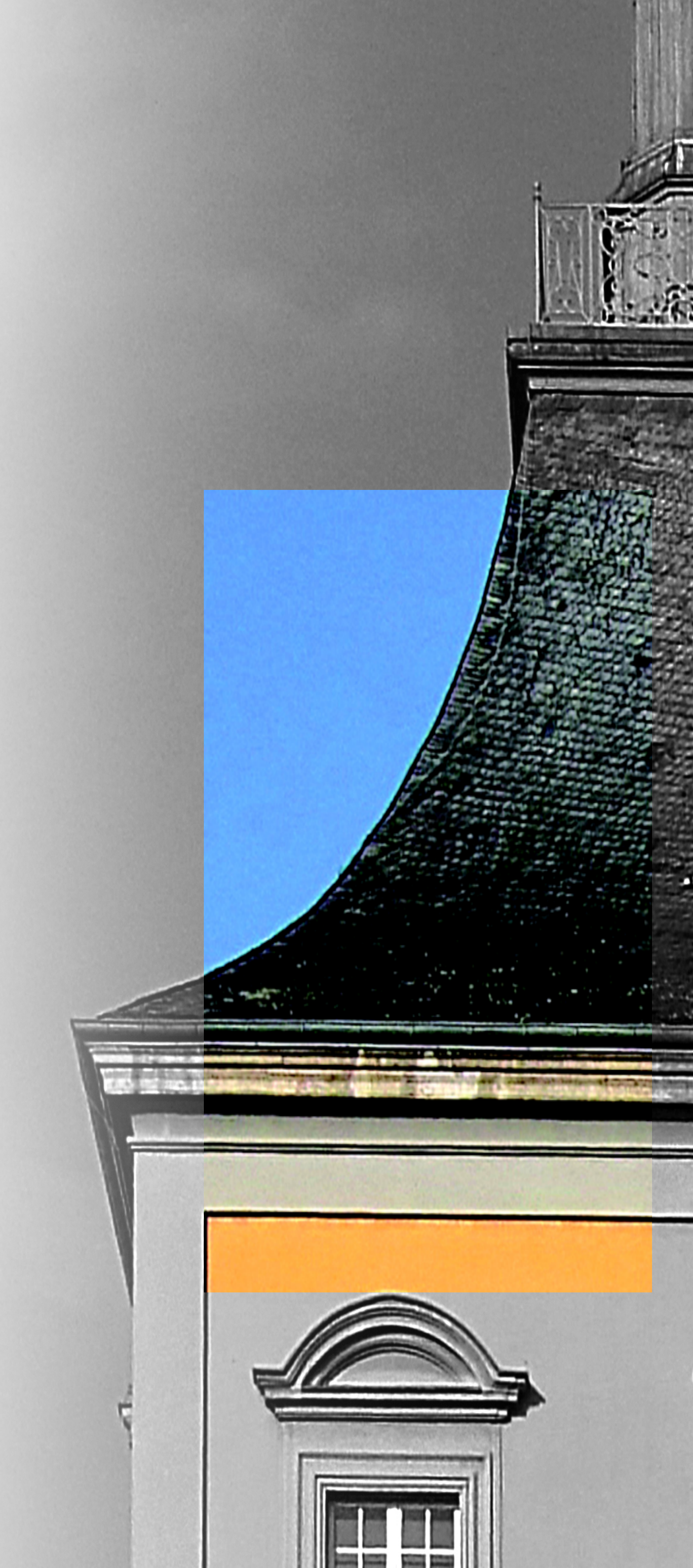
Heavy-Fermion Systems and Some *Exotic* Examples

Marvin Lenk (AG Kroha)

CMT Journal Club Kickoff Meeting
19 Oct 2022 – Bonn



Outline

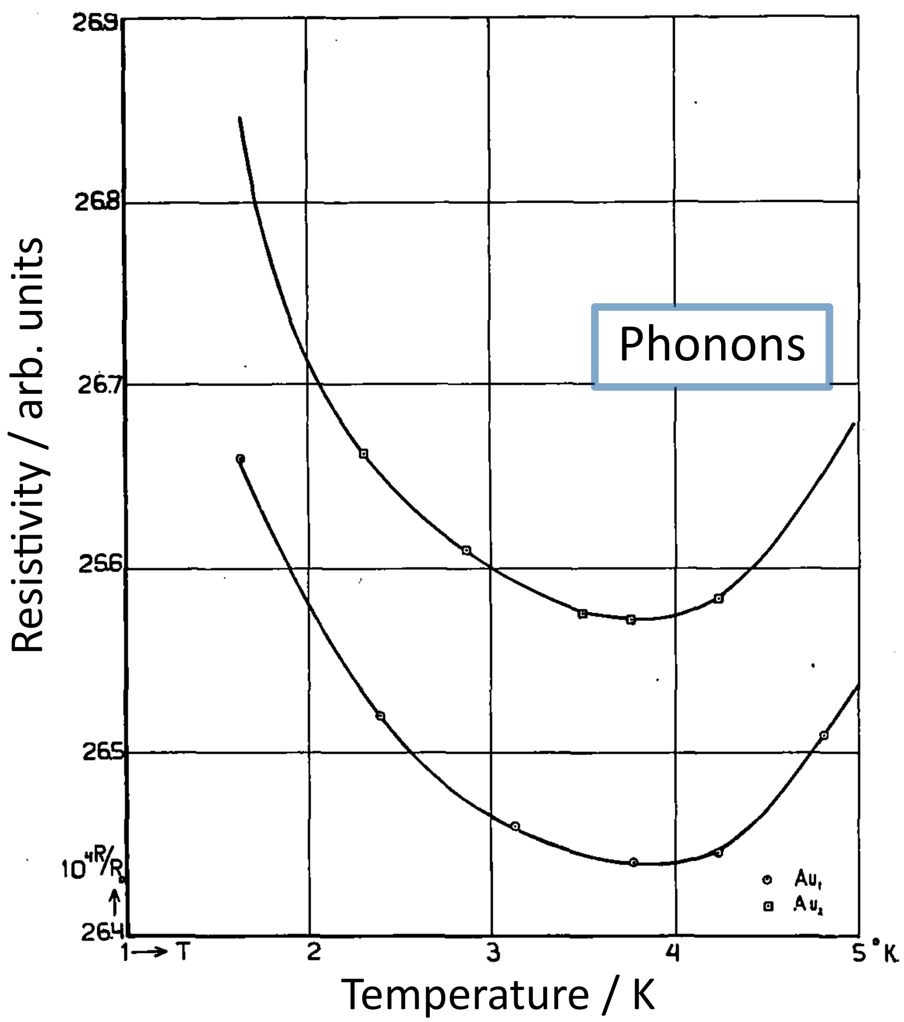
1. Single impurity physics

2. Lattice impurity physics

3. Solving impurity systems

4. Selected research results

The Kondo effect



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Physica 1.7-12 (1934), pp. 1115–1124

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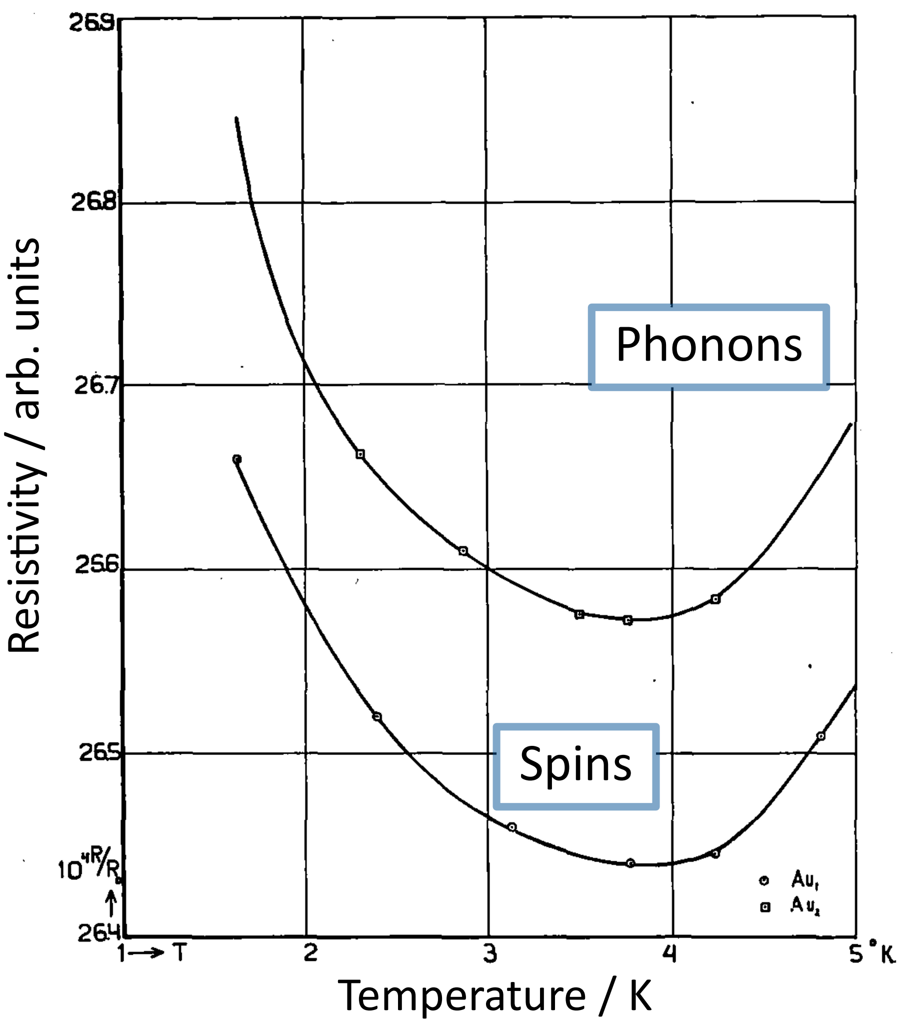

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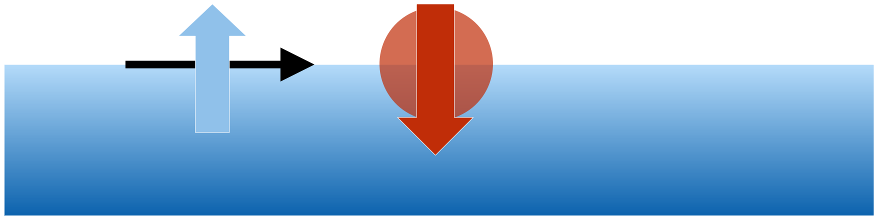

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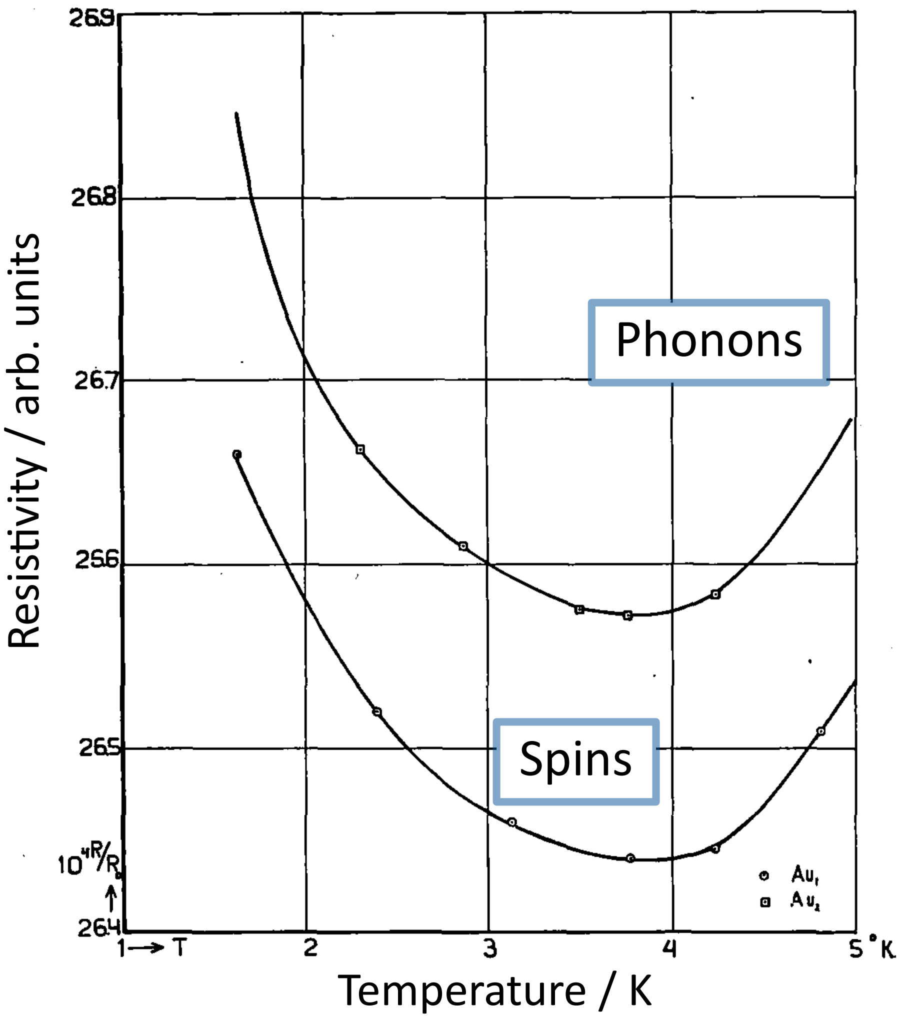

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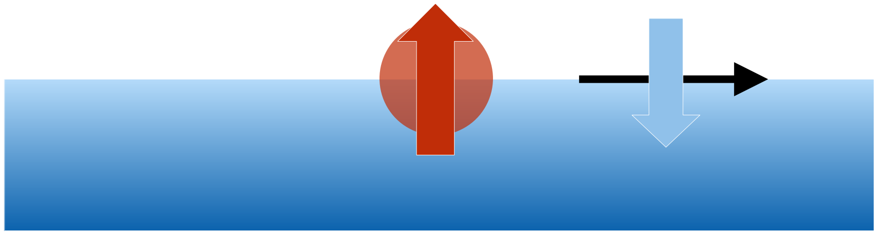

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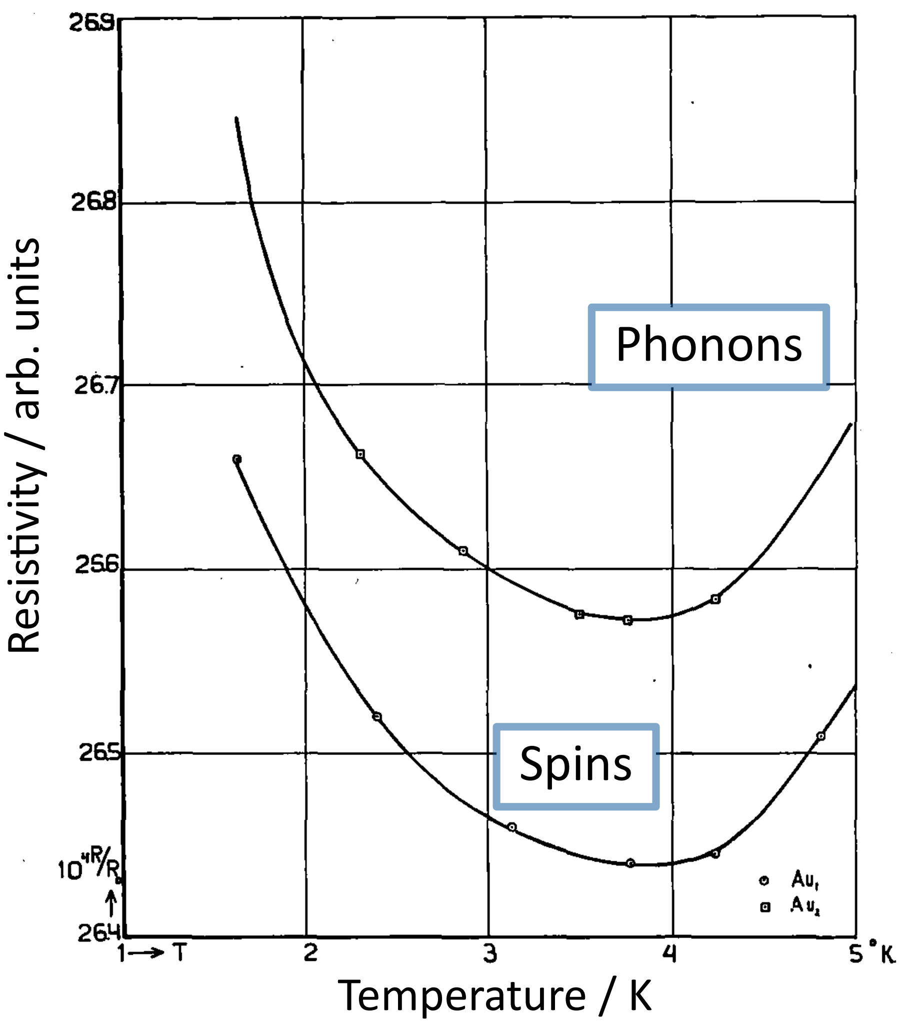

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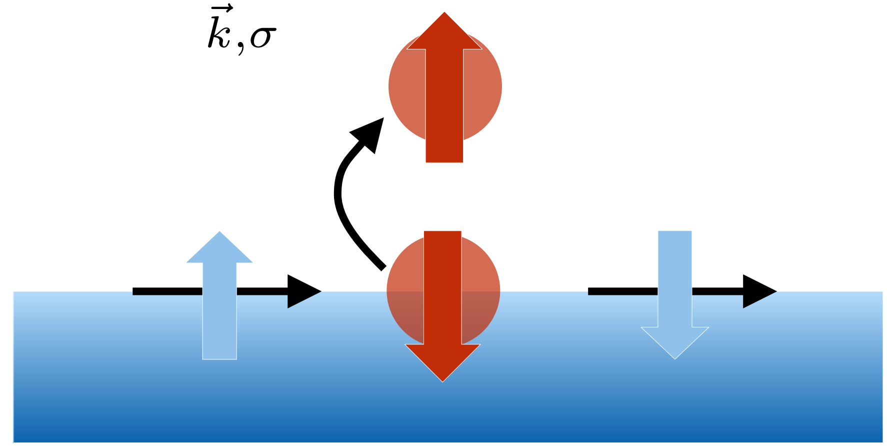

$$J(T) = J_0 \left[1 - 2J_0 \rho(\epsilon_F) \ln(T/D)\right]$$

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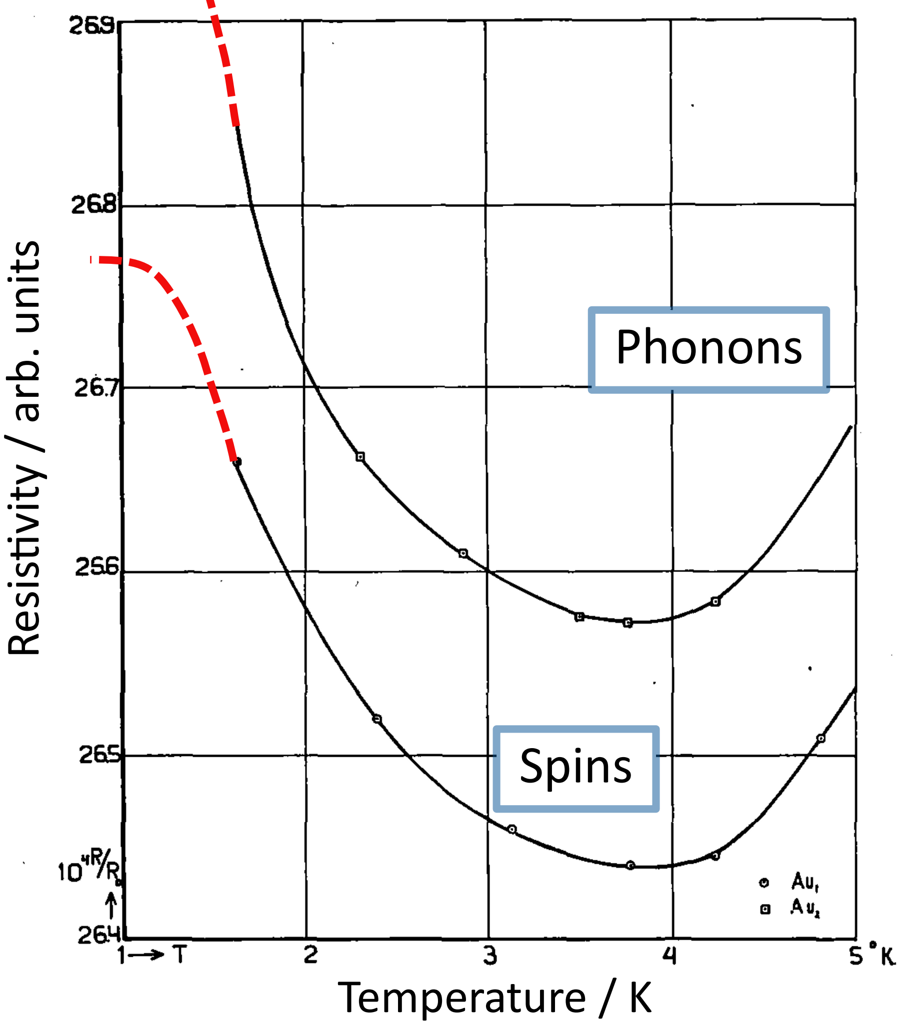

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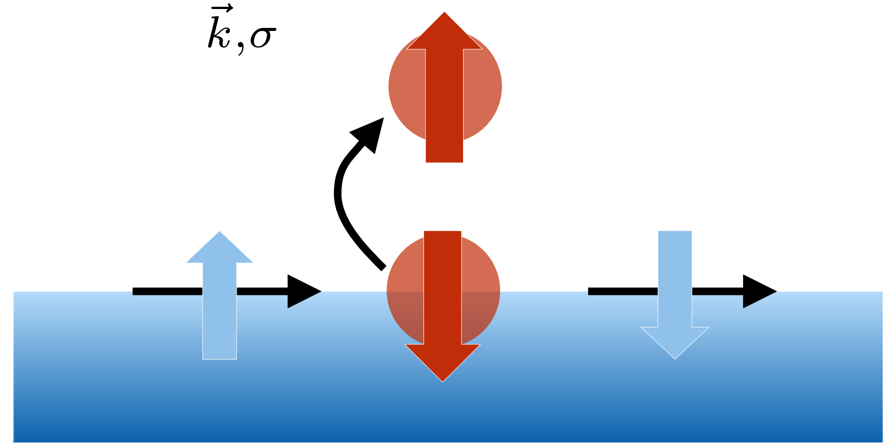
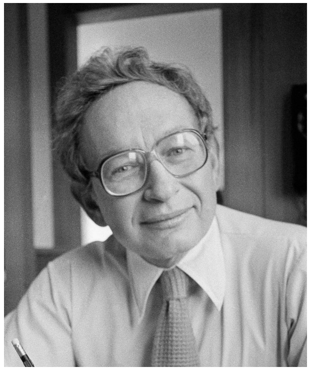


$$J(T) = J_0 \left[1 - 2J_0 \rho(\epsilon_F) \ln(T/D)\right]$$

$$T_K = D e^{-\frac{1}{2\rho(\epsilon_F)} J_0}$$



Phil Anderson (1961)

„Localized Magnetic States in Metals“

$$\hat{H}_c = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma}$$

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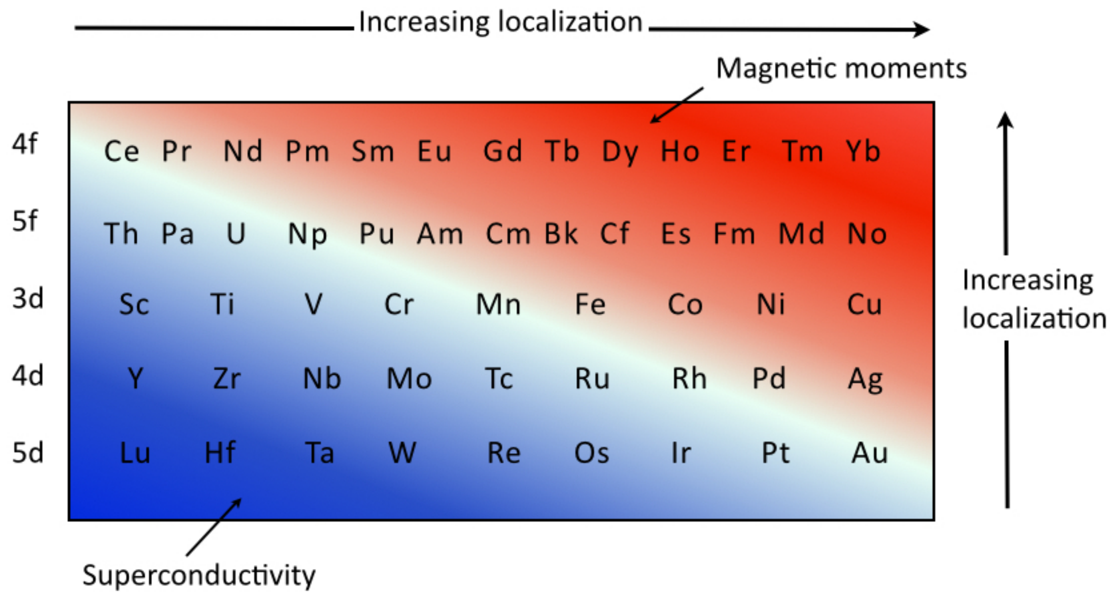

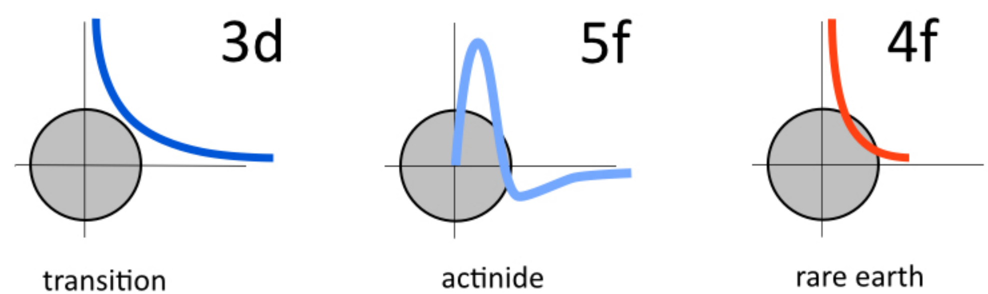

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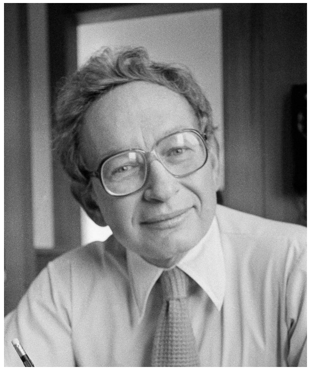
Anderson's Impurity Model



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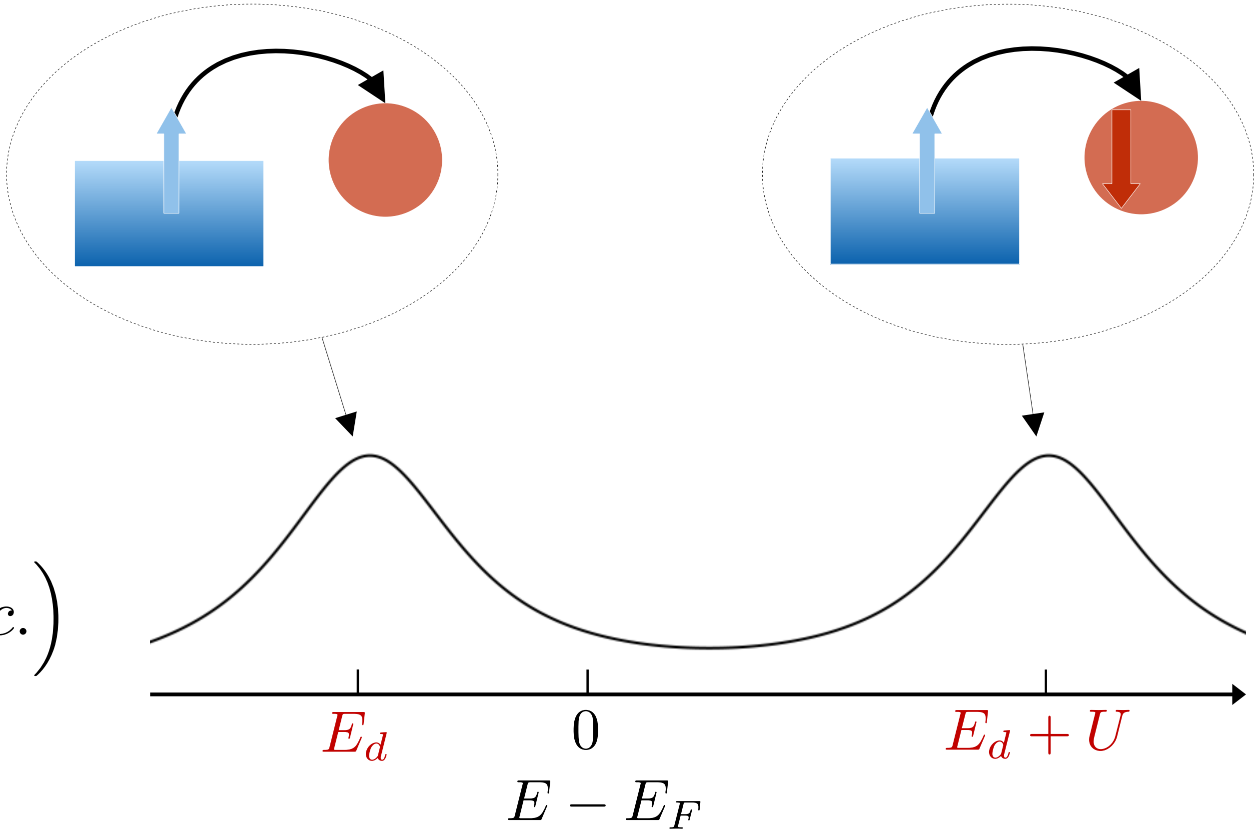
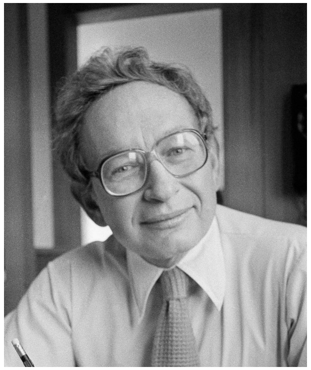
<u>Impurity density of states (sketch)</u>





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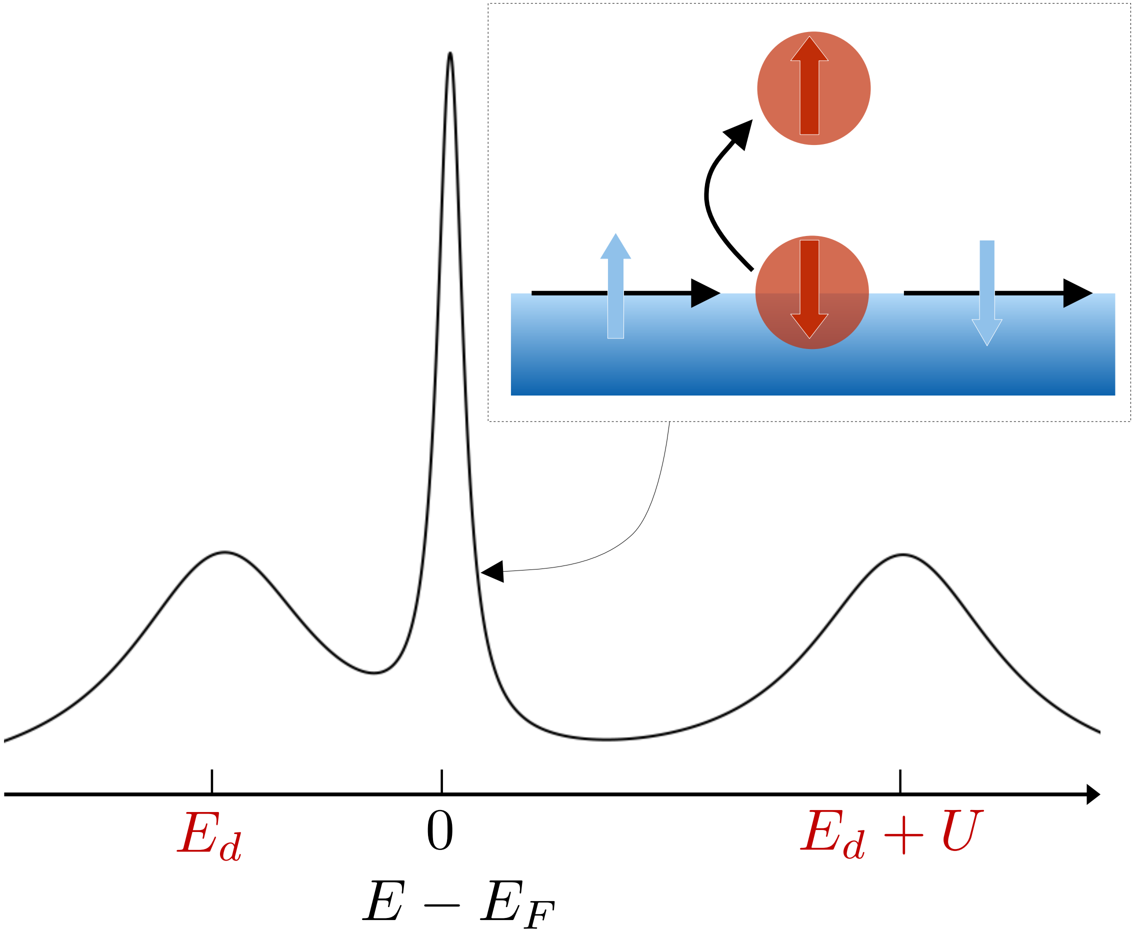

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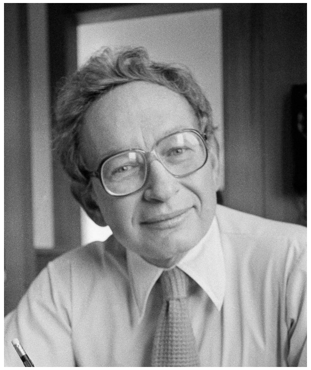

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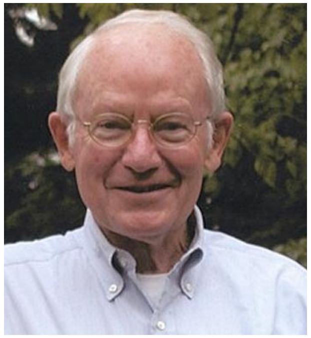
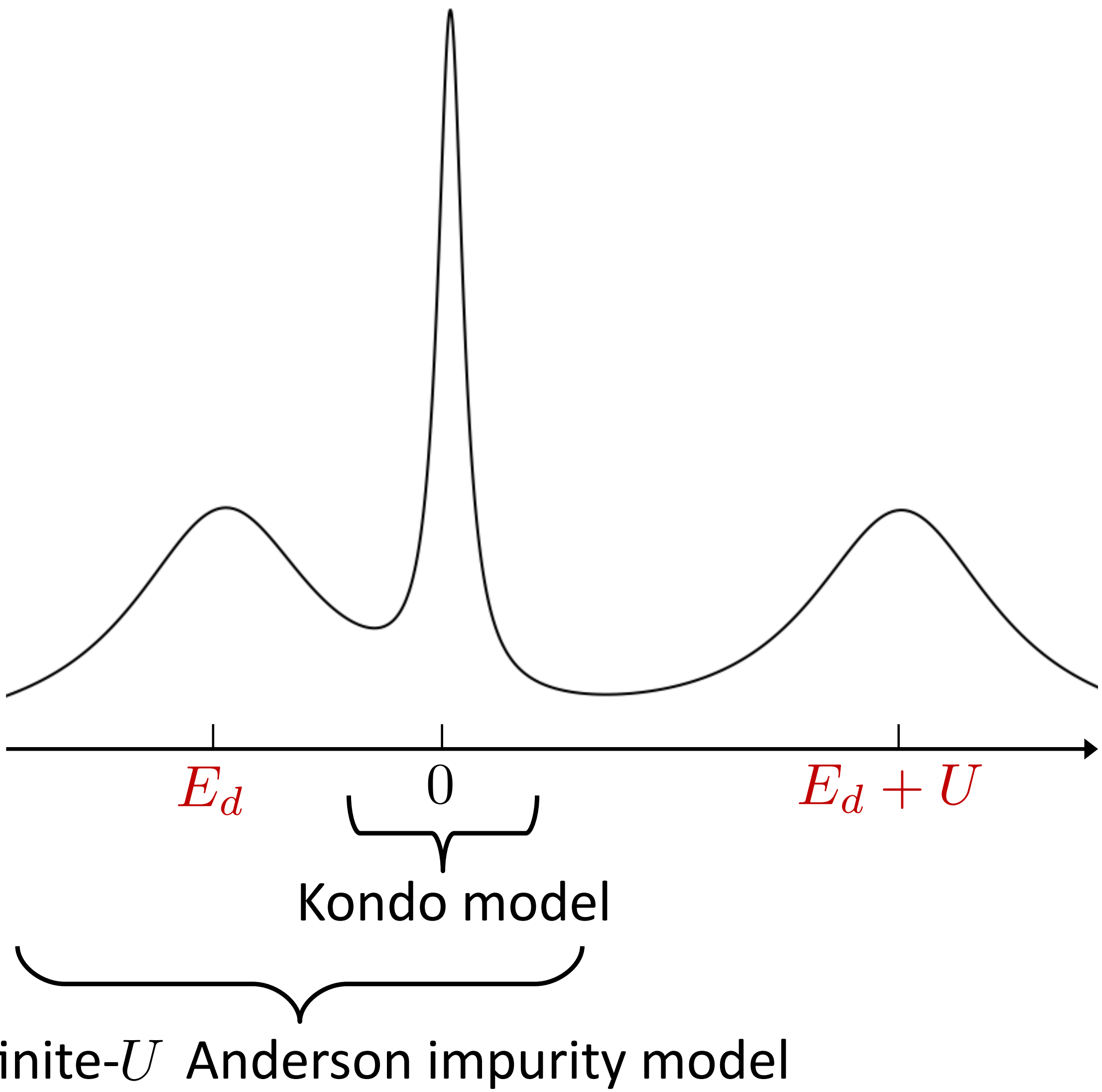


John Schrieffer
Peter Wolff
(1966)

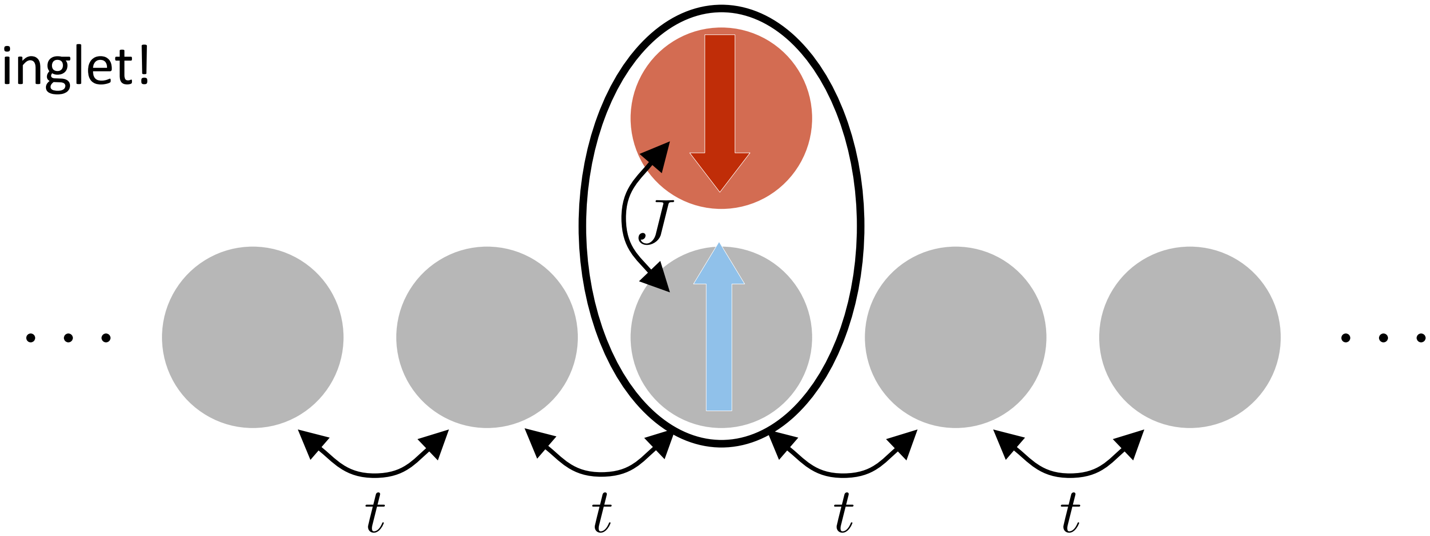
„Relation between the Anderson and Kondo Hamiltonians“

Impurity density of states (sketch)



Kondo model: strong antiferromagnetic coupling at $T = 0$.

Ground state is spin singlet!



Philippe Nozières (1974)

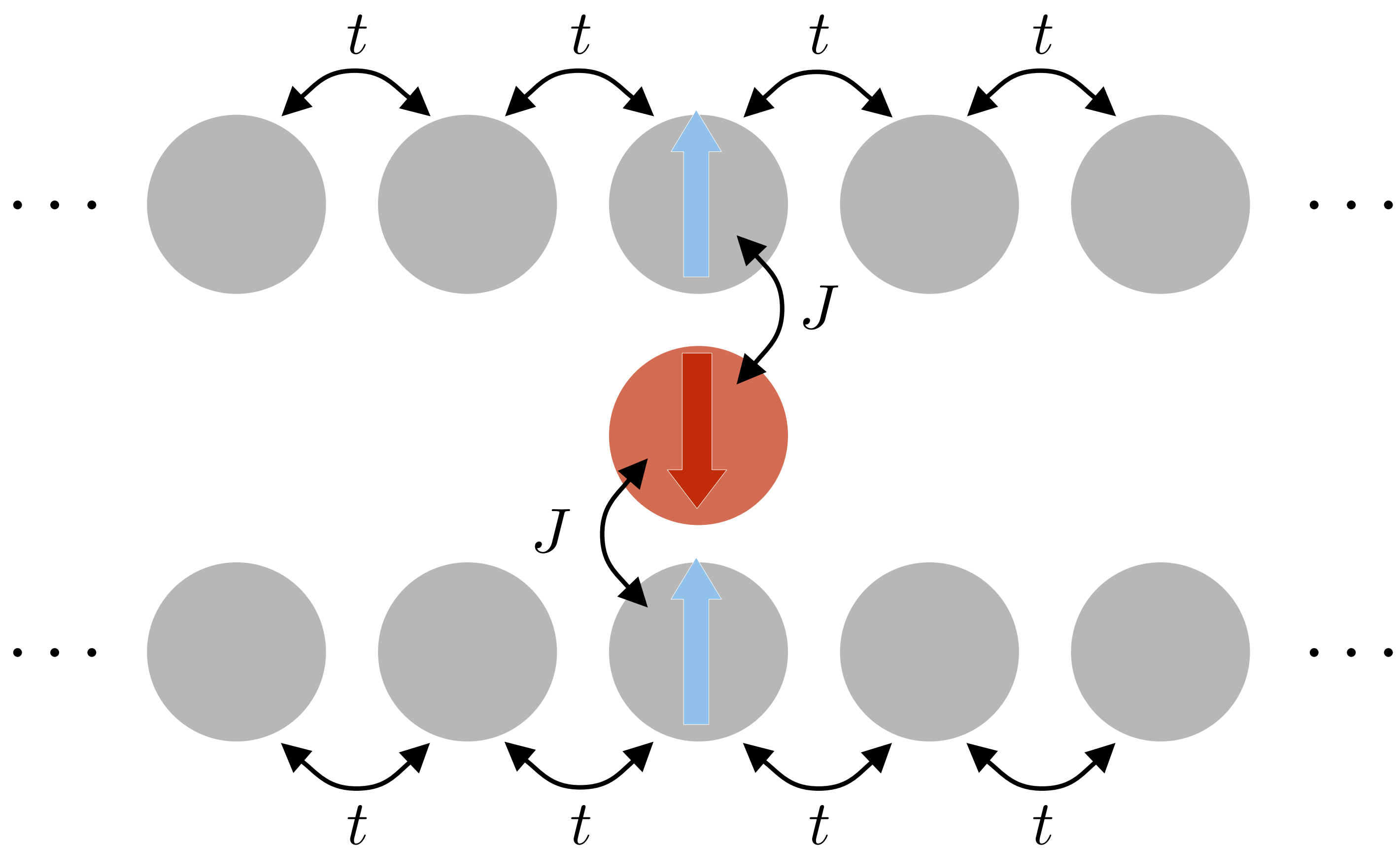
Ground state of the Kondo model gives rise to Landau Fermi-liquid.

Why? Hopping is a small perturbation to the singlet ground state, giving rise to Landau quasi-particles in a straightforward way.

Is there a situation in which this is **not** the case?

Ground States and *Exotic* Effects

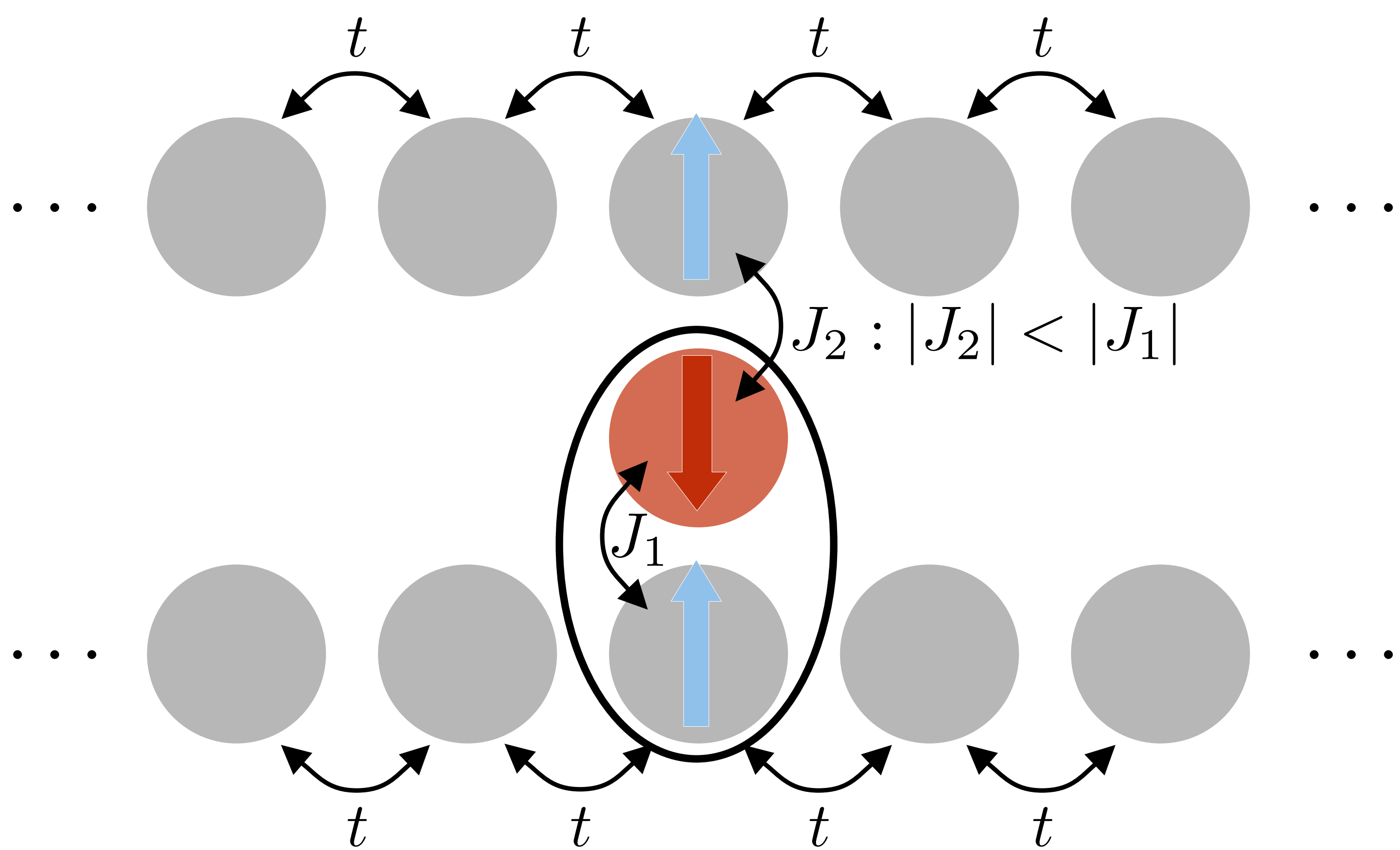
Consider a case, where the impurity is getting screened by two channels.



What is the ground state? It will be degenerate!
The formation of a FL is not possible anymore.

Ground States and *Exotic* Effects

Multi-channel Kondo systems are rare, the slightest asymmetry leads to one channel dominating the ground state.



Channel degree of freedom **must** be conserved in the scattering process.
Real-life realization: Quadrupolar Kondo systems.

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2. **Lattice impurity physics**

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Kondo Insulators: More *Exotic* Effects

The SIAM can be extended to a lattice of impurities.

$$\hat{H}_{\mathrm{PAM}} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} + \sum_{i,\sigma} E_d \hat{d}^{\dagger}_{i\sigma} \hat{d}_{i\sigma} + \sum_{i} U \hat{n}^{d}_{i\uparrow} i \hat{n}^{d}_{\downarrow}$$

$$+ \sum_{i,\mathbf{k},\sigma} \left(V_{i\mathbf{k}} e^{i\mathbf{k}\mathbf{x}_i} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{d}_{i\sigma} + h.c. \right)$$

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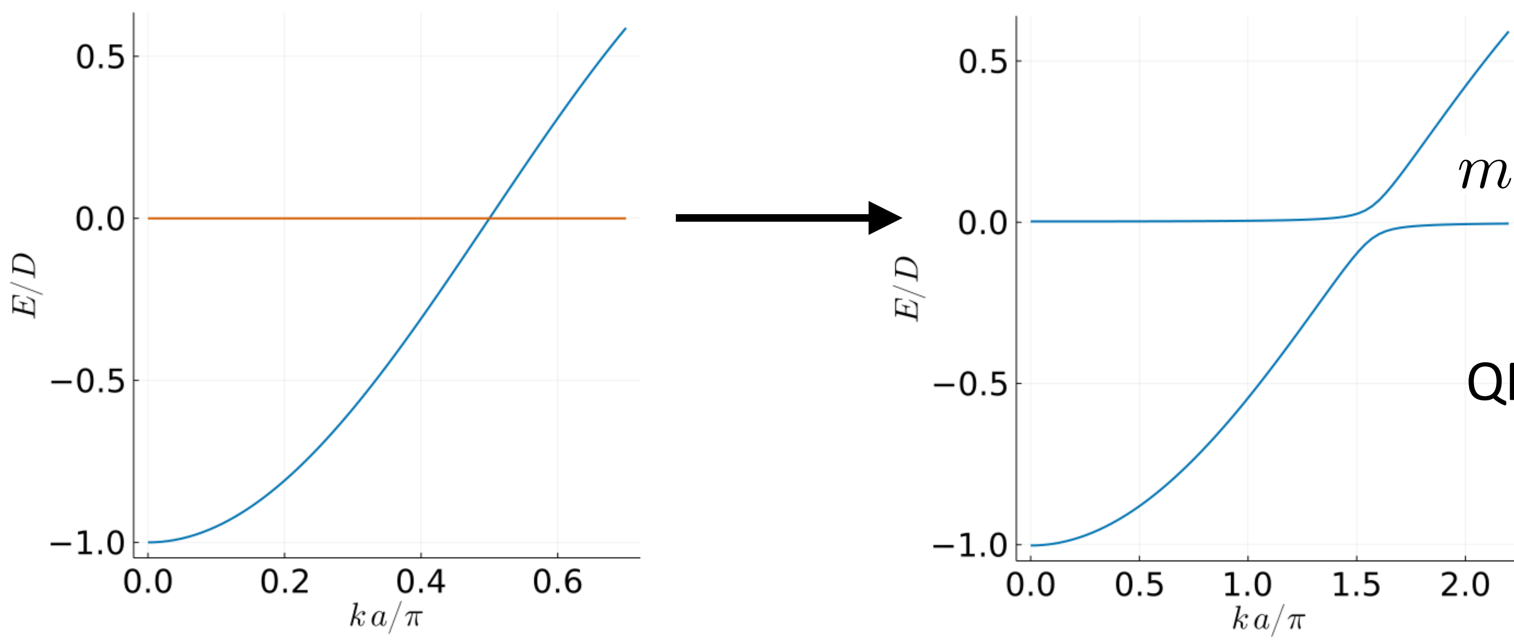
Impurities can now form multiple singlets, potentially a flat band (coherence!).



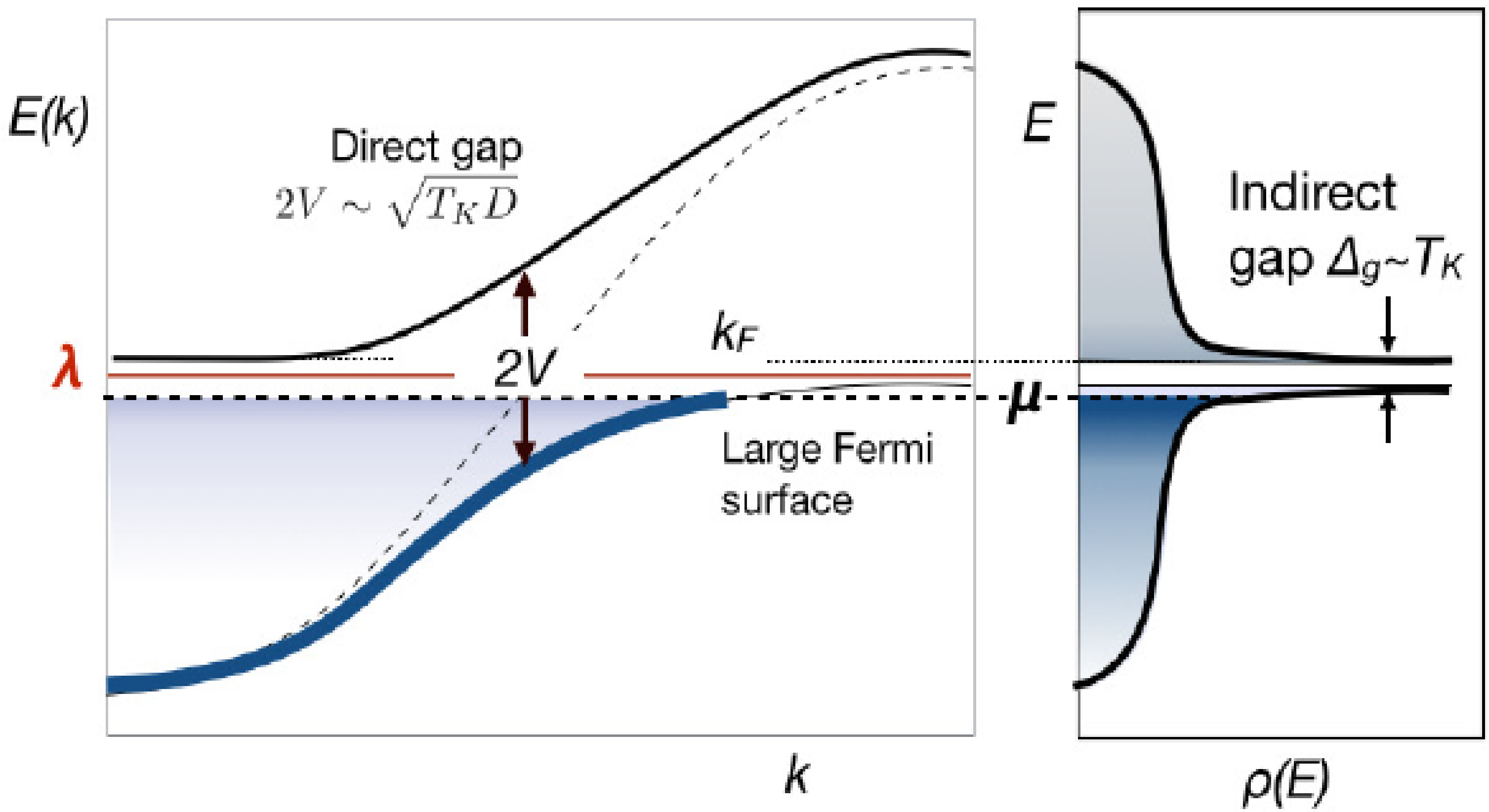
$m^* \approx 10^2 \ldots 10^3\, m_e$

QP binding energy

$\sim T_K \ll D$

Kondo Insulators: More *Exotic* Effects

This effect can fully deplete the Fermi-edge at low temperatures, leading to a narrow-gap Kondo insulator.



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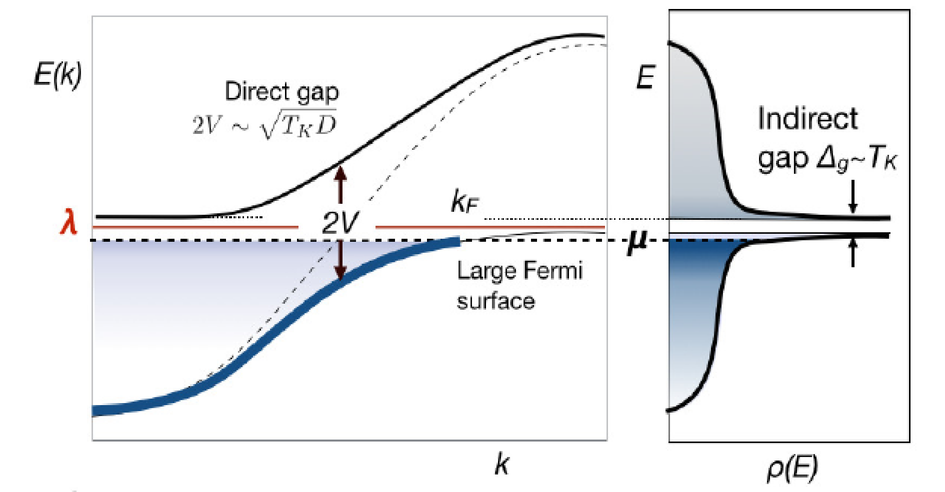
Kondo insulator:

Hybridization opens gap.



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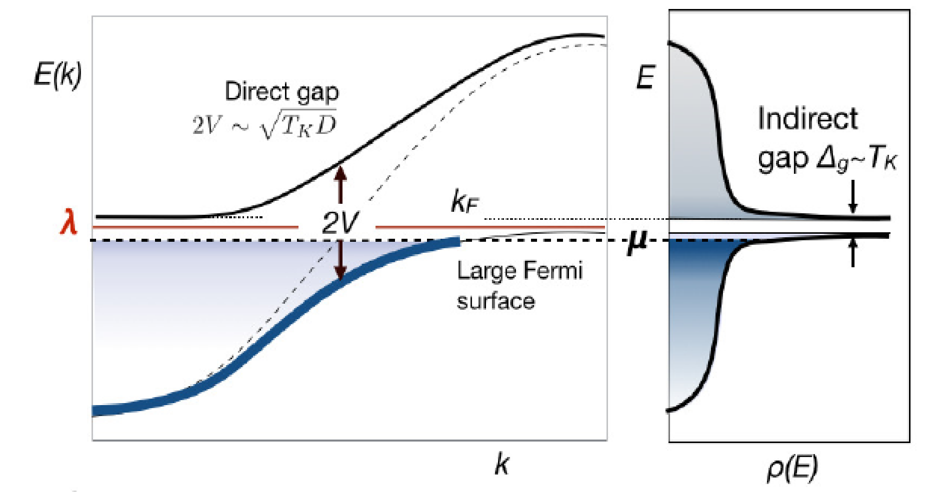

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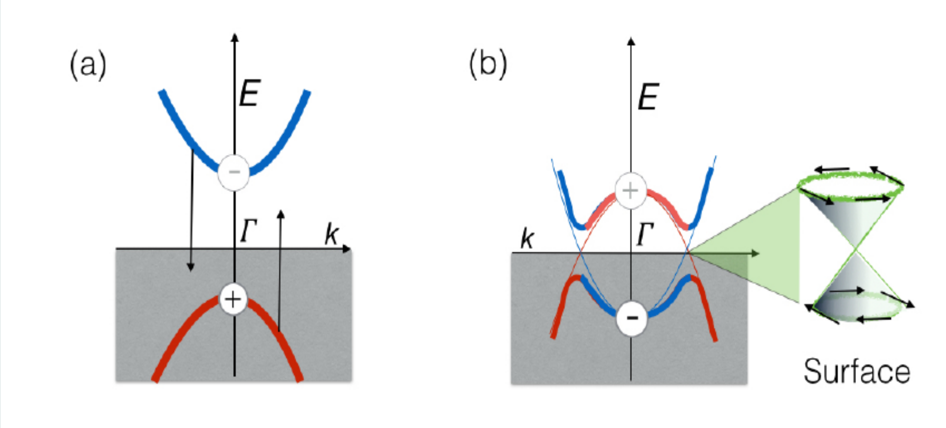
Topological insulator:

Two bands with opposite parity.
Band inversion → bulk insulator.



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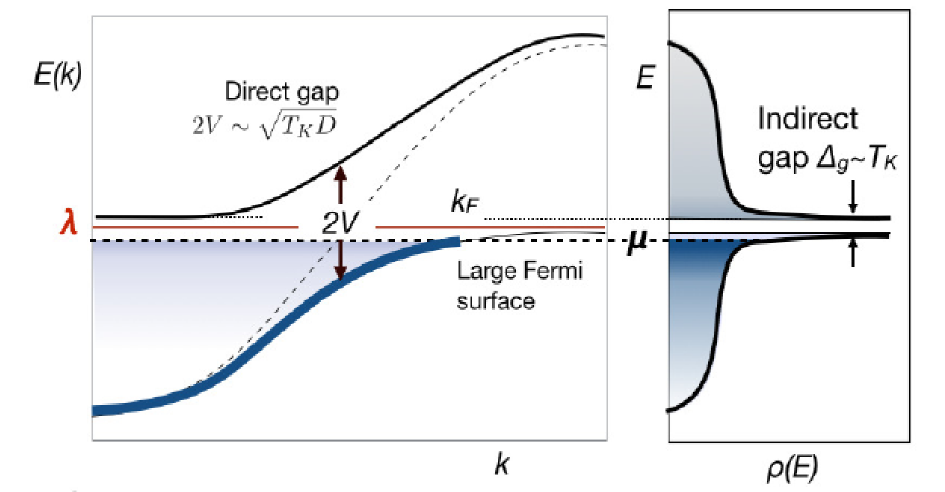

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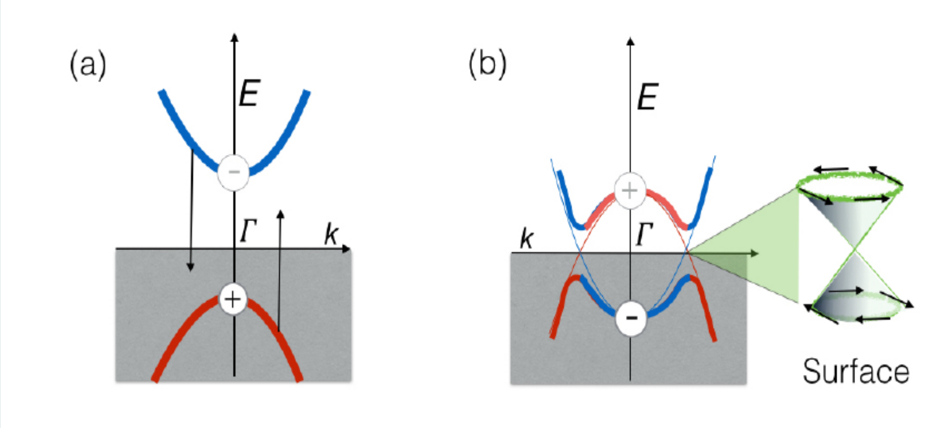

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M. Dzero et al. (2009):

Simple model for TKIs with single metallic band hybridizing with Kramers doublet, opposite parity, **strong SO coupling**:

PAM + topological hybridization

$$V_{\vec{k},\sigma\sigma'} = V_0(\vec{S}_{\vec{k}}\vec{\sigma})_{\sigma\sigma'}$$

$$\vec{S}_{\vec{k}} = \begin{pmatrix} \sin k_x a \\ \sin k_y a \\ \sin k_z a \end{pmatrix} \quad \vec{\sigma} = \begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{pmatrix}$$

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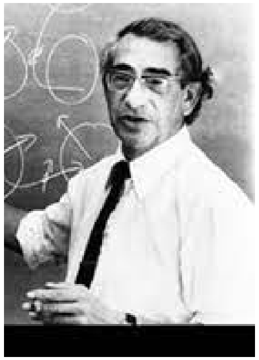
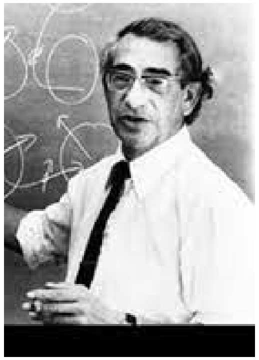


John Hubbard (1963)
Derivation of the Hubbard model for s-bands:

$$\hat{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Dynamical Mean-Field Theory



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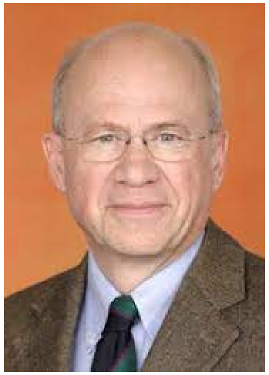

Walter Metzner, Dieter Vollhardt (1988)

Infinite dimensional Hubbard model gives exactly local self-energy, good approximation for 3 dimensions.

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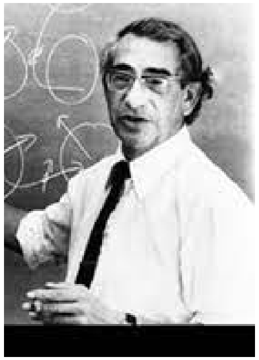

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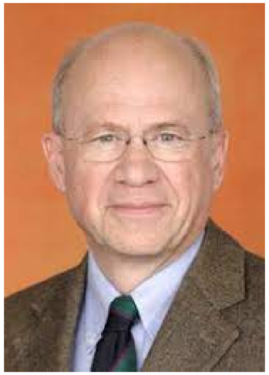

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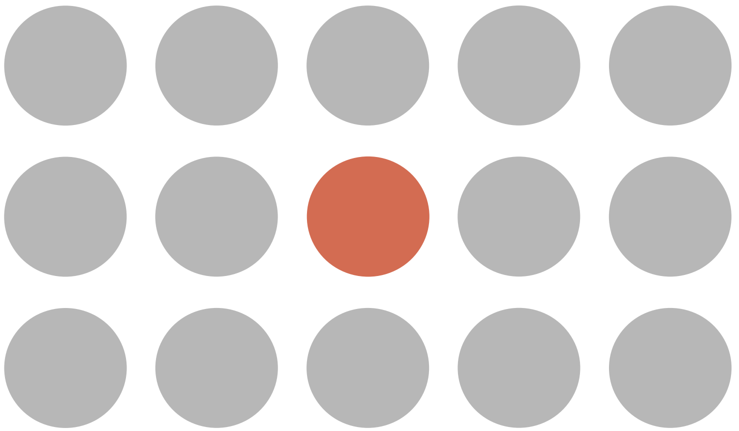
Anoine Georges, Gabriel Kotliar (1991)

Exact mapping of an infinite dimensional Hubbard model onto an effective SIAM:
Dynamical mean-field theory (DMFT)

Cavity construction:

Single out a single site in the lattice.

Hopping to neighbors is an effective hybridization between the local site and the surrounding effective bath.



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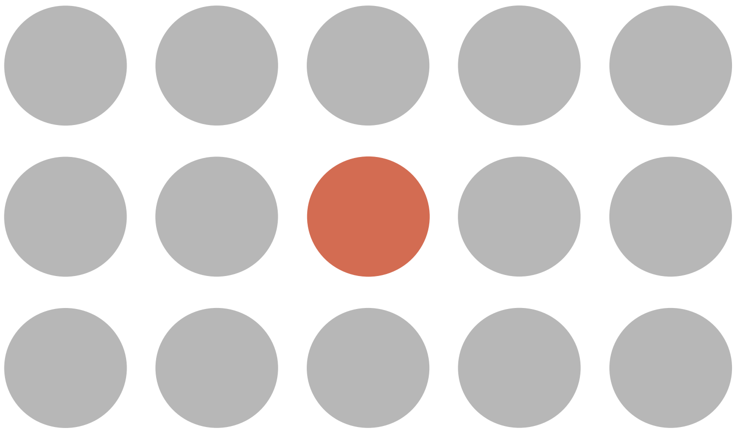

local electron background $G^c(\omega)$

impurity solver (NCA)

local $\Sigma^c(\omega) = V G^d(\omega) V^\dagger$

DMFT assumption

$$\mathcal{G}^c_{\vec{k}}(\omega) = \left(\omega - \epsilon^c_{\vec{k}} - \Sigma^c(\omega)\right)^{-1}$$

momentum sum

local full $\mathcal{G}^c(\omega)$

cavity construction

Solving the SIAM

Different approaches to solve the single impurity Anderson model (SIAM):

- Bethe Ansatz
- Conformal field theory mappings
- Renormalization Group techniques (NRG, fRG, DMRG, perturbative RG)
- Quantum Monte-Carlo (in various flavors)
- Exact diagonalization
- Slave-boson mean-field (SBMF)
- Non-crossing approximation (NCA) and higher orders
- Conserving T-matrix approximations

In our group, we mostly use Slave-boson based methods, mainly NCA.

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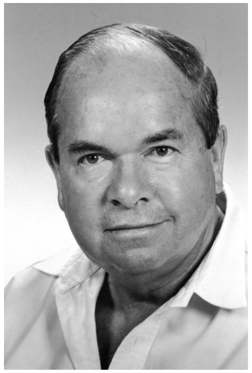
What are Slave-bosons and why do we need them?

Auxiliary particles

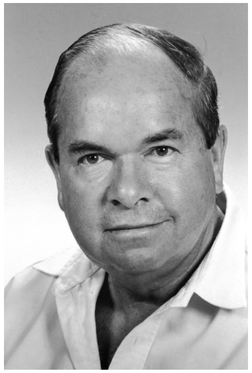


Alexej Abrikosov (1965)
Pseudo-fermion representation for spins in the Kondo model.

$$\hat{\vec{S}}_n = \hat{a}^\dagger_{n\beta} \vec{S}_{\beta\beta'} \hat{a}_{n\beta'}$$

Hilbert-space is enhanced, projection onto physical space is necessary!

Auxiliary particles



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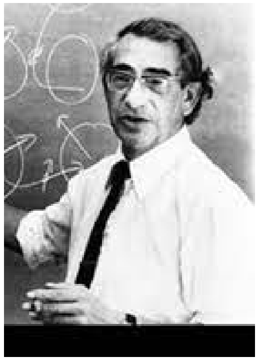

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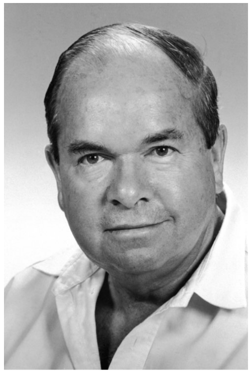
Problem: degenerate bands (e.g. d- and f-bands) can have more than two electrons on-site! Not easily impementable.

Solution: Use operators for individual valence states.

$$\hat{X}_{a,b} = |a\rangle \langle b| \equiv \hat{c}^\dagger_{\sigma_1} \dots \hat{c}^\dagger_{\sigma_n} \hat{c}_{\sigma_1} \dots \hat{c}_{\sigma_m}$$ for fermions!

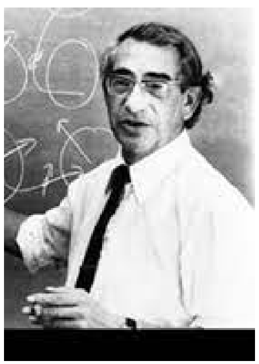
Problem: non-canonical commutation relations...



Alexej Abrikosov (1965)
Pseudo-fermion representation for spins in the Kondo model.

$$\hat{\vec{S}}_n = \hat{a}^\dagger_{n\beta} \vec{S}_{\beta\beta'} \hat{a}_{n\beta'}$$

Hilbert-space is enhanced, projection onto physical space is necessary!



John Hubbard (1963)
Derivation of the Hubbard model for s-bands, proposal of valence-state operators w. Non-canonical commutators:

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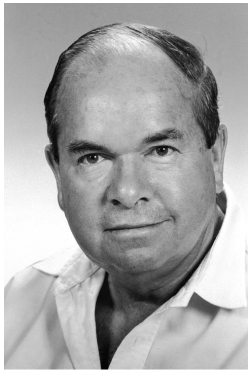
Auxiliary particles



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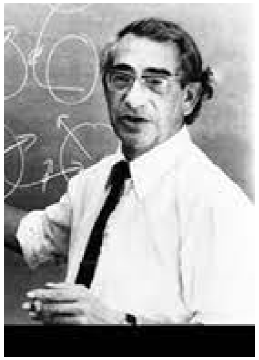

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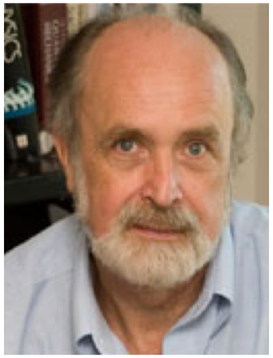
Piers Coleman (1983) based on Steward Barnes (1976)
Application of the Hubbard operators to the SIAM

$$\hat{X}_{0,0} = |0\rangle \langle 0| \,, \; \hat{X}_{\sigma,\sigma'} = |\sigma\rangle \langle \sigma'|$$

Auxiliary particles (slave-bosons and pseudo-fermions)

$$b^\dagger |\mathrm{vac}\rangle = |0\rangle \,, \; \hat{f}^\dagger_\sigma |\mathrm{vac}\rangle = |\sigma\rangle \; \Rightarrow \hat{X}_{0,0} = \hat{b}^\dagger \hat{b}, \; \dots$$



Auxiliary particles

$$\hat{H}_{SIAM} \xrightarrow[U\to\infty]{} \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k},\sigma} \hat{c}_{\mathbf{k},\sigma} + \sum_{\sigma} E_d \, \hat{X}_{\sigma,\sigma} + V \sum_{\mathbf{k},\sigma} (\hat{c}^{\dagger}_{\mathbf{k},\sigma} \hat{X}_{0,\sigma} + \text{h.c.})$$

Represent the Hubbard operators via auxiliary particles

$$\hat{X}_{0,0} = \hat{b}^{\dagger} \hat{b} \qquad \hat{X}_{\sigma,\sigma'} = \hat{f}^{\dagger}_{\sigma} \hat{f}_{\sigma'} \qquad \hat{X}_{0,\sigma} = \hat{b}^{\dagger} \hat{f}_{\sigma} \qquad \hat{X}_{\sigma,0} = \hat{f}^{\dagger}_{\sigma} \hat{b}$$

They have to satisfy the holonomic constraint

$$\hat{Q} = \hat{b}^{\dagger} \hat{b} + \sum_{\sigma} \hat{f}^{\dagger}_{\sigma} \hat{f}_{\sigma} = \mathbb{1}$$

Which can be implemented using a chemical potential $\lambda(\hat{Q} - \mathbb{1}), \ \lambda \to \infty$

Auxiliary particles

In terms of the auxiliary particles, we get

$$\hat{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k},\sigma} \hat{c}_{\mathbf{k},\sigma} + \sum_{\sigma} E_d \, \hat{f}^\dagger_\sigma \hat{f}_\sigma + V \sum_{\mathbf{k},\sigma} (\hat{c}^\dagger_{\mathbf{k},\sigma} \hat{b}^\dagger \hat{f}_\sigma + \mathrm{h.c.}) + \lambda(\hat{Q} - \mathbb{1})$$

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Grand canonical expectation values can be decomposed into sub-sectors

$$\begin{aligned}
\langle \hat{A}\hat{Q} \rangle_G &= \frac{1}{Z_G} \mathrm{tr} \left(\hat{A}\hat{Q} e^{-\beta(\hat{H} + \lambda(\hat{Q} - \mathbb{1}))} \right) \\
&= \frac{1}{Z_G} \Big[0 \, e^{\beta\lambda} \mathrm{tr} \left(\hat{A} e^{-\beta \hat{H}} \right)_{Q=0} + 1 \, e^{0} \mathrm{tr} \left(\hat{A} e^{-\beta \hat{H}} \right)_{Q=1} \\
&\qquad + 2 \, e^{-\beta\lambda} \mathrm{tr} \left(\hat{A} e^{-\beta \hat{H}} \right)_{Q=2} + 3 \, e^{-2\beta\lambda} \mathrm{tr} \left(\hat{A} e^{-\beta \hat{H}} \right)_{Q=3} + \dots \Big]
\end{aligned}$$

Auxiliary particles

In terms of the auxiliary particles, we get

$$\hat{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k},\sigma} \hat{c}_{\mathbf{k},\sigma} + \sum_{\sigma} E_d \, \hat{f}^\dagger_\sigma \hat{f}_\sigma + V \sum_{\mathbf{k},\sigma} (\hat{c}^\dagger_{\mathbf{k},\sigma} \hat{b}^\dagger \hat{f}_\sigma + \text{h.c.}) + \lambda(\hat{Q} - \mathbb{1})$$

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In particular, we get

$$\langle \hat{Q} \rangle_G = \frac{1}{Z_G} \left[0 + \mathrm{tr}\left(1 \cdot e^{-\beta \hat{H}} \right)_{Q=1} + \mathcal{O}\left(e^{-\beta\lambda} \right) \right]$$

Auxiliary particles

Grand canonical expectation values can be decomposed into sub-sectors

$$\langle \hat{A}\hat{Q}\rangle_G = \frac{1}{Z_G}\mathrm{tr}\left(\hat{A}\hat{Q}e^{-\beta(\hat{H}+\lambda(\hat{Q}-\mathbb{1}))}\right)$$
$$= \frac{1}{Z_G}\Big[0\,e^{\beta\lambda}\mathrm{tr}\left(\hat{A}e^{-\beta\hat{H}}\right)_{Q=0} + 1\,e^{0}\mathrm{tr}\left(\hat{A}e^{-\beta\hat{H}}\right)_{Q=1}$$
$$+ 2\,e^{-\beta\lambda}\mathrm{tr}\left(\hat{A}e^{-\beta\hat{H}}\right)_{Q=2} + 3\,e^{-2\beta\lambda}\mathrm{tr}\left(\hat{A}e^{-\beta\hat{H}}\right)_{Q=3} + \dots\Big]$$

In particular, we get

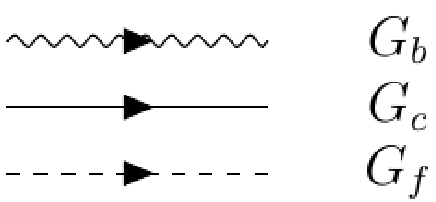
$$\langle \hat{Q}\rangle_G = \frac{1}{Z_G}\left[0 + \mathrm{tr}\left(1\cdot e^{-\beta\hat{H}}\right)_{Q=1} + \mathcal{O}\left(e^{-\beta\lambda}\right)\right]$$

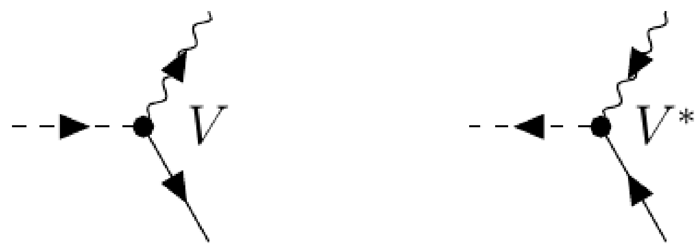
This allows us to write canonical, i.e. physical, expectation values as

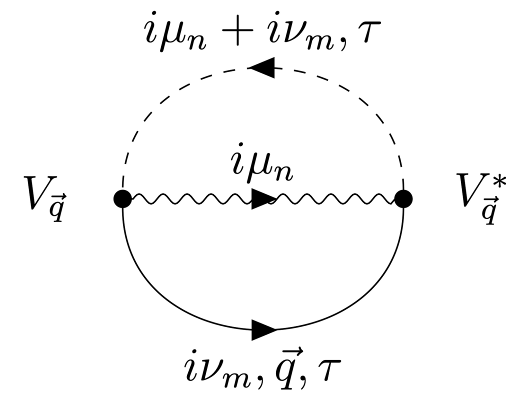
$$\langle \hat{A}\rangle_C = \lim_{\lambda\to\infty}\frac{\langle \hat{A}\hat{Q}\rangle_G}{\langle \hat{Q}\rangle_G}$$

The Non-Crossing Approximation

Expansion of the Luttinger-Ward functional to the lowest order in the hybridization.







$$\boxed{G = G^0 + G^0 \Sigma G}$$

The self-energies are then given by functional derivatives w.r.t. Green functions, i.e. cutting lines in diagrams.

Grand canonical conduction electron self-energy vanishes in the limit $\lambda \to \infty$

$$\mathrm{Im}\,\Sigma_f^A(\sigma,\omega) = \pi |V|^2 \int_{-\infty}^{\infty} d\epsilon\, \big(1 - n_F(\epsilon)\big) A_b(\omega - \epsilon) A^0_{c,\sigma}(\epsilon)$$

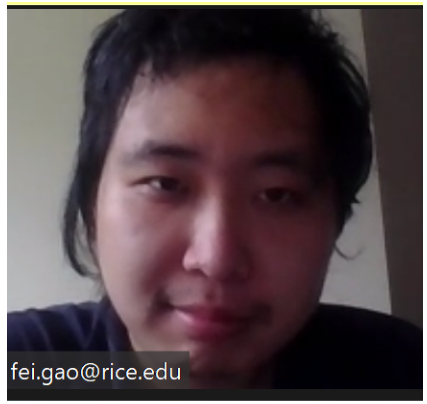
$$\mathrm{Im}\,\Sigma_b^A(\omega) = 2\pi |V|^2 \int_{-\infty}^{\infty} d\epsilon\, n_F(\epsilon) A_f(\epsilon + \omega) A^0_c(\epsilon)$$

Outline

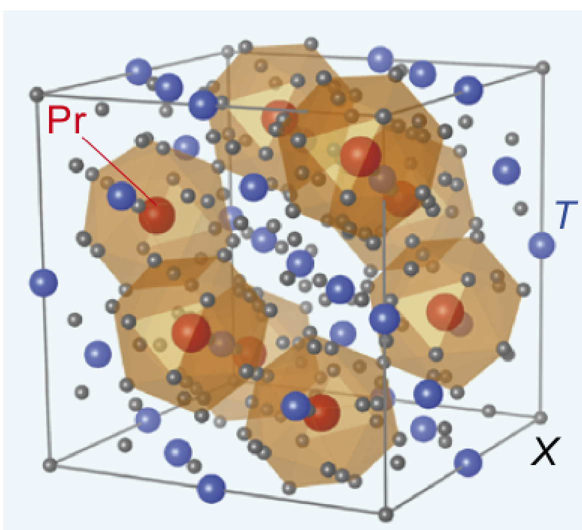
1. Single impurity physics
2. Lattice impurity physics
3. Solving impurity systems
4. **Selected research results**

Quadrupolar Kondo in PrV_2Al_{20}

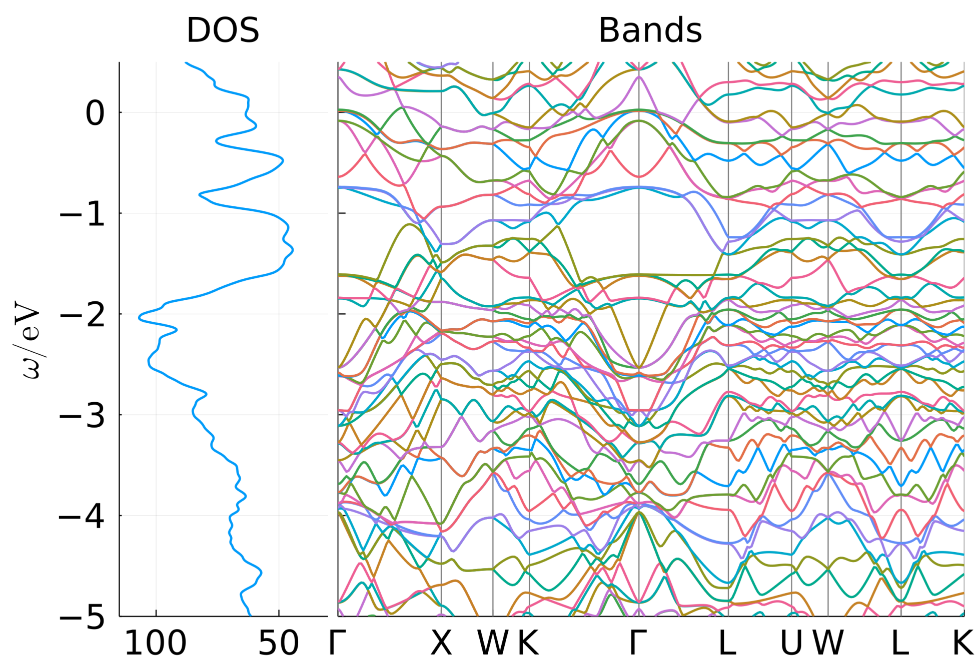
Collaboration with Rice University in Houston, Texas



RICE



T. Onimaru, H. Kusunose, J. Phys. 85 2016

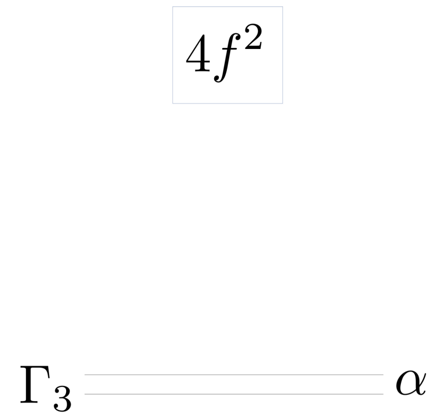


Valence fluctuations & CEF

Large coordination number of Pr:
$4f^2$ electrons with small CEF splitting.

Point group is T_d, Eigenstates are:
Γ_1 singlet, Γ_3 doublet, Γ_4 & Γ_5 triplets.

Not Kramers degenerate!
Quadrupolar mag. moment.



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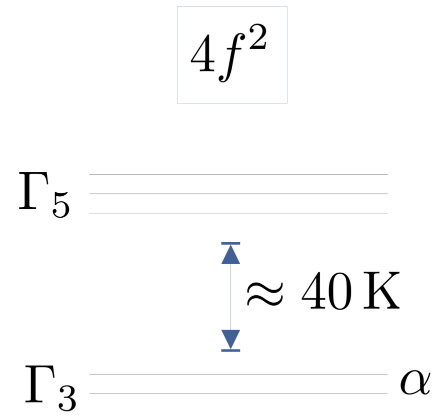

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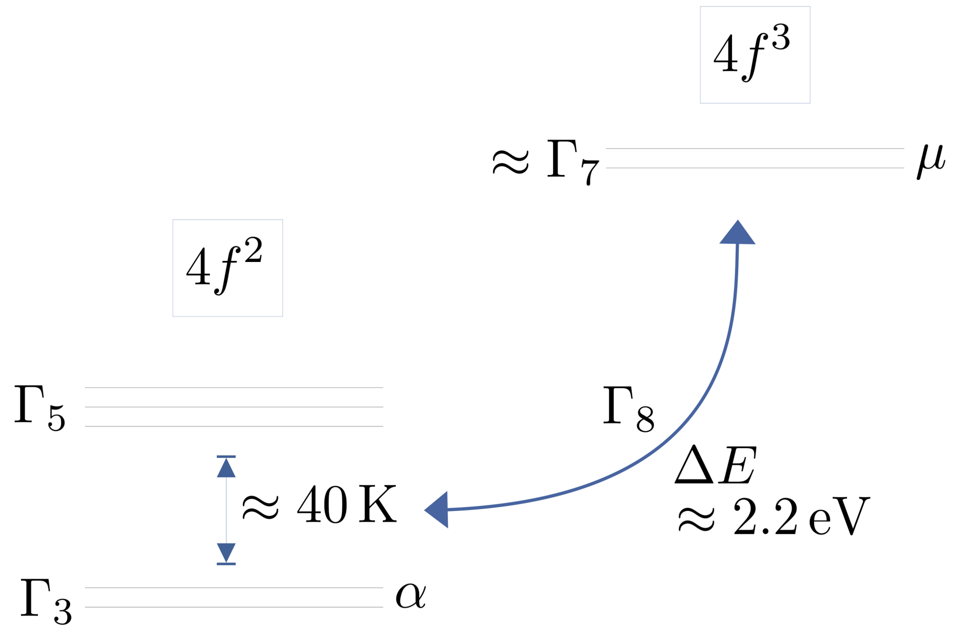
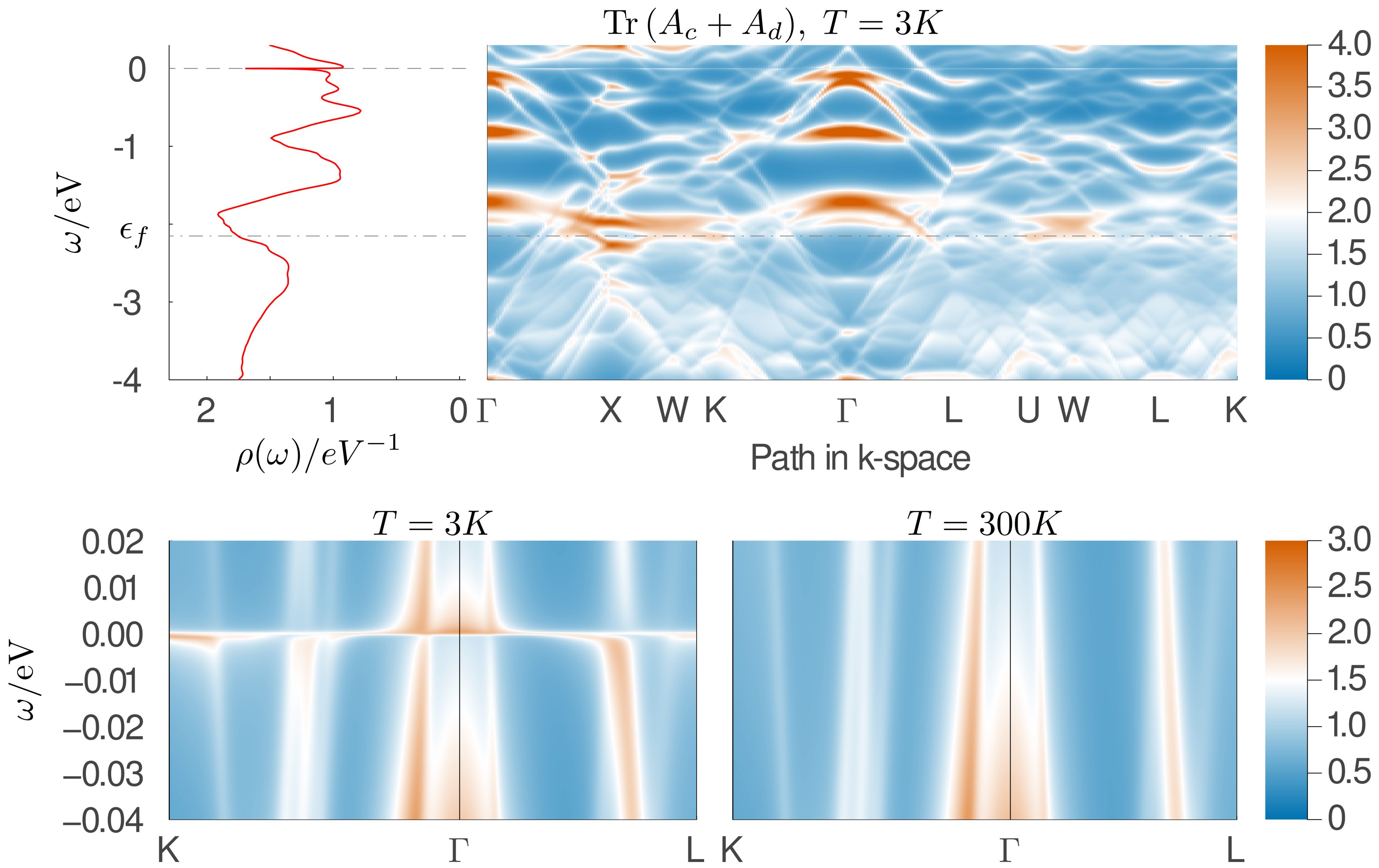


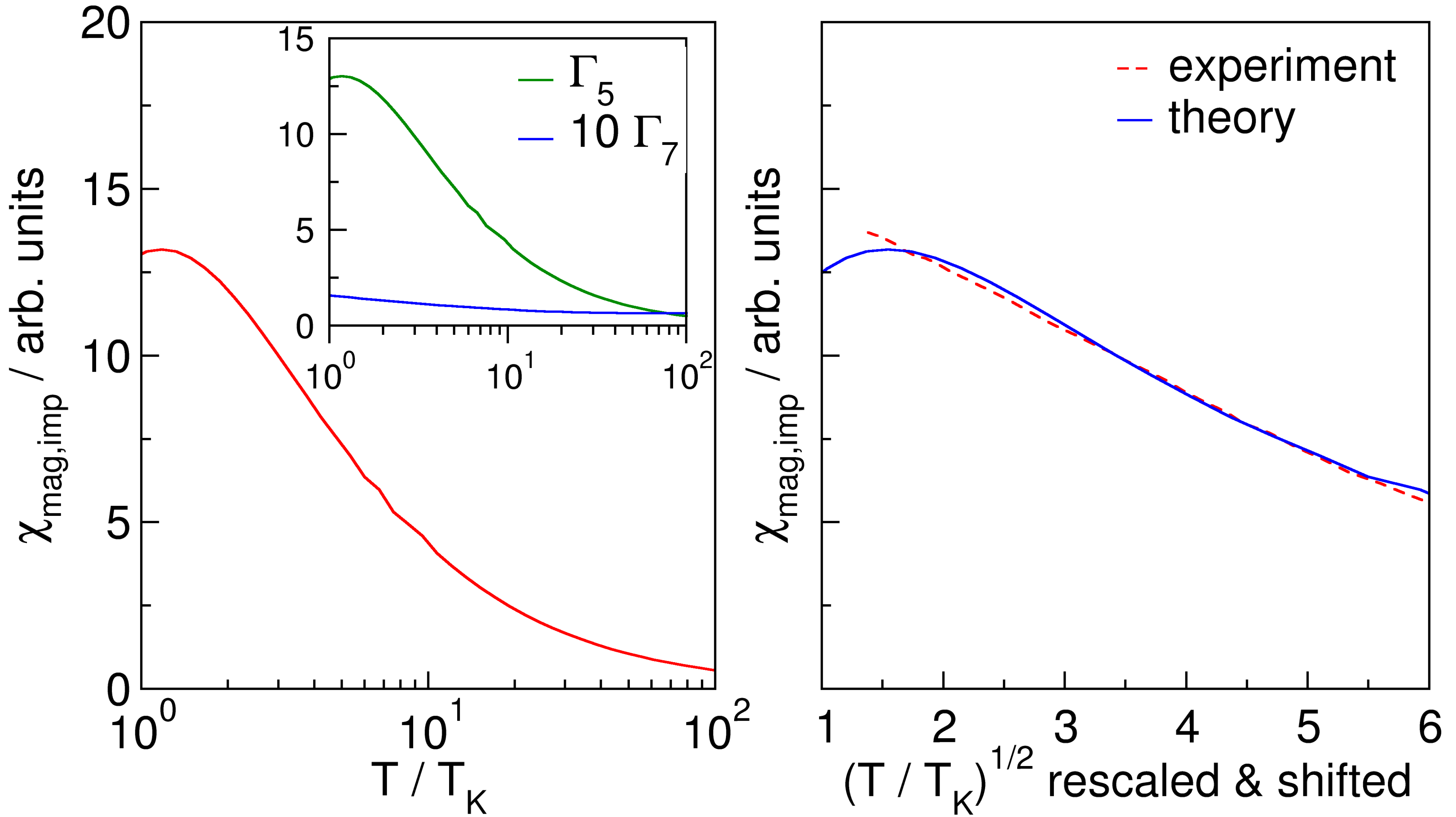
The $4f^2$ configuration fluctuates with $4f^3$, CEF ground state similar to $4f^1$:
Kramers degenerate Γ_7 state with dipole moment.

Strong hybridization with Vanadium d-orbital conduction electrons:
Quadrupolar 2-channel Kondo effect.

DMFT results

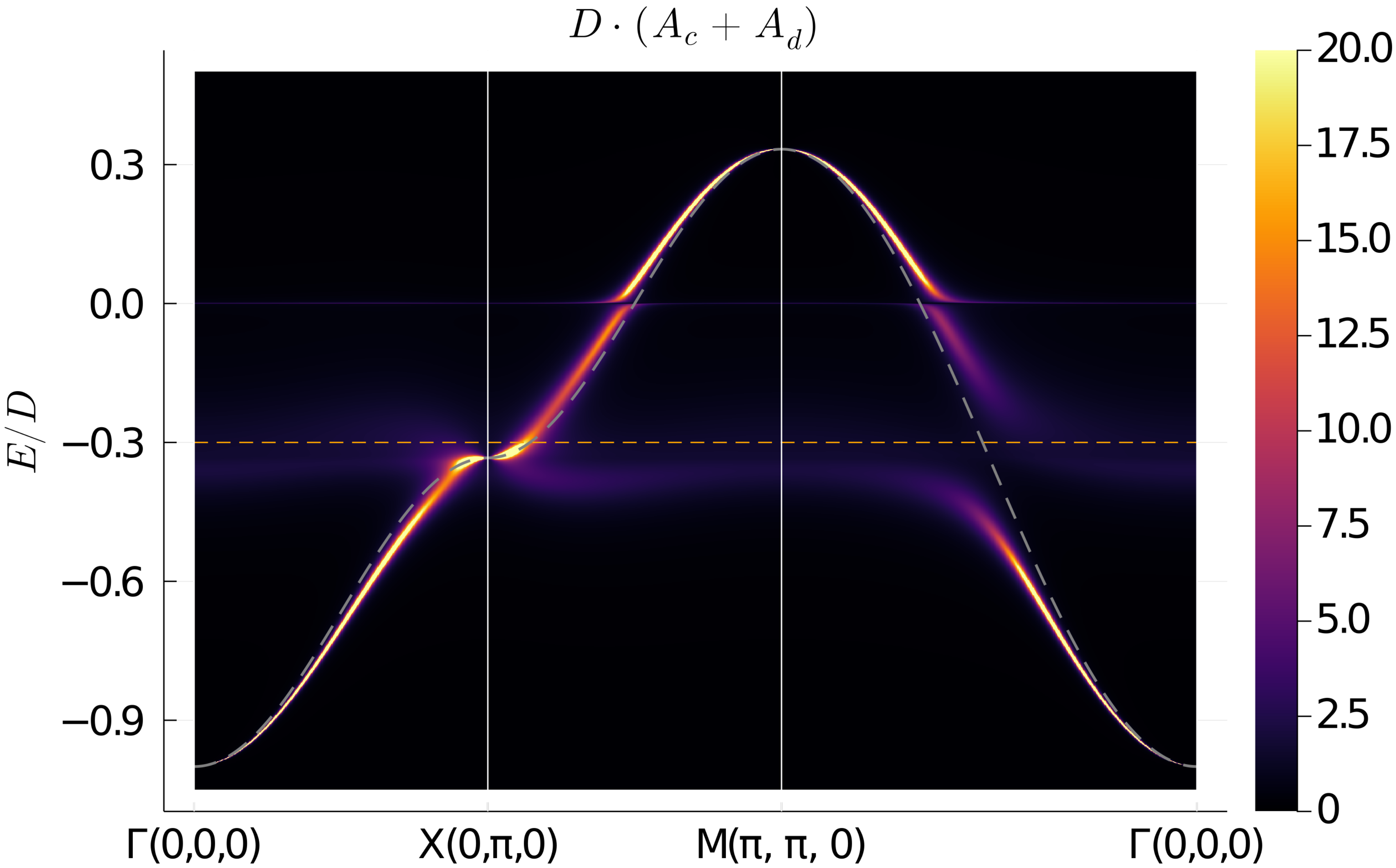


Magnetic susceptibility



PRELIMINARY!

Bulk DMFT for TKIs



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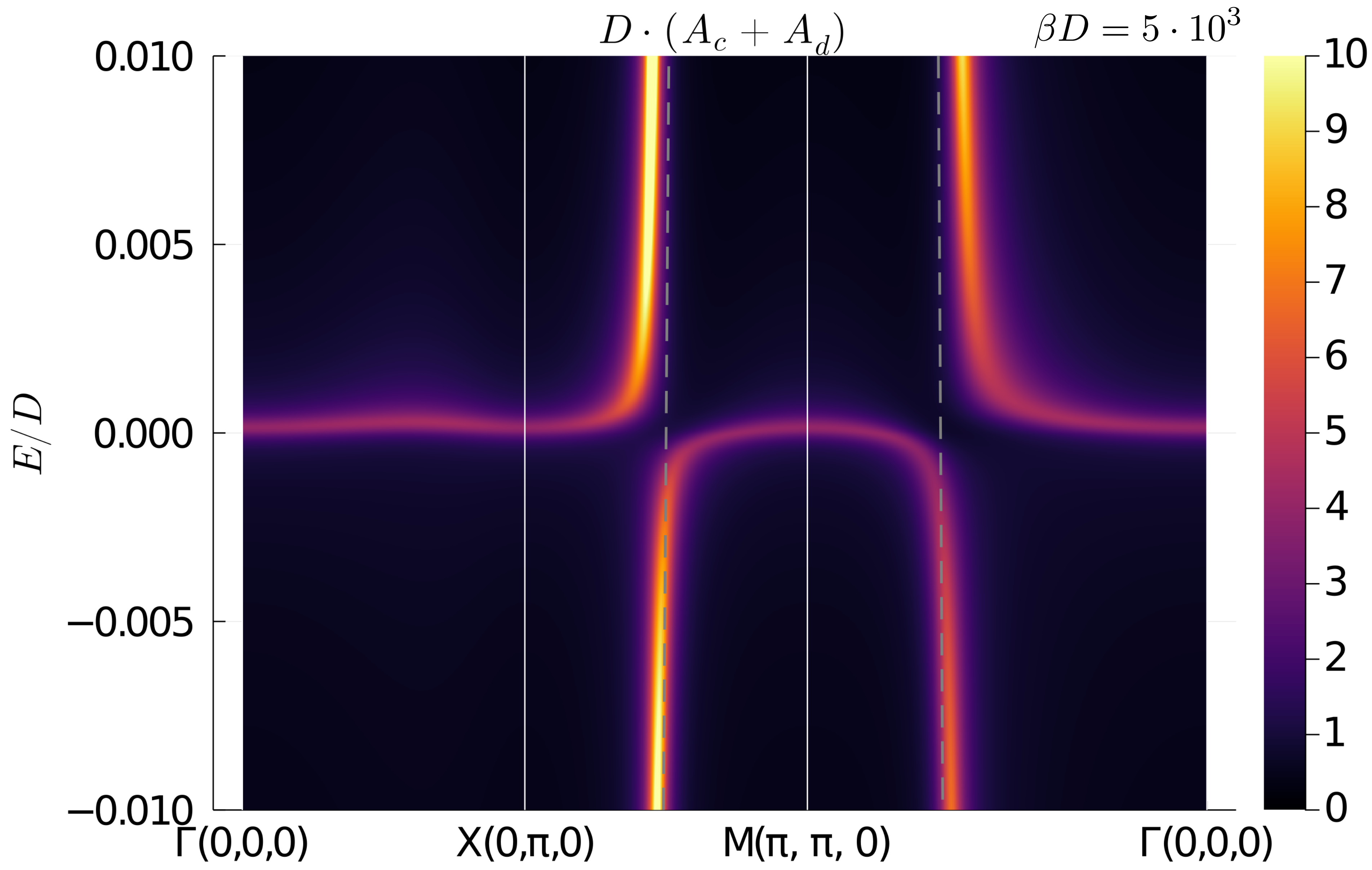

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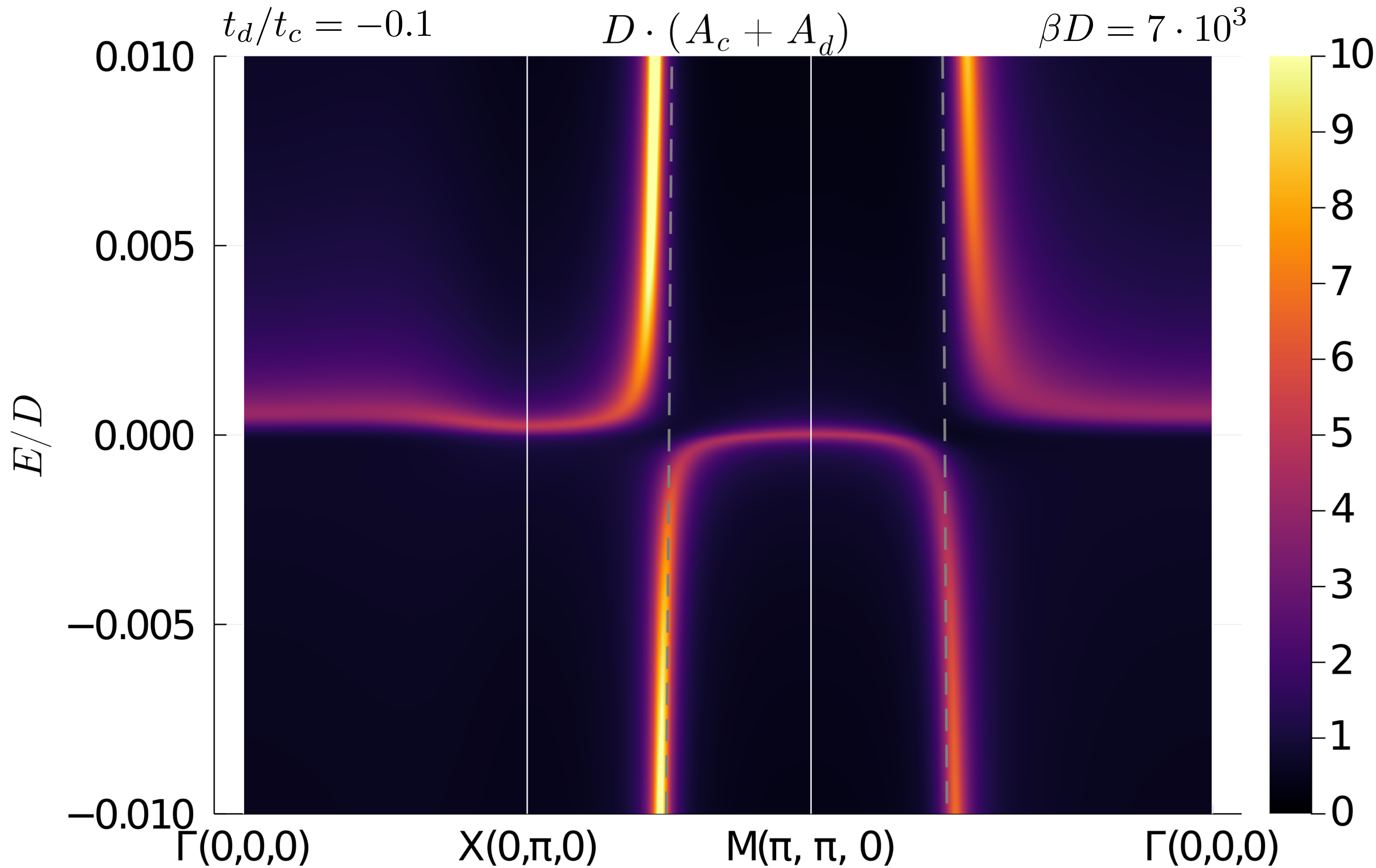

Thank you!

Backup