Lecture Notes

Introduction to Strongly Correlated Electron Systems

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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

Strongly Correlated Electron Systems (SCES)

What is it?

Systems where the interactin between electrons is very large (mainly Coulomb repulsion). This includes most of transition metal compounds with partially filled 3d orbitals as well as compounds with partially filled 4f orbitals, e.g. Heay fermion systems.
Localization of d, f orbitals enhances Coulomb interaction between electrons with their spin, charge, orbital and lattice degrees of freedom.

⇒ **Existence of several competing ground (ordered) states that are sensitive to control parameters, e.g. doping, pressure, magnetic field.**

⇓

Electronic correlations ⇒ unique materials and device properties

comparison of γ_{th} with experimental γ values

m^*

$$\frac{m^*}{m} \equiv \frac{\gamma}{\gamma_{th}}$$

Metal	γ	γ_{th}	Metal	γ	Metal	γ
Li	1.63	0.749	Fe	5.0	$CeAl_3$	1600
Na	1.38	1.094	Co	4.7	$CeCu_6$	1500
K	2.08	1.668	Ni	7.1	$CeCu_2Si_2$	1100
Cu	0.69	0.505	La	10	$CeNi_2Sn_2$	600
Ag	0.64	0.645	Ce	21	UBe_{13}	1100
Au	0.69	0.642	Er	13	U_2Zn_{17}	500
Al	1.35	0.912	Pt	6.8	YbBiPt	8000
Ga	0.60	1.025	Mn	14	$PrInAg_2$	6500

$\gamma / \gamma_{th} \approx 1-1.5$

mainly s-electrons, broad bands

$\gamma / \gamma_{th} \approx 10-30$

partially filled d-bands

$\gamma / \gamma_{th} \approx 100-1000$

heavy fermion compounds 4 f (5f)-orbitals strong electron-electron correlations SCES

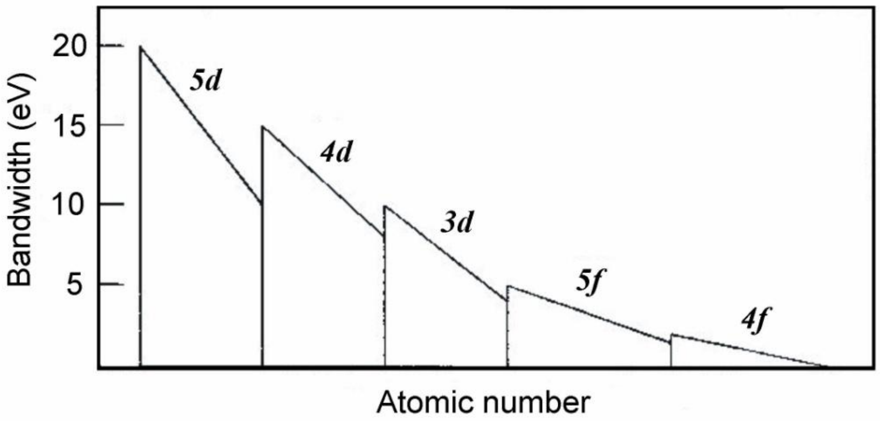
Why m^* is so large in some 4f and 5f electron system?

No answer from the band theory (one electron approximation), neglecting electron-electron interactions. This will be discussed in Chapter II (b).

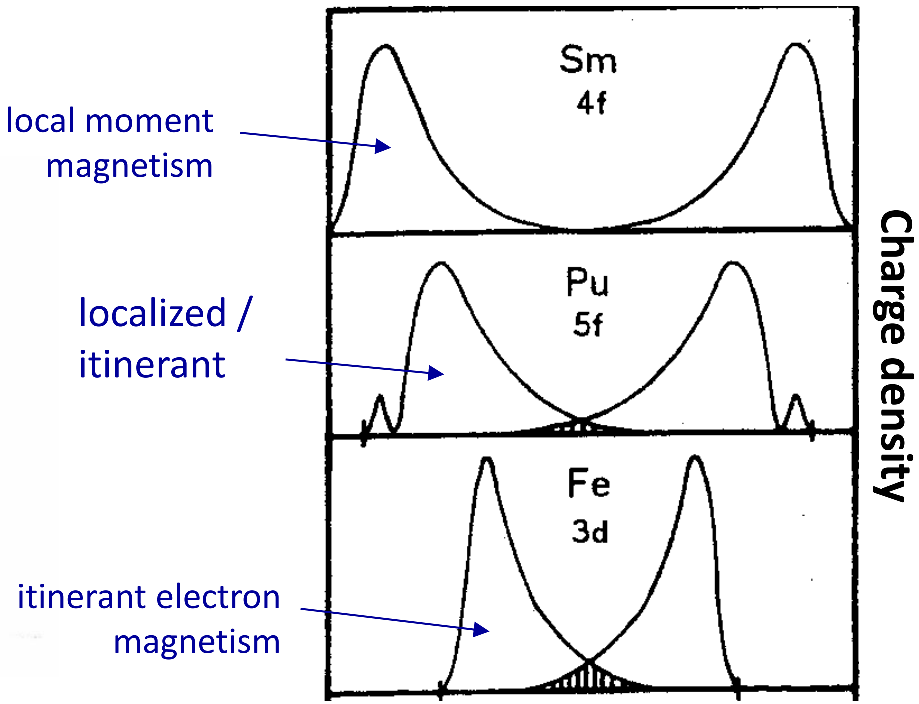
Why expecting unusual ground states in correlated 4f (5f)-electron metallic systems?

→ **Origin of strong electron correlations**

Magnetic states in metallic systems



Bandwidth of the metallic state



Interatomic distance

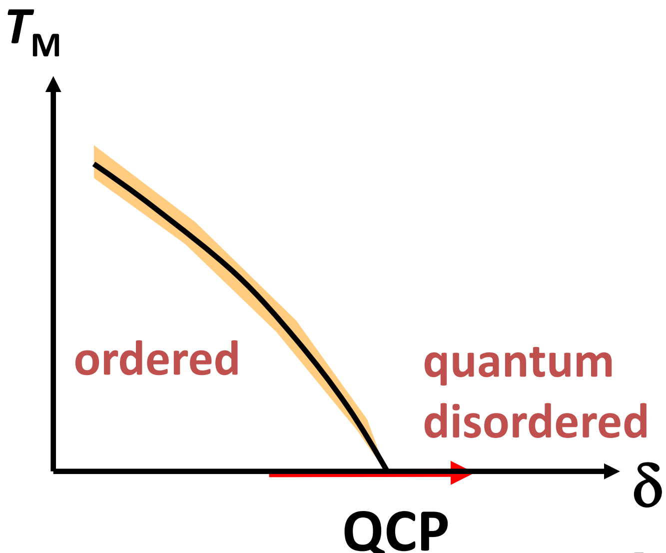
Degree of overlap of valence orbitals determines the nature of magnetism

Heavy fermion metallic systems

Intermetallic Ce (4f), Yb (4f) and U(5f) - compounds

local moments → **itinerant moments**

increasing hybridization between localized states and conduction electrons



Control parameters

crossover

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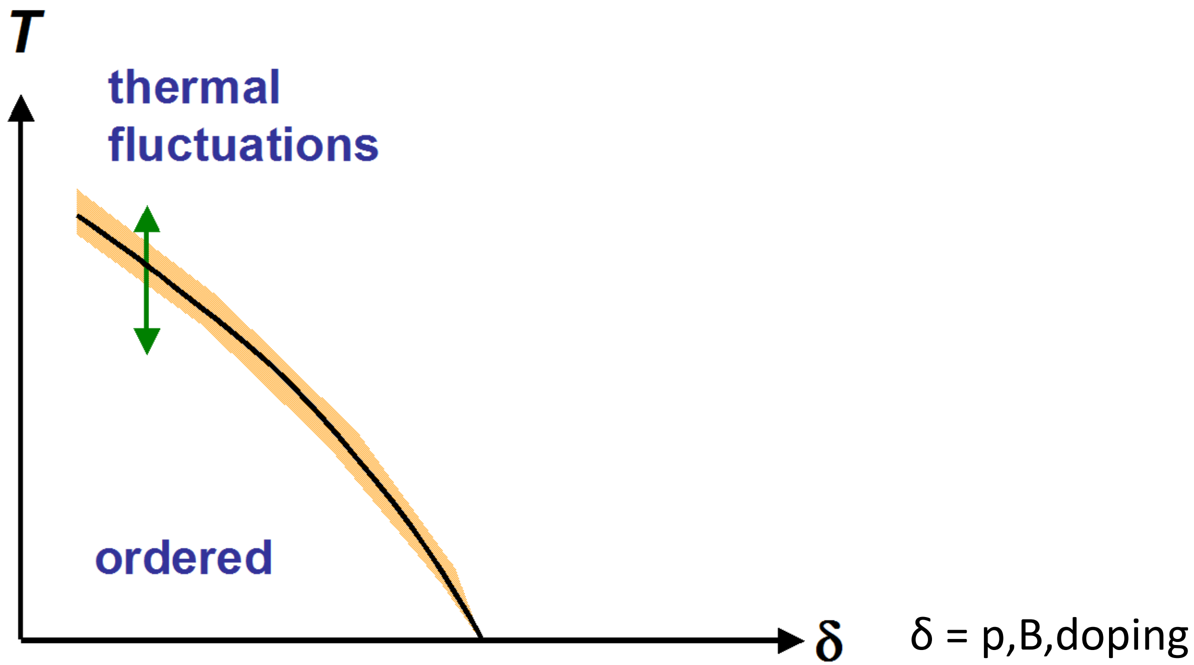
<u>unusual ground states</u>:

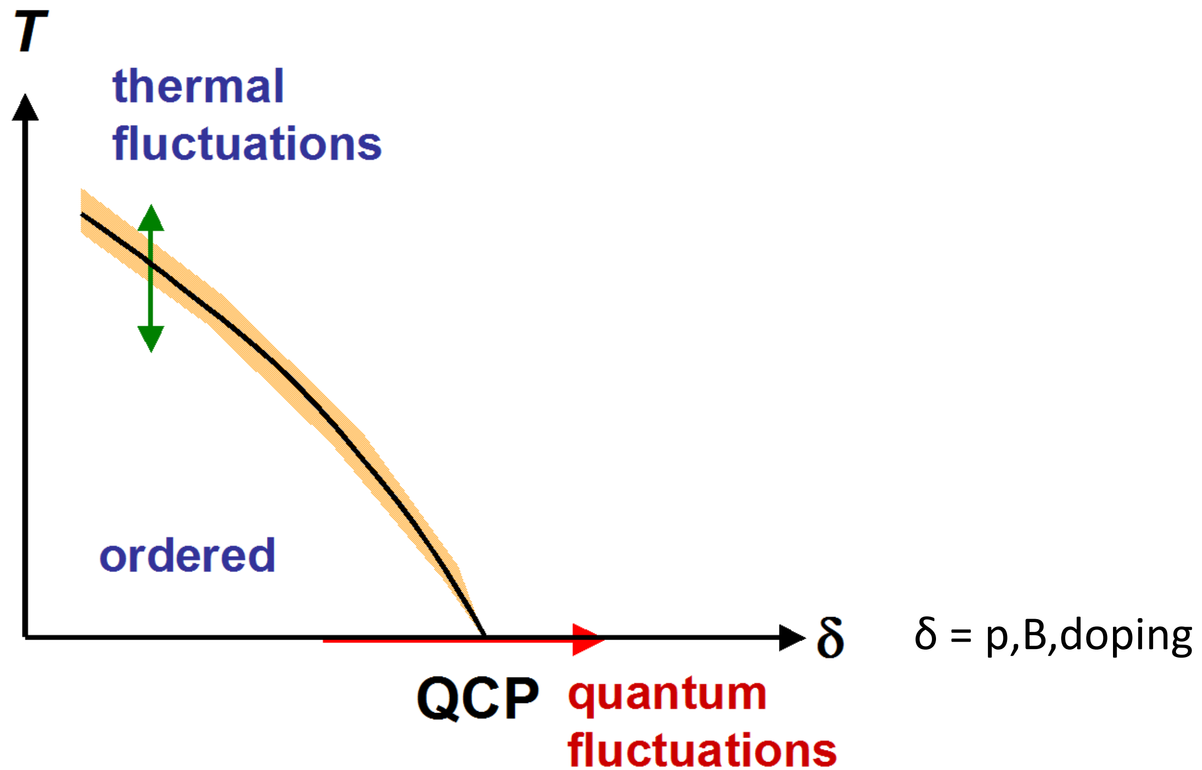
Fermi-liquid, Non-Fermi-liquid, heavy fermions, new magnetic and unconventional superconducting states

Quantum Phase Transitions



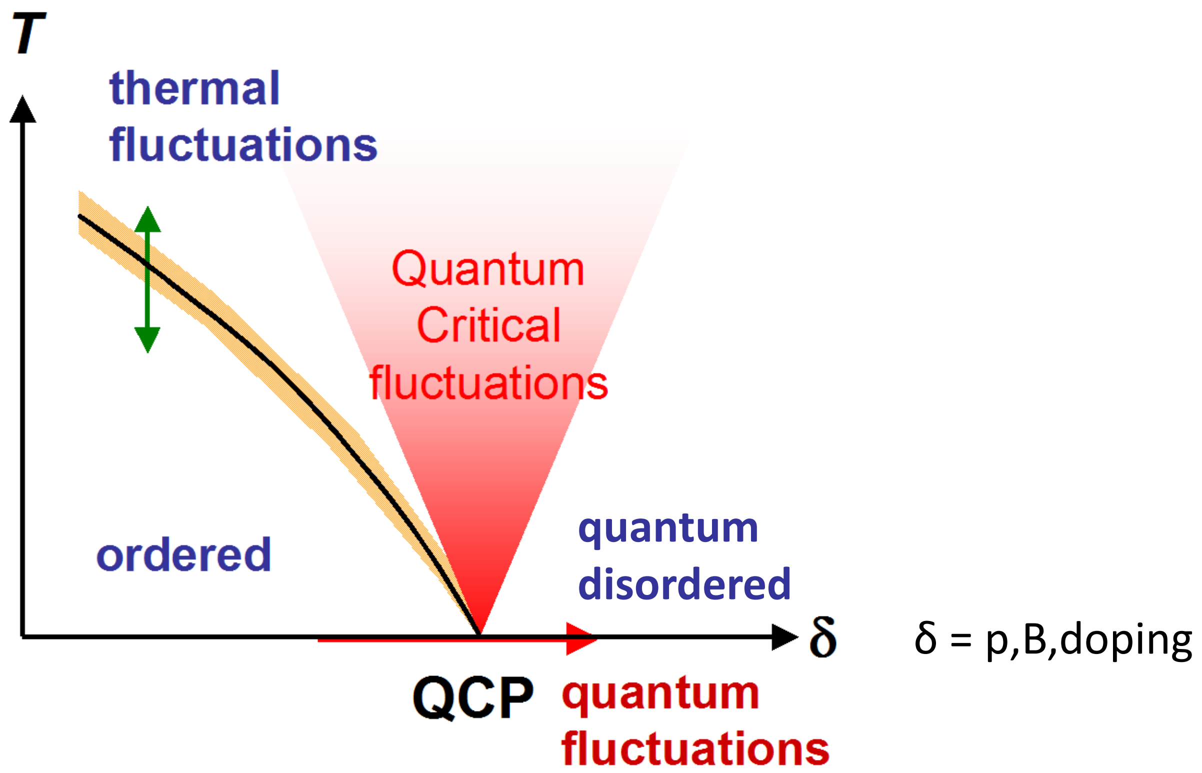
- classical phase transition: driven by thermal fluctuations

Quantum Phase Transitions



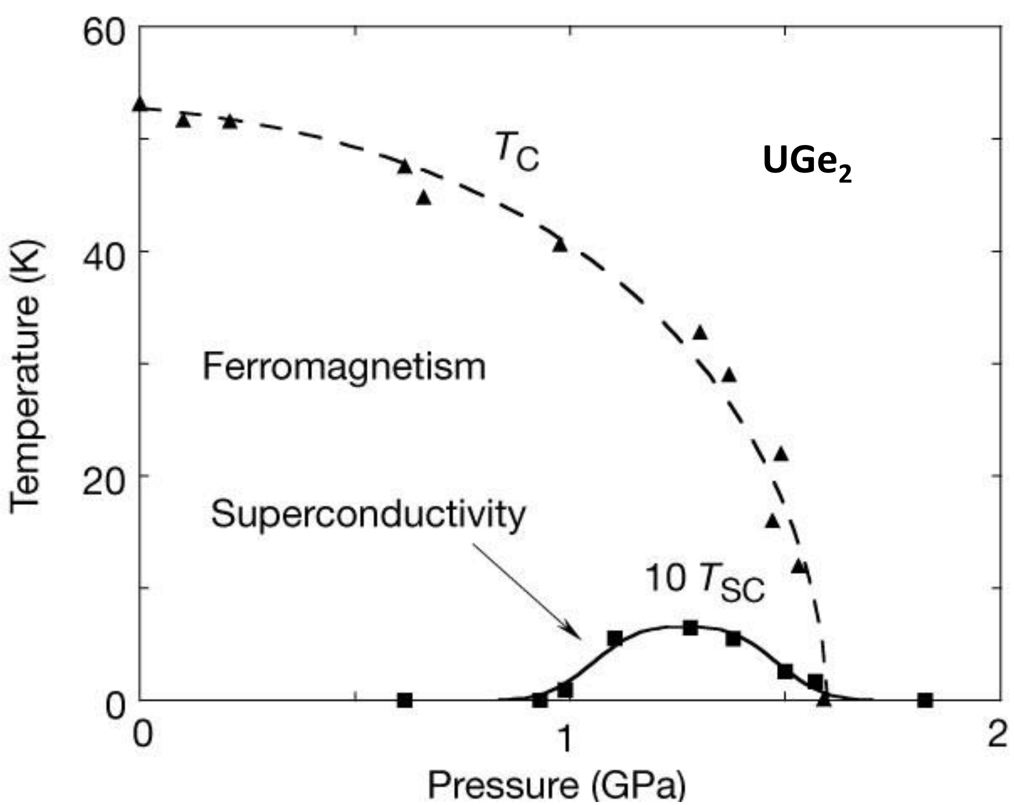
- classical phase transition: driven by thermal fluctuations
- quantum phase transition: driven by quantum fluctuations

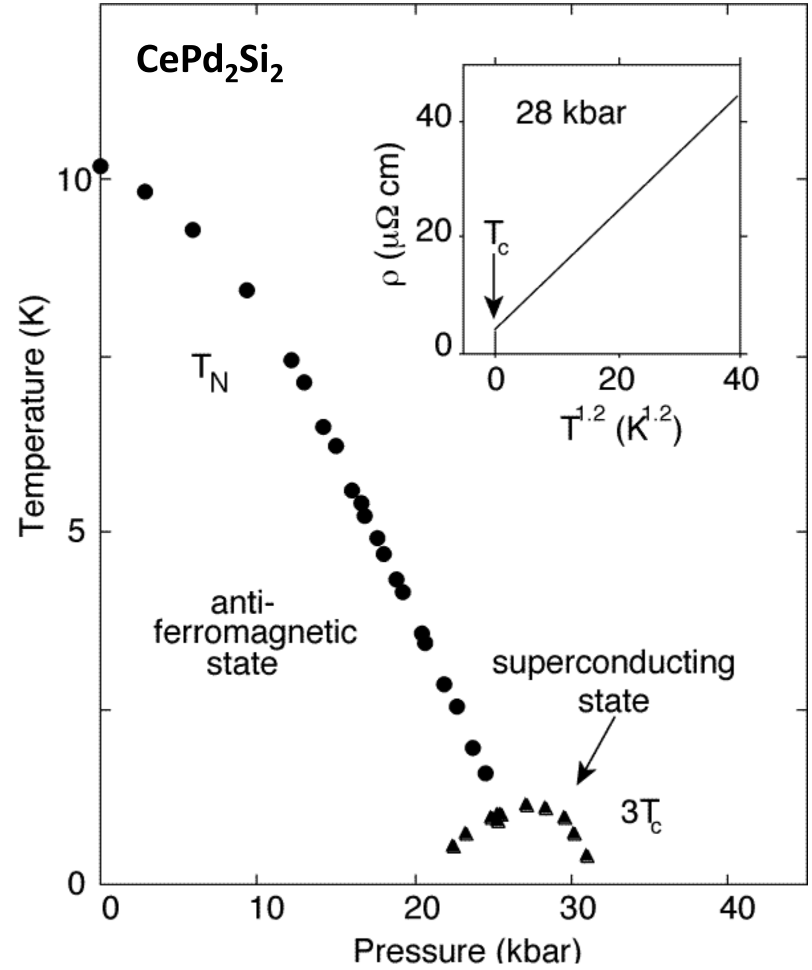
Quantum Phase Transitions



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

Metallic systems on the border of intinerant electron magnetism





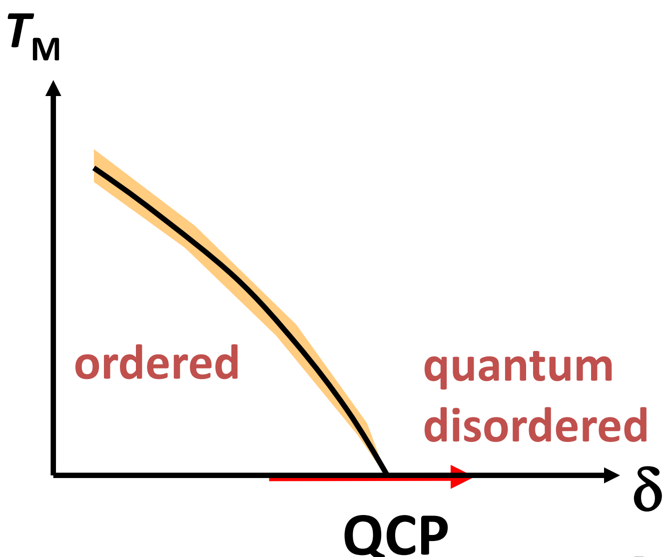
S. S. Saxena et al., Nature 406, 587 (2000) N. D. Mathur et al., Nature 394, 39 (1998)

Heavy fermion metallic systems

Intermetallic Ce (4f), Yb (4f) and U(5f) - compounds

local moments → **itinerant moments**

increasing hybridization between localized states and conduction electrons



Control parameters

crossover

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ground states:

Fermi-liquid, Non-Fermi-liquid, heavy fermions, new magnetic and unconventional superconducting states

To understand the physics underlying heavy fermion systems

1- first we shortly discuss Landau Fermi-liquid theory (Landau,1957)

2- second the Kondo effect (Kondo 1964)

Landau Fermi-liquid theory (Landau,1957)

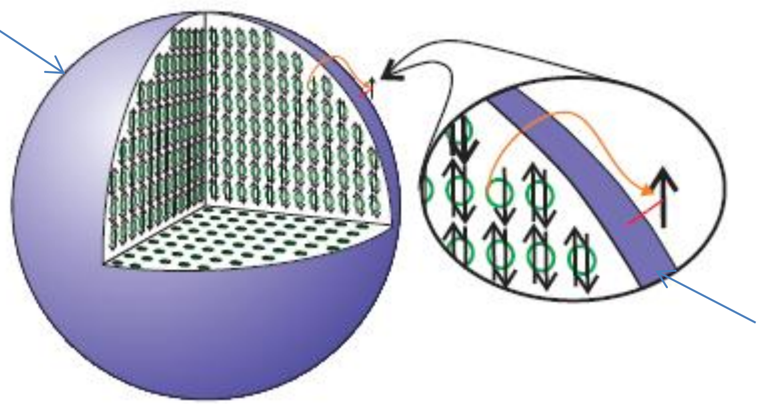
Description of the ground state of metals with interacting fermions

complicated electron systems where electron electron interactions are important can be **renormalized to** the model of a **free electron gas**; there is a 1:1 correspondence between the quasi-particles and the excitations of the non-interacting Fermi gas

Excitations of system with strongly interacting electrons ⟷ (1:1 correspondence) ⟷ Free electron gas

Landau Fermi-liquid Theory

Weakly excited states in the ground state of a metallic system can be described in terms of elementary excitation (paricle-hole exitation), or **quasiparticles (QP). QP (Fermions with S=1/2) have effective mass m* and only finite (long) life time near** E_F



A particle-hole excitation is made by promoting an electron from a state below E_F to an empty one above it.

Landau Fermi liquid Theory: origin of energy change

First, when a low-energy excited quasiparticle moves there will now be a back-flow in the filled Fermi sea as the quasiparticle `pushes' the ground state out of the way. This modies the inertial mass of the quasiparticle

⟹ $m \to m^*$ and thus their energy.

Note that this mass modification (renormalization) is **in addition to** that due to the effect of the crystal lattice| which produces a **band mass** as well as due to the **change of the mass induced by interactions with phonons**.

Second, the interaction between excited quasiparticles leads to a modification of the energy of the ground state.

What is the energy of quasiparticles?; see board

Landau Fermi-liquid: calculation of the quasiparticle energy

Landau Fermi-liquid theory

* **quasiparticle concept**:

- Consider non-interacting system; ⇒ the occupation of single particle states $|\vec{k}\sigma\rangle$ with momentum $\vec{k}$ is given by:

distribution function →

$$\boxed{n^{T=0}_{\vec{k}\sigma} = \theta(k_F - k)}, \quad \theta(x): \text{the step function (Fermi-Dirac function)} \qquad (1)$$

k_F is determined by the density of particles:

$$n = \sum_{\vec{k}\sigma} n^{T=0}_{\vec{k}\sigma} = \frac{k_F^3}{3\pi^2}$$

- interacting system:

interaction between particle is adiabatic (very slow!) ⇒ assume that the low energy excitation spectrum is in one-to-one correspondence with the Fermi gas spectrum ⇒ Fermi liquid ⇒ low energy single particle excitations of the Fermi-liquid with $\vec{k}, \sigma$ are called quasiparticles.

The energy of the quasiparticles:

amount of energy by which the total energy E of the system increases, if a quasiparticle is added to the unoccupied state $|\vec{k}\sigma\rangle$ ⇒

$$\epsilon_{\vec{k}\sigma} = \frac{\partial E}{\partial n_{\vec{k}\sigma}} \quad \text{——— (2)}$$

↑ change of the distribution function (eq. 1)

* Consequence of the interaction:

the ~~energy~~ single particle energies depend on the state of the system

$$\Rightarrow \quad \epsilon_{\vec{k}\sigma} = \epsilon_{\vec{k}\sigma}\{n_{\vec{k}'\sigma'}\}$$

⇒ the energy of a single low energy quasiparticle added to the ground state:

$$\Rightarrow \quad \epsilon_{\vec{k}\sigma}\{n^{T=0}_{\vec{k}'\sigma'}\} = v_F (k - k_F) \quad \text{——— (3)}$$

↑ Fermi Velocity

$$v_F = \frac{\hbar \vec{k}_F}{m^*}$$

$$\Rightarrow \quad \epsilon_{\vec{k}\sigma} = \frac{\hbar k_F}{m^*}(k - k_F) \quad \text{——— (3)'}$$

m^* determines the density of states at E_F

$$\Rightarrow \boxed{D^*(E_F) = \frac{m^* k_F}{2\pi^2 \hbar^2}}$$ renormalized density of states — (4)
(renormalized mass)

- The effect of interaction with other excited quasiparticles on the energy of a specific quasiparticle may be expressed in terms of 2 particle-interaction function or FL interaction $f_{\vec{k}\sigma, \vec{k}'\sigma'}$

$$\Rightarrow \boxed{\delta\epsilon_{\vec{k}\sigma} = \sum_{\vec{k}\sigma} f_{\vec{k}\sigma, \vec{k}'\sigma'} \, \delta n_{\vec{k}'\sigma'}} \quad (\delta n_{\vec{k}\sigma} = n_{\vec{k}\sigma} - n^0_{\vec{k}\sigma})$$ — (5)

$\delta\epsilon_{\vec{k}\sigma}$: Energy shift of quasiparticle

$f_{\vec{k}\sigma, \vec{k}'\sigma'}$: invariant with respect to exchange of $\vec{k}$ and $\vec{k}'$

- the total energy of quasiparticle (renormalized particle energy)

$$\tilde{\epsilon}_{\vec{k}\sigma} = \epsilon_{\vec{k}\sigma} + \delta\epsilon_{\vec{k}\sigma}$$

$$\Rightarrow \quad = \boxed{\epsilon_{\vec{k}\sigma} + \sum_{\vec{k}'\sigma'} f_{\vec{k}\sigma, \vec{k}'\sigma'} \, \delta n_{\vec{k}'\sigma'}}$$ — (6)

for isotropic system with short-range interaction the FL interaction only depends on the angle θ between $\vec{k}$ and $\vec{k}'$ and on the relative spin orientation of σ and σ'

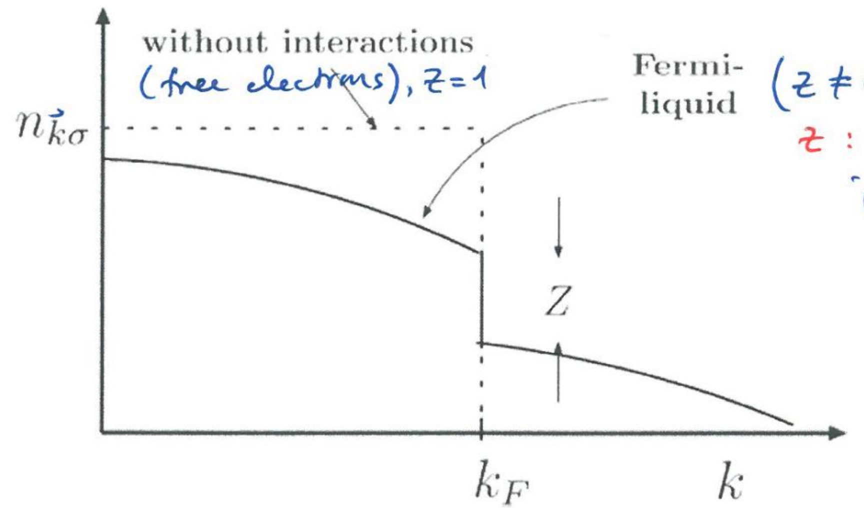
Landau Parameters

$$= \quad f_{\vec{k}\sigma\vec{k}'\sigma'} = \frac{1}{2D(E_F)} \sum_{l=0}^{\infty} (2l+1) \underbrace{P_l(\cos\theta)}_{\text{Legendre polynomials}} \left[F_l^s + \sigma\sigma' F_l^a \right]$$

F_l^s and F_l^a are dimensionless symmetric and antisymmetric Landau parameters which characterize the effect of interaction on the quasiparticle energy.

For Galilean invariant systems the Ladau parameter F_l^s and the effective mass m^* are related through:

$$\boxed{m^*/m = 1 + F_l^s/3}$$

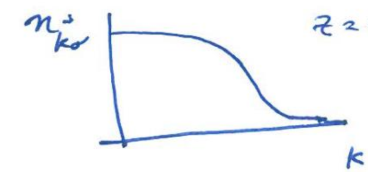


$(Z \neq 0,\ Z \leq 1)$

Z : weight of the "real" electrons in the quasiparticles

if $Z = 0$

$\Rightarrow$ non FL !



The jump, Z, is often considered as the order parameter of the FL

$(0 < Z \leq 1)$

$$G(\omega, \vec{k}) = \frac{Z}{\omega - \epsilon(\vec{k}) + i\Gamma}$$ (Γ life time of excited electrons, $\Gamma \sim \frac{1}{\tau}$)

Green function

Predections of LFL theory ($T \ll T_F$)

(1) Specific heat : $C_V = \frac{\pi^2}{3} k_B^2 D^*(E_F) T = \gamma T \Rightarrow \boxed{C_V = C_V^{free} \cdot \frac{m^*}{m}}$ $\left(D^*(E_F) = \left(\frac{k_F}{2\pi^2 \hbar^2} \right) \cdot m^* \right)$

m^* renormalized mass

$D^*(E_F)$ = renormalized density of states at E_F

(2) Spin susceptibility : $\chi_p = \frac{\mu_B^2 D^*(E_F)}{1 + F_0^a} \Longrightarrow \boxed{\chi_p = \chi_p^{free} \frac{m^*/m}{(1 + F_0^a)}}$

(3) Compressibility : $\kappa = \frac{D^*(E_F)}{(1 + F_0^s)} \Longrightarrow \kappa = \kappa^{free} \cdot \frac{m^*/m}{(1 + F_0^s)}$

Note : * (1), (2), and (3) are affected by mass renormalization m^*

* (2) and (3) are affected in addition by Ladau parameters (F_0^a, F_0^s)

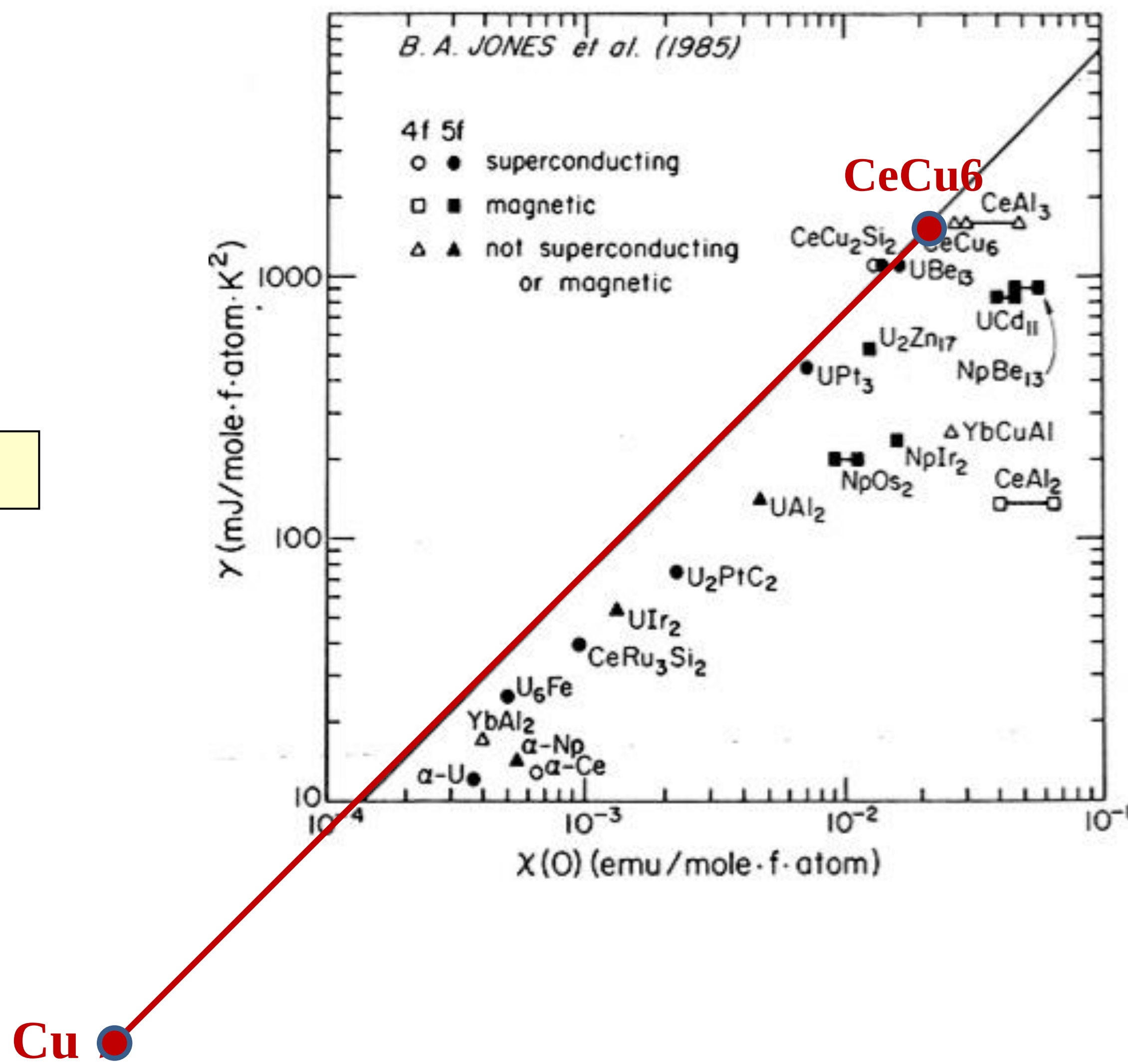
$\Rightarrow$ affected by the interaction of quasiparticles.

Wilson's ratio (R) :

$$R = \frac{\chi_p}{C/T} = \frac{4\pi^2 k_B^2}{3 (g \mu_B)^2} \cdot \frac{\chi_p}{\gamma} = 1 \text{ for free electron gas}$$

$R \simeq 1$, observed for heavy fermions systems, despite that m^* or $D^*(E_F)$ vary by more than a factor 100 ! $\Rightarrow$ Ground state can be described by LFL theory

Wilson s Ratio, R : γ / T



(4) electrical resistivity :

Consequence of locality appears in the transport properties ⇒ electron-electron scattering

$$\rho(T) = \rho_0 + A T^2 \qquad A \sim D^*(E_F)^2$$

ρ_0 ↑ residual resistivity

A ↖ electron-electron interaction coeffiecent

--⇒ large in heavy fermions (very small in conventional metals)

Kadawaki-Woods ration (1986)

$$A \propto D^*(E_F)^2 \quad \text{and} \quad C = \gamma T \qquad (\gamma \propto D^*(E_F))$$

⇒ A/γ^2 expected to be material independent ⇒ observed in heavy fermions

Note : Scaling relations for heavy fermions

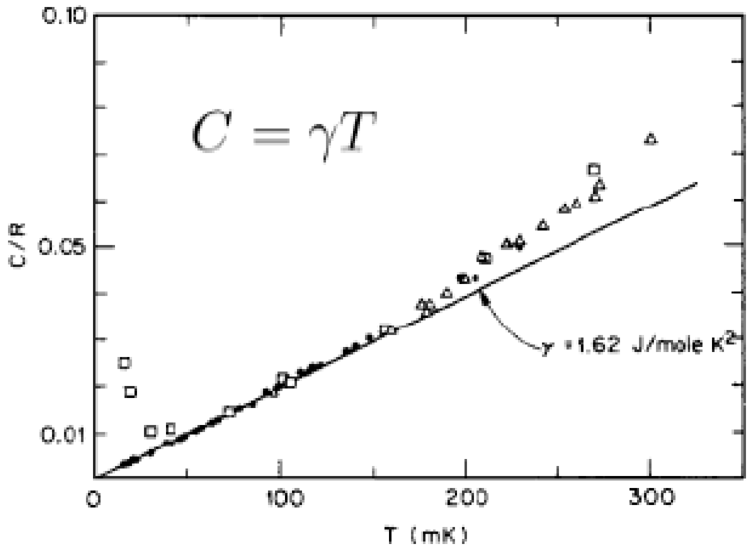
$$\boxed{\chi/\gamma \simeq \text{Const} \quad \text{and} \quad A/\gamma^2 \simeq \text{Const}}$$

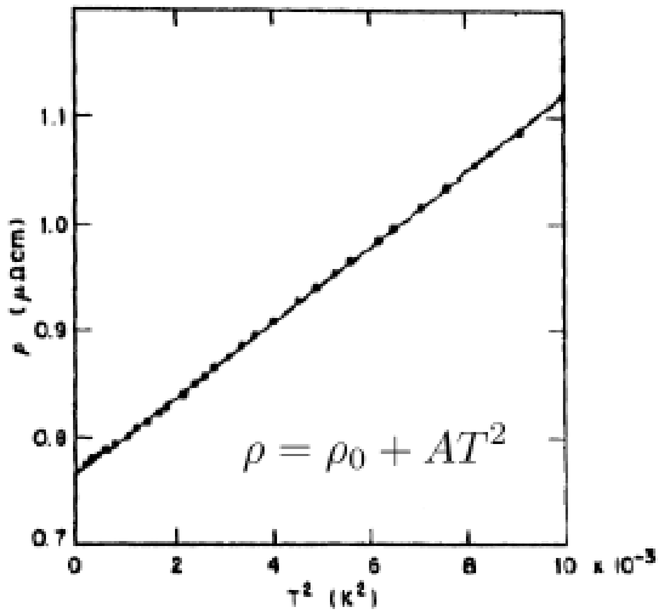
for a wide range of heavy fermions

⇒ excellent support for FL picture of heavy electrons !

Fermi liquid behavior in some heavy fermion systems (4f and 5f electron systems)

Example : $CeAl_3$

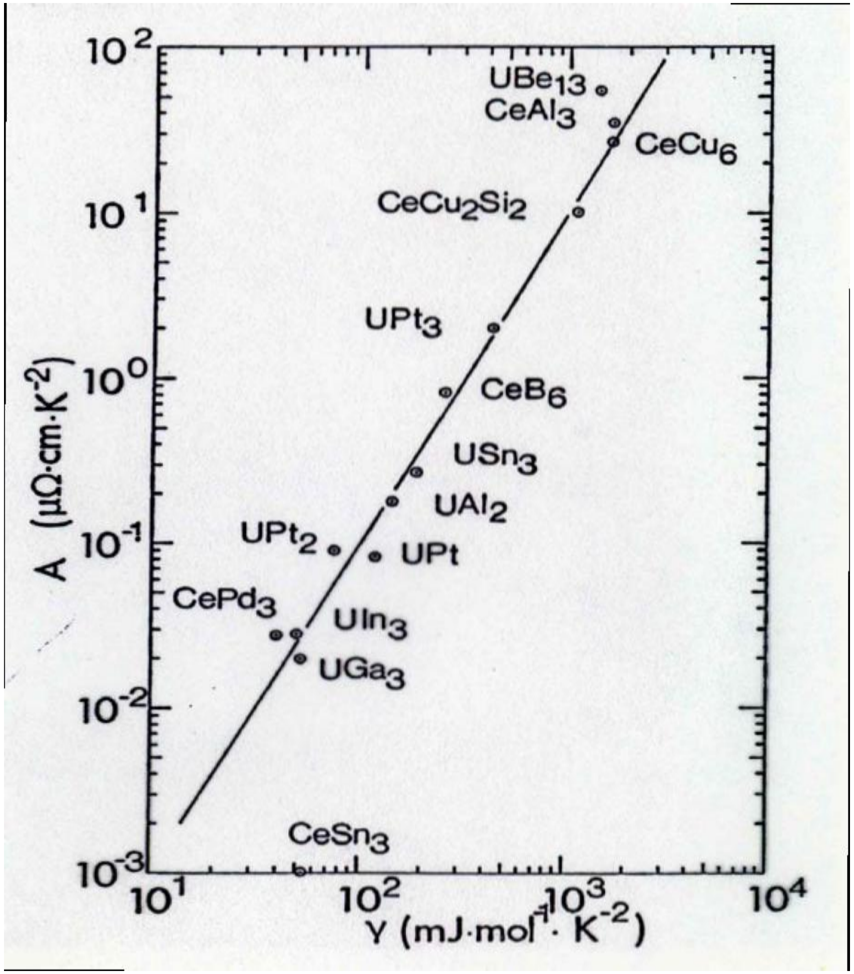




electron-electron scattering

Kadowaki-Woods plot (1986)

$$\frac{A}{\gamma^2}$$ is constant and material-independent



Observed for a large number of heavy fermion systems

Table 2 Experimental and free electron values of electronic heat capacity constant γ of metals

(From compilations kindly furnished by N. Phillips and N. Pearlman. The thermal effective mass is defined by Eq. (38).)

Observed γ in mJ mol^{-1} K^{-2}.
Calculated free electron γ in mJ mol^{-1} K^{-2}
m_{th}/m = (observed γ)/(free electron γ).

Li 1.63 0.749 2.18	Be 0.17 0.500 0.34											B	C	N
Na 1.38 1.094 1.26	Mg 1.3 0.992 1.3											Al 1.35 0.912 1.48	Si	P
K 2.08 1.668 1.25	Ca 2.9 1.511 1.9	Sc 10.7	Ti 3.35	V 9.26	Cr 1.40	Mn(γ) 9.20	Fe 4.98	Co 4.73	Ni 7.02	Cu 0.695 0.505 1.38	Zn 0.64 0.753 0.85	Ga 0.596 1.025 0.58	Ge	As 0.19
Rb 2.41 1.911 1.26	Sr 3.6 1.790 2.0	Y 10.2	Zr 2.80	Nb 7.79	Mo 2.0	Tc —	Ru 3.3	Rh 4.9	Pd 9.42	Ag 0.646 0.645 1.00	Cd 0.688 0.948 0.73	In 1.69 1.233 1.37	Sn (w) 1.78 1.410 1.26	Sb 0.11
Cs 3.20 2.238 1.43	Ba 2.7 1.937 1.4	La 10.	Hf 2.16	Ta 5.9	W 1.3	Re 2.3	Os 2.4	Ir 3.1	Pt 6.8	Au 0.729 0.642 1.14	Hg(α) 1.79 0.952 1.88	Tl 1.47 1.29 1.14	Pb 2.98 1.509 1.97	Bi 0.008

Possible causes:

- e-ph interaction
- e-e interaction

Heavy fermions:
$m^* \sim 1000\ m$

UBe_3 , $CeAl_3$, $CeCu_2Si_2$.

To understand the physics underlying heavy fermion systems

1- first we shortly discuss Landau Fermi-liquid theory (Landau,1957); and

2- the Kondo effect (Kondo 1964)

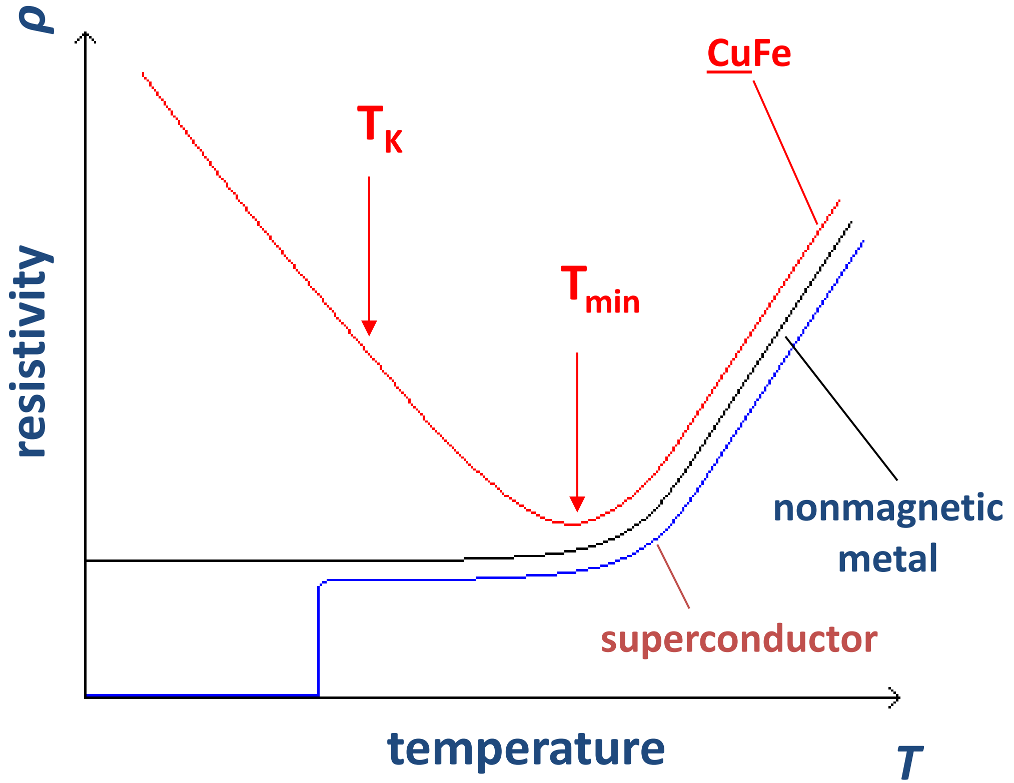
The Kondo Effect

What is the Kondo Effect?

Anomalous resistivity behavior

Experimental observation (1930s):

Anomalous temperature dependence of the resistivity ρ at low temperatures in **very diluted** magnetic alloys, e.g. CuFe, AuFe, CuMn with 10 ppm ... 1 at%



- **minimum in $\rho(T)$**
- **logarithmic increase** of the resistivity below a characteristic temperature T_K

Theoretical explanaition by Jun Kondo, 1964

⇒ Kondo effect

Jun Kondo, japanese theoretician

Explained the Kondo effect in 1964

Short notes to electrical conductivity in mettals

Electrical conductivity of metals

$$\sigma = \frac{ne^2\tau}{m} \quad \text{or} \quad \rho = \frac{1}{\sigma} = \frac{m}{ne^2\tau}$$

with

$$D(E_F) = \frac{3}{2}\frac{N}{E_F}$$

$$N = \frac{2}{3}D(E_F)E_F$$

and

$$E_F = \frac{P_F^2}{2m}$$

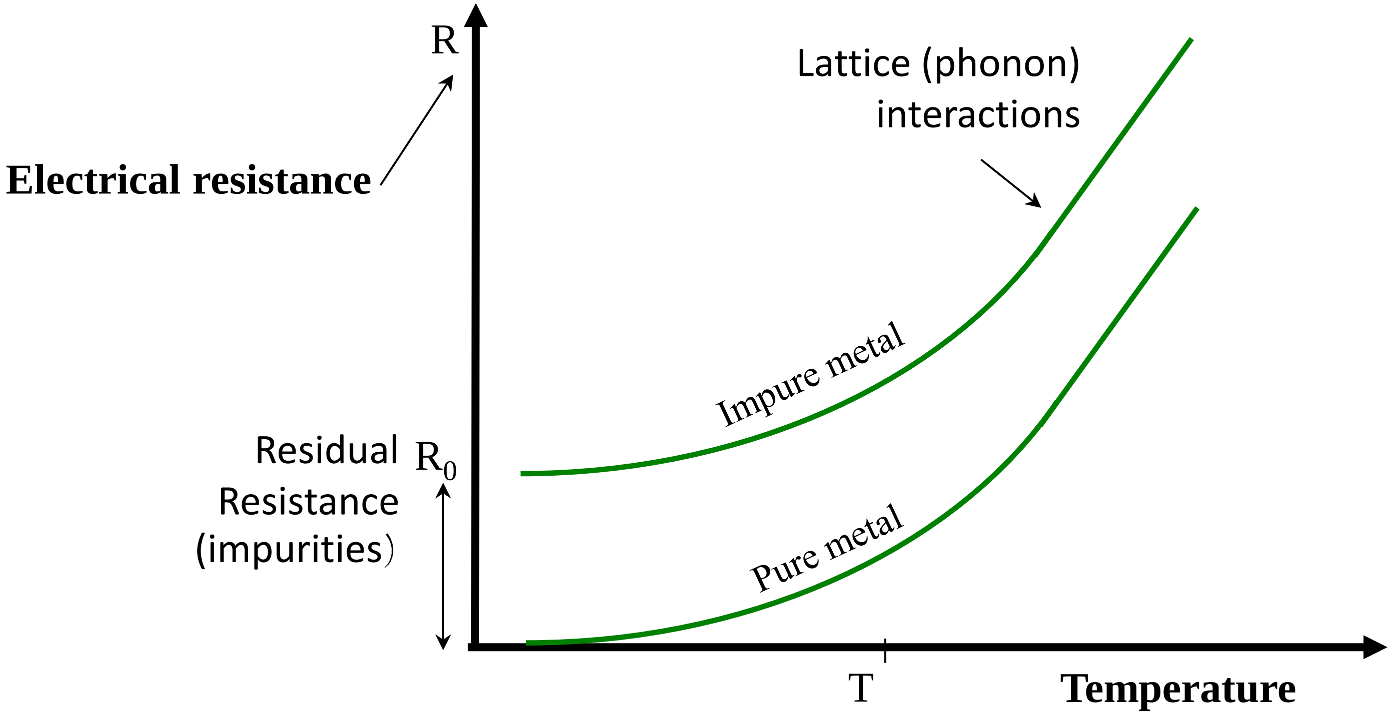
$$E_F = \frac{m^2}{2m}\frac{V_F^2}{} = \frac{1}{2}mV_F^2$$

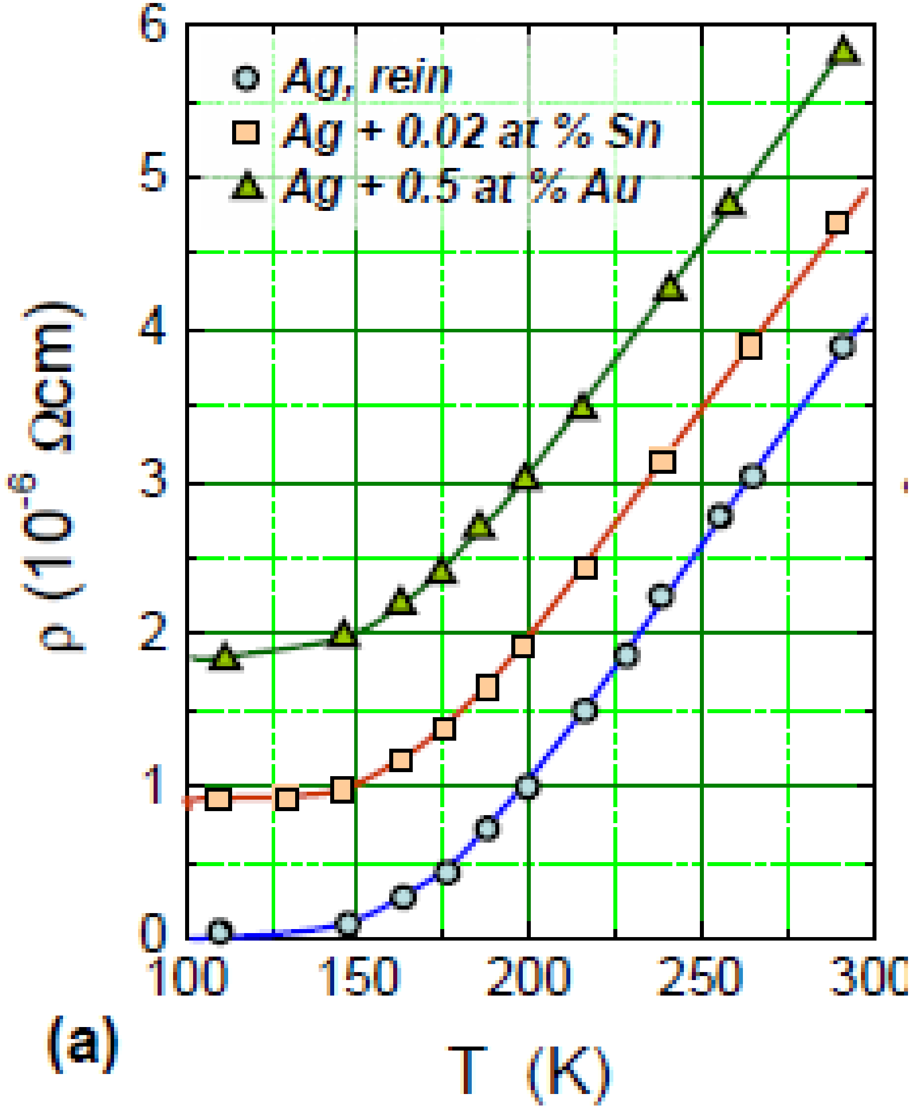
$$\Rightarrow \quad \sigma = \frac{1}{3}e^2V_F^2.\tau.D(E_F) \quad \textbf{or} \quad \sigma = \frac{ne^2\tau(E_F)}{m^*}$$

Density of states at the Fermi level!!

Temperature dependence of the resistance in metals

- **Metallic R vs T**
  - **e-p scattering (lattice interactions) at high temperature**
  - **Impurities at low temperatures**





Ag, rein
Ag + 0.02 at % Sn
Ag + 0.5 at % Au
ρ (10⁻⁶ Ωcm)
0
1
2
3
4
5
6
100
150
200
250
300
T (K)

(a)

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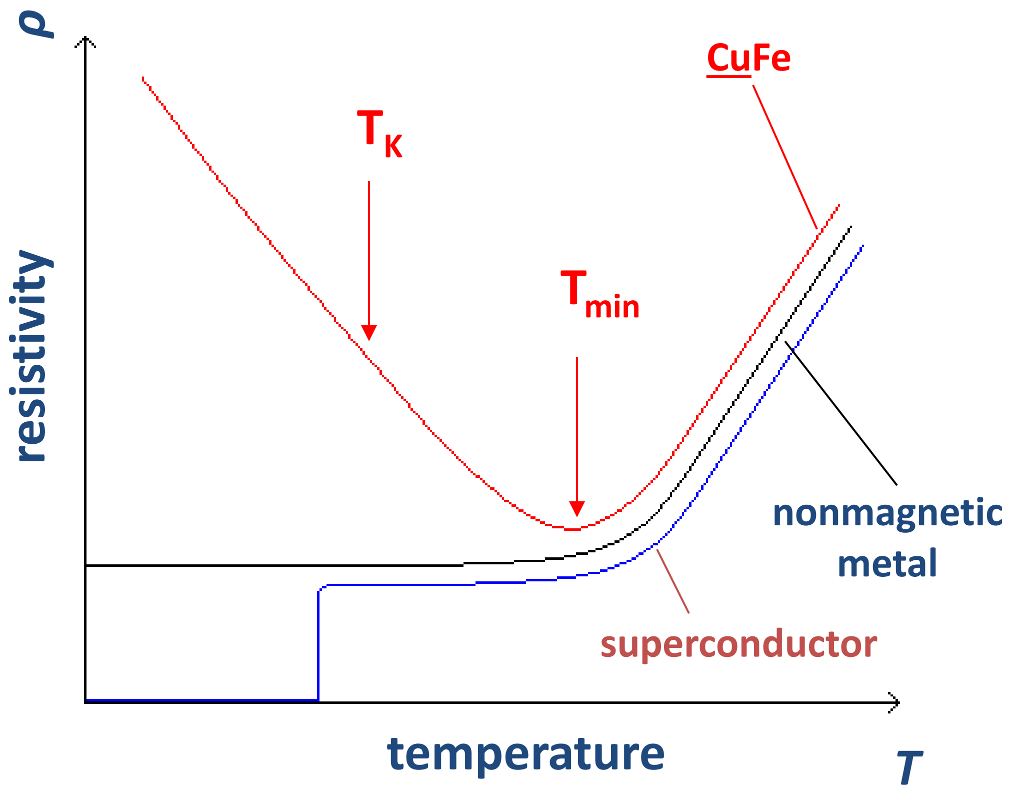


- **minimum in $\rho(T)$**
- **logarithmic increase** of the resistivity below a characteristic temperature T_K

Theoretical explanaition by Jun Kondo, 1964

⇒ Kondo effect

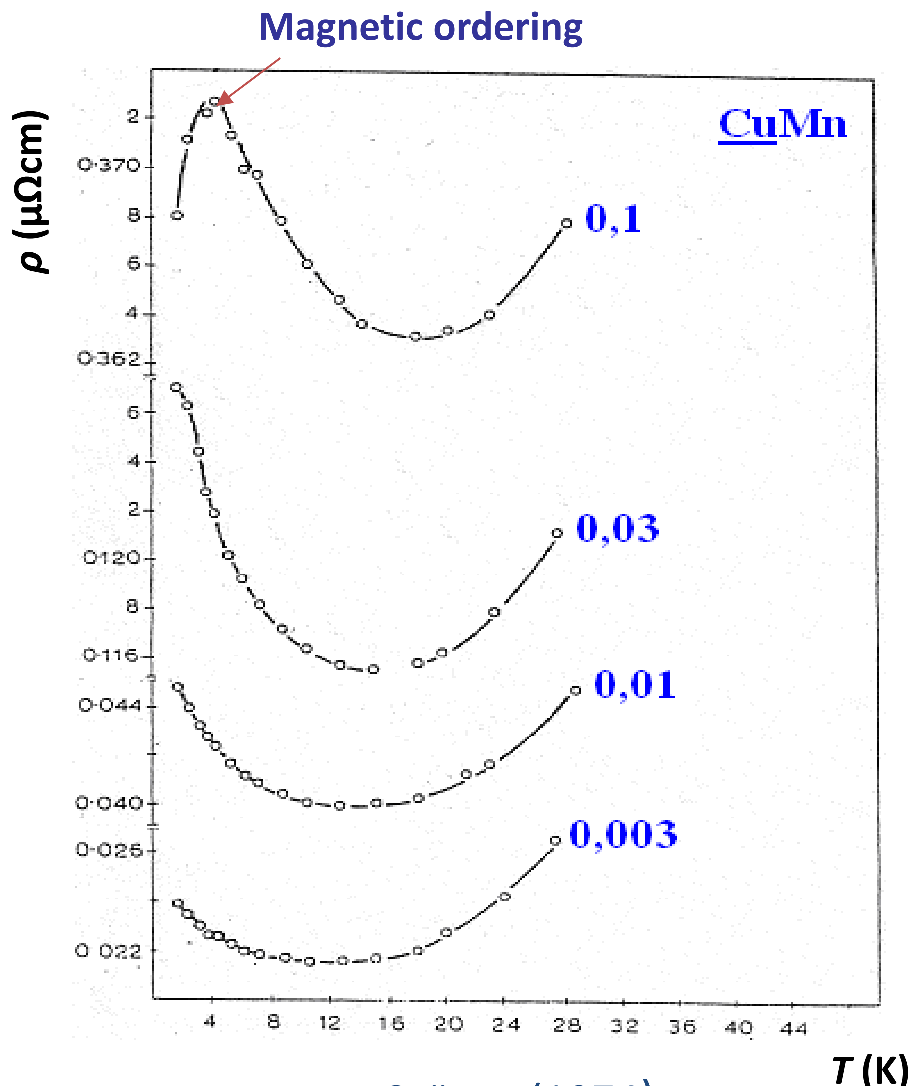
Concentration dependence of T_{min}

T_{min} depends on the **concentration** of the magnetic impurity, example: CuMn

- **Value** of ρ_{min} is **proportional** to Mn concentration
- **Temperature** T_{min} **weakly** depends on Mn concentration

⬇

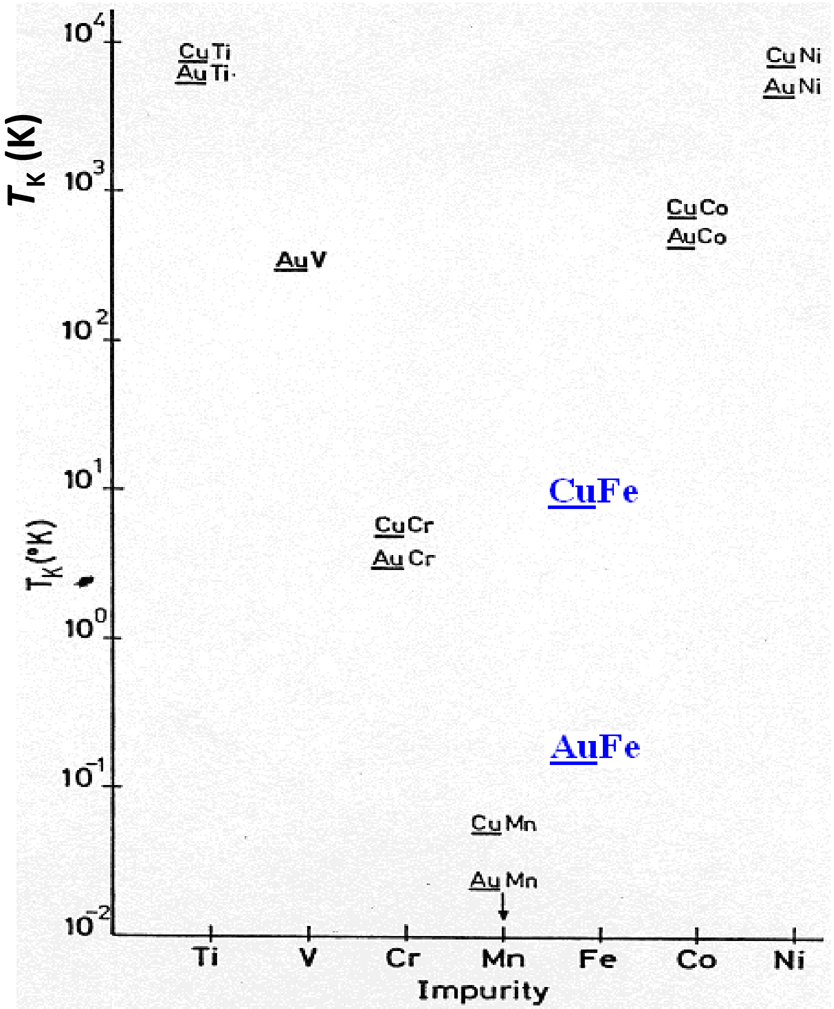
Anomalous behavior is not caused by interaction of magnetic impurities with each other!



Grüner (1974)

Dependence of T_K on the matrix

Kondo temperature T_K depends on the **nonmagnetic matrix (e.g. Au, Cu)** in which the magnetic impurities are embedded



Rizzuto (1974)

***T_K* varies strongly** for the same type of impurity **upon changing the matrix**

Large interaction between the conduction electrons of the matrix and the magnetic impurities!

example:

AuFe **CuFe**

T_K: 0,4K << 30K

How to deal with the interaction between localized electrons (e.g. d or f electrons) and itinerant (conduction **)**
electrons

What happens if we put magnetic impurites (e.g. Mn, Fe)
in nomagnetic metals (e.g. Cu, Au)?; and

What are the condition for moment formation?

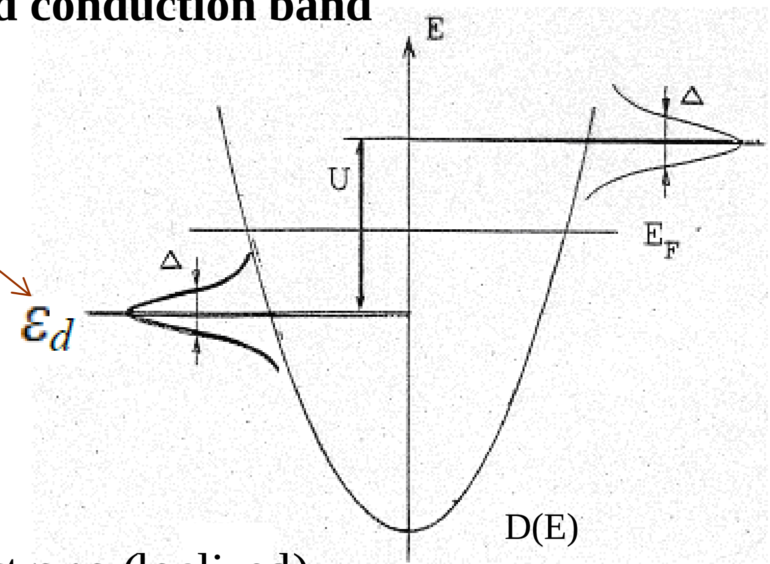
Anderson model, Phys. Rev. 124, 41 (1961)

The Anderson model (961)

hybridization between mpurity level and conduction band

$\Rightarrow$ magnetic impurity d-level exhibits finite life time $\Rightarrow$ finite width Δ

$\Rightarrow \Delta = \pi V_k^{\,2} D(E_F)$



conduction s electrons $\quad$ d electrons (loalized)

$$H_A = \sum_{k\sigma} \varepsilon(k) c^\dagger_{k\sigma} c_{k\sigma} + \sum_{\sigma} \varepsilon_d c^\dagger_{d\sigma} c_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} +$$

$$\sum_{k\sigma} V_k c^\dagger_{k\sigma} c_{d\sigma} + V_k^* c^\dagger_{d\sigma} c_{k\sigma}$$

Coulomb repulsion between d electros

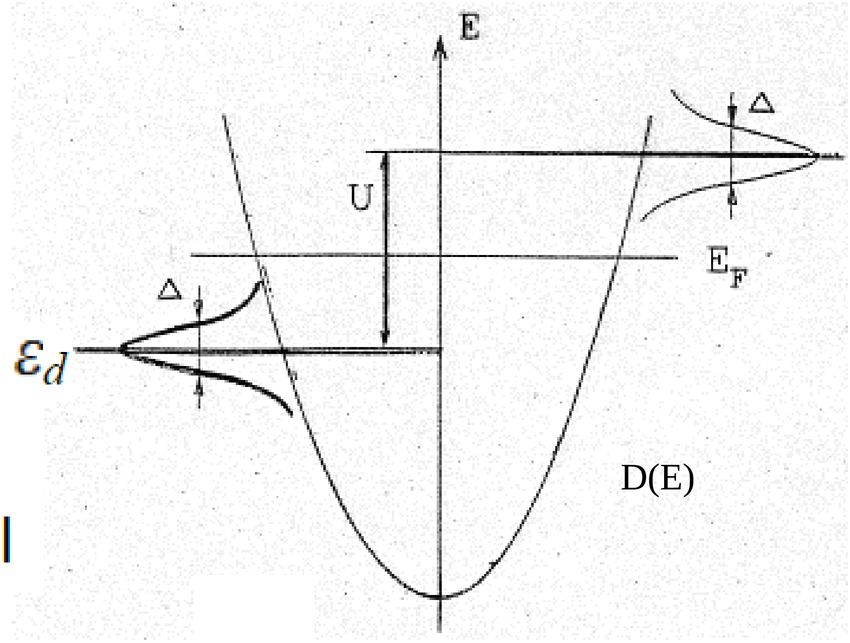
hybridization between local d electrons and conduction s electrons (Δ)

Strong Coulomb interaction U leads to local moment formation

moment formation when: :

$\varepsilon_d < E_F$ with $\Delta << |\varepsilon_d - E_F|$, and

$\varepsilon_d + U > E_F$ with $\Delta << |\varepsilon_d + U - E_F|$



(i) impurity level is mainly occupied by a single electron (spin= ½); and (ii) the hybridization is small enough to keep the spin localized at the impurity level

Kondo model

Schrieffer-Wolff-Transformation):

Hybridization Matrix element

$V_{\vec{k}} \longrightarrow J$

$H_{Anderson} \longrightarrow H_{Kondo}$

effective exchange interaction between local spins and spins of conduction electrons

$$H = \sum_{\vec{k}\sigma} \varepsilon(k) c^{\dagger}_{k\sigma} c_{k\sigma} + J \vec{s} \cdot \vec{S}$$

local spin $\vec{S} = \frac{1}{2}$ (located at $\vec{r} = 0$)

$s = \frac{1}{2} \sum_{\vec{k}\vec{k}'} c^{+}_{\vec{k}\sigma} \vec{\tau}_{\sigma\sigma'} c_{\vec{k}'\sigma'}$ ($\vec{\tau}_{\sigma\sigma'}$ = vector of Pauli matrices)

exchange coupling $J = 2V^2 \left(\frac{1}{|\epsilon_d|} + \frac{1}{\epsilon_d + U} \right)$

$$H_K = \underbrace{\sum_{\vec{k}.\sigma} \epsilon(\vec{k}) c^{+}_{\vec{k}\sigma} a_{\vec{k}\sigma}}_{\text{conduction electrons}} + J \sum_{kk'} \left[\underbrace{\left(c^{+}_{\vec{k}'\uparrow} c_{\vec{k}\uparrow} - c^{+}_{\vec{k}'\downarrow} c_{\vec{k}\downarrow} \right) S_z}_{\text{scattering without spin-flip}} - \underbrace{\left(c^{+}_{\vec{k}'\downarrow} c_{\vec{k}\uparrow} S^{+} - c^{+}_{\vec{k}'\uparrow} c_{\vec{k}\downarrow} S^{-} \right)}_{\text{with spin-flip}} \right]$$

pertubation theory:

2nd Born approximation ➡

calculation of the **transition probability** per time unit from an initial into the final state for all possible scattering processes

Results of the Kondo model

electrical resistivity $\rho(T)$:

$$\rho = a \cdot T^5 + c \cdot \rho_P + c \cdot \rho_M = a \cdot T^5 + c \cdot \rho_P + c \cdot \rho_B \left[(1 + 2 \cdot J \cdot D(E_F) \cdot \ln(D/k_B T) \right]$$

phonons | **defect scattering** | **Kondo** | **temperature independent, from 1st Born approximation**

***D*(E_F): density of states of conduction electrons per spin at the Fermi level**
***D*: band width of conduction band ($D \approx E_F$)**

$$\rho_B = \frac{3\pi m J^2 S(S+1)}{2e^2 \hbar n E_F}$$

c: concentration of magnetic impurities
m: electron mass
n=*N*/*V*: density of electrons

(a) Magnetic contribution to the electrical resistivity

$\rho_M \propto J \cdot \ln(D/k_B T)$

⬇

Logarithmic increase at low temperatures!

(b) Minimum in $\rho(T)$:

$\partial\rho/\partial T = 0$

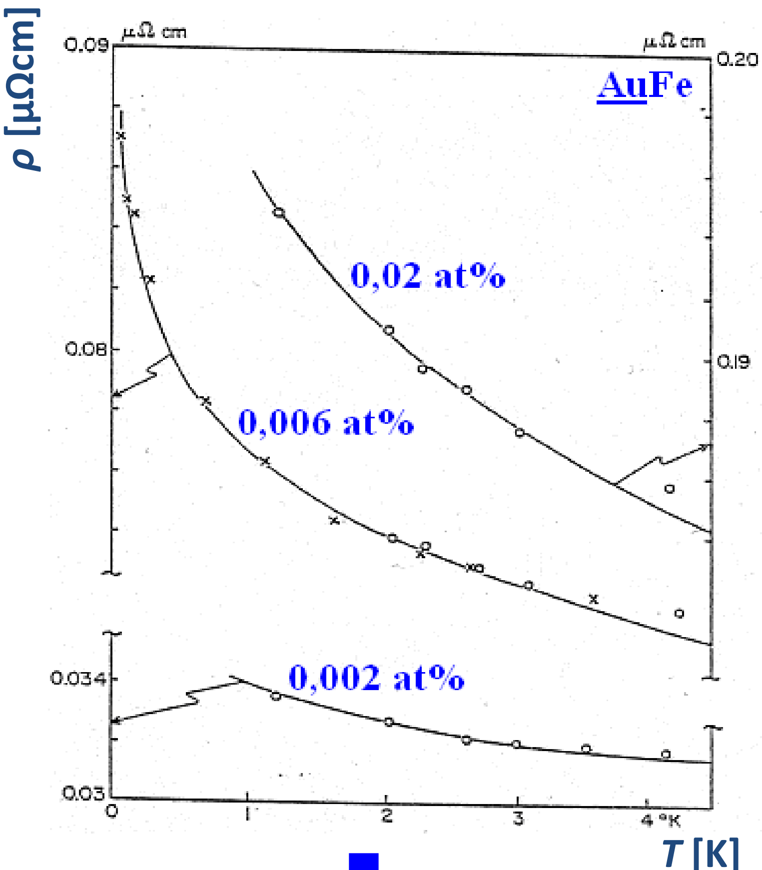
$\Rightarrow T_{min} = (2|J|\rho_B N(E_F)/5a)^{1/5} c^{1/5}$

⬇

T_{min} weakly depends on the concentration!

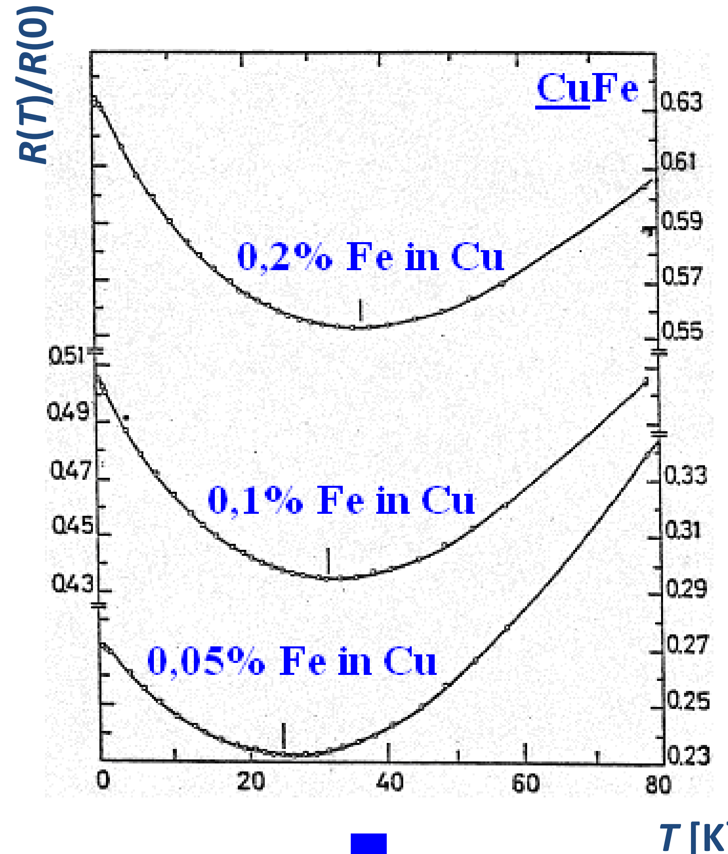
Comparison with experiment

MacDonald *et al.* (1962)



very good
Description by
Kondo model

Franck *et al.* (1961)



$T_{min} \propto c^{1/5}$ in agreent with
Kondo model

(c) Kondo temperature

$$T_K \propto D e^{-\frac{1}{|J| D(E_F)}}$$

$\rho(T)/\rho(0)$ versus T/T_K shows **universal** behavior (holds also for $\chi(T)/\chi(0)$...)

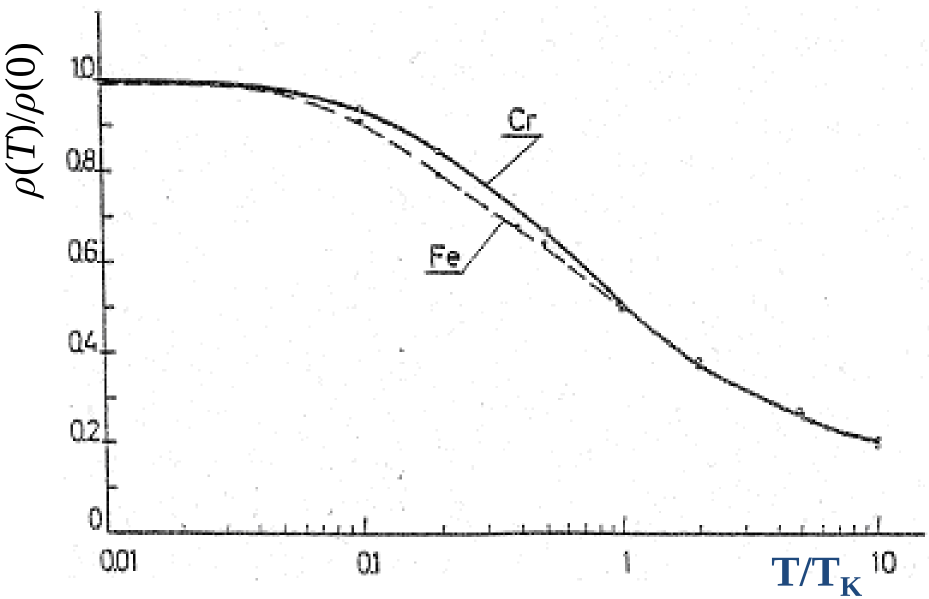
⬇

***T_K* is a new energy scale!**

c) Kondo-Temperatur T_K is very sensitive **to changes** in $|J|\cdot D(E_F)$, weak dependence on D

⬇

Explanation of very different values of T_K



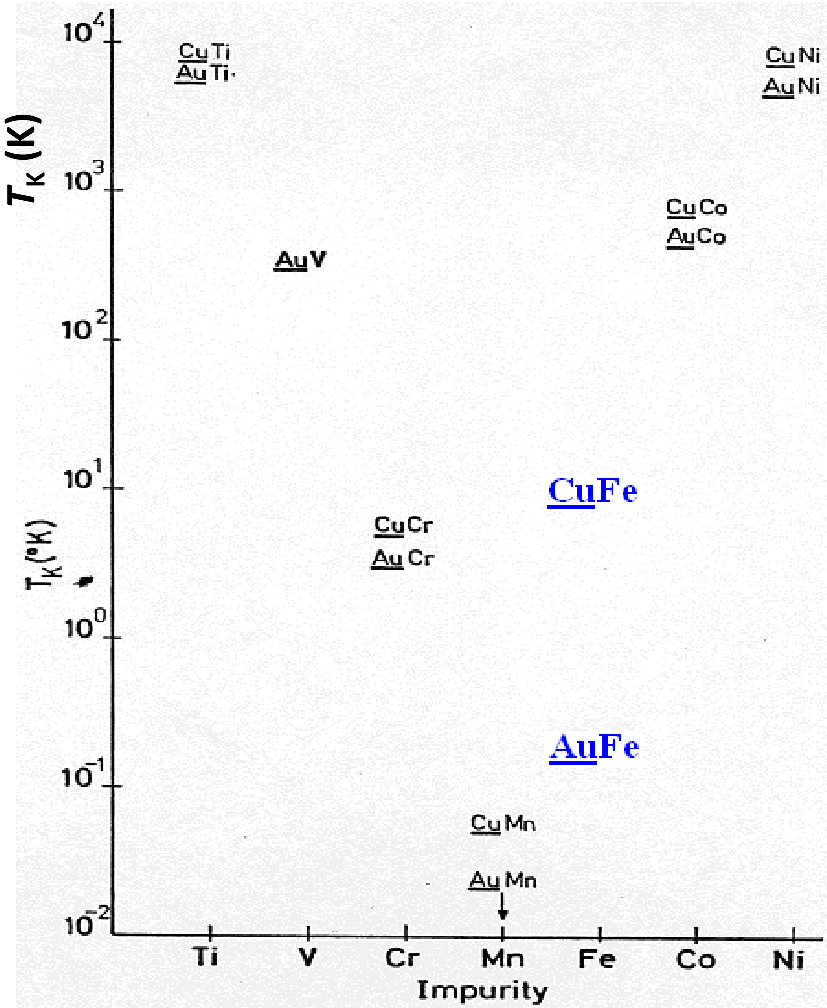
Example: D=5eV

$|J|\cdot D(E_F)$=**0,1** → T_K=**2,6K**

$|J|\cdot D(E_F)$=**0,2** → T_K=**390K**

Dependence of T_K on the matrix

Kondo temperature T_K depends on the **nonmagnetic matrix (e.g. Au, Cu)** in which the magnetic impurities are embedded



Rizzuto (1974)

***T_K* varies strongly** for the same type of impurity **upon changing the matrix**

↓

Large interaction between the conduction electrons of the matrix and the magnetic impurities!

example:

	AuFe	CuFe
T_K:	0,4K	<< 30K

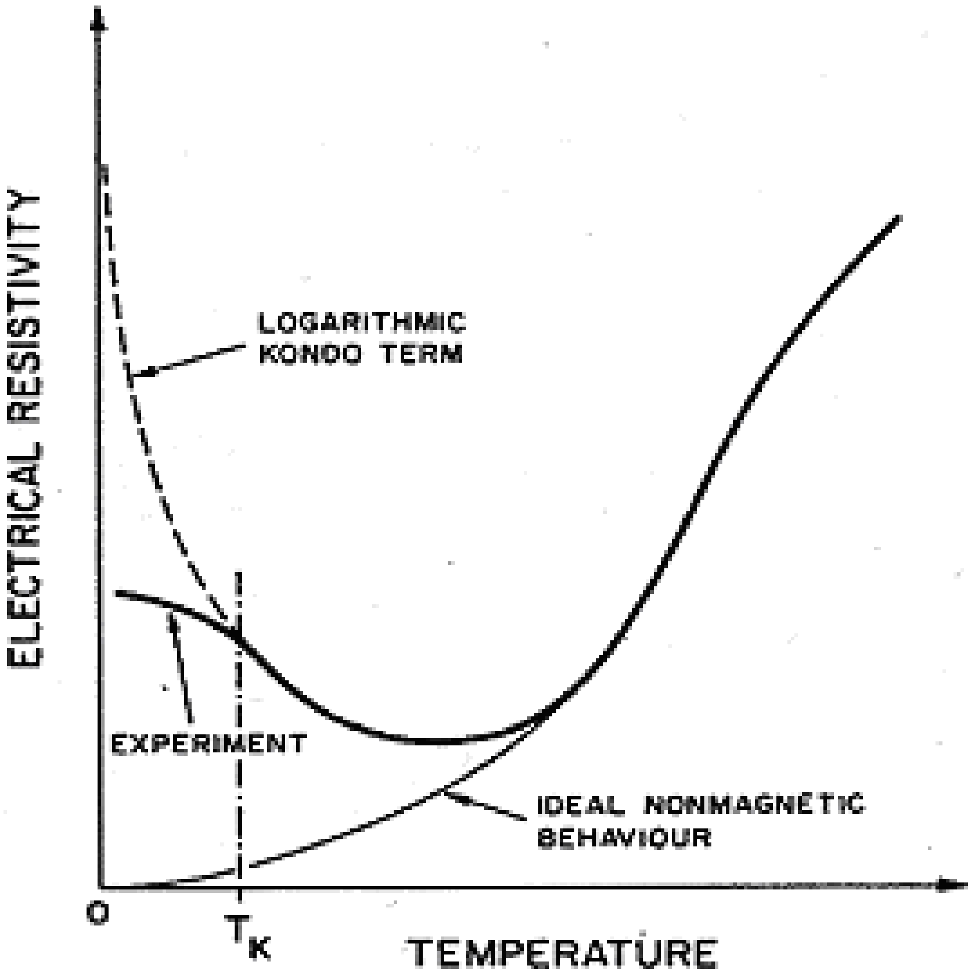
From the Kondo effect to the Kondo problem?

Unphysical increase of $\rho_M \propto J \cdot \ln(k_B T/D) \rightarrow \infty$ as $T \rightarrow 0$!
Experiment: ρ_M finite for $T \rightarrow 0$. This is called the Kondo-Problem!

⬇

Theory: approximation not valid for $T << T_K$

No description of the experimental data at $T << T_K$



What happend at $T \ll T_K$?

We consider physical quantities which which contain the spin degree of freedom

$\Rightarrow$ Magnetic suszeptibility $\chi(T)$ und specific heat $c_V(T)$ at low temperatures (**$T \ll T_K$**)

1. Magnetic Suszeptibiliy:

***T>T_K*: Curie-Weiss-behavior**

⇒ Local magnetic moments

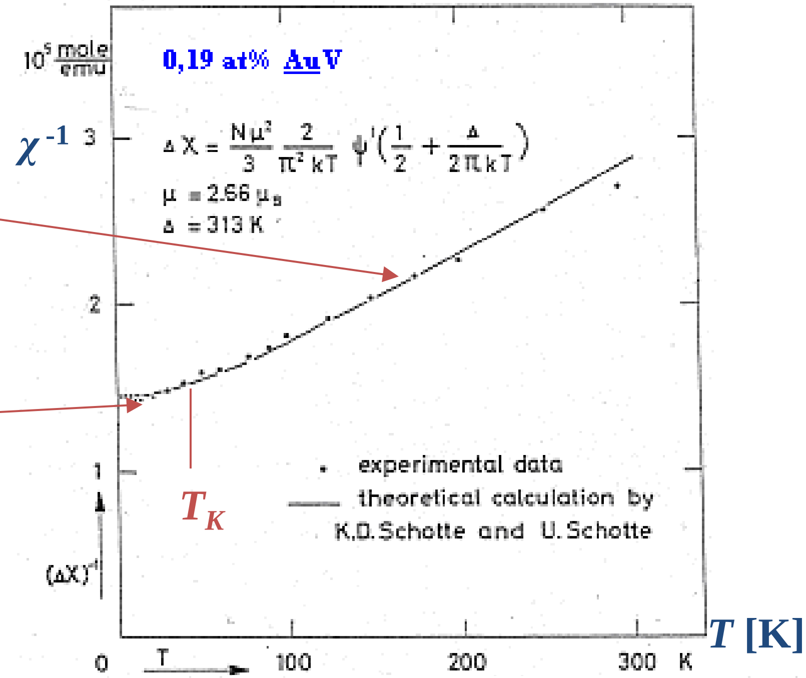
***T<T_K*: Pauli-Suszeptibility**

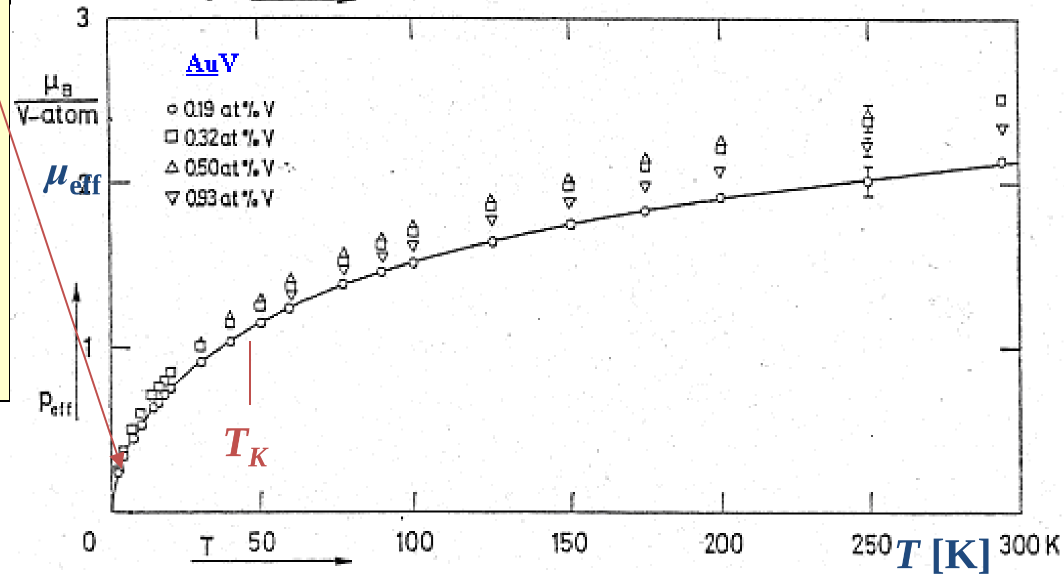
$\chi(T)=const$

μ_{eff} (magnetic impurity) ≈ 0 for $T \rightarrow 0$

⬇

At T_K: magnetic → nonmagnetic crossover, but no phase transition





Van Dam *et al.* (1972)

2. Specific heat:

Entropy change ΔS_{Ent} between T=0 und T=∞

$$\Delta S_{Ent} = \int_0^\infty \frac{c_V}{T}\, dT = R \ln(2S+1)$$

Experimentell:

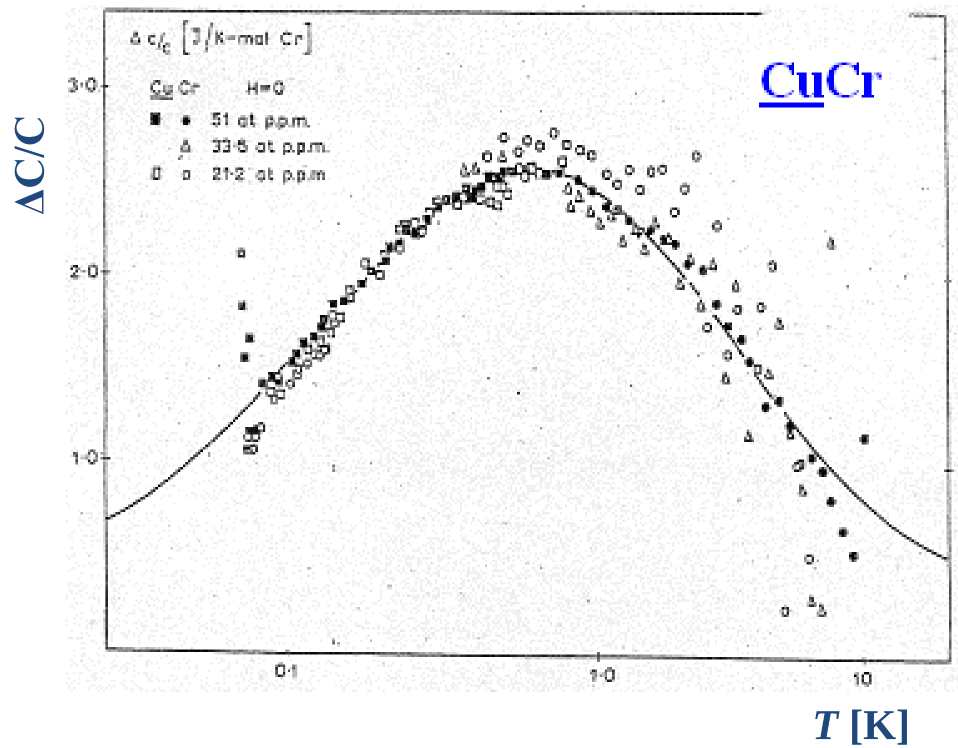
$\Delta S_{Ent} = R \cdot \ln 4 \Rightarrow$ Spin S=3/2

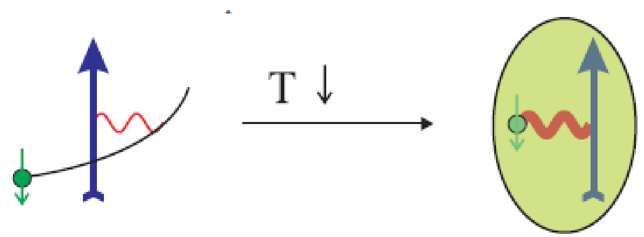
from $\chi(T)_{T>>T_K} \Rightarrow S$=3/2

$\Rightarrow S$=0 für T=0

Magnetic impurity at $T \rightarrow 0$ nonmagnetic with mit S=0 (Singlet) ground state

Triplett and Phillips (1971)





Physical picture: crossover magnetic ↔ nonmagnetic

Interaction between the Spins of conduction electrons with impurity spins
⇒ Spin correlations

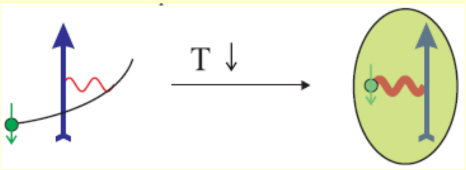
Strong resonace scattering of conduction electrons by the local moments

Formation of an (Abrikosov-Suhl) resonance at E_F of width $k_B T_K$

Logarithmic increase of ρ below T_K

***$T \ll T_K$*:**

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:

$$k_B T_K = D e^{-\frac{1}{|J| N(E_F)}}$$

Crossover:
magnetic ↔ nonmagnetic
weak ↔ strong coupling

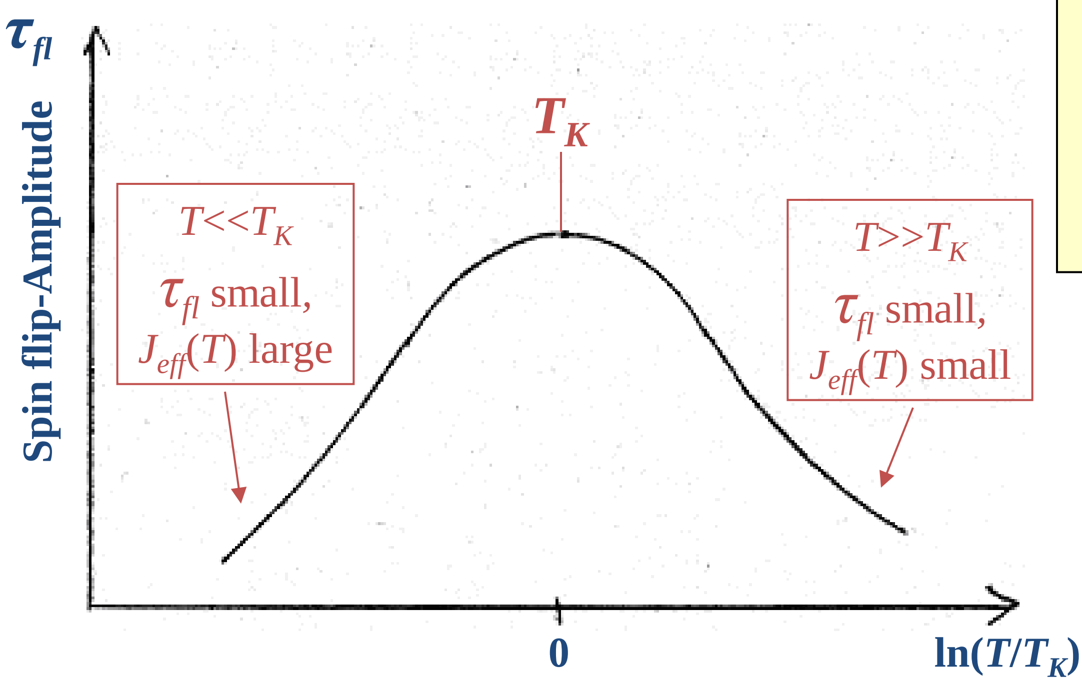
Comparison with results of the BCS Theory:

$$k_B T_c = 1{,}14\ \hbar\omega_c\ \exp(\ -1/N(E_F)\ V_0)$$

$$k_B T_K = D e^{-\frac{1}{|J|N(E_F)}}$$

Something to the dynamic:

$J \rightarrow J_{eff}(T)$ ← **Temperature dependence of effective coupling increases with decreasing temperature**



$T \rightarrow 0$: Spin flip frozen

⬇

Singlet state,
can be brocken up with energy $\hbar\omega \geq k_B T_K$ (e.g. Neutron scattering) (**Singlet-Triplet-excitation)**

Physical picture: crossover magnetic ↔ nonmagnetic

Interaction between the Spins of conduction electrons with impurity spins
⇒ Spin correlations

Strong resonace scattering of conduction electrons by the local moments

↓

Formation of an (Abrikosov-Suhl) resonance at E_F of width k_BT_K

↓

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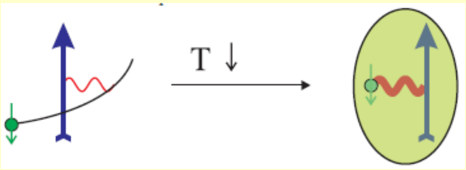

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