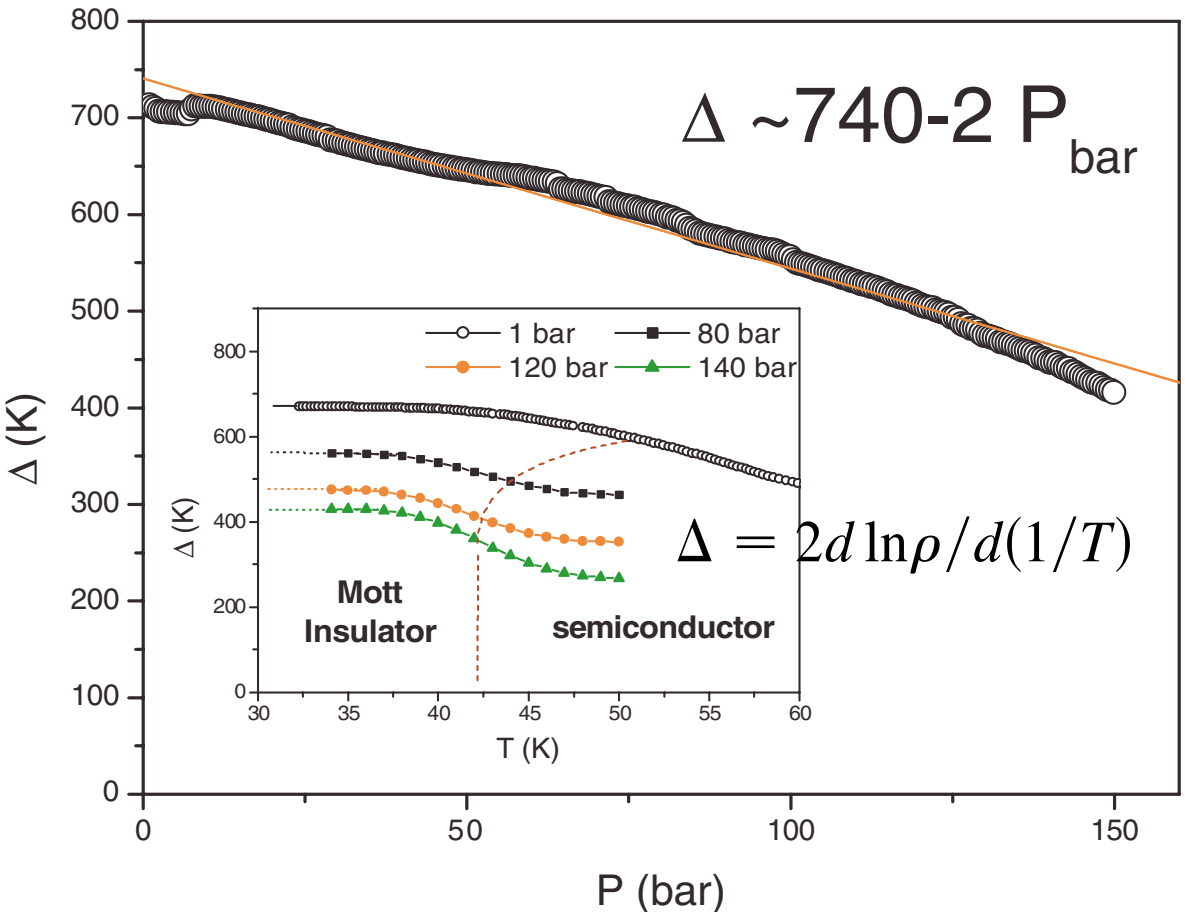
- Divergence of A (extrapolated) when Mott gap still large.
- T_coh << Δ

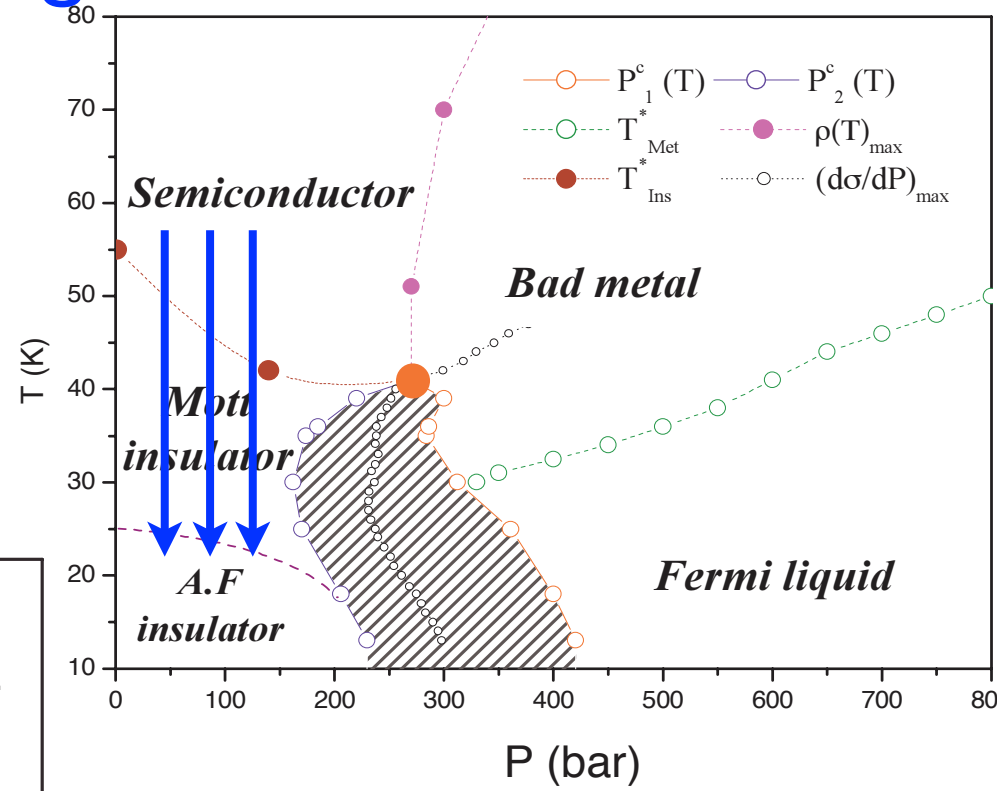
Insulating regime

- At low temperature, activation law

$$\rho \sim \exp(\Delta/2T)$$

- Semi-conductor regime

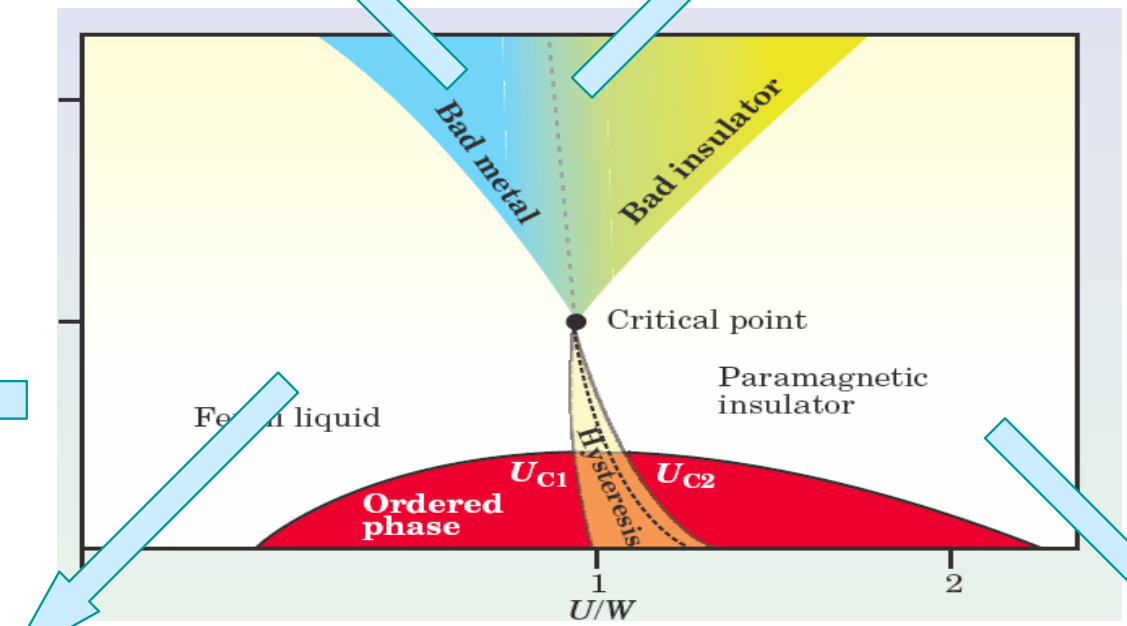




- Δ still large close to coexistence
- Mott transition not driven by closure of the gap.

Various regimes around the critical point

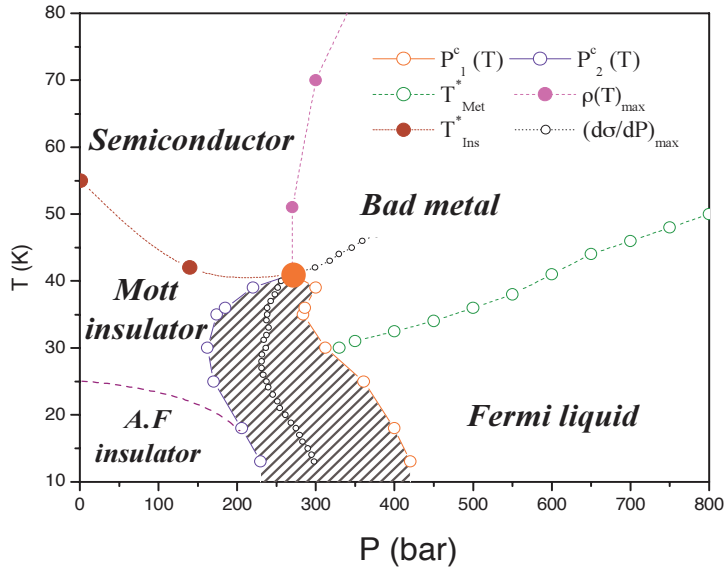
T/W

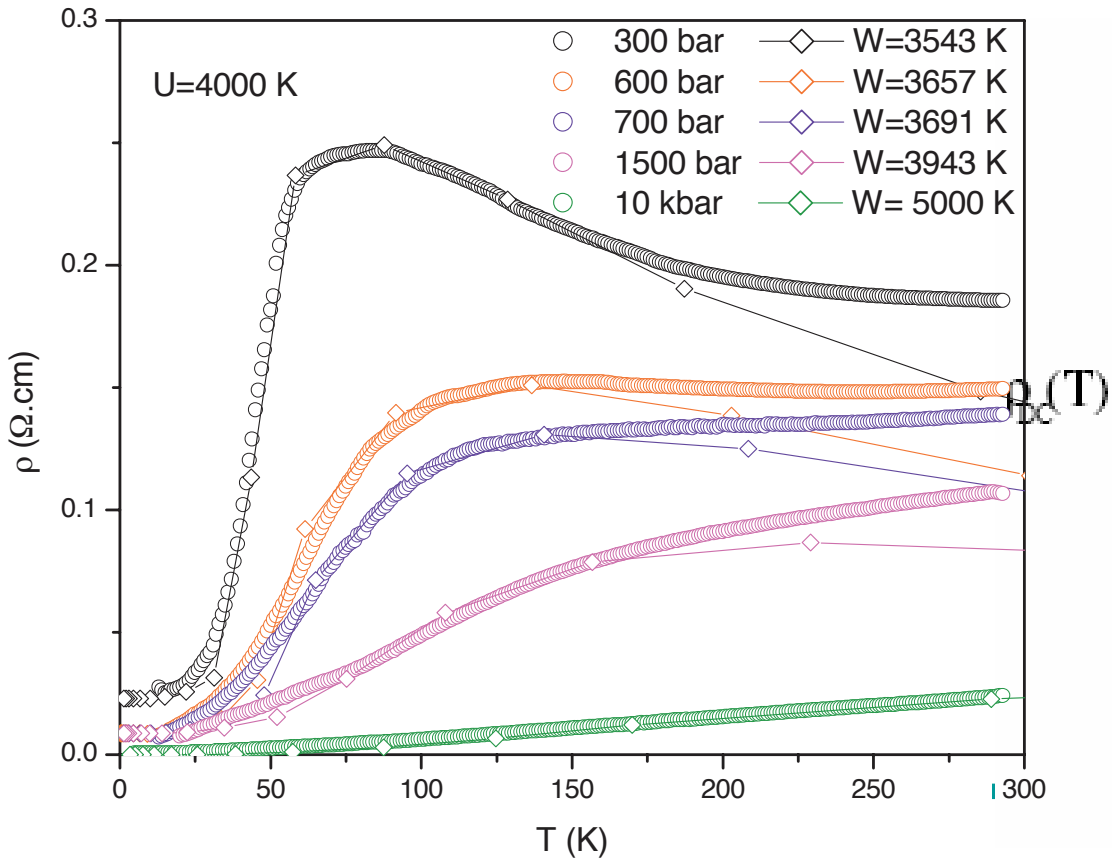


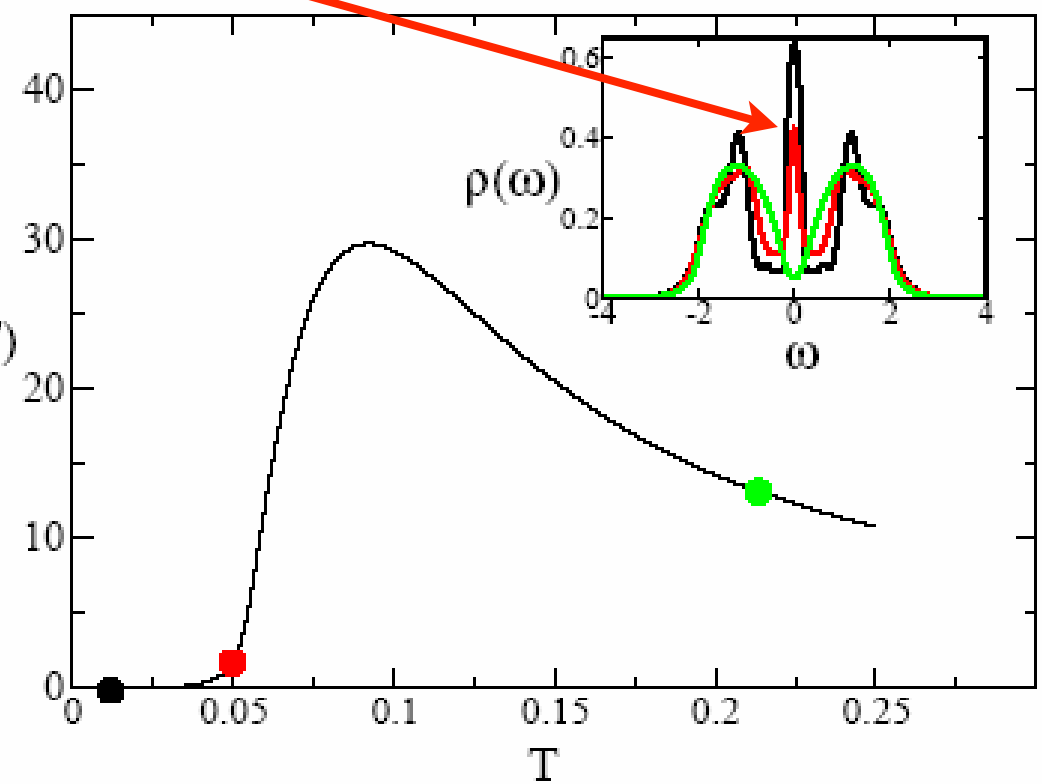
Sketchs of the spectral density

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



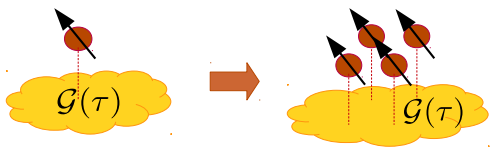




DMFT : a family of approximations

DMFT, a family of approximations

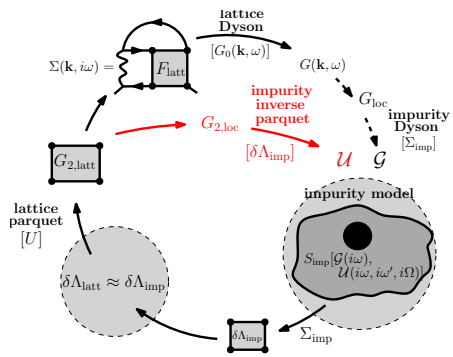
- Cluster DMFT



Control, short range correlation

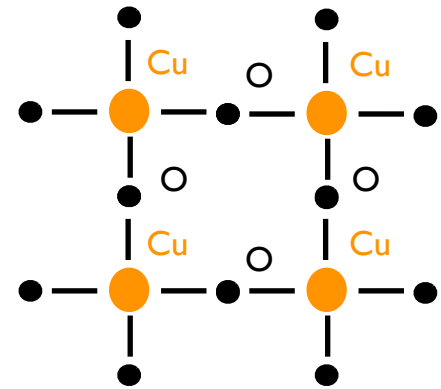
- Beyond cluster DMFT

Self-consistency on vertex
Dual fermions/bosons, Trilex, DΓA



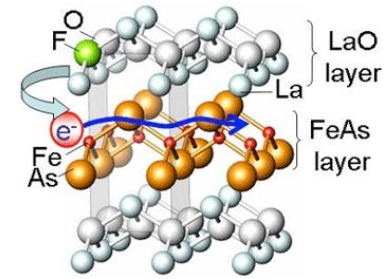
- Multiband/realistic systems

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



- Self-consistency in large unit cell (Cu + 2 O)
  $\Sigma_{ab}(\omega)$ a 3x3 matrix
- Impurity model on Cu, 1 band : $\Sigma^{\rm imp}(\omega)$ 1x1 matrix

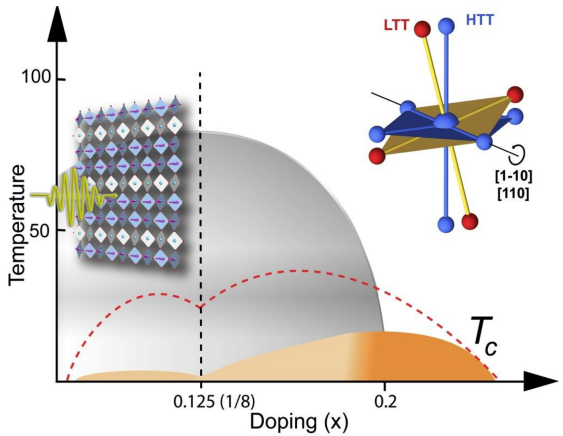
- DFT + DMFT



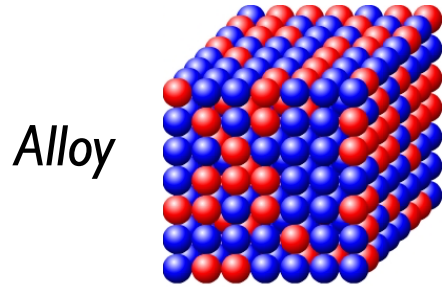
- Interface with electronic structure codes (project on Wannier functions, etc).

DMFT, a family of approximations

- Non equilibrium

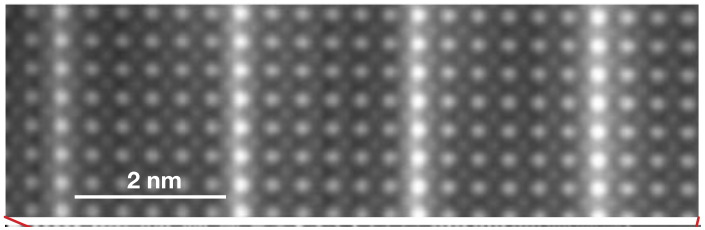


- Disordered systems



- Two impurity models

- Correlated interfaces.



$SrTiO_3/LaTiO_3$

Ohtomo et al, Nature 2002

- One impurity per layer

Outline

- Lecture 1 : Introduction to DMFT
  - Why DMFT ?
    - Introduction to Mott transition.
    - Introduction to Quantum Impurity models.
  - DMFT equations.
  - A classic : solution of DMFT for 1 band 1/2 filling Hubbard model
- Lecture 2 : Multiorbital DMFT. Clusters.
- Lecture 3 : Impurity solvers
- Lecture 4 : Introduction to TRIQS & Hands-on

Thank you for your attention