**Lecture Notes** 

# Introduction to Strongly Correlated Electron Systems

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**Mohsen Abd-Elmeguid** 

**II. Institute of Physics, University of Cologne, Germany** 

# Introduction to strongly correlated electron systems

## **I. Introduction**

Brief summary of electrons in solids, origin of strong electron correlations

## **II.** Classes of strongly correlated electron systems

#### (a) Transition metal compounds: 3d-electrons

- Hubbard model, Mott insulator, metal-insulator transition
- Spin, charge, and orbital degrees of freedom and ordering phenomena, selected materials
- Pressure effect on the ground state properties of transition metal compounds

#### (b) Heavy fermion systems: 4f (5f) – electrons

- Landau Fermi-liquid model, Kondo effect, heavy fermion systems, non-Fermi liquid, quantum phase transitions, selected materials

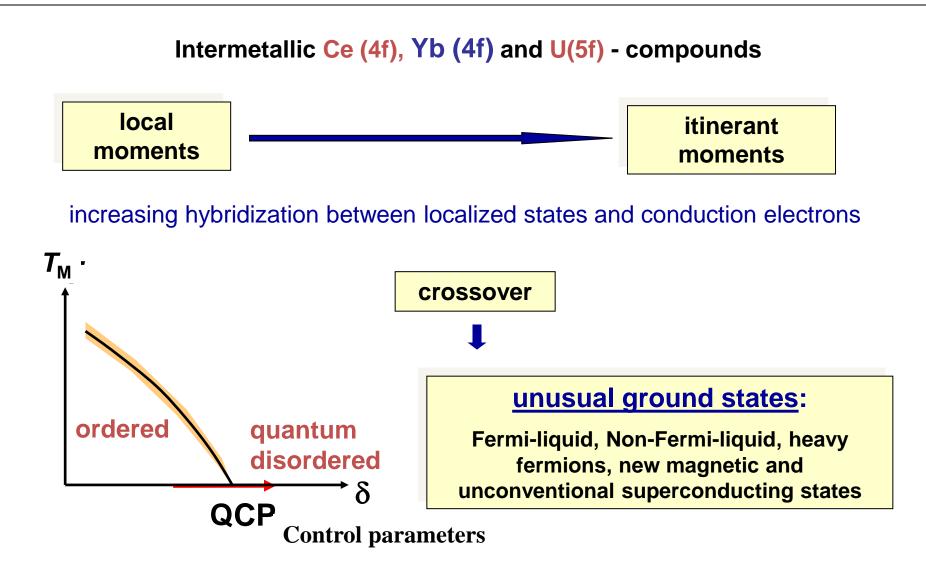
- Pressure effect on the ground state properties of heavy fermion compounds

#### (c) Nanoscale structures:

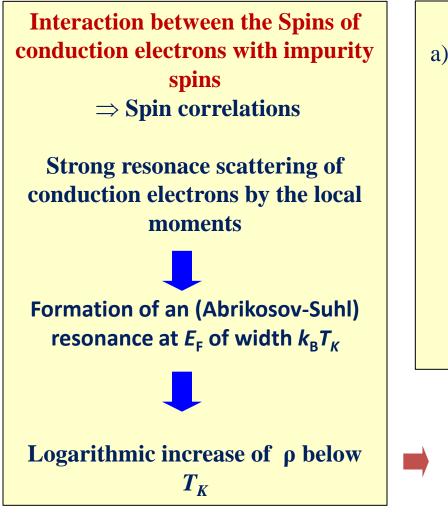
- Quantum confinement, unusual properties for potential applications

### **III. Summary and open discussion**

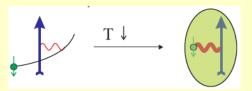
## Heavy fermion metallic systems



## Physical picture: crossover magnetic ↔ nonmagnetic



a) impuity magnetic Moment is screend by the Spins of conduction electrons. This leads to formation of a local Singlet state



b) Energy lowering due to formation of a Kondo-state:  $_{1}_{K_{B}}T_{K} = De^{-\frac{1}{|J|N(E_{F})}}$ 

Crossover: magnetic ↔ nonmagnetic weak ↔ strong coupling

# Kondo effect in concentrated alloys

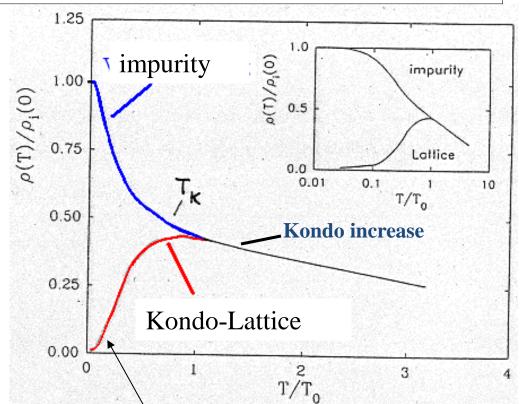
Kondo-lattice systems (heavy fermions)

# **Properties of Kondo-Lattice systems (Heavy Fermions)**

#### Electrical resistivity: deviation from single ion behavior

**Periodicity of the lattice** 

Coherent scattering of conduction electrons on magnetic impurities



resonace type increase of the density of state at Fermi level.

Formation of an Abrikosov-Suhl resonance at  $E_{\rm F}$ 

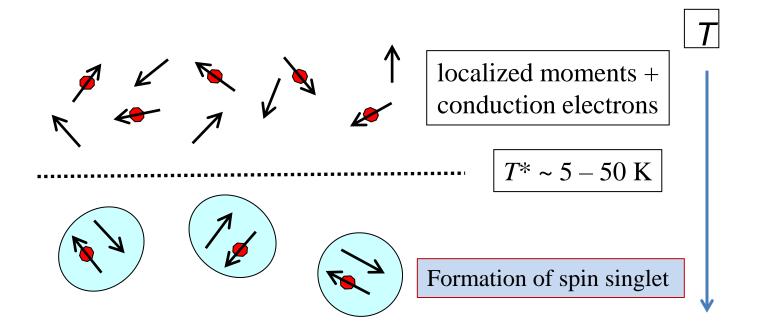
$$T \rightarrow 0:$$
  

$$\rho(T) = \rho_0 + AT^2$$
  
(Fermi-liquid state)

 $A \propto [D(E_F)^2]$ (electron-electron interaction)

## **Kondo-lattice systems (heavy fermions)**

Lattice of certain *f*-electrons (most Ce, Yb or U) in metallic environment Ce<sup>3+</sup>:  $4f^1$  (J = 5/2), Yb<sup>3+</sup>:  $4f^{13}$  (J = 7/2) partially filled inner 4f/5f shells  $\rightarrow$  localized magnetic moment CEF splitting  $\rightarrow$  effective S=1/2



# **Kondo-lattice systems (heavy fermions)**

characeristic temperature  $T^*$ 

*T* >>*T*\*: local moment behavior

*T* << *T*\*: nonmagnetic heavy fermion liquid (Fermi liquid grond state)

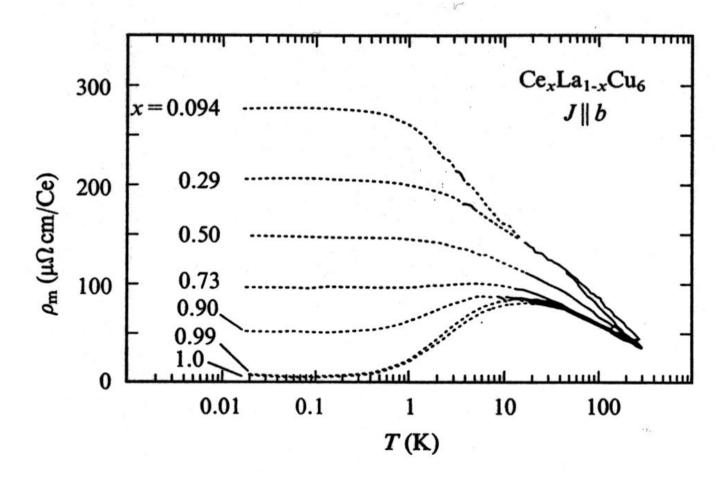
## See board!

Properties of heavy fermion systems

mormal metal heavy fermion system Characteristic Temp. T\*:  $\frac{g_{1}}{f_{0}} = \frac{g_{0} - T^{2}}{30 \text{ K}} T$   $\frac{g_{0}}{f_{0}} = \frac{g_{0} + AT^{2}}{30 \text{ K}} A \text{ remylight}$   $A \sim \delta^{2}$  $p_{o}$  T  $p_{o}$  T T T TT>To : local moment behavior X(T) -> Curie-Weiss' P(T) - InT (Kondo! T&T nonmagnetic heavy  $X \uparrow f$  lokalisiert  $T_N X = \frac{R}{T+\Theta}$  $X - X_{o} \times \mathcal{X}_{o} \neq D(\mathcal{E}_{\mathcal{F}}), high!$  $X = \frac{H}{T + \Theta}$ fermion liquid =) FL ground soft with large D(EF) X Pauli 5-100K -----→T 10K X(T) dm d I 𝔅(T), 𝔅 𝔍 𝑘<sup>™</sup> 𝔬 ⊥ 𝑘<sup>™</sup> 𝔅  $\stackrel{C}{=} \gamma \cdot T_{+} \beta T^{3}$   $\forall \neq D(E_{F})$ Yo Yo Very light T\* 2 K S(T) d S (T)~  $\mathcal{S}(\tau) \ll A T^2, A \sim \partial_{y}^2$ 1. 8~1mJ/(Kimol)\_2 Wilson's radio Ra 1 -> show some examples.

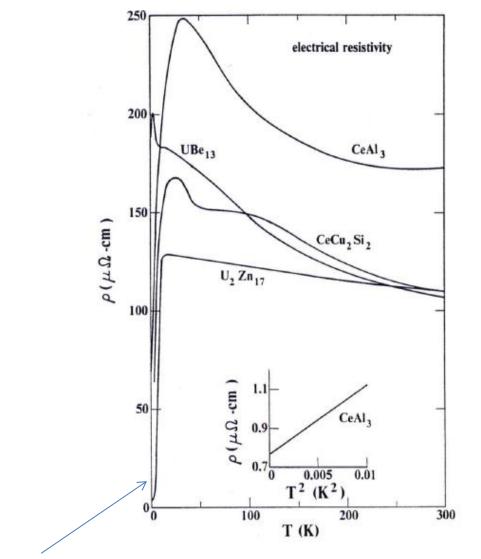
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Development of coherent scattering in Ce-based alloy



Onuki and Komatsubara (1987)

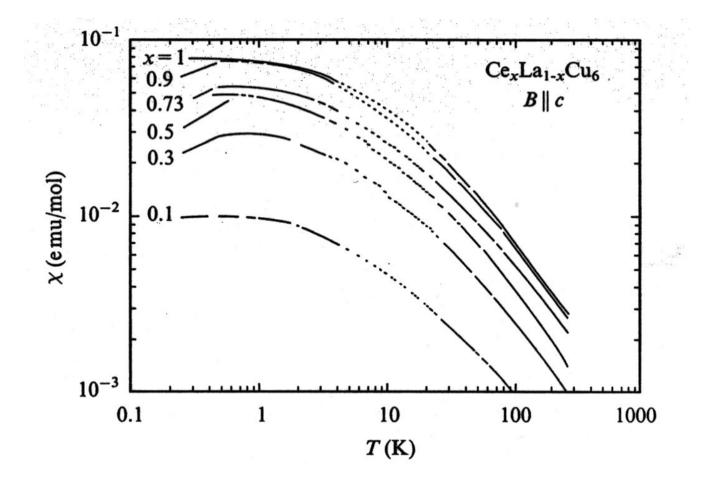
#### Kondo-Lattice, heavy fermion systems





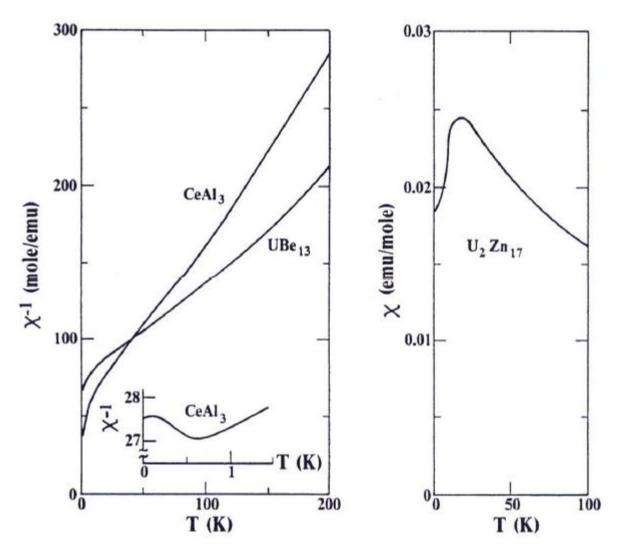
After Fisk, Ott, Rice & Smith 86

**Coherent heavy fermions** 



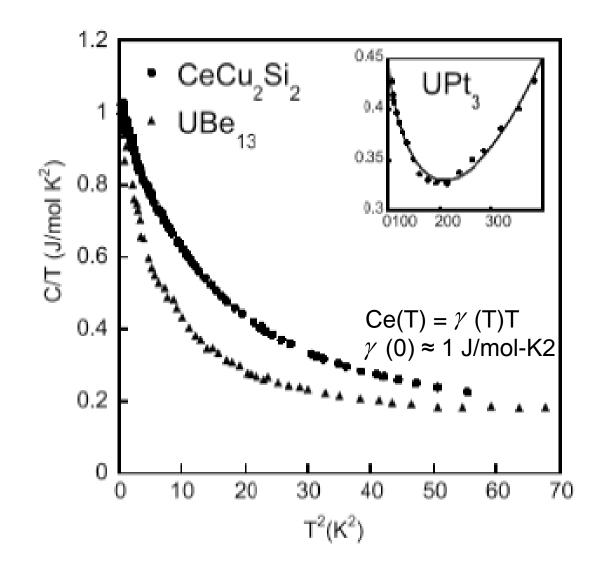
Onuki and Komatsubara (1987)

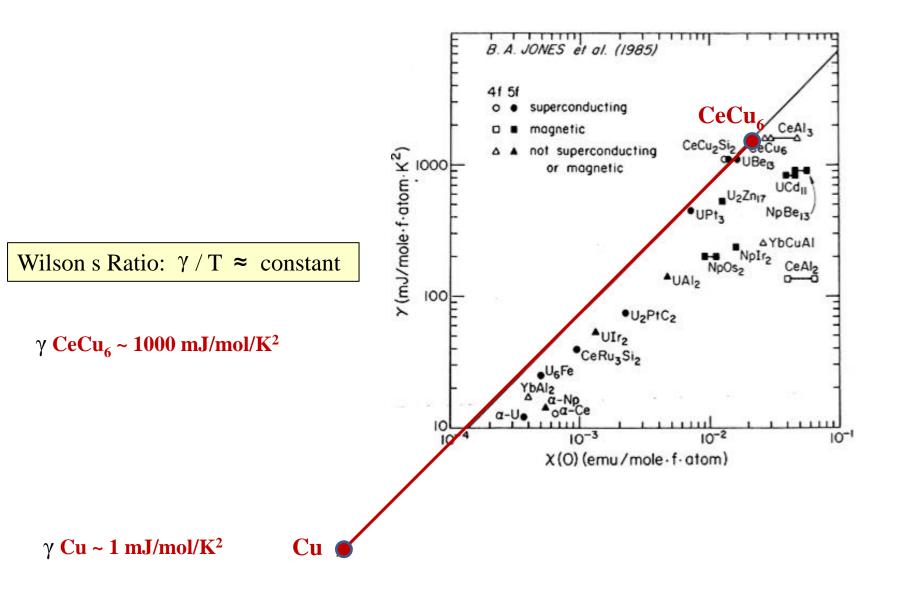
#### magnetic susceptibility



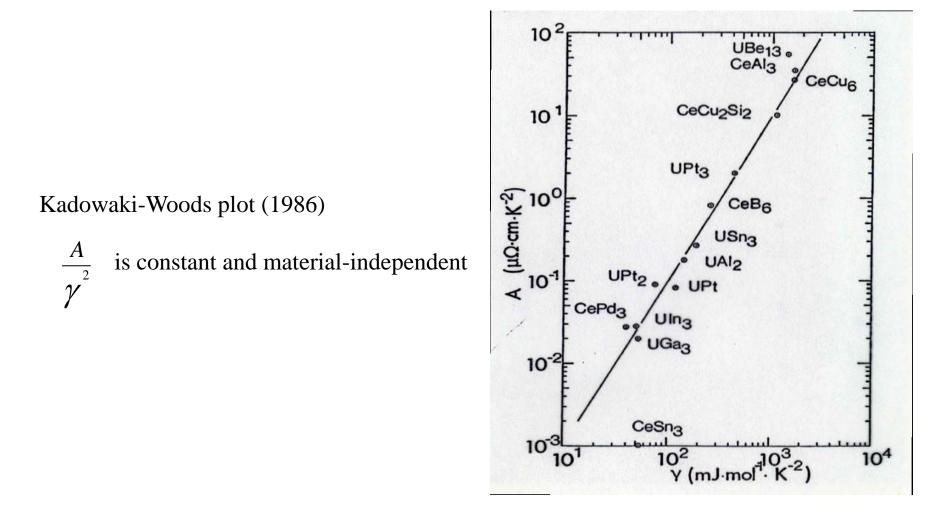
After Fisk, Ott, Rice & Smith 86

 $C/T = \gamma$  vs T2 for CeCu2Si2, UBe13, and UPt3  $\longrightarrow$  very high  $\gamma$  (effective mass!)





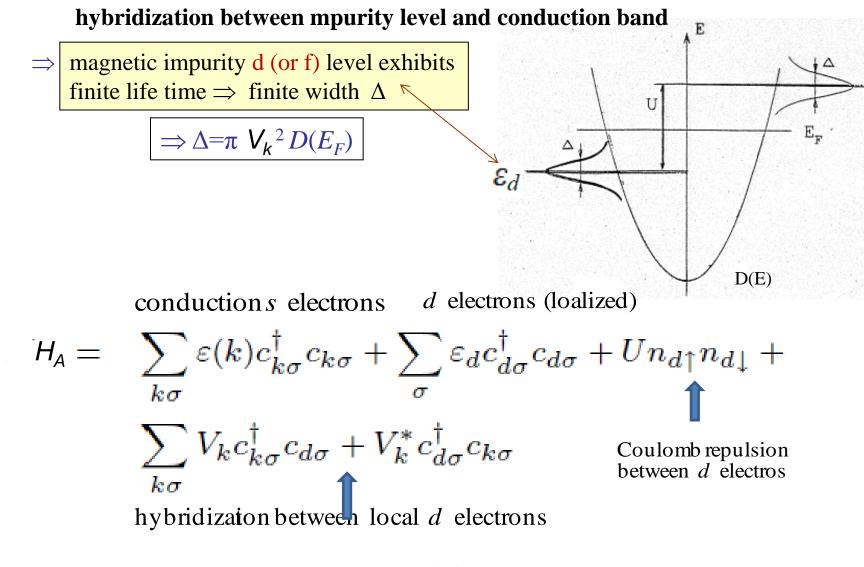
### electron-electron scattering



Observed for a large number of heavy fermion systems

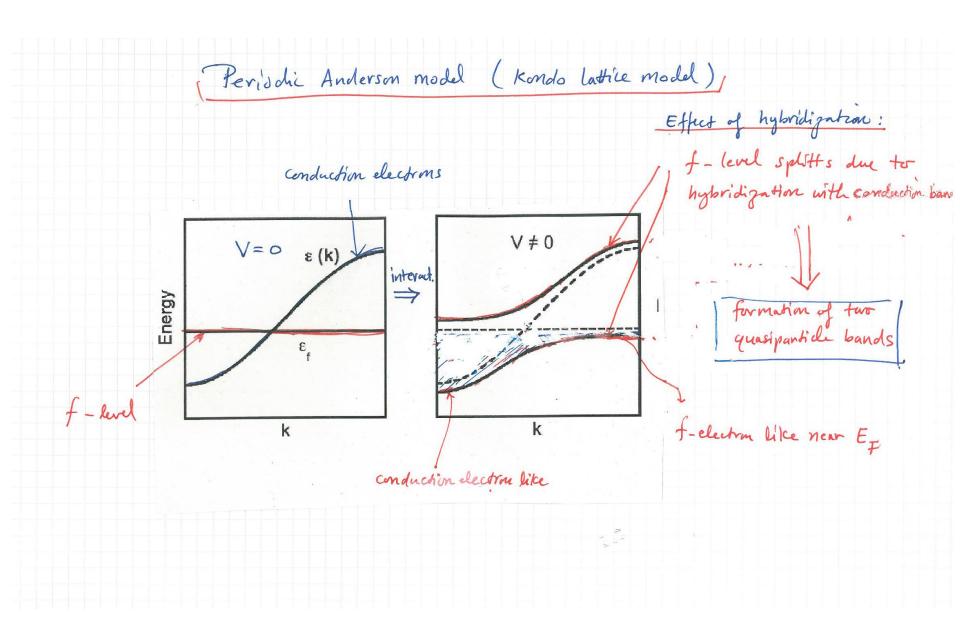
## Theoretical description of heavy fermions Kondo-lattice model

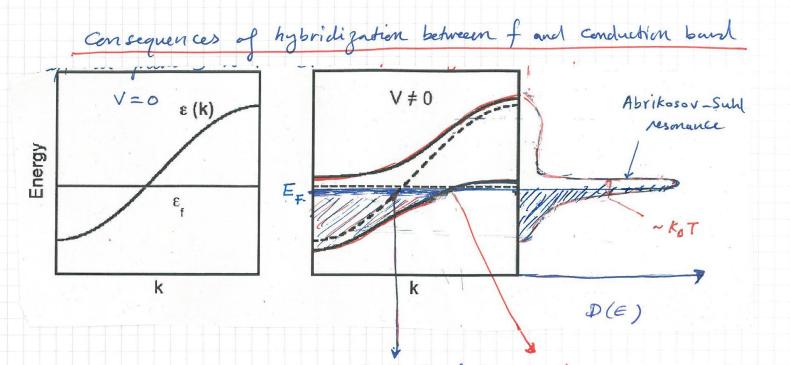
#### The Anderson model (961)



and conduction s electrons  $(\Delta)$ 

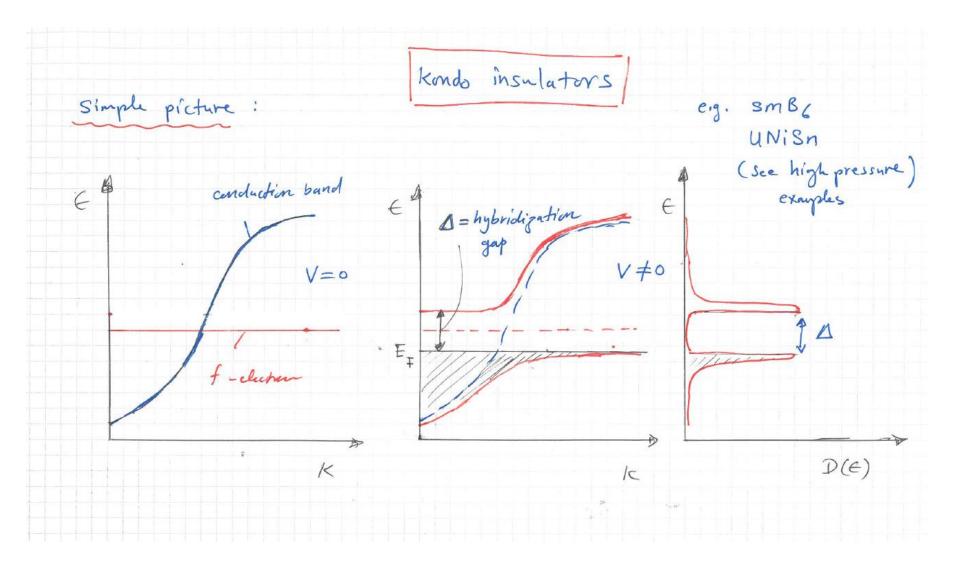
Theoretical description of them heavy fermines generalizing the single impurity Anderson model Kondo-lattile model: (periodic Anderson model) to a lattice of localized of cristals f. Coulomb repulsion between f electrons hybridization between f and conduction band. local f moments if : is U large and E is negative uning Schrieffer-Will transformation => Kondo lattice model:  $\mathcal{H} = \sum_{k=0}^{t} c_{k} c_{k} c_{k} + J \sum_{i} S_{i} S_{i} - S_{i}$   $J = 2V^{2} \left( \frac{1}{1 + \frac{1}{\epsilon_{f} + \mu}} \right) 70$   $kondo coupling = \frac{1}{2} \left( \frac{1}{1 + \frac{1}{\epsilon_{f} + \mu}} \right) 70$ - Ly





KF (conduction clec.) KF (conduction electron + f electr.)

★ a FL ground state can be expected if the local moments are screened by a lattice generalization of the Kondo effect. The onset of kundo screening at T to Tk \* the resulting FL ; formed below a coherence temperature Tcoh ; Tcoh < Tk => coherent scattering of conduction dectron by the local f moments => resonance type increase of the density if states at E => formation of an Abrikosov-Suhl resonance at E with width ~ k<sub>B</sub>Tk => high density if states => high effective mass m\* 1



Consequences of hybridigation:  
=> f - electrons participate to the Fermi surface (FS)  
=> harge values of the Fermi surface  

$$V_{FS} = 4\pi^{3} (n_{c} + n_{F}) [, n_{c} = n_{c} + f - electrons$$
further comments:  
\* T > T\_{ch} => local moments exsist => System has a Fermi values  
described by cond. electrons => V\_{FS} = 4T n\_{c} (undly small)  
\* T ~ T\_{ch} : The FS fluctuates strongly => resistivity is enhanced  
T\_{ch} (=> resistivity maximum (experimentel point of view)  
\* T < T\_{ch} := screening of local moments:  
=> FL behavior in the Kondo lattice  
=> FL behavior in the Kondo lattice  
=> fluctuates of the FL maybe magnetic order  
=> other competitors of the FL maybe magnetic frastration,  
spin glaes and Spin liquid

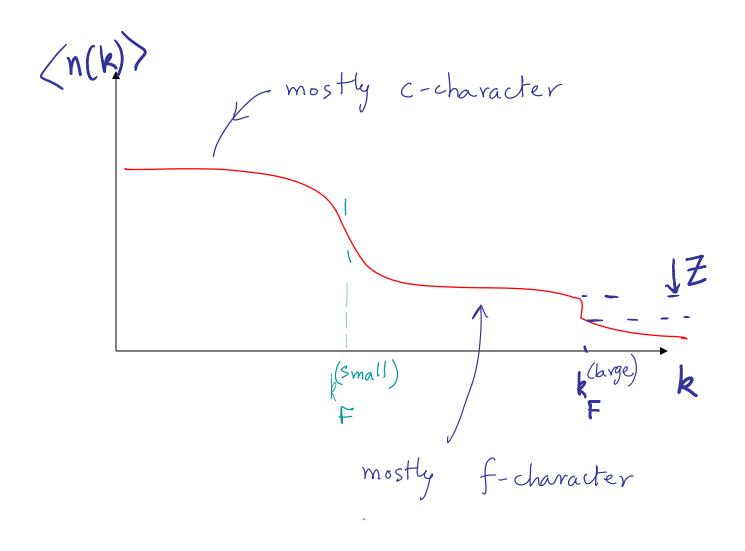
## **Experimental support for description of heavy fermion metals by Landau Fermi Liquid Theory**

-The volume of the Fermi surface includes the f electrons.

-The measured quasiparticle mass accounts for the enhanced specific heat.

Both these observations confirm the success of Fermi liquid theory.

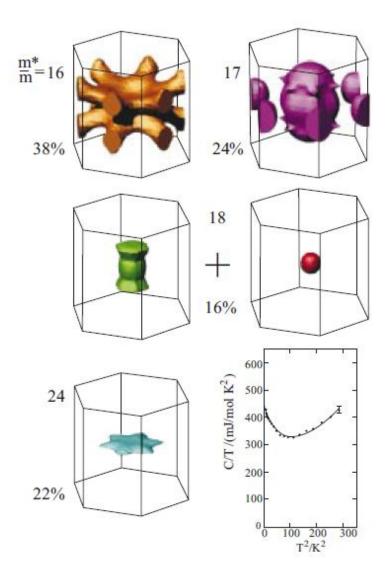
## Momentum distribution



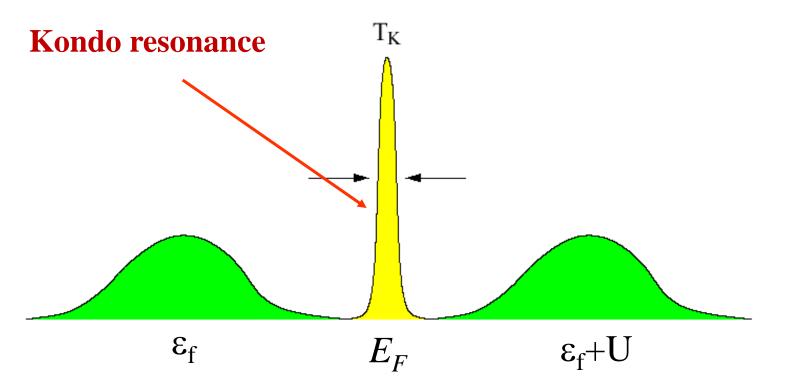
#### The f electrons participate to the Fermi surface

#### Example: UPt3

Figure 7: The consistency of the Fermi liquid description has been demonstrated in UPt3. The Fermi surface sheets (from Julian and McMullan 1998) and Effective mass of the quasiparticles have been mapped out by de Haas van Alphen measurements (Taillefer and Lonzarich 1988). They confirm that the *5f3 electrons* are absorbed into the Fermi liquid and that the quasiparticle masses are consistent with the mass enhancements measured in specific heat (after Stewart *et al.* 1984). The percentages reflect the contribution from quasiparticles on each sheet to the total specific heat.

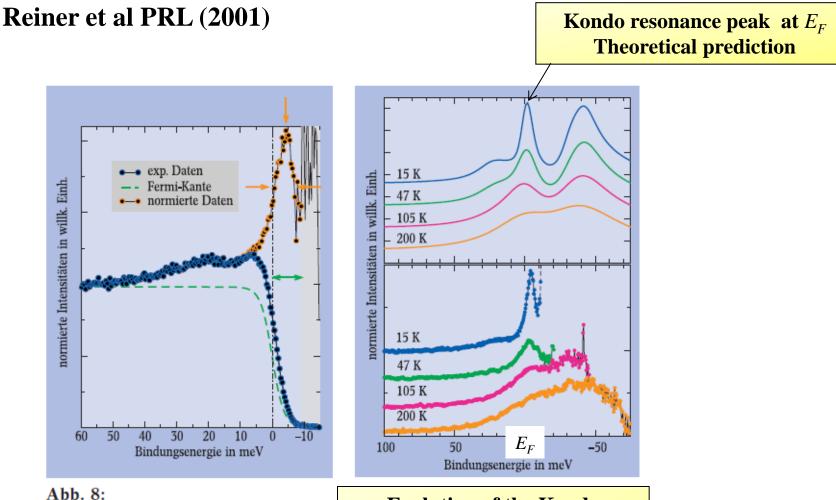


can we observe the Kondo resonance experimentally?



Formation of an (Abrikosov-Suhl) resonance at  $E_{\rm F}$  of width  $k_{\rm B}T_K$ 

## **High-resolution photoemission spectroscopy of CeCu2Si2**



Hochaufgelöstes Photoemissionsspektrum an  $CeCu_2Si_2$  bei T=11 K in der Nähe der Fermi-Energie, vor und nach einer Normierung auf die Fermi-Verteilung. Nach der Normierung wird die Existenz der scharfen Kondo-Resonanz deutlich, deren Breite und Energie nur wenige Millielektronenvolt beträgt. Evolution of the Kondo resonance peak at  $E_F$ at low temperatures

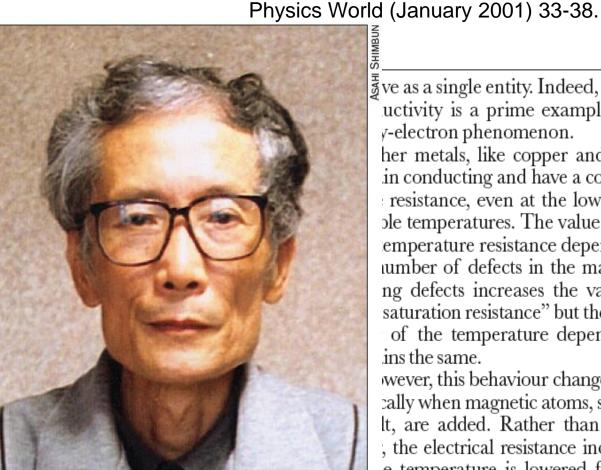
# Kondo Effect in Mesoscopic Systems

Nanotechnology has rekindled interest in the Kondo effect, one of the most widely studied phenomena in condensed-matter physics

# **Revival of the Kondo effect** Leo Kouwenhoven and Leonid Glazman,

WHY would anyone still want to stu physical phenomenon that was di ered in the 1930s, explained in the 1 and has been the subject of nume reviews since the 1970s? Although Kondo effect is a well known and w studied phenomenon in conder matter physics, it continues to car the imagination of experimentalist theorists alike.

The effect arises from the interac between a single magnetic atom, as cobalt, and the many electrons otherwise non-magnetic metal. Suc impurity typically has an intrinsic a lar momentum or "spin" that inte with the electrons. As a result, the m motion description of the grater is

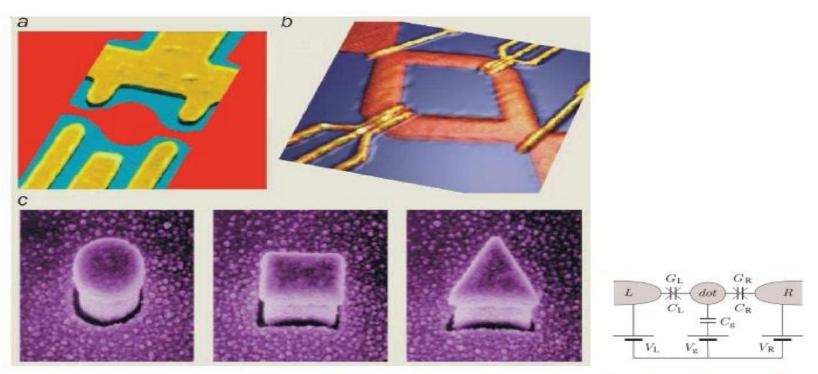


∛ve as a single entity. Indeed, supeructivity is a prime example of a

y-electron phenomenon. her metals, like copper and gold, in conducting and have a constant resistance, even at the lowest acole temperatures. The value of the emperature resistance depends on number of defects in the material. ng defects increases the value of saturation resistance" but the charof the temperature dependence ins the same.

wever, this behaviour changes dracally when magnetic atoms, such as lt, are added. Rather than satur-, the electrical resistance increases tomporature is lowered further

Quantum dots – mesoscopically fabricated, tunneling of single electrons from contact reservoir controlled by gate voltage



Regions that can hold a few hundred electrons! Can drive a current through these! This *is* Nano!

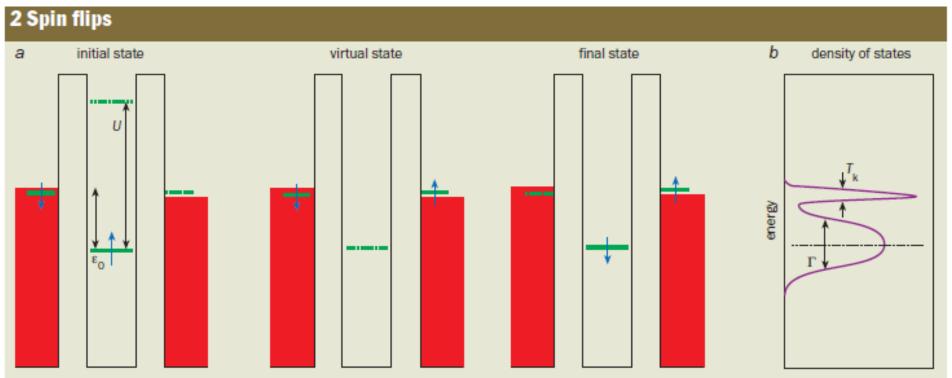
How is conduction related to the Kondo effect?

#### Physics World (January 2001) 33-38

# 1 The Kondo effect in metals and in quantum dots

(a) As the temperature of a metal is lowered, its resistance decreases until it saturates at some residual value (blue). Some metals become superconducting at a critical temperature (green). However, in metals that contain a small fraction of magnetic impurities, such as cobalt-in-copper systems, the resistance increases at low temperatures due to the Kondo effect (red). (b) A system that has a localized spin embedded between metal leads can be created artificially in a semiconductor quantum-dot device containing a controllable number of electrons. If the number of electrons confined in the dot is odd, then the conductance measured between the two leads increases due to the Kondo effect at low temperature (red). In contrast, the Kondo effect does not occur when the dot contains an even number of electrons and the total spin adds up to zero. In this case, the conductance continuously decreases with temperature (blue).

#### Physics World (January 2001) 33-38



(a) The Anderson model of a magnetic impurity assumes that it has just one electron level with energy  $\varepsilon_0$  below the Fermi energy of the metal (red). This level is occupied by one spin-up electron (blue). Adding another electron is prohibited by the Coulomb energy, *U*, while it would cost at least  $|\varepsilon_0|$  to remove the electron. Being a quantum particle, the spin-up electron may tunnel out of the impurity site to briefly occupy a classically forbidden "virtual state" outside the impurity, and then be replaced by an electron from the metal. This can effectively "flip" the spin of the impurity. (*b*) Many such events combine to produce the Kondo effect, which leads to the appearance of an extra resonance at the Fermi energy. Since transport properties, such as conductance, are determined by electrons with energies close to the Fermi level, the extra resonance can dramatically change the conductance.

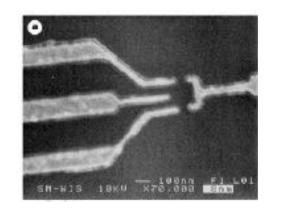
# Kondo effect in quantum dot

 $\epsilon_d + U$ 

ε<sub>d</sub>

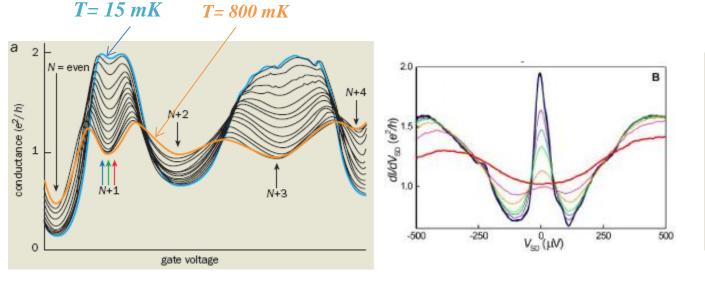
 $V_{\underline{SP}}$ 

Vg

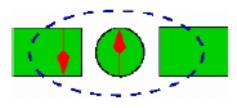


Single quantum dot

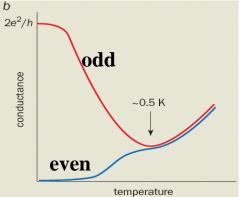
Goldhaber-Gorden et al. nature 391 156 (1998)



**Coulomb blockade** 



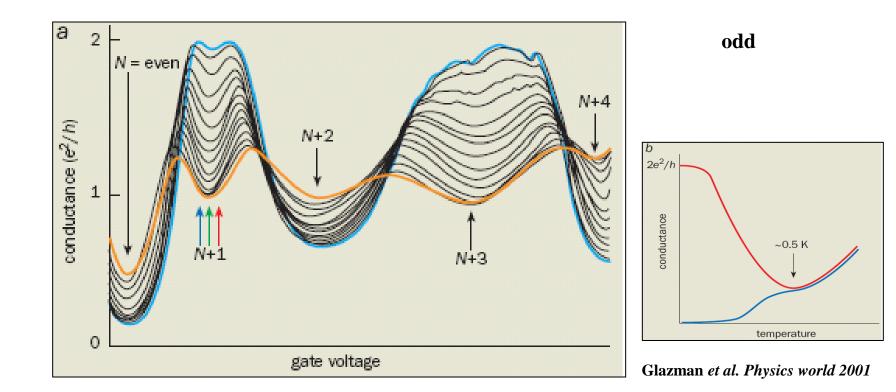
Kondo effect



#### conductance anomalies

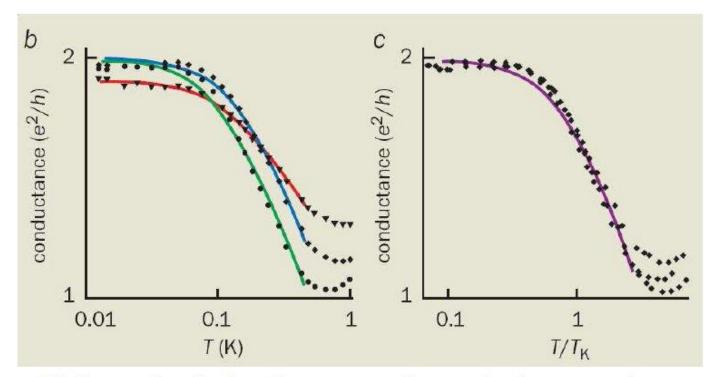
#### Glazman et al. Physics world 2001

L.Kouwenhoven et al. science 289, 2105 (2000)



L.Kouwenhoven et al. science 289, 2105 (2000)

#### Quantized conductance vs temperature



Universal relation between dimensionless conductance and temperature!

Gate voltage is used to tune  $T_K$ ; measurements at 50 to 1000 mK.

# 3 Single magnetic impurities under the microscope b a

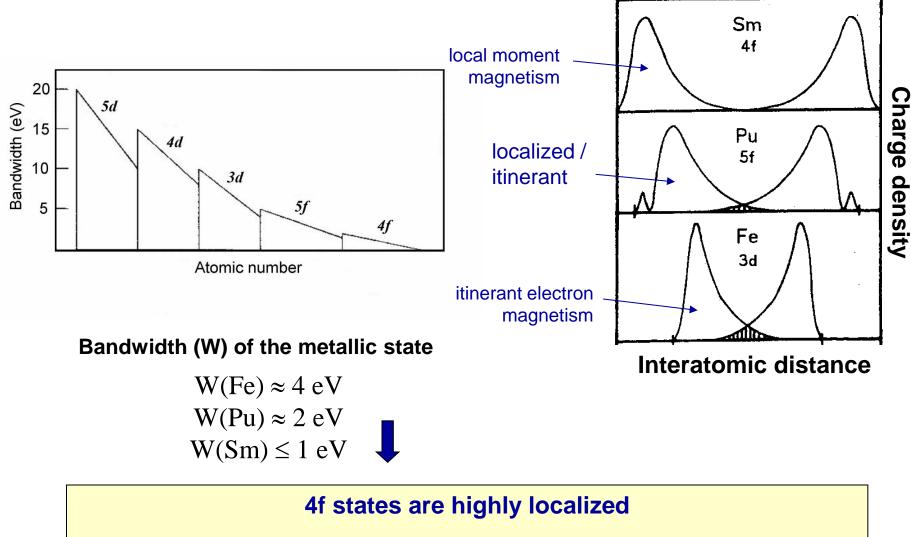
(a) By manipulating cobalt atoms on a copper surface, Don Eigler and colleagues at IBM have placed a single cobalt atom at the focal point of an ellipse built from other cobalt atoms (bottom). The density of states (top) measured at this focus reveals the Kondo resonance (left peak). However, elliptical confinement also gives rise to a second smaller Kondo resonance at the other focal point (right) even though there is no cobalt atom there. (b) Meanwhile, Mike Crommie and co-workers have measured two Kondo resonances produced by two separate cobalt atoms on a gold surface (top). When two cobalt atoms are moved close together using an STM, the mutual interaction between them causes the Kondo effect to vanish (data not shown).

# Question:

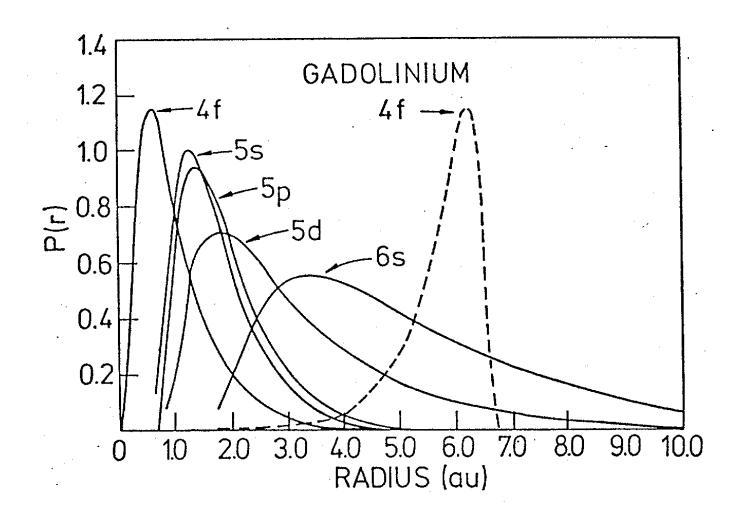
# What happens if the Kondo lattice system is magnetically ordered?

First step

We consider magnetic interaction between localized 4f moments in a metallic systems!



No direct interaction possible!

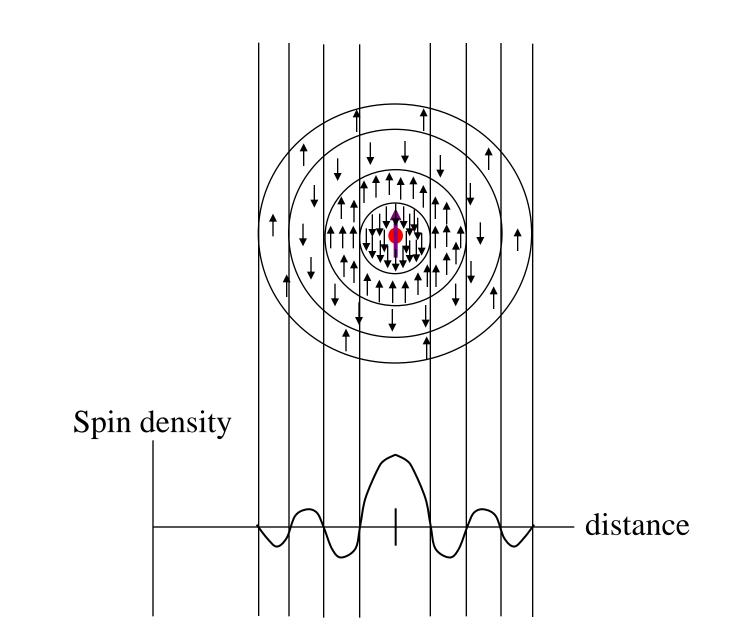


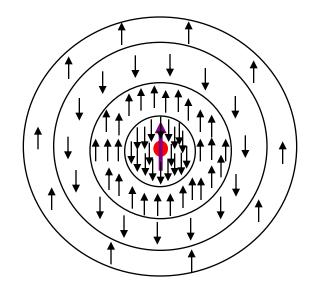
# Exchange in Rare Earths (4f electrons)

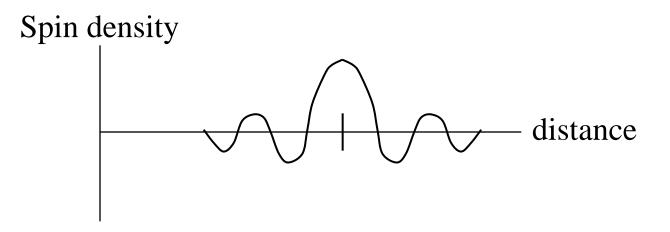
• Indirect exchange between 4f moments occurs:

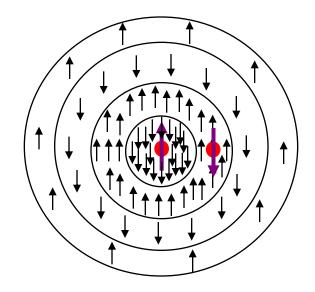
This type of exchange was first proposed by **R**uderman and **K**ittel and later extended by **K**asuya and **Y**osida to give the theory now generally know as the **RKKY** interaction.

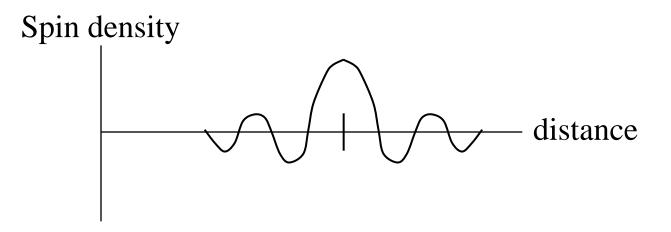
It is the dominant exchange interaction in metals where there is little or no direct overlap between neighboring magnetic electrons

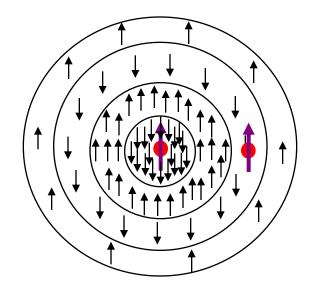


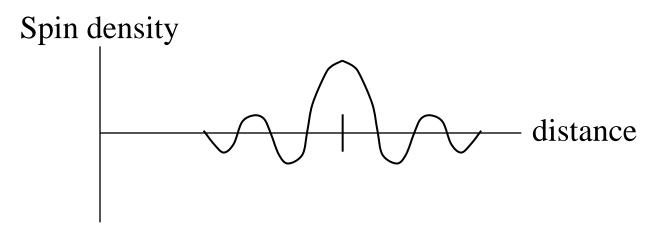


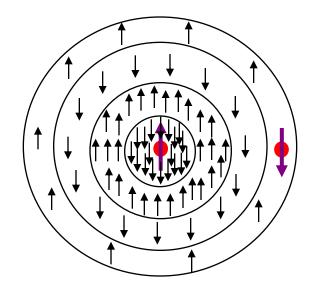


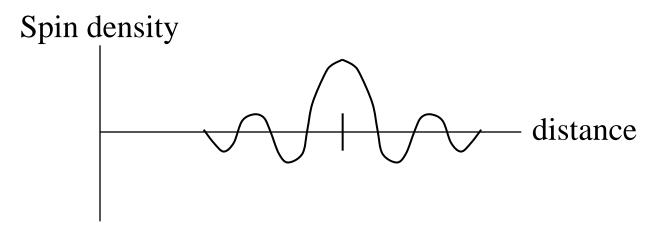












#### **RKKY** interaction: Description

Local moments (Spin  $S_i$ ) in a sea of conduction electrons with itinerant spin s(r)

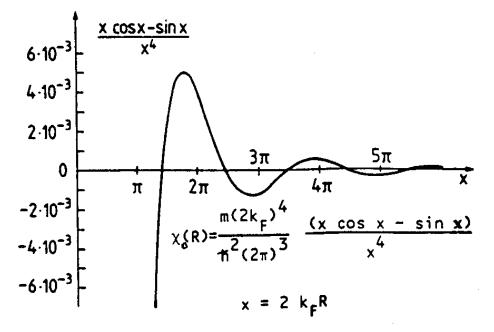
$$J(r) = 6\pi Z J N(E_F) \left[ \frac{\sin(2k_F r)}{(2k_F r)^4} - \frac{\cos(2k_F r)}{(2k_F r)^3} \right]$$

Ζ

J

k<sub>F</sub>

r



number of electrons / atom s-d exchange interaction  $D(E_F)$ DOS at Fermi energy Fermi momentum distance between impurities

=> Oscillations of value and sign

P.H. Dederichs in: Magnetismus von Festkörpern und Grenzflächen, 24. IFF Ferienkurs, Jülich 1993

#### Question:

#### What happens if the Kondo lattice system is magnetically ordered?

#### second step

# We consider in Kondo lattice the relatave strength of RKKY interaction and that of the Kondo effect

#### **Theoretical description**

Kondo-lattice-system: periodical arrangement of localized 4f- moments in a metallic matrix

#### **Competition between:**

Intrasite (on-site) interaction: Kondo-Effect  $E_{K} = k_{B}T_{K}$   $\Rightarrow$  screening of the magnetic moments  $\Rightarrow$  nonmagnetic ground state

Intersite interaction: **RKKY**,  $\mathbf{E}_{\mathbf{RKKY}} = \mathbf{k}_{\mathbf{B}}\mathbf{T}_{\mathbf{RKKY}}$ 

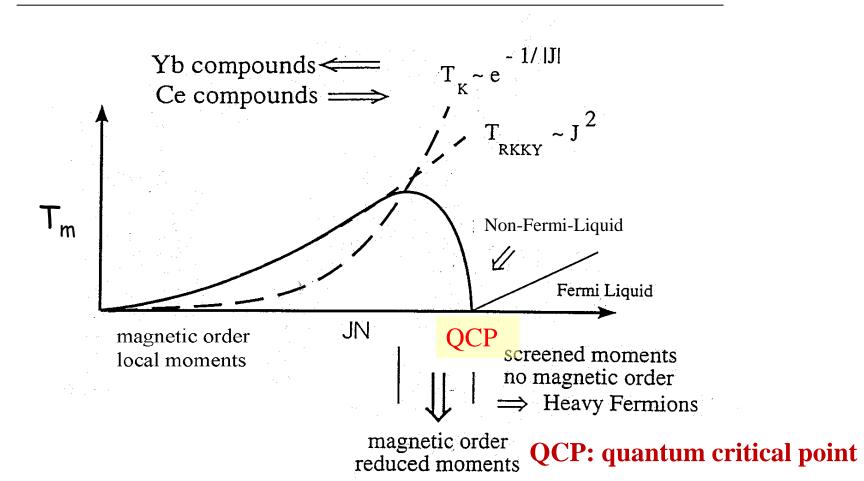
 $\Rightarrow$  long range magnetic order

 $T_{K} \sim exp(-1/N(E_{F})J)$ 

 $T_{RKKY} \sim N(E_F) J^2$ 

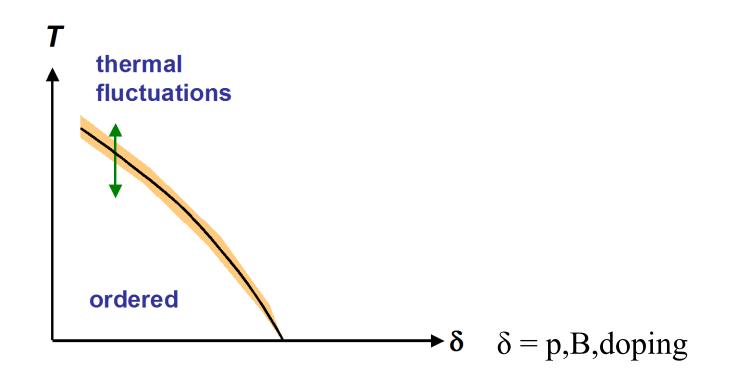
J: interaction between fand conduction electrons

#### Doniach Model (Doniach 1977)



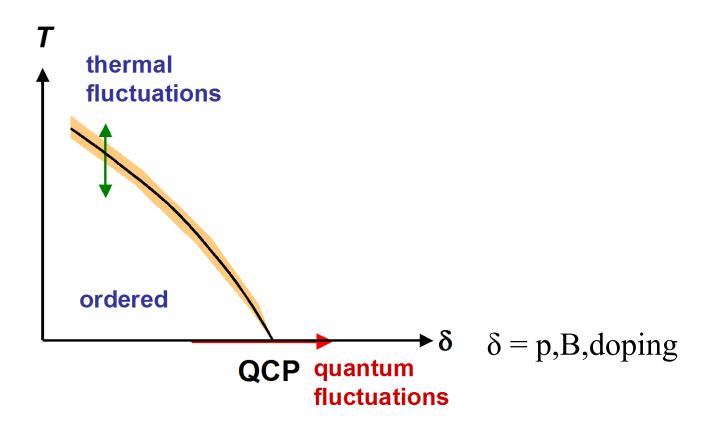
The main result ... is that there should be a **second-order transition at zero temperature (at QCP)**, as the exchange coupling J is varied, between an antiferromagnetic ground state for weak J and a Kondo-like state in which the local moments are quenched.

#### **Quantum Phase Transitions**



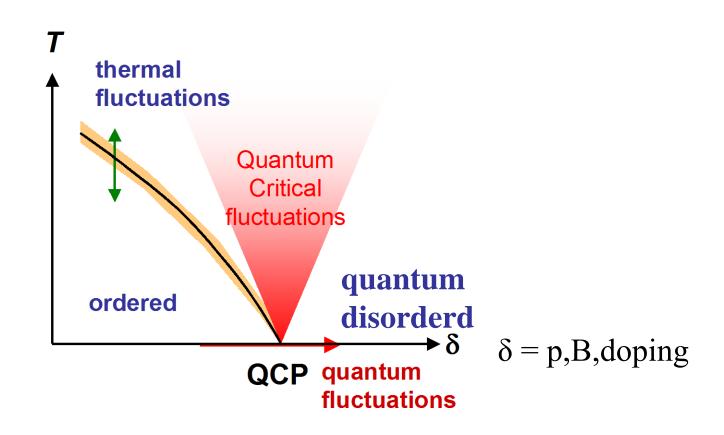
#### classical phase transition: driven by thermal fluctuations

#### **Quantum Phase Transitions**



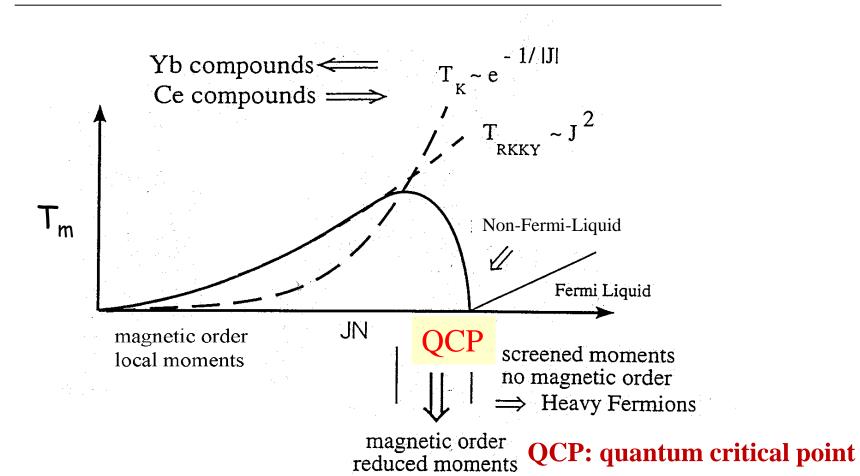
- classical phase transition: driven by thermal fluctuations
- quantum phase transition: driven by quantum fluctuations

#### **Quantum Phase Transitions**



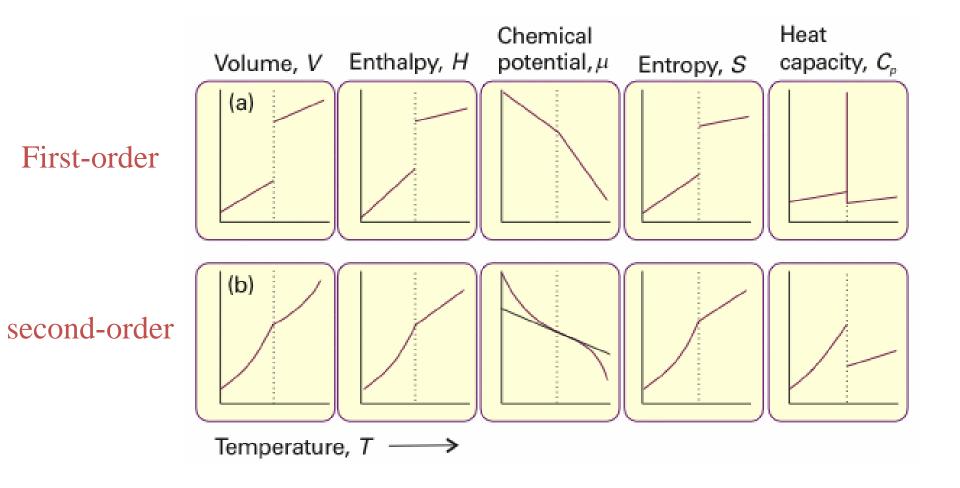
- classical phase transition: driven by thermal fluctuations
- quantum phase transition: driven by quantum fluctuations

#### Doniach Model (Doniach 1977)

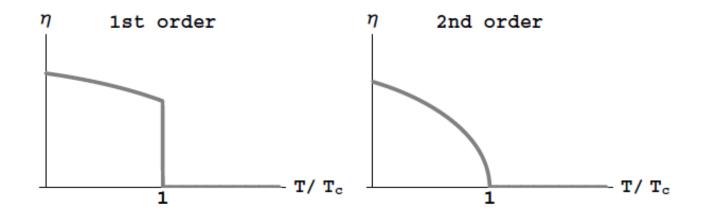


The main result ... is that there should be a **second-order transition at zero temperature (at QCP)**, as the exchange coupling is varied, between an antiferromagnetic ground state for weak *J* and a Kondo-like state in which the local moments are quenched.

#### **Types of Phase Transitions**



#### **Order parameter of a phase transition**

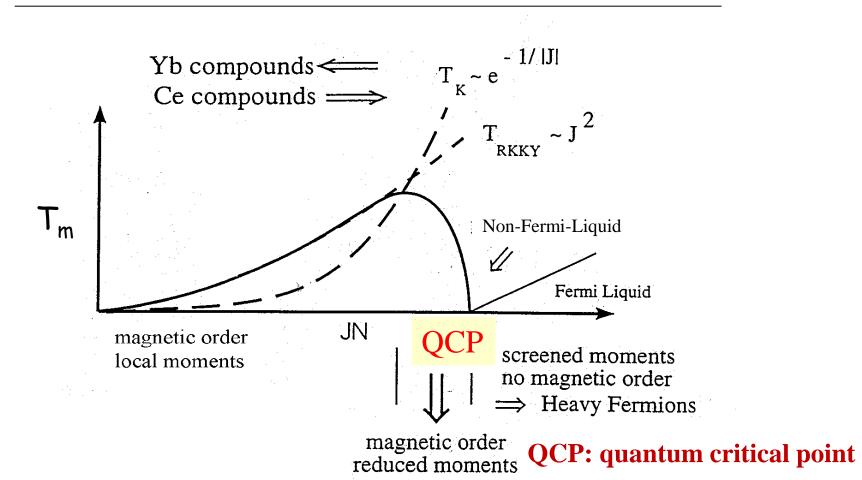


#### Partial list of transitions and order parameters

Transition	Order parameter		
Liquid-gas	density		
Ferromagnetic	magnetization		
Ferroelectric	polarization		
Superconductors	complex gap parameter		
Siperfluid	condensate wave function		
Phase Separation	concentration		

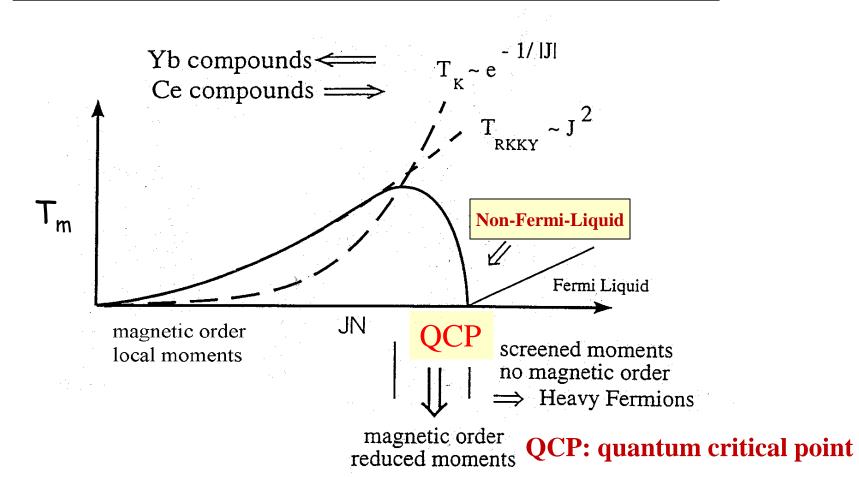
L. P. Kadanoff et al., Rev. Mod. Phys., 39 (1967), 395.

#### **Doniach Model (Doniach 1977)**



The main result ... is that there should be a **second-order transition at zero temperature (at QCP)**, as the exchange coupling is varied, between an antiferromagnetic ground state for weak J and a Kondo-like state in which the local moments are quenched.

#### Doniach Model (Doniach 1977)



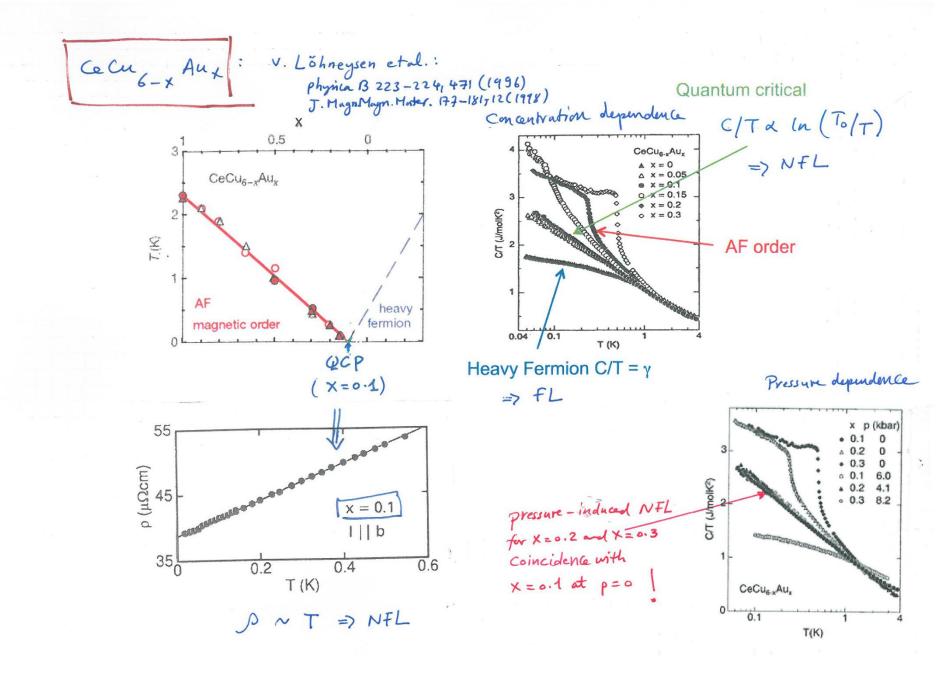
**Consequence:** The nature of the ground state of the system strongly depends on the relative strength of RKKY interaction and Kondo effect.

Non - Fermi liquid behavior at magnotic quantum phase transitions (here a brief discussion, for theoretical description see : H. v. Löhneysen et al., Rev. Mod. Phys. 79, 1015(2007) General aspects : NFL behavior has been observed in U, Ce, 16 intermetallic componds: S-chemically substituted : e.g. V U Pdz, Ucus Pdx, ..... (disordered systems) - Stoichiometeric (p=o)=> UBe, CeCoIns, YbRh2Siz, .... (proximity to QCP) P70 (pressure tuned) => CeIn3, CePd2Siz, UGe2, -... ifferent nontes to NFL behavior ! distribution of the Kondo temperature \* NFL behavior due to disorder : (disdribution of J and or  $D(E_{\mp})$ . (see Stewart, Rev. Mod. Phys. 73, 797 (2001) \* multi-channel Kondo effect : 78,743(2006) f-electron spin is overscreened by the spins of Conduction electrons => antiferromagnetic superexchange interaction with electrons \* proximity to a QCP => induced by quantum fluctuations

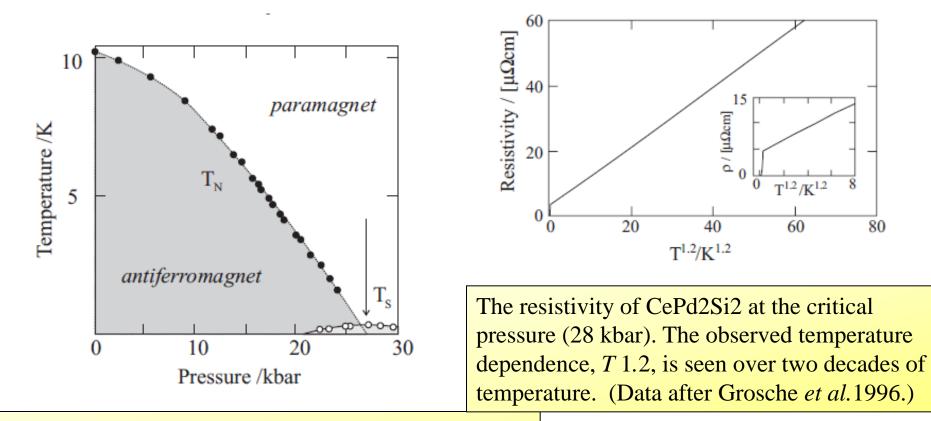
\* Physical properties: Weak power low, logarithmic divergences in NFL Tat how temperatures (TKT\_): -electric resistivity, S~ at with 1 ≤ x ≤ 1.6 non-quadratic - Specific heat divided by T, C/T~ (n(To/T) ( diverging - magnetic susceptibility, X: X ~ (n (To/T) Note that -: The appreciable T-dependence below To ... => lower energy scale than Fermi liquid!

few comments to proximity to a QCP: \* At the QCP, the low temperature thermodynamics is determined by collective modes corresponding to fluctuations of the order parameter, rather than by single-fermion excitations as in FL => NFL properties arise. \* NFL can also occurs near quantum spin-glass or superconducting transitions. \* A quantum phase transition (like thermal or classical phase transition) is Characterized by a diverging correlation length 2 and a diverging relation time Z. However : @ the critical fluctuations are quantum fluctuations rather than thermal fluctuations, and @ contrary to classical critical point? the dynamic and static behavior of a QCP ar coupled together. =) a system at a QCP will be affected in the same way by either a finite frequency or a finite temperature.

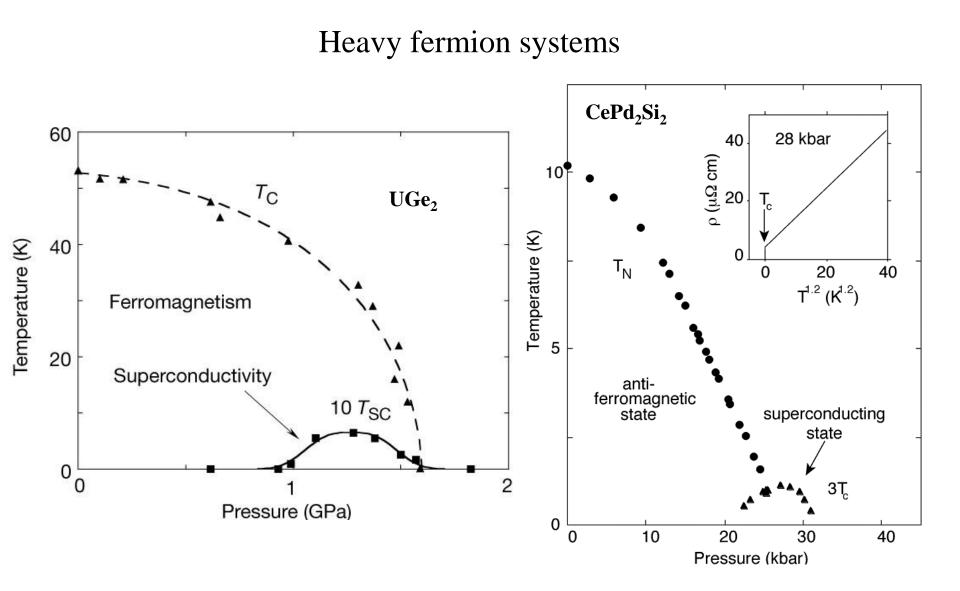
Туре	Material	$T^*$	$T_c, x_c, B_c$	Properties	ρ	$\gamma_n$ $mJmol^{-1}K^{-2}$
Metal	$CeCu_6$	10K	-	Simple HF Metal	$T^2$	1600
	$CeCu_2Si_2$	20K	$T_c = 0.17 \text{K}$	First HFSC	$T^2$	800-1250
Super- conductors	$UBe_{13}$	$2.5\mathrm{K}$	$T_c = 0.86 { m K}$	$\begin{array}{c} {\rm Incoherent} \\ {\rm metal} {\rightarrow} {\rm HFSC} \end{array}$	$ ho_c \sim 150 \mu \Omega { m cm}$	800
	$CeCoIn_5$	38K	$T_c=2.3\mathrm{K}$	Quasi 2D HFSC	Т	750
Kondo	$Ce_3Pt_4Bi_3$	$T_\chi \sim 80 K$	-	Fully Gapped KI	$\sim e^{\Delta/T}$	-
Insulators	CeNiSn	$T_\chi\sim 20K$	-	Nodal KI	Poor Metal	-
Quantum	$CeCu_{6-x}Au_x$	$T_0 \sim 10 K$	$x_c = 0.1$	Chemically tuned QCP	Т	$\sim rac{1}{T_0} \ln \left( rac{T_0}{T}  ight)$
Critical	$YbRh_2Si_2$	$T_0\sim 24K$	$B_{\perp} = 0.06 \mathrm{T}$ $B_{\parallel} = 0.66 \mathrm{T}$	Field-tuned QCP	Т	$\sim rac{1}{T_0} \ln \left( rac{T_0}{T}  ight)$
SC +	$UPd_2Al_3$	110K	$T_{AF}{=}14\mathrm{K},$ $T_{sc}{=}2\mathrm{K}$	AFM + HFSC	$T^2$	210
other Order	$URu_2Si_2$	$75\mathrm{K}$	$T_1 = 17.5 \text{K},$ $T_{sc} = 1.3 \text{K}$	Hidden Order & HFSC	$T^2$	120/65



#### Examples for non Fermi-liquid (NFL) behavior: CePd2Si2

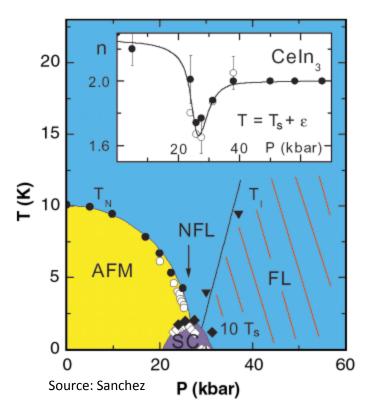


CePd2Si2: a low temperature antiferromagnet. Under pressure the antiferromagnetism can be suppressed to zero temperature giving a quantum critical point. Not only non-Fermi liquid behavior but also there is a superconducting transition (after Julian *et al.* 1996, Mathur *et al.* 1998)



#### S. S. Saxena et al., Nature 406, 587 (2000) N. D. Mathur et al., Nature 394, 39 (1998)

Rich Phase Diagrams Exhibiting both NFL behavior and superconductivity.



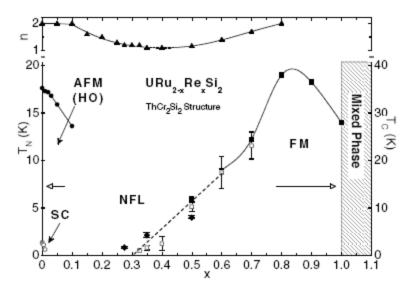
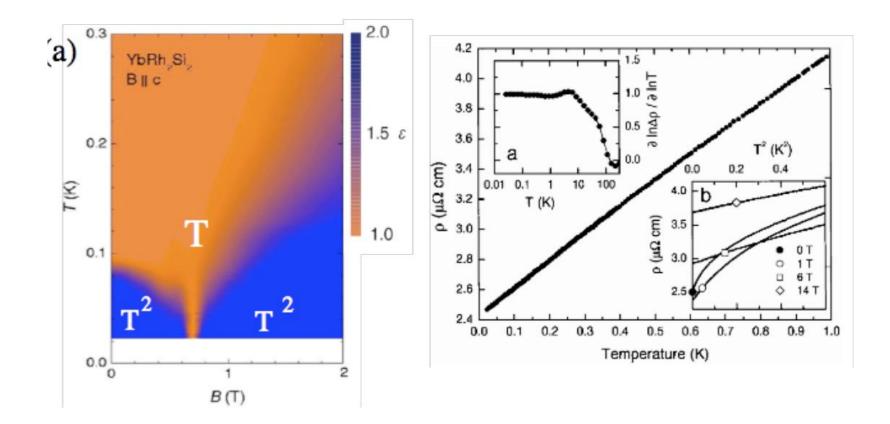


FIG. 1. The power-law exponent of  $\rho(T)$ , *n*, is shown in the top part of the diagram.

	Y <sub>1-x</sub> U <sub>x</sub> Pd (NFL)	Fermi Liquid
Heat Capacity	$C \sim -Tln(T)$	$C = \gamma T$
Conductivity	$\rho \sim \rho_0 + AT^{1.1}$	$\rho = \rho_0 + AT^2$
Magnetic	$\chi_{\rm m}$ ~ $\alpha$ - $\beta T^{1/2}$	$\chi_{\rm m} = \beta$
Susceptibility		Source: Seaman et al.

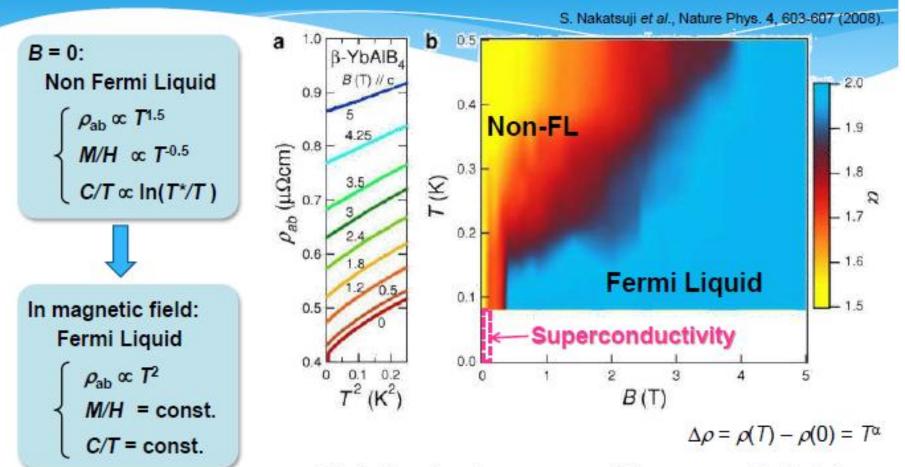
#### YbRh2Si2:

#### Field-induced quantum critical point



J. Custers et al., Nature 424, 524 (2003)

# NFL behavior @ B = 0 in $\beta$ -YbAlB<sub>4</sub>



FL behavior is recovered in magnetic field.

QCP at B = 0 under P = 0?

Normally, we have to tune *B* or *P* or doping to approach QCP. ex) YbRh<sub>2</sub>Si<sub>2</sub>, CeCoIn<sub>5</sub>, CeCu<sub>5.9</sub>Au<sub>0.1</sub>, ...