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Frustration and competition of interactions in the Kondo lattice: beyond the Doniach's diagram

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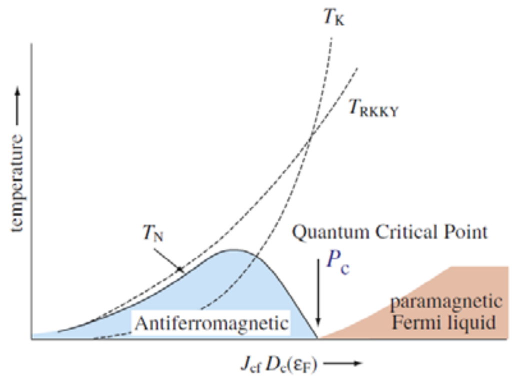
1- The S=1 Kondo lattice: coexistence of ferromagnetism and Kondo effect in underscreened Kondo lattice
Collaboration: C. Thomas, J.R. Iglesias, A. da Rosa Simoes, N. Perkins, B. Coqblin ; Phys Rev B, to be published

2- The frustrated Kondo lattice: Kondo singlets vs. Dimer singlets
Collaboration: B.H. Bernhard, B. Coqblin

1. The Kondo lattice: S=1/2 vs S=1

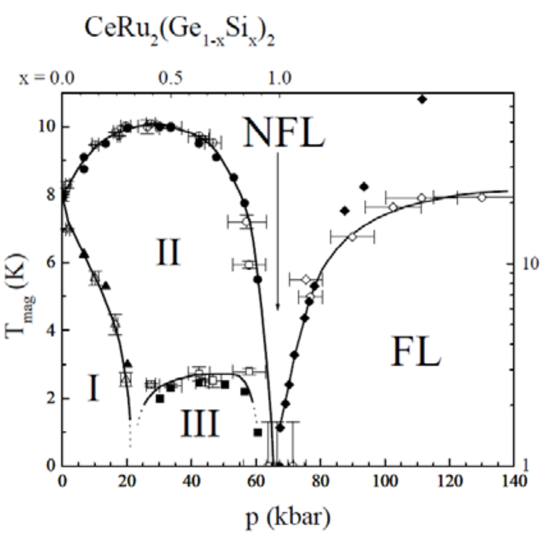
$$H = \sum_{k,\sigma} \varepsilon_k n_{k\sigma} - J_K \sum_i \vec{S_i} \cdot \vec{\sigma_i}$$



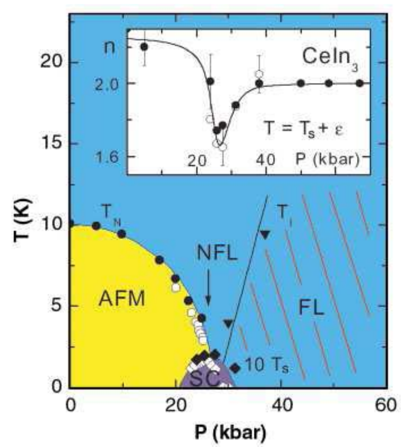
Doniach's diagram of the Kondo lattice <u>**(S=1/2)**</u> ***(Doniach 1977)***

$T_K \propto 1/\rho \exp(-1/\rho J_K)$; $T_N \propto \rho J_K^2$

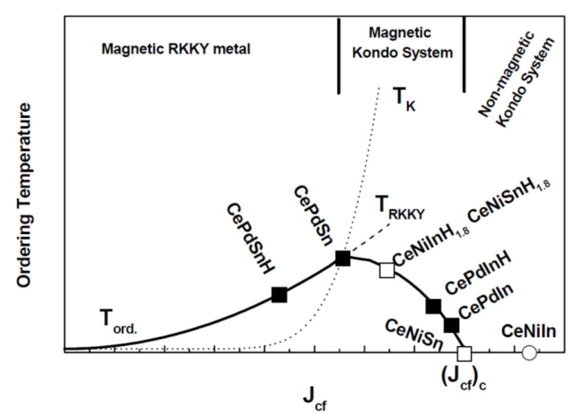
Mainly used to describe Ce compounds



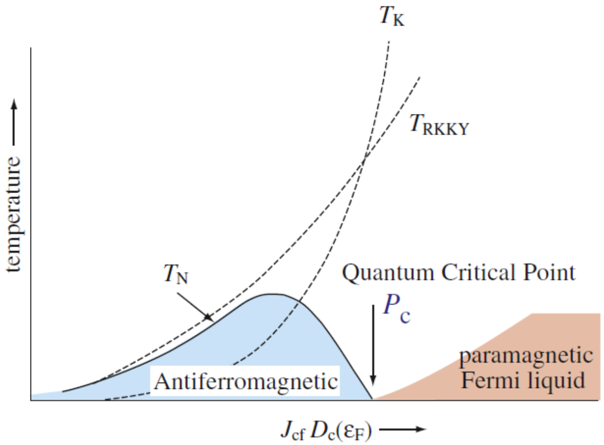
S. Süllow et al, 1999



G. Knebel et al, 200



B. Chevalier et al, 2005

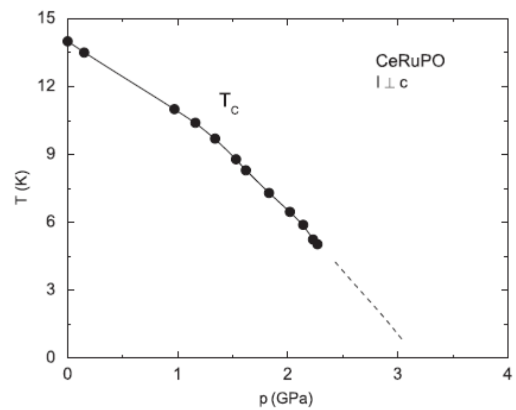


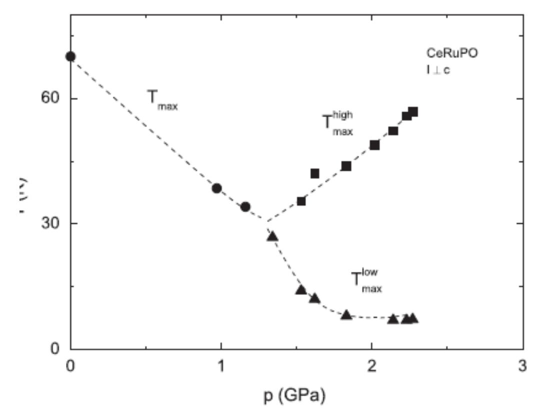
Competition between Kondo and RKKY exchange interactions in Ce compounds

⇒ Magnetic state is usually AF with small T_N

⇒ **very few ferromagnetic Kondo Ce compounds :**

CeRuPO
(*M. Macovei et al, 2009*)

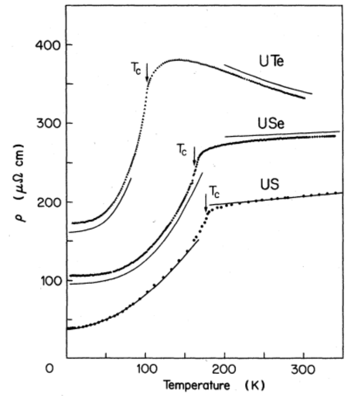




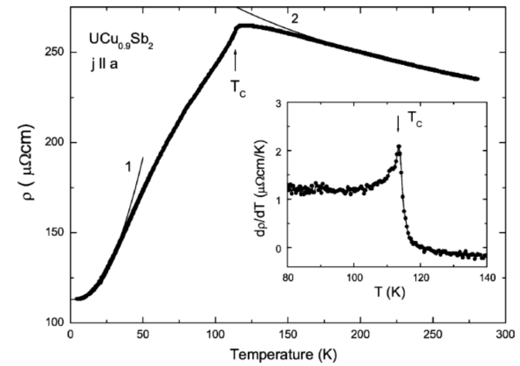
Why so few ferromagnetic Ce Kondo lattices?: Kondo effect is destroyed by the internal field

In Ce effective moment S_{eff} =1/2. The situation is different in S=1 systems

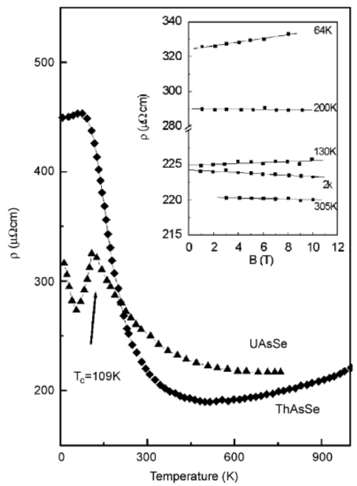
Coexistence of ferromagnetism and Kondo effect in U and Np compounds: Logarithmic variation of resistivity above T_C



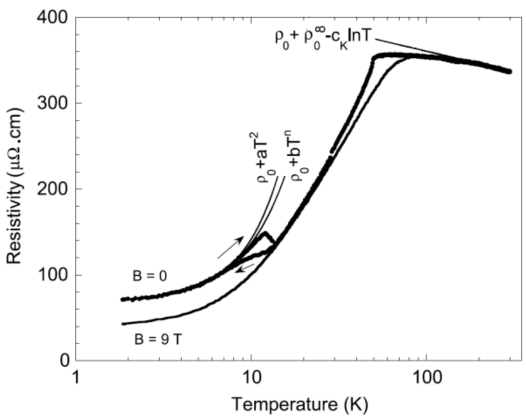
J. Schoenes et al, 1984



J. Schoenes et al, 2007



Bukowski et al, 2005



$NpNiSi_2$

Colineau et al, 2008

Systems not described by the S=1/2 Kondo lattice: number of 5f-electrons >1⇒ S>1/2

The S=1 Kondo impurity

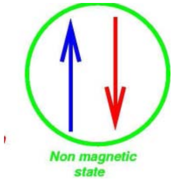
P. Nozieres and A. Blandin (1980): « Kondo effect in real metals »

<u>2 important parameters</u>: - the spin S of the impurity

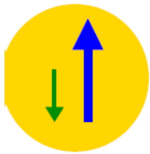
- the number n of orbital channels

<u>3 cases</u>:

- <u>n = 2S</u> : ground state is non degenerate (Kondo singlet) . Fermi liquid



- <u>n < 2S</u> : Kondo impurity is underscreened. Below T_K, effective spin S' = S-n/2 . S' is coupled ferromagnetically to conduction electrons. Incomplete Kondo effect.

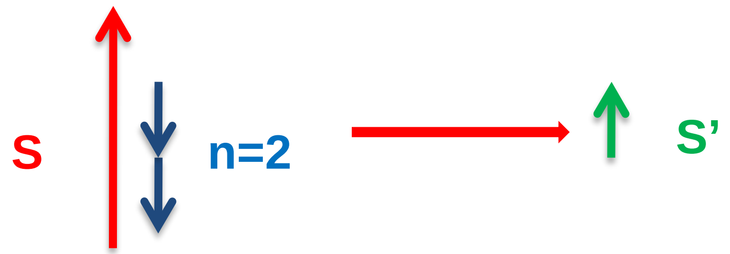


- <u>n > 2S</u>: overscreening. Non-Fermi liquid. Complete quenching ? $S' \neq 0$?

The underscreened Kondo lattice

- Coexistence of ferromagnetism and Kondo effect is possible:

S' = S-n/2 ≠ 0 ⇒ residual spins interact through exchange interactions.



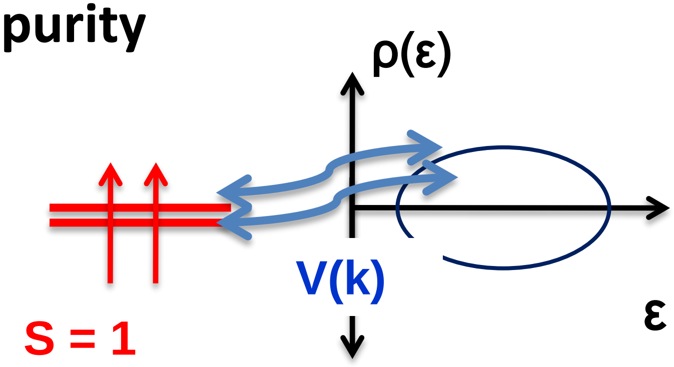
S' is weakly coupled to conduction electrons ⇒ RKKY coupling

-Description through an Anderson lattice with

2 localized electrons on each site ⇒ S=1 impurity

- Localized orbitals coupled to a non

degenerate band (n=1)



Schrieffer-Wolff transformation

Anderson lattice with 2 f-orbitals per site and 2 electrons in f-orbitals

⇒ Effective S=1 Kondo lattice model

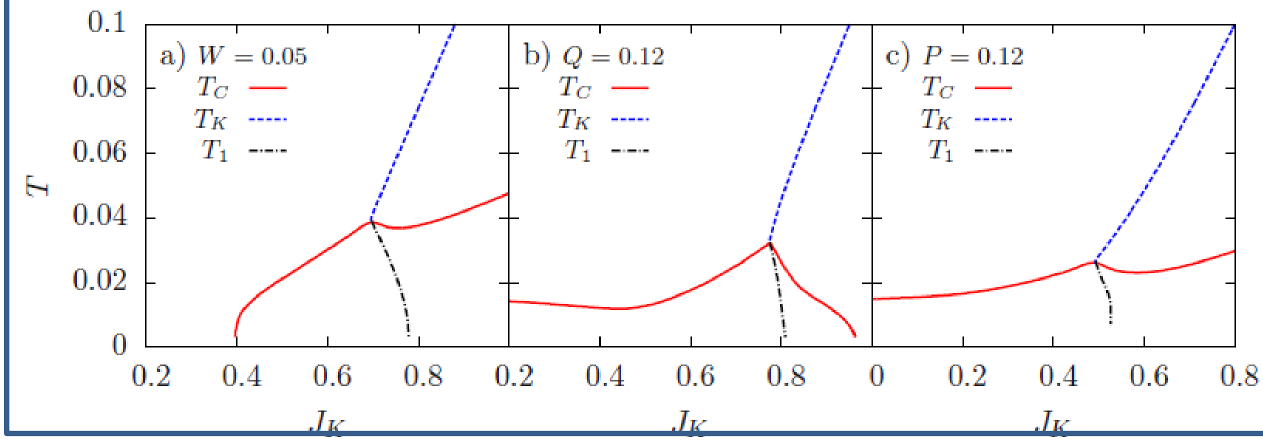
Hamiltonian $H = H_c + H_K + H_J + H_f$

- H_c **conduction electrons band**
- H_K **Kondo coupling :** $-J_K \vec{S_i} . \vec{\sigma}_i$ ($J_K < 0$) **and** $|S| = 1$
- H_J **Magnetic intersite exchange (RKKY):** $-J_{ij} \vec{S}_i . \vec{S}_j$ **(ferro)**
- H_f **Effective f-band (width:** $W_f \propto J_K$ **)**

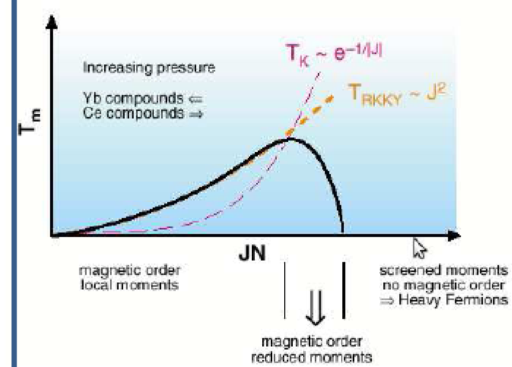
Mean-field approach

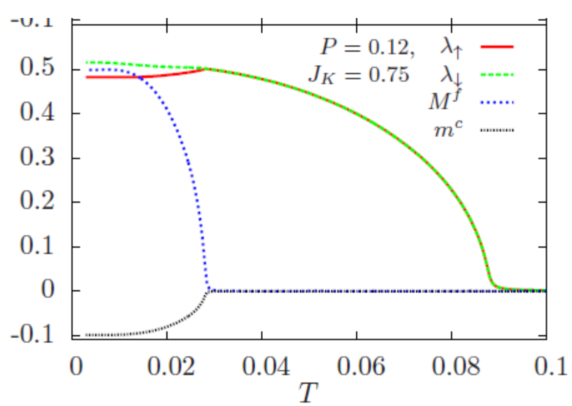
- **Magnetizations** ***M*** **of f-electrons and** ***m*** **of conduction electrons**
- **Kondo parameters:** $\lambda_i = \langle f_i^+ c_i \rangle$ **(spin-dependent in ferro phase)**

Some possible phase diagrams for the underscreened Kondo lattice



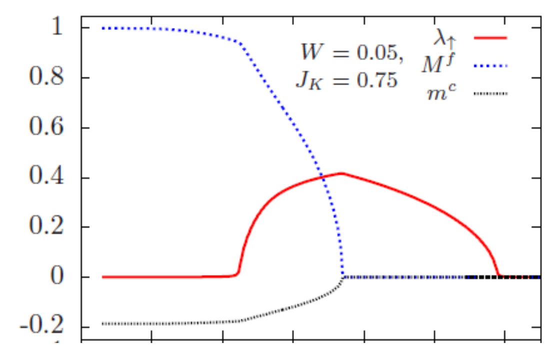
Doniach's diagram





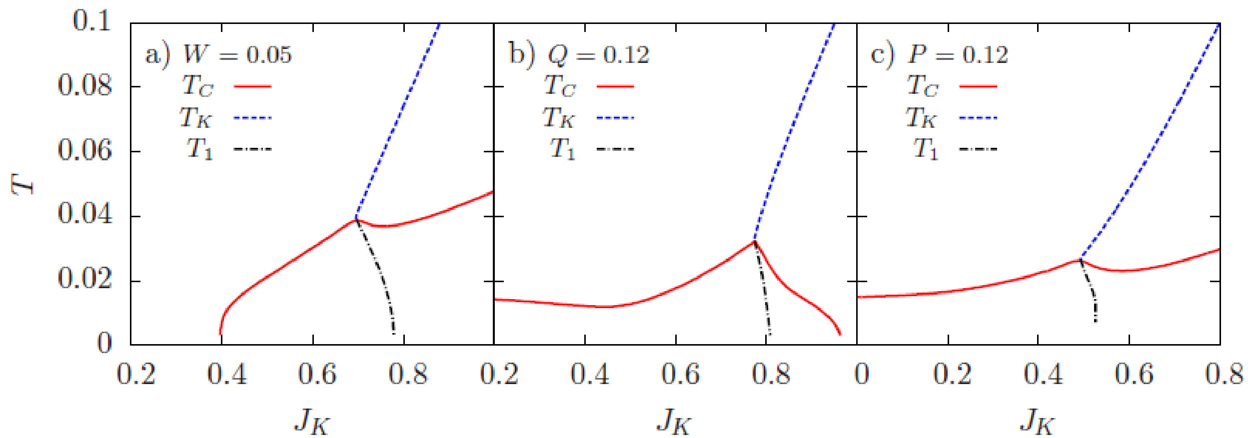
$T_K > T_c$: ferromagnetic ordering of the screened magnetic moments (S')

F + K — **K**



Re-entrant case: at low T, Kondo effect is destroyed by internal field

F — **F+K** — **K**



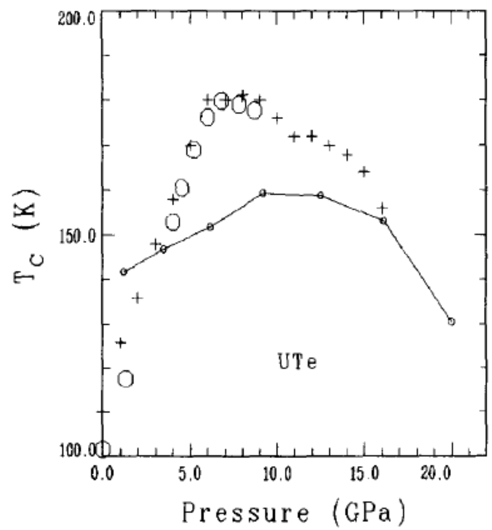
Possible model for UTe, $UCuSb_2$, $UCoSb_2$, $NpNiSi_2$, Np_2PdGa_3 …

-Large Curie temperature

-Nb. of 5f electrons > 2

-Kondo effect in resistivity

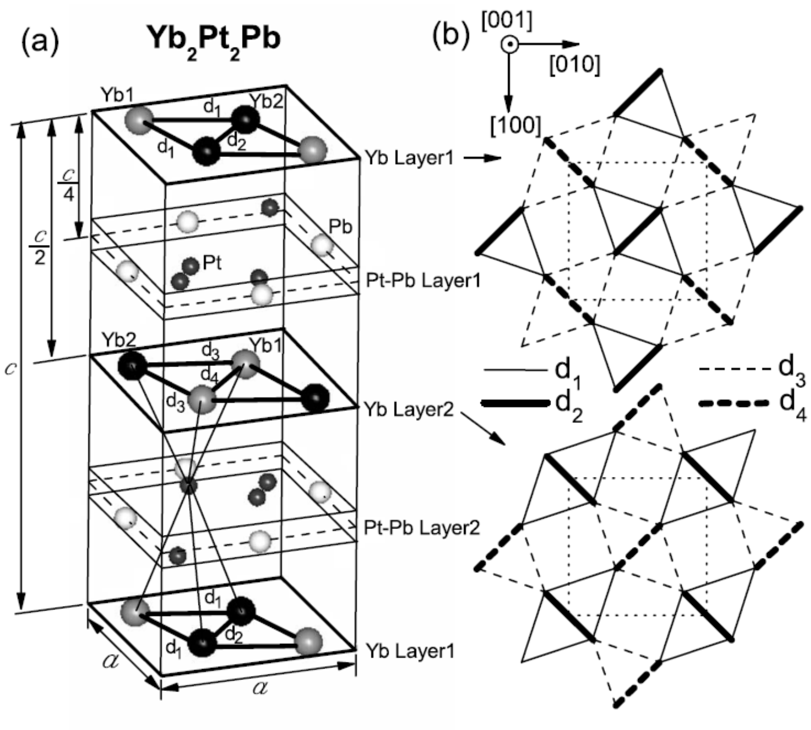
-Magnetic moment < $5f^2$

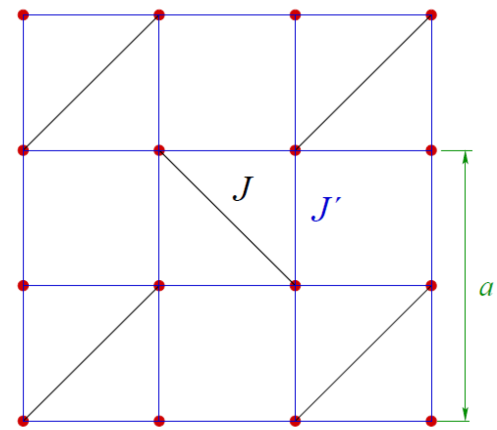


Sheng & Cooper, 1996

2- Frustrated Kondo lattice *(Collaboration: B. H. Bernard, B. Coqblin)*

Intermetallics with Shastry-Sutherland lattice:



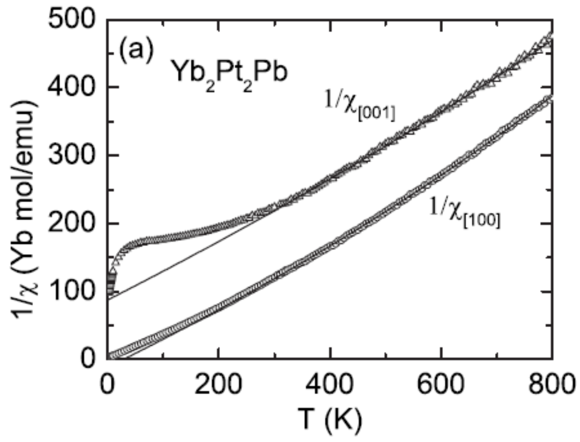


Topology similar to Shastry-Sutherland

GS: RVB singlets if J/J' ≳ 1.6

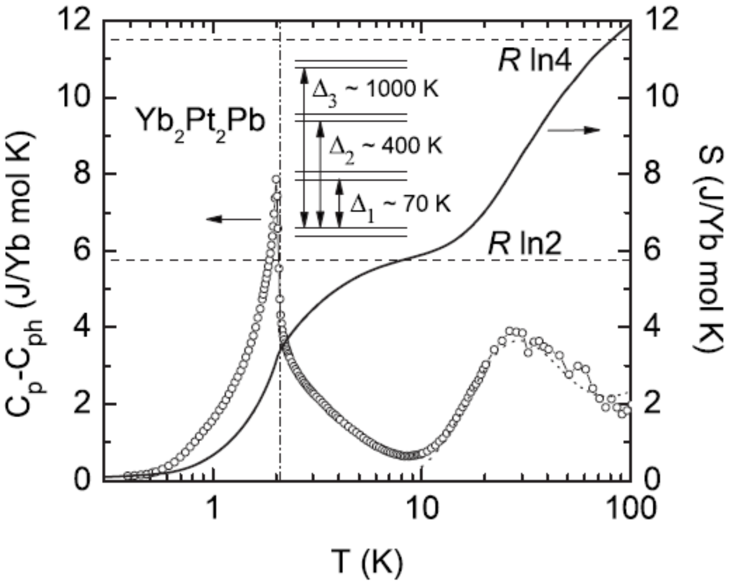
Yb_2Pt_2Pb *(Kim et al 2008)*, Ce_2Pd_2Sn *(J. Sereni at al, 2009)*

Experimental evidence of frustration and Kondo effect (*Kim et al 2008*)



Frustration:

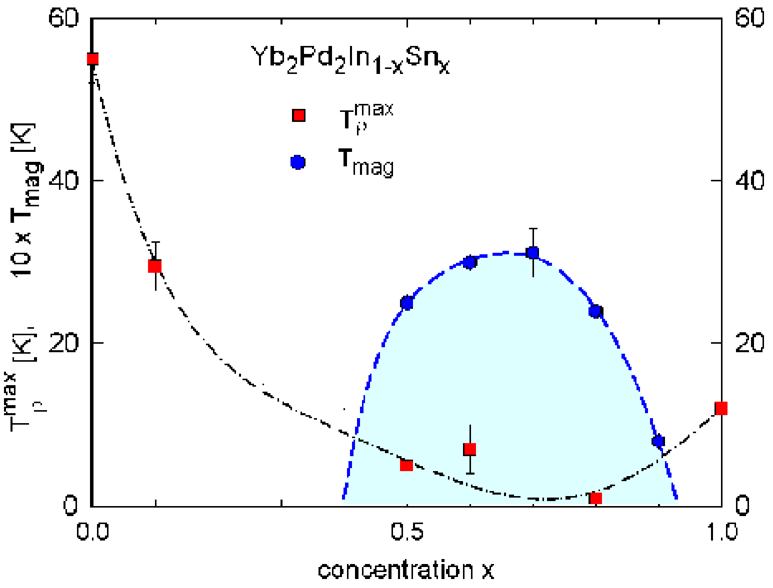
- T_N = 2°K, Θ_p = 217K
- Long wave spiral state
- Magnetic fluctuations above T_N

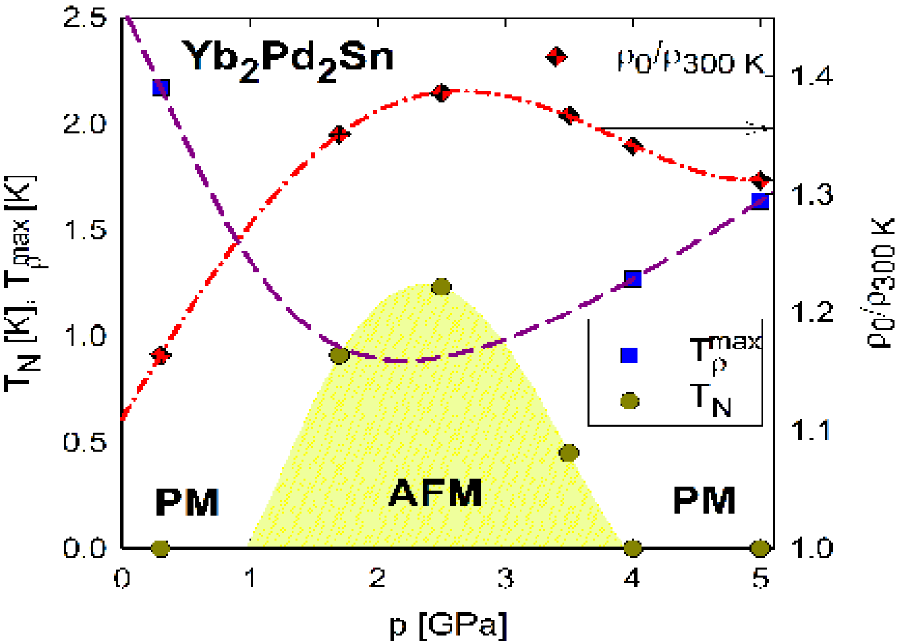


Kondo:

- γ = 311 mJ $mole^{-1}$ K^{-2}
- resistivity

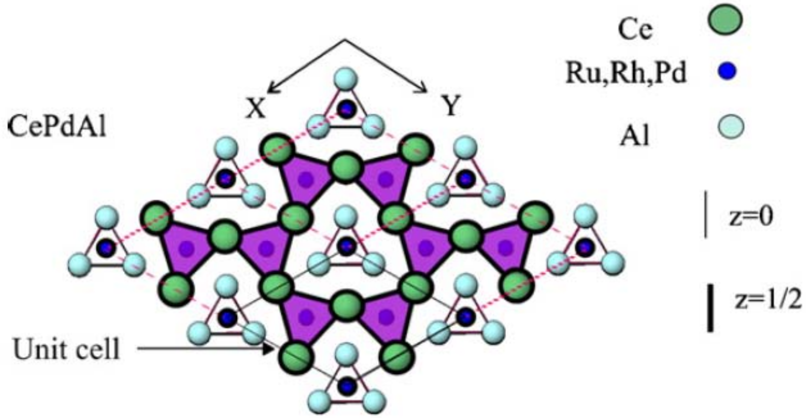
Yb_2Pd_2Sn: 2 magnetic-non-magnetic transition as a function of x or pressure *(Bauer et al, 2008)*

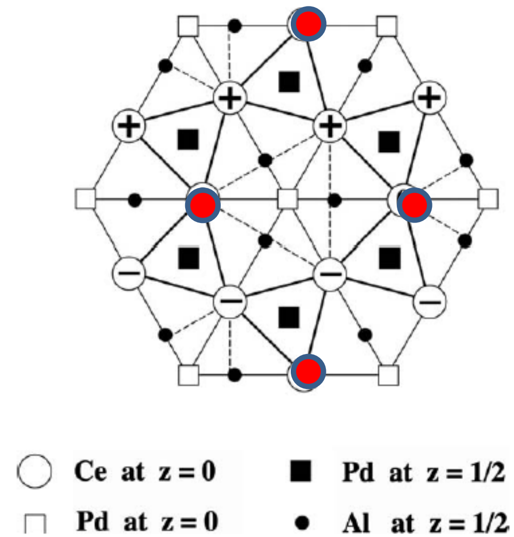




T_ρ^{max}: 'coherence temperature'

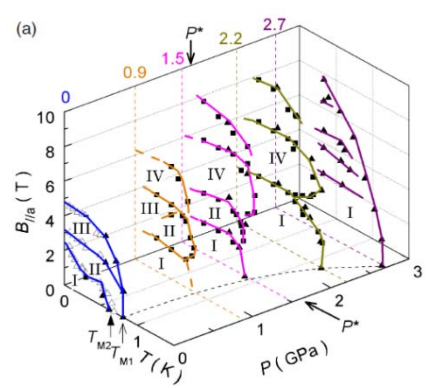
Quasi-Kagome Kondo lattice systems : YbAgGe, YbPtAl, CePdAl…





Dönni et al, 1996

Evidence for Kondo effect: magnetic structure contains magnetic and non-magnetic (Kondo) Ce sites



Frustration + Kondo effect:

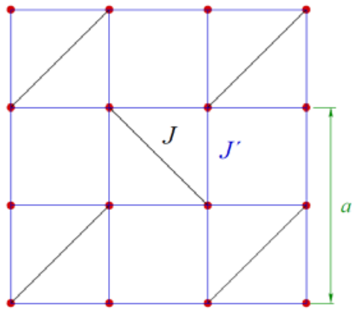
Complicated phase diagrams

YbAgGe (*H. Kubo et al, 2010)*

Kondo lattice in frustrated structure:

- Kondo effect ⇒ local singlet
- Frustration ⇒ non-local singlet

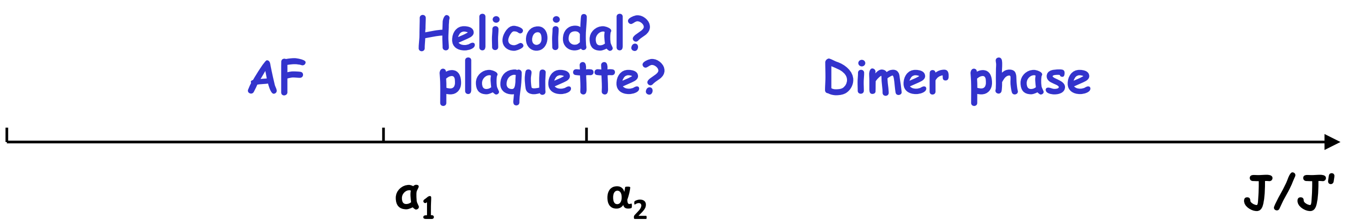
$$H = \sum_{<ij>} J \vec{S_i} . \vec{S_j} + \sum_{<ik>} J' \vec{S_i} . \vec{S_k}$$



In Shastry-Sutherland lattice:

- local singlets on strong bonds (J>>J')
- magnetic order if J<<J'
- intermediate phase

Possible phase diagram of Heisenberg spins on Shastry-Sutherland lattice



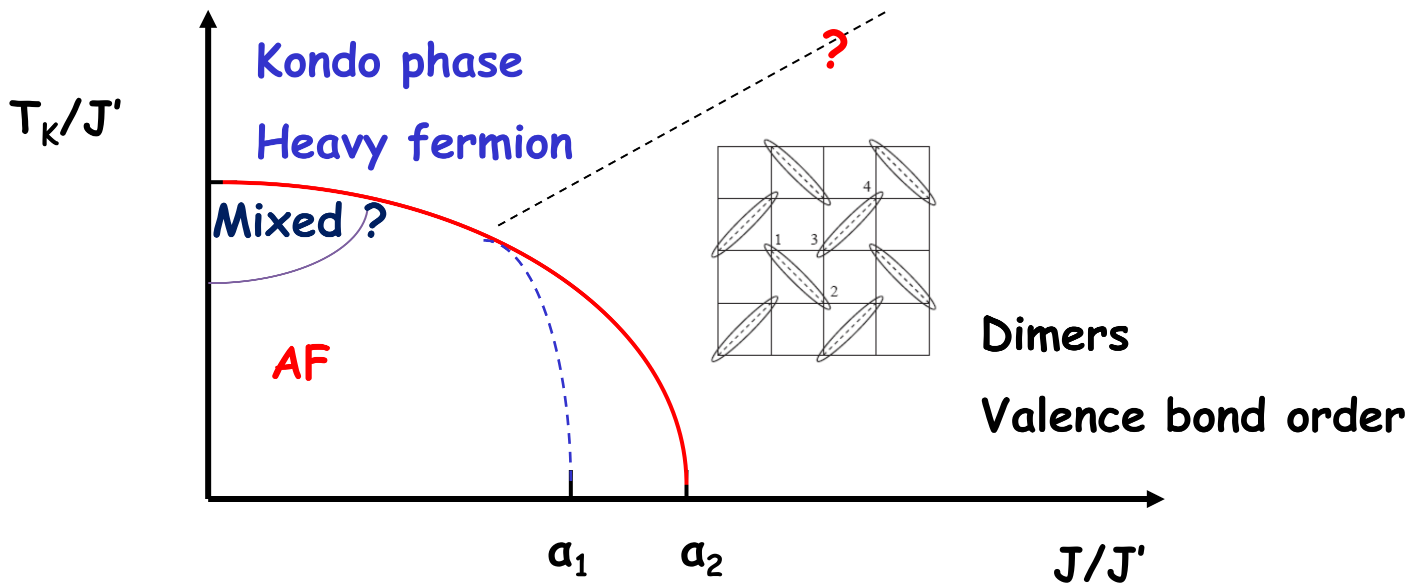
$\alpha_1 \approx 1.2$

$\alpha_2 \approx 1.6$

Kondo lattice: Heisenberg spins + conduction electrons

C. Lacroix, B.H. Bernhard

$$H = \sum_{<ij>} J\vec{S_i}.\vec{S_j} + \sum_{<ik>} J'\vec{S}_i.\vec{S_k} - J_K\sum_i \vec{S_i}.\vec{\sigma_i} + \sum_k \varepsilon_k n_{k\sigma}$$



Description within Kondo lattice model :

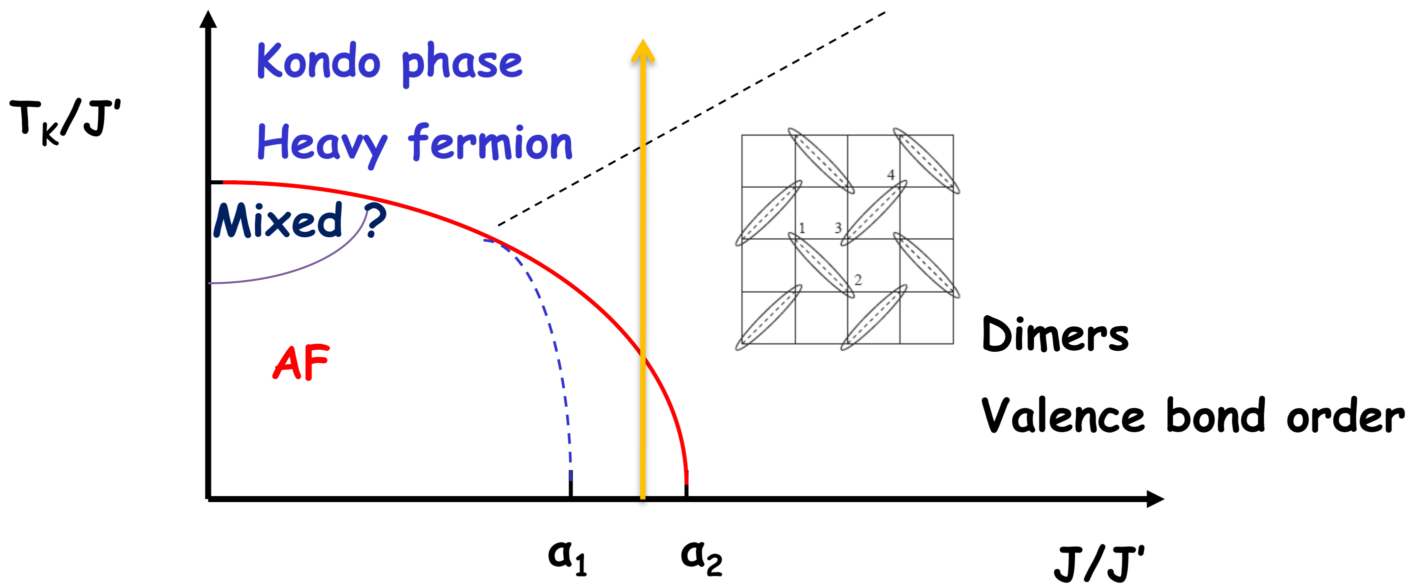
-Dimer correlations $\Gamma_{ij} = \langle f^+_{i\sigma} f_{j\sigma}\rangle$ (valence bond parameter)

-Kondo correlations $\lambda = \langle f^+_{i\sigma} c_{i\sigma}\rangle$ (local f-c correlations)

-Magnetic order: $M = \langle S_{iz}\rangle$, $m = \langle \sigma_{iz}\rangle$ (f and c magnetizations)

Kondo lattice: Heisenberg spins + conduction electrons

C. Lacroix, B.H. Bernhard



Increase of T_K/J' (pressure): AF ⟶ Dimer phase ⟶ Kondo phase

2 quantum critical points?

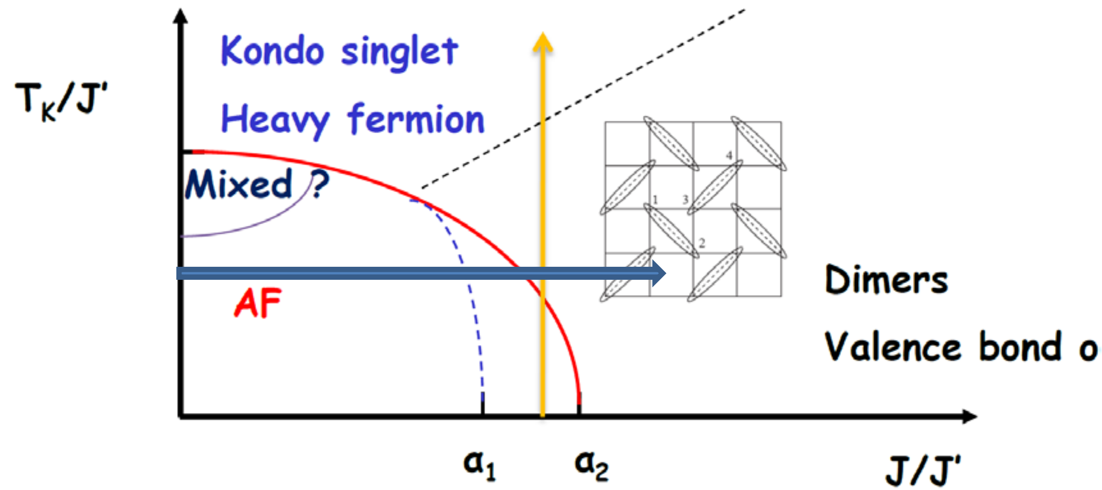
-Dimer correlations

$$\Gamma_{ij} = \langle f_{i\sigma}^{+} f_{j\sigma} \rangle \quad (\Gamma, \Gamma')$$

-Kondo correlations

$$\lambda = \langle f_{i\sigma}^{+} c_{i\sigma} \rangle$$

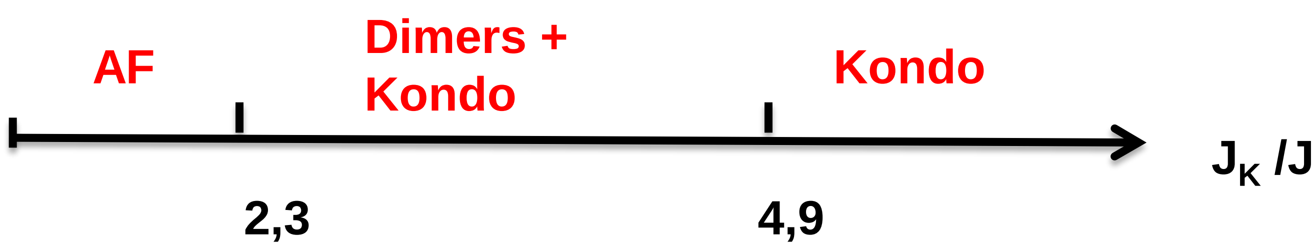
-Magnetic moment $M(q)$



Comparison of several possible ground states

$J_K = 6J$

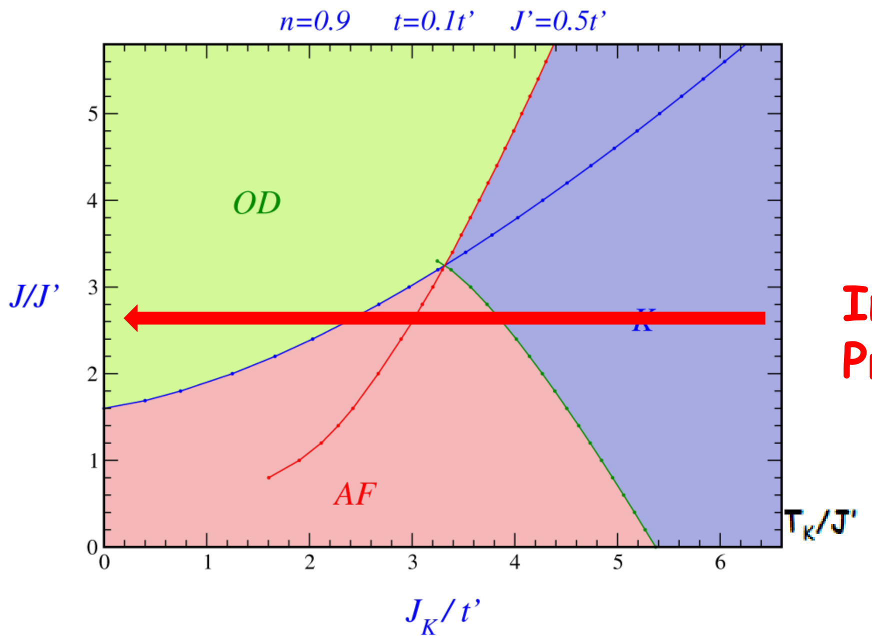
J = J'

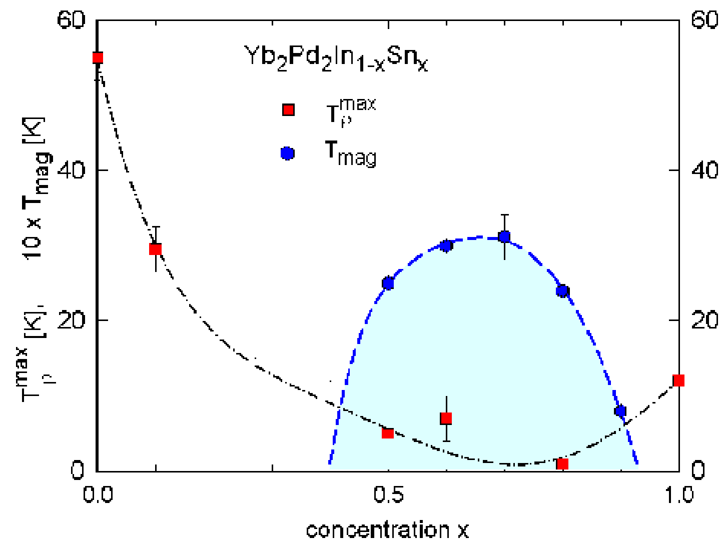


2 quantum critical points under pressure?

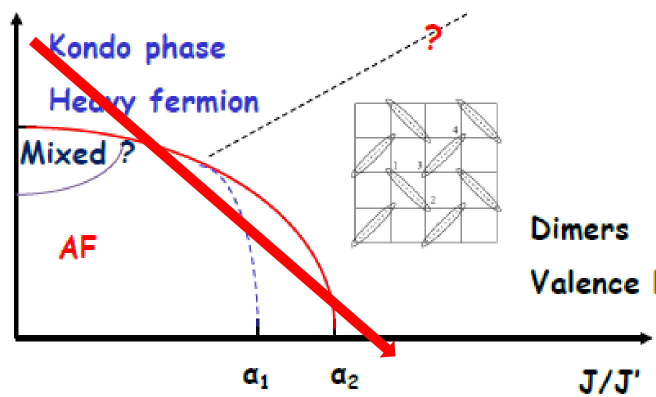
Some results for the Shastry-Sutherland lattice

OD: dimers phase
AF: long range antiferromagnet
K: Kondo phase





Increasing Pressure



In Yb compounds T_K usually decreases with pressure

2 quantum critical points

Summary

<u>Phase diagrams of the Kondo lattice in 2 different situations:</u>

- S=1 underscreened Kondo lattice: coexistence of ferromagnetism and Kondo effect ⇒ application to actinides compounds

- Kondo lattice on frustrated lattice: 2 possible origins for a non-magnetic GS ⇒ frustrated Ce and Yb compounds
Possibility of 2 different QCP in the same system

Kondo lattice problem is still an active field of research for more than 30 years (Doniach's diagram 1977).