Autumn School on Correlated Electrons: Correlations and Phase Transitions

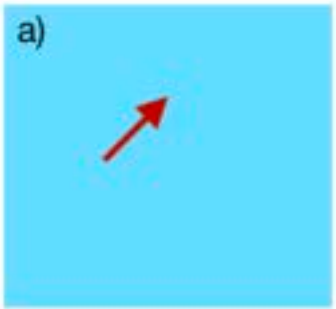
Jülich 16.-20.9. 2024

Competition between Kondo Effect and RKKY Coupling

Stefan Kettemann, Constructor University Bremen, Germany

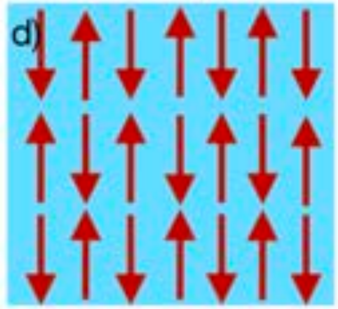
Lecture Notes of the Autumn School on Correlated Electrons 2024,
published in Correlations and Phase Transitions, Band/Volume 14
edited by Eva Pavarini and Erik Koch
Verlag des Forschungszentrums Jülich

1.Introduction



Dilute
magnetic moments
in a metal: Kondo Effect

Example:
dilute
Fe-impurities in Ag



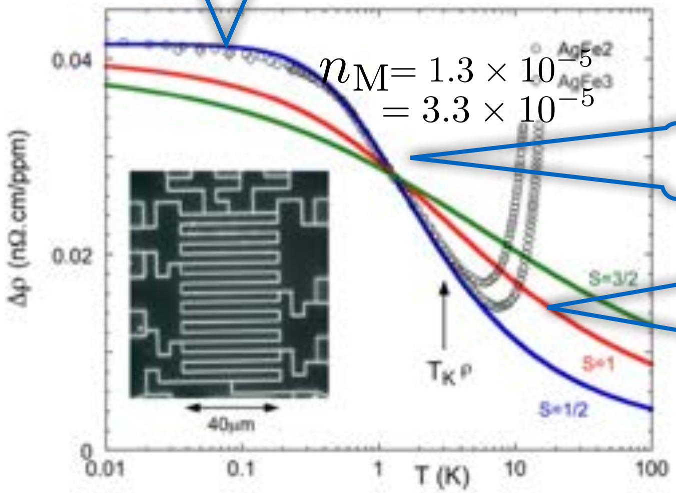
Dense, ordered lattice
of magnetic moments in
Heavy Fermion Materials
like $CeAl_3$

Saturation of resistivity ρ at Low T: Fermi Liquid

$n_M = 1.3 \times 10^{-5}$
$= 3.3 \times 10^{-5}$

Kondo enhanced resistivity

Resistivity Minumum

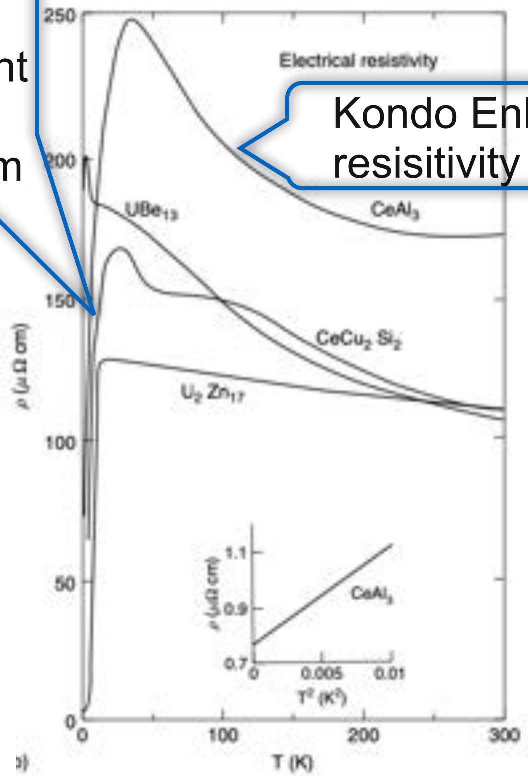


F.Mallet, et al Phys. Rev. Lett. 97, 226804 (2006).

Sharp Drop of resisitivity ρ

when coherent Heavy Fermions form

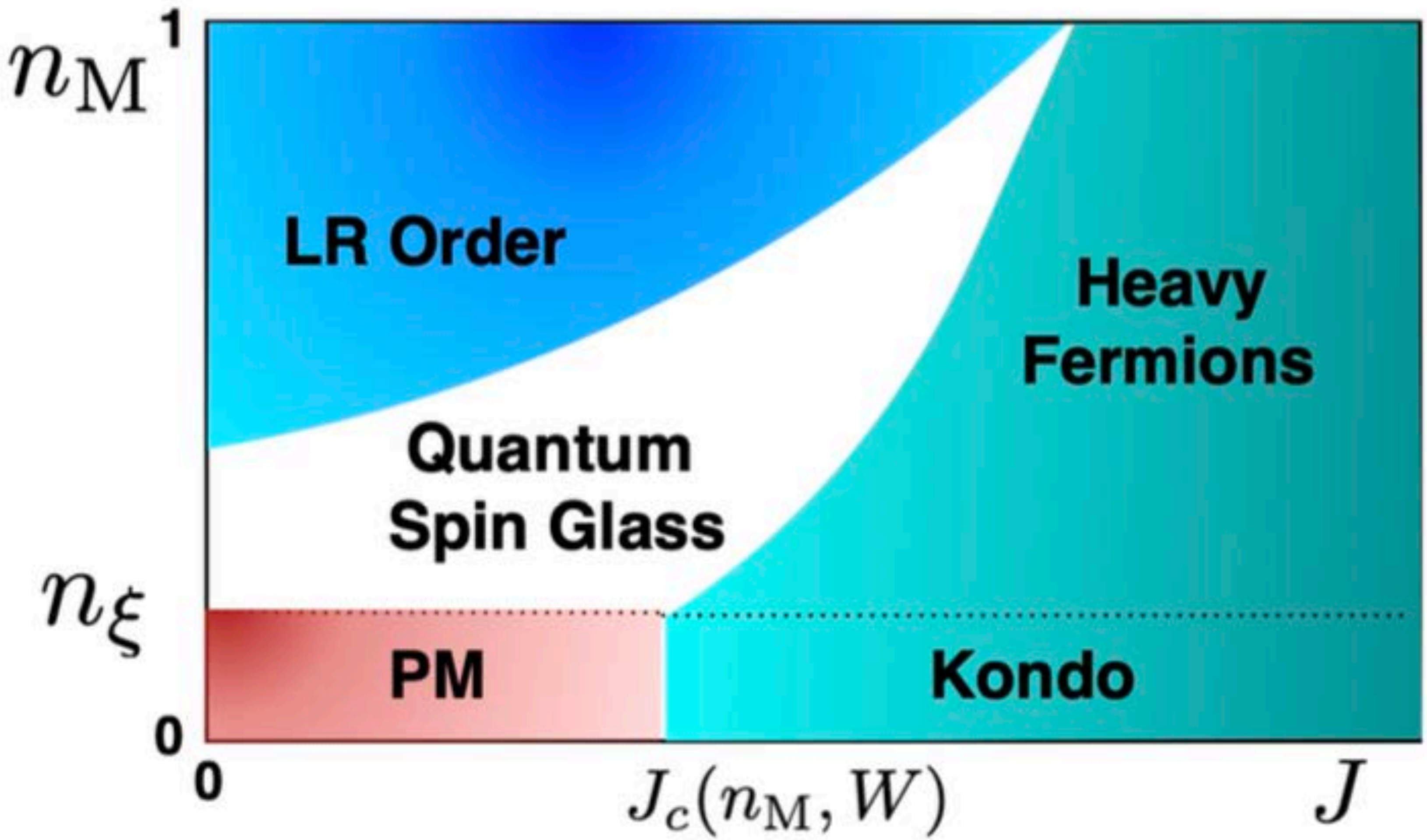
Kondo Enhanced resisitivity



J.L. Smith and P.S. Riseborough, *J. Mag. Mat.* 47–48, 1985

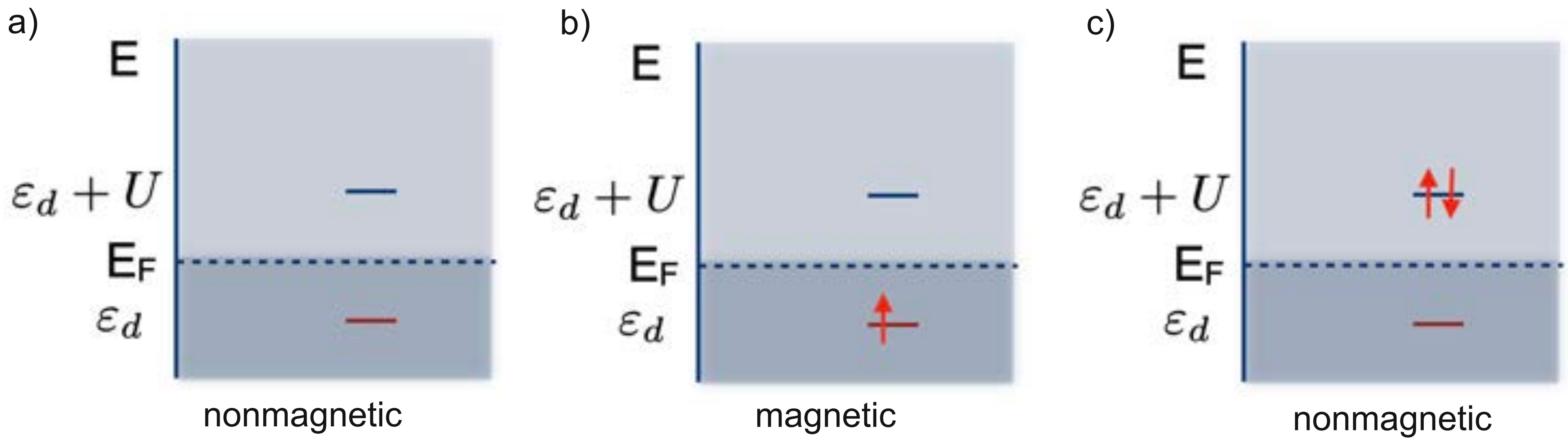
1. Introduction
2. Formation of magnetic moments
3. Kondo effect: screening of magnetic moments
4. RKKY coupling between magnetic moments
5. Spin competition:
   a) the Doniach diagram
   b) Kondo lattice
   c) Kondo-RKKY-Renormalization Group
6. Spin competition in presence of a spectral (pseudo) gap
   a) Band insulator, semiconductor
   b) Pseudo gap semimetal (Graphene, Topological Insulator,...)
7. Spin competition in the presence of disorder
   a) Distribution of Kondo temperature and RKKY couplings
   b) Anderson localization - local spectral gaps
   c) Multifractality - local pseudo gaps
   d) Doniach diagram of disordered systems
8. Conclusions and open problems

T=0K Quantum Phase Diagram



n_M	concentration of localized magnetic moments	W	Disorder Strength	J	exchange coupling between local moment and conduction electron spins

2. Formation of magnetic moments in Metals



A localized (d- or f-) level with energy ε_d can a) remain unoccupied, b) be filled with one electron of either spin $\sigma = +, -$ or doubly occupied with 2 electrons of opposite spin (Pauli Principle), costing repulsion energy U >0.

Thus, the condition for formation of magnetic moments, is that the level remains singly occupied b), requiring $\varepsilon_d < 0$ and $\varepsilon_d + U > 0$ or $U > -\varepsilon_d$ relative to the Fermi Energy E_F=0

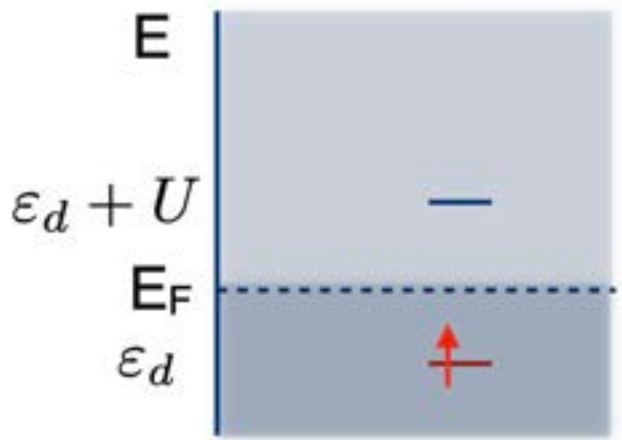
Notation: an electron in the d-level is removed, created by the Fermion operators $d_\sigma \, , \, d_\sigma^+$

The number of electrons of spin $\sigma = +, -$ in the d-level is obtained with the number operator

$$\hat{n}_{d\sigma} = d_\sigma^+ d_\sigma$$

P. W. Anderson, Phys. Rev. 124, 41 (1961).

Fermi Sea



Fermi Sea: Conduction band states filled up to Fermi energy E_F
with single Electron energy E_n , given by solution of Schrödinger equation

$$\left(\frac{\mathbf{p}^2}{2m} + V(\mathbf{r})\right)\psi_n(\mathbf{r}) = E_n\psi_n(\mathbf{r})$$

with potential $V(\mathbf{r})$ due to impurities, material imperfections, Hartree potential and confinement.

Notation: an electron is removed, created in state n by the Fermion operators $c_{n\sigma}, c^+_{n\sigma}$

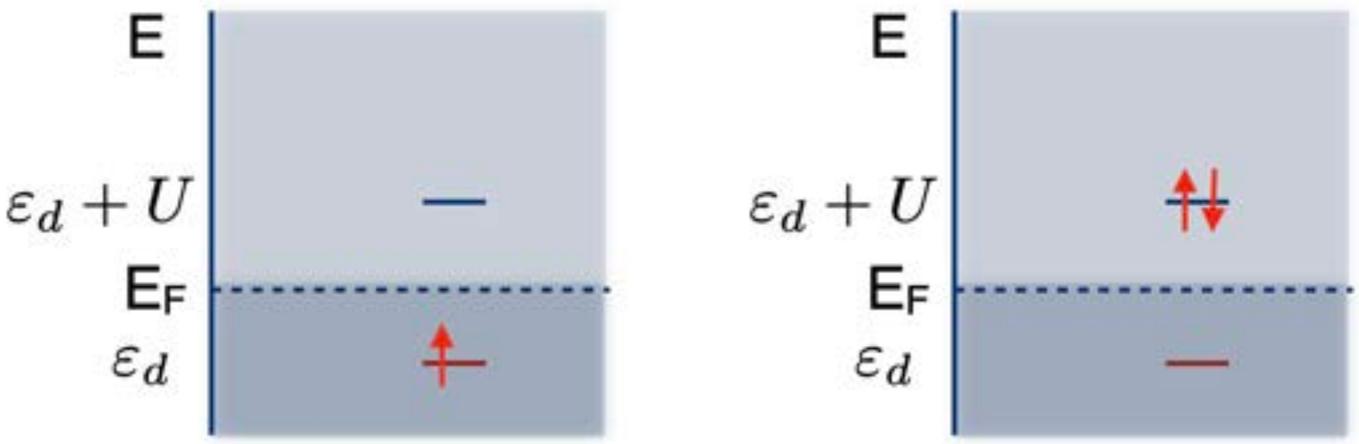
The number of electrons of spin $\sigma = +, -$ in that state is obtained with the number operator

$$\hat{n}_{n\sigma} = c^+_{n\sigma} c_{n\sigma}$$

We assume, if not stated otherwise $E_{n\sigma} = E_n$

P. W. Anderson, Phys. Rev. 124, 41 (1961).

Coupling to the Fermi Sea



Thus, the Hamiltonian of electrons in the conduction band and the d-(or f-) level is given by

$$H = \sum_{n,\sigma} E_{n\sigma}\hat{n}_{n\sigma} + \sum_{\sigma} \varepsilon_{d\sigma}\hat{n}_{d\sigma} + U\hat{n}_{d+}\hat{n}_{d-} + \sum_{n,\sigma}\left(t_{nd}c^{+}_{n\sigma}d_{\sigma} + t_{dn}d^{+}_{\sigma}c_{n\sigma}\right)$$

The d-levels hybridize with the conduction band states with matrix elements

$$t_{dn} = t^{*}_{nd}$$

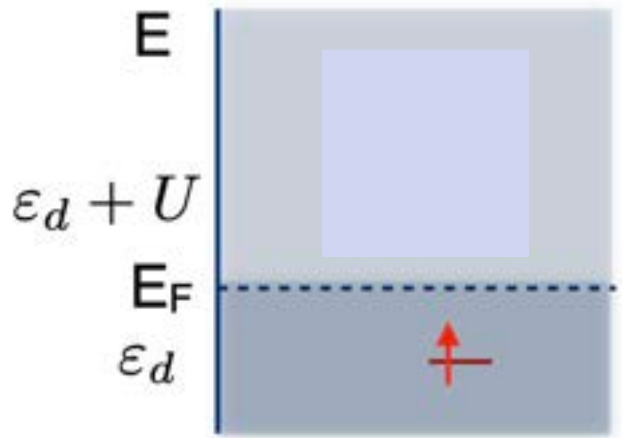
which are matrix elements of the impurity Atomic potential

$$t_{dn} = \langle d|\hat{V}_A|n\rangle = \int d^d r\, \phi^{*}_{d}(\mathbf{r})\, V_A(\mathbf{r})\psi_n(\mathbf{r})$$

where $\phi^{*}_{d}(\mathbf{r}), \psi_n(\mathbf{r})$ are the wave functions amplitudes of the d-level and the conduction band state, respectively, at position **r**

P. W. Anderson, Phys. Rev. 124, 41 (1961).

Kondo Hamiltonian



Projecting out the high energy, nonmagnetic states (unoccupied and doubly occupied d-level), -the so called Schrieffer-Wolff transformation- one gets the Kondo Hamiltionian

$$H_K = \sum_{n,\sigma} E_n \hat{n}_{n\sigma} + \sum_{n,n'} J_{nn'} \left[\underbrace{S^+ c^+_{n+} c_{n'-} + S^- c^+_{n-} c_{n'+}}_{\text{Spin Flip}} + \underbrace{S_z (c^+_{n+} c_{n'+} - c^+_{n-} c_{n'-})}_{\text{Zeeman-splitting}} \right]$$

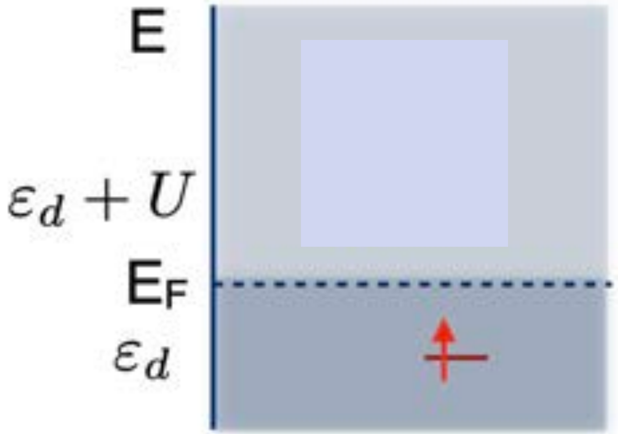
where $\mathbf{S}$ is the spin S=1/2- operator of the localized magnetic moment, with $S^\pm = S_x \pm \imath S_y$

and the matrix elements of the exchange coupling are found to be

$$J_{nn'} = t_{nd}\, t_{dn'} \left(\frac{1}{U + \varepsilon_d - E_{n'}} + \frac{1}{-\varepsilon_d + E_n} \right)$$

J. R. Schrieffer and P. Wolff, Physical Review 149, 491 (1966).

Symmetric Kondo Hamiltonian



For $\epsilon_d = -U/2$ the Kondo Hamiltonian simplifies to

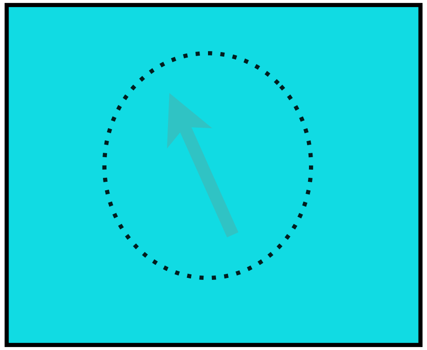
$$H_K^0 = \sum_{n,\sigma} E_n \hat{n}_{n\sigma} + J\vec{\mathbf{S}}\vec{\mathbf{s}}(\mathbf{r}),$$

with exchange coupling $J = 4t^2/U > 0$ antiferromagnetic

where we defined the conduction band spin density operator $\vec{\mathbf{s}}_{\alpha\beta}(\mathbf{r}) = \sum_{n,n'} \psi^*_{n'}(\mathbf{r})\psi_n(\mathbf{r})c^+_{n\alpha}c_{n'\beta}\vec{\sigma}_{\alpha\beta}$

J. R. Schrieffer and P. Wolff, Physical Review 149, 491 (1966).

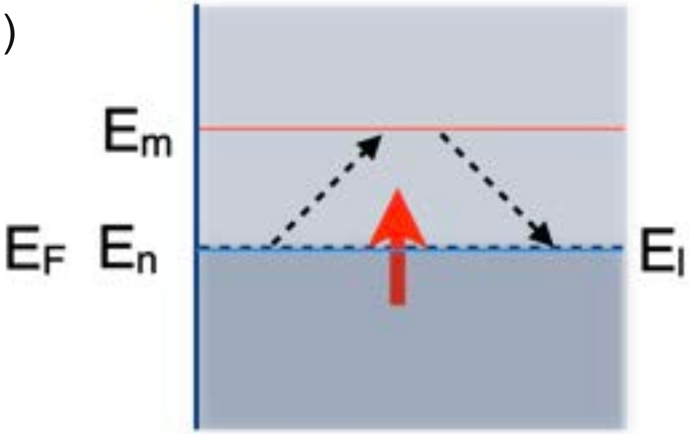
Kondo effect:
screening of magnetic moments
by conduction electron spins



Corrections to the Exchange Coupling in Perturbation Theory

corrections to the exchange coupling matrix elements J_{nl} between states at Fermi energy n, l :

a)

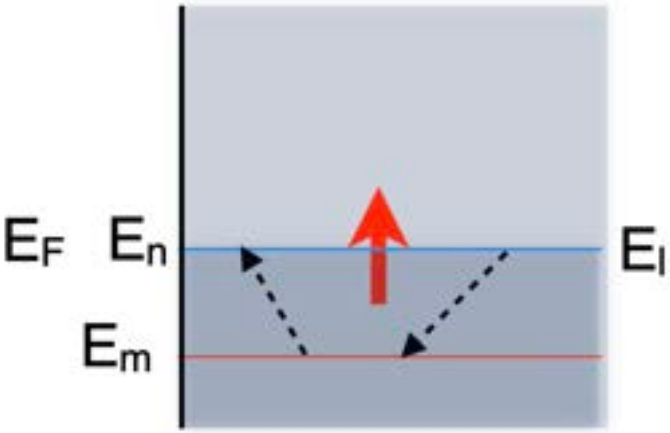


due to electron excitations caused by J via intermediate state m, if not occupied $\sim (1 - f(E_m))$

with Fermi distribution function

$$f(E_m) = \frac{1}{1 + \exp(\frac{E_m - E_F}{k_B T})}$$

b)



and due to hole excitations via intermediate state m, if occupied $\sim f(E_m)$

yielding corrections to the exchange coupling matrix elements:

$$\tilde{J}_{nl} = J_{nl}\left[1 + \frac{J}{2N}\sum_{m,\sigma}\frac{Vol.|\psi_m(\mathbf{r})|^2}{E_m - E_F}\tanh\left(\frac{E_m - E_F}{2T}\right)\right]$$

J. Kondo, Prog. Theor. Phys 32, 37 (1964)

Kondo Minimum of Resistivity

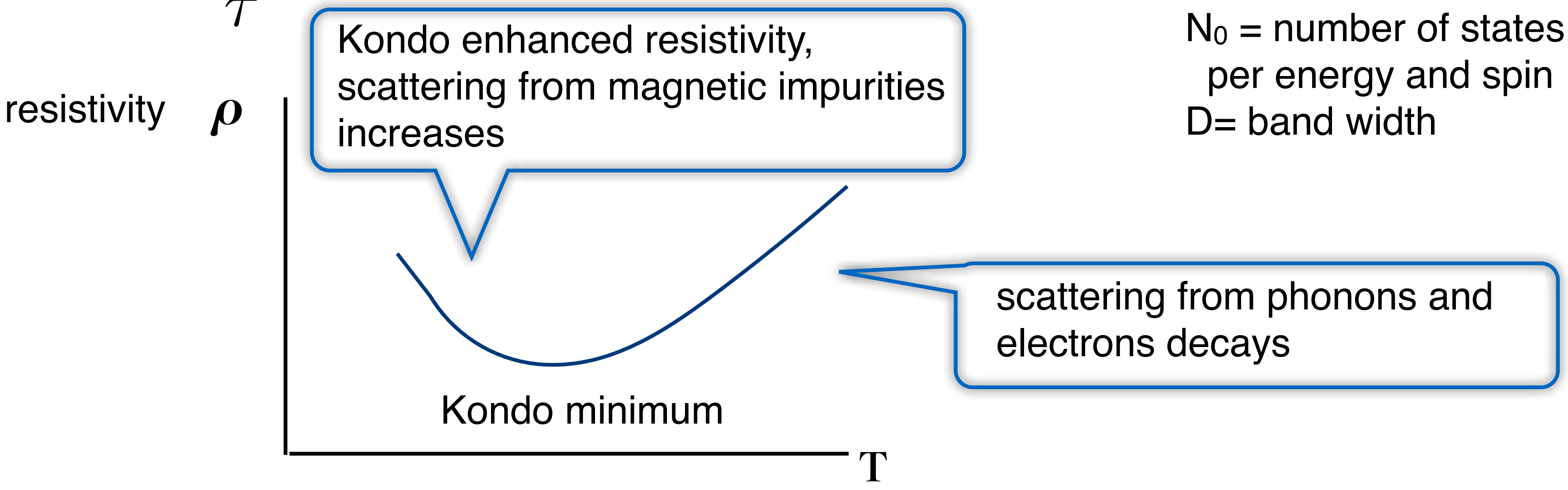
Corrections to exchange coupling matrix elements

$$\tilde{J}_{nl} = J_{nl}\left[1 + \frac{J}{2N}\sum_{m,\sigma}\frac{Vol.|\psi_m(\mathbf{r})|^2}{E_m - E_F}\tanh\left(\frac{E_m - E_F}{2T}\right)\right]$$

may become large at low temperature, and even diverge in the zero temperature limit.
→Scattering rate $1/\tau$ from magnetic impurity becomes larger at lower temperature.

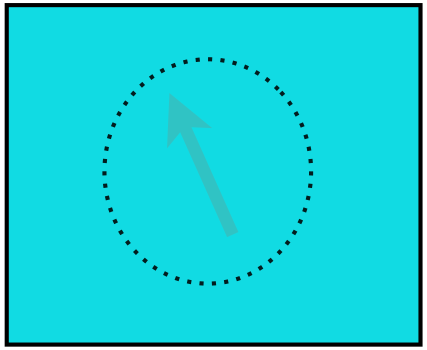
$$\rho \sim \frac{1}{\tau} \sim \tilde{J}^2 = J^2(1 + 2JN_0 \ln D/T)^2$$

N_0 = number of states per energy and spin
D= band width



J. Kondo, Prog. Theor. Phys 32, 37 (1964)

Kondo Temperature



Corrections to exchange coupling matrix elements

$$\tilde{J}_{nl} = J_{nl}\left[1 + \frac{J}{2N}\sum_{m,\sigma}\frac{Vol.|\psi_m(\mathbf{r})|^2}{E_m - E_F}\tanh\left(\frac{E_m - E_F}{2T}\right)\right]$$

Kondo temperature = Temperature when correction is as large as bare exchange coupling

$$\boxed{1 = \frac{J}{2N}\sum_{n,\sigma}\frac{L^d|\psi_n(\mathbf{r})|^2}{E_n - E_F}\tanh\left(\frac{E_n - E_F}{2T_{\mathrm{K}}(\mathbf{r})}\right)},$$

Nagaoka-Suhl (1-loop) equation for the Kondo temperature

$$T_{\mathrm{K}}(\mathbf{r})$$

of a magnetic moment at position **r**

J. Kondo, Prog. Theor. Phys 32, 37 (1964)

Y. Nagaoka, Phys. Rev. 138, 1112 (1965).

H. Suhl, Phys. Rev. A 138, 515 (1965).

Alternative Way to derive Kondo Effect: Poor Man's Scaling

Integrating successively high energy excited states at energy scale Λ above and below Fermi energy yields renormalized coupling $\tilde{J}(\Lambda)$ governed by RG equation

$$\frac{d\tilde{J}}{d\ln\Lambda} = -\tilde{J}^2(N(\mathbf{r},\epsilon_F+\Lambda)+N(\mathbf{r},\epsilon_F-\Lambda))$$

Integration over energy scale Λ from band width to Kondo temperature $T_{\mathrm{K}}(\mathbf{r})$
=Temperature when correction is as large as bare exchange coupling

$$1 = J\int_0^D dEN(E,\mathbf{r})\frac{1}{E-E_F}\tanh\left(\frac{E-E_F}{2T_{\mathrm{K}}(\mathbf{r})}\right)$$

same as Nagaoka-Suhl (1-loop) equation with number of states per energy and spin defined by

$$N(\mathbf{r},E) = \frac{Vol.}{2N}\sum_{n,\sigma}|\psi_n(\mathbf{r})|^2\delta(E-E_n)$$

with Vol. = volume of the material, and N the number of states

Kondo Temperature in clean Metal

In a metal without impurities, the number of states is the same everywhere, and assuming that it weakly depends on energy we can substitute

$$N(\mathbf{r}, E) \approx N(E_{\mathrm{F}}) = N_0$$

Thus, the Nagaoka-Suhl (1-loop) equation becomes

$$1 = J N_0 \int_0^D dE \frac{1}{E - E_F} \tanh\left(\frac{E - E_F}{2T_{\mathrm{K}}}\right)$$

Approximating

$$\tanh(x) \rightarrow \mathrm{sign}(x) \text{ for } |x| > 1$$

we can perform the integral and get

$$1 \approx J\ 2N_0 \ln(D/T_K)$$

giving the Kondo temperature

$$T_{\mathrm{K}}^0 = cD \exp(-\frac{1}{2N_0 J})$$

where c=0.57 by performing the integral more accurately

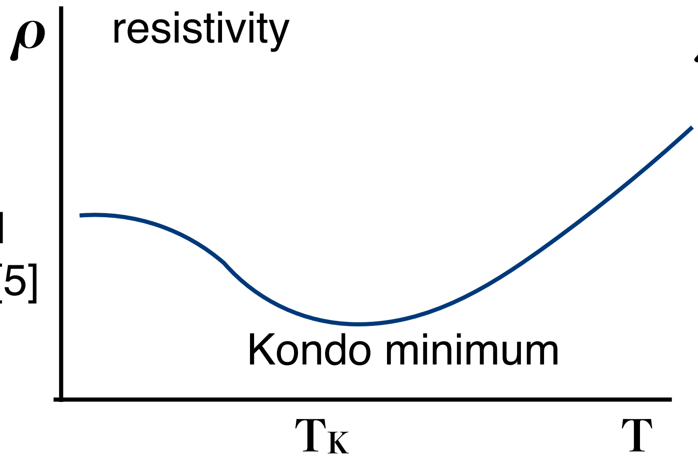
Beyond Perturbation theory

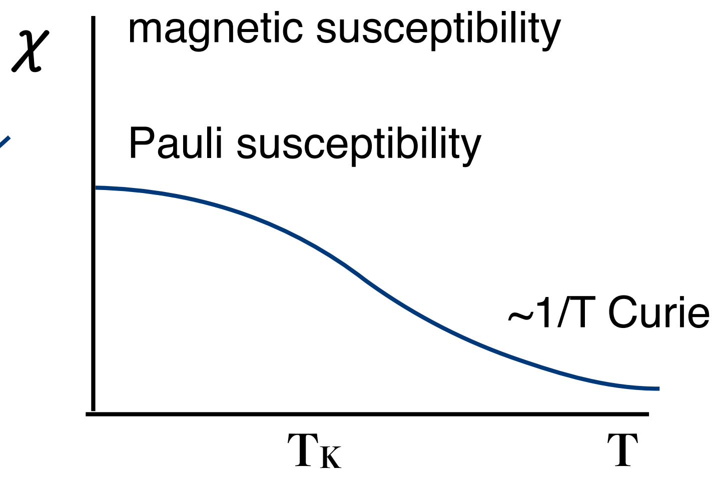
Perturbation theory breaks down at Kondo temperature $T_{\mathrm{K}}(\mathbf{r})$
Instead:

- Wilson numerical renormalization group (numerical) [1,2]
- exact Bethe-Ansatz (analytical) [3,4]

→ At low T a new state is formed, where magnetic moemnts **screened**.
Mass of conduction electron **renormalized**. Reformation of Fermi liquid [5].
Scattering rate from magnetic impurities converges to unitary limit.
Contribution of magnetic moments to resistivity, magnetic susceptibility, etc.
universal functions of T/T_K and H/T_K (H= magnetic field)

Kondo renormalized Fermi liquid [5]

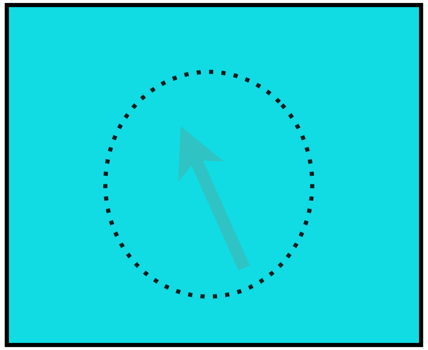




1. K. G. Wilson, Rev. Mod. Phys. 47, 773 (1975).
2. H. R. Krishna-murthy, J. W. Wilkins, and K. G. Wilson, Phys. Rev. B 21, 1003 (1980); ibid. 21, 1044 (1980).
3. A. M. Tsvelick and P. B. Wiegmann, Adv. Phys. 32, 453 (1983).
4. N. Andrei, K. Furuya, and J. H. Lowenstein, Rev. Mod. Phys. 55, 331 (1983).
5. P. Nozières, J. de Phys. C, 37, 1 (1976).

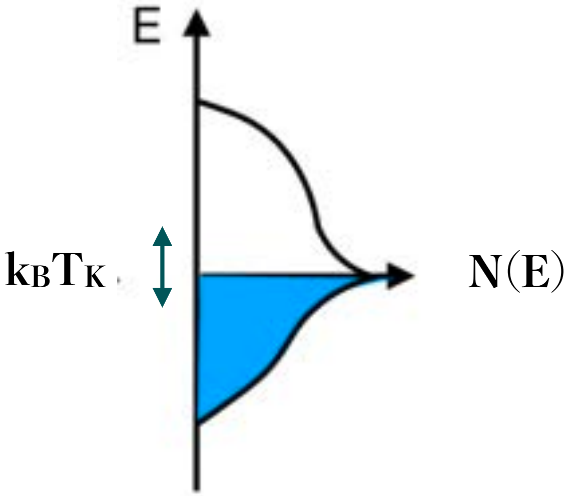
Kondo Screening

Thus, at temperatures T below the Kondo temperature T_K
the magnetic impurity becomes screened by a cloud of conduction electron spins.



Kondo Cloud

Conduction Electron Scattering from magnetic impurity leads to enhanced density of states at Fermi energy, the Kondo Peak of width $k_B T_K$

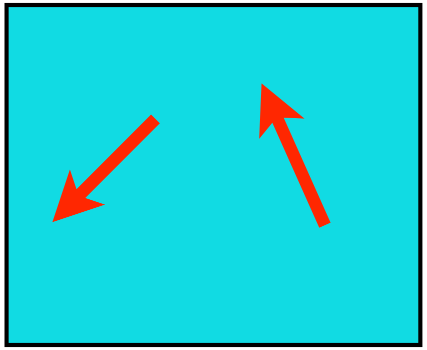


Kondo Peak

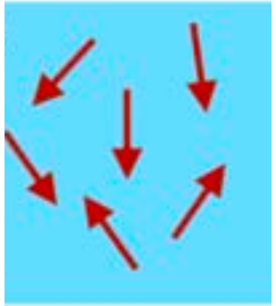
H. Suhl, Phys. Rev. A 138, 515 (1965).

P. Nozières, J. de Phys. C, 37, 1 (1976).

RKKY coupling between magnetic moments



Anderson model for M Magnetic Moments



Consider M localized level sites at different positions $\mathbf{r}_j$

$$H = \sum_{n,\sigma} E_{n\sigma}\hat{n}_{n\sigma} + \sum_{j,\sigma}\varepsilon_{d_j\sigma}\hat{n}_{d_j\sigma} + \sum_{j} U_j \hat{n}_{d_j+}\hat{n}_{d_j-} + \sum_{n,j,\sigma}\left(t_{nd_j}c^{+}_{n\sigma}d_{j\sigma} + t_{d_jn}d^{+}_{j\sigma}c_{n\sigma}\right)$$

Summation j over M localized levels at different positions

Performing the Schrieffer-Wolff transformation one gets the **Kondo Hamiltionian** of M magnetic moments immersed into a Fermi sea:

$$H_K = \sum_{n,\sigma} E_n\hat{n}_{n\sigma} + \sum_{j,n,n'} J_{j,nn'}\left[S^{+}_{j}c^{+}_{n+}c_{n'-} + S^{-}_{j}c^{+}_{n-}c_{n'+} + S_{jz}(c^{+}_{n+}c_{n'+} - c^{+}_{n-}c_{n'-})\right]$$

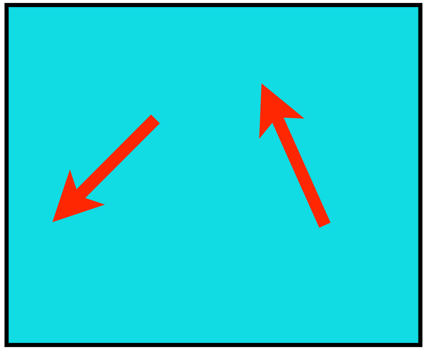
with exchange couplings $J_{j;nn'} = t_{nd_j}\,t_{d_jn'}\left(\frac{1}{U_j + \varepsilon_{d_j} - E_{n'}} + \frac{1}{-\varepsilon_{d_j} + E_n}\right).$

For $\epsilon_{d_j} = -U_j/2$ for all j= 1,...,M we get the Symmetric Kondo Model of M magneti moments:

$$H_K = \sum_{n,\sigma} E_n\hat{n}_{n\sigma} + \sum_{j} J_j \vec{\mathbf{S}}_j \vec{\mathbf{s}}(\mathbf{r_j}) = H_0 + H_J,$$

with $J_j = 4t_j^2/U_j > 0$

RKKY coupling between magnetic moments



Let us calculate the correction to the thermodynamic potential at finite temperature T

$$\Delta\Omega = -T \ln\left(\mathrm{Tr}[e^{-\int_0^{1/T} H_J(\tau)d\tau - H_0/T}]/Z_0\right)$$

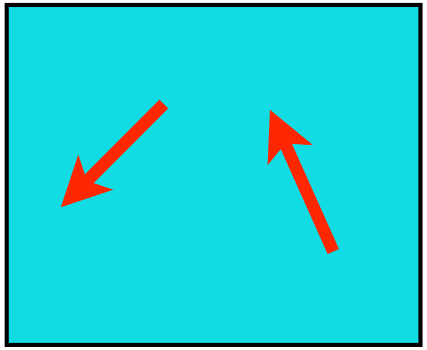
with the partition function of the system without magnetic momnents $Z_0 = \mathrm{Tr}[e^{-H_0/T}]$

with $H_0 = \sum_{n,\sigma} E_n \hat{n}_{n\sigma}$

with the exchange coupling to magnetic moments as the correction

$$H_J = \sum_j J_j \vec{\mathbf{S}}_j \vec{\mathbf{s}}(\mathbf{r_j})$$

RKKY coupling between magnetic moments



Expansion of the thermodynamic potential to 2nd order in H_J yields

$$\Delta\Omega = -\frac{1}{2}T \sum_{i,j;\alpha\beta\gamma\delta} J_i J_j \int_0^{1/T}\int_0^{1/T} d\tau_1 d\tau_2 \left\langle \vec{\mathbf{S}}_i \vec{\sigma}_{\alpha\beta} \vec{\mathbf{S}}_j \vec{\sigma}_{\gamma\delta} T_\tau [c^\dagger_{i\alpha}(\tau_1) c_{i\beta}(\tau_1) c^\dagger_{j\gamma}(\tau_2) c_{j\delta}(\tau_2)] \right\rangle$$

where $\langle \ldots \rangle = Tr[\ldots \exp(-H_0/T)]/Z_0$

and we assumed that the conduction electron spins are not in a polarized state $\langle \vec{\mathbf{s}}(\mathbf{r}) \rangle = 0$

Using Wick's theorem to decouple the expectation value and $\sum_{\alpha\beta} \mathbf{S}_i \vec{\sigma}_{\alpha\beta} \mathbf{S}_j \vec{\sigma}_{\beta\alpha} = \mathbf{S}_i \cdot \mathbf{S}_j$

one can write the correction in terms of a Heisenberg Hamiltonian of coupled spins

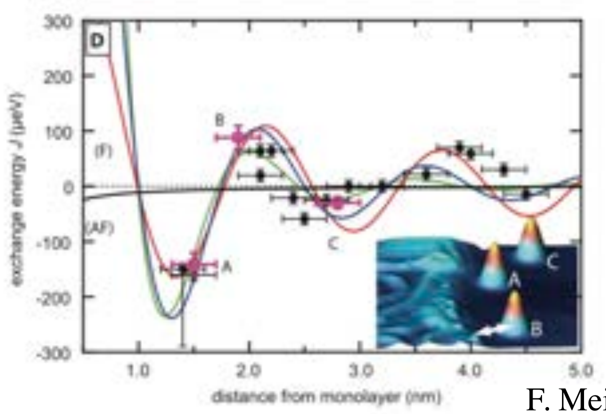
$$H_{RKKY} = \sum_{i,j} J_i J_j \chi_{ij} \vec{\mathbf{S}}_i \vec{\mathbf{S}}_j,$$

where the coupling is the RKKY-coupling, given by

$$J_{\mathrm{RKKY}}(\mathbf{r}_{ij}) = J_i J_j \chi_{ij} = J_i J_j \frac{V_a^2}{4\pi} \mathrm{Im} \int dE f(E) \sum_{n,l} \frac{\psi_n^*(\mathbf{r}_i)\psi_n(\mathbf{r}_j)}{E - E_n + i\epsilon} \frac{\psi_l(\mathbf{r}_i)\psi_l^*(\mathbf{r}_j)}{E - E_l + i\epsilon}$$

with $V_a = L^d/N$

RKKY coupling between magnetic moments



Spin resolved STM of Magnetic Adatoms on Metal Surface.
Lines: analytical Eq. (1) in d=1,2,3 dimensions

F. Meier, L. Zhou, J. Wiebe and R. Wiesendanger, Science 320, 82 (2008)

$$H_{RKKY} = \sum_{i,j} J_i J_j \chi_{ij} \vec{\mathbf{S}}_i \vec{\mathbf{S}}_j,$$

$$J_{\mathrm{RKKY}}(\mathbf{r}_{ij}) = J_i J_j \chi_{ij} = J_i J_j \frac{V_a^2}{4\pi} \mathrm{Im} \int dE f(E) \sum_{n,l} \frac{\psi_n^*(\mathbf{r}_i)\psi_n(\mathbf{r}_j)}{E - E_n + i\epsilon} \frac{\psi_l(\mathbf{r}_i)\psi_l^*(\mathbf{r}_j)}{E - E_l + i\epsilon}$$

F.e. in a clean metal, inserting plain wave states $\psi_n(\mathbf{r}_i) \sim \exp(i\mathbf{k}\mathbf{r}_i)$

One finds at large distances $k_{\mathrm{F}} r_{ij} \gg 1$ where $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$

$$J^0_{\mathrm{RKKY}}(\mathbf{r}_{ij}) \to -c_d N_0 J_i J_j \sin(2k_{\mathrm{F}} r_{ij} + d\pi/2) \frac{V_a}{r_{ij}^d} \quad (1)$$

where d is the dimension and $c_2 = 1/\pi, c_3 = 1/(2\pi)$

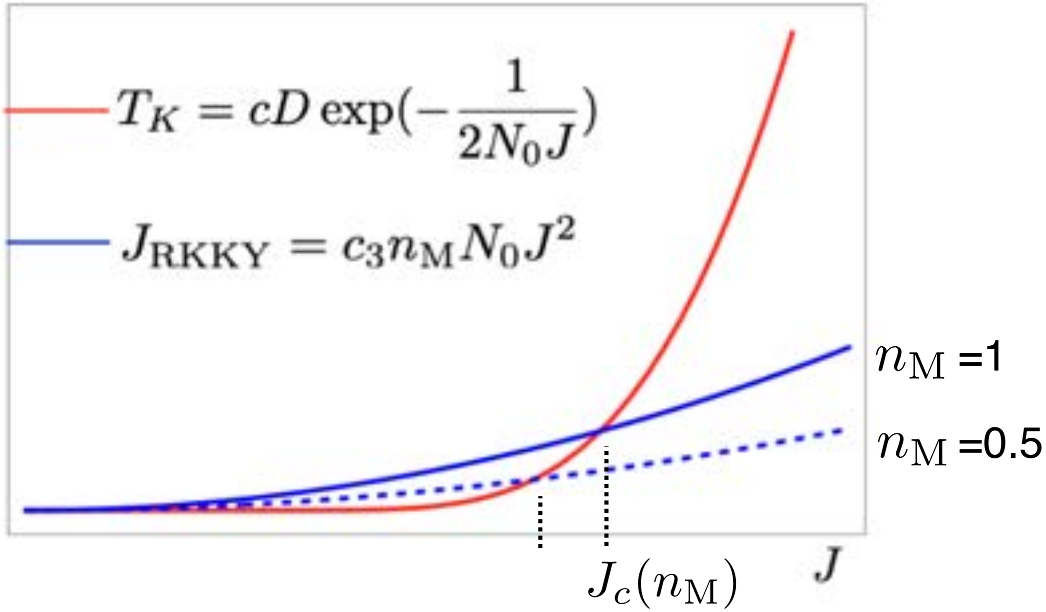
D. N. Aristov, Phys. Rev. B 55, 8064-8066 (1997).

Spin competition

a) the Doniach diagram
b) Kondo lattice
c) Kondo-RKKY-Renormalization Group

Competition between Kondo effect and RKKY

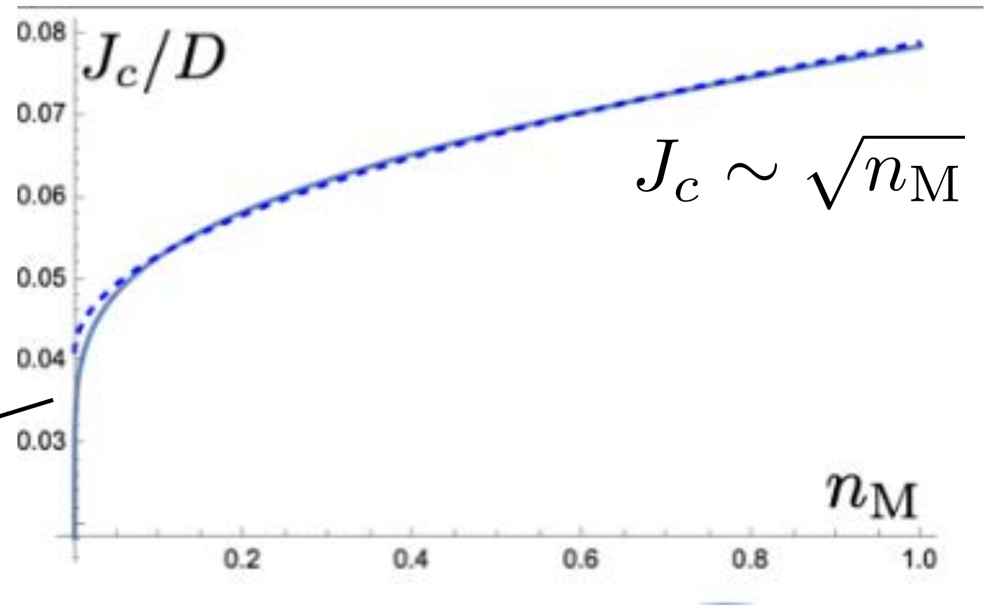
For a clean metal, inserting plain wave states, let us compare the Kondo temperature T_K with the typical RKKY-coupling at a distance R, where $n_{\mathrm{M}} = R^{-d}$ is the density of magnetic moments:



Thus, above a critical exchange coupling $J_c(n_{\mathrm{M}})$ the Kondo screening by the conduction electrons wins over the RKKY-coupling. We note that $J_c(n_{\mathrm{M}})$ increases with the density of magnetic moments $n_{\mathrm{M}} = R^{-d}$

Critical Coupling: Dependence on Density of Magnetic Moments

$$J^0_{\mathrm{RKKY}} = c_3 n_{\mathrm{M}} N_0 J_c^2 = T^0_{\mathrm{K}} = cD\exp(-\frac{1}{2N_0J_c}) \quad \text{with} \quad N_0 = \frac{1}{D}$$

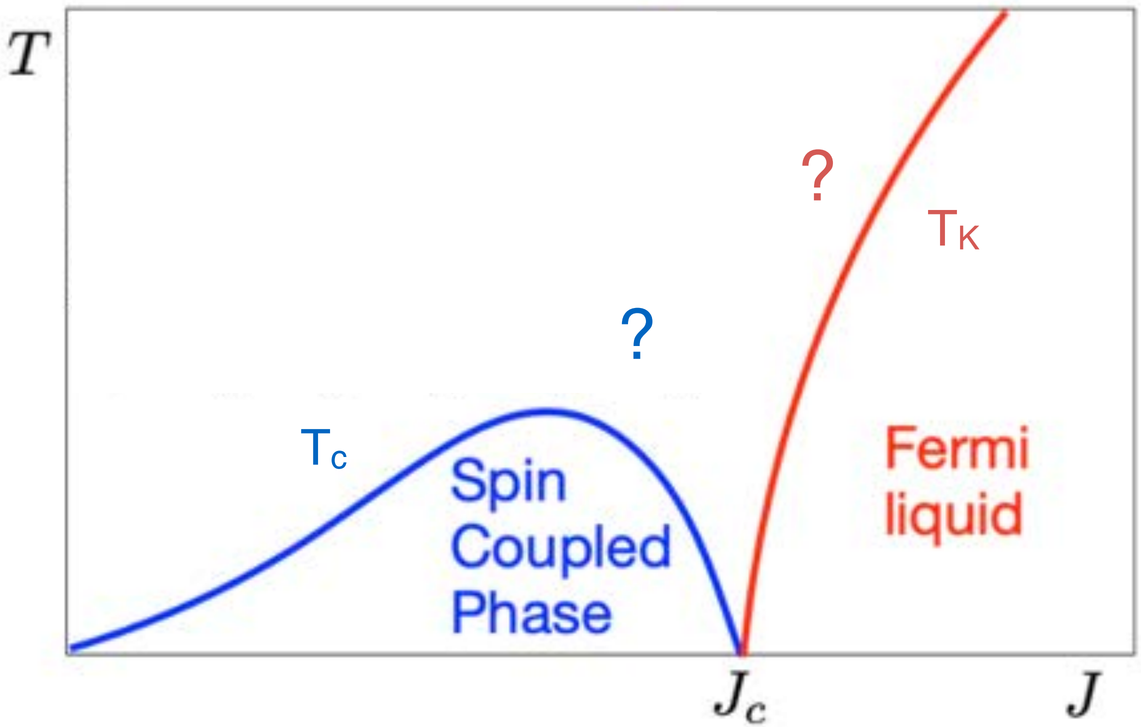


exact solution

(available in closed form in terms of the Lambert-W special function)

Doniach diagram:

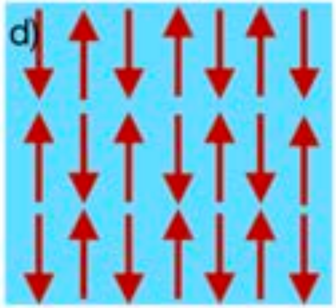
Doniach argued that the critical exchange coupling $J_c(n_{\mathrm{M}})$marks a quantum phase transition, where the ordering temperature T_c of the spin coupled phase and the temperature at which Kondo screening sets in T_K suppressed:



However, the Doniach argument does not yield a theory for the suppresion of T_c, and T_K nor does it yield information on the **quantum state** in which the system settles for given J.

S. Doniach, Physica B+C 91 231(1977).

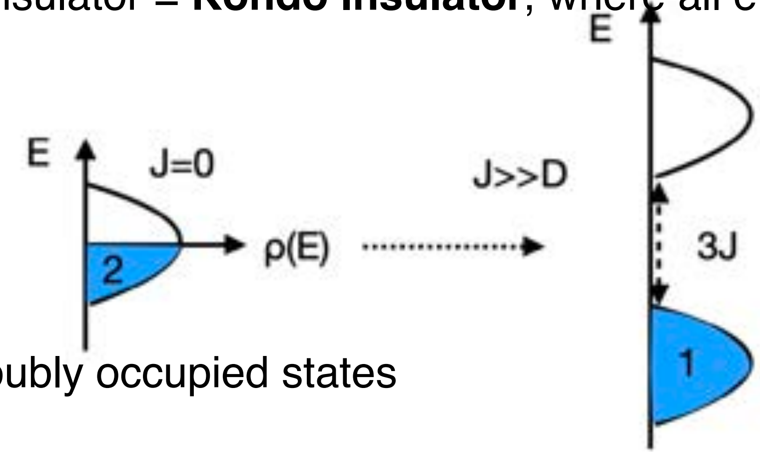
The Kondo lattice for $J > J_c$



Let's consider very strong coupling J >>D.
Then, each of the M=N localized spin grabs one conduction electron spin forming a localized singlet $|0_i\rangle = 1/\sqrt{2}(|\uparrow_{di}\rangle|\downarrow_{ci}\rangle - |\downarrow_{di}\rangle|\uparrow_{ci}\rangle)$ of energy $E_{0i} = -(3/2)J$

For M=N, ground state is product state of singlets $|\psi_0\rangle = \prod_{i=1}^{N} |0_i\rangle$

Transfer of 1 electron from site i to j,
leaves site i unoccupied, site j doubly occupied.
that costs energy $\Delta E_q = 2\ 3/2\ J = 3J$
Thus, the system is an insulator = **Kondo Insulator**, where all electrons are **localized**

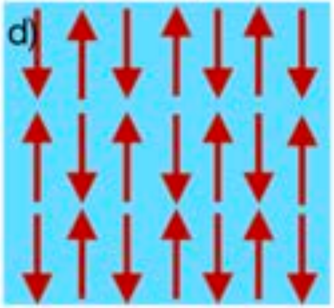


2= doubly occupied states

1=singly occupied states

P. Coleman, in Band/Volume 5
Many-Body Physics: From Kondo to Hubbard
Inhaltsverzeichnis
Lecture Notes of the Autumn School on Correlated Electrons 2015 Pavarini, Eva; Koch, Erik; Coleman, Piers (Eds.) 2015

The Kondo lattice for $J_c < J < D$



At intermediate coupling $J_c < J < D$ and dense lattice of magnetic moments, N=M a generalised Kondolattice Hamiltonian with degeneracy $N_K \gg 1$, the Coqblin- Schrieffer Hamiltonian was solved, performing a $1/N_K$ -expansion. In mean field approximation the Energy dispersion is

$$\tilde{E}_n = \frac{1}{2}(E_n + \tilde{\epsilon}_d) \pm \frac{1}{2}\sqrt{(E_n - \tilde{\epsilon}_d)^2 + 4V^2}$$

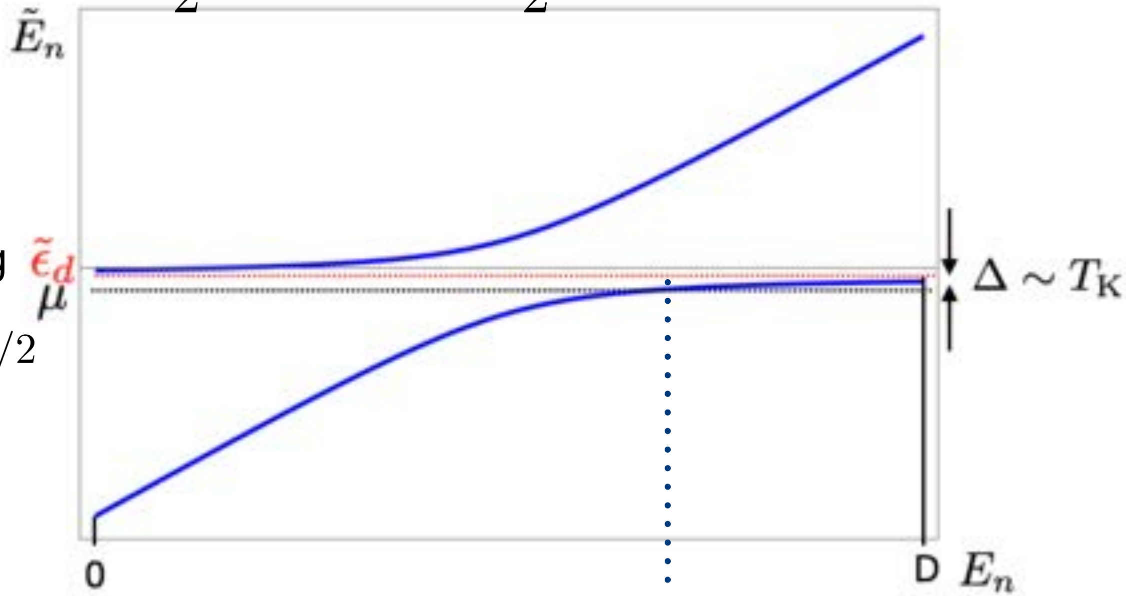
with mean field parameter

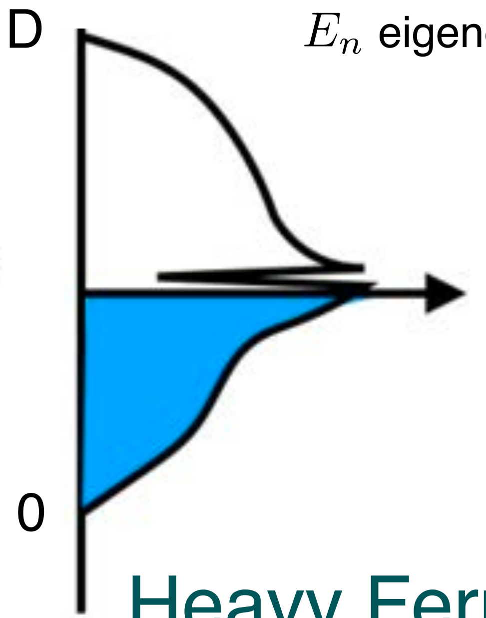
$$V^2 = DT_{\rm K}/4$$

E_n eigenenergies for J=0

setting $\tilde{\epsilon}_d$

$\tilde{\epsilon}_d = D/2$





Flat band→ heavy mass→ Heavy Fermions !

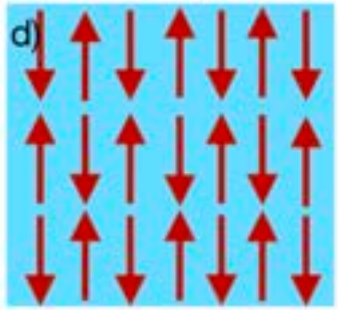
B. Coqblin and J. R. Schrieffer, Phys. Rev. 185, 847 (1969)..

Read, N. and Newns, D.M. J. of Phys. C 29, L1055 (1983); J. of Phys. C 16, 3274 (1983).

A. Auerbach, and K. Levin, Phys. Rev. Lett. 57, 877(1986).

Heavy Fermions:

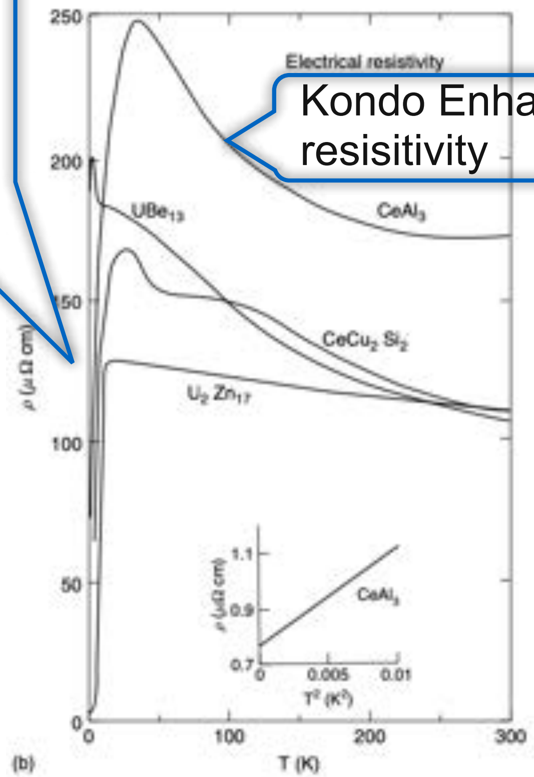
Low temperature Fermi liquid
of heavy Fermions
with heavy mass upto m=1000 m_e



Dense, ordered lattice
of magnetic moments in
Heavy Fermion Materials
like $CeAl_3$

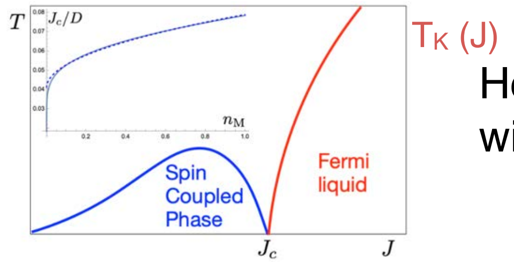
Sharp Drop of
resisitivity ρ
when coherent
Heavy
Fermions form

Kondo Enhanced
resisitivity



J.L. Smith and P.S. Riseborough, *J. Mag. Mat.* 47–48, 1985

Kondo-RKKY-Renormalization Group



How can we derive T_K (J) with RKKY-coupling?

Recall: Kondo temperature has been derived by calculating renomalization of exchange coupling

$$\frac{d\tilde{J}}{d\ln\Lambda} = -\tilde{J}^2\left(N(\mathbf{r},\epsilon_F+\Lambda)+N(\mathbf{r},\epsilon_F-\Lambda)\right)$$

But: this does not take into account RKKY Coupling!

Including the RKKY coupling we rather get

$$\frac{d\tilde{J}_i}{d\ln\Lambda} = -\tilde{J}_i^2\sum_{\alpha=\pm}N(\mu+\alpha\Lambda,\mathbf{r}_i)$$

$$+\frac{4}{\pi}\tilde{J}_i^2 J_i^0 \sum_{\alpha=\pm}\sum_{j\neq i} J_j^0 \mathrm{Im}[e^{i\mathbf{k}_F\mathbf{r}_{ij}}\chi_c(\mathbf{r}_{ij},\mu+\alpha\Lambda) \quad G_c^R(\mathbf{r}_{ij},\mu+\alpha\Lambda)\chi_f(\mathbf{r}_j,\mu+\alpha\Lambda)$$

A. Nejati, K. Ballmann, and J. Kroha, Phys. Rev. Lett. 118, 117204 (2017).

J. Kroha, Interplay of Kondo effect and RKKY interaction, in

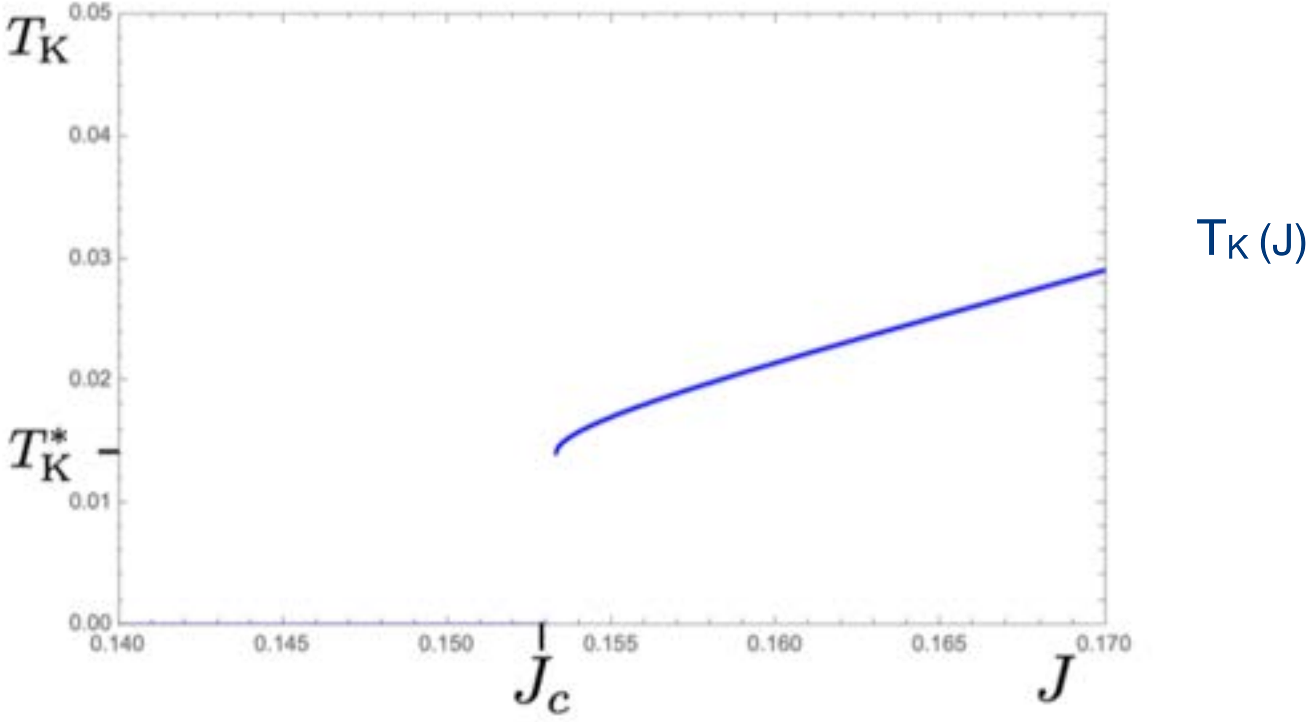
The Physics of Correlated Insulators, Metals, and Superconductors Modeling and Simulation,

Eds. E. Pavarini, Erik Koch, R. Scalettar, and R. M. Martin (eds.), Vol. 7 (Verlag des Forschungszentrum Jülich, 2017).

Kondo-RKKY-Renormalization Group

Solution:

- RKKY Coupling indeed reduces Kondo temperature:



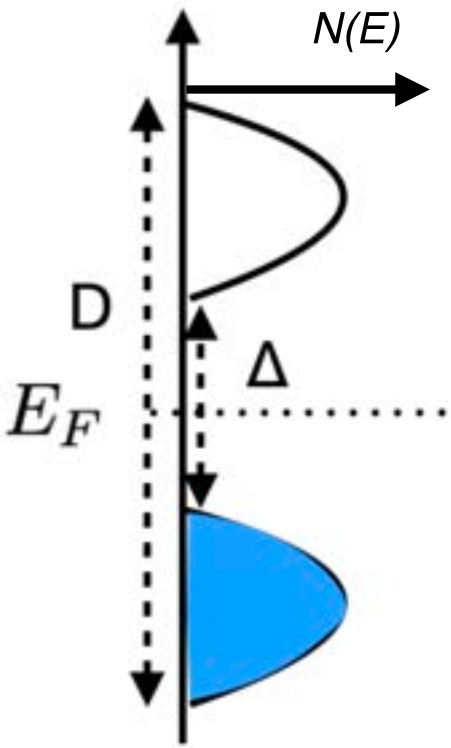
- Critical coupling J_c same as with Doniach Argument
- But: Kondo temperature finite at J_c before it jumps to zero

$$T_K^* = T_K(J_c) = e^{-1} T_K^0(J_c)$$

Spin competition in presence of a spectral (pseudo) gap

a) Band insulator, semiconductor
b) Pseudo gap semimetal

Kondo Effect in a
Band insulator or semiconductor



Kondo temperature in metal:

$$T_{\rm K}^0 = cD\exp(-\frac{1}{2N_0 J})$$

with $N(\mathbf{r}, E) \approx N(E_{\rm F}) = N_0$

In Insulator, undoped semiconductor:

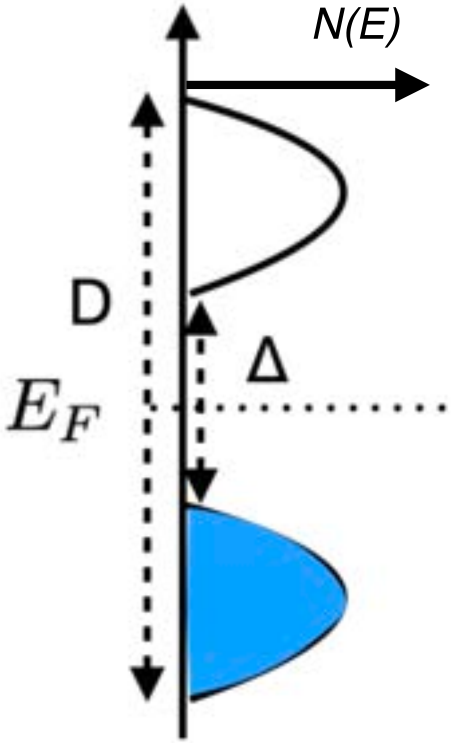
$$N(E_F) = 0$$

$$\rightarrow T_{\rm K} = 0 \quad ?$$

But: assumption $N(\mathbf{r}, E) \approx N(E_{\rm F}) = N_0$

is wrong when there is a spectral gap!

Kondo Effect in a
Band insulator or semiconductor



Rather derive Kondo temperature from Nagaoka-Suhl equation:

$$1 = J \int_0^D dE N(E, \mathbf{r}) \frac{1}{E - E_F} \tanh\left(\frac{E - E_F}{2T_{\mathrm{K}}(\mathbf{r})}\right)$$

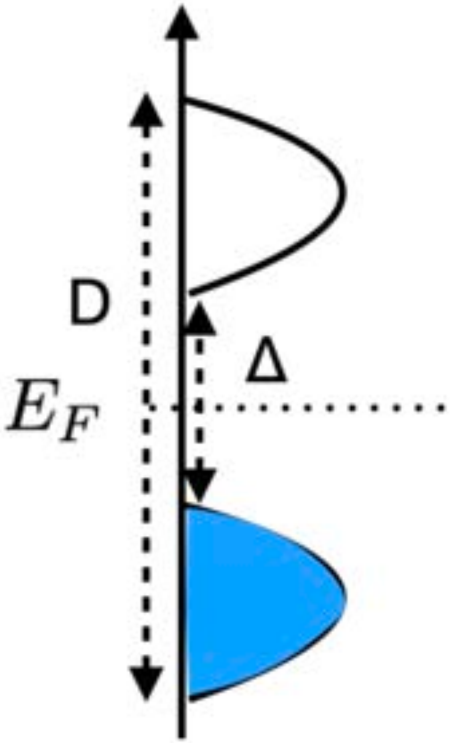
keeping the energy dependence of *N(E),* one finds a finite Kondo temperature T_K only for sufficiently strong $J > J_c$

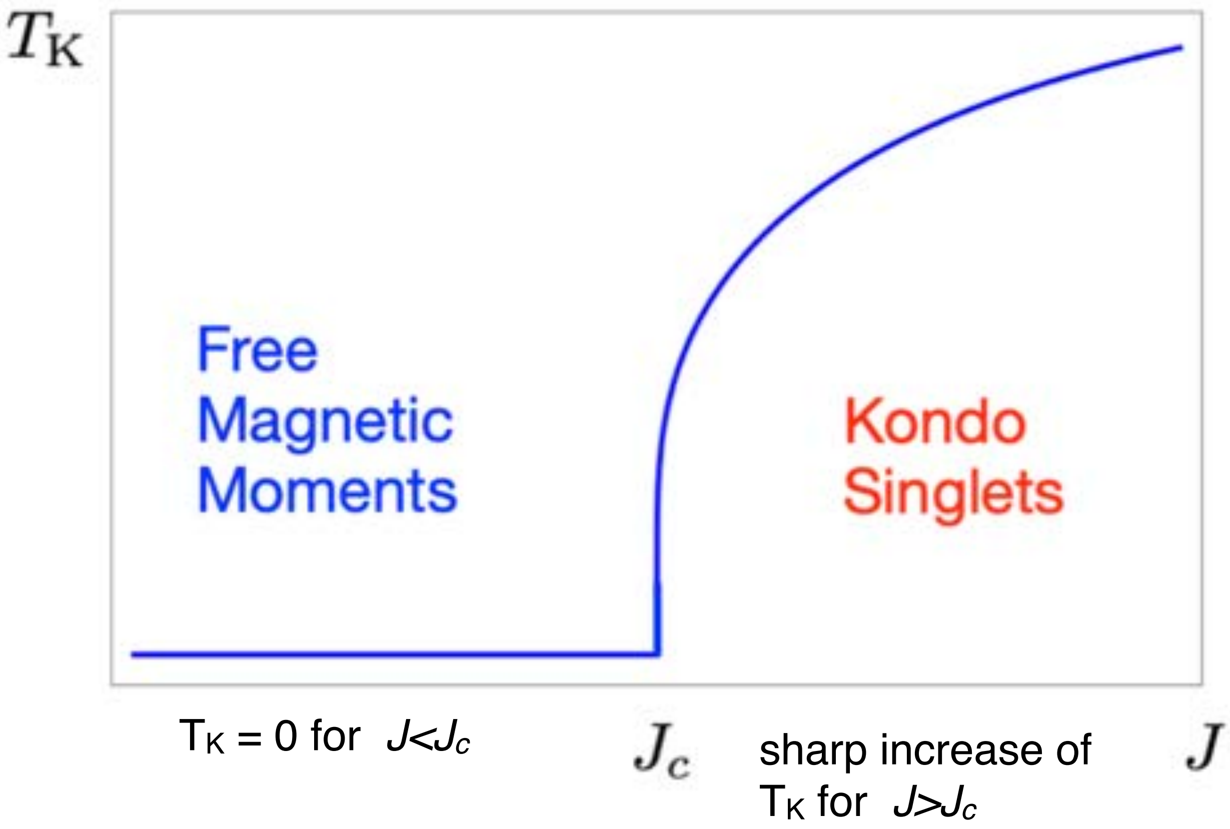
where J_c decreases with increasing energy gap Δ:

$$J_c = \frac{1}{2N_0} \frac{1}{\ln(D/\Delta)}.$$

where we asuumed density of states constant N_0 in both bands, separated by energy gap Δ

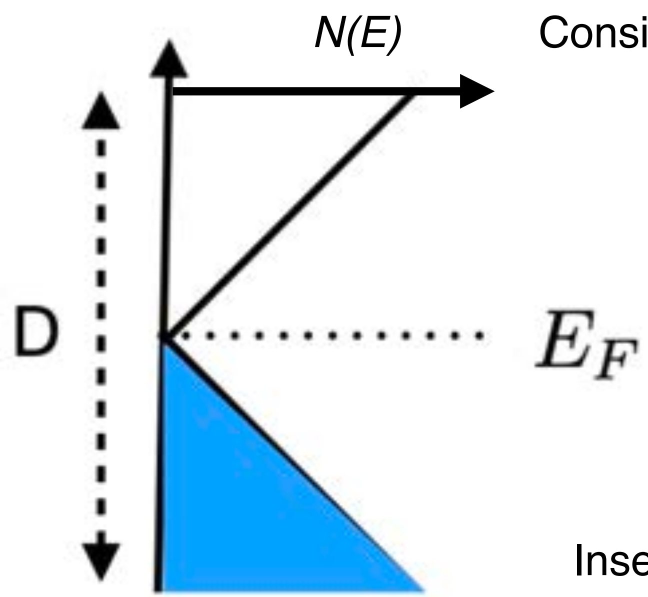
Kondo Effect in a
Band insulator, semiconductor





$$T_K \approx \frac{\Delta}{2\ln(4N_0 J/(J/J_c - 1))}$$

Kondo Effect in Materials with Pseudogap like Graphene, Topological Insulator



Consider a Material with a Pseudogap at the Fermi Energy:

$$N(E) = N_0 \left| \frac{E - E_F}{D/2} \right|^{\beta}$$

For example in Graphene and Topological Insulator: β=1

Thus,

$$N(E_F) = 0$$

Insertion in Nagaoka-Suhl equation:

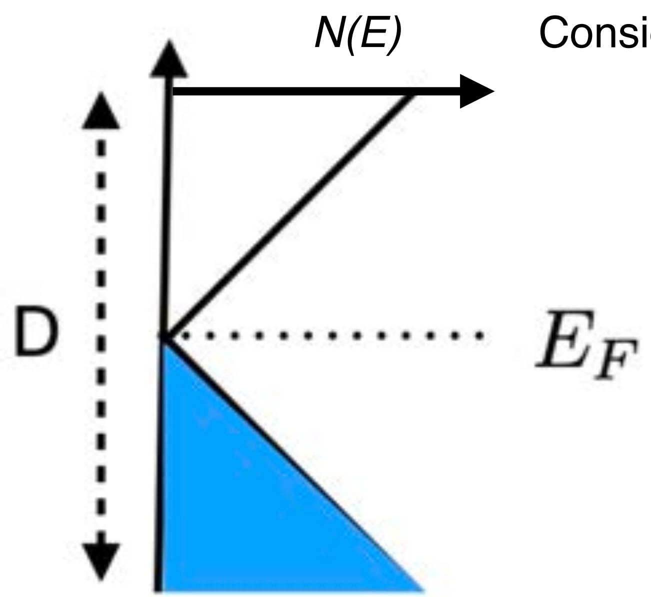
$$1 = J \int_0^D dE N(E, \mathbf{r}) \frac{1}{E - E_F} \tanh\left(\frac{E - E_F}{2T_{\mathrm{K}}(\mathbf{r})}\right)$$

keeping the energy dependence of *N(E),* one finds a finite Kondo temperature T_K only for sufficiently strong $J > J_c^{PG}$

with

$$J_c^{PG}(\beta) = \frac{\beta}{2N_0}$$

Kondo Effect in Materials with Pseudogap like Graphene, Topological Insulator



Consider a Material with a Pseudogap at the Fermi Energy:

$$N(E) = N_0 \left| \frac{E - E_F}{D/2} \right|^{\beta}$$

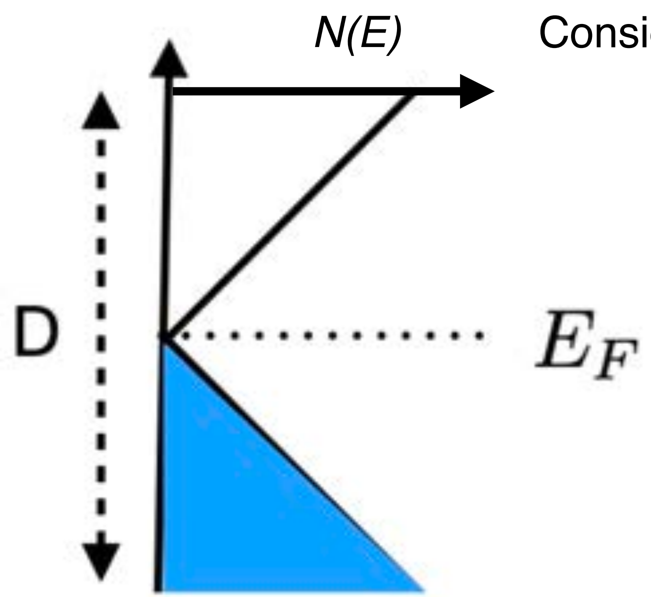
Finite Kondo temperature T_K for sufficiently strong $J > J_c^{PG}$

$$J_c^{PG}(\beta) = \frac{\beta}{2N_0}$$

given by

$$T_K = \frac{D}{2} \left(1 - \frac{J_c^{PG}(\beta)}{J} \right)^{1/\beta}$$

RKKY-Coupling in Materials with Pseudogap



Consider a Material with a Pseudogap at the Fermi Energy:

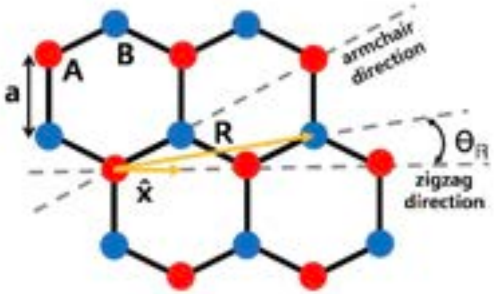
$$N(E) = N_0 \left| \frac{E - E_F}{D/2} \right|^\beta$$

RKKY-coupling becomes at long distance

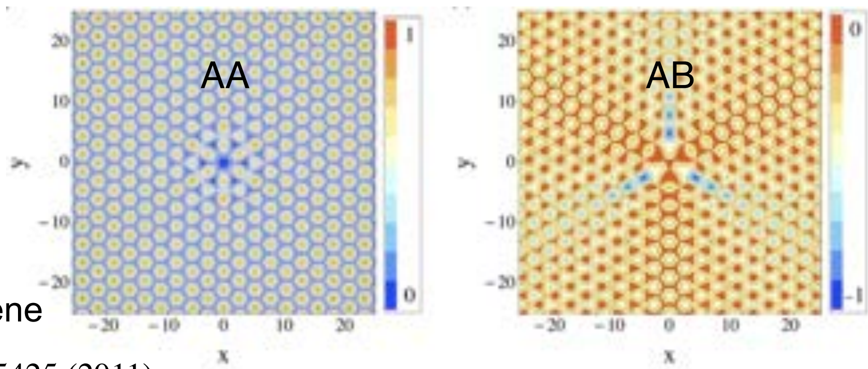
$$J_{\mathrm{RKKY}}(\mathbf{R}) = \frac{g(\mathbf{R})}{R^{d+\beta}}$$

Example: Graphene d=2, β=1

$$g_{AA}(\mathbf{R}) = -J^2(1 + \cos(\Delta\mathbf{K} \cdot \mathbf{R}))$$
$$g_{AB}(\mathbf{R}) = J^2 3(1 - \cos(\Delta\mathbf{K} \cdot \mathbf{R} - 2\theta_R)).$$



where
$$\Delta\mathbf{K} = \mathbf{K}^+ - \mathbf{K}^-$$



$\mathbf{K}^+, \mathbf{K}^-$ reciprocal lattice vectors of the 2 Dirac points in graphene

M. Sherafati and S. Satpathy, Phys. Rev. B 83, 165425 (2011).

H.Y. Lee, E. R. Mucciolo, G. Bouzerar, S. Kettemann, Phys. Rev. B 86, 205427 (2012).

H.Y. Lee, J.H. Kim, E. R. Mucciolo, G. Bouzerar, S. Kettemann, Phys. Rev. B 85, 075420 (2012).

Spin competition in Graphene, Topological Insulator

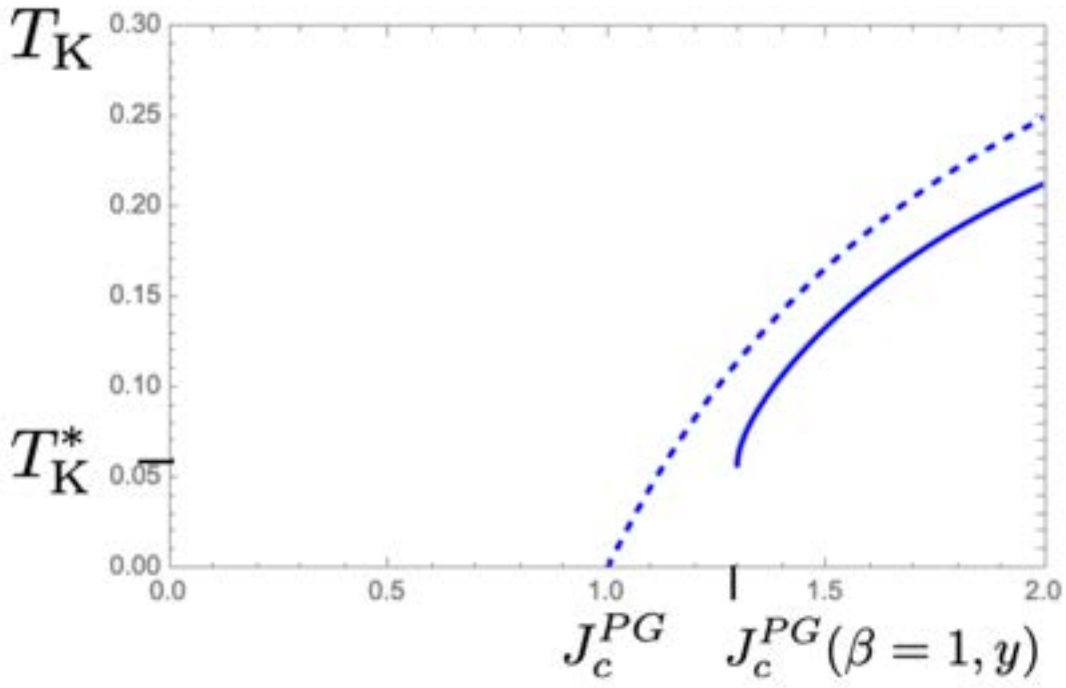
Kondo RG with RKKY Coupling:

- increase of critical coupling

$$J_c^{PG}(\beta=1,y_1) = J_c^{PG}\frac{1-\sqrt{1-4\sqrt{ky_1}}}{2\sqrt{ky_1}}$$

with $k = \ln(\sqrt{2}+1)$

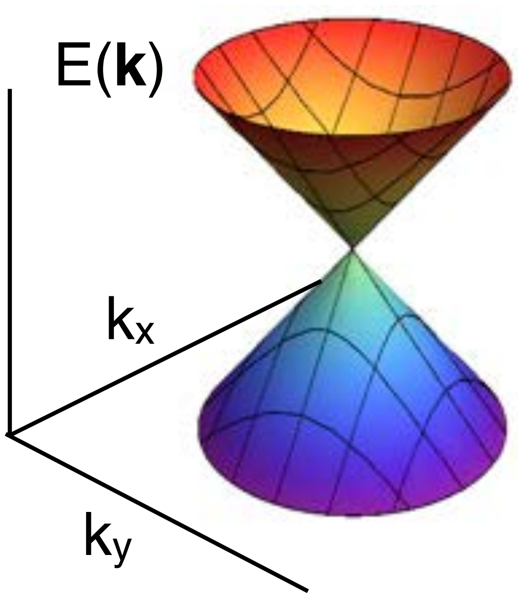
y_1 = dimensionless RKKY coupling for pseudogap power β=1

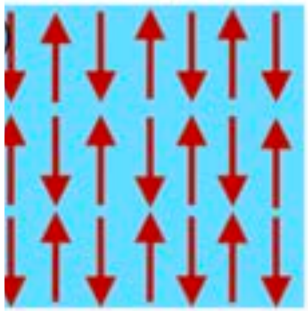


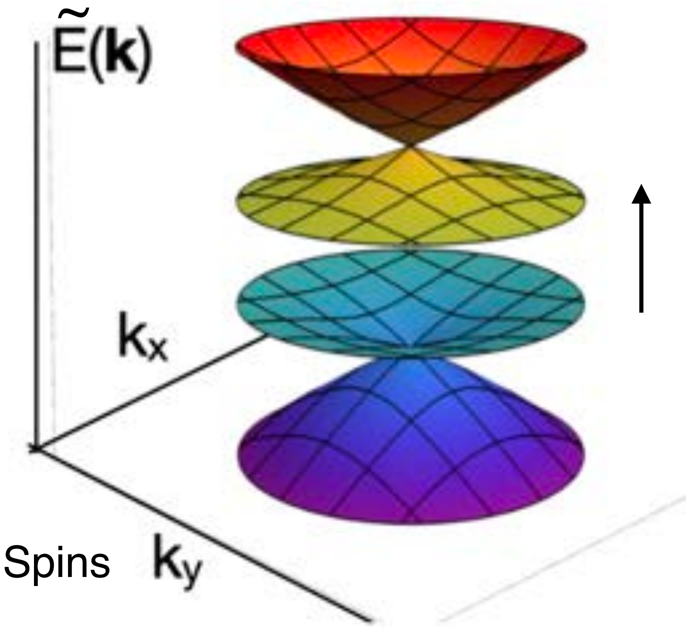
Stronger suppression of T_K, Jump to zero at critical coupling.

$$T_K^* = \frac{D}{4}\left(1-\frac{J_c^{PG}}{J_c^{PG}(\beta=1,y_1)}\right)$$

Emergence of Heavy Fermions from a massless Fermi Sea







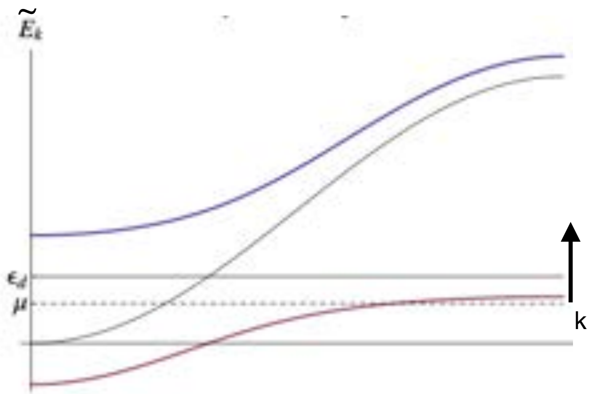
direct band gap!

coupled to lattice of Kondo Spins

$$E(\mathbf{k}) = c|\mathbf{k}|$$

$$\tilde{E}(\mathbf{k}) = \frac{1}{2}(E(\mathbf{k}) + \tilde{\epsilon}_d) \pm \frac{1}{2}\sqrt{(E(\mathbf{k}) - \tilde{\epsilon}_d)^2 + 4V^2}$$

as opposed to Kondo lattice coupled to massive Fermi sea:



indirect band gap!

H. Y. Lee, S. Kettemann, Phys. Rev. B 91, 205109 (2015)

Spin competition in the presence of disorder

a) Distribution of Kondo temperature and RKKY couplings
b) Anderson localization - local spectral gaps
c) Multifractality - local pseudo gaps
d) Doniach diagram of disordered systems

Schrödinger Equation with random potential V(r)

$$\left(\frac{\mathbf{p}^2}{2m} + V(\mathbf{r})\right)\psi_n(\mathbf{r}) = E_n\psi_n(\mathbf{r})$$

$$\left(\frac{\mathbf{p}^2}{2m} + V(\mathbf{r})\right)\psi_n(\mathbf{r}) = E_n\psi_n(\mathbf{r})$$

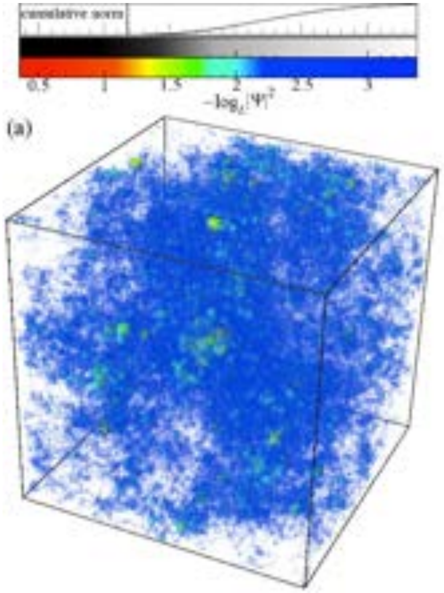
f.e. assuming a white noise, uncorrelated potential

$$\langle V(\mathbf{r})\rangle = 0 \qquad \langle V(\mathbf{r})V(\mathbf{r}')\rangle = \frac{1}{2\pi\rho(\epsilon_F)\tau}\delta(\mathbf{r}-\mathbf{r}')$$

with elastic scattering rate $1/\tau$

yields spatially distributed Wave function Intensity $|\psi_n(\mathbf{r})|^2$

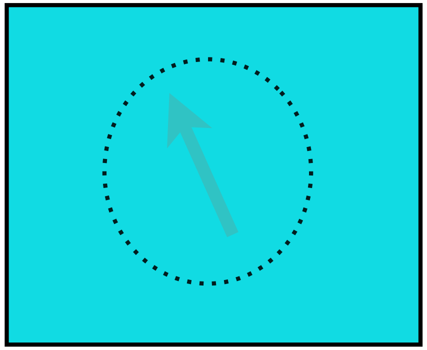
Metal



extended state

Rodriguez, Vasquez, Slevin, Römer, 2011

Kondo Temperature



$$1 = \frac{J}{2N} \sum_{n,\sigma} \frac{L^d |\psi_n(\mathbf{r})|^2}{E_n - E_F} \tanh\left(\frac{E_n - E_F}{2T_\mathrm{K}(\mathbf{r})} \right),$$

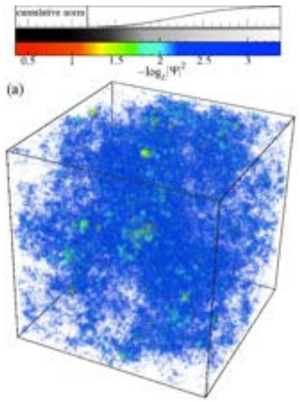
Nagaoka-Suhl (1-loop) equation for the Kondo temperature

$$T_\mathrm{K}(\mathbf{r})$$

of a magnetic moment at position **r**

spatial distribution of

Wave function Intensity



distribution of

Kondo temperature

$$T_\mathrm{K}(\mathbf{r})$$

J. Kondo, Prog. Theor. Phys 32, 37 (1964)

Y. Nagaoka, Phys. Rev. 138, 1112 (1965).

H. Suhl, Phys. Rev. A 138, 515 (1965).

Distribution of Kondo temperature: Width

In a disordered metal, the Kondo temperature is different at every position, depending on the local intensities.
It is thereby distributed with finite width

$$\delta T_K \approx T_K^{(0)} \begin{cases} \frac{c_3}{(E_F\tau)\sqrt{\beta}} \left[\ln\left(\frac{1}{\tau\, T_K^{(0)}}\right)\right] & \text{in } d=3, \\ \frac{1}{\sqrt{3\pi E_F \tau \beta}} \left[\ln\left(\frac{1}{\tau\, T_K^{(0)}}\right)\right]^{3/2} & \text{in } d=2, \\ 2\sqrt{\frac{\pi\sqrt{3}}{k_F^2 A \beta}} (\tau T_K^{(0)})^{-1/4} & \text{in quasi } 1-\text{D wire of crosssection } A, \end{cases}$$

$\beta = 1$ with time reversal symmetry

$\beta = 2$ broken time reversal symmetry (due to magnetic field)

S. Kettemann, E. R. Mucciolo, JETP Lett. 83, 240 (2006).

T. Micklitz, A. Altland, T. A. Costi, A. Rosch, Phys. Rev. Lett. 96, 226601 (2006).

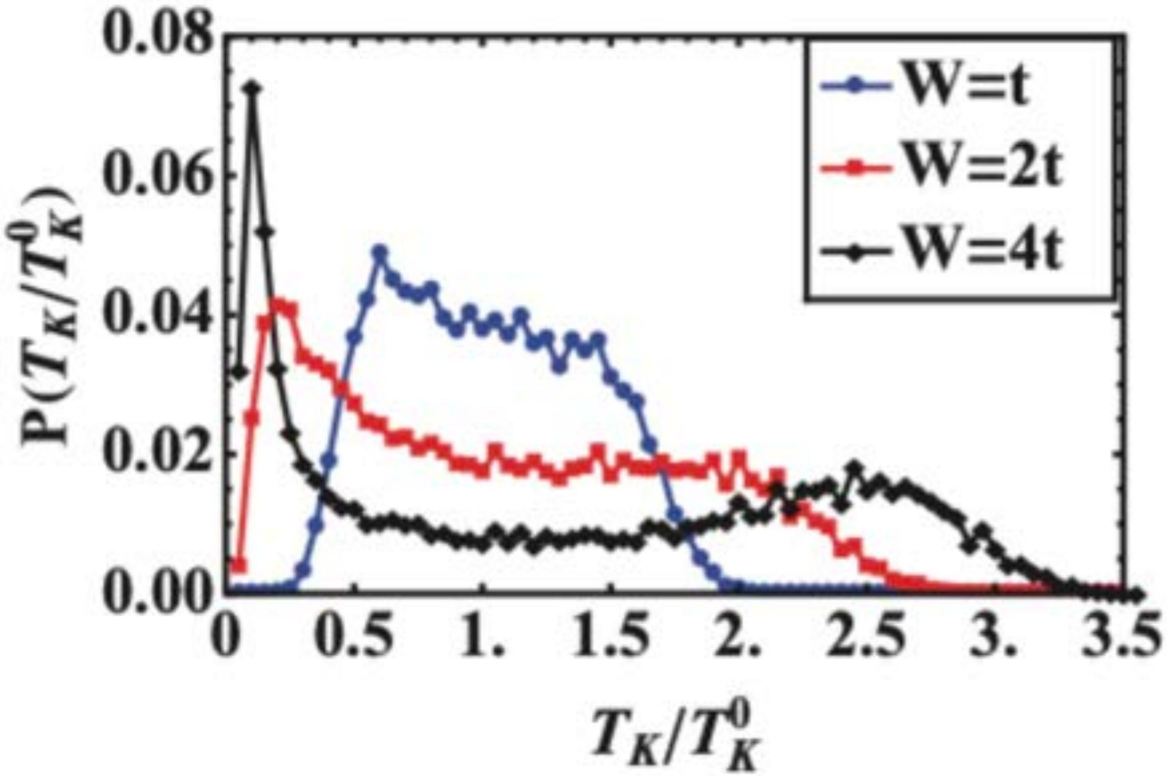
S. Kettemann, E. R. Mucciolo, Phys. Rev. B75, 184407 (2007).

Distribution of Kondo temperature

F.e. for 2D Anderson tight binding model on square lattice
with uncorrelated disorder potential

$$H^0 = -t \sum_{\langle ij \rangle} \left(c_i^\dagger c_j + \text{h.c.} \right) + \sum_i V_i \, c_i^\dagger c_i$$

with box distribution of width W: $V_i \in [-W/2, W/2]$



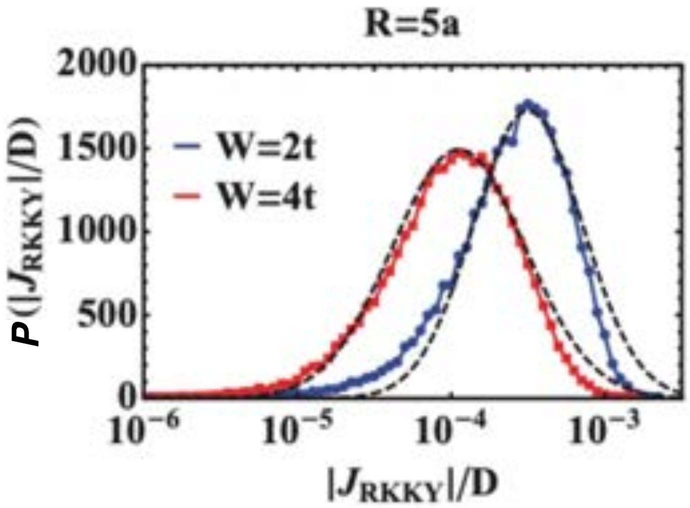
H. Y. Lee, S. Kettemann, Phys. Rev. B 89, 165109 (2014).

Distribution of RKKY couplings

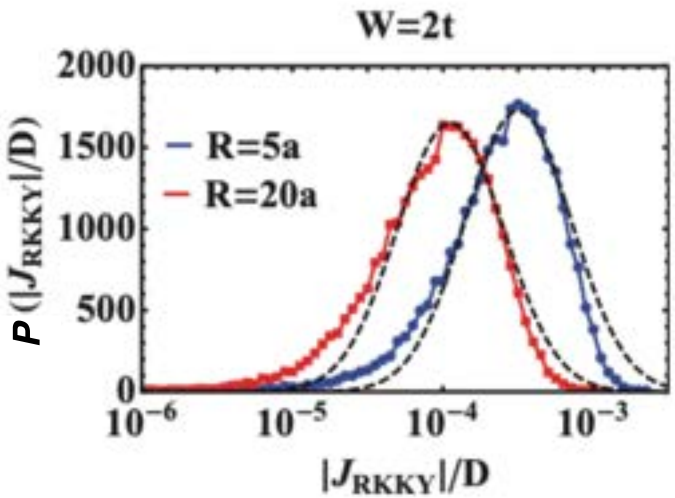
$$J_{\rm RKKY}(\mathbf{r}_{ij}) = J_i J_j \chi_{ij} = J_i J_j \frac{V_a^2}{4\pi} \mathrm{Im} \int dE f(E) \sum_{n,l} \frac{\psi_n^*(\mathbf{r}_i)\psi_n(\mathbf{r}_j)}{E - E_n + i\epsilon} \frac{\psi_l(\mathbf{r}_i)\psi_l^*(\mathbf{r}_j)}{E - E_l + i\epsilon}$$

distribution of absolute value of the RKKY coupling at T=0K for 2D Anderson tight binding model

at fixed distance



at fixed disorder



Dashed lines: lognormal distribution with fitted parameters

$$P(x = \ln(|J_{RKKY}|/D) = \exp(-(x - x_0)^2/(2\sigma^2))/(\sqrt{2\pi}\sigma)$$

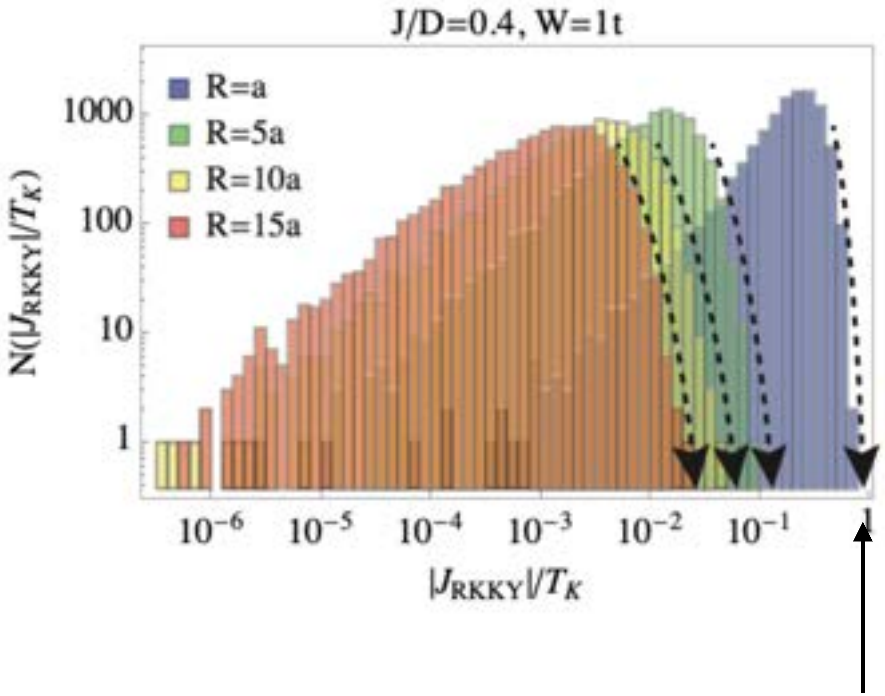
H. Y. Lee, S. Kettemann, Phys. Rev. B 89, 165109 (2014).

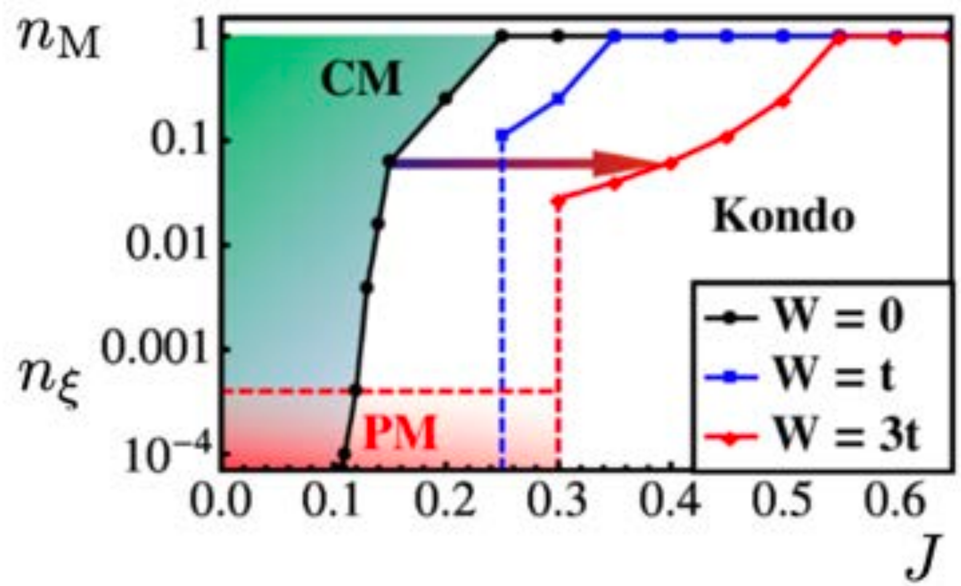
Doniach diagram of disordered systems

Extending the Doniach argument to disordered systems

derive the

distribution of the ratio of both energy scales, $J_{\mathrm{RKKY}}(r_{ij})/T_{\mathrm{Ki}}$





Sharp cutoff! allows to find distance R so that $J_{\mathrm{RKKY}}(r_{ij})/T_{\mathrm{Ki}} < 1$

so that Kondo wins at all sites i

Repeating it for different J, and R, we can draw a phase diagram density of magnetic moments n_{M} versus J.

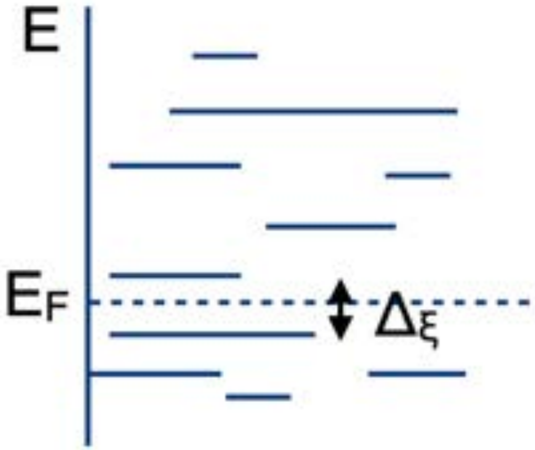
$n_{\mathrm{M}} = 1/R^2$

CM= Phase with Coupled Moments
PM= paramagnetic moments

H. Y. Lee, S. Kettemann, Phys. Rev. B 89, 165109 (2014).

Anderson localization - local spectral gaps

Disorder can localize Eigenfunctions, the so called **Anderson localization**



Then, the spectrum is discrete, with a local level spacing $$\Delta_\xi = \frac{1}{\rho(E)\xi(E)^d}$$

where $\xi(E)$ is the localization length of an Eigenfunction at energy E

P.W. Anderson, Phys. Rev. 109 (1958) 1492;

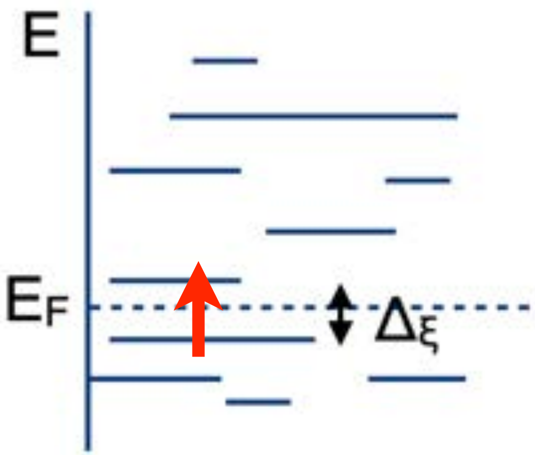
P. W. Anderson, Nobel Lectures in Physics 1980, 376 (1977).

B. Kramer, and A. MacKinnon, Reports on Prog. Phys. 56, 1469 (1993).

K. B. Efetov, Supersymmetry in Disorder and Chaos, (Cambridge University Press, Cam- bridge,1997).

Anderson localization - local spectral gaps quench Kondo screening

Disorder can localize Eigenfunctions, the so called **Anderson localization**



Thus the Kondo impurity sees a local gap

$$\Delta_\xi = \frac{1}{\rho(E)\xi(E)^d}$$

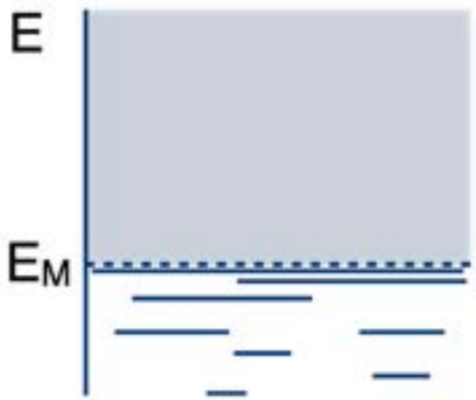
and becomes Kondo screened only for $J > J_c$

$$J_c = \frac{1}{2N_0}\frac{1}{\ln(D/\Delta_\xi)}. \quad N_0 = V_a \rho(E)/2$$

S. Kettemann and M. E. Raikh, Phys. Rev. Lett. 90, 146601 (2003).

Anderson Metal-Insulator transition

mobility edge



extended states

critical state

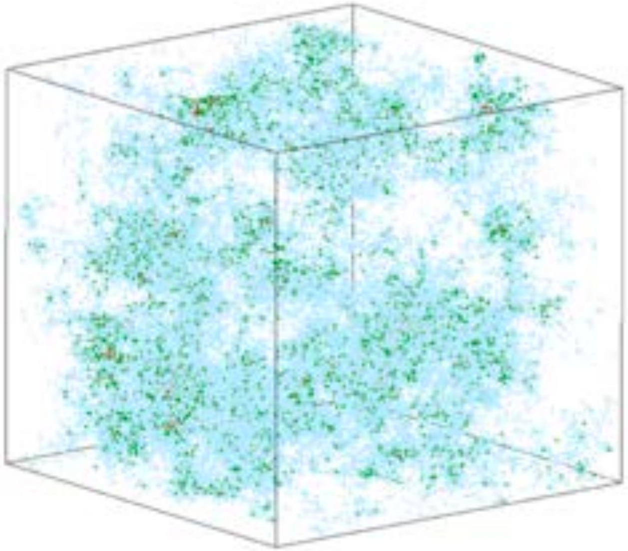
localized states

2nd order transition:

diverging localization length

$$\xi(E) \sim (E - E_{\mathrm{M}})^{-\nu}$$

critical state at 3D Anderson MIT



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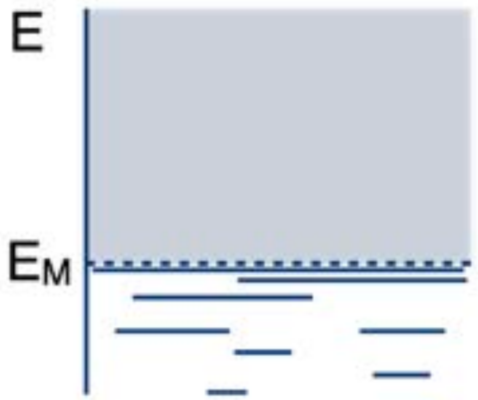
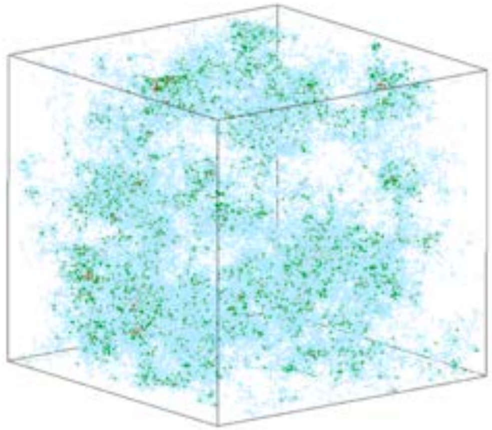
S. Kettemann, Special Issue in memory of K. B. Efetov, Ann. Phys. 456, 169306 (2023).

Multifractality





$$P_q = L^d \langle\, |\psi_l(\mathbf{r})|^{2q} \rangle \sim L^{-d_q(q-1)}$$

fractal: $d_q = d^* \neq d$

multifractal: $d_q = d^*(q)$

then, non-Gaussian Distribution f.e. log normal $P(|\psi_l(\mathbf{r})|^2) \sim L^{\alpha_\psi - (\alpha_\psi - \alpha_0)^2/(2\eta)}$

with $\alpha_\psi = -\ln |\psi_l(\mathbf{r})|^2 / \ln L$

$d_q = d - q(\alpha_0 - d)$ and $\eta = 2(\alpha_0 - d)$

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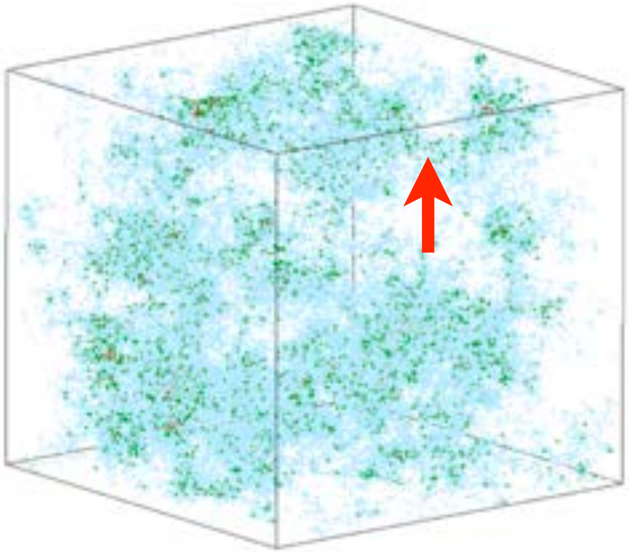
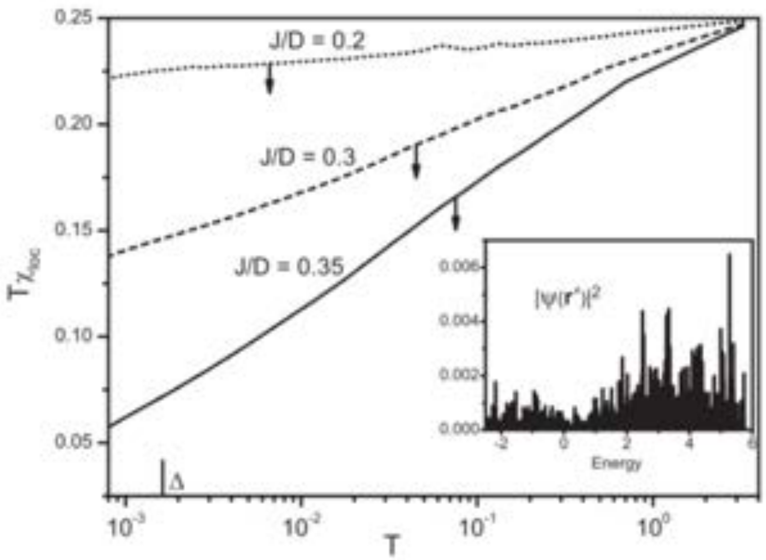
Multifractality - local pseudo gaps





conditional intensity in critical state

$$I_\alpha = L^d \langle |\psi_l(\mathbf{r})|^2 \rangle_{|\psi_M(\mathbf{r})|^2 = L^{-\alpha_\psi}} \sim \left| \frac{E_l - E_M}{E_c} \right|^{\beta_\alpha}$$

with power $\beta_\alpha = (\alpha_\psi - \alpha_0)/d$

→ power law suppressed intensity for $\beta_\alpha > 0$

→ Kondo spin sees at some sites pseudogaps → Kondo screening quenched for $J < J_c$

$$J_c(\beta_\alpha) = \beta_\alpha D/2$$

A. Zhuravlev, I. Zharekeshev, E. Gorelov, A. I. Lichtenstein, E. R. Mucciolo, and S. Kettemann, Phys. Rev. Lett. 99, 247202 (2007).

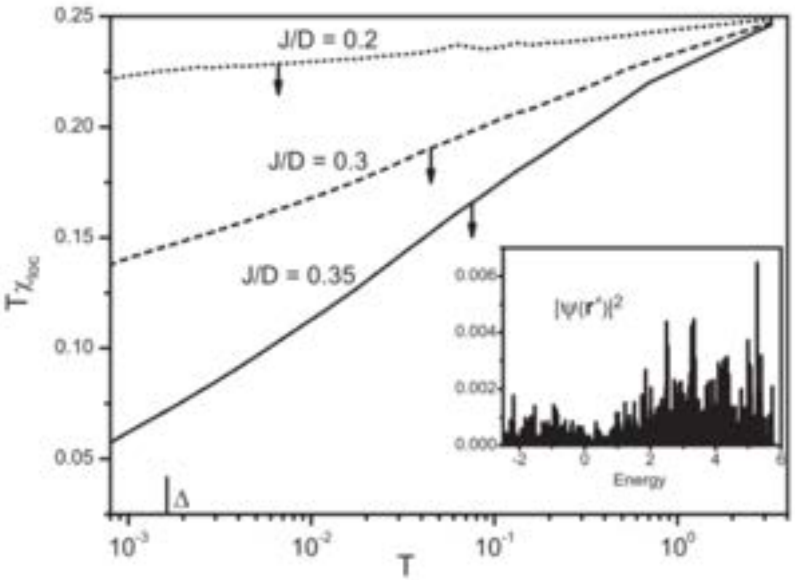
S. Kettemann, E. R. Mucciolo, and I. Varga, Phys. Rev. Lett. 103, 126401, (2009).

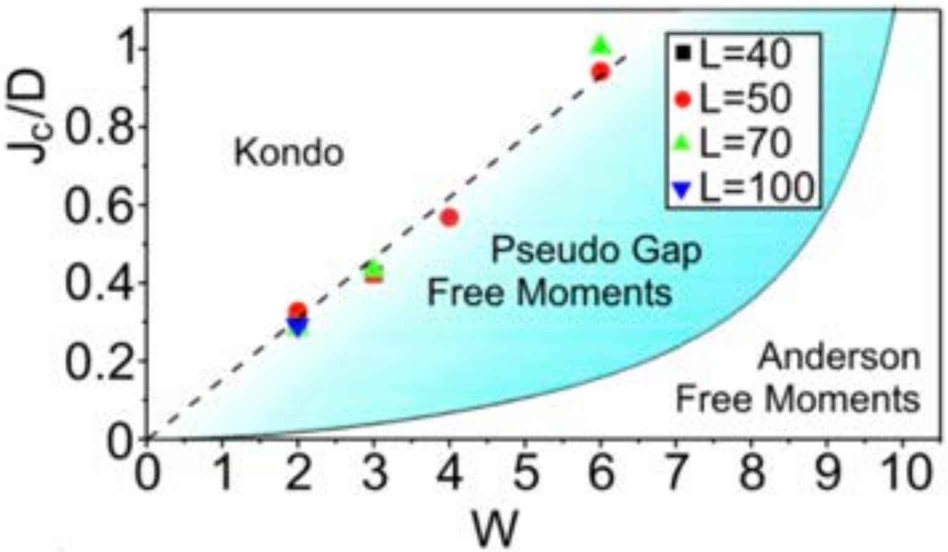
S. Kettemann, E. R. Mucciolo, I. Varga, K. Slevin, Phys. Rev. B 85, 115112 (2012).

Multifractality - local pseudo gaps

→ Kondo spin sees locally pseudogap → Kondo screening quenched for $J < J_c$

→ Free moments for $J < J_c$





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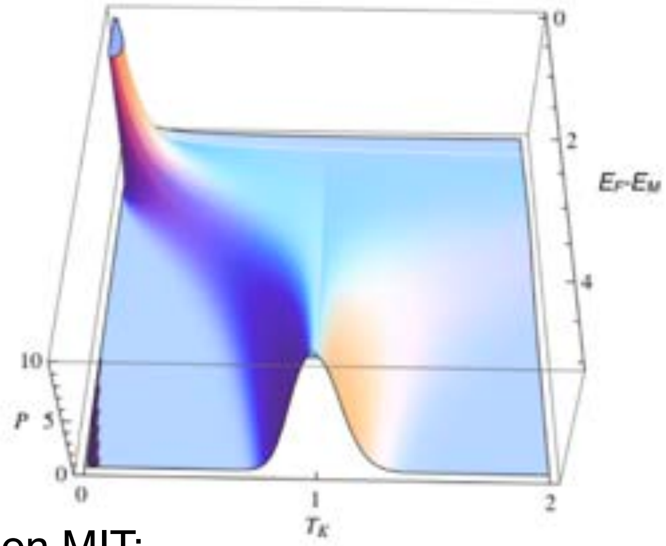
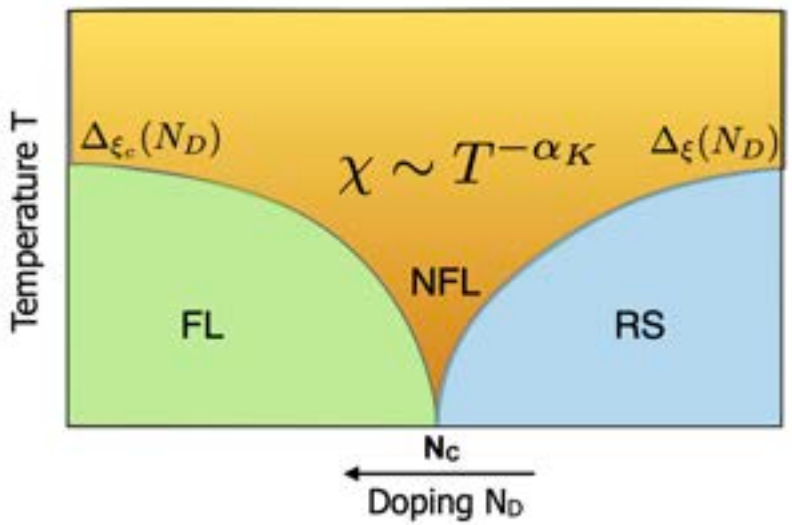
Multifractality - Universal Non-Fermi Liquid Magnetic Suceptibility





at Anderson MIT:

$$P(0 < T_K \ll T_K^0) \sim T_K^{-\alpha_K}$$ with power $\alpha_K = 1 - \eta/(2d)$

with $\eta = 2(\alpha_0 - d)$

Magnetic Susceptibility from magnetic moments

$$\chi(T) \sim n_{FM}(T)/T$$

with $n_{FM}(T) = n_M \int_0^T dT_K P(T_K)$ ➡ $\chi(T) \sim \left(\frac{T}{E_c}\right)^{-\alpha_K}$

A. Zhuravlev, I. Zharekeshev, E. Gorelov, A. I. Lichtenstein, E. R. Mucciolo, and S. Kettemann, Phys. Rev. Lett. 99, 247202 (2007).

S. Kettemann, E. R. Mucciolo, and I. Varga, Phys. Rev. Lett. 103, 126401, (2009).

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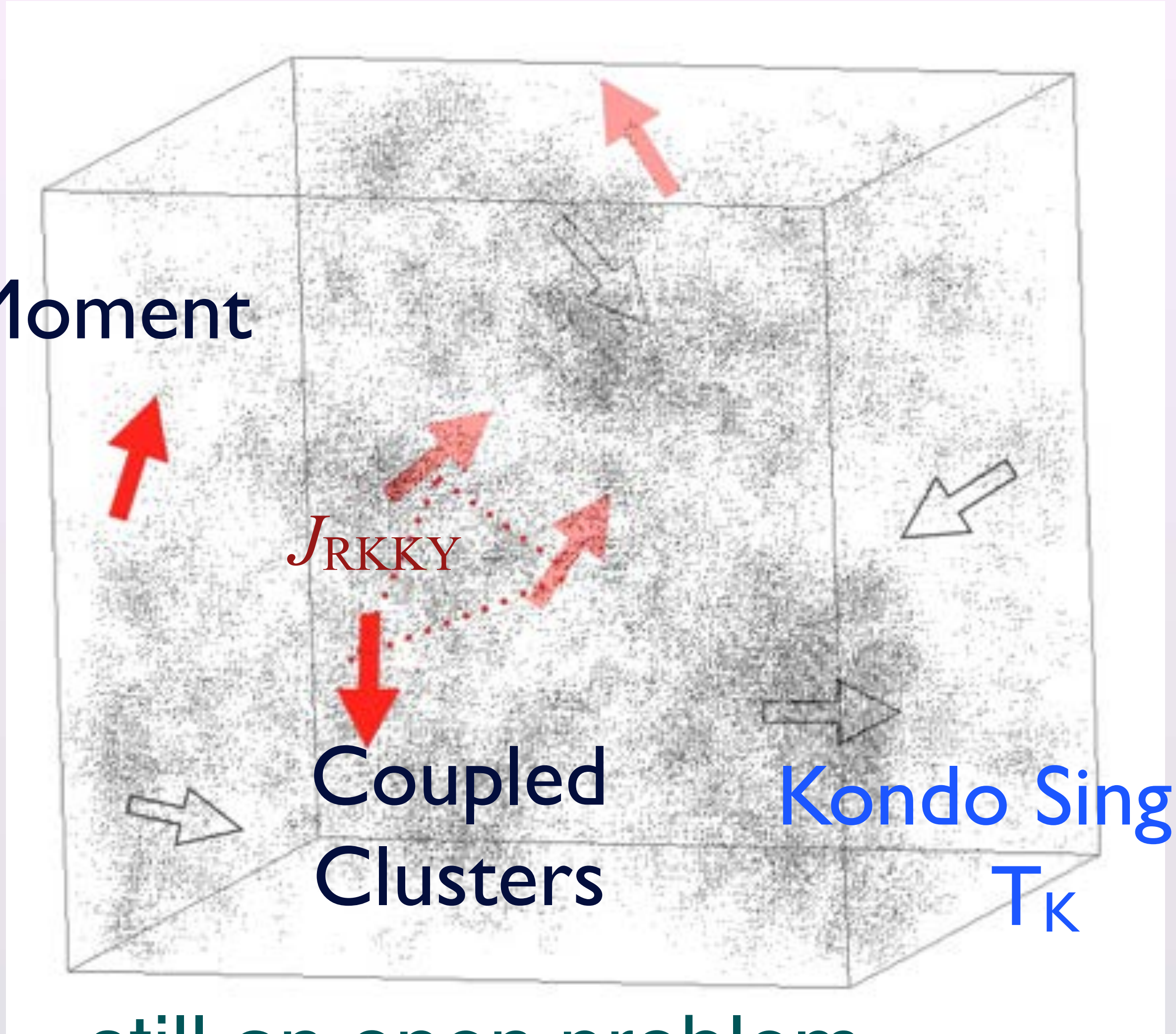
K. Slevin, S. Kettemann, T. Ohtsuki, Eur. Phys. J. B 92, 281(2019).

Competition between Kondo Effect and RKKY Coupling at the Anderson-Metal-Insulator Transition



still an open problem...

For some progress see
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Other Approaches to Dilute Kondo Systems

Mean field theories of the Kondo lattice with an added RKKY coupling term: Transition between AFM, Spin Glass and Kondo Phases.

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Other Approaches to Dilute Kondo Systems

Quantum Monte Carlo methods

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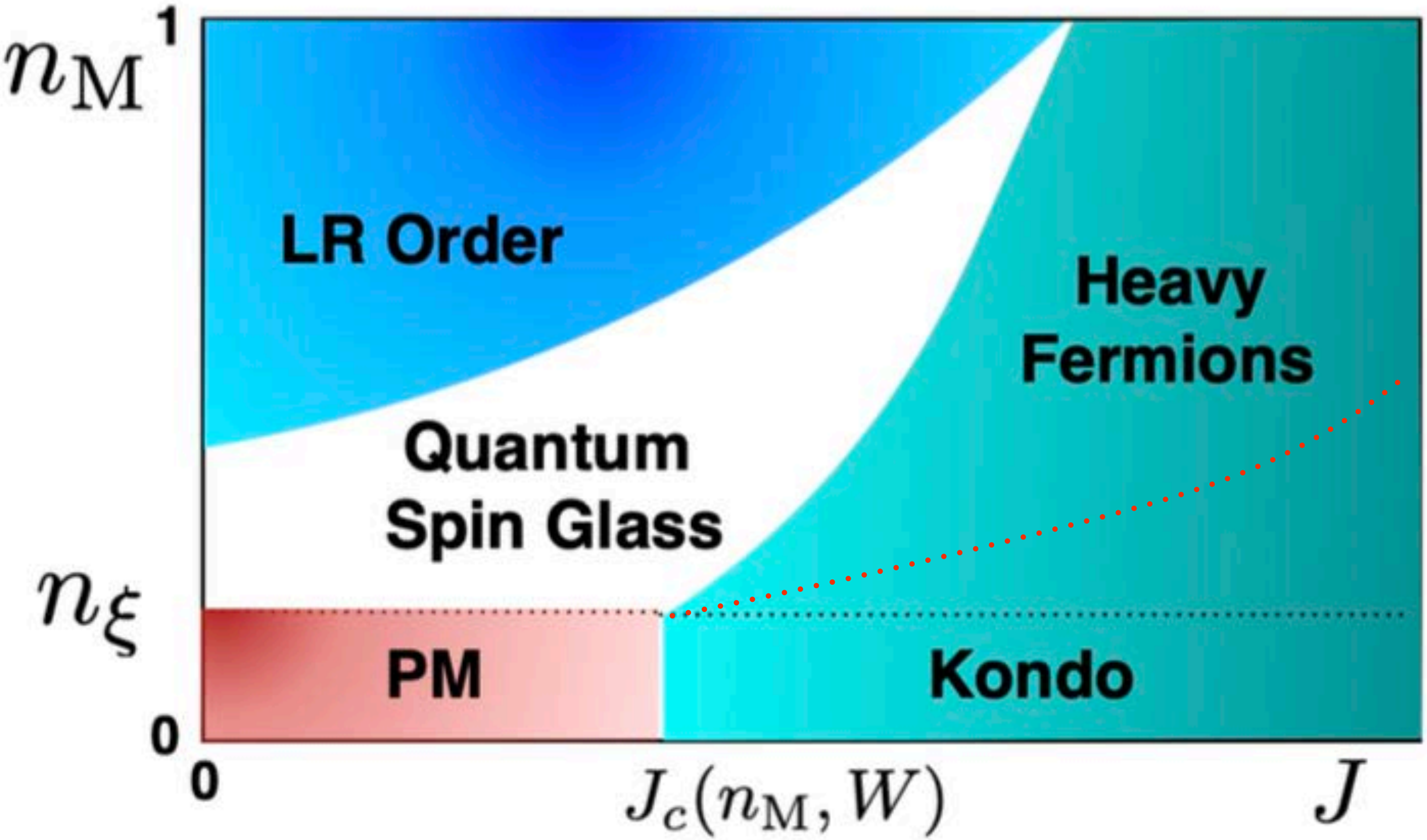
Cluster extensions of the numerical renormalization group method

A. K. Mitchell, P. G. Derry, and D. E. Logan, Phys. Rev. B 91, 235127 (2015).

Conclusions

- Quantum Phas transition between LR Ordered and Heavy Fermion State due to RKKY-Kondo Competition
- RG for Kondo with RKKY-Coupling
- Kondo temperature jumps at transition



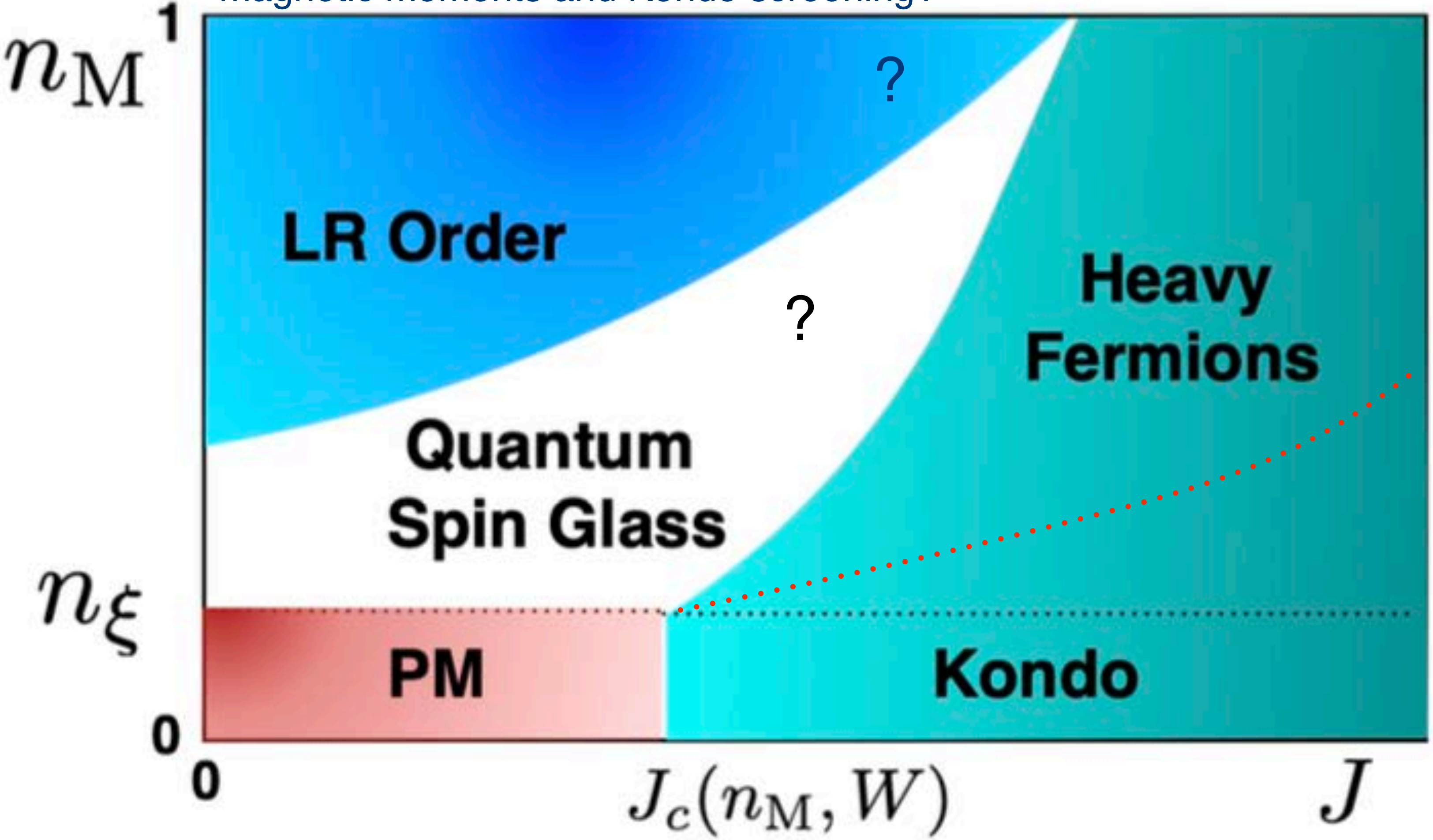
- Coherence transition to low temperature Fermi Liquid with heavy quasiparticles in Kondo lattice systen with low resistivity
- Kondo Fermi liquid with enhanced resistivity

- Critical coupling increases with m.m. density as $J_c \sim \sqrt{n_M}$
- Disorder in dilute system prevents LR order
- Quantum Spin Glass phase emerges
- Paramagnetic Phase of T=0K free moments in very dilute system

Open problems

Is the LR order transition due to

- ordering of emerging local moments?
- spin-density wave transition?
- inhomogenoeous coexcistence of ordered magnetic moments and Kondo screening?



?

- Crossover?
- Transition?

- FInite Temperature Phase transitions?
- Classical Spin Glass?
- (Quantum) Spin Liquid?
- critical spin liquid?
- Griffiths phase?

?

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