Introduction to DMFT

Plan of the lectures

Toulouse, May-June 2007

O. Parcollet

1. Introduction : DMFT and the Mott transition
2. Derivation of the DMFT equations. Impurity solvers.
3. Cluster methods and applications.
4. Realistic computation in DMFT (with S. Biermann)

Introduction to DMFT

Lecture I : DMFT and the Mott transition

Toulouse, May 24th 2007

O. Parcollet

1. Mott transition.
2. Quantum impurity models.
3. Introduction to Dynamical Mean Field Theory
4. The classic result : Mott transition in a single site DMFT.
5. Advertisement for next lectures...

General references

- ***DMFT, extensions and applications.***
  - A. Georges, G. Kotliar, W. Krauth and M. Rozenberg, Rev. Mod. Phys. 68, 13, (1996).
  - G. Kotliar, S.Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, C.A. Marianetti, Rev. Mod. Phys. 78, 865 (2006)
- ***Metal Insulator transitions.***
  - M. Imada, A.Fujimori, Y. Tokura Rev. Mod. Phys. 70, 1039 (1998)
- ***Quantum impurity models.***
  - "The Kondo problem to heavy fermions", A.C. Hewson, Cambridge University Press (1993).

Fermi liquid theory

- Standard metal at low temperature.
- Effective theory with fermionic quasiparticle (spin 1/2, charge -e), effective mass m*, residu Z. *(Landau, 50's)*
- Determines low-T physics, e.g. $\rho(T) \propto T^2, \chi(T) \propto cte, C_v \propto T$
- Picture valid below the <u>coherence scale</u> : $\omega, T < T_{\mathrm{coh}}$

- Explain success of "one body" methods, in particular in ab-initio calculations of the electronic structure (e.g. DFT et al.).
- *Textbooks : Pines-Nozières; Abrikosov, Gorkov, Dzyaloshinski*

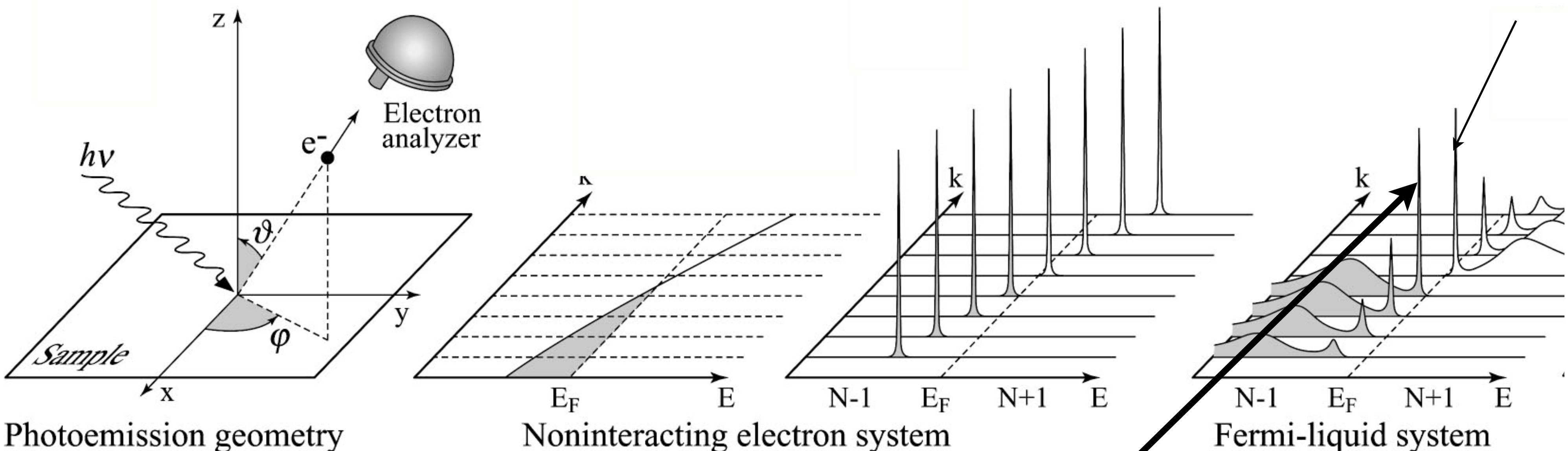
Spectral function

- Spectral function. Can be measured in photoemission experiments.

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

ARPES

Z<1



Quasi-particle-peak

Local spectral function

- Local component of the spectral function

$$G(\omega) = -i\int dt e^{i\omega t}\theta(t)\sum_k \langle[c(k,t), c^\dagger(k,0)]\rangle$$
$$= \int d\epsilon \frac{\rho(\epsilon)}{\omega - \epsilon + i0^+}$$

- Can be measured in STM experiments.
- G(ω) will be the central object of DMFT method.

Hubbard model

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

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

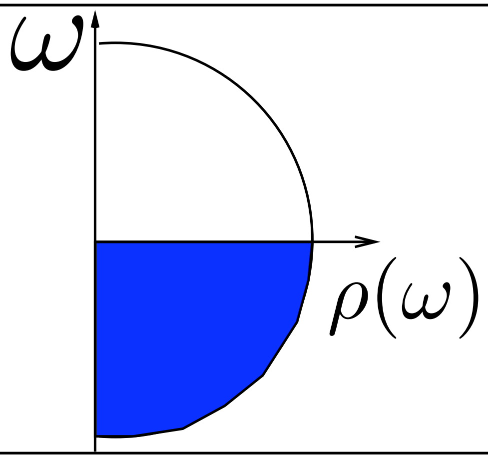
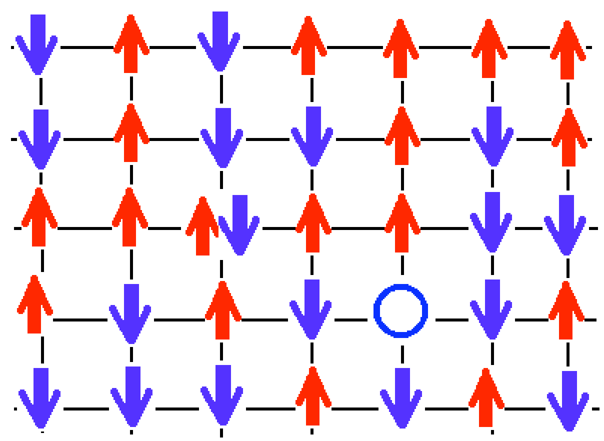
Kinetic term

Interaction term
local Coulomb

- A toy-model for strongly correlated systems.
- Plays a role similar to the Ising model in classical statistical physics.
- Parameters :
  - hopping t, frustration t'/t (lattice shape), Coulomb repulsion U
  - doping δ (chemical potential μ), temperature T.
- Half filling : 1 electron/site in average : δ=0

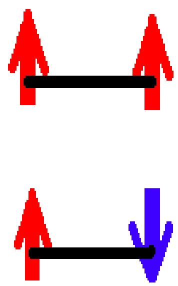
Mott transition

- Metal-Insulator transition due to interactions *(Mott, 49)*.
- Hubbard model : 2 solvable limits (δ=0, ph symmetric, μ = U/2)

U=0 : half-filled band Metal	U/t large : charge motion frozen Mott Insulator
	
Easy in k-space	Easy in real space Charge gap ~ U

Mott insulators

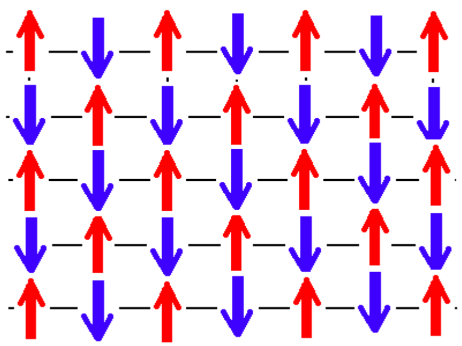
- Spin-spin interaction (Heisenberg exchange)



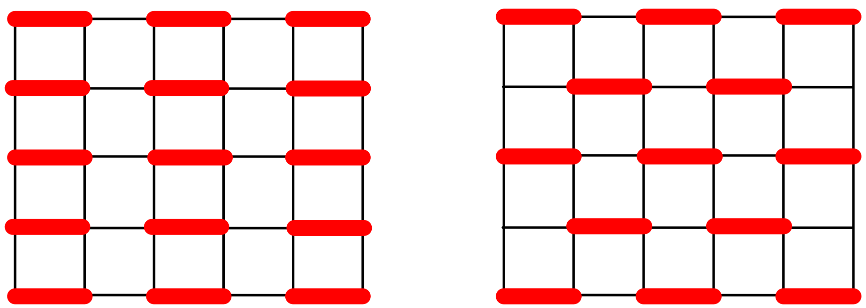
$$J_{AF} = \frac{4t^2}{U}$$

- Mott insulators with various spin orders:

AF, spin liquids, VBS, depending on the lattice



AF order



Valence Bond Solids

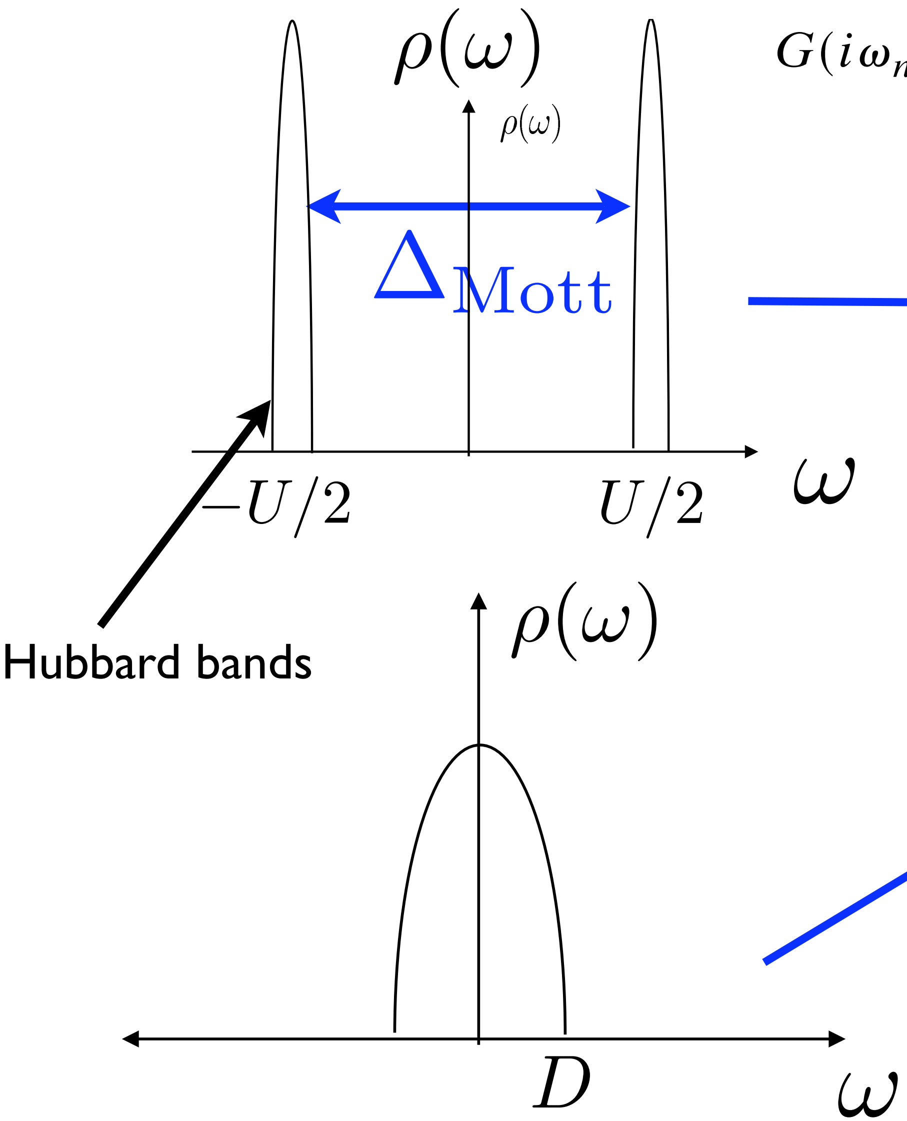
Introduction : G. Misguich and C.Lhuillier cond-mat/0310405

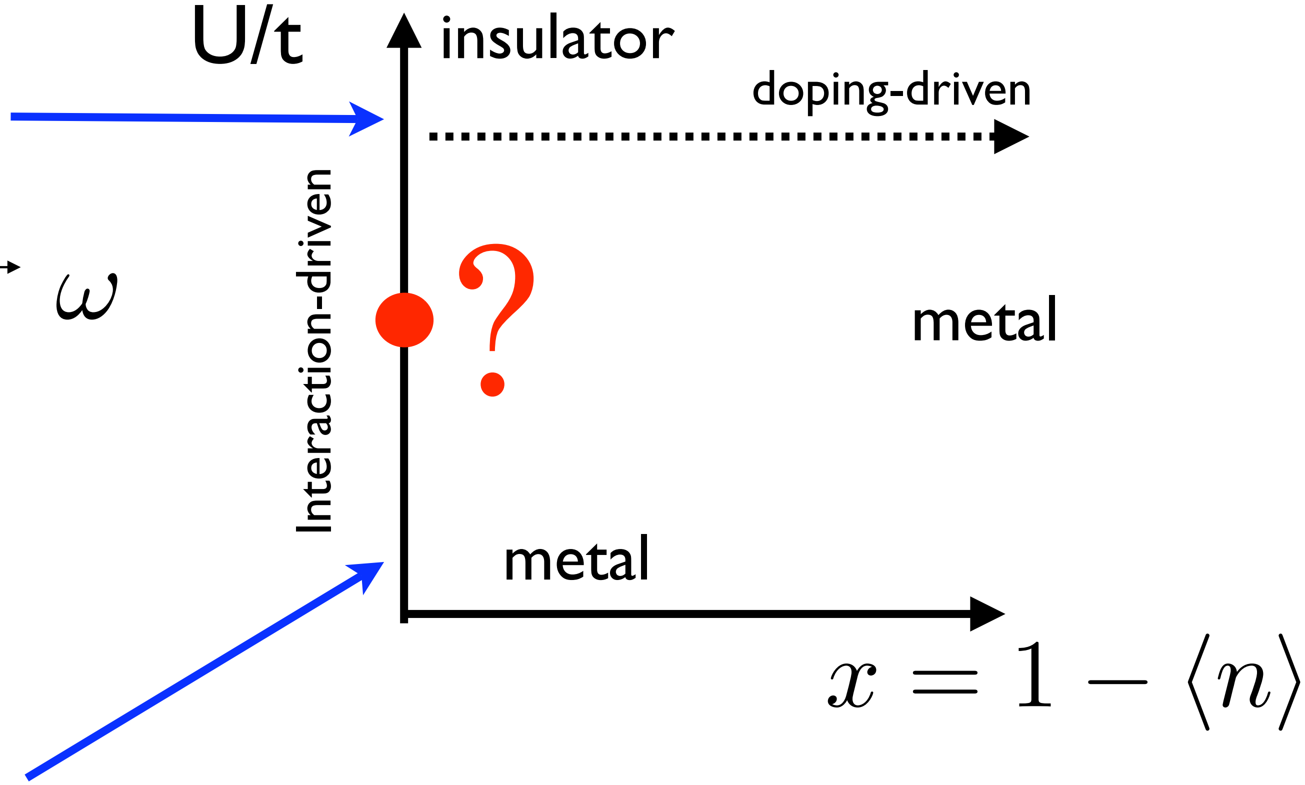
Mott transition (2)

- An intermediate coupling problem

➡ How is the metal destroyed close to a Mott transition ?

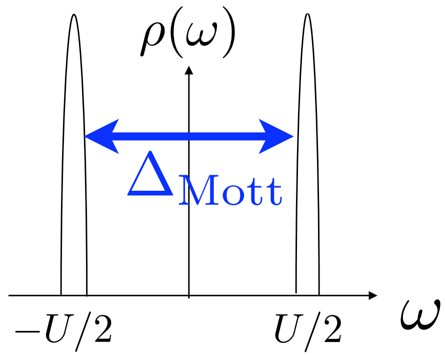
$$G(i\omega_n)_{\mathrm{at}} = \frac{1/2}{i\omega_n + U/2} + \frac{1/2}{i\omega_n - U/2}.$$

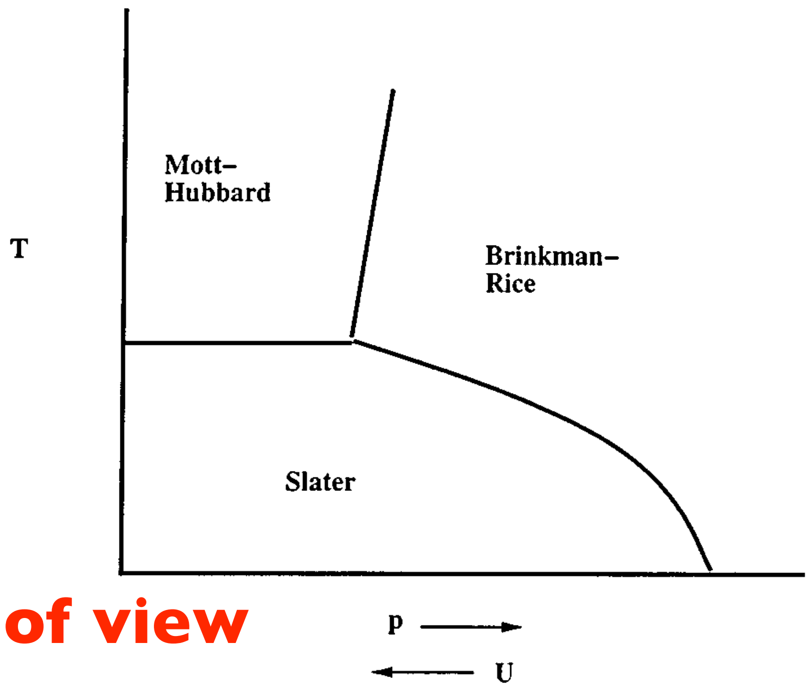




Simple mechanisms for Mott transition

- Brinkman-Rice
  - Destruction of the Fermi liquid. $Z \to 0, m^* \to \infty$
  - Simple theory : slave bosons.
- Mott-Hubbard
  - Closure of the Mott gap. $\Delta_{\mathrm{Mott}} \to 0$
- Slater
  - AF order.
    Reduction of the Brillouin zone.

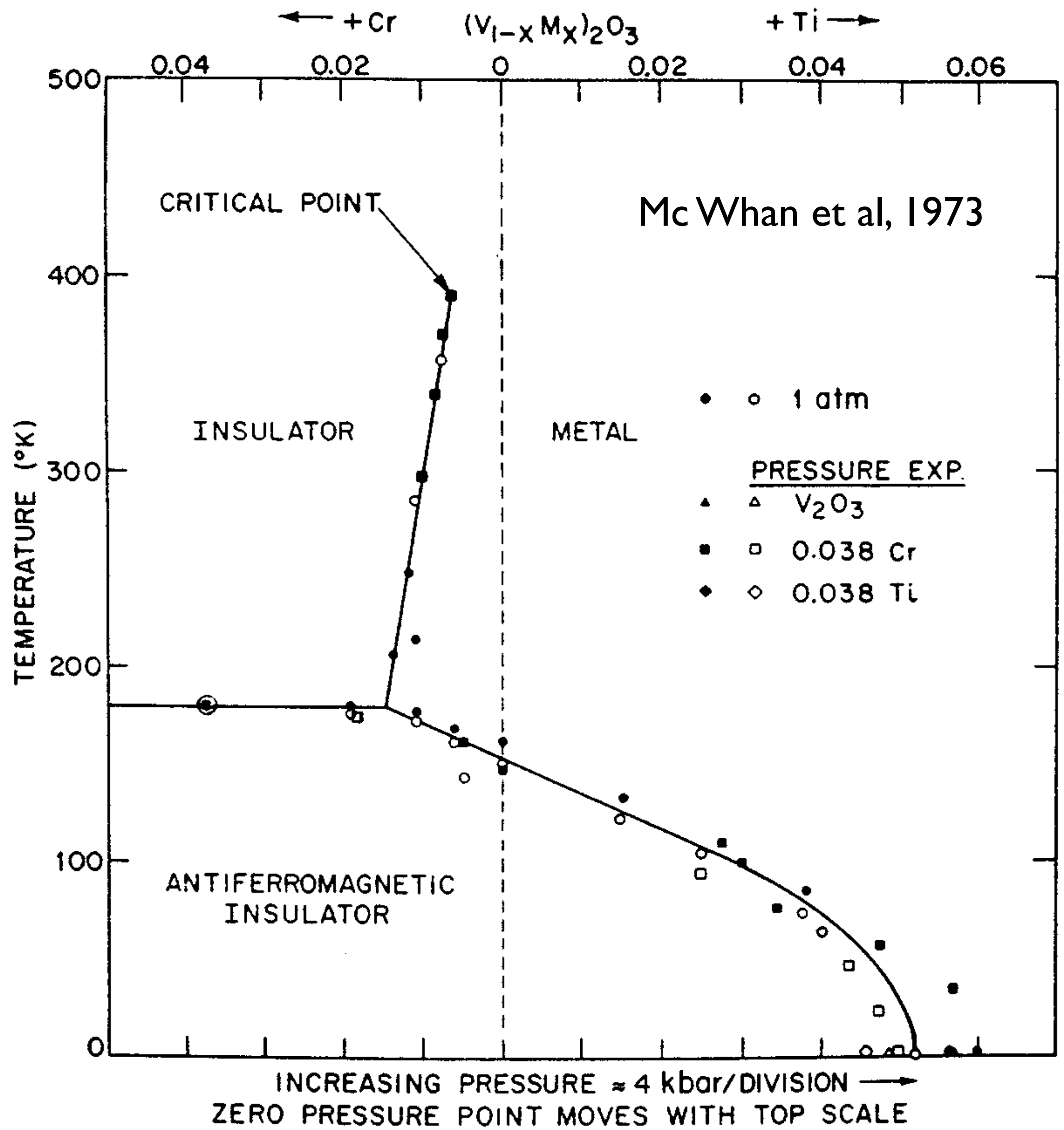




DMFT will unify these points of view

What about experiments ?

Experiments : V_2O_3



- Lattice size changes at transition.
- Early theory : *C.Castellani et al. PRL 43 1957 (1979)*

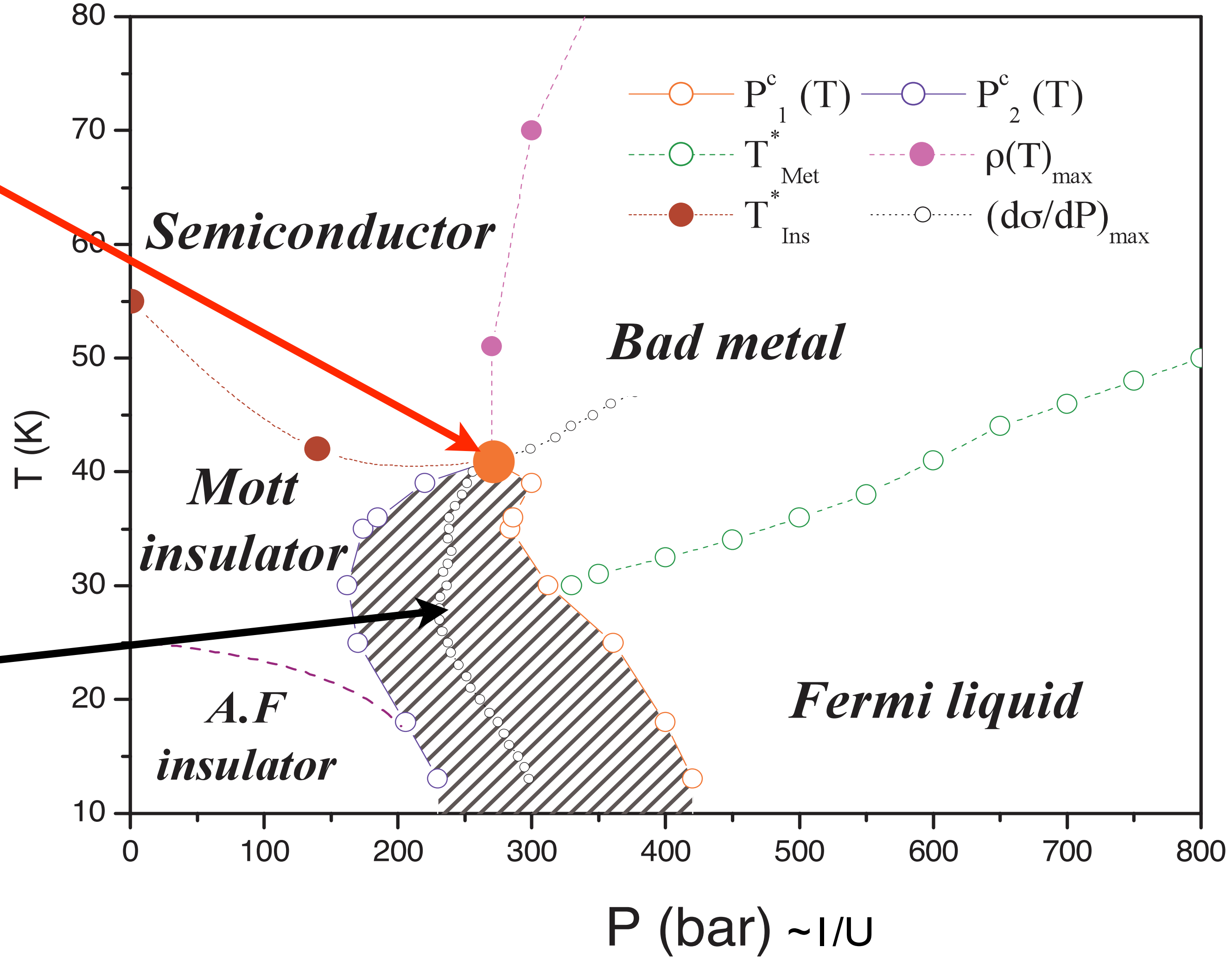
First order transition of purely electronic nature ?

Organics (resistivity measurements)

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

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

Critical Point



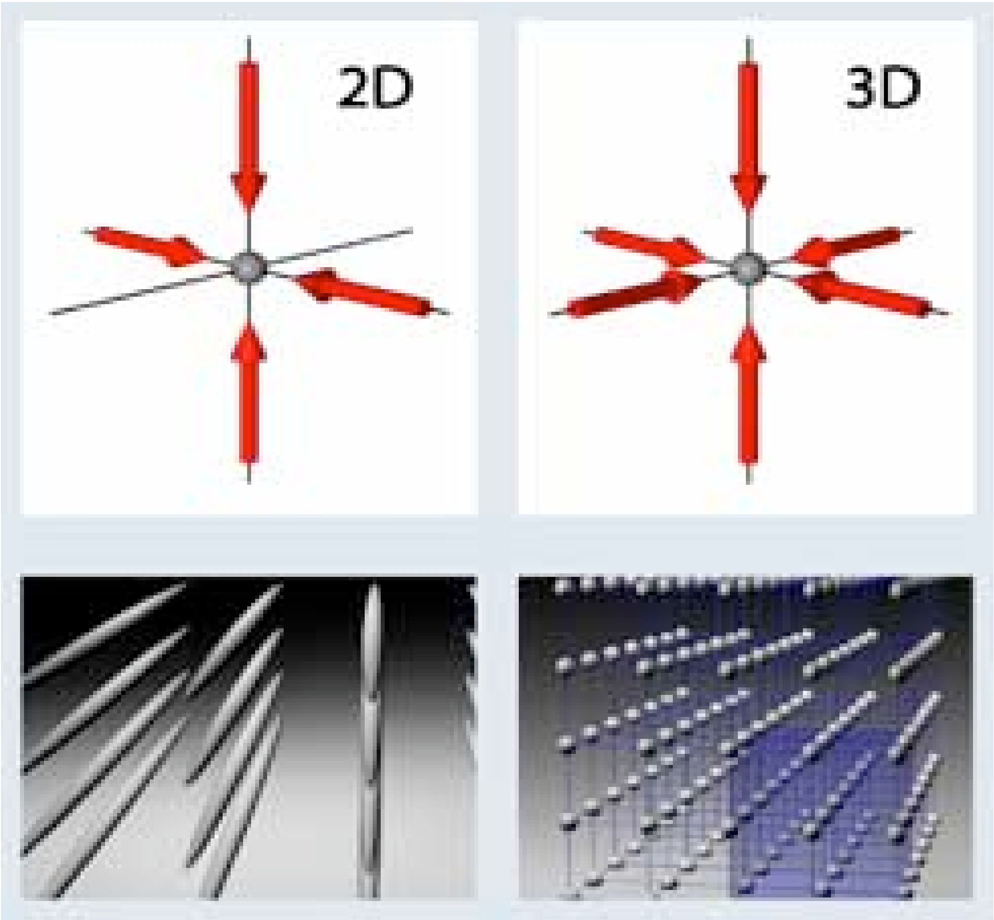
First order transition

P. Limelette, P. Wzietek, S. Florens, A. Georges, T.A. Costi, C. Pasquier, D. Jérome, C. Meziere, P. Batail PRL 91, 016401 (2003)

Mott transition in ultra-cold atoms (I)

- Controled realisation of (bosonic) Hubbard model in optical lattices *(Jaksch et al, PRL 81 (1998) 3108)*

Standing wave with lasers



$$V_{opt}(\vec{r}) = V_0 \sum_{i=1}^{3} \sin^2(k_L\, x_i)$$

$$k_L = \frac{2\pi}{\lambda}; \quad \lambda = \text{wavelength}$$

↓ *Wannier basis*

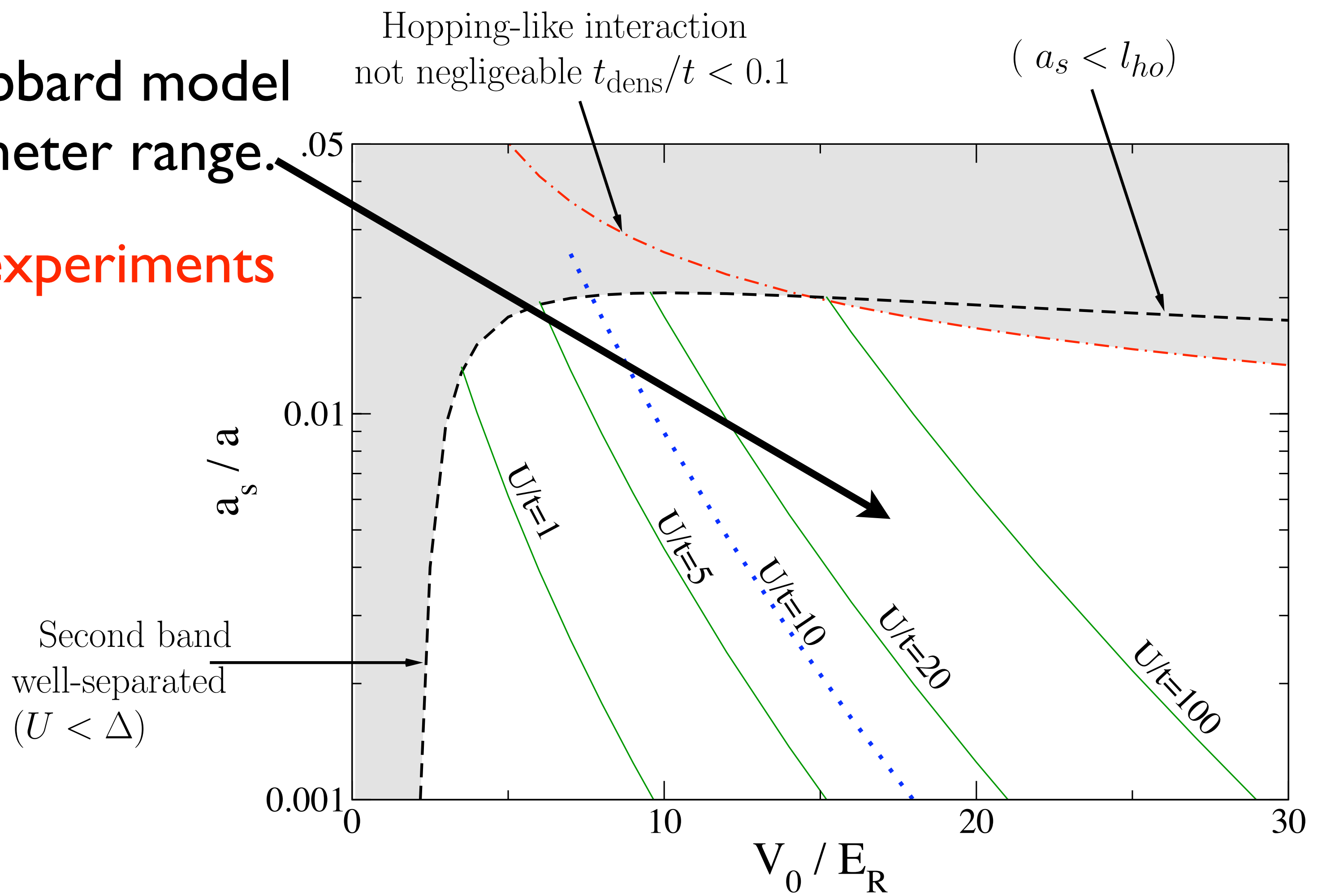
Bosonic Hubbard model

$$H = -\underbrace{\sum_{i,j} t_{ij} b_i^\dagger b_j}_{\text{Optical Lattice}} + \underbrace{U \sum_i n_i(n_i - 1)}_{\text{Feshbach resonance}}$$

- U/t tunable in experiments

Mott transition in ultra-cold atoms (2)

- Mapping to Hubbard model for some parameter range.
- U/t tunable in experiments

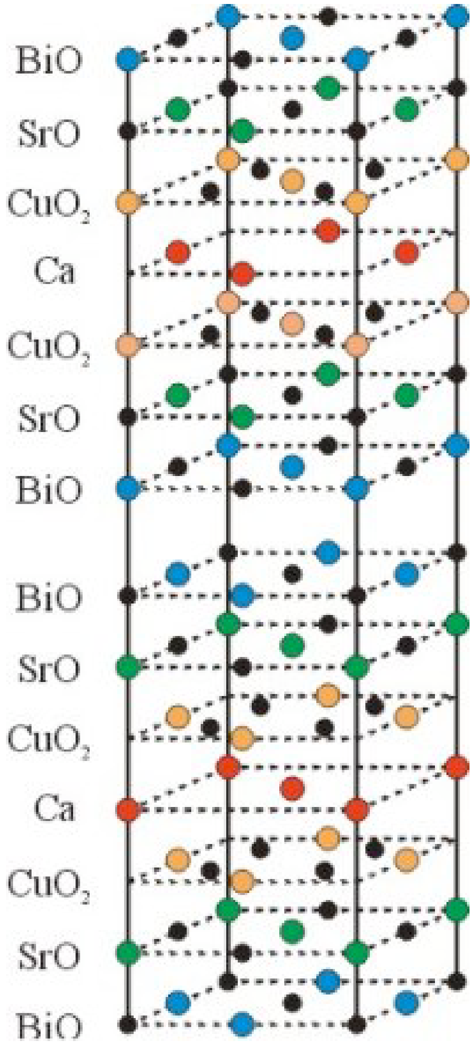


- Observation of the Mott transition by varying the depth of the optical potential *(M. Greiner et al., Nature 2002, vol 415 p 39).*

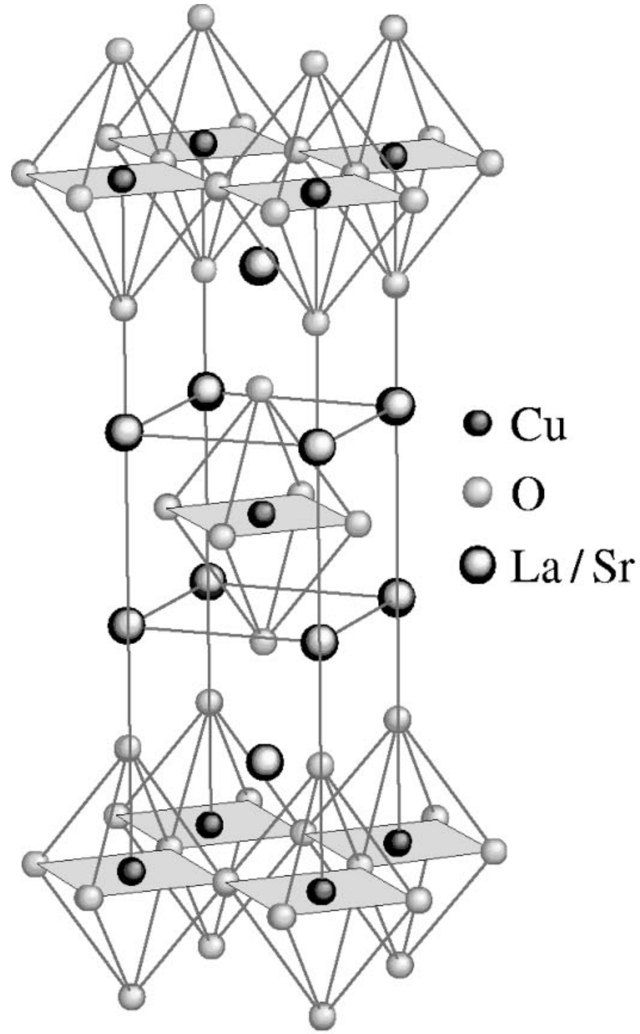
Doping driven Mott transition

High temperature superconductors

- A family of copper oxides: $\mathrm{La}_{2-x}\mathrm{Sr}_x\mathrm{CuO}_4,\ \mathrm{Bi}_2\mathrm{Sr}_2\mathrm{CaCu}_2\mathrm{O}_{8+\delta}$, ...

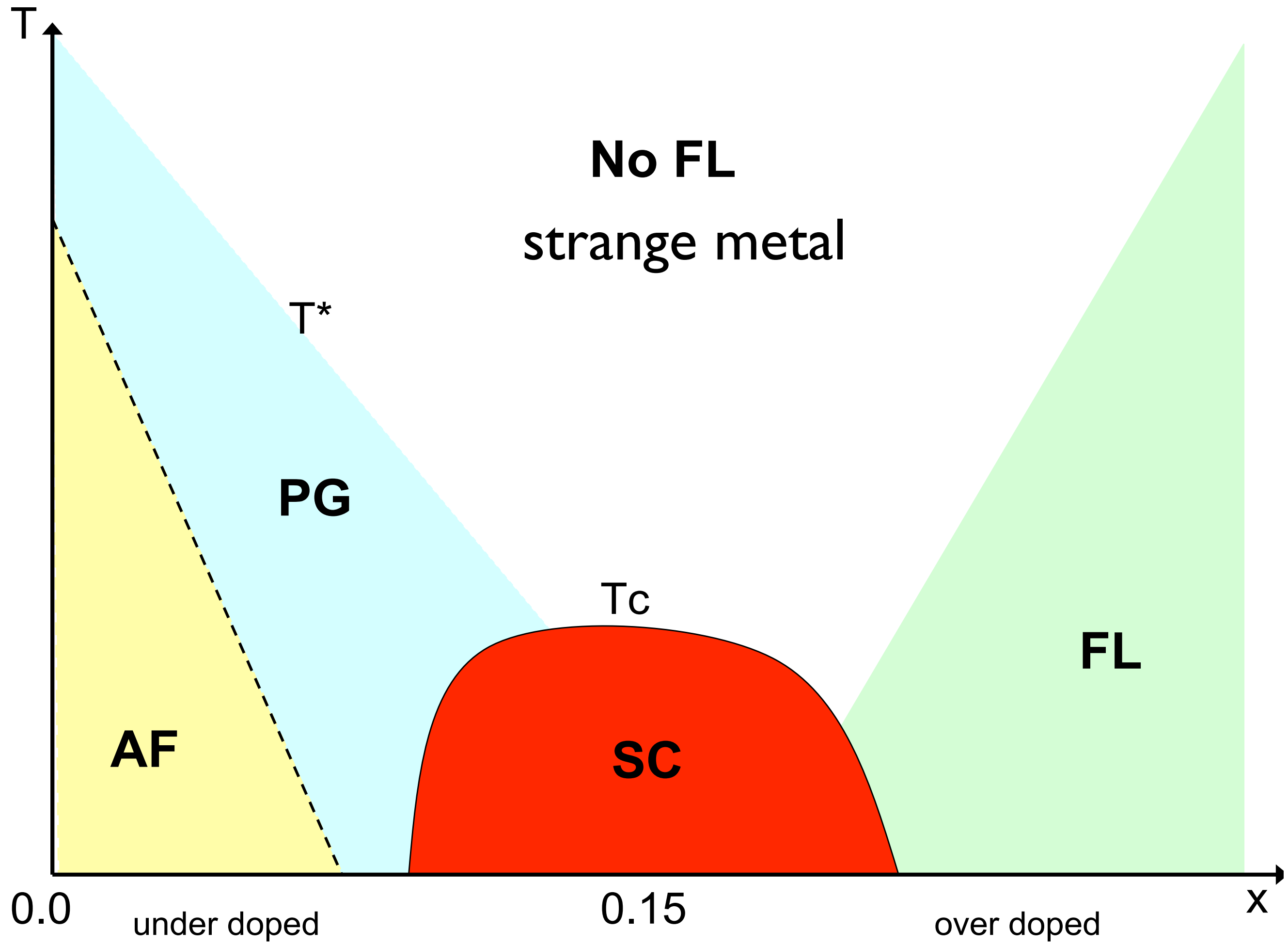


Cu-O plane structure



High temperature superconductors

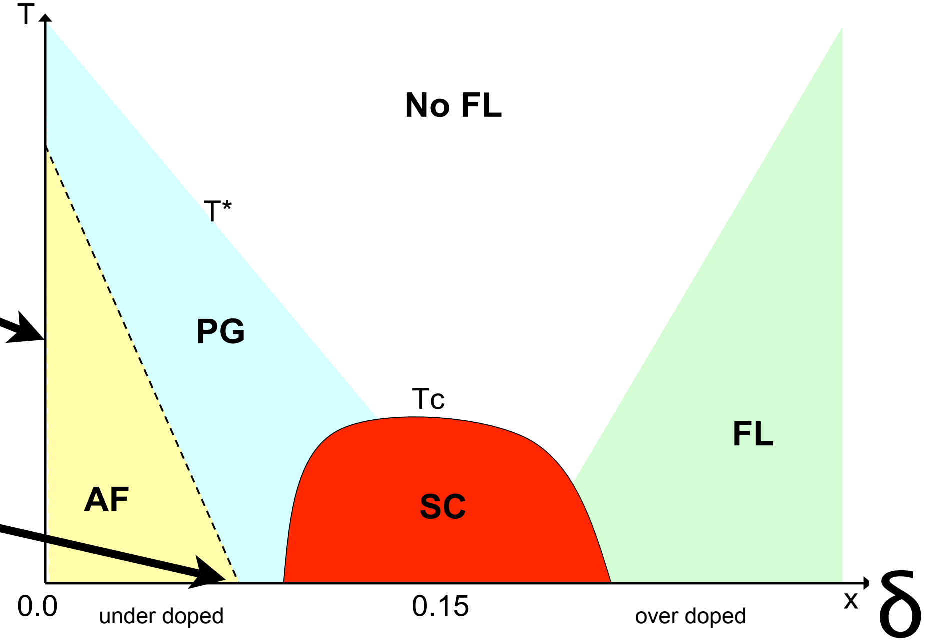
- A generic phase diagram, with 5 regions :



Parent compound is a Mott Insulator.

δ=0 : AF Mott insulator
J = 1500K

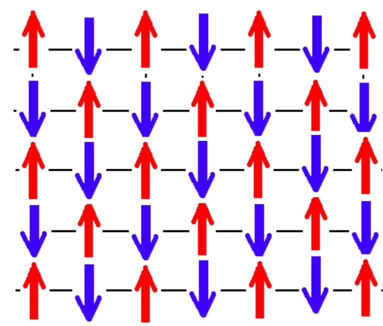
Quickly destroyed at small δ



Neutron scattering

- detect magnetic order
- mesure spin susceptibility :

$$\chi(k,\omega) \propto \int dxdte^{i(kx-\omega t)}\langle S(t,x)S(0,0)\rangle$$



AF order

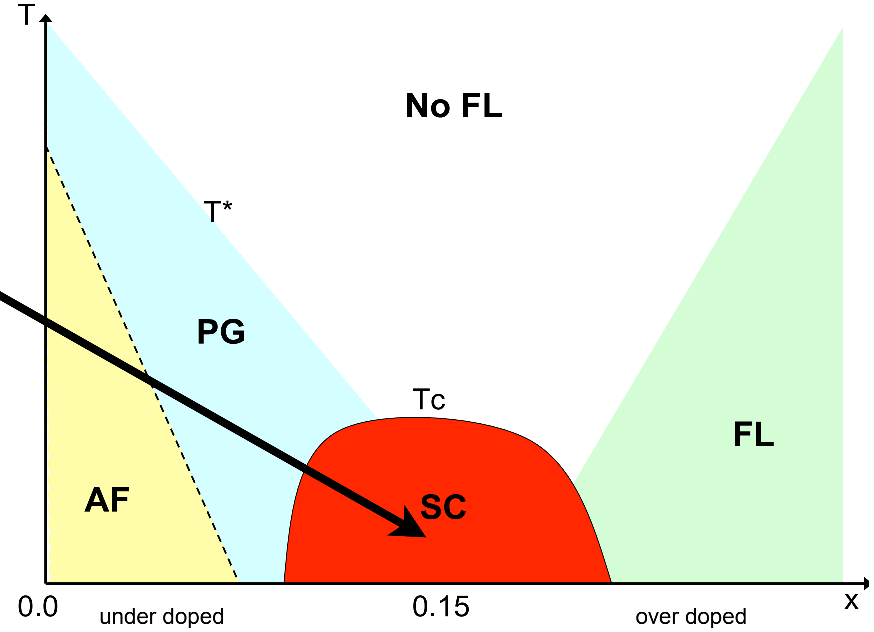
Superconducting phase

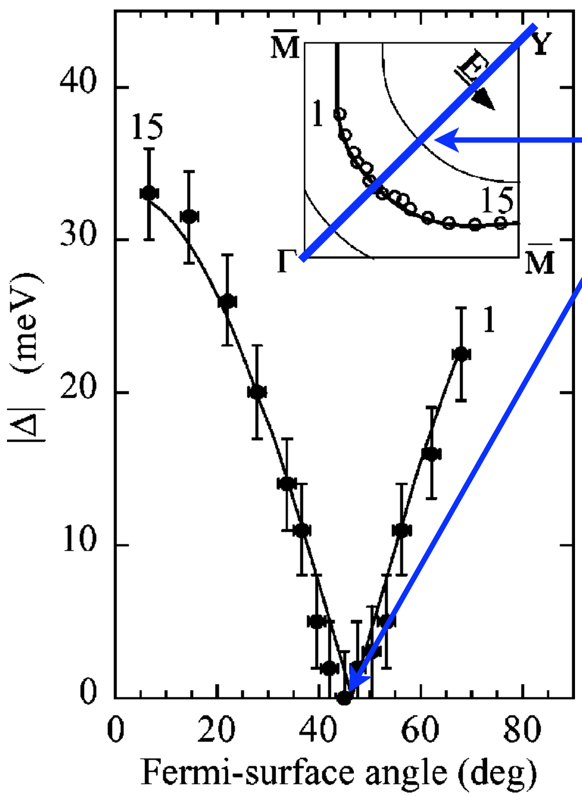
- Cooper pairs (as in BCS)
- d-wave gap and order parameter

$$\Delta(k) \propto \Delta_0 \left(cos(k_x) - cos(k_y) \right)$$

- Deviation from BCS: (?)

$$\Delta_0(x) \not\propto T_c(x)$$



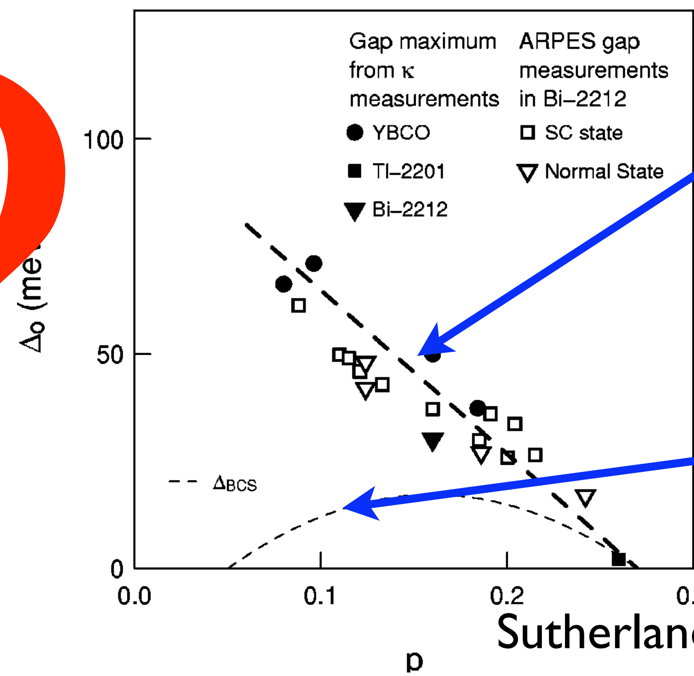


Nodal direction

← ARPES

Ding et al, 1996

?



T*

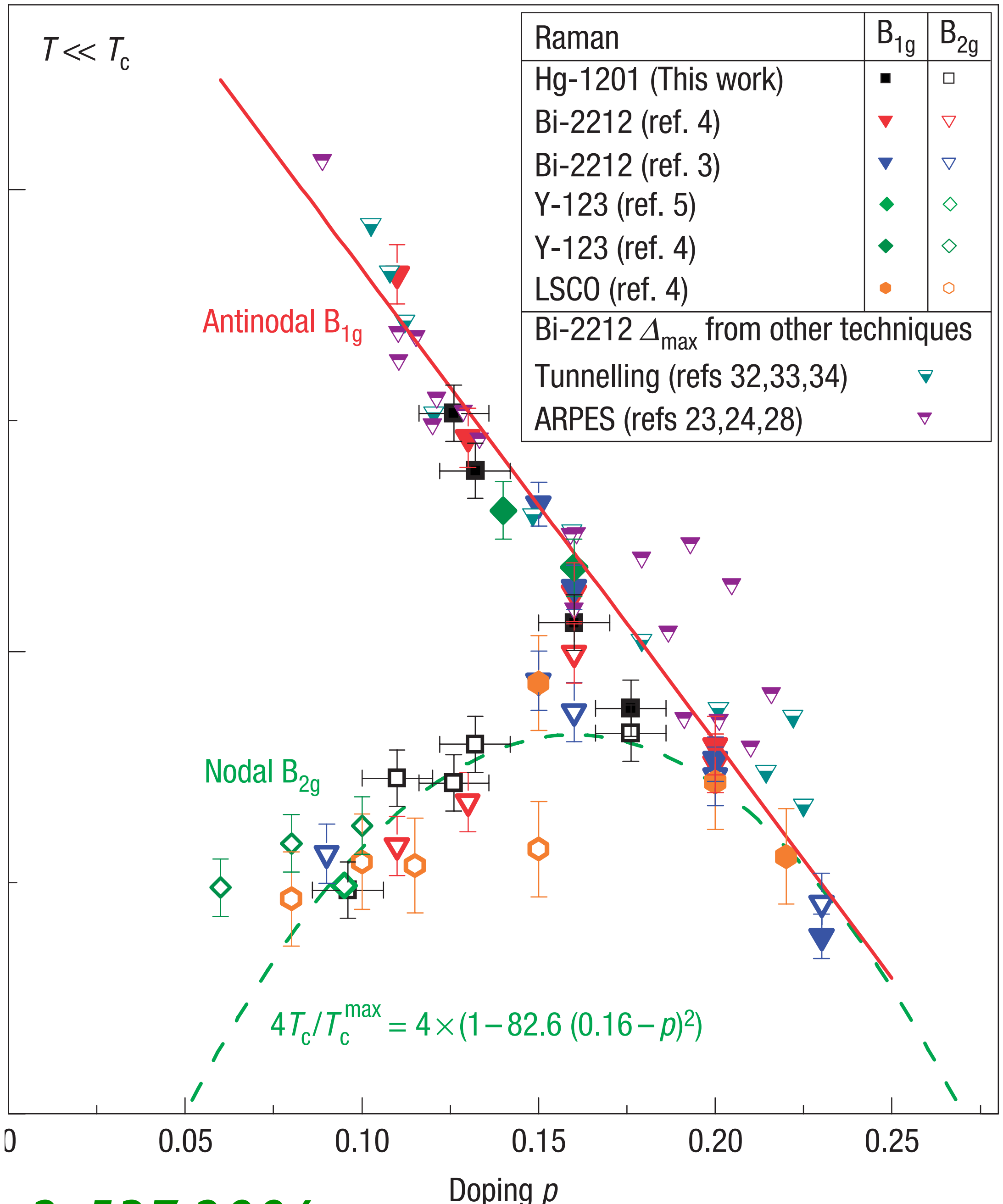
Tc

Sutherland, PRB2003

Two energy scales in SC phase

- Raman experiments.
- Mesure the gap around the node and at the antinode.

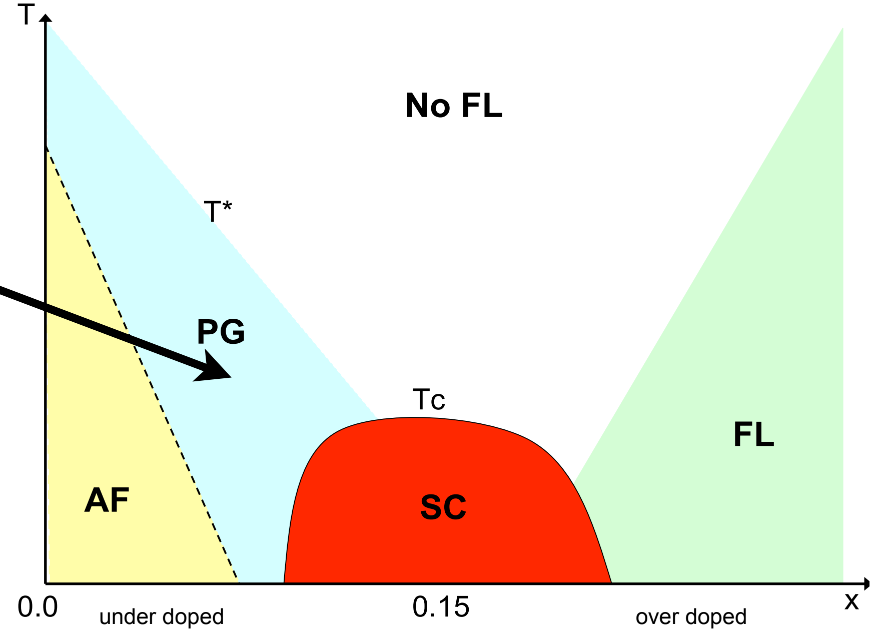
Lecture 3

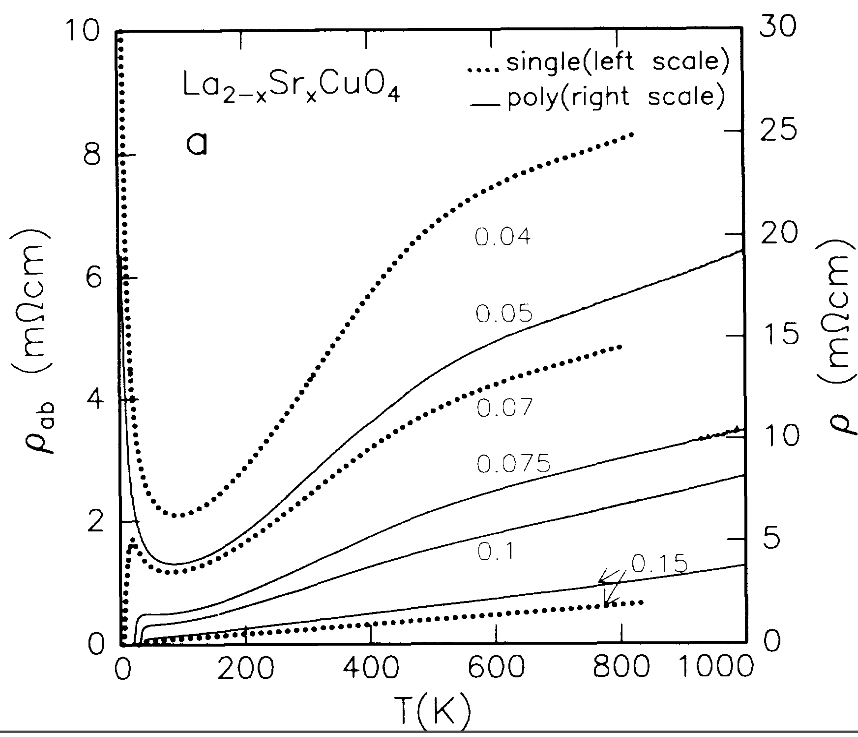


M. LeTacon et al., Nature Physics, 2, 537,2006

Pseudo-gap region (I)

- *<u>Pseudo-gap</u>* for T<T* (crossover) observed in various quantities : transport, NMR, specific heat ...





In-plane resistivity

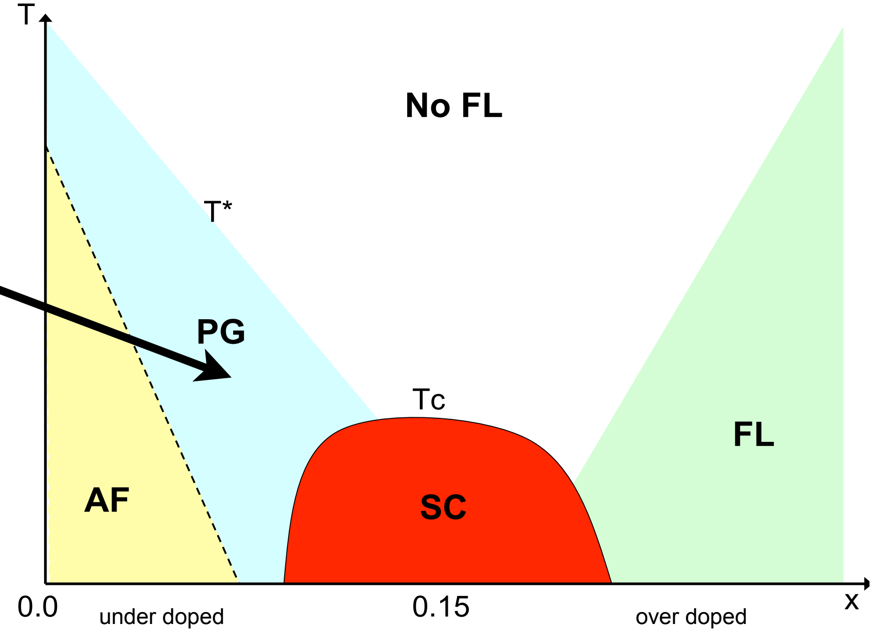
Takagi, PRL 92

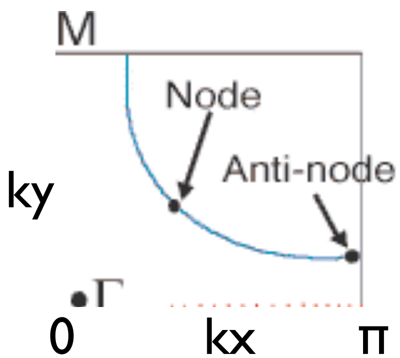
Pseudo-gap region (II)

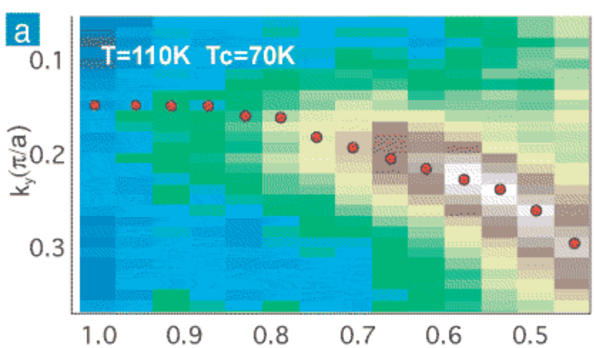
- Fermi “arcs” (ARPES)

➡ Fermi liquid below and above coherence scale ? Variations of along the Fermi surface of

$$Z, m^*, T_{\rm coh}$$

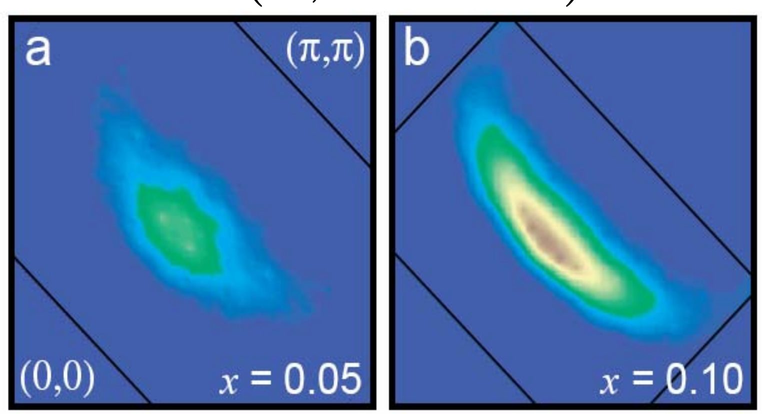






Bi2212 : Kanigel et al. 2,447 (2006)

$$A(k, \omega = 0^+)$$

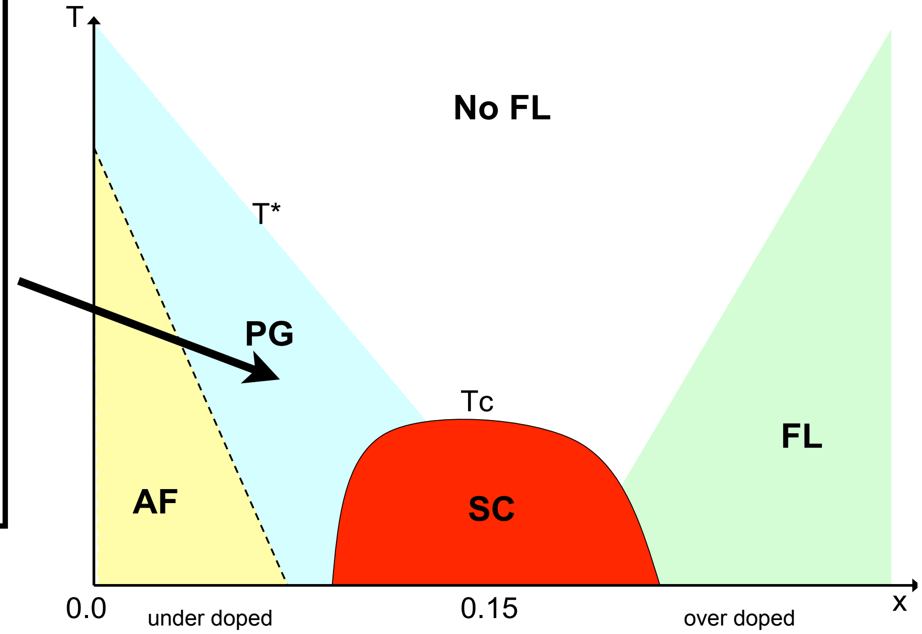


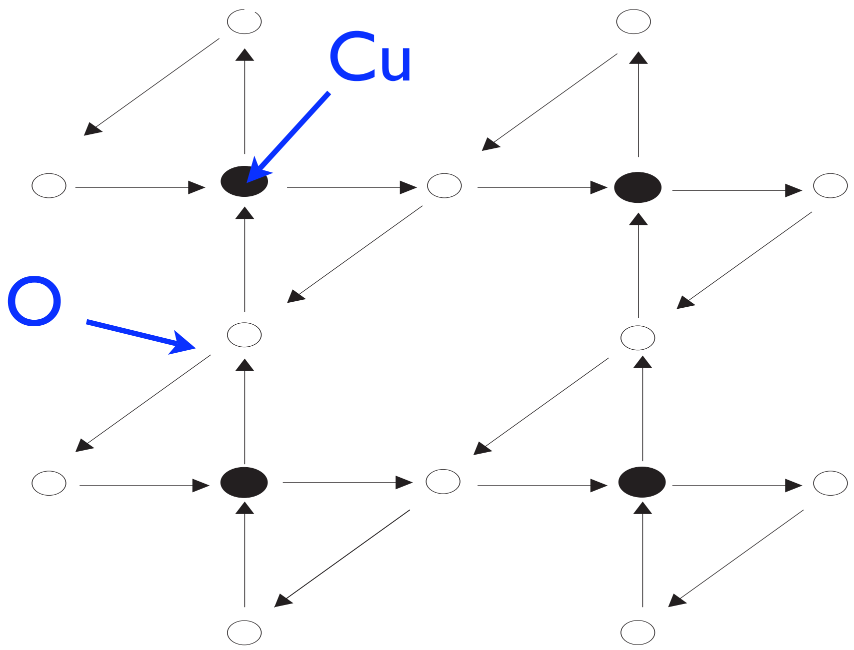
Shen et al. Science 307, 901 (2005)

Pseudo-gap region (III)

<u>*An ordered phase ?*</u>

- Polarized neutrons diffraction :
B. Fauque, Y. Sidis, V. Hinkov, S. Pailhes, C.T. Lin, X. Chaud, Ph. Bourges, PRL 96, 197001 (2006)
- Hidden order : local current ?
(C.Varma e.g. cond-mat/0507214)



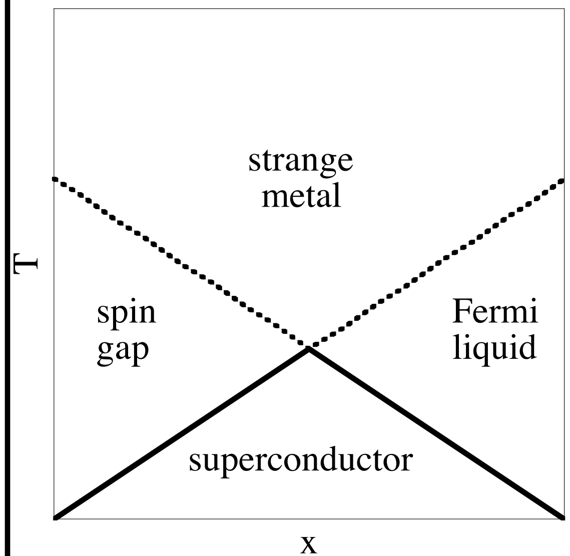


Local current in the unit cell (Varma's proposal)

Beyond Hubbard model ?

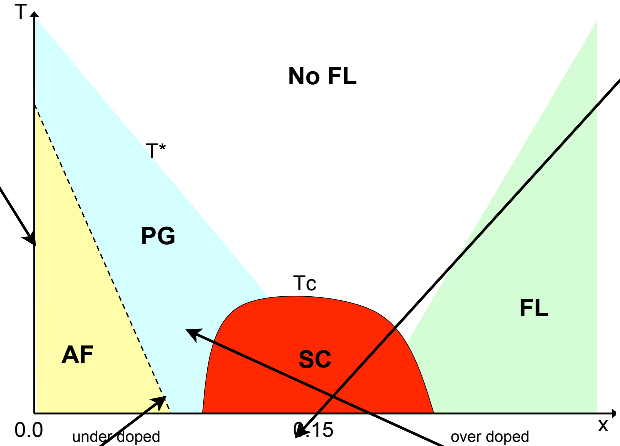
Many theoretical approaches !

Doped Mott insulator

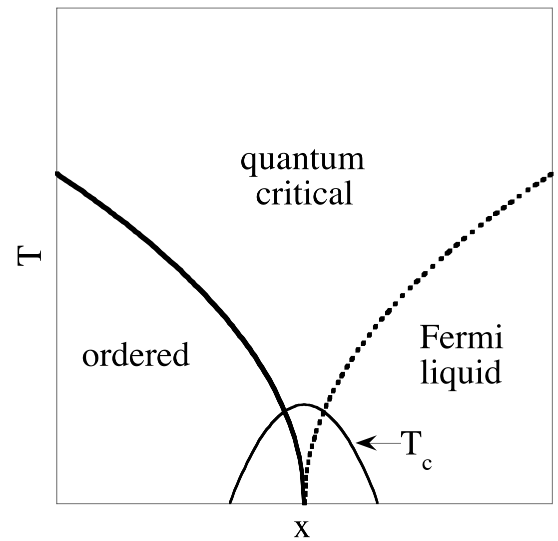


- RVB (Anderson 87)
- Kotliar-Liu (88)

Prediction of d-SC !



Quantum phase transition hidden below the SC.



Critical AF fluctuations ?

?

Cooper Pair fluctuations ?

Mott transition : what should a theory describe ?

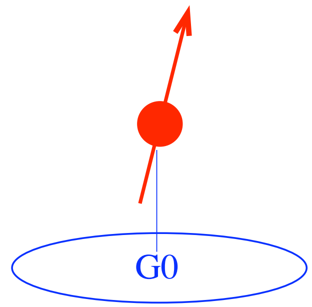
- Mechanism of the Mott transition (phase diagram, first order transition and critical point ?).
- How is a metal (or d-SC) destroyed close to Mott transition ?
- Various microscopic models (e.g. many bands)
- Various competing orders : AF, d-SC, DDW, local currents (?)
- Variations of Z, m*, lifetime, coherence temperature versus T, δ and along the Fermi surface.
- Fermi liquid above coherence temperature (pseudogap in high Tc ?)
- Non trivial Mott insulators (frustrated magnets, RVB, VBS ?)

➡ Dynamical Mean Field Methods ?

Outline

1. Mott transition.
2. Quantum impurity models.
3. Introduction to Dynamical Mean Field Theory

Quantum impurity models



- Isolated magnetic impurity in a metal.
- *Kondo model*

$$H = \sum_{k\sigma\alpha} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + J_K \overrightarrow{S} \cdot \sum_{\substack{kk' \\ \sigma\sigma'}} c^\dagger_{k\sigma} \vec{\sigma}_{\sigma\sigma'} c_{k'\sigma'}$$

<u>*Schrieffer-Wolf*</u>

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

- *Anderson model*

$$H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{\sigma} \epsilon_d d^\dagger_\sigma d_\sigma + U n_{d\uparrow} n_{d\downarrow} + \sum_{k\sigma} V_{k\sigma} \left(c^\dagger_{k\sigma} d_\sigma + h.c. \right)$$

They are correlated many-body problems.

How to solve them ? See Lecture 2.

Action versus Hamiltonian form

- An equivalent formulation obtained by integrating the fermions

$$H = \sum_{k\sigma} \epsilon_{k\sigma} c^\dagger_{k\sigma} c_{k\sigma} + \sum_{\sigma} \epsilon_d d^\dagger_\sigma d_\sigma + U n_{d\uparrow} n_{d\downarrow} + \sum_{k\sigma} V_{k\sigma} \left(c^\dagger_{k\sigma} d_\sigma + h.c. \right)$$

$$\updownarrow$$

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

Hybridisation $\longrightarrow$ $\Delta_\sigma(i\omega_n) \equiv \sum_k \frac{|V_{k\sigma}|^2}{i\omega - \epsilon_{k\sigma}}$

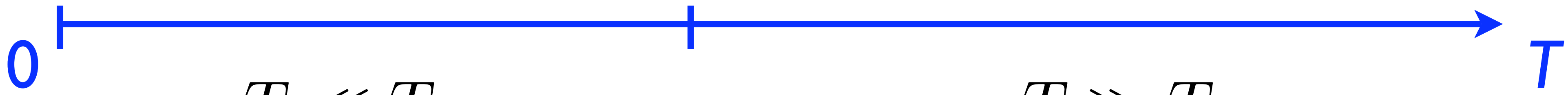
Bath $\longrightarrow$ $G^{-1}_{0\sigma}(i\omega_n) \equiv i\omega_n + \epsilon_d - \Delta_\sigma(i\omega_n)$

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

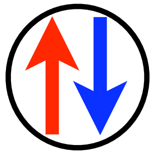
Kondo effect

- Screening of the Kondo impurity by the metallic bath

Kondo temperature $T_K \sim De^{-1/J\rho_0}$ dos at the Fermi level



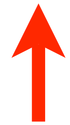
$T \ll T_K$



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

- Local Fermi liquid (Nozières)
- Strong coupling picture : singlet

$T \gg T_K$



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

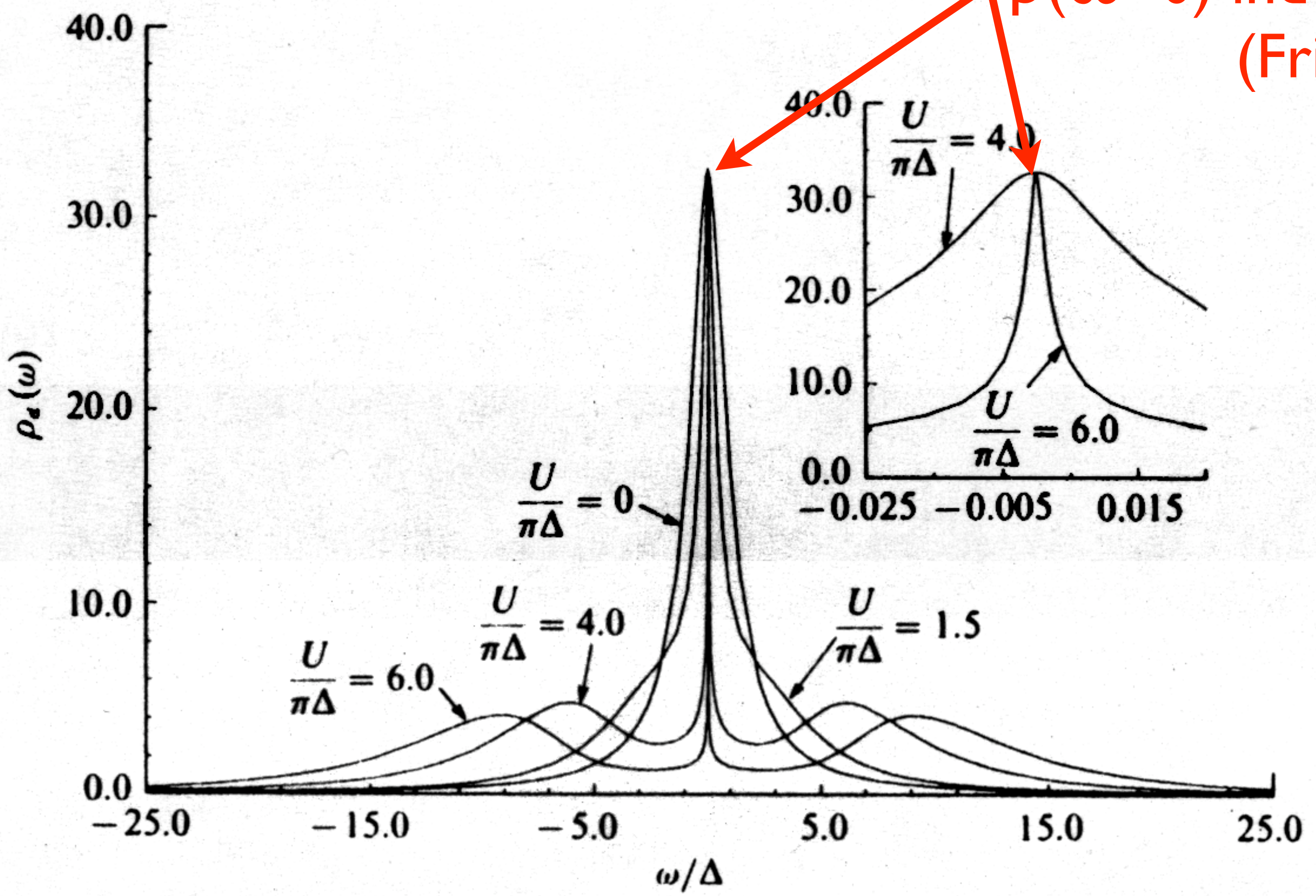
- Free spin (Curie law)

Kondo-Abrikosov-Suhl resonance

- Sharp resonance in the spectral function of *d* at the Fermi level, of width T_K , for $T \ll T_K$

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

$\rho(\omega=0)$ independent of U (Friedel)



- QP peak, Hubbard bands analogous to lattice.
- With DMFT, this analogy transformed into a formalism

Outline

1. Mott transition.
2. Quantum impurity models.
3. Introduction to Dynamical Mean Field Theory

Mean Field Theory

- *Ising model* (Weiss) : A single spin in an effective field.
- Derivation : e.g. large dimension limit on hypercubic lattice.

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

Generalisation for quantum models ?

Dynamical Mean Field Theory

- *Ising model* (Weiss) : A single spin in an effective field.
- *Quantum spin glass* (Bray-Moore, 80)

  A single quantum spin in a fluctuating field (in imaginary time)

  Close to a QCP, we must keep the (long time) dynamics.
- *Fermionic Hubbard model* (Kotliar-Georges, 92)

  Anderson impurity model coupled to an effective band

  determined self-consistently

$$H = \underbrace{\epsilon_0 \sum_{\sigma=\uparrow,\downarrow} c_\sigma^\dagger c_\sigma + U n_\uparrow n_\downarrow}_{\text{Local site}} + \underbrace{\sum_{k,\sigma=\uparrow,\downarrow} V_k d_{k\sigma}^\dagger c_\sigma + h.c. + \sum_{k,\sigma=\uparrow,\downarrow} \epsilon_k d_{k\sigma}^\dagger d_{k\sigma}}_{\text{Coupled to an effective electronic bath}}$$

DMFT equations (1 site, 1 orbital Hubbard)

Lecture 2

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

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

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

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

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

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

$$G_c(\tau) = -\langle T c(\tau) c^\dagger(0) \rangle_{S_{eff}}$$

$$S_{\text{eff}} = -\int_0^\beta c^\dagger_\sigma(\tau) G_0^{-1}(\tau - \tau') c_\sigma(\tau') + \int_0^\beta d\tau U n_\uparrow(\tau) n_\downarrow(\tau)$$

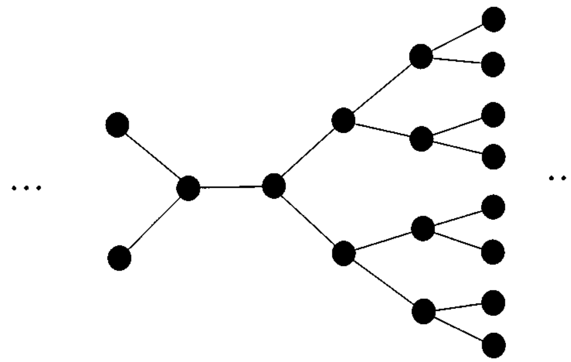
$$G_0(i\omega_n) = \mathcal{F}_{\text{lattice}}[G_c](i\omega_n)$$: Self-consistency condition

Solution of the quantum impurity model

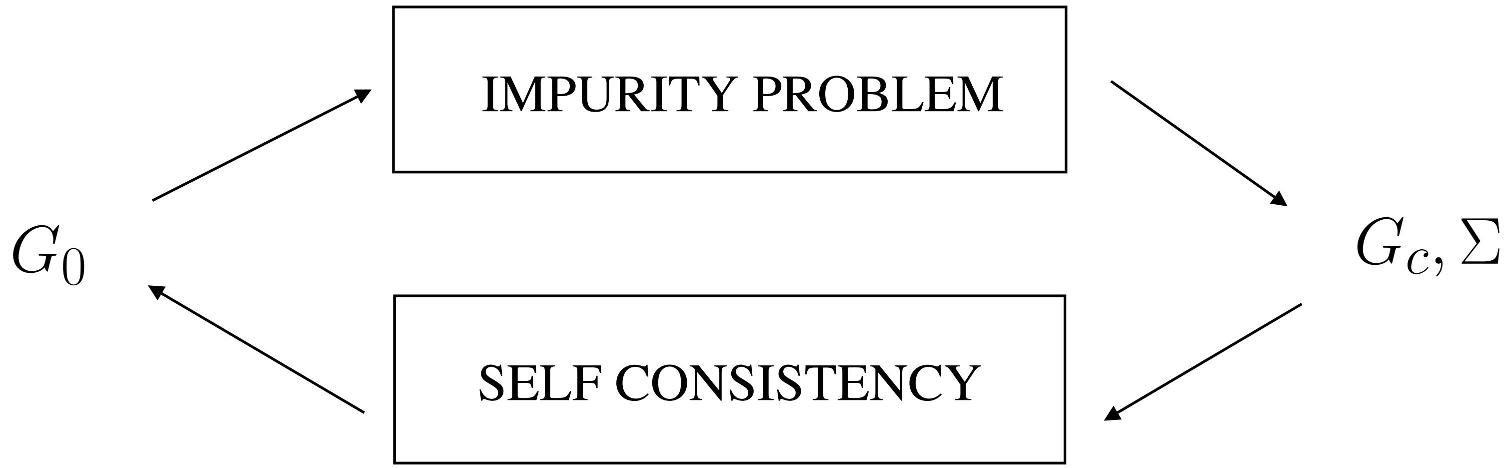
- Bethe lattice with connectivity (z→∞)

$$\Delta(i\omega_n) = t^2 G_c(i\omega_n)$$

$$G_0^{-1}(i\omega_n) = i\omega_n + \mu - \Delta(i\omega_n)$$



DMFT loop



- In practice, iterative loop is always convergent !
- *All the hard work in DMFT lies in the impurity solver !*
  See Lecture 2 for various methods to solve the impurity problem.

Lattice quantities in DMFT

- The self-energy on the lattice is local :

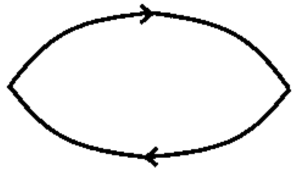
$$G_{\text{latt}}(k,\omega) = \frac{1}{\omega + \mu - \epsilon_k - \Sigma_{\text{latt}}(k,\omega)}$$

$$\Sigma_{\text{latt}}(k,\omega) = \Sigma_{\text{impurity}}(\omega) \equiv G_0^{-1} - G_c^{-1}$$

- Therefore effective mass and Z are related : $Z = \frac{m}{m^*}$
- G on the lattice is not local. There is a Fermi surface in metallic regimes.
- Finite temperature lifetime, Z are constant along the FS.

Resistivity calculation in DMFT

- One shows that there is no vertex correction : simple particle-hole buble (with full propagators) in current-current correlator.



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

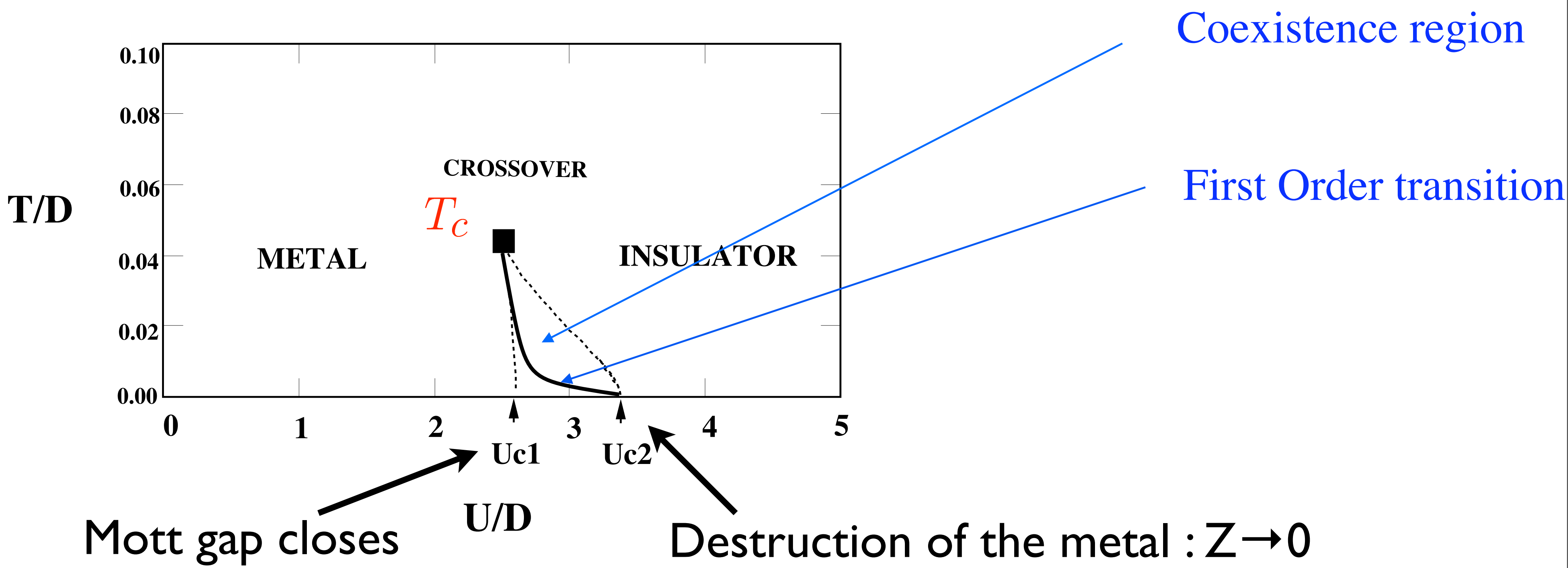
$$\mathrm{Re}\ \sigma(\omega + i0^+) = \pi \frac{e^2}{\hbar a d}\int_{-\infty}^{+\infty} d\epsilon \int_{-\infty}^{+\infty} d\nu\ D(\epsilon)\rho(\epsilon,\nu) \times \rho(\epsilon,\nu' + \omega)\,\frac{f(\nu) - f(\nu+\omega)}{\omega}$$

- Need a computation of $\Sigma(\omega)$ at real frequencies.

What does DMFT tell us about the Mott transition ?

Phase diagram

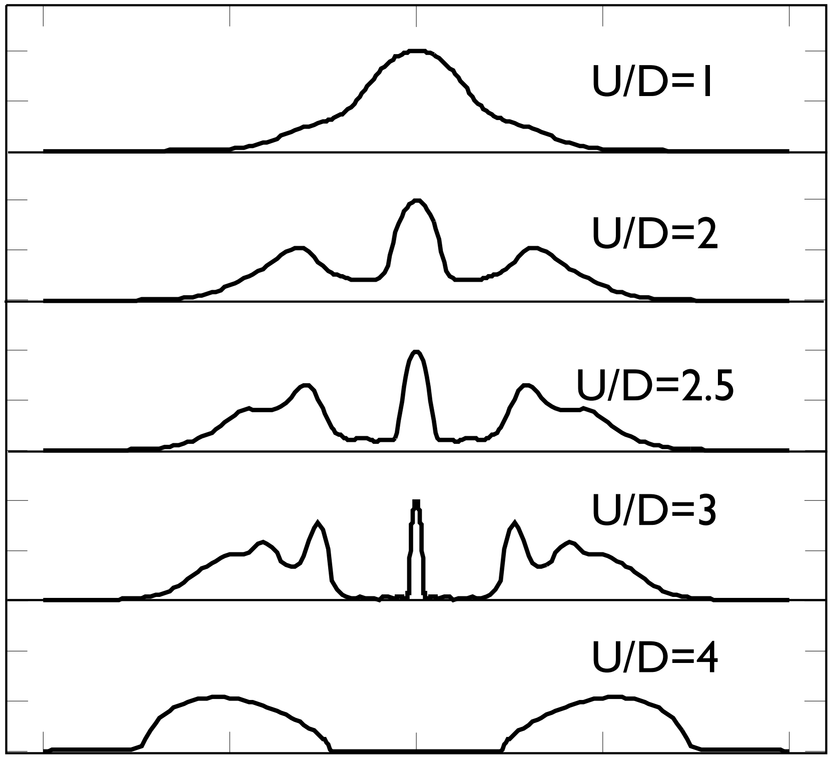
- Hubbard model at half-filling (δ=0). D is half-bandwidth.
- Frustrated model (paramagnetic phase).
  Frustration is essential, otherwise hidden by Néel phase.
  Self-consistency depends only on the d.o.s on the lattice.



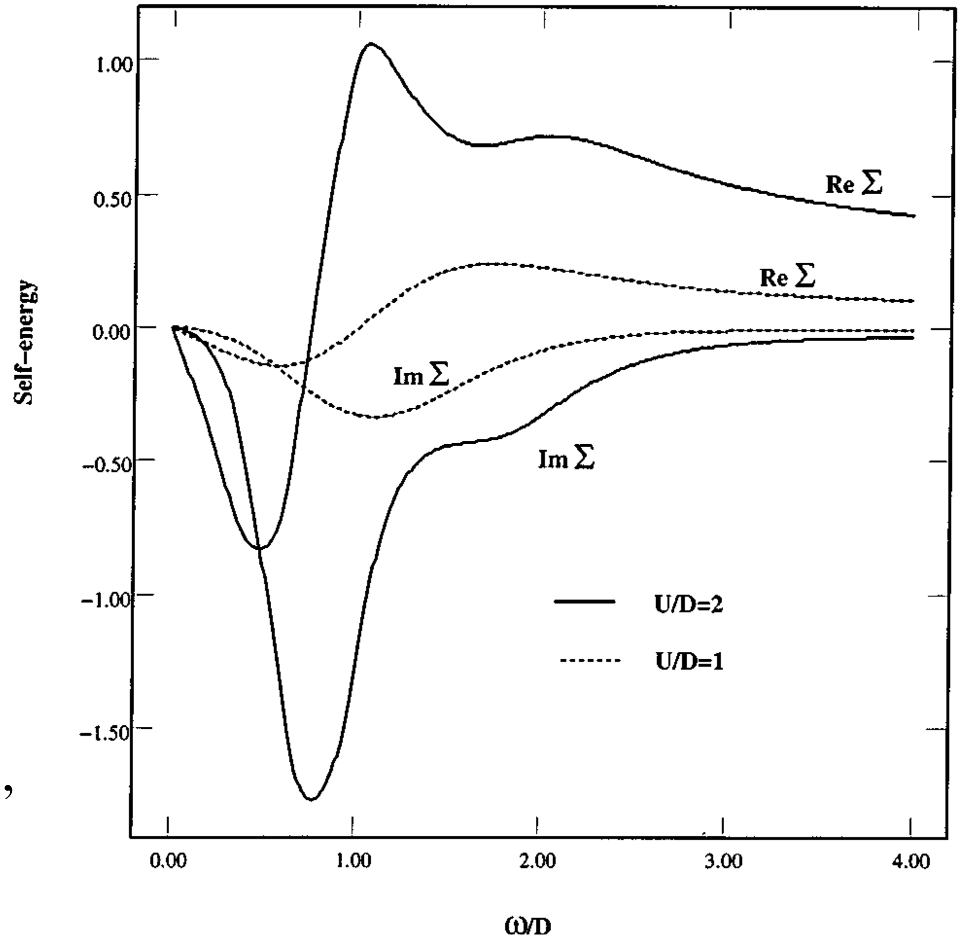
2 solutions

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

Spectral function



Self-energies in metal



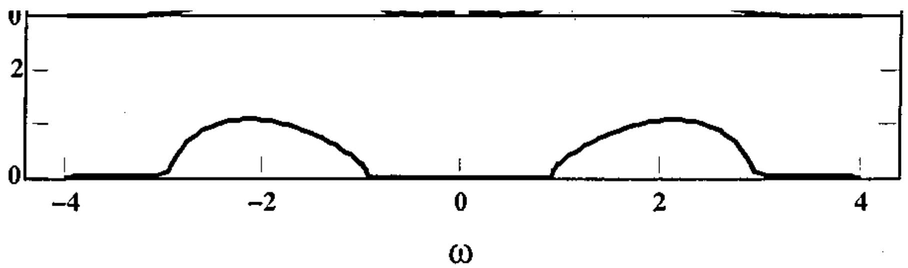
$$\mathrm{Re}\Sigma(\omega+i0^+) = U/2 + (1-1/Z)\omega + O(\omega^3),$$

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

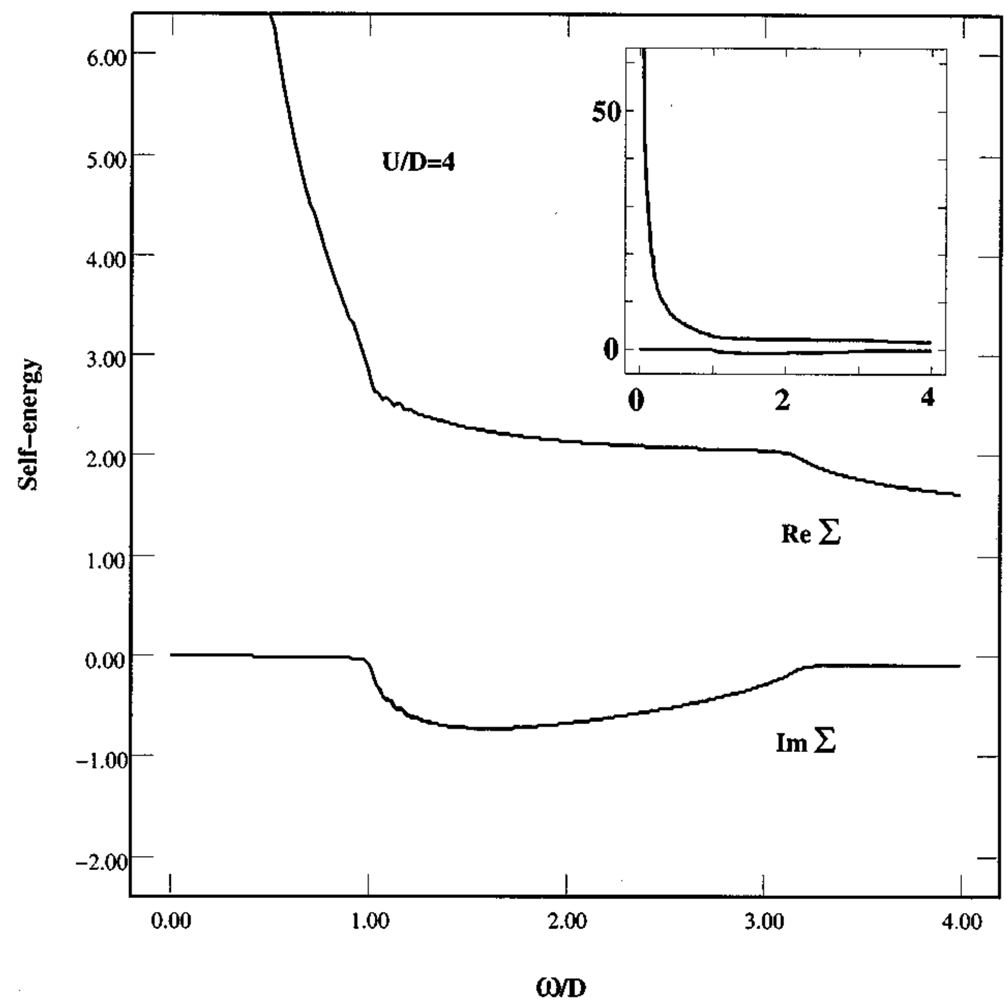
2 solutions

- Insulating solution : $\Delta(0) = 0$: gapped bath $\Rightarrow$ no Kondo effect

Spectral function (U/D=4)



Self-energies in insulator



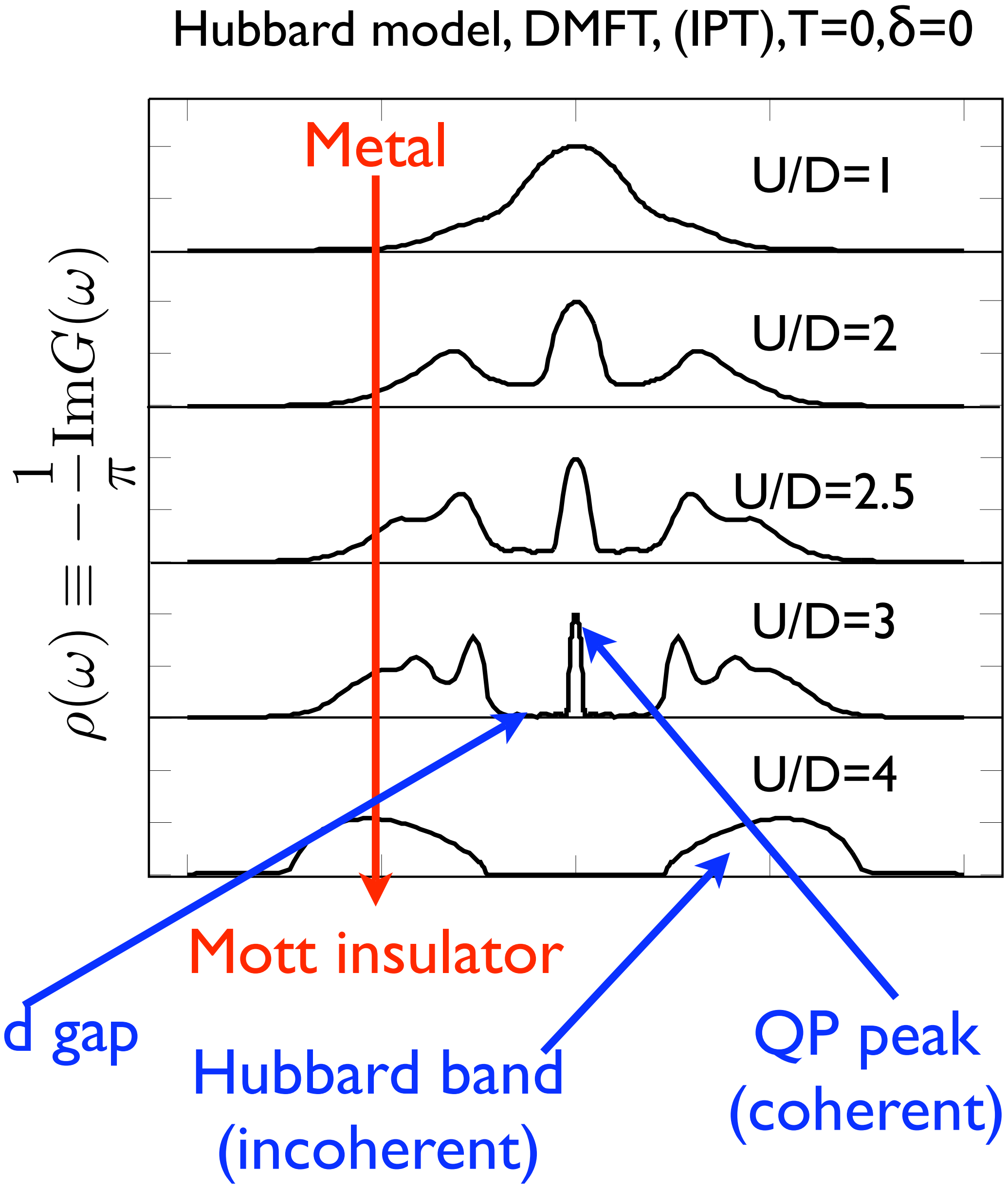
Atomic limit

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

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

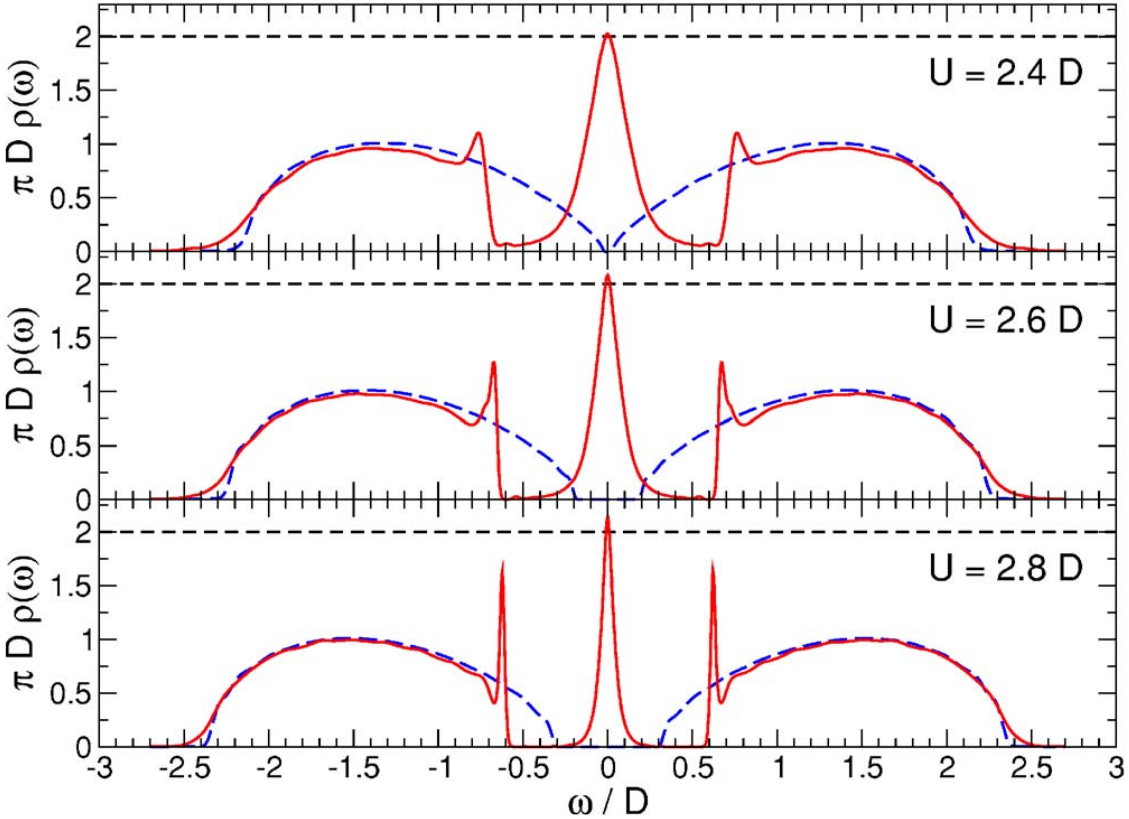
Why do we need a Dynamical Mean Field ?

- Fermi liquid with low coherence scale : $\epsilon_F^* = ZD$
- Coherent and incoherent part
- Transfer of spectral weight from low to high ω
- Beyond a low energy quasi-particle description (slave bosons)
- Price : solve a quantum impurity model.



A Kondo peak in a preformed gap

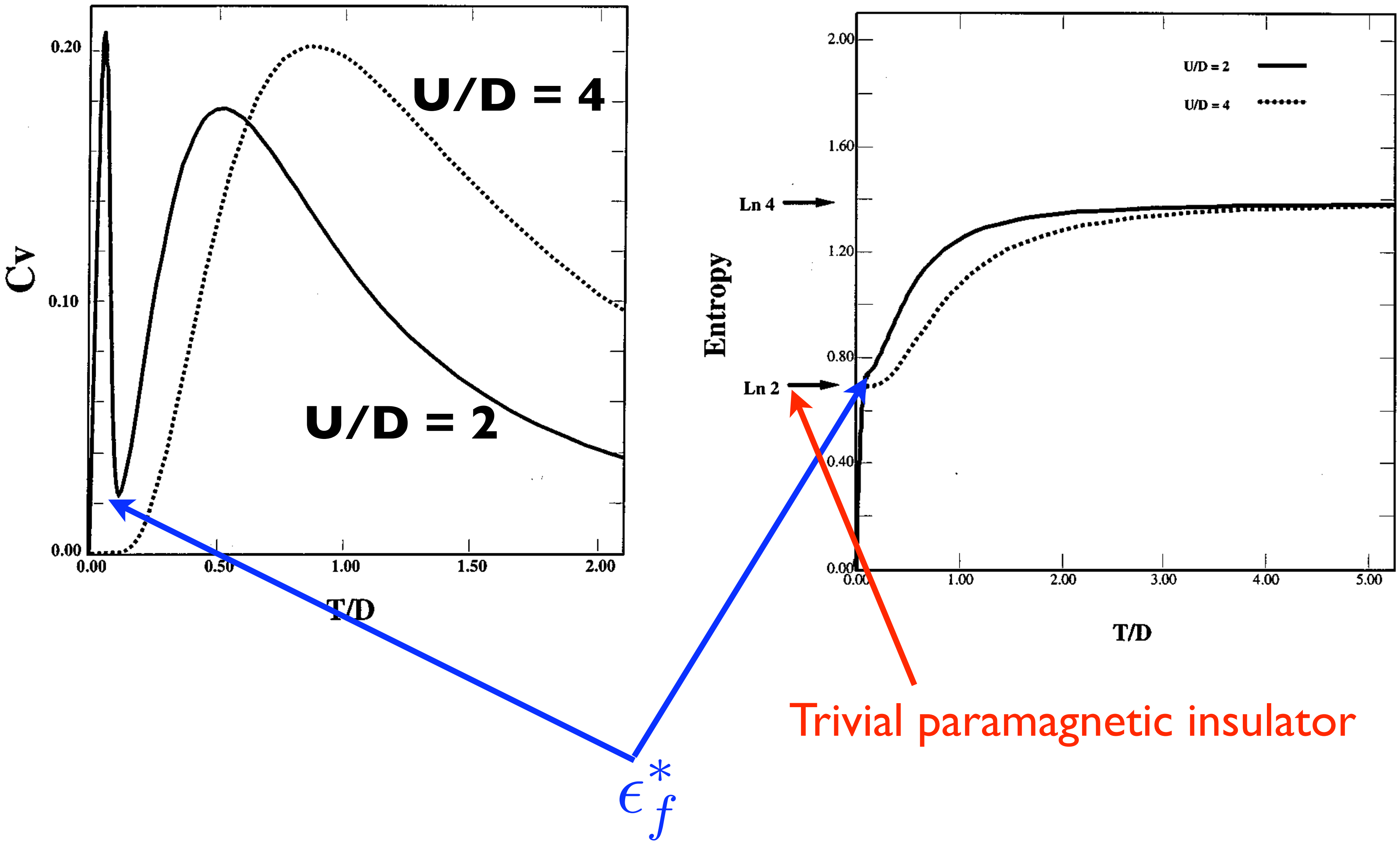
- *A. Georges, G. Kotliar, 1992*
- Clear in modern DMRG calculation (Cf lecture 2).



M. Karski et al PRB 72, 113110, 2005

Illustration of the low-coherence temperature

- Thermodynamics quantities (Cf lecture 2 for equations)



Role of the frustration

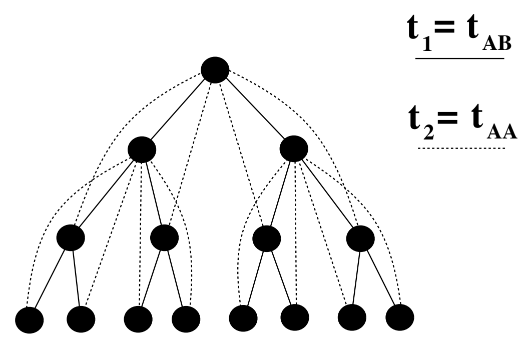
- Computation of AF in DMFT (two sublattices e.g. Bethe Lattice)

$$G_{0A\sigma}^{-1}(i\omega_n) = i\omega_n + \mu - t^2 G_{B\sigma}(i\omega_n) \qquad \sigma = \uparrow, \downarrow \qquad G_{B\sigma} = G_{A\bar{\sigma}}$$

- DMFT : paramagnetic equations = equations for a frustrated model

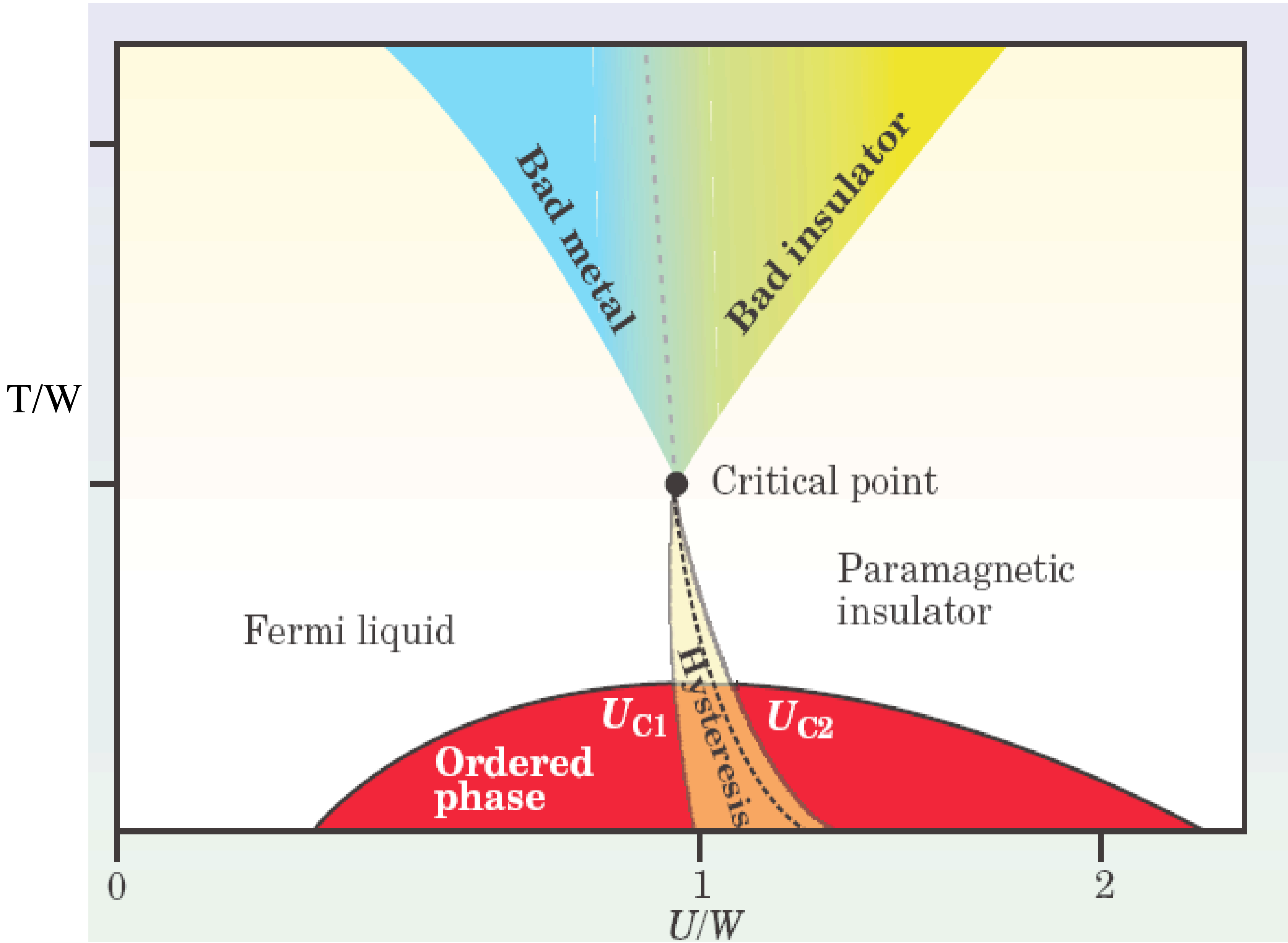
Example of the Bethe lattice with second neighbour

$$G_0^{-1}(i\omega_n) = i\omega_n + \mu - (t_1^2 + t_2^2) G(i\omega_n)$$

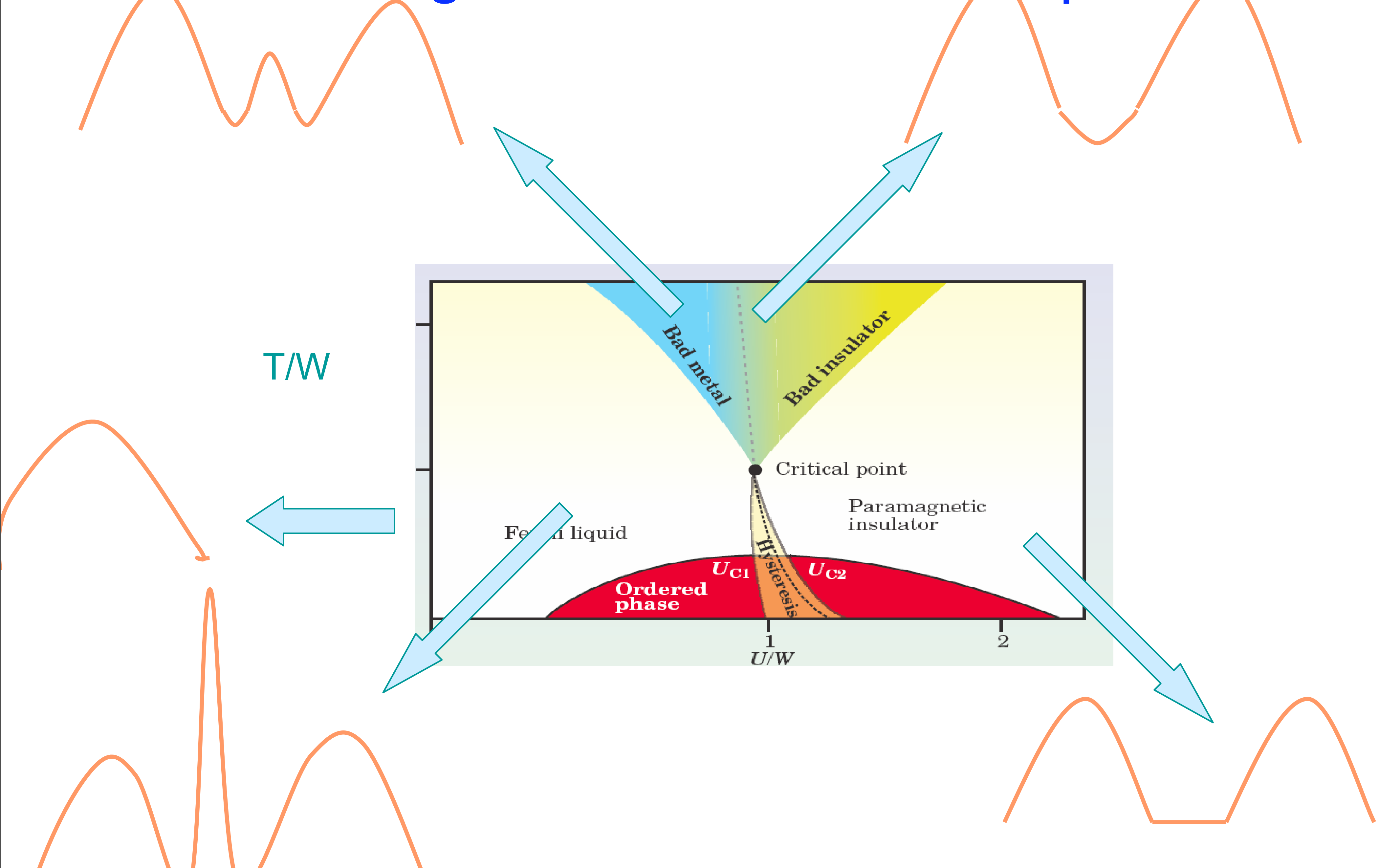


$\Longrightarrow$ In DMFT, simply solve the paramagnetic equations.

Complete generic phase diagram



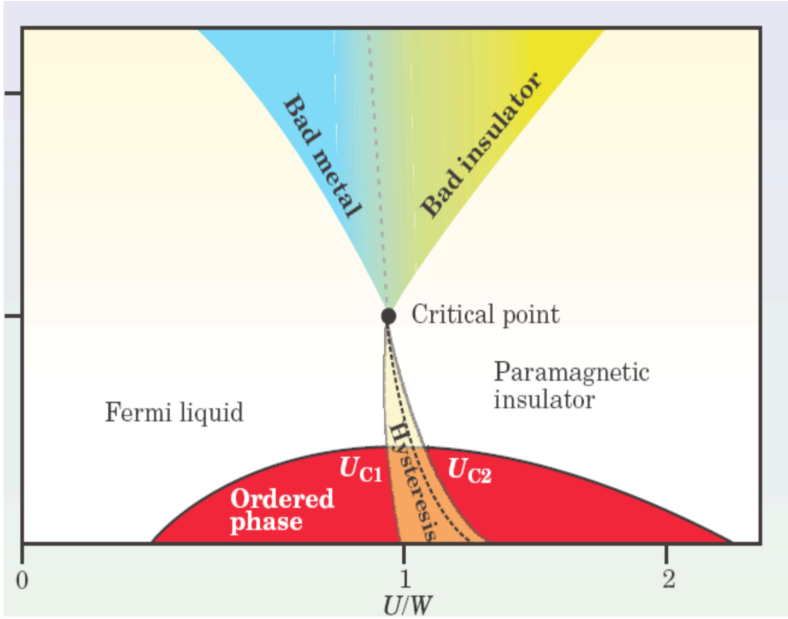
Various regimes around the critical point

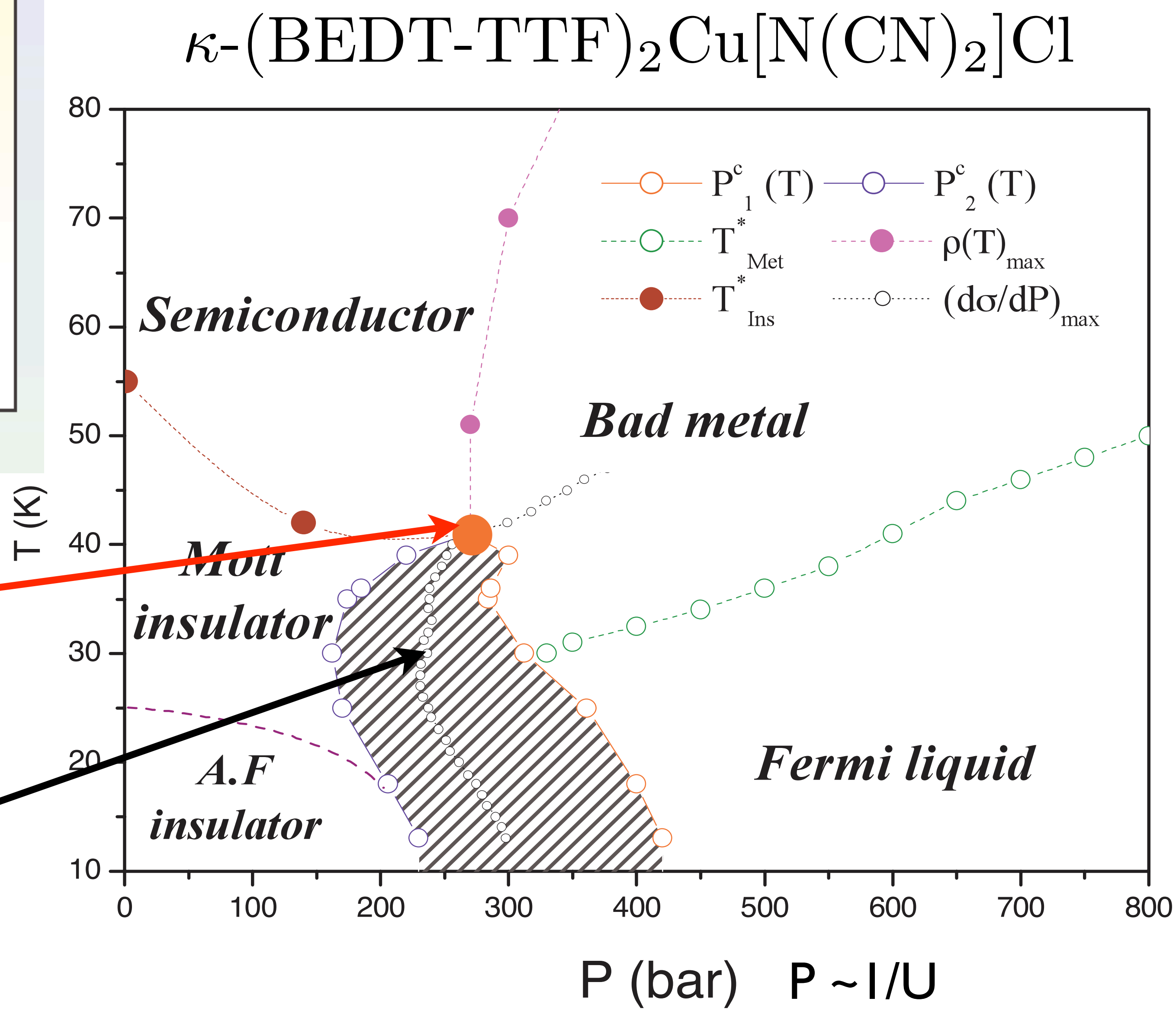


Sketchs of the spectral density

Comparison with experiments

Comparison with organics : phase diagram





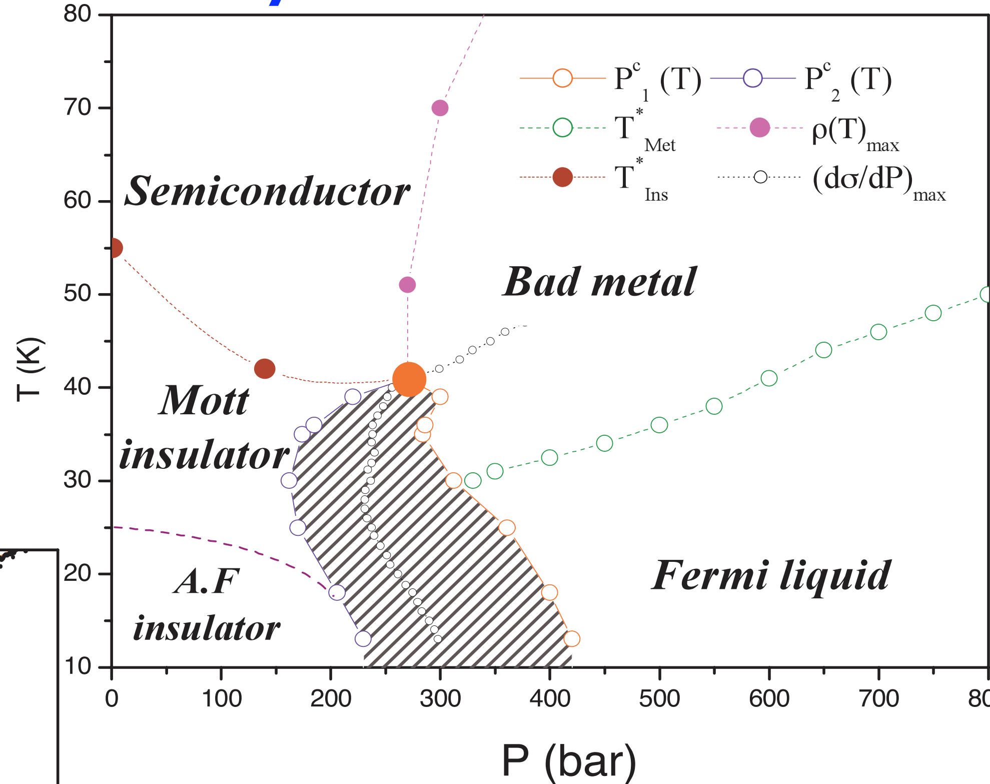
Critical Point

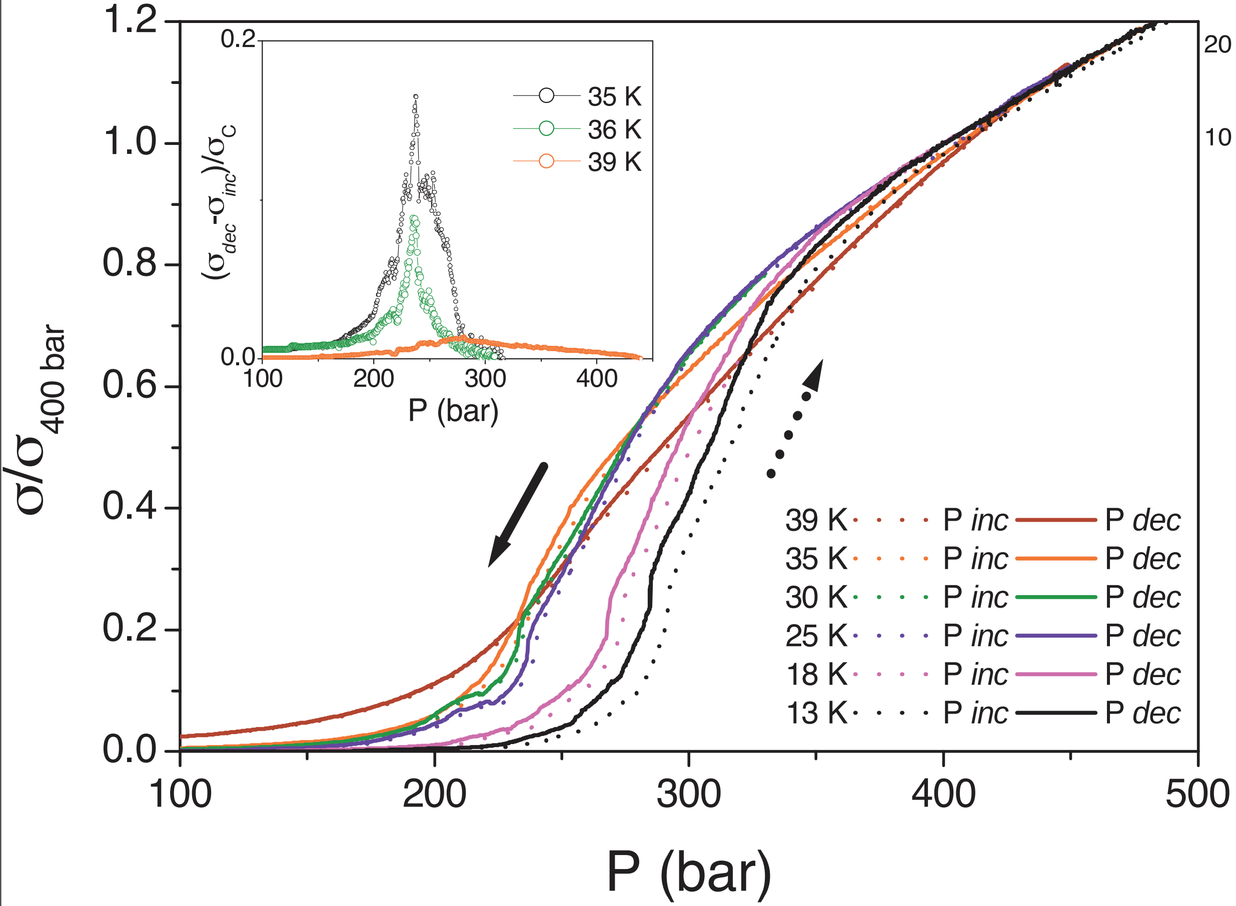
First order transition

P ~1/U

P. Limelette, P. Wzietek, S. Florens, A. Georges, T.A. Costi, C. Pasquier, D. Jérome, C. Meziere, P. Batail
PRL 91, 016401 (2003)

Experimental evidence for hysteresis



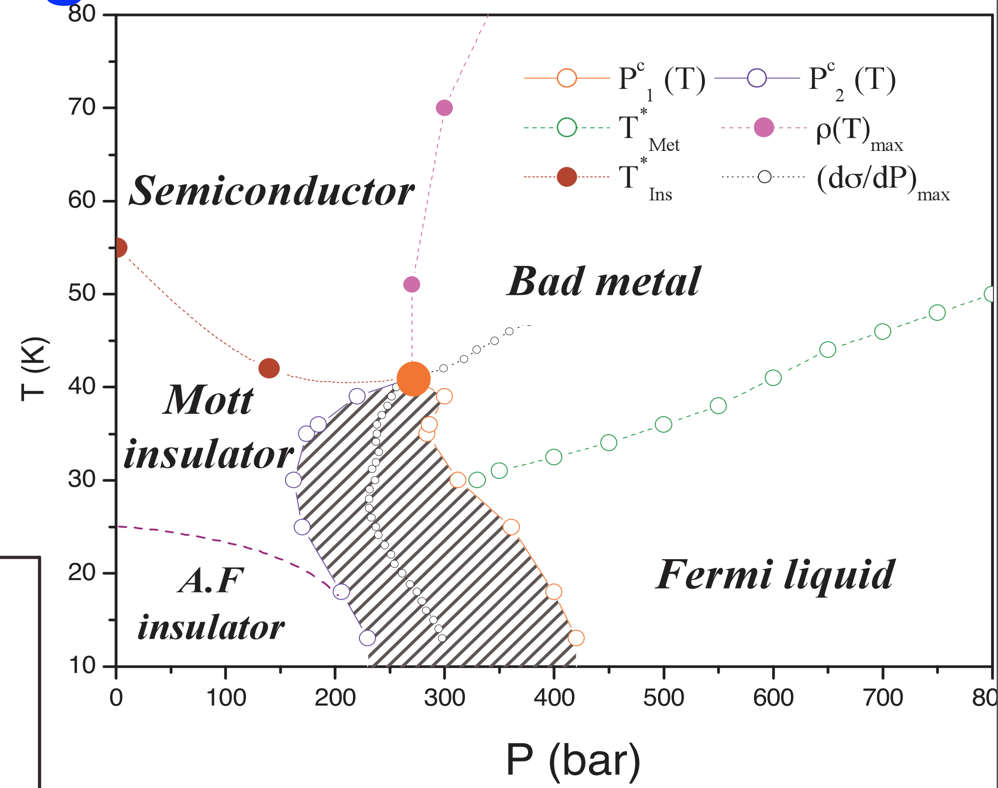


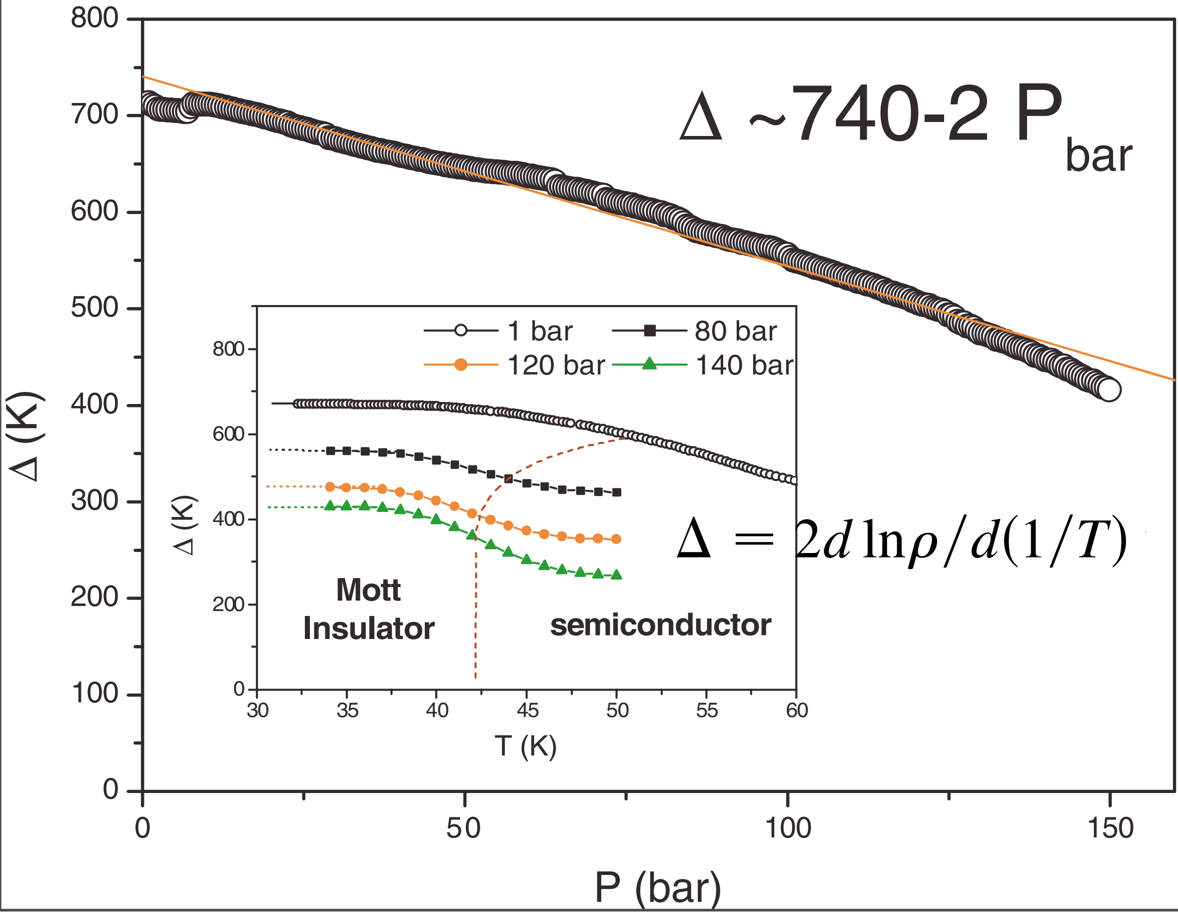
Insulating regime

- At low temperature, activation law

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

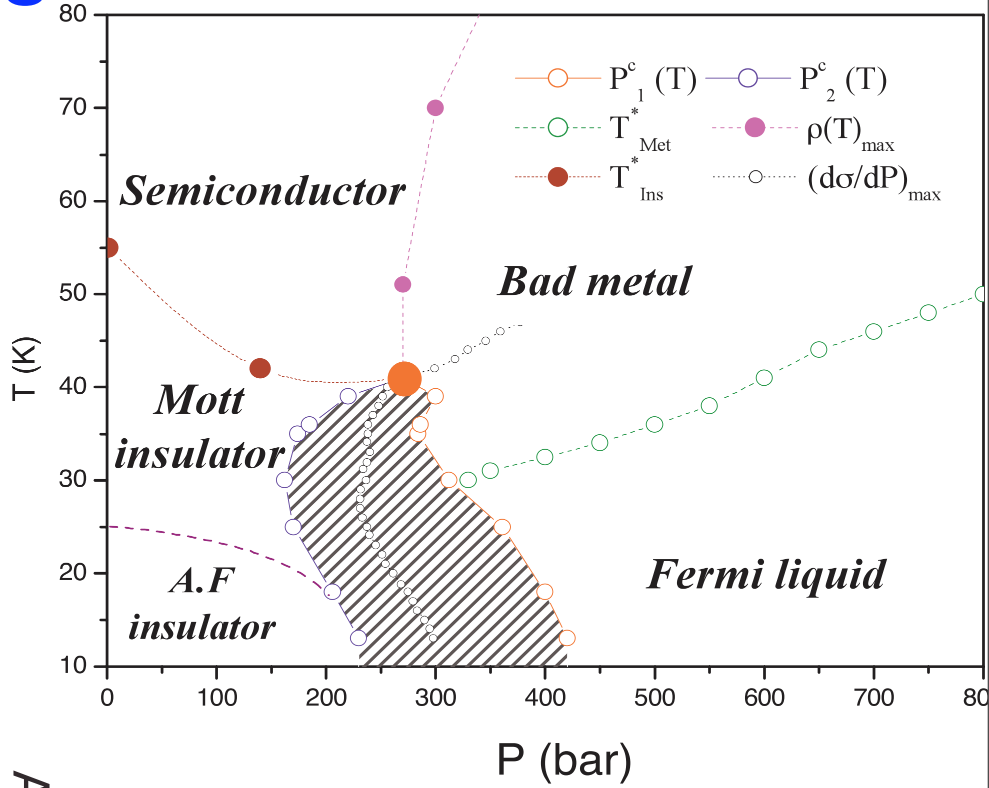
- Semi-conductor regime





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

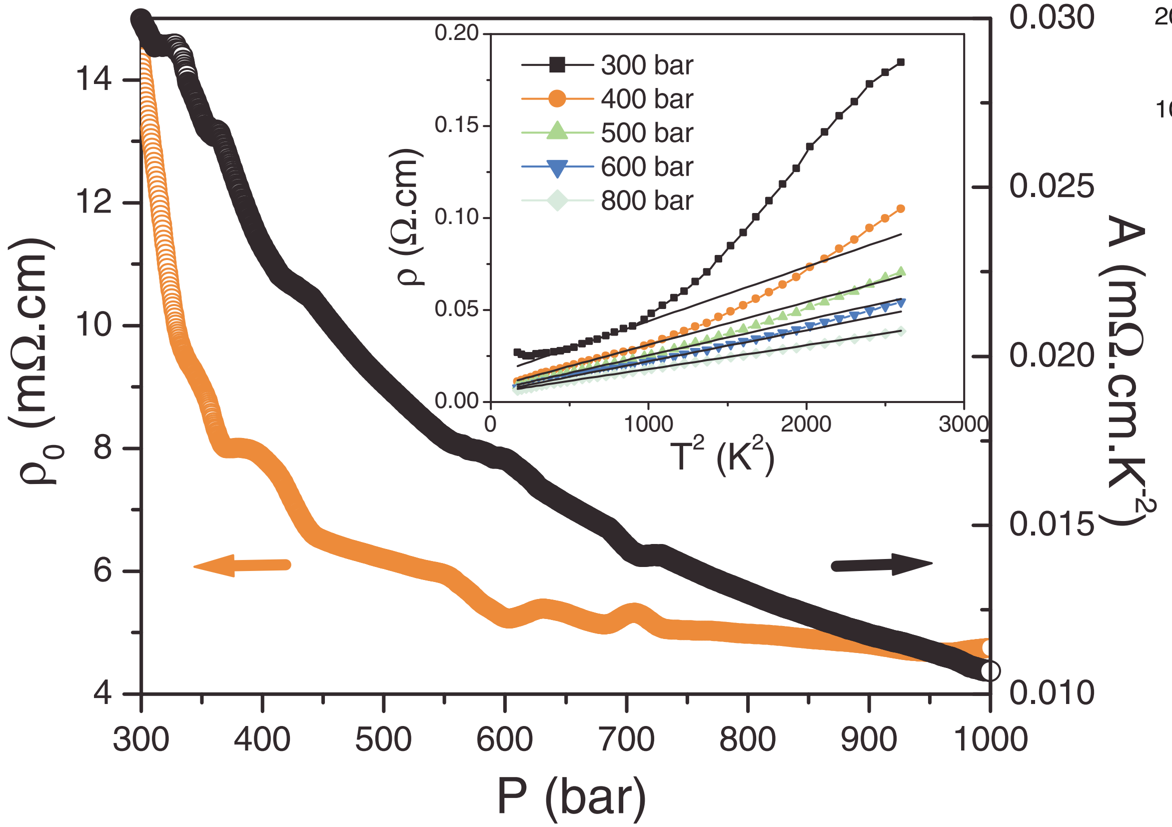
Metallic regime



- At low temperature, Fermi liquid

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

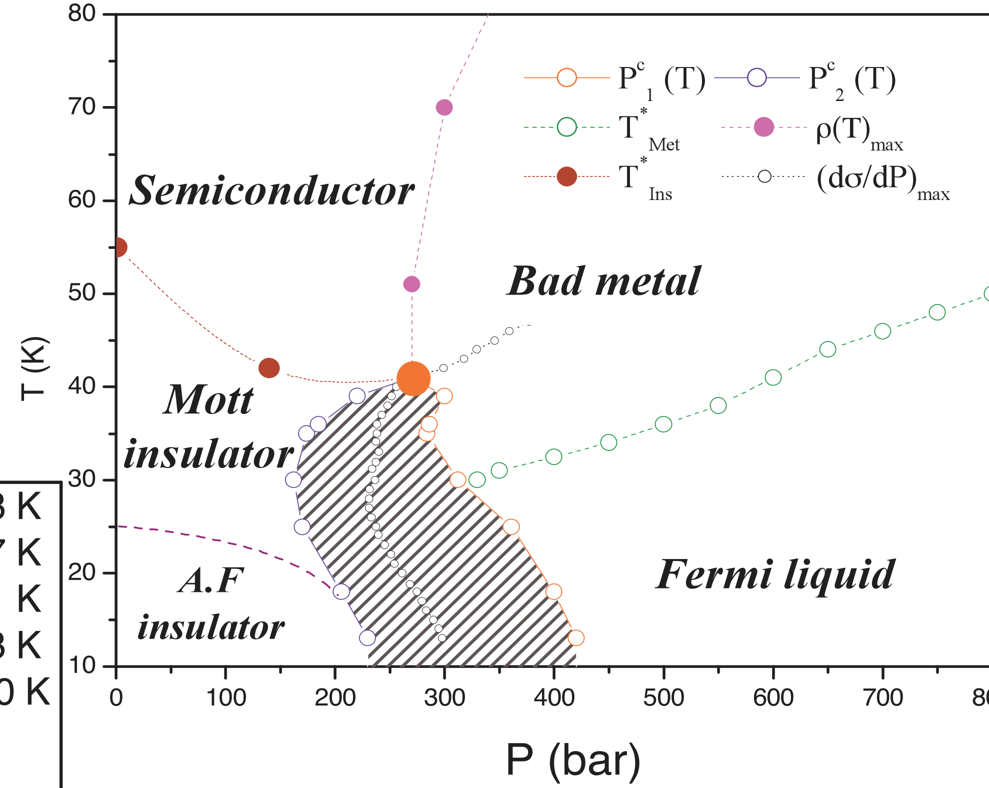
$$A(P)T_{coh}^2 \approx const$$

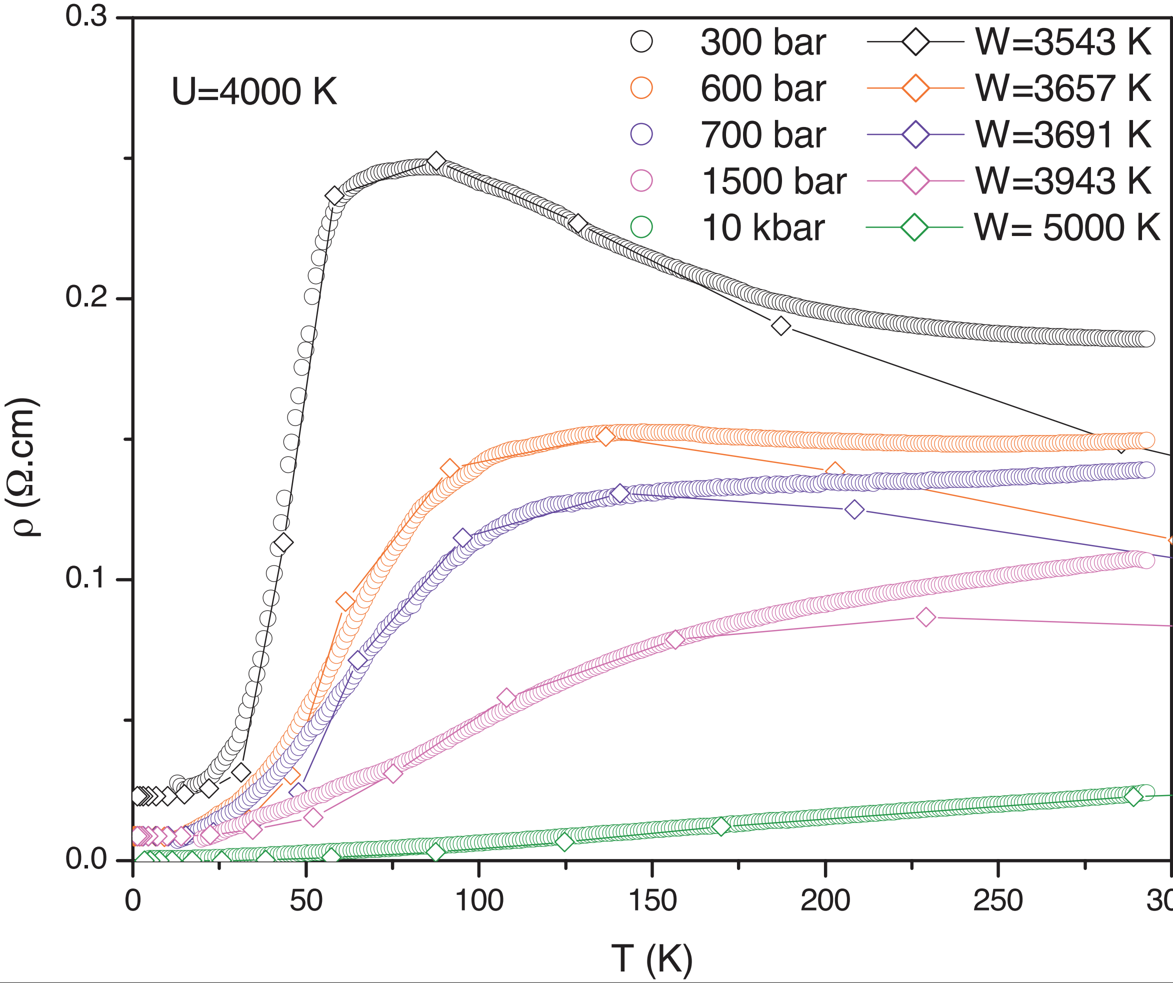


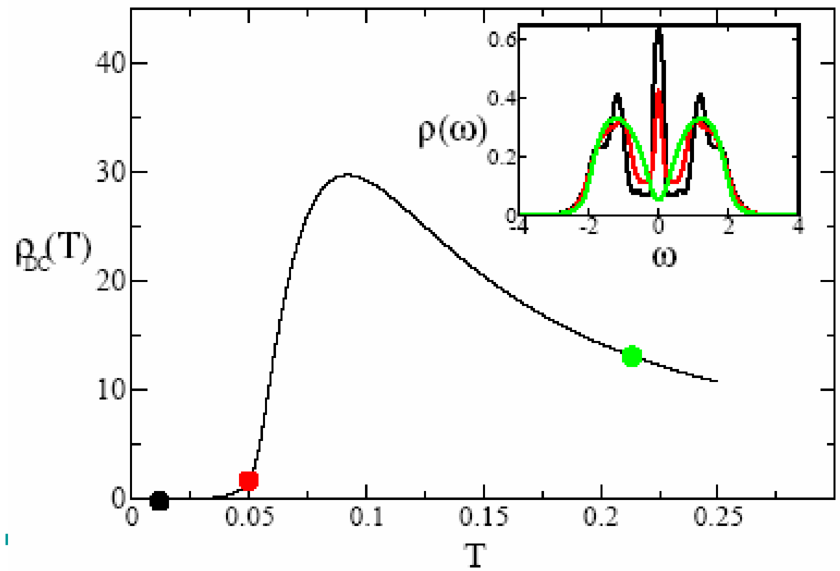
- Divergence of A (extrapolated) when Mott gap still large.
- T_coh << Δ

Bad metal regime. Comparison with DMFT

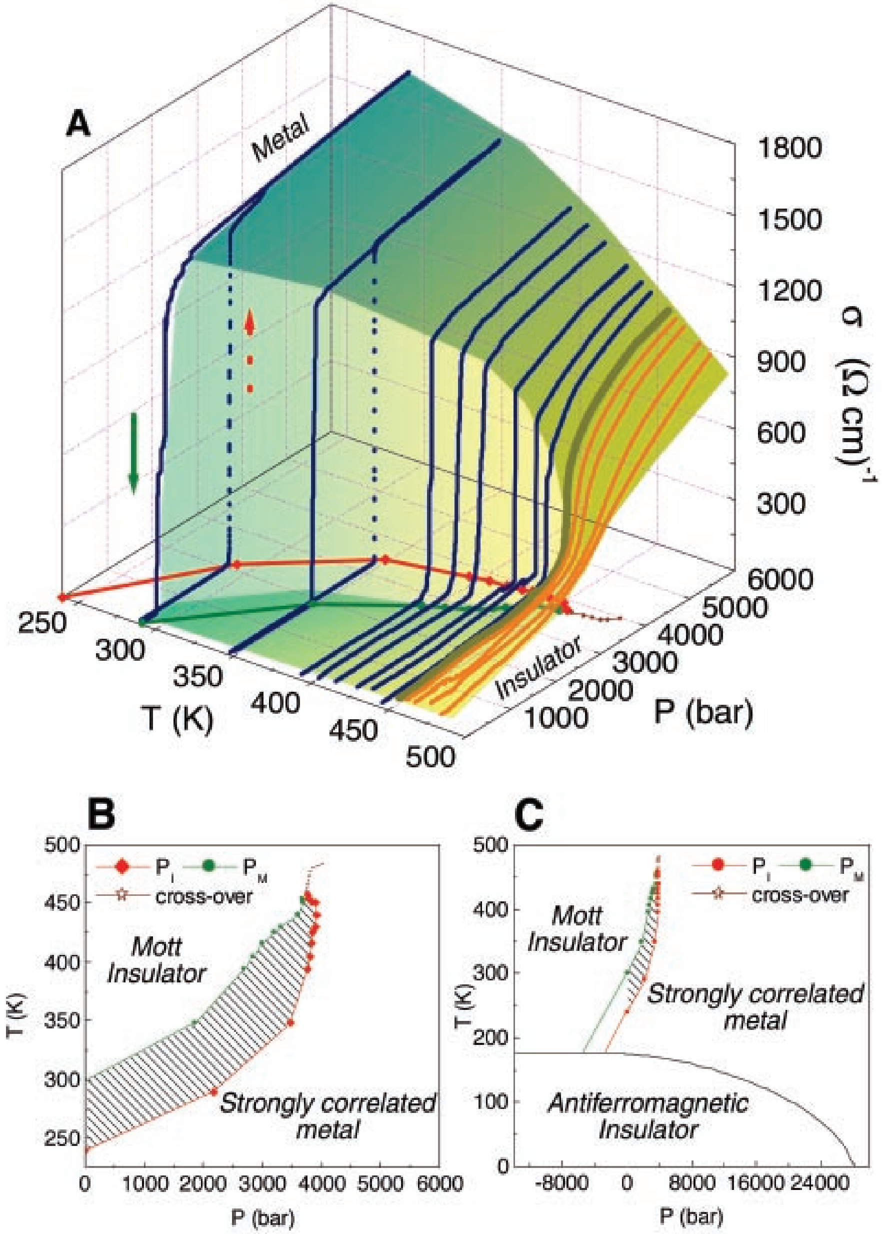
- Bethe lattice, NRG solver
- Adjusted parameters :
  D, ρ(T=0), global scale and U.



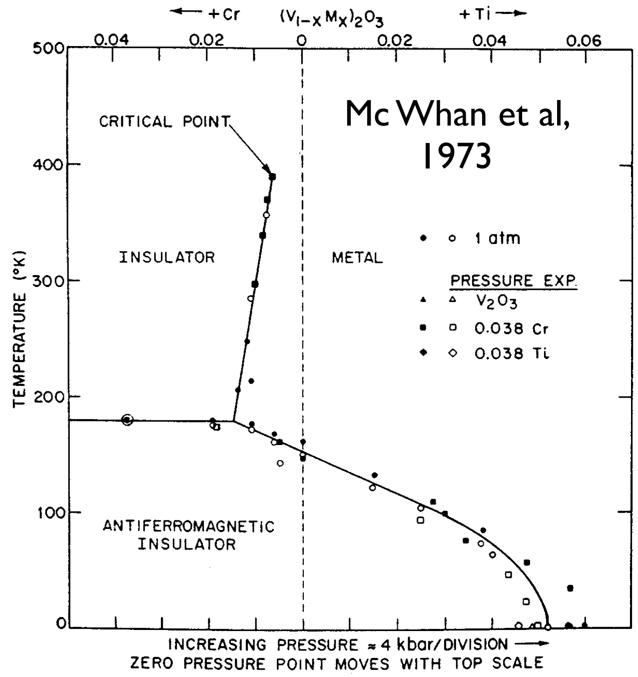




Critical point : V_2O_3



Resistivity under pressure.

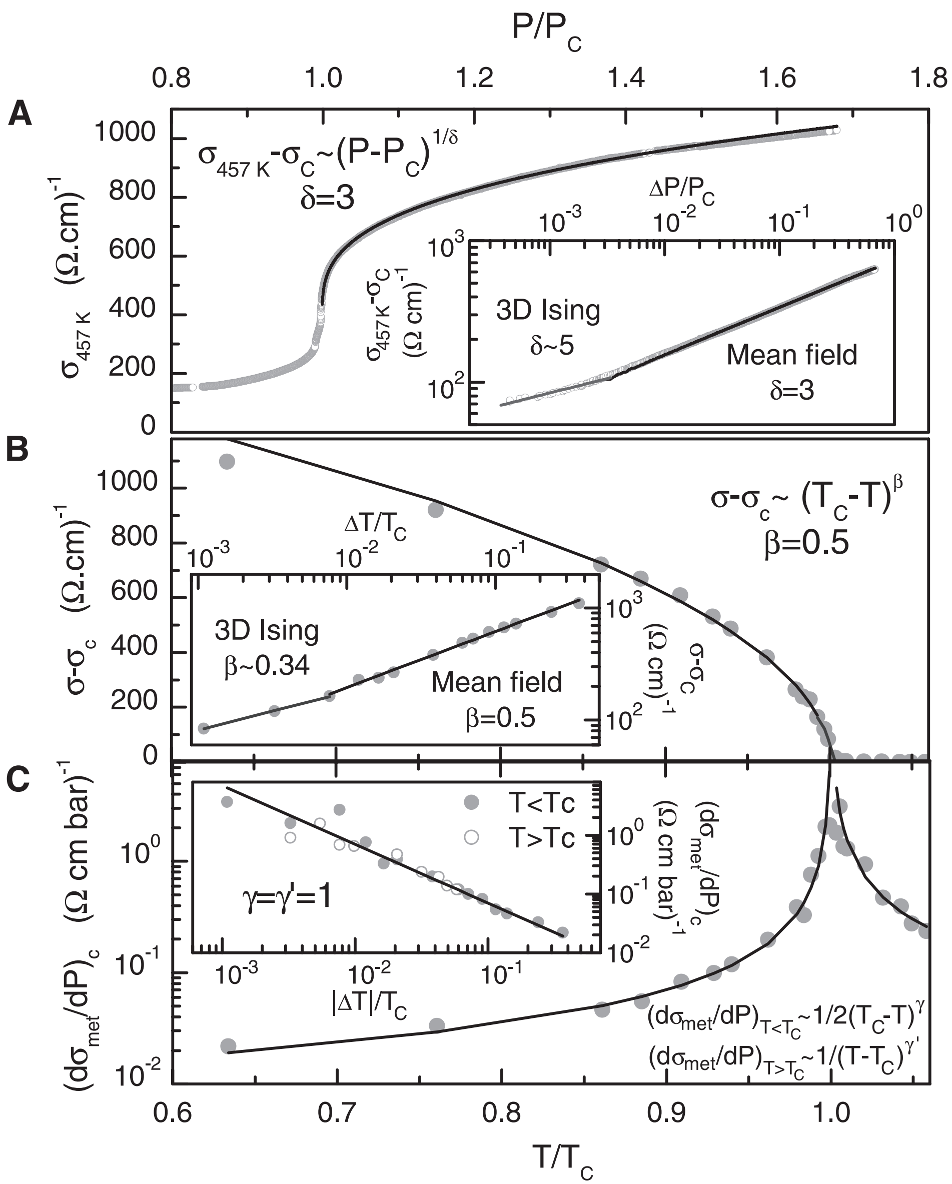


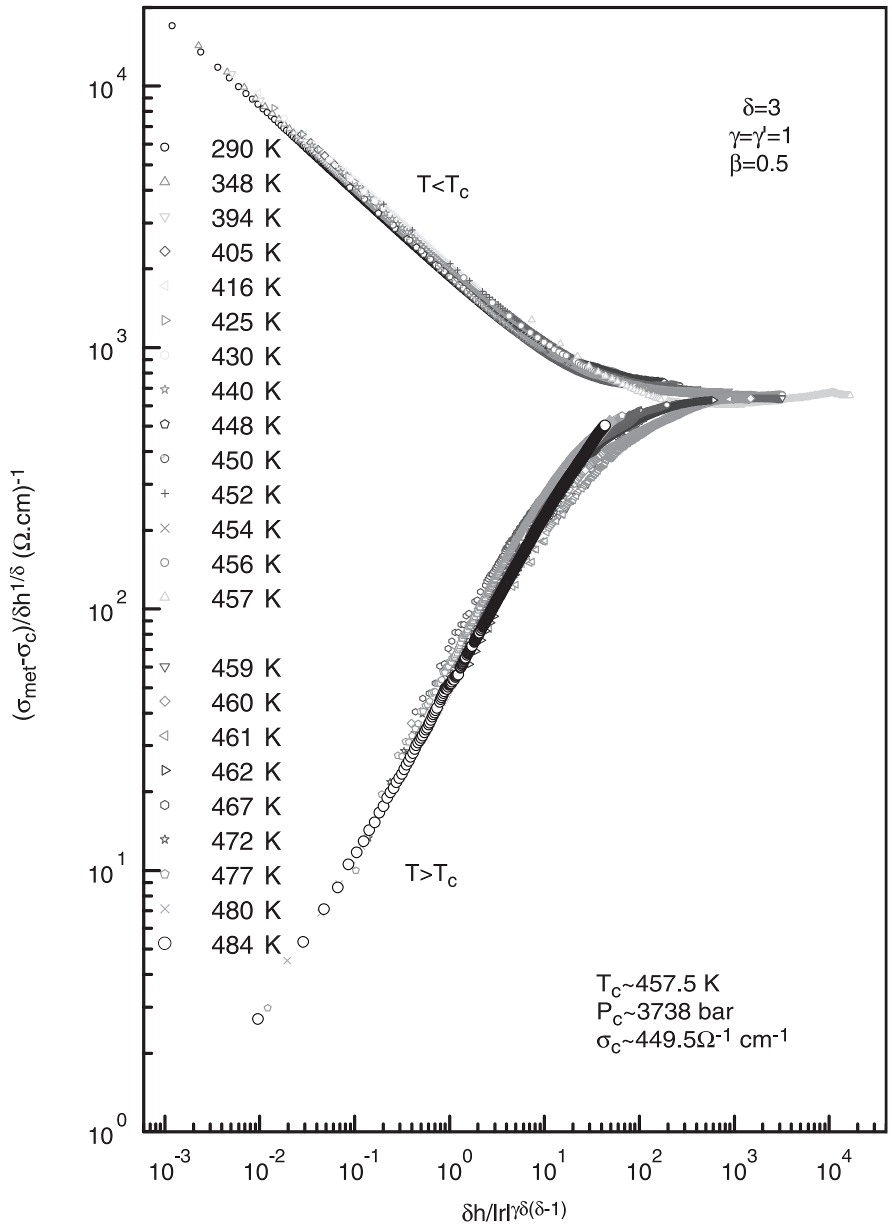
P. Limelette, A. Georges, D. Jérome, P. Wzietek, P. Metcalf, J.M. Honig, Science 302, 89 (2003)

Critical regime

DMFT : Ising universality class *G. Kotliar.E. Lange, M.J. Rozenberg, PRL84 5180 (2000).*

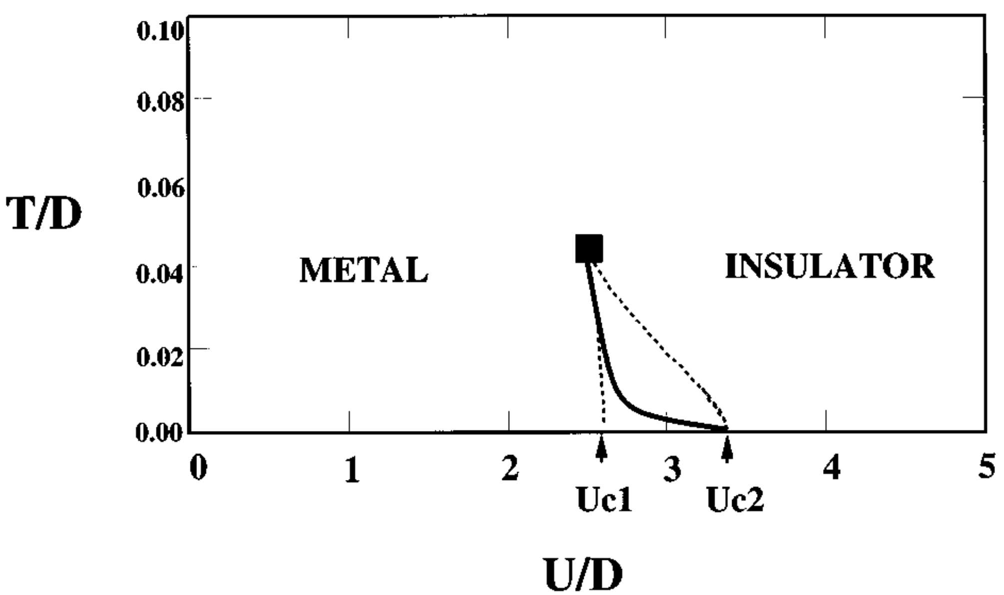
$$r \sim T - T_c,\ h \sim P - P_c$$



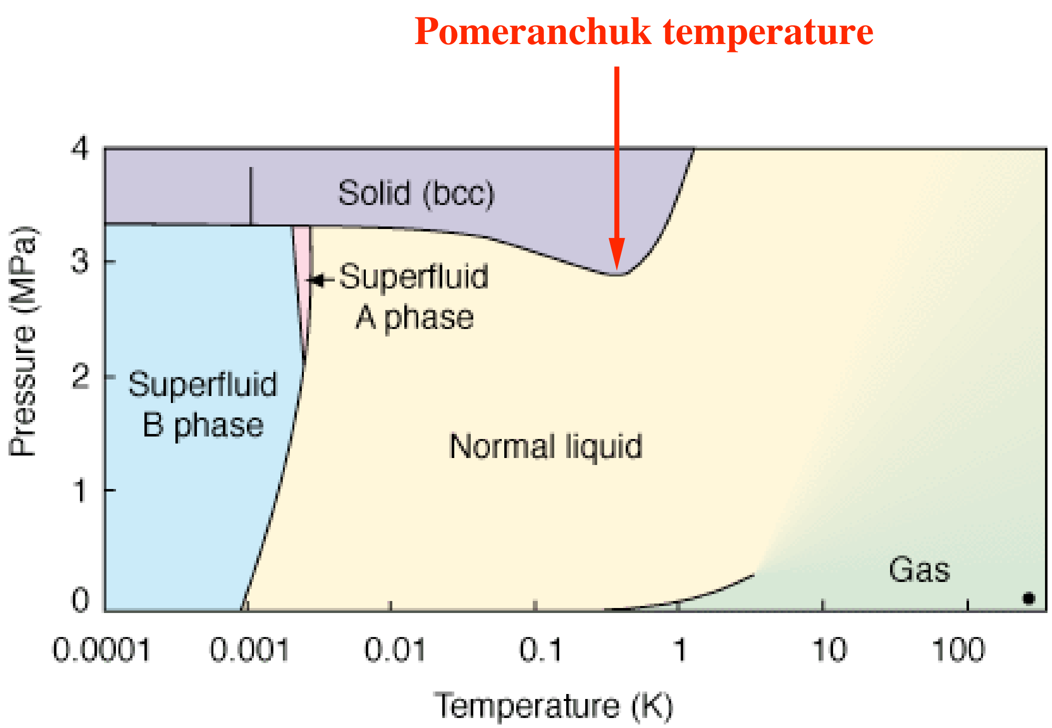


Analogous to Pomeranchuk effect

- Entropy of the localized phase > Entropy of the liquid
- One can increase localization by heating
- Real of artefact of a too simple paramagnetic insulator ?
- A possible test in cold fermions....



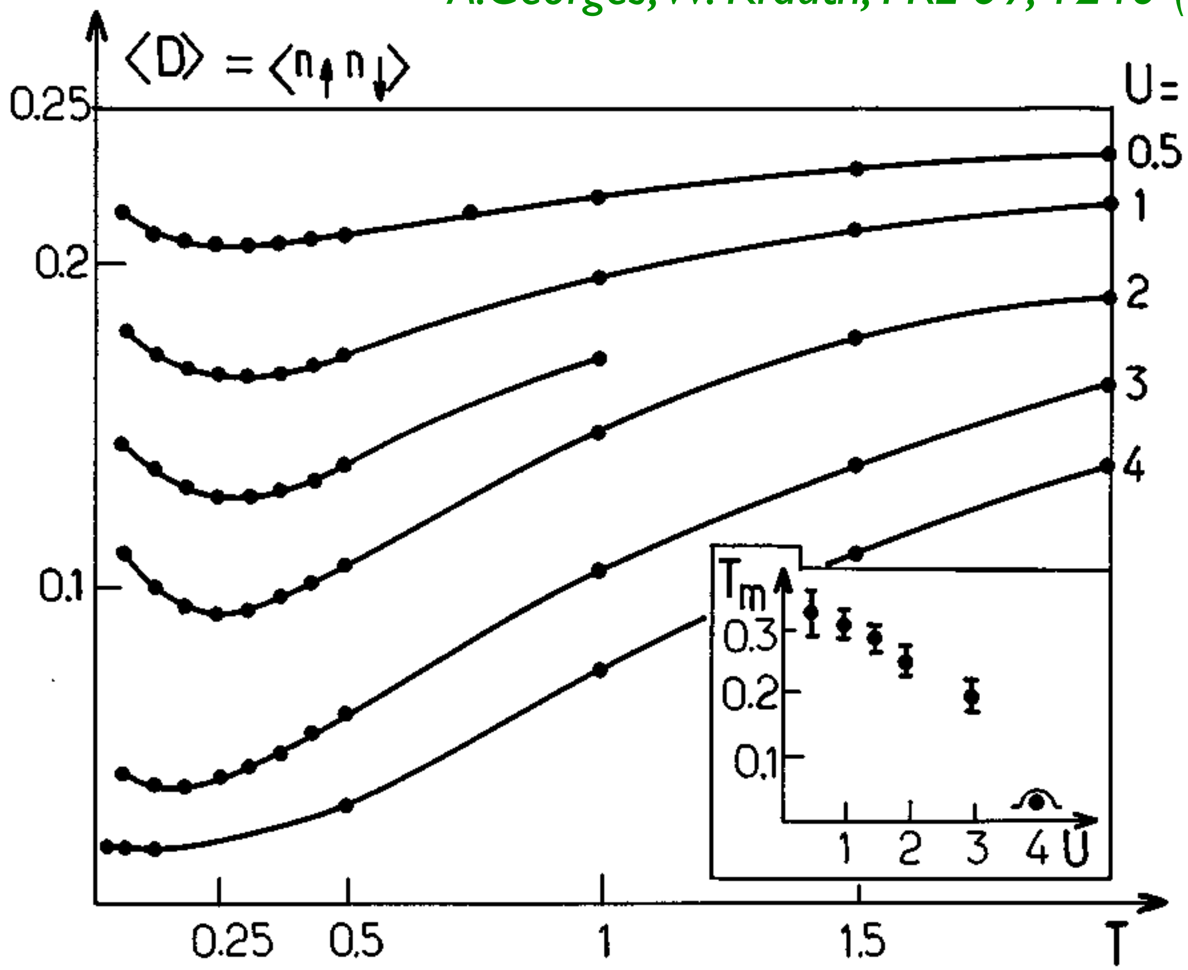
He3 phase diagram



Signature of Mott transition in double occupancy

A.Georges, W. Krauth, PRL 69, 1240 (1992)

$$d \equiv \langle n_{i\uparrow} n_{i\downarrow} \rangle$$

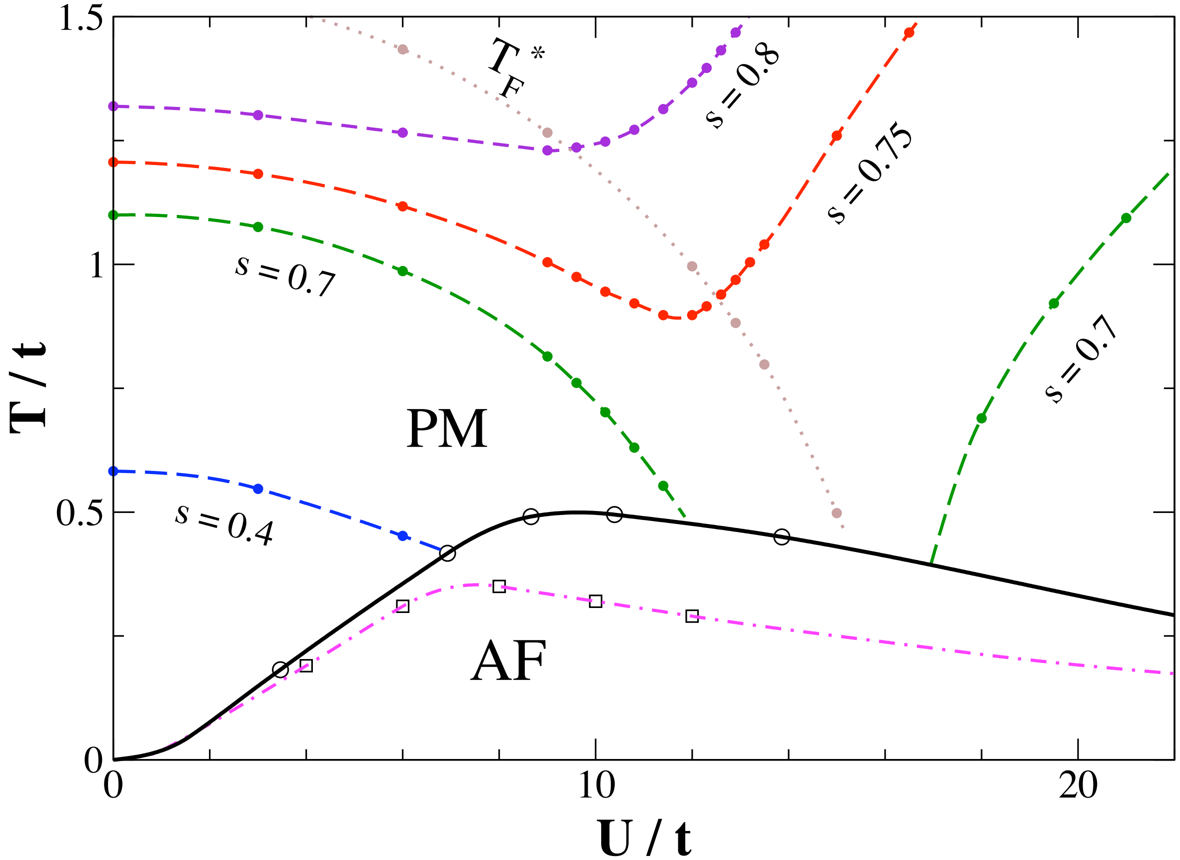


- There is a minimum for metallic values.

Interaction-Induced Adiabatic Cooling

- A relation between entropy per site s and double occupancy :
- Isentropic curves determined by variations of d !

$$\frac{\partial s}{\partial U} = -\frac{\partial d}{\partial T} \qquad s(T_i(U), U) = cte \Longrightarrow c(T_i)\,\frac{dT_i}{dU} = T_i\,\frac{\partial d}{\partial T}|_{T=T_i}$$



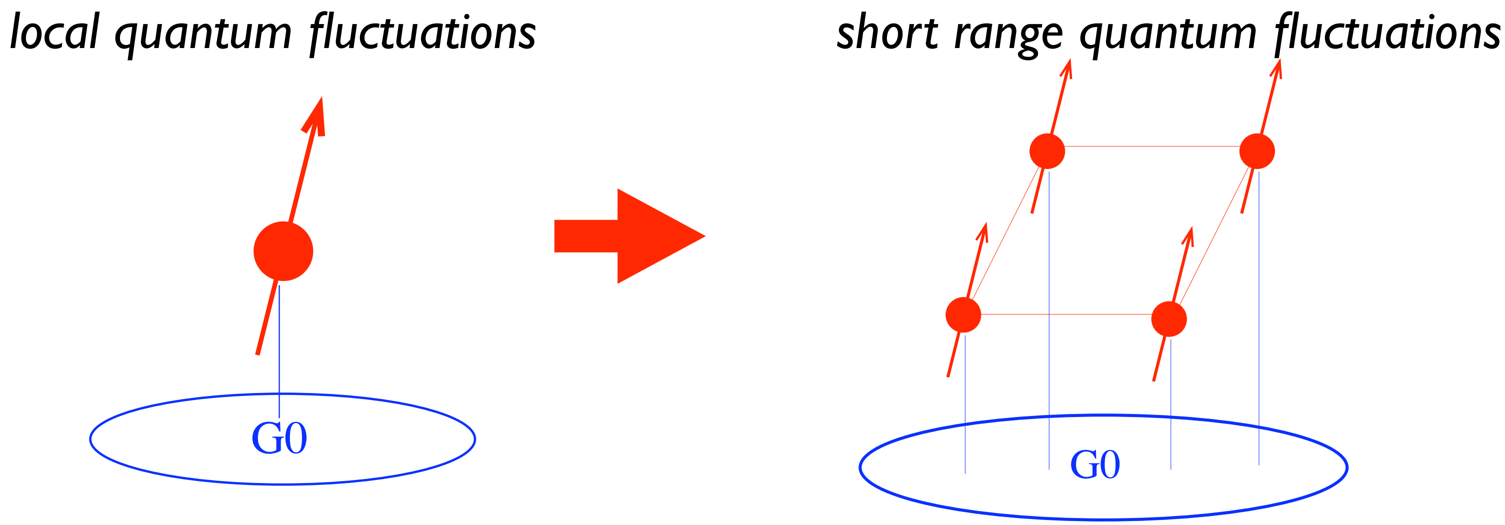
Isentropic lines

F. Werner, O. Parcollet, A. Georges, and S. R. Hassan PRL 95, 056401 (2005)

Beyond Hubbard model and 1 site DMFT ?

Cluster extensions of DMFT

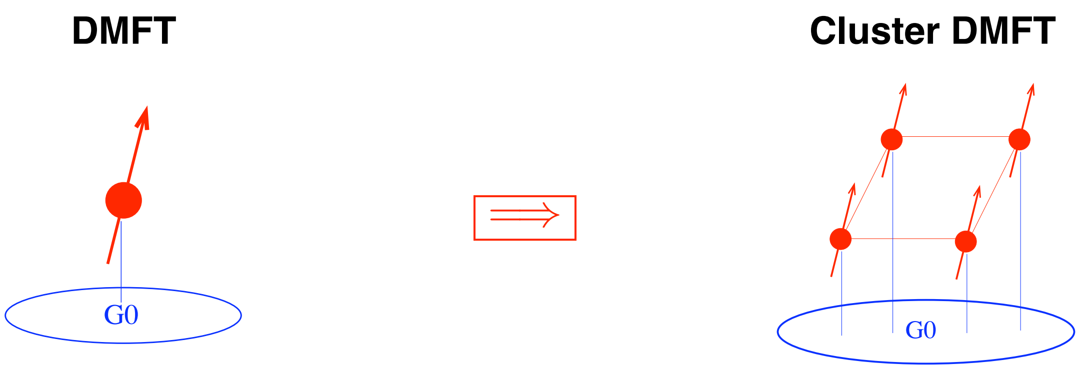
Lecture 3

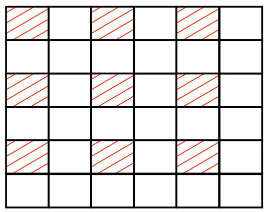


- Reintroduce k-dependence of $\Sigma(k,\omega)$:
  variations of Z, effective mass, lifetime along the Fermi surface.
- Describe d-wave supraconductors.
- Applications to high-Tc and to heavy fermions.
- Non trivial paramagnetic insulators (frustrated magnets ?)

Cluster extensions : CDMFT

- 4 Anderson impurities coupled to an effective bath





Superlattice

$$S_{\text{eff}} = -\iint_0^{\beta} d\tau d\tau' c^{\dagger}_{\mu}(\tau) G^{-1}_{0,\mu\nu}(\tau,\tau') c_{\nu}(\tau') + \int_0^{\beta} d\tau U (n_{i\uparrow} n_{i\downarrow})(\tau)$$

$$G_{c\mu\nu}(\tau) = -\langle T c_{\mu}(\tau) c^{\dagger}_{\nu}(0)\rangle_{S_{\text{eff}}} \qquad 1 \leq \mu,\nu \leq 4$$

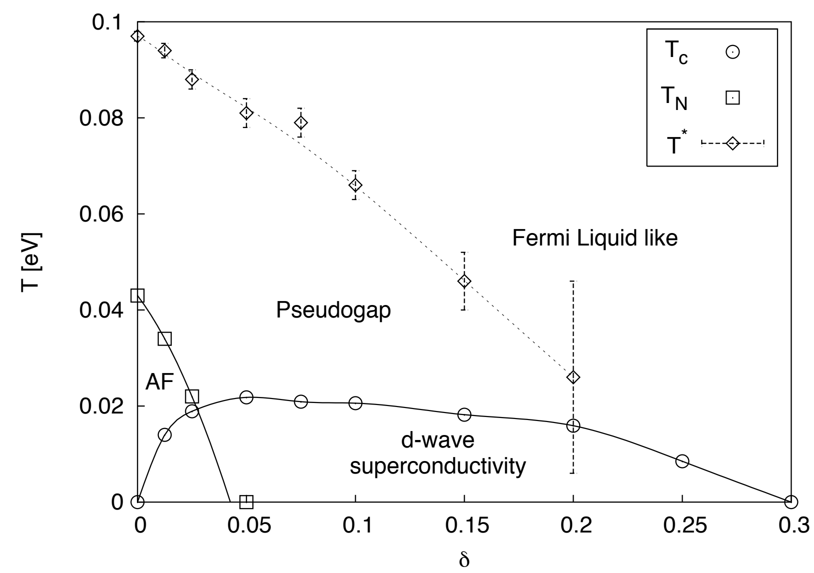
$$\Sigma_c = G_0^{-1} - G_c^{-1}$$

$$G_0^{-1}(i\omega_n) = \left[\sum_{K \in R.B.Z.}' \left(i\omega_n + \mu - \hat{t}(K) - \Sigma_c(i\omega_n) \right)^{-1} \right]^{-1} + \Sigma_c(i\omega_n)$$

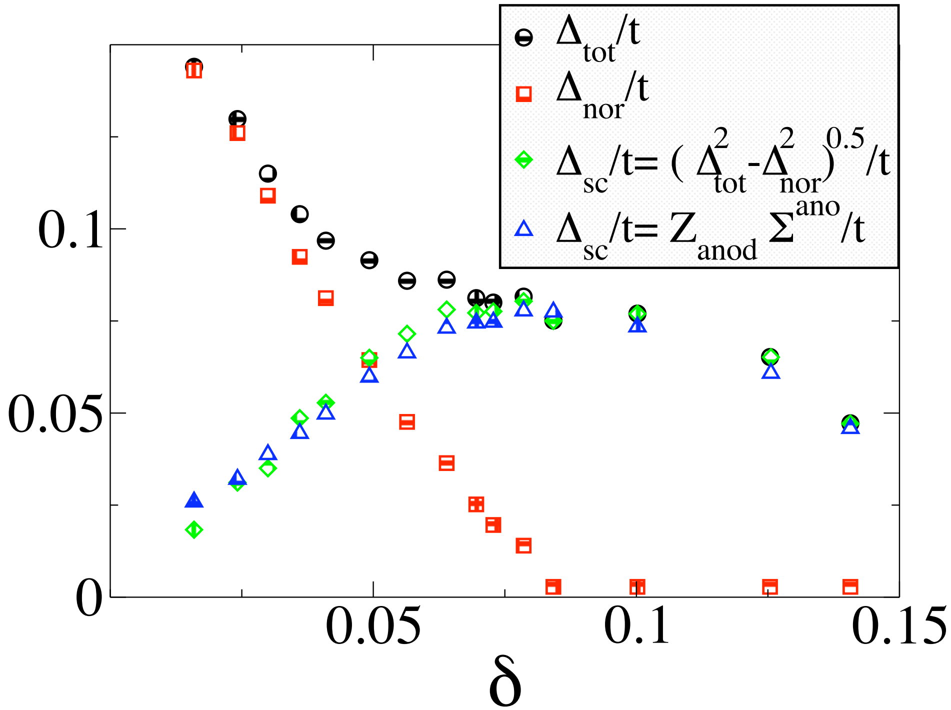
CDMFT equations

Cluster DMFT and high-Tc ...

M. Jarrell et al (2001)



- Phase diagram of Hubbard model



- Two gaps in the SC phase close to Mott transition

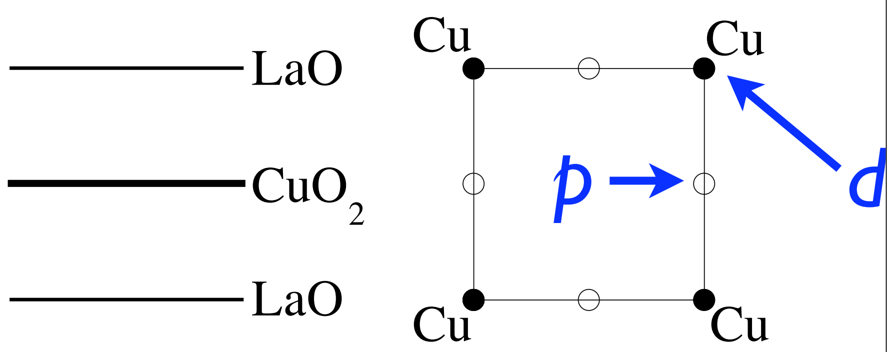
M. Civelli, M. Capone, A. Georges, K. Haule, O. Parcollet, T. D. Stanescu, G. Kotliar arXiv:0704.1486

Cluster extensions of DMFT : heavy fermions

- Heavy fermion problem. Periodic Anderson model
- DMFT maps e.g. 2 Anderson impurities to the lattice problem
  - Multiple impurities model have richer physics due to competition between Kondo screening and RKKY interaction
  - Local QCP $\rightarrow$ QCP of the lattice model ??

Towards more realism...

- Multiorbital models. Possibility of orbitally selective Mott transition
- 3 bands for cuprates (d-p orbitals).



- Use a better t(k)
- Mix DFT and DMFT : Lecture 4.

Conclusion lecture 1

- Introduction to Mott transition, impurities and DMFT formalism
- Mott transition in DMFT in the simplest case
- Compares nicely to experiments

- Next time :
  - Derivation of the DMFT equations ?
  - How to solve quantum impurity models ?