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Interplay of
Kondo effect and RKKY interaction

Hans Kroha
University of Bonn

Autumn School on Correlated Electrons:
Correlated Insulators, Metals, and Superconductors FZ Jülich, 27.09.2017

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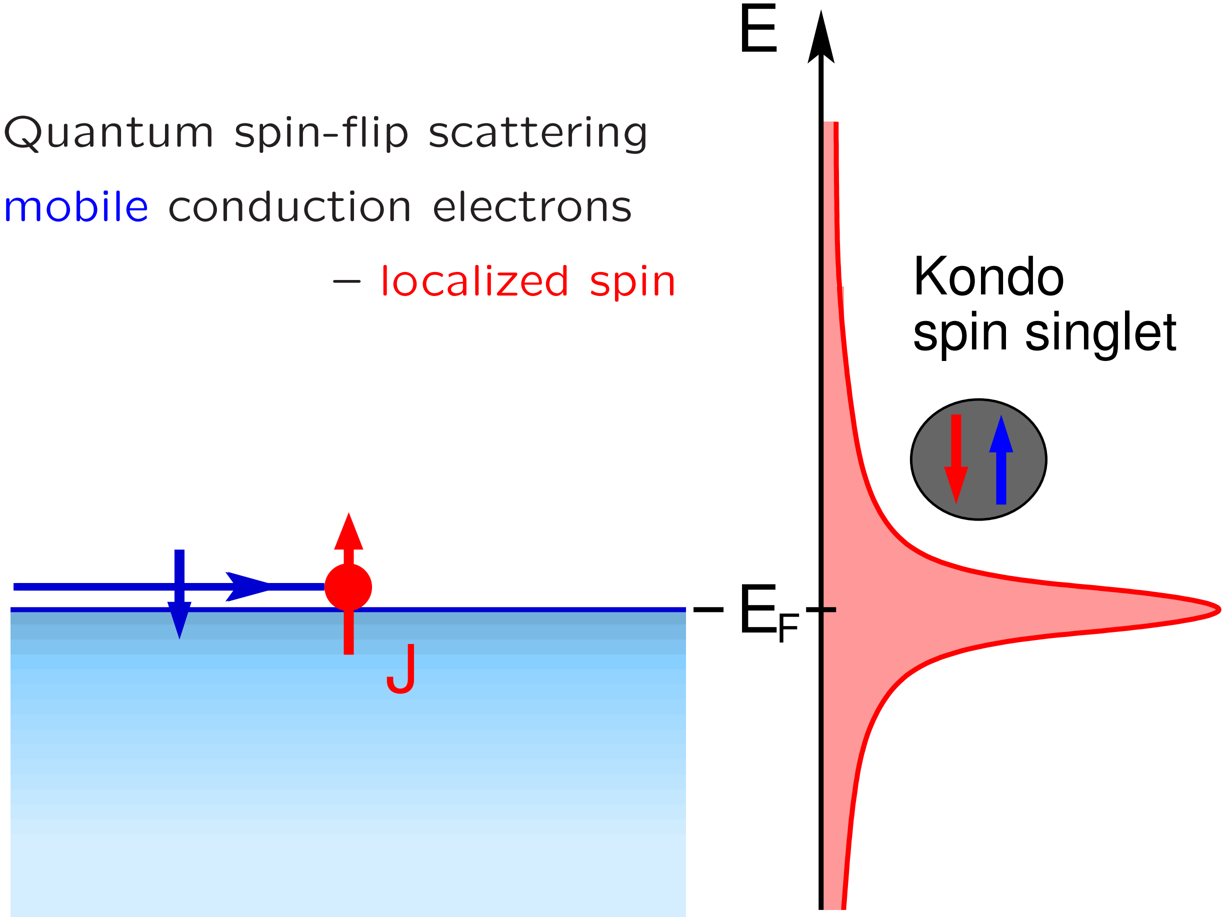
Kondo effect

Quantum spin-flip scattering

mobile conduction electrons

– localized spin



Resonant scattering

of electrons at Fermil level:

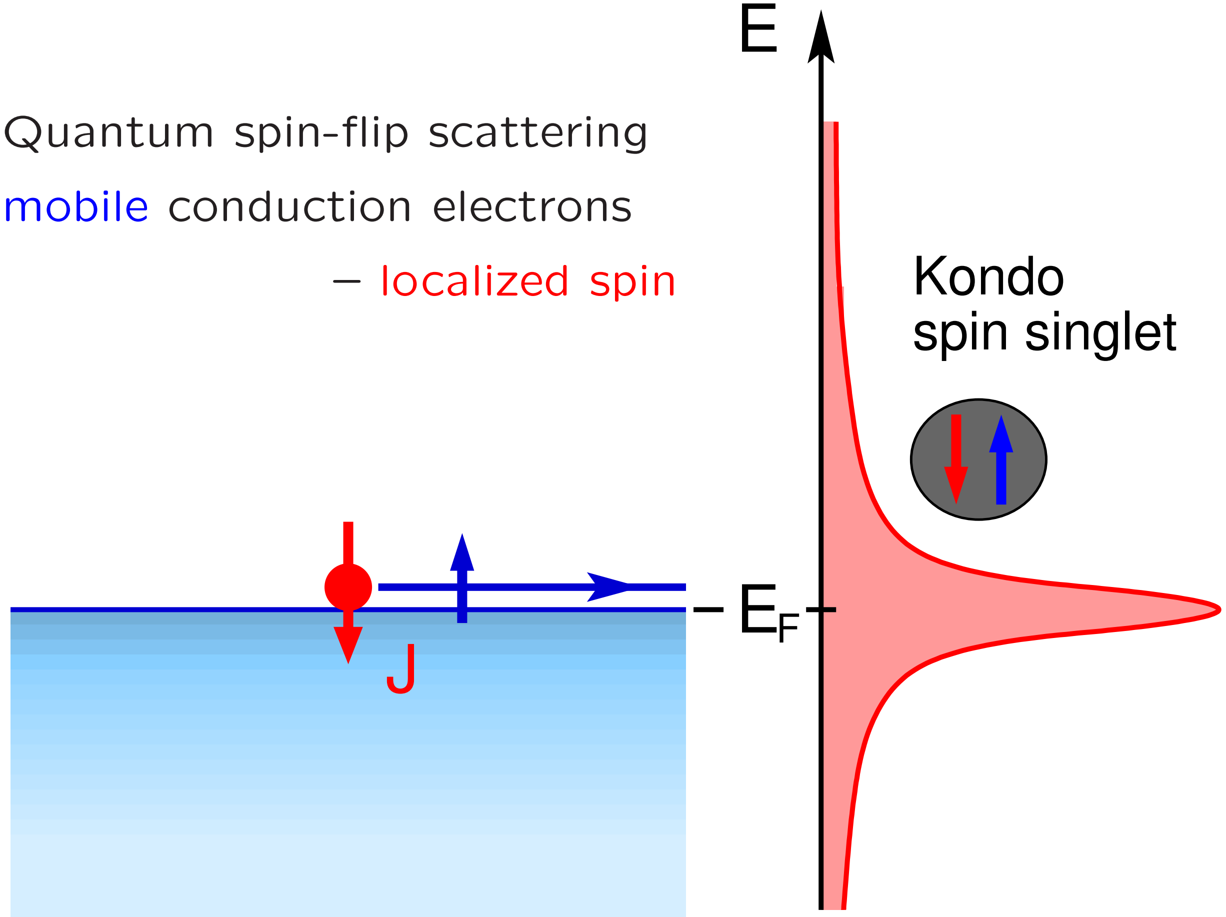
- Narrow resonance at E_F
- $T \to 0$: Strong AF coupling
- c-f spin singlet for $T < T_K$
  Binding energy T_K

Kondo effect

Quantum spin-flip scattering

mobile conduction electrons

– localized spin



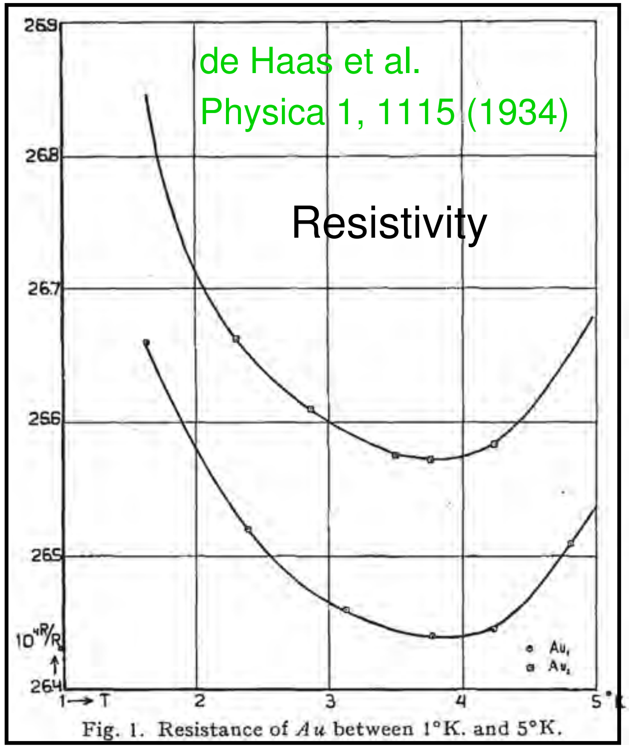
Resonant scattering

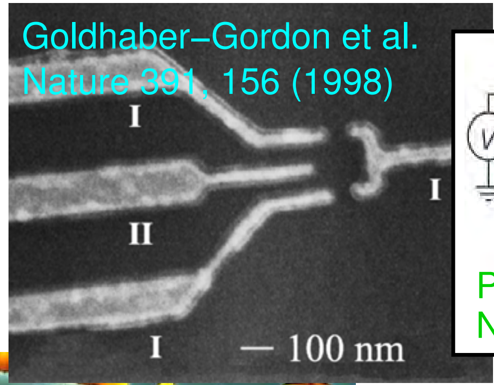
of electrons at Fermil level:

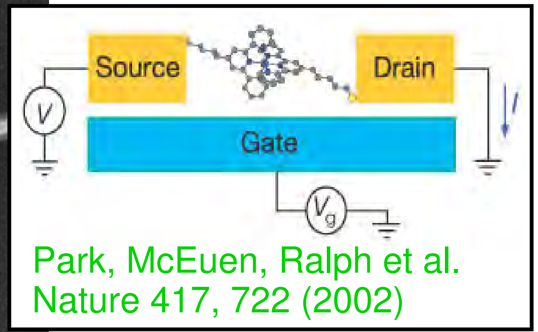
- Narrow resonance at E_Fx
- $T \to 0$: Strong AF coupling
- c-f spin singlet for $T < T_K$

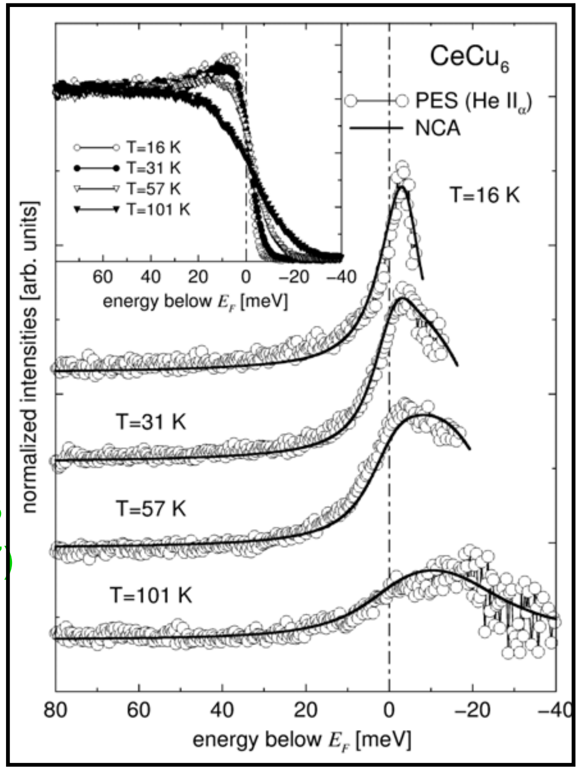
  Binding energy T_K

Kondo systems and experimental signatures



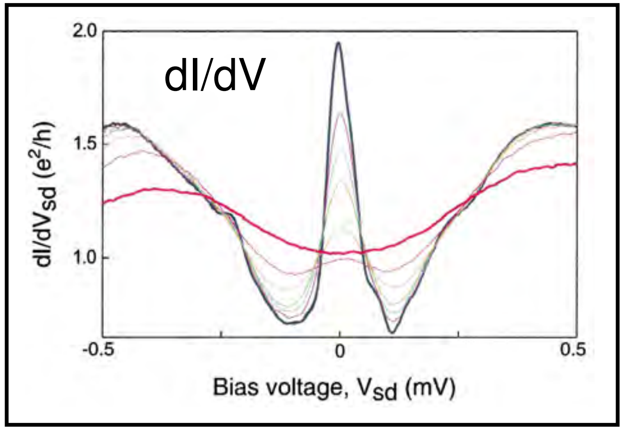






Photoemission

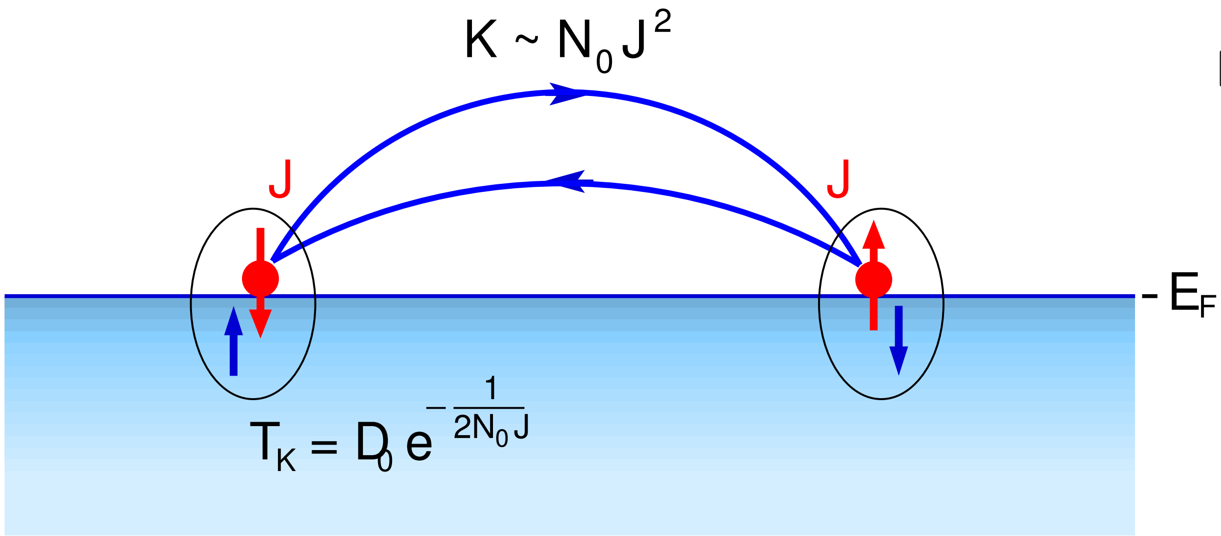
Ehm et al., Phys Rev B 76, 0415117 (2007)



Van der Wiel, Tarucha, Kouwenhoven et al. (2000)

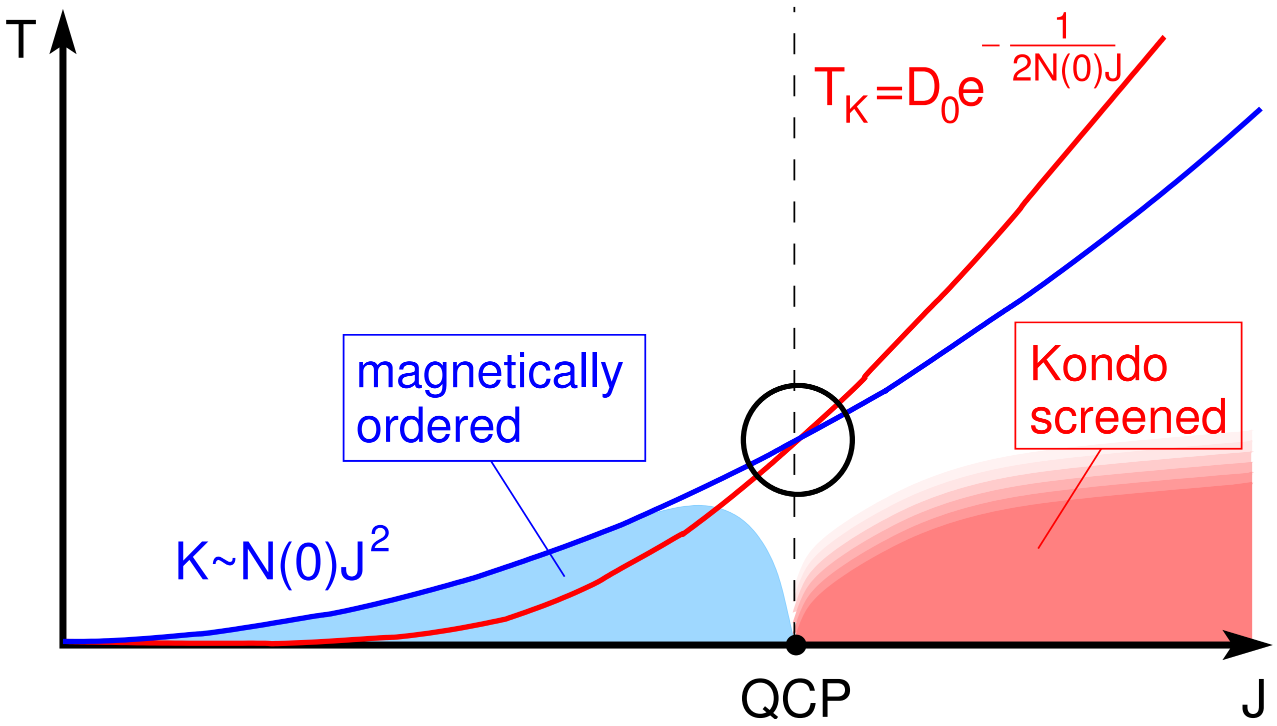
Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction:

Coupling between local spins mediated by conduction electron sea



Long-range interaction

Competition between Kondo singlet formation and RKKY interaction (Doniach 1977)

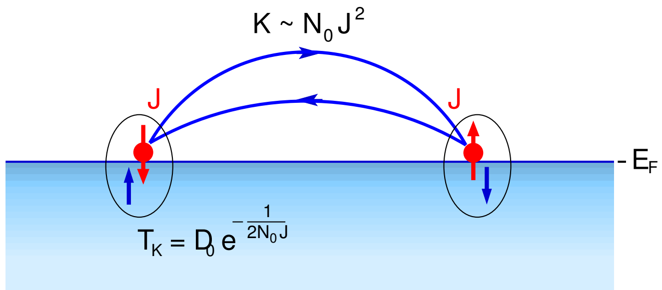


General believe:
Kondo destruction driven by critical fluctuations

- **Local or AF OP fluctuations** coupling to the heavy fermions [Si (2001), Coleman (2001)]; [Wölfle, Abrahams, Schmalian (2011)]
- **Fermi surface fluctuations** due to Kondo collapse, fractionalization [Senthil, Vojta, Sachdev (2004)]
- **Kondo breakdown due to RKKY interaction alone**

Outline

- Kondo effect
  - Perturbation theory
  - Renormalization group

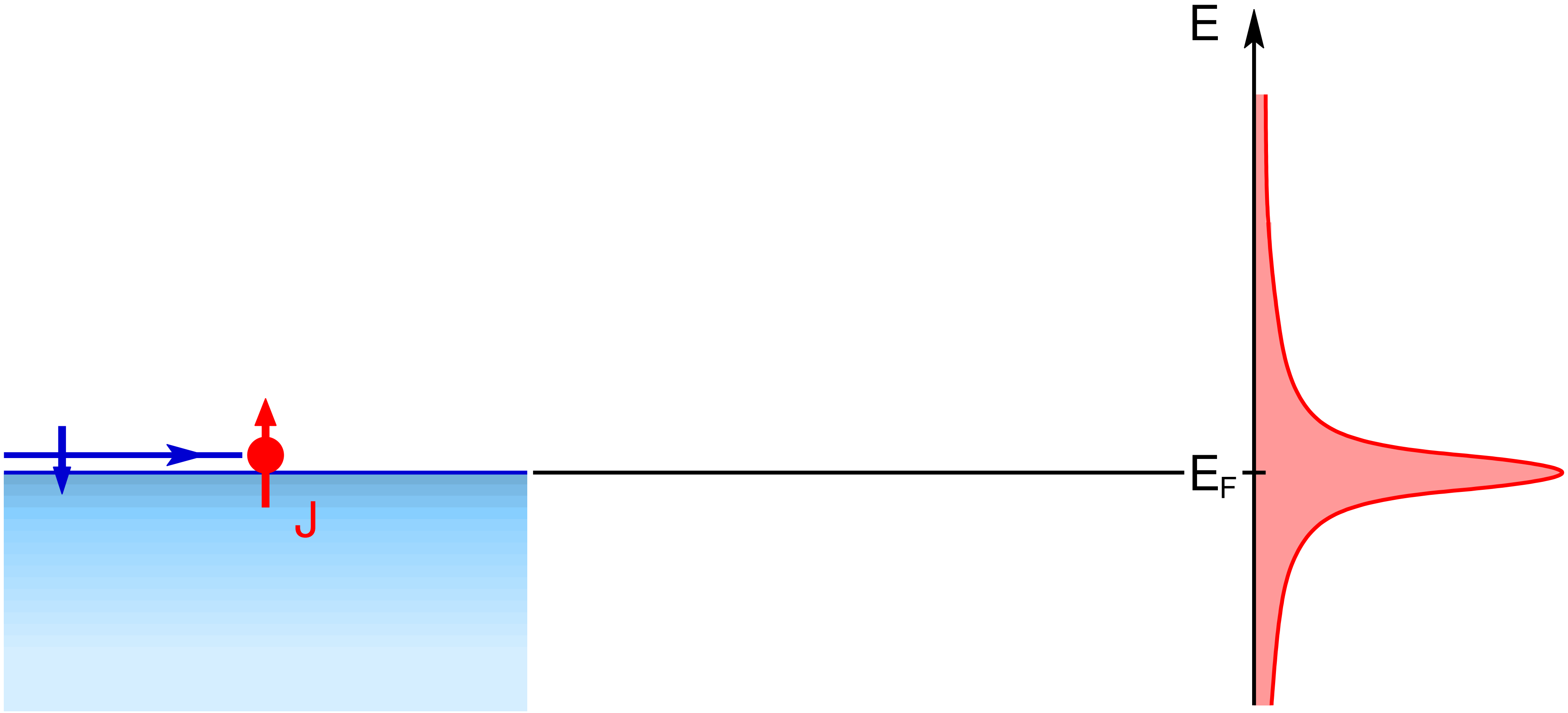


- RKKY interaction

- Competition: local Kondo and long-range RKKY interaction
  - Renormalization group: "How to measure Euler's constant"
  - Experiments

Localized spin in a metal:

$$H = \sum_{k\sigma} \varepsilon_k \, c^\dagger_{k\sigma} c_{k\sigma} \; + \; \mathbf{J} \sum_{kk'\sigma\sigma'} c^\dagger_{k\sigma} \left(\vec{S} \cdot \vec{\sigma}\right) c_{k'\sigma'}$$



Kondo effect

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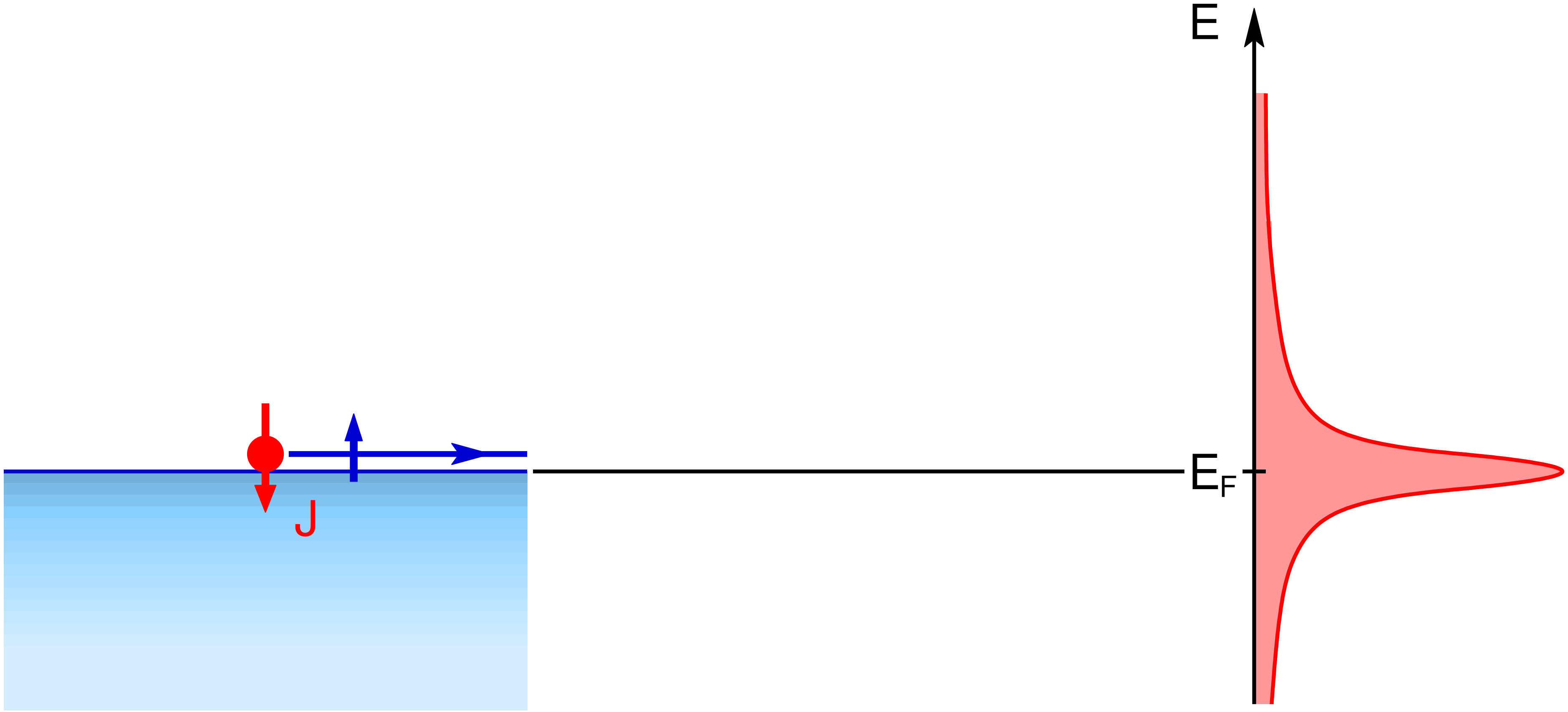

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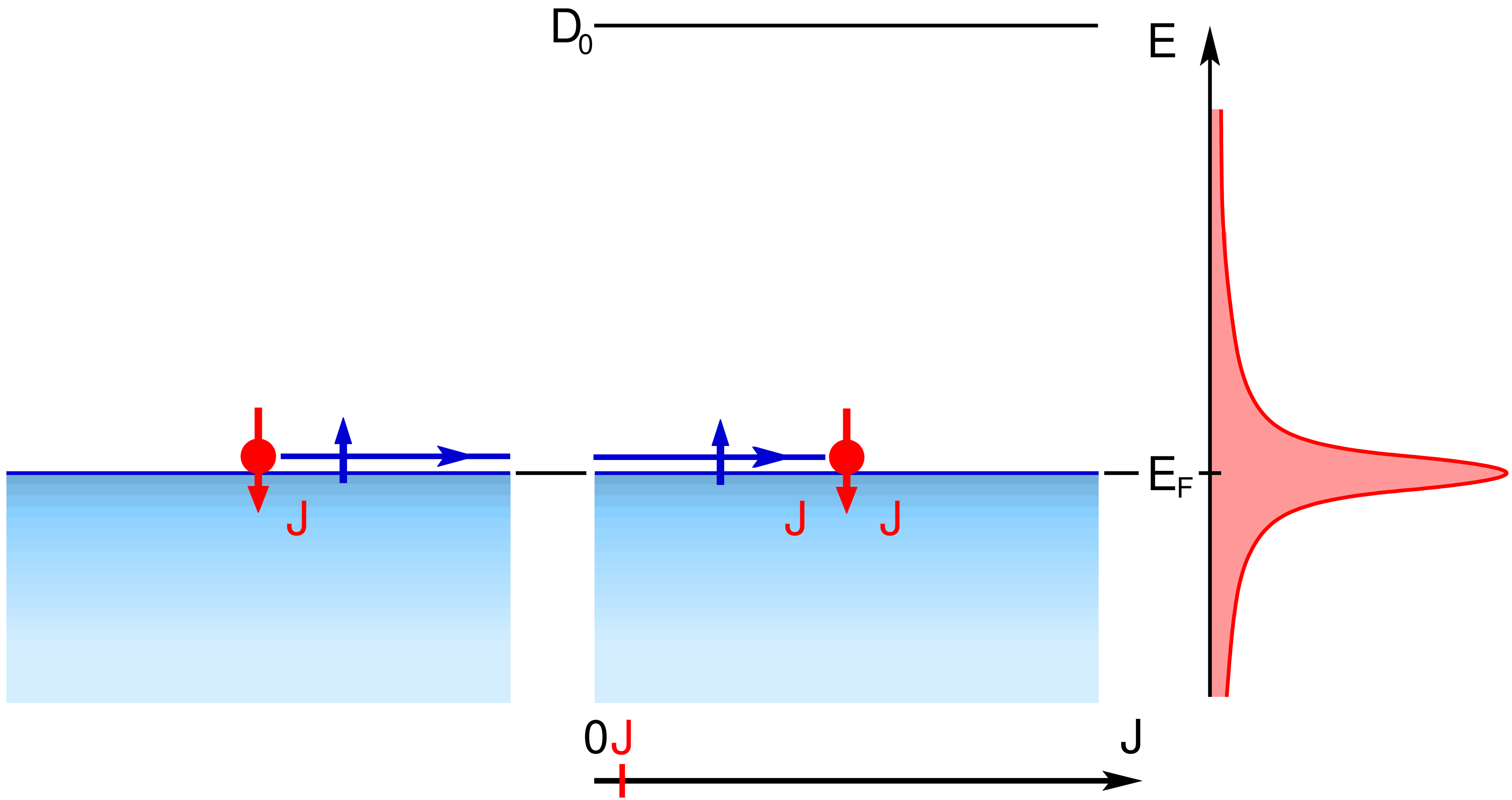

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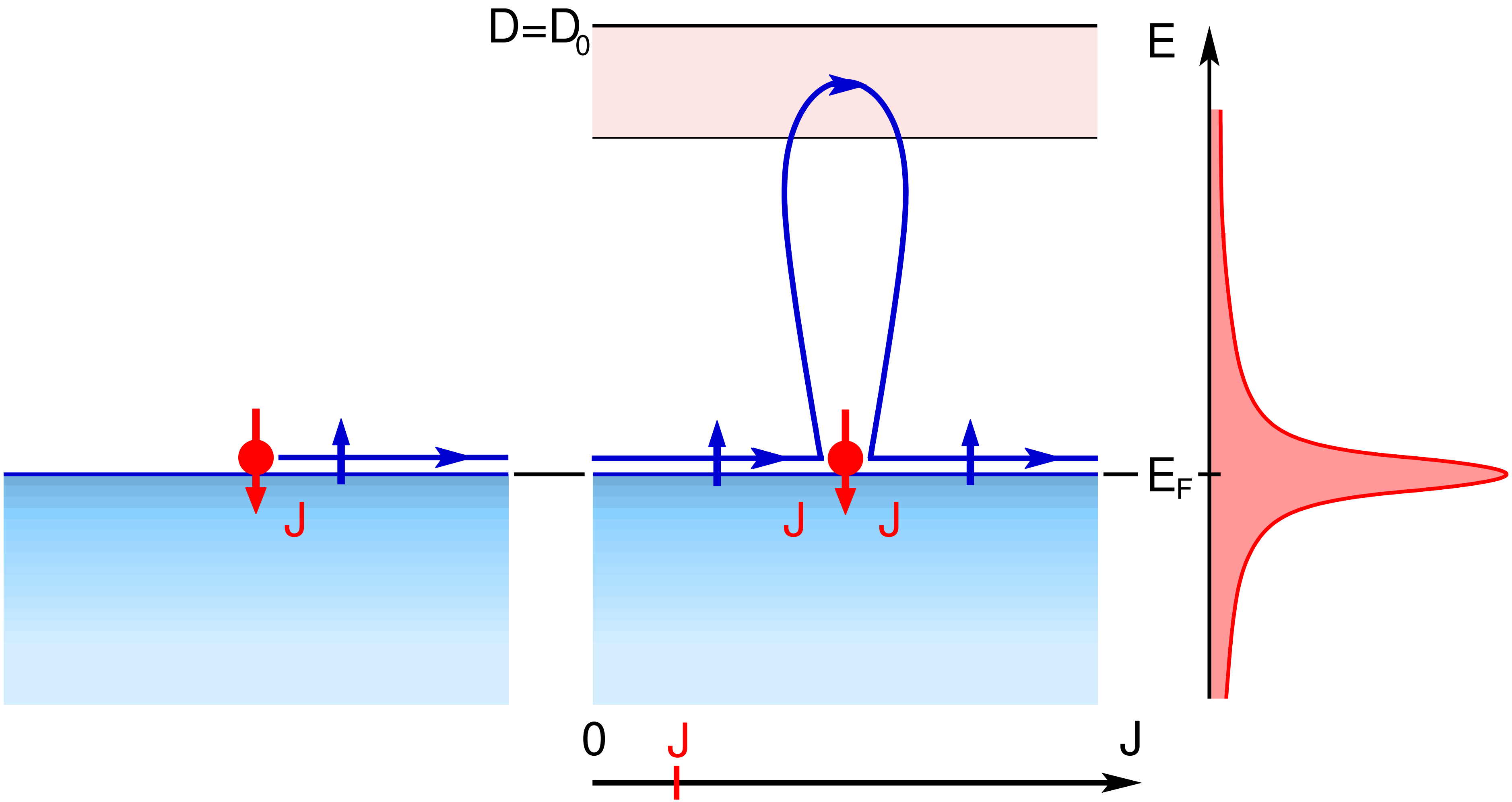

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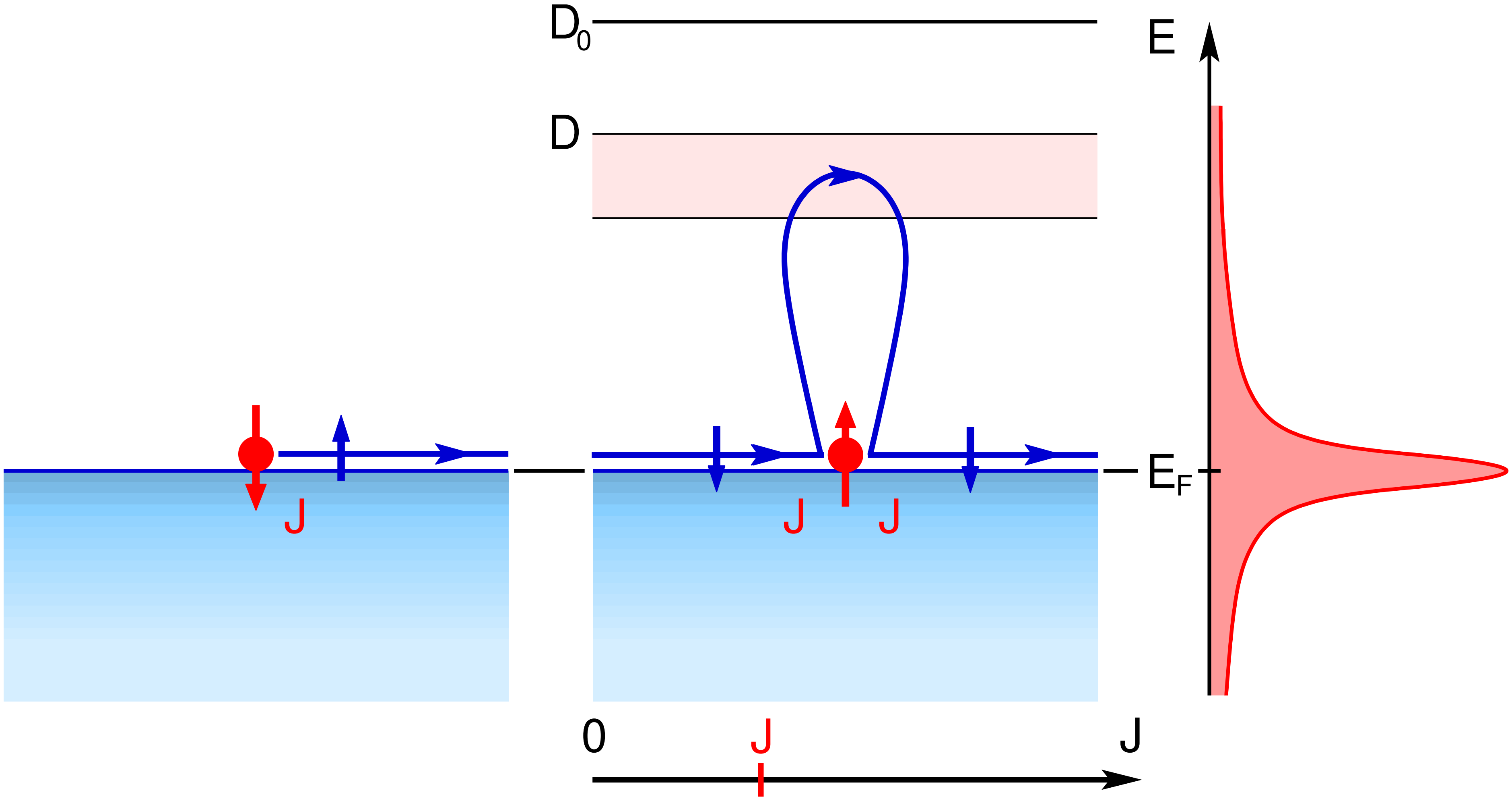

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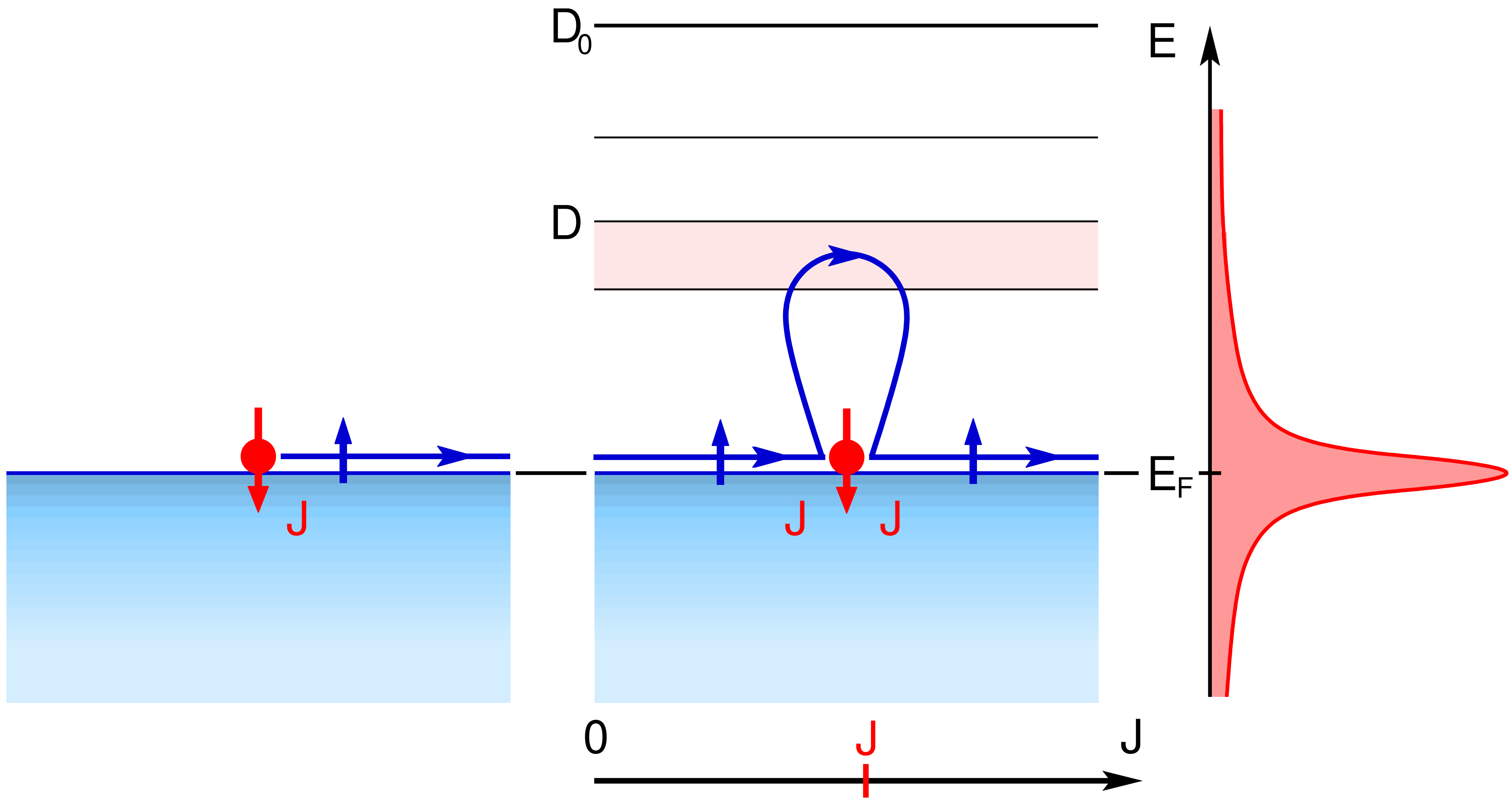

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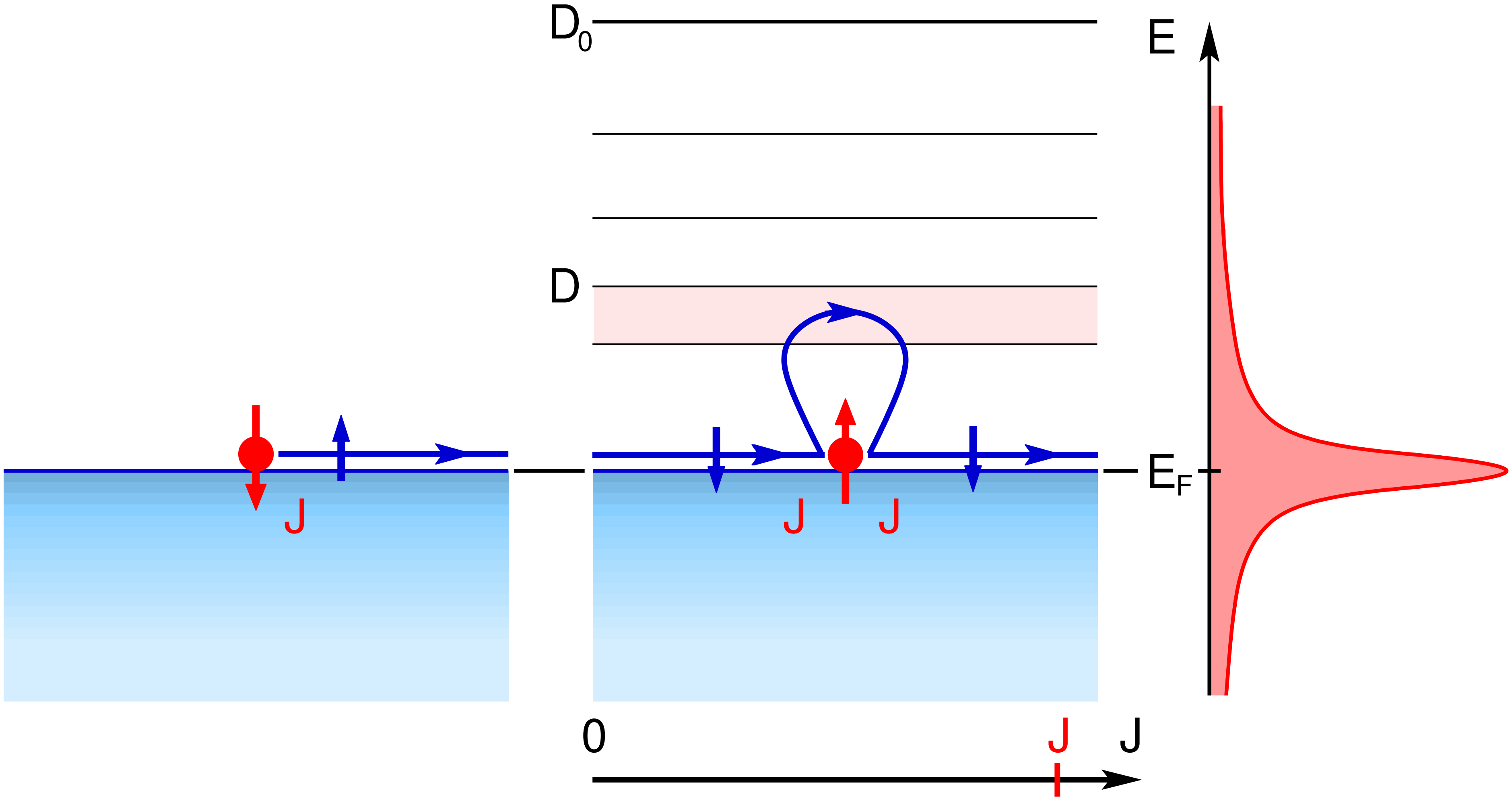

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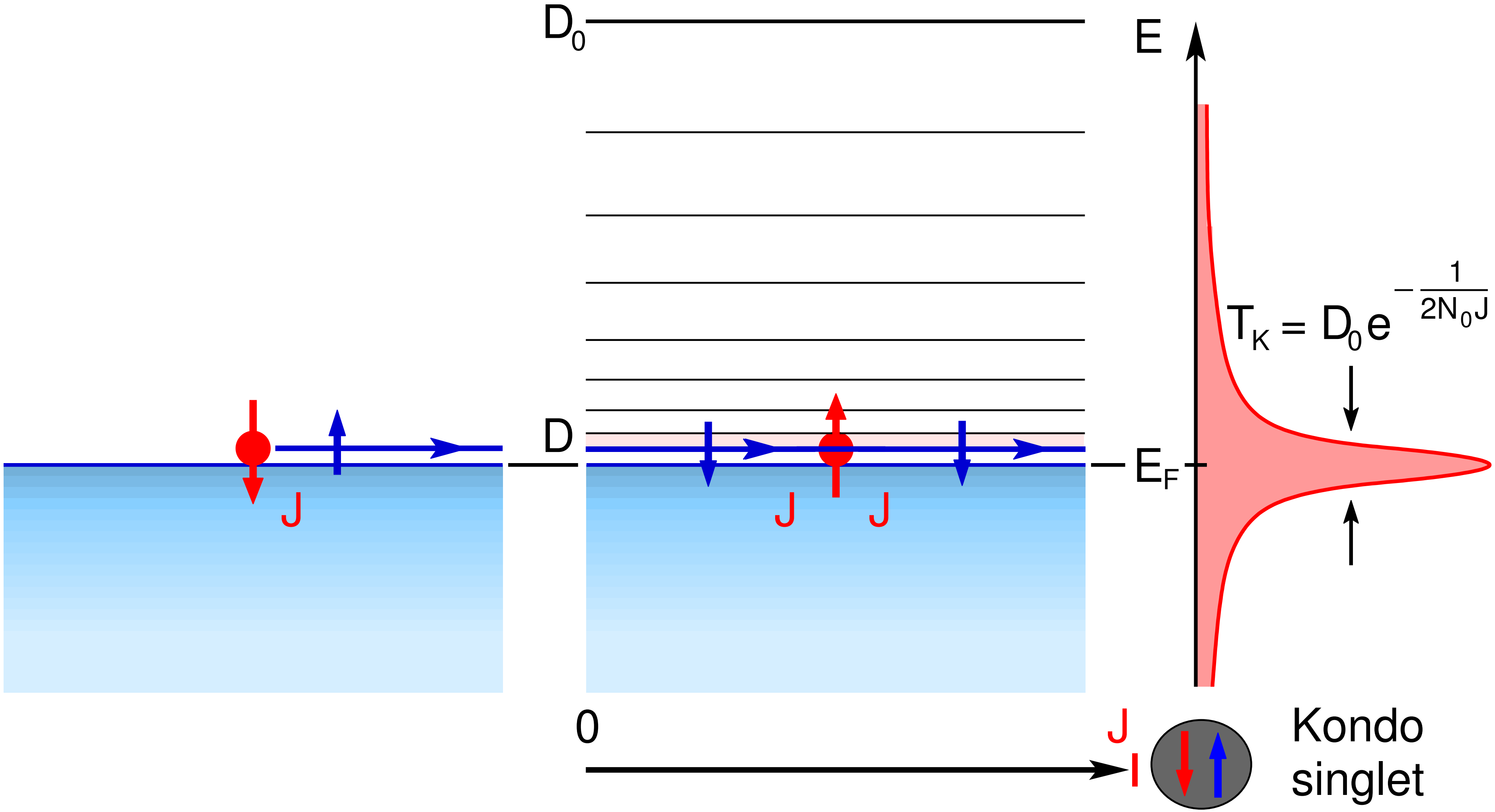
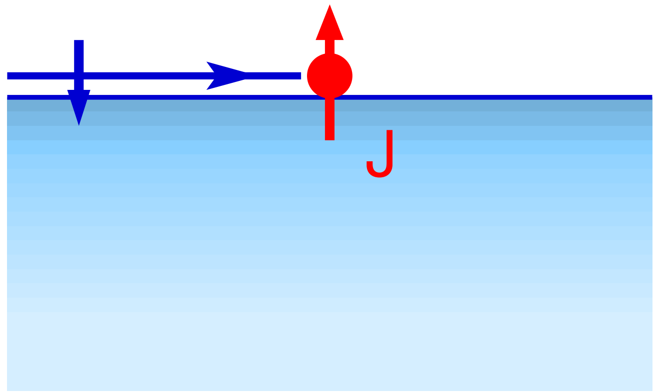


Localized spin in a metal



$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + J_0\, \vec{\hat{S}} \cdot \vec{\hat{s}}$$

$$\vec{\hat{s}} = \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} c^{\dagger}_{\mathbf{k}\sigma}\, \vec{\sigma}_{\sigma\sigma'}\, c_{\mathbf{k}'\sigma'}$$

$\vec{\hat{S}}$: impurity spin

$\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)^T$: vector of Pauli matrices, $[\sigma_i, \sigma_j] = 2\mathrm{i}\, \varepsilon^{ijk}\, \sigma_k$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Pseudofermion representation of spin

$$\hat{\vec{S}} = \frac{1}{2}\sum_{\tau,\tau'} f^{\dagger}_{\tau}\,\vec{\sigma}_{\tau\tau'}\,f_{\tau'}$$

$$\hat{S}^{+} = f^{\dagger}_{\uparrow}\,f_{\downarrow} \qquad \hat{S}^{-} = f^{\dagger}_{\downarrow}\,f_{\uparrow} \qquad \hat{S}_{z} = \frac{1}{2}\left[f^{\dagger}_{\uparrow}\,f_{\uparrow} - f^{\dagger}_{\downarrow}\,f_{\downarrow}\right]$$

With operator constraint

$$\hat{Q} = \sum_{\sigma} f^{\dagger}_{i\sigma} f_{i\sigma} = \mathbb{1}$$

to restrict the dynamics to the physical spin Hilbert space $\{|\uparrow\rangle, |\downarrow\rangle\}$.

Abrikosov 1964

Kondo effect: Pseudofermion representation

Projection onto the physical Hilbert space

Grand canonical density matrix with respect to $Q = 0, 1, 2$:

$$\hat{\rho}_G = \frac{1}{Z_G} \mathrm{e}^{-\beta(H+\lambda Q)}$$

$$Z_G = \mathrm{tr}\left[\mathrm{e}^{-\beta(\hat{H}+\lambda\hat{Q})}\right] \qquad \beta = \frac{1}{k_B T}$$

Expectation value observable $\hat{A}$ acting on the impurity spin space (Q−grand canonical):

$$\langle \hat{A} \rangle_G(\lambda) = \mathrm{tr}[\hat{\rho}_G \hat{A}]$$

Projection onto the physical subspace $Q = 1$:

$$\langle \hat{A} \rangle := \frac{\mathrm{tr}_{Q=1}\left[\hat{A} e^{-\beta \hat{H}}\right]}{\mathrm{tr}_{Q=1}\left[e^{-\beta \hat{H}}\right]} = \lim_{\lambda \to \infty} \frac{\mathrm{tr}\left[\hat{A} e^{-\beta[\hat{H}+\lambda(\hat{Q}-1)]}\right]}{\mathrm{tr}\left[\hat{Q} e^{-\beta[\hat{H}+\lambda(\hat{Q}-1)]}\right]} = \lim_{\lambda \to \infty} \frac{\langle \hat{A} \rangle_G(\lambda)}{\langle \hat{Q} \rangle_G(\lambda)}$$

Computational rules

$$G_{c\mathbf{k}\sigma}(i\omega_n) = \frac{1}{i\omega_n - \varepsilon_{\mathbf{k}}}$$

$$G^G_{f\sigma}(i\omega_n) = \frac{1}{i\omega_n - \lambda}, \quad \omega_n = \frac{\pi}{\beta}(2n+1)$$

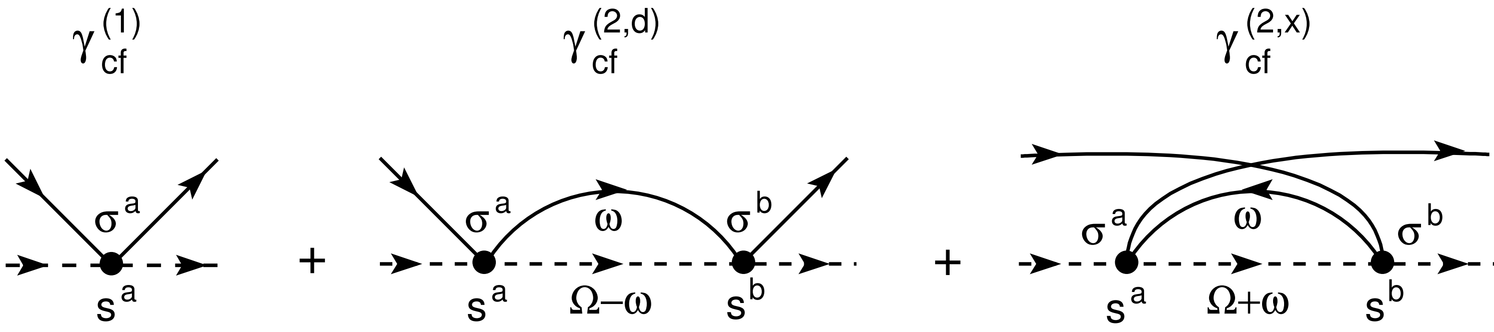
(1) Calculate first in the $Q-$grand canonical ensemble.
$\longrightarrow$ Feynman diagrams valid.

(2) Take the limit $\lambda \to \infty$.

(3) Each integral along a pseudofermion branch cut carries a factor $e^{-\beta\lambda}$ and, thus, vanishes in this limit.

(4) Each diagram contributing to the projected $\langle \hat{A} \rangle$, contains exactly one closed pseudofermion loop per impurity site:
The factor $e^{-\beta\lambda}$ cancels in the numerator and denominator of $\langle \hat{A} \rangle$.
Higher order loops vanish by virtue of rule (3).

Perturbation theory



$$\hat{\gamma}_{cf} = \frac{1}{2} J_0\,(\mathbf{s}\cdot\sigma)\left[1 + N(0)J_0 \int_{-D_0}^{D_0} d\varepsilon\, \frac{1-2f(\varepsilon)}{\varepsilon} + \mathcal{O}(J_0^2)\right]$$

$$\approx \frac{1}{2} J_0\,(\mathbf{s}\cdot\sigma)\left[1 + 2N(0)J_0 \ln\left(\frac{D_0}{T}\right) + \mathcal{O}(J_0^2)\right]$$

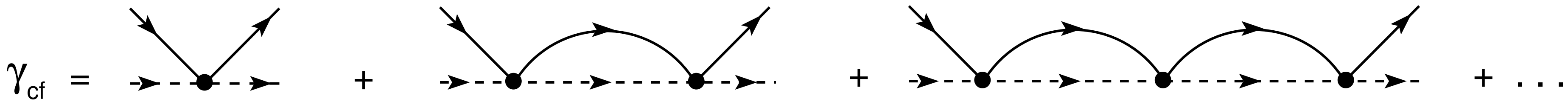
Breakdown of perturbation theory for $T < T_K$:

$$T_K = D_0\, \mathrm{e}^{-1/(2N(0)J_0)}$$

Kondo effect

Universality

Partial resummation of perturbation theory



$$N(0)\tilde{J} = 2N(0)J_0\left[1 + 2N(0)J_0 \ln\left(\frac{D_0}{T}\right) + \left(2N(0)J_0 \ln\left(\frac{D_0}{T}\right)\right)^2 + \ldots\right]$$

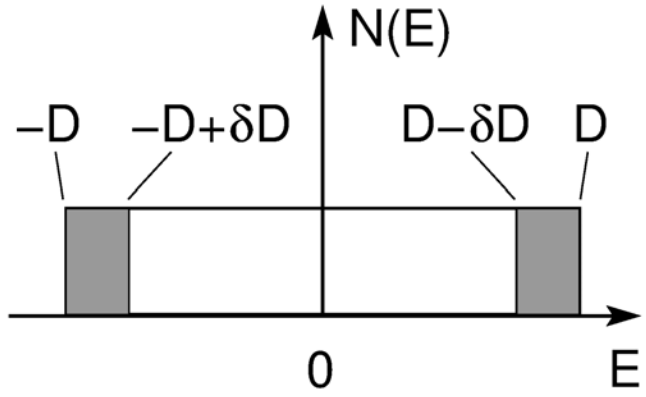
$$= \frac{2N(0)J_0}{1 - 2N(0)J_0 \ln\left(\frac{D_0}{T}\right)} = \frac{1}{\ln\left(\frac{T}{T_K}\right)}$$

The resummed vertex depends on system parameters only implicitly through the single energy scale T_K!

$$T_K = D_0\, e^{-1/(2N(0)J_0)}$$

Renormalization group

Universality implies:
Since physical observables (γ_{cf}) depend on system parameters (J, D) only through a (yet unknown) scale $T_K(J, D)$, systems with
different bandwidths D and
appropriately chosen couplings J
must be equivalent.



→ Systems with high band cutoff D and low band cutoff D must be connected with each other.

→ Calculate low-energy properties by successive, infinitesimal cutoff reduction.

→ Renormalization group (RG) flow
"Running" coupling $J(D)$.

Kondo effect: Renormalization group

Perturbative computation of the RG flow:

$$\hat{\gamma}_{cf} = \hat{\gamma}_{cf}^{(1)} + \hat{\gamma}_{cf}^{(1)}\, G\, \hat{\gamma}_{cf}$$

$$\begin{aligned}
\hat{\gamma}_{cf} &= \hat{\gamma}_{cf}^{(1)} + \hat{\gamma}_{cf}^{(1)}\, [P_{\delta D} G]\, \hat{\gamma}_{cf} + \hat{\gamma}_{cf}^{(1)}\, [(1 - P_{\delta D}) G]\, \hat{\gamma}_{cf} \\
&= \hat{\gamma}_{cf}^{(1)} + \hat{\gamma}_{cf}^{(1)}\, [P_{\delta D} G] \left\{ \hat{\gamma}_{cf}^{(1)} + \hat{\gamma}_{cf}^{(1)}\, [(P_{\delta D} + (1 - P_{\delta D}))\, G]\, \hat{\gamma}_{cf} \right\} \\
&\qquad + \hat{\gamma}_{cf}^{(1)}\, [(1 - P_{\delta D}) G]\, \hat{\gamma}_{cf} \\
&= \hat{\gamma}_{cf}^{(1)\prime} + \hat{\gamma}_{cf}^{(1)\prime}\, [(1 - P_{\delta D}) G]\, \hat{\gamma}_{cf} \quad + \quad \mathcal{O}(P_{\delta D}^2),
\end{aligned}$$

with renormalized coupling

$$\hat{\gamma}_{cf}^{(1)\prime} = \hat{\gamma}_{cf}^{(1)} + \hat{\gamma}_{cf}^{(1)}\, [P_{\delta D} G]\, \hat{\gamma}_{cf}^{(1)} =: \hat{\gamma}_{cf}^{(1)} + \delta \hat{\gamma}_{cf}^{(1)}.$$

Perturbative computation of the RG flow:

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Kondo effect: Renormalization group

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&= \widehat{\gamma}^{(1)'}_{cf} + \widehat{\gamma}^{(1)'}_{cf}\,[(1-P_{\delta D})G]\,\widehat{\gamma}_{cf} \quad + \quad \mathcal{O}(P^2_{\delta D}),
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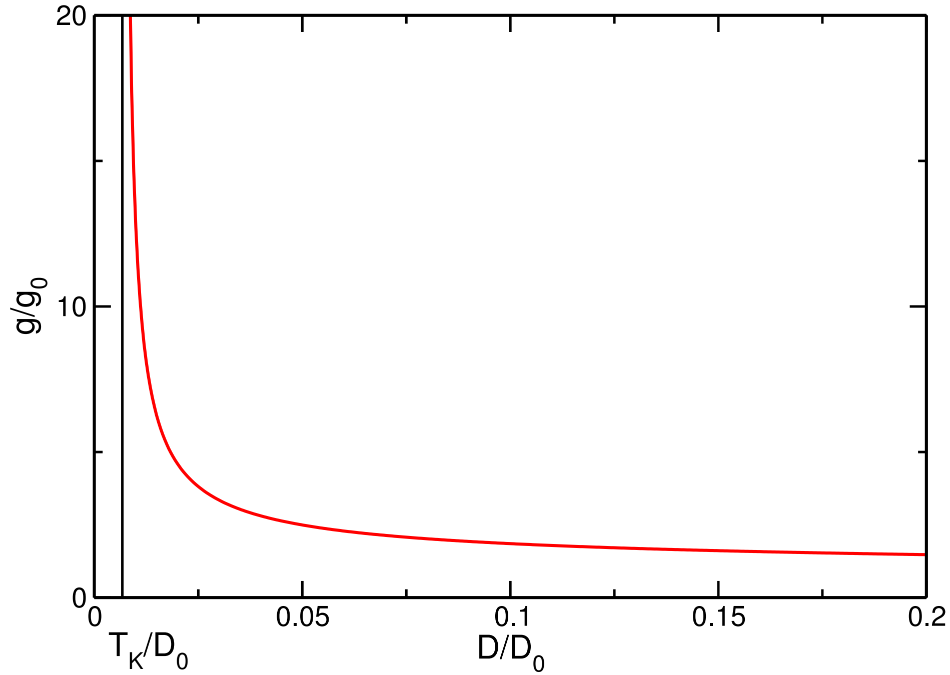
Kondo effect: Renormalization group

RG equation:

$$dg = -\frac{d}{dD}\left[g^2 \int_{-D}^{D} d\varepsilon\, \frac{1-2f(\varepsilon)}{\varepsilon}\right]\delta D = -\frac{2g^2}{D}\,\delta D$$

$$g(D) = \frac{g_0}{1+2g_0 \ln(D/D_0)}$$



Divergence at $T_K = D_0\, e^{-1/(2N(0)J_0)}$

→ Kondo singlet formation for $T < T_K$.

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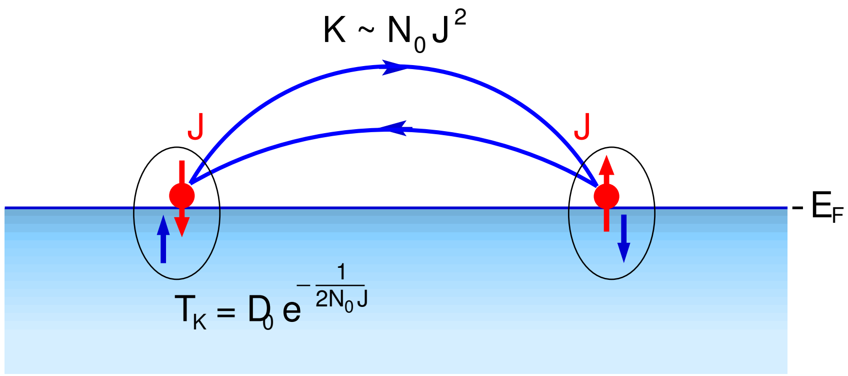


Kondo lattice Hamiltonian

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}}\, c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + J_0 \sum_i \hat{\mathbf{S}}_i \cdot \hat{\mathbf{s}}_i$$

The operator coupling the conduction electrons and the localized f-spin $\mathbf{S}_j$ at a site $j \neq i$,

$$H_j^{(cf)} = J_0 \hat{\mathbf{S}}_j \cdot \hat{\mathbf{s}}_j$$

acts as a perturbation for the localized f-spin at a site i,
because it involves the conduction electron sea.

Leading order perturbation theory in the non-local perturbation $j \neq i$, tracing out the conduction electrons only:

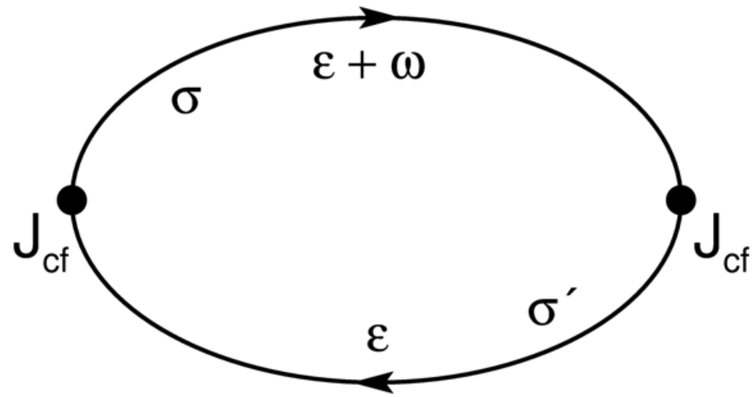
Time evolution operator (interaction picture):

$$\hat{U} = \hat{T} e^{-\int_0^\beta d\tau H_j^{cf}(\tau)} = 1 - \int_0^\beta d\tau H_j^{cf}(\tau) \quad + \mathcal{O}(J_0^2)$$

→ Hamiltonian operator for the f-spin at site i:

$$H_{ij}^{(2)} = J_0\, \hat{\mathbf{S}}_i \cdot \hat{\mathbf{s}}_i - J_0^2 \left. \langle (\hat{\mathbf{S}}_i \cdot \hat{\mathbf{s}}_i)(\hat{\mathbf{S}}_j \cdot \hat{\mathbf{s}}_j) \rangle_c \right|_{\omega=0} \qquad H_{ij}^{RKKY}$$

$\hat{\mathbf{S}}_i - \hat{\mathbf{S}}_j$ coupling Hamiltonian:



$$H_{ij}^{RKKY} = -\frac{J_0^2}{4} \sum_{\alpha,\beta=x,y,z} \sum_{\sigma\sigma'} \hat{S}_i^{\alpha}\, \sigma^{\alpha}_{\sigma\sigma'} \sigma^{\beta}_{\sigma'\sigma}\, \hat{S}_j^{\beta} \Pi_{ij}^{\sigma\sigma'}(0),$$

with the conduction electron density propagator between the sites i and j

$$\Pi_{ij}^{\sigma\sigma'}(i\omega) = -\frac{1}{\beta} \sum_{\varepsilon_n} G_{ji\,\sigma}(i\varepsilon_n + i\omega) G_{ij\,\sigma'}(i\varepsilon_n) \quad \text{or}$$

$$\Pi_{ij}^{||}(0) = \frac{1}{2} \sum_{\sigma} \Pi_{ij}^{\sigma\sigma}(0) = -\sum_{\sigma} \int d\varepsilon\, f(\varepsilon)\, A_{ij\,\sigma}(\varepsilon) \mathrm{Re} G_{ij\,\sigma}(\varepsilon)$$

$$\Pi_{ij}^{\perp}(0) = \frac{1}{2} \sum_{\sigma} \Pi_{ij}^{\sigma\,-\sigma}(0) = -\sum_{\sigma} \int d\varepsilon\, f(\varepsilon)\, A_{ij\,\sigma}(\varepsilon) \mathrm{Re} G_{ij\,-\sigma}(\varepsilon) \ ,$$

RKKY interaction

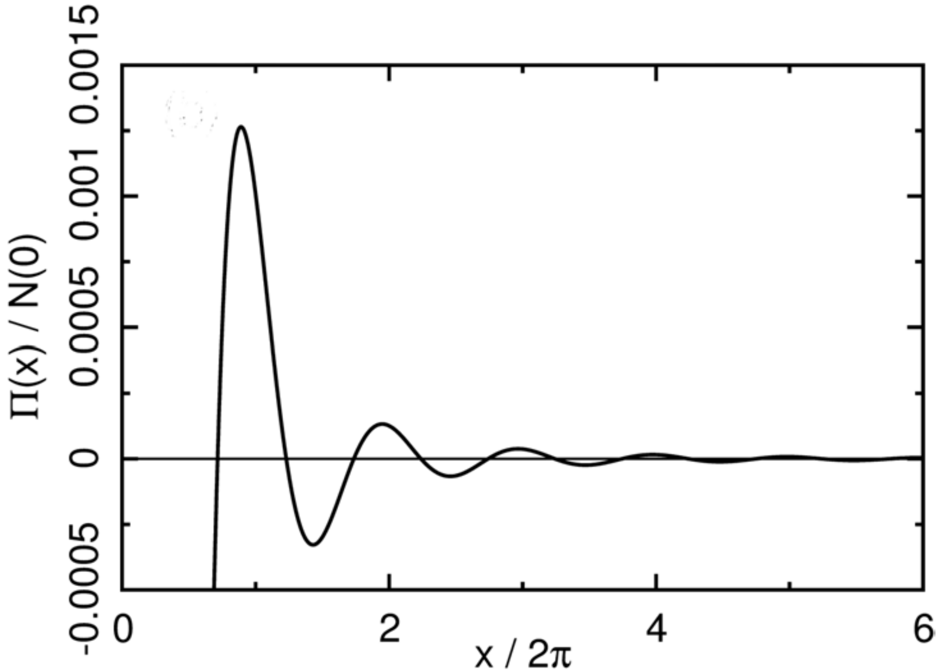
RKKY interaction Hamiltonian:

$$H^{RKKY} = \sum_{i\neq j} H_{ij}^{RKKY} = -\sum_{i,j}\left[K_{ij}^{||}\,\hat{S}_i^z\hat{S}_j^z + K_{ij}^{\perp}\left(\hat{S}_i^x\hat{S}_j^x + \hat{S}_i^y\hat{S}_j^y\right)\right]$$

$$K_{ij}^{||} = \frac{1}{2}J_0^2\Pi_{ij}^{||}(0)\ , \qquad K_{ij}^{\perp} = \frac{1}{2}J_0^2\Pi_{ij}^{\perp}(0)$$

in general, anisotropic for a magnetized conduction band.

Isotropic case



$$\Pi_r^{\sigma\sigma'}(\omega + i0) = \left[N(0)\,\frac{\sin(x) - x\cos(x)}{4x^4} + \mathcal{O}\left(\left(\frac{\omega}{\varepsilon_F}\right)^2\right)\right] \sim \frac{1}{x^d}$$

$$\pm \; i \left[\frac{1}{\pi}N(0)\,\frac{1-\cos(x)}{x^2}\,\frac{\omega}{\varepsilon_F} + \mathcal{O}\left(\left(\frac{\omega}{\varepsilon_F}\right)^3\right)\right]$$

with $x = 2k_F r$, $r = |\mathbf{r}_i - \mathbf{r}_j|$.

Interplay of

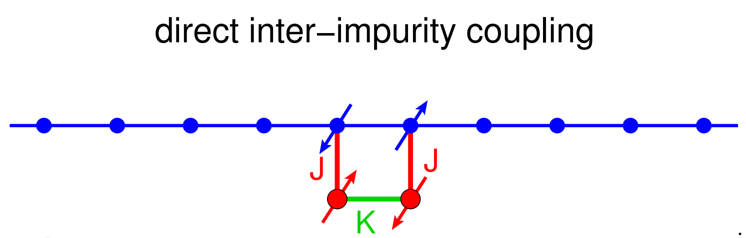
Kondo effect and RKKY interaction

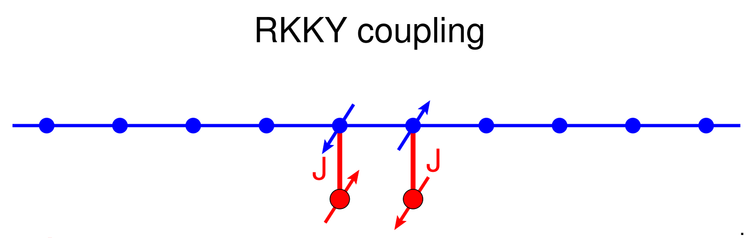
Importance of RKKY-mediated spin coupling

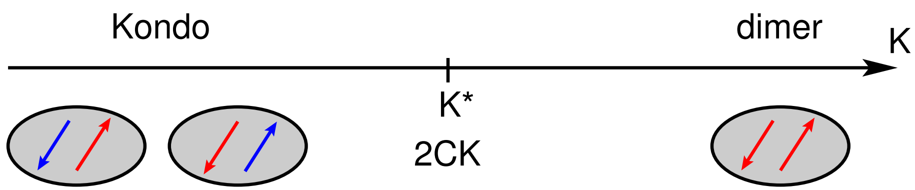
RKKY coupling usually dominates over direct dipole coupling →

Kondo lattice model:

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + J_0 \sum_{\{i\}} \mathbf{S}(\mathbf{x}_i) \cdot \mathbf{s}(\mathbf{x}_i) \qquad J_0 > 0$$







Jones, Varma, Wilkins, PRL **61**, 125 (1988)
Affleck, Ludwig, Jones, PRB **52**, 9528 (1995)
Sela, Affleck, PRL **103**, 087204 (2009)
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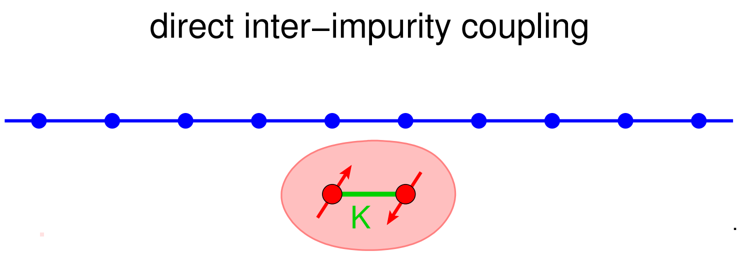

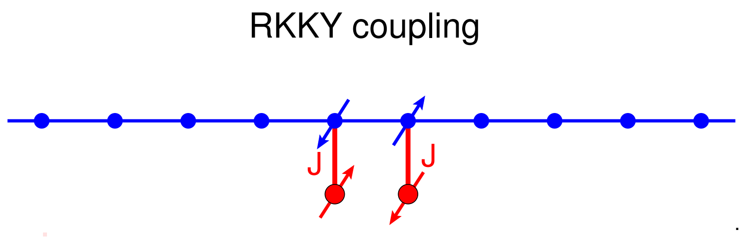

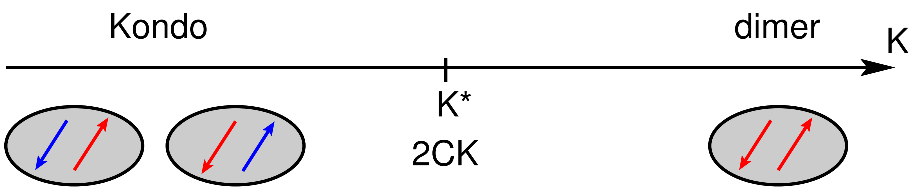

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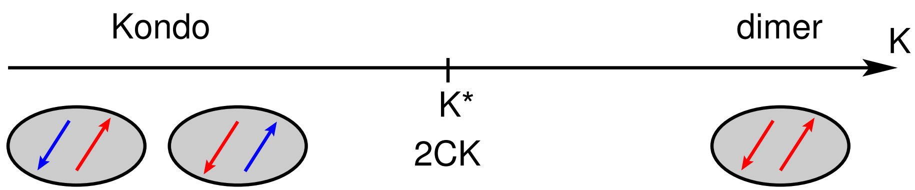

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RKKY does not allow for a dimer coupling–decoupling transition.

$\rightarrow$ New type of Kondo breakdown transition?

Observable in local susceptibility and spectroscopy.

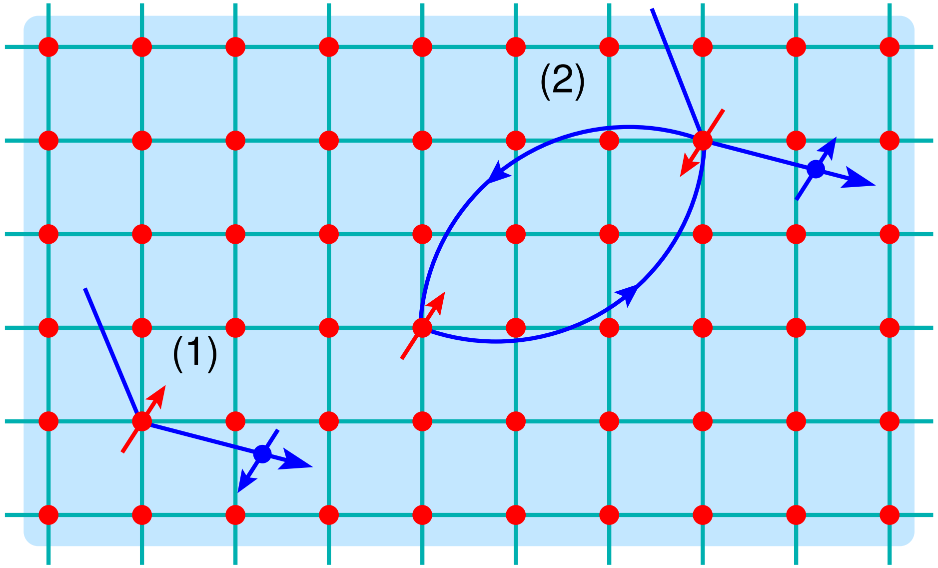
RG with RKKY interaction

Renormalization of the total conduction electron–local spin vertex Γ_{cf}

Multi-impurity Kondo system:

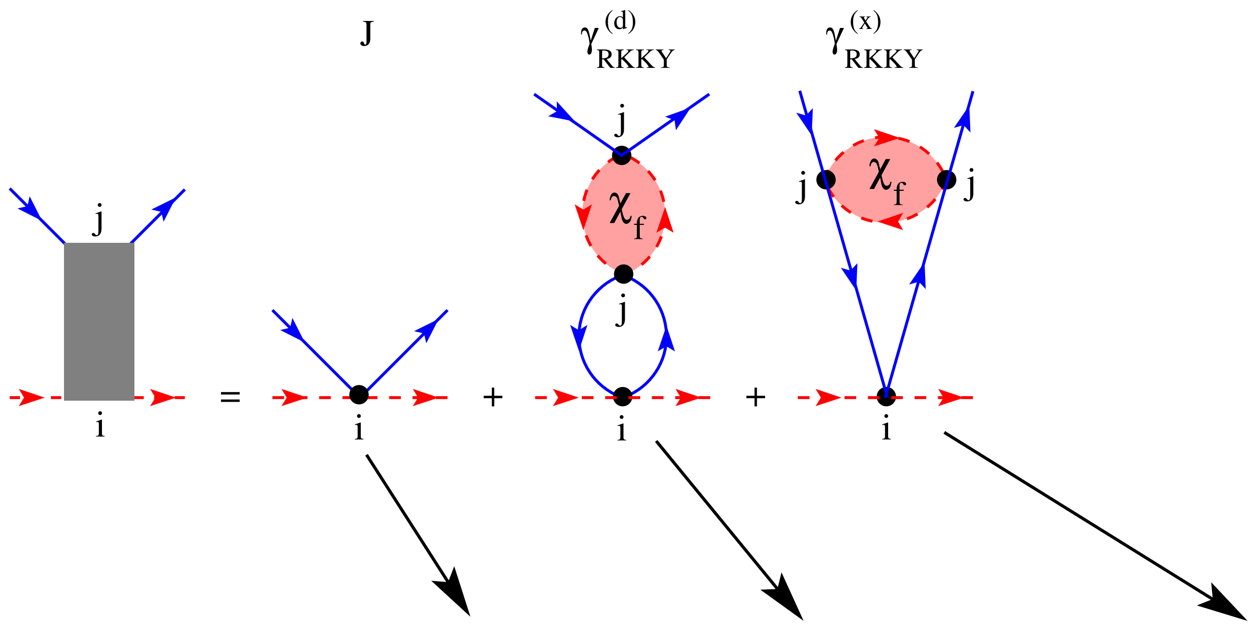
Γ_{cf} is strictly local in the f-spin coordinate,
but acquires non-local contributions in the c-electron coordinate
via RKKY interaction with surrounding spins.

The RKKY f-spin – f-spin vertex has no RG flow.



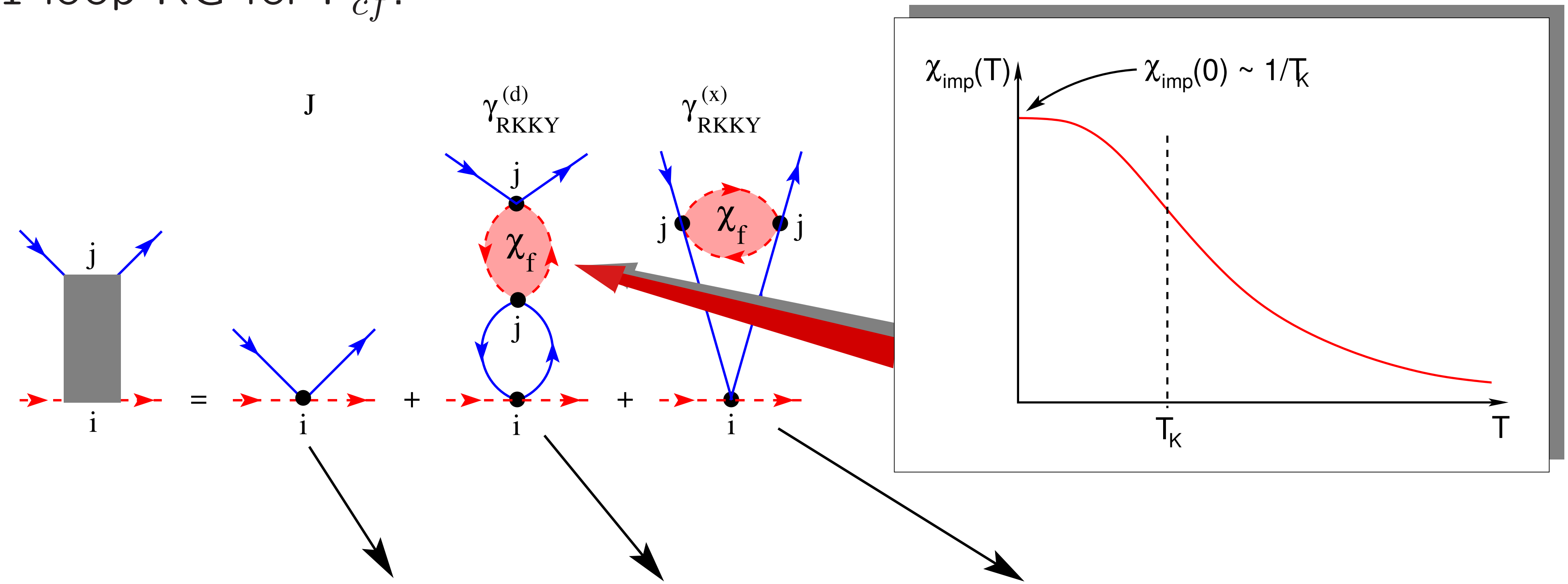
– Lattice coherence
– Critical OP fluctuations
to be included later.

1-loop RG for Γ_{cf}:



$$\hat{\Gamma}_{fc}(\mathbf{x}_i, \mathbf{x}_j, i\Omega) = \left[J\delta_{ij} + \gamma^{(d)}_{RKKY}(\mathbf{r}_{ji}, i\Omega) + \gamma^{(x)}_{RKKY}(\mathbf{r}_{ji}, i\Omega) \right] \mathbf{S}(\mathbf{x}_i) \cdot \mathbf{s}(\mathbf{x}_j)$$

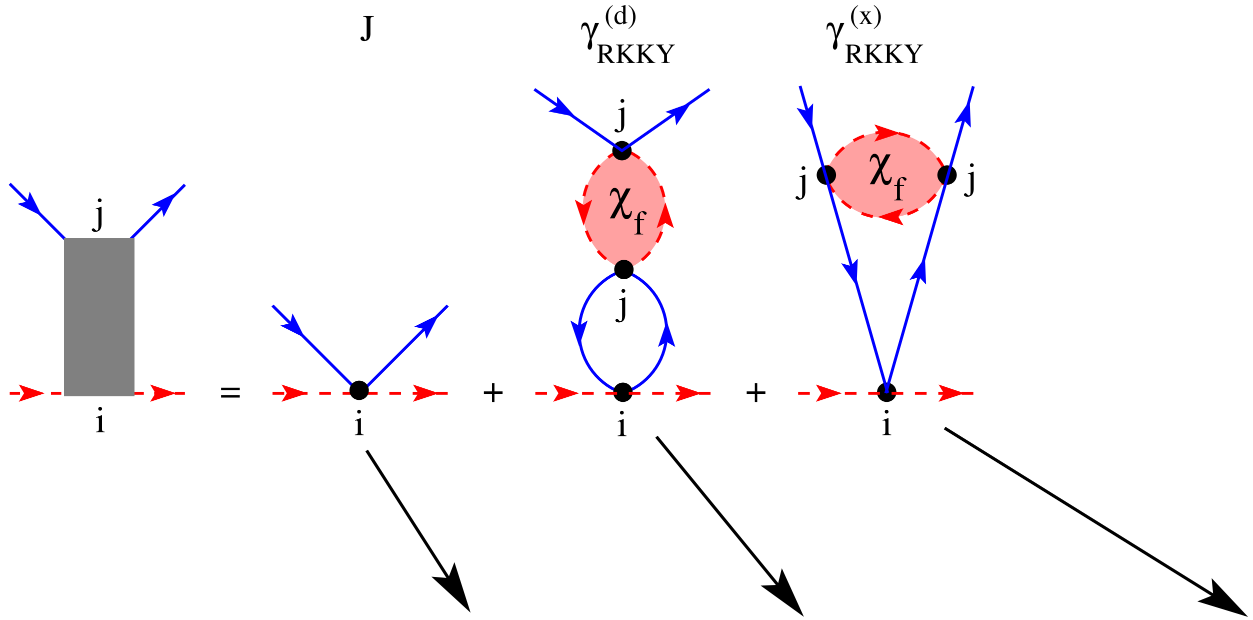
1-loop RG for Γ_{cf}:



$$\hat{\Gamma}_{fc}(\mathbf{x}_i, \mathbf{x}_j, i\Omega) = \left[J\delta_{ij} + \gamma^{(d)}_{RKKY}(\mathbf{r}_{ji}, i\Omega) + \gamma^{(x)}_{RKKY}(\mathbf{r}_{ji}, i\Omega) \right] \mathbf{S}(\mathbf{x}_i) \cdot \mathbf{s}(\mathbf{x}_j)$$

$$\chi_f(\Omega \pm i0) = \frac{(g_L \mu_B)^2 W}{\pi T_K} \frac{1}{\sqrt{1 + (\Omega/T_K)^2}} \left(1 \pm \frac{2i}{\pi} \text{arsinh} \frac{\Omega}{T_K} \right)$$

1-loop RG for Γ_{cf}:



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RG with RKKY interaction

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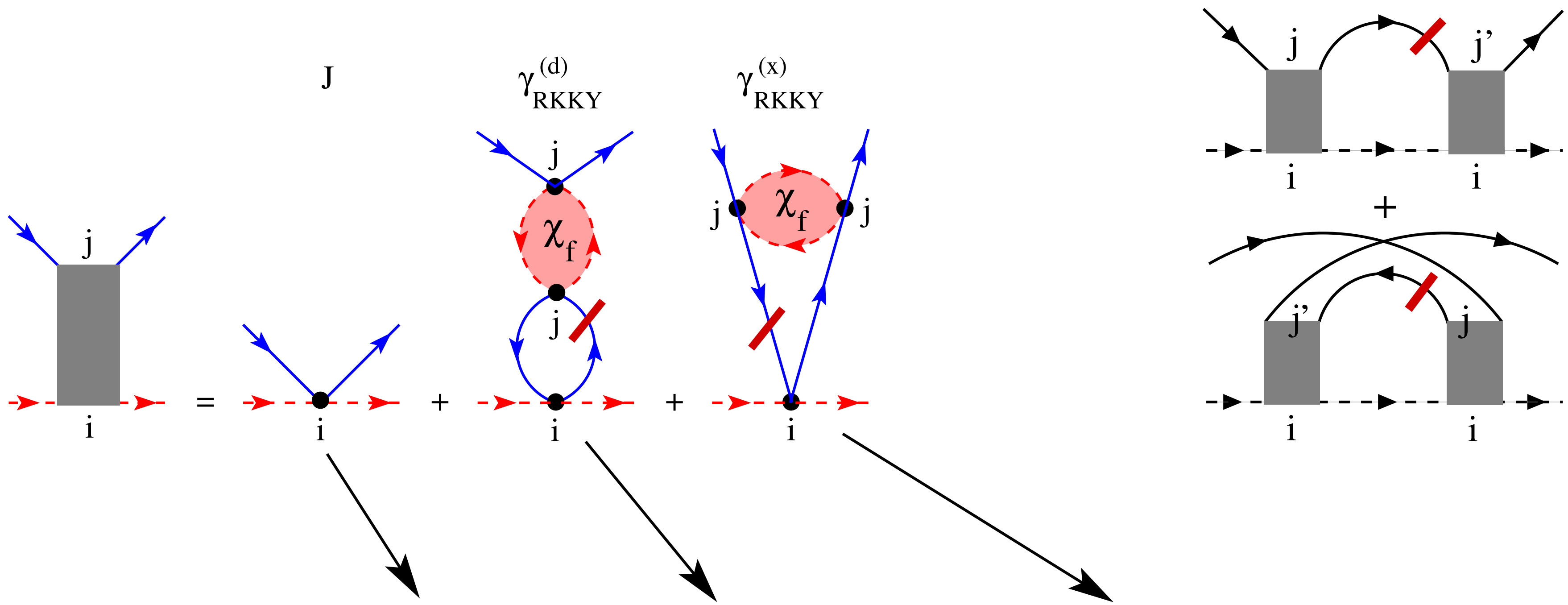
1-loop RG for Γ_{cf}:



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RG with RKKY interaction

RG equation:

$$\frac{\mathrm{d}g}{\mathrm{d}\ln D} = -2g^2 \left(1 - y\, g_0^2 \, \frac{D_0}{T_K} \frac{1}{\sqrt{1+(D/T_K)^2}}\right) \qquad g = N_0 J, \quad g_0 = N_0 J_0$$

RKKY parameter: $y = -\frac{W}{(k_F a)^3} \int_{k_F a}^{\infty} dx \; (1 - \cos x) \; \frac{x \cos x - \sin x}{x^4} > 0$

RKKY contribution perturbatively controlled, since $T_K(y)$ remains finite.

Screening scale determined selfconsistently by the divergence of the RG equation:

$$\frac{T_K(y)}{T_K(0)} = \exp\left(-y\, \alpha\, g_0^2 \, \frac{D_0}{T_K(y)}\right)$$

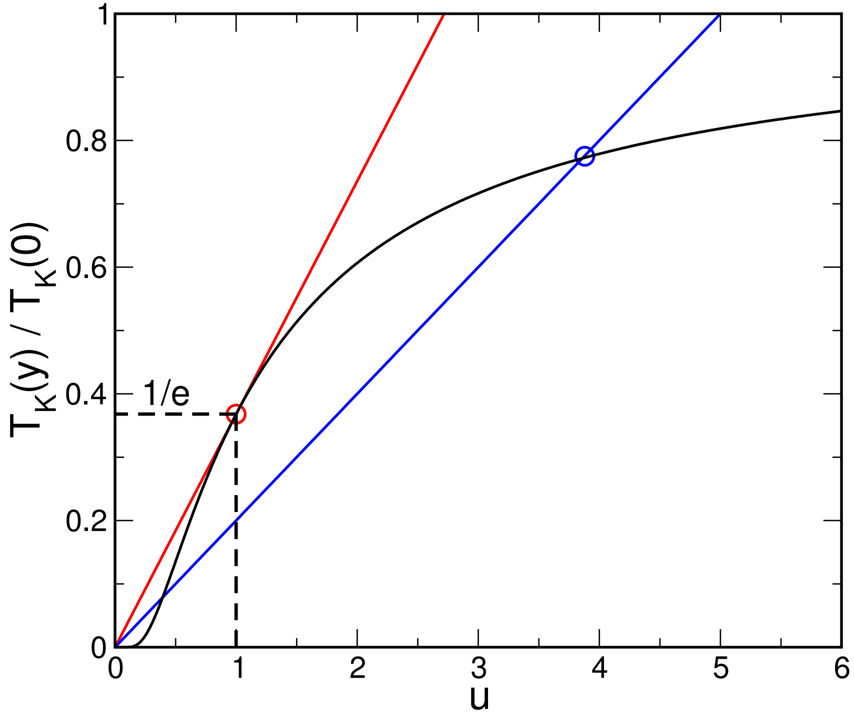
Rescaling: $u := \frac{T_K(y)}{y\,\alpha\,g_0^2\,D_0}$ $\quad s = \frac{\alpha\,g_0^2\,D_0}{T_K(0)}$

$$\frac{T_K(y)}{T_K(0)} = y\,s\,u = \exp\left(-\frac{1}{u}\right)$$

Kondo breakdown for $u = 1$

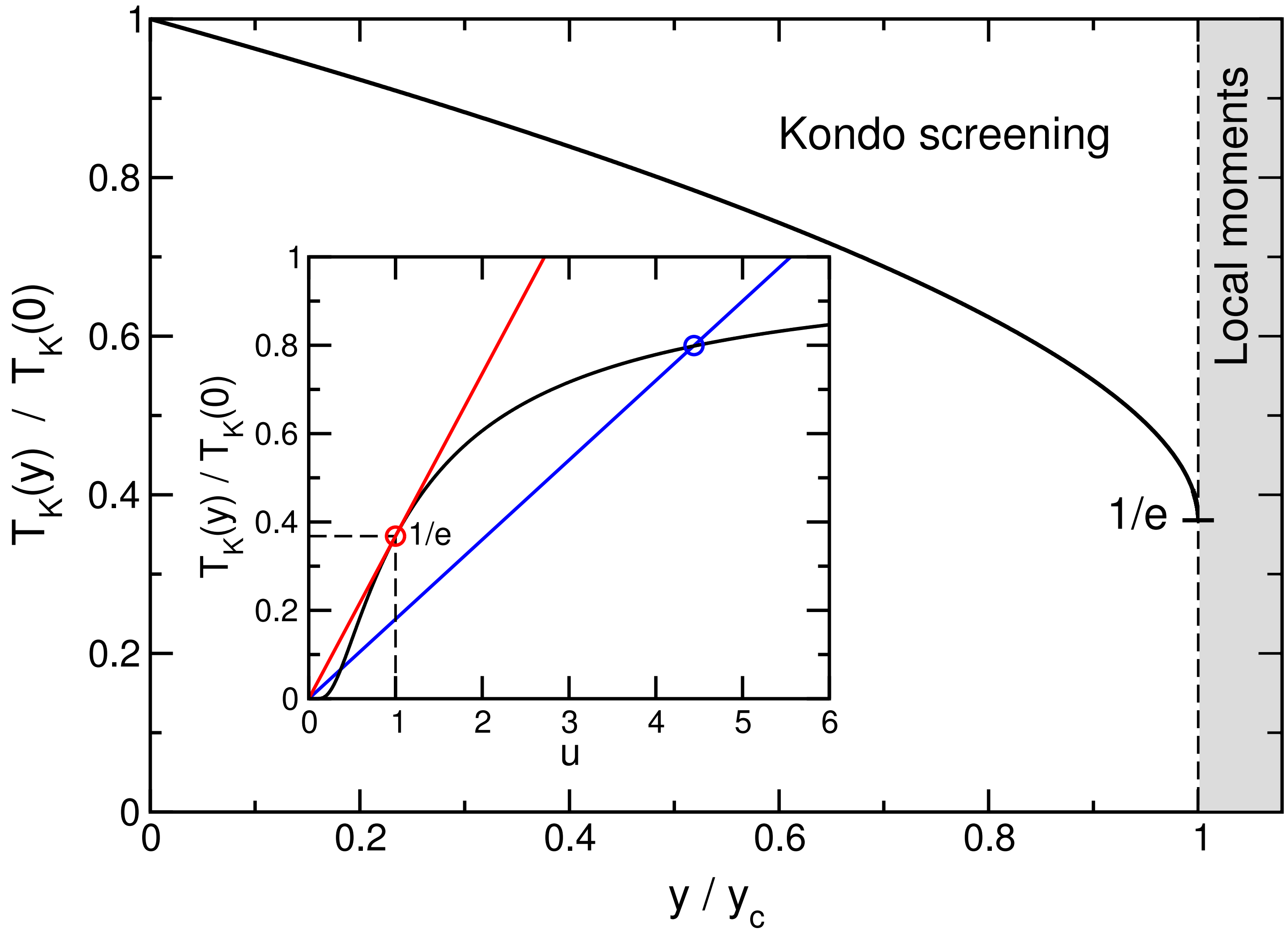
Universal breakdown ratio:

$$\frac{T_K(y_c)}{T_K(0)} = \frac{1}{e} \approx 0.368$$



- Universal ratio robust against
  - details of band structure, DoS, higher order RKKY (absorbed in y)
  - precise form of soft cutoff in χ_{cf} (absorbed in α, here: $\alpha = 2\ln(1+\sqrt{2})$).
- In presence of magnetic instability of the Fermi sea, the ratio $T_K(y_{max})/T_K(0)$ takes a smaller value, but remains finite.

RG with RKKY interaction: universality



Nejati, Ballmann, Kroha, PRL **118**, 117204 (2017); arXiv:1612.03338

Expt: Kondo destruction in a 2-impurity system

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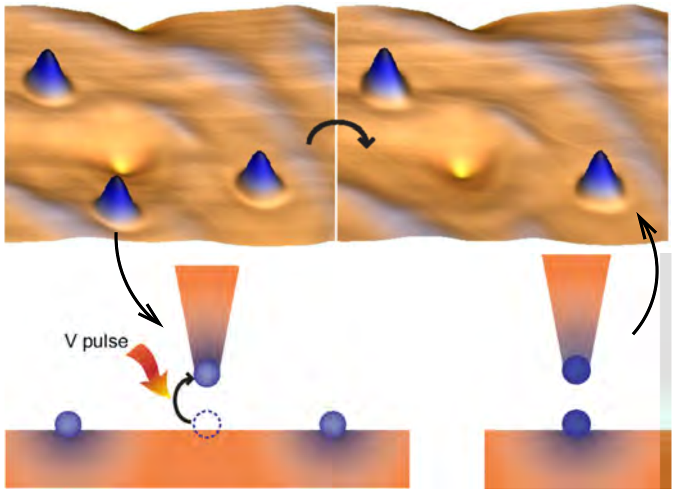
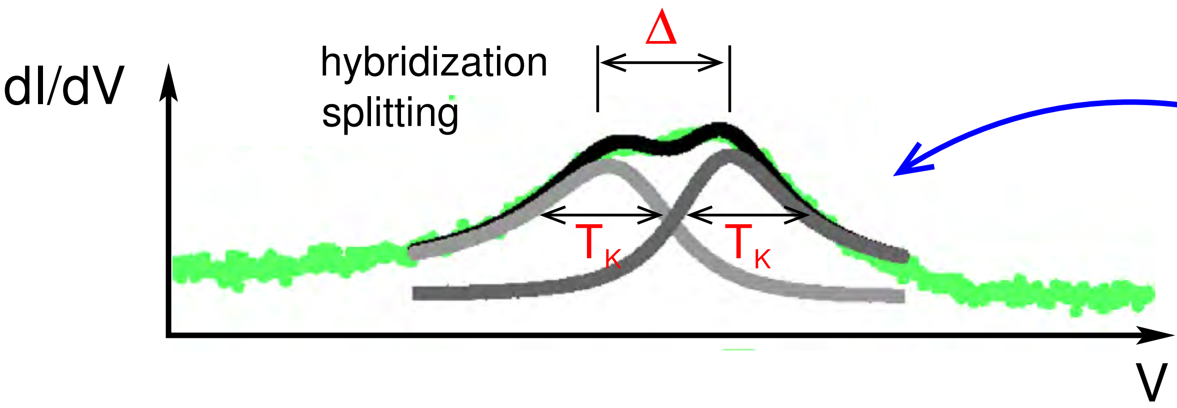
Scanning tunneling spectroscopy
on a tunable Co 2-impurity system

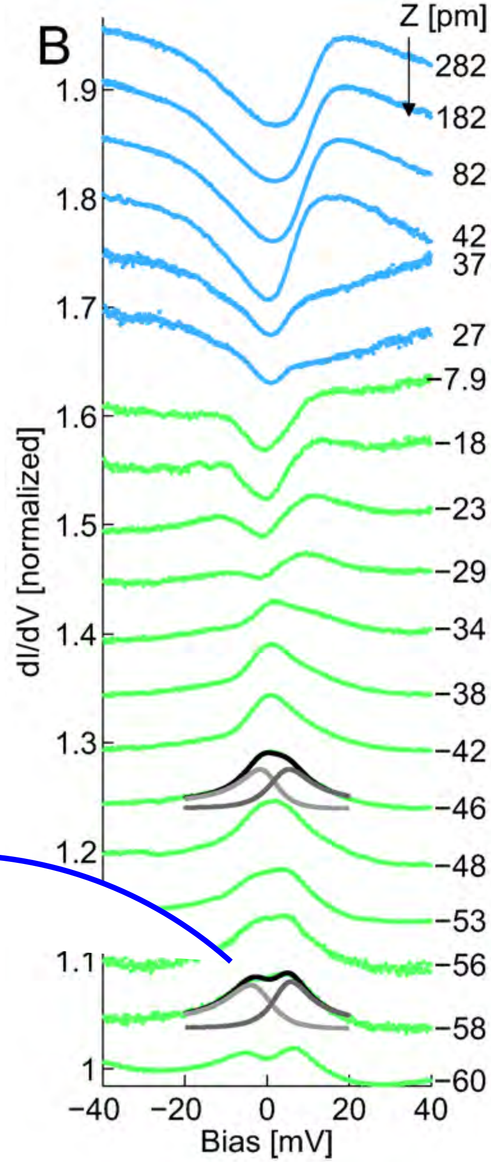


Fano fit:

$$G = A\frac{(\omega_+ + q)^2}{\omega_+^2 + 1} + A\frac{(\omega_- + q)^2}{\omega_-^2 + 1}$$

$$\omega_\pm = \frac{V \pm \Delta/2}{T_K}$$





Bork, Zhang, Diekhöner, Simon, Borda, Kroha, Wahl, Kern, Nature Phys. **7**, 901 (2011)

Ujsághy, Kroha, Szunyogh, Zawadowski, PRL **85**, 2557 (2000)

Expt: Kondo destruction in a 2-impurity system

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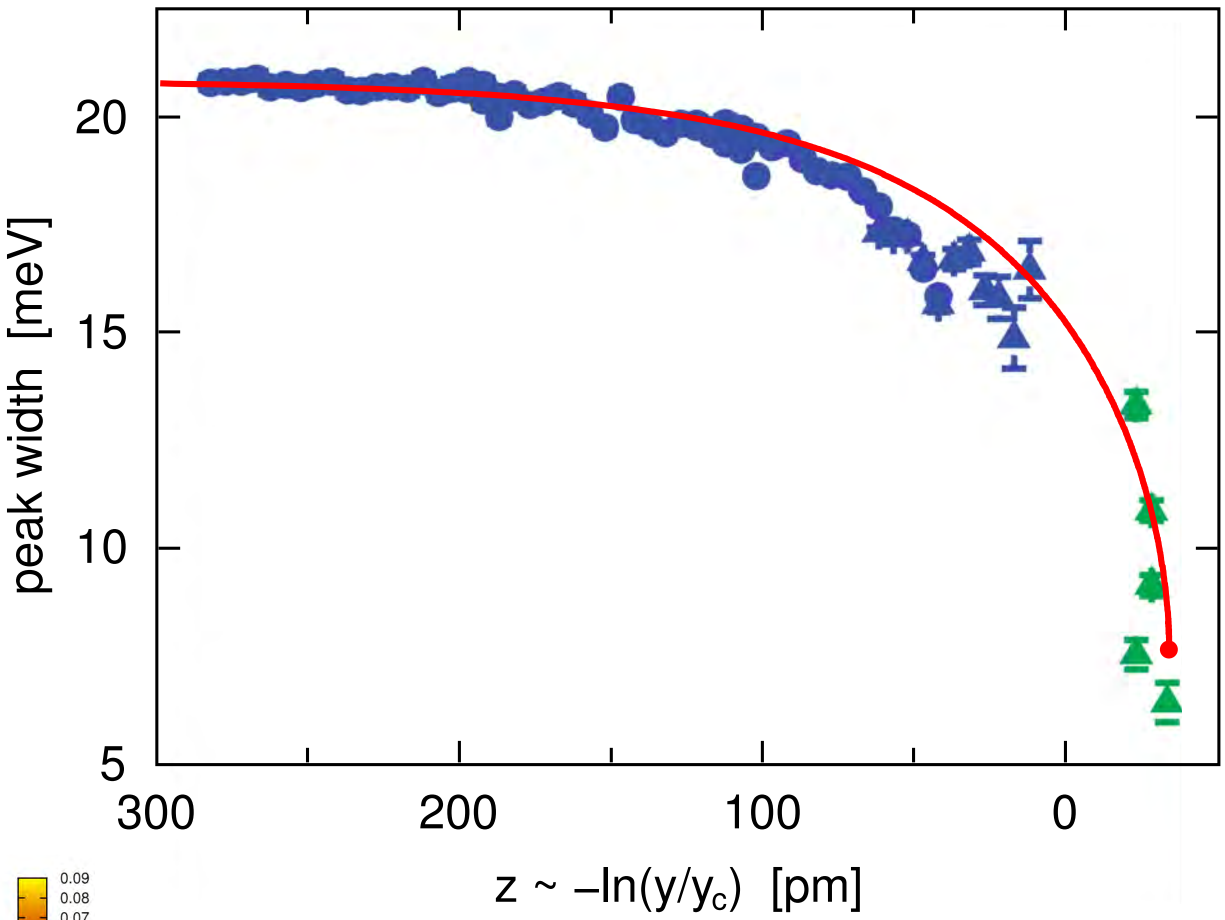

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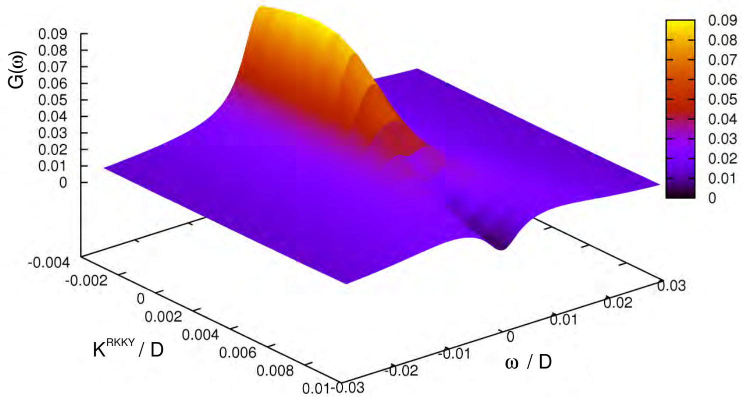


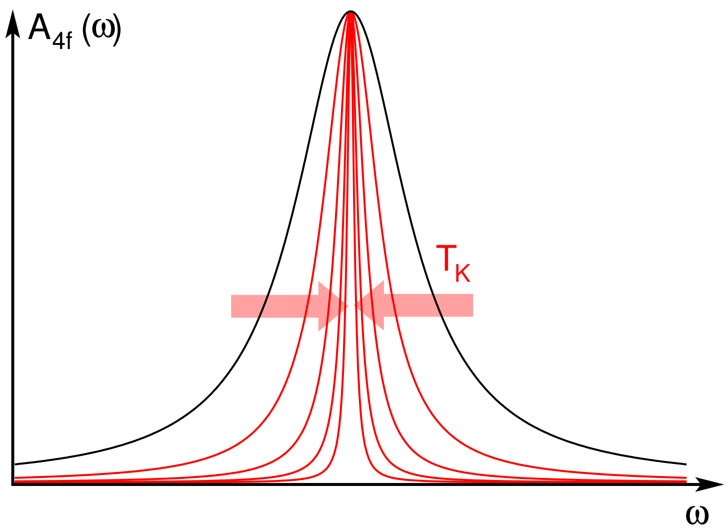
NRG: RKKY-splitting of Kondo resonance

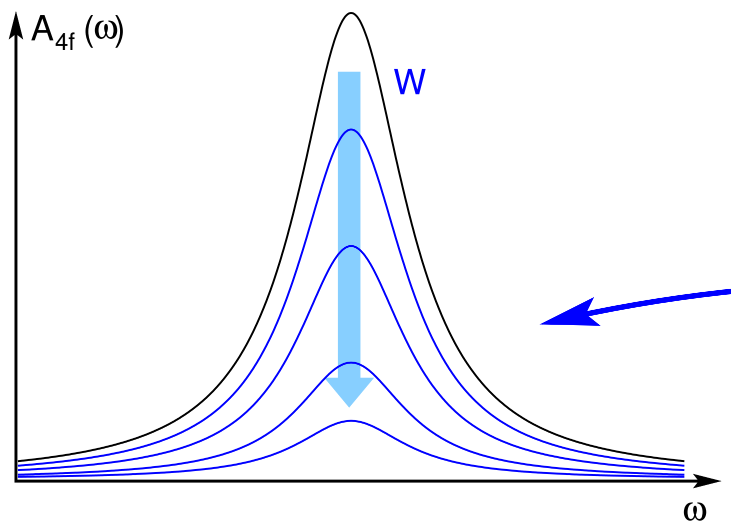
(L. Borda)

Possible RKKY-induced QC scenario

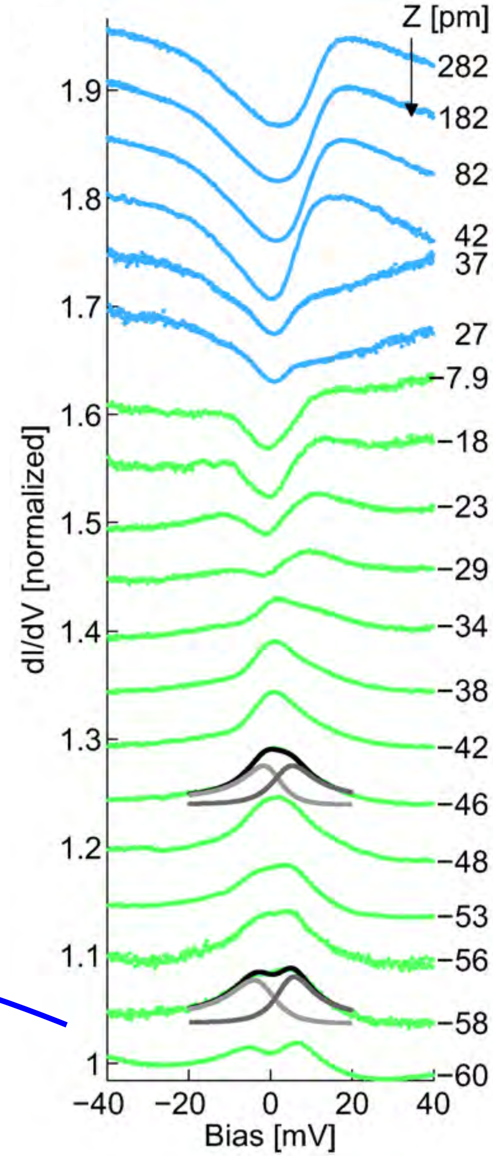
Kondo resonance destruction

$W \to 0$ compatible with ω/T scaling





$$A_{4f}(\omega) = \frac{W \; T_K^2}{\omega^2 + T_K^2}$$



Conclusions

RG for Kondo screening and break-down in presence of RKKY interaction.

- Kondo breakdown even without magnetic ordering.

  Universal break-down ratio $T_K(y_{max})/T_K(0) = 1/e$,

  robust against non-critical perturbations.

- The selfconsistent treatment of all Kondo sites is reminiscent of a DMFT, but includes long-range RKKY interaction.

- Mathematical definition of the Kondo lattice temperature $T_K(y)$.

- Further work:
  - Apply methods that allow calculating spectral functions (NRG) to the selfconsistent scheme.
  - Include magnetic ordering instability by constructing effective Heisenberg model of residual moments in the ordered phase.

Thanks!

Uni Bonn

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