NHSCP 2014@ISSP

ISSP International Workshop

New Horizon of Strongly Correlated Physics

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ISSP, The University of Tokyo

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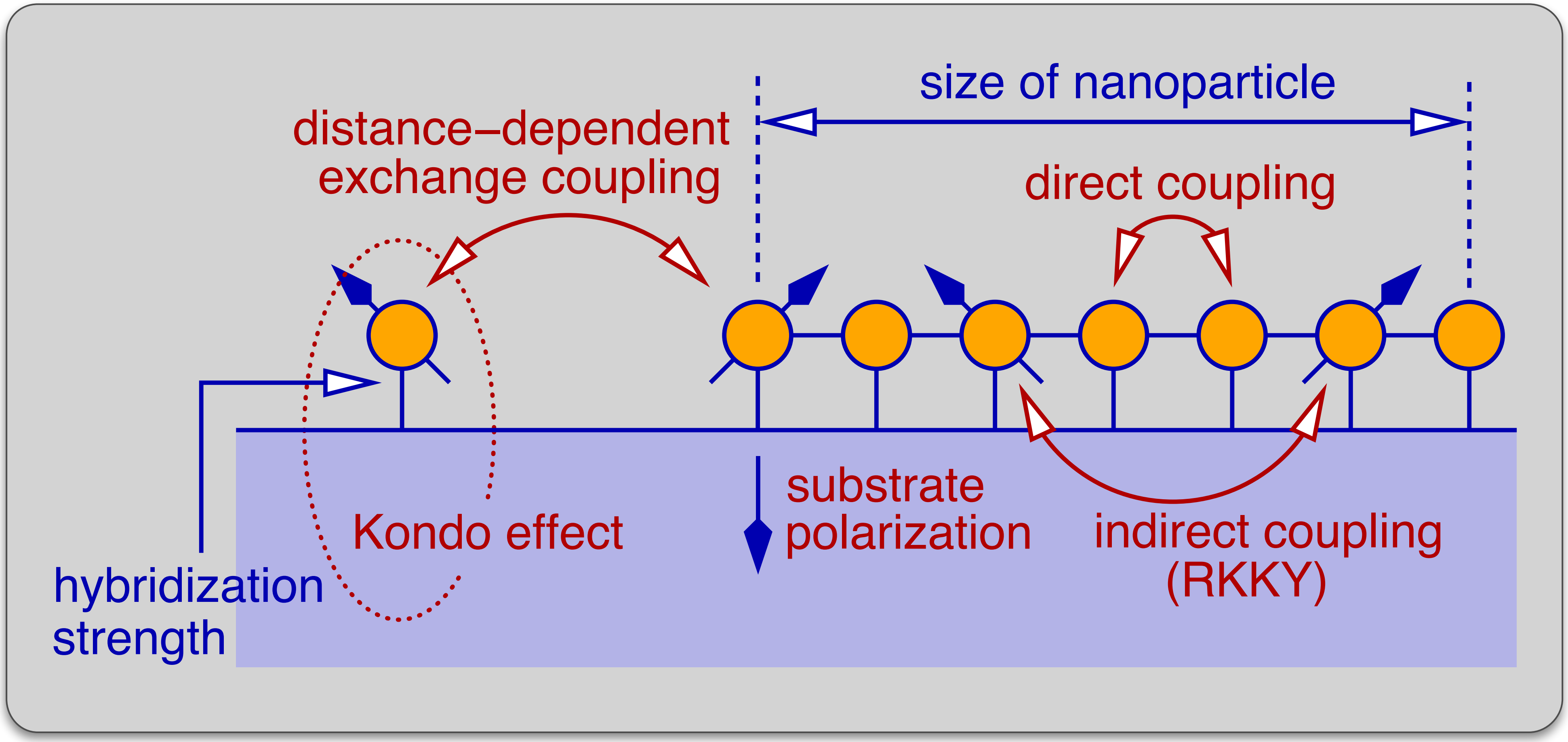
Inverse Indirect Magnetic Exchange



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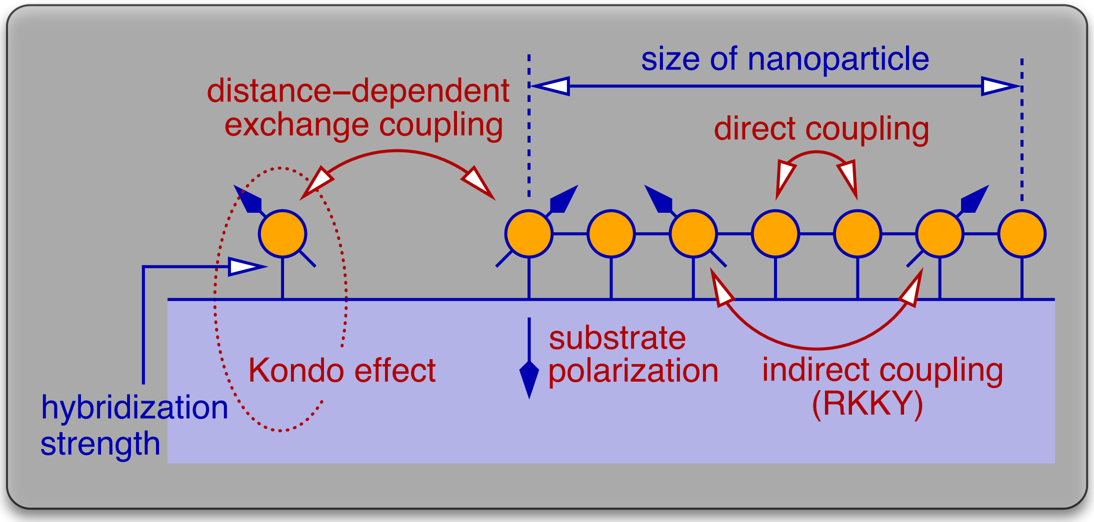
Inverse Indirect Magnetic Exchange

Contents:

- Kondo effect and RKKY
- physical systems
- IIME - main idea
- exact diagonalization
- DMRG in D=1 dimension
- real-space DMFT:
  D=2 nanostructures
- 4-th order perturbation theory:
  IIME effective Hamiltonian
- IIME off half-filling and at T>0
  static mean field and DMFT/QMC
- flat-band ferromagnetism?



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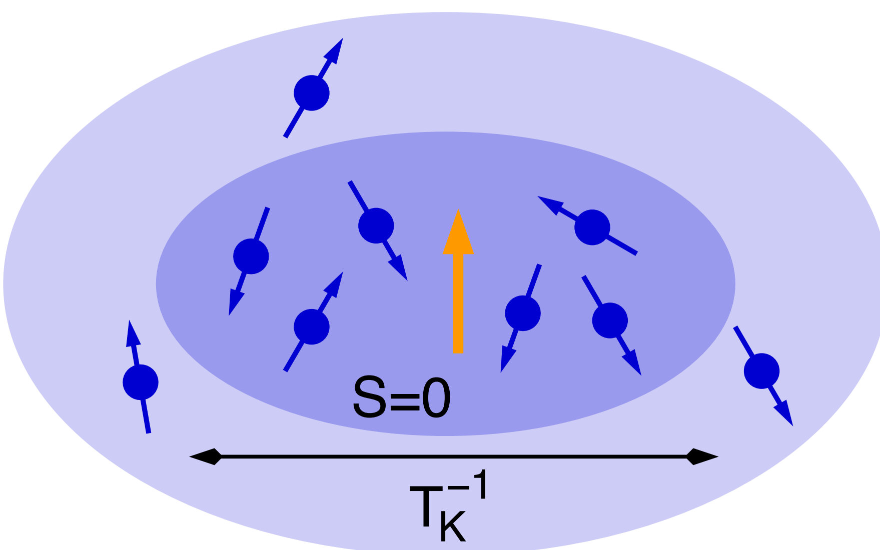
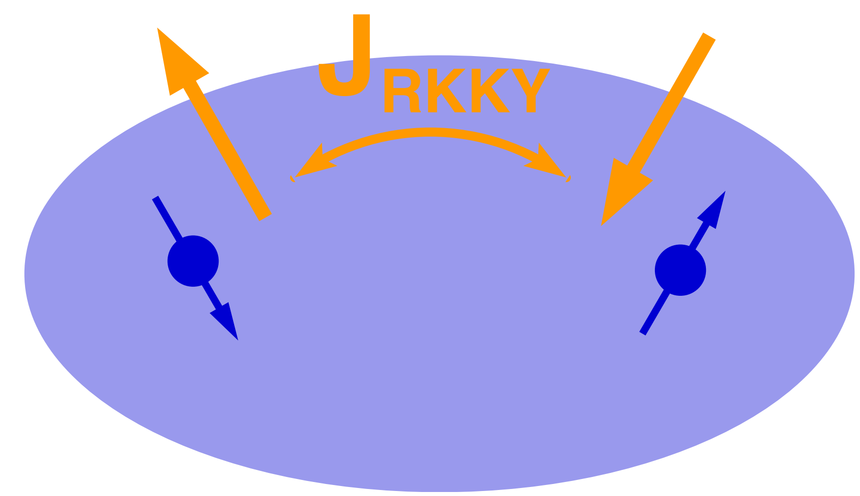
Kondo vs. RKKY

Kondo screening

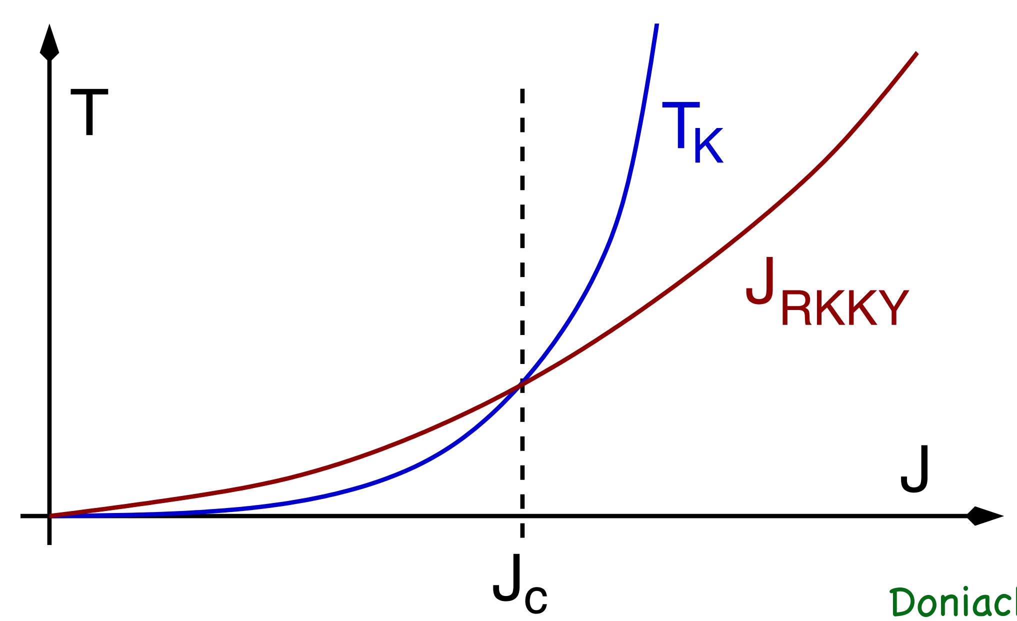


$$T_K \propto e^{-1/J\rho_0}$$

indirect magnetic exchange



$$J_{ij}^{\mathrm{RKKY}} \propto (-1)^d \, J^2 \, \frac{1}{d}$$



Doniach diagram

Doniach (1977)

Confined structures: The Kondo box

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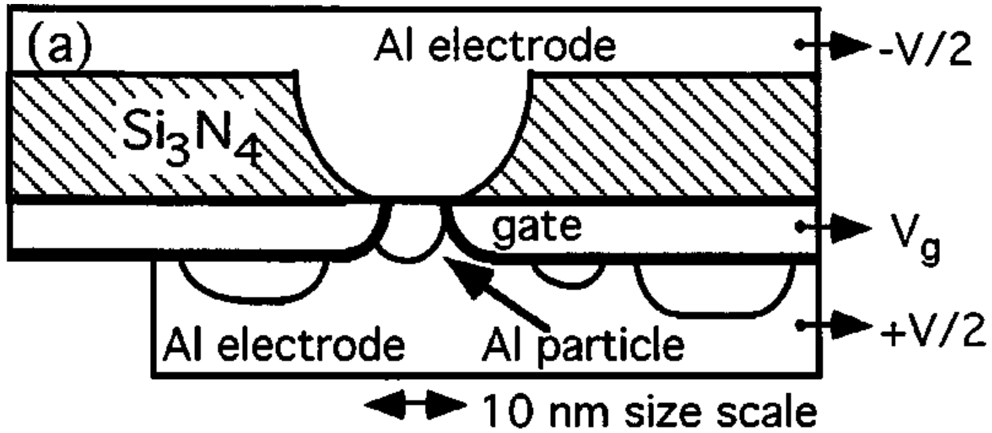
Thimm, Kroha, von Delft (1999)

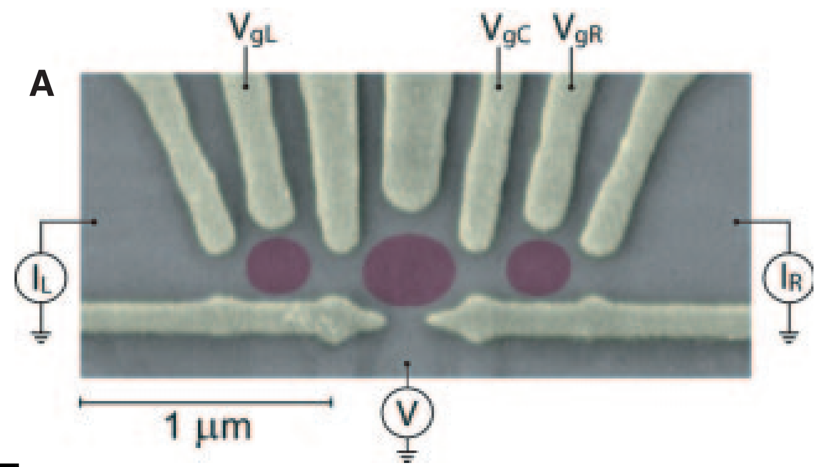
resonance splitting and odd/even effects

$$T_K \sim \Delta \qquad \Delta \approx 0.5 - 60\ \mathrm{K} \quad \text{for} \quad V \approx (15\mathrm{nm})^3 - (3\mathrm{nm})^3$$

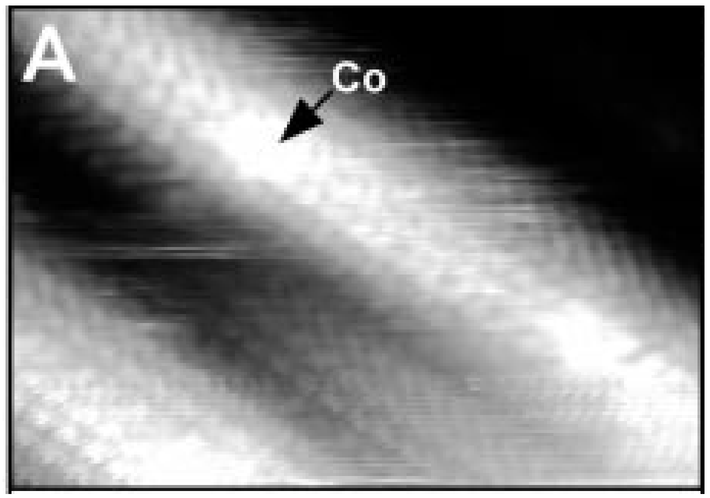
- metallic grains (Al nanoparticles)
- metallocene molecules (Ce, Yb in carbon rings)
- Co clusters in small carbon nanotube pieces
- small QD (spin 1/2) coupled to large QD



Ralph, Black, Tinkham (1995)

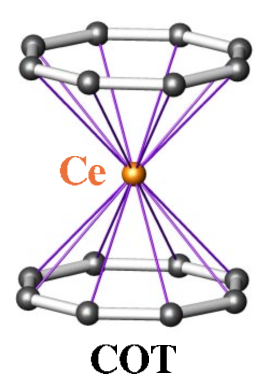


Craig et al. (2006)

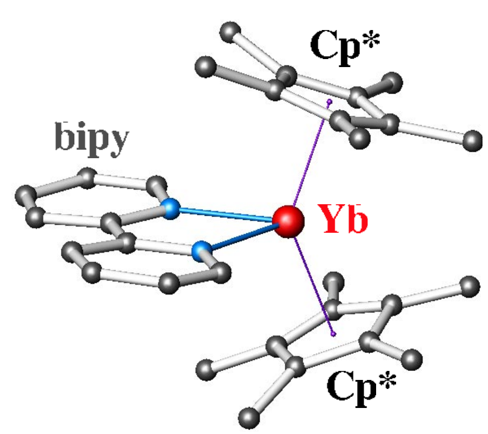


Odom et al. (2000)

$Ce(COT)_2$



$Cp^*{}_2Yb(bipy)$



Booth et al (2005)

Magnetic atoms on metallic surfaces: Kondo effect

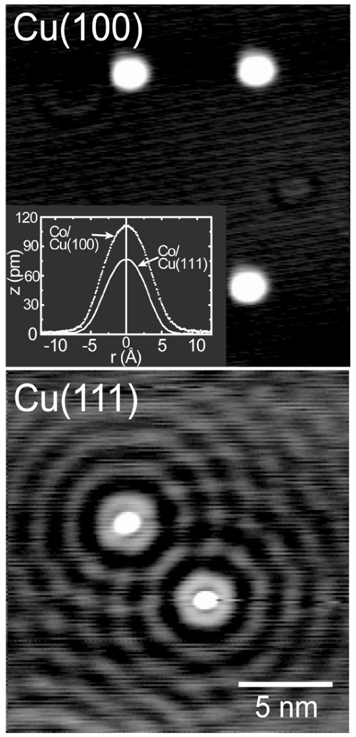
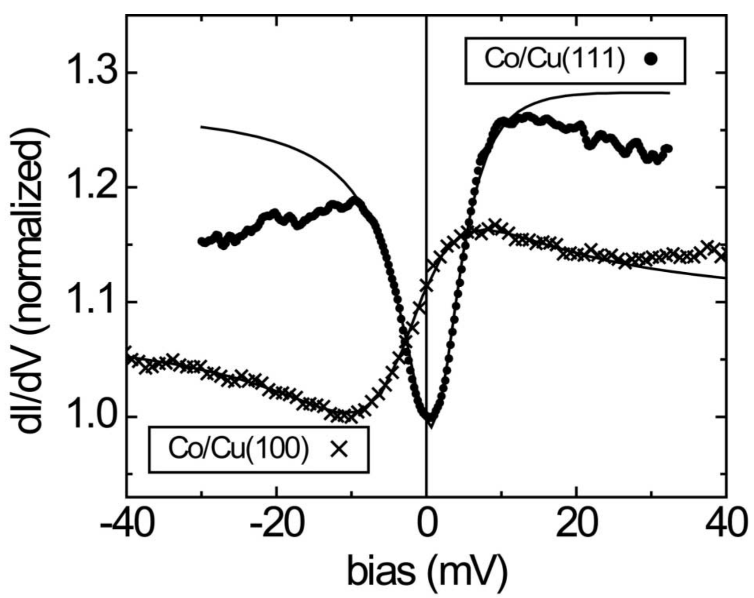


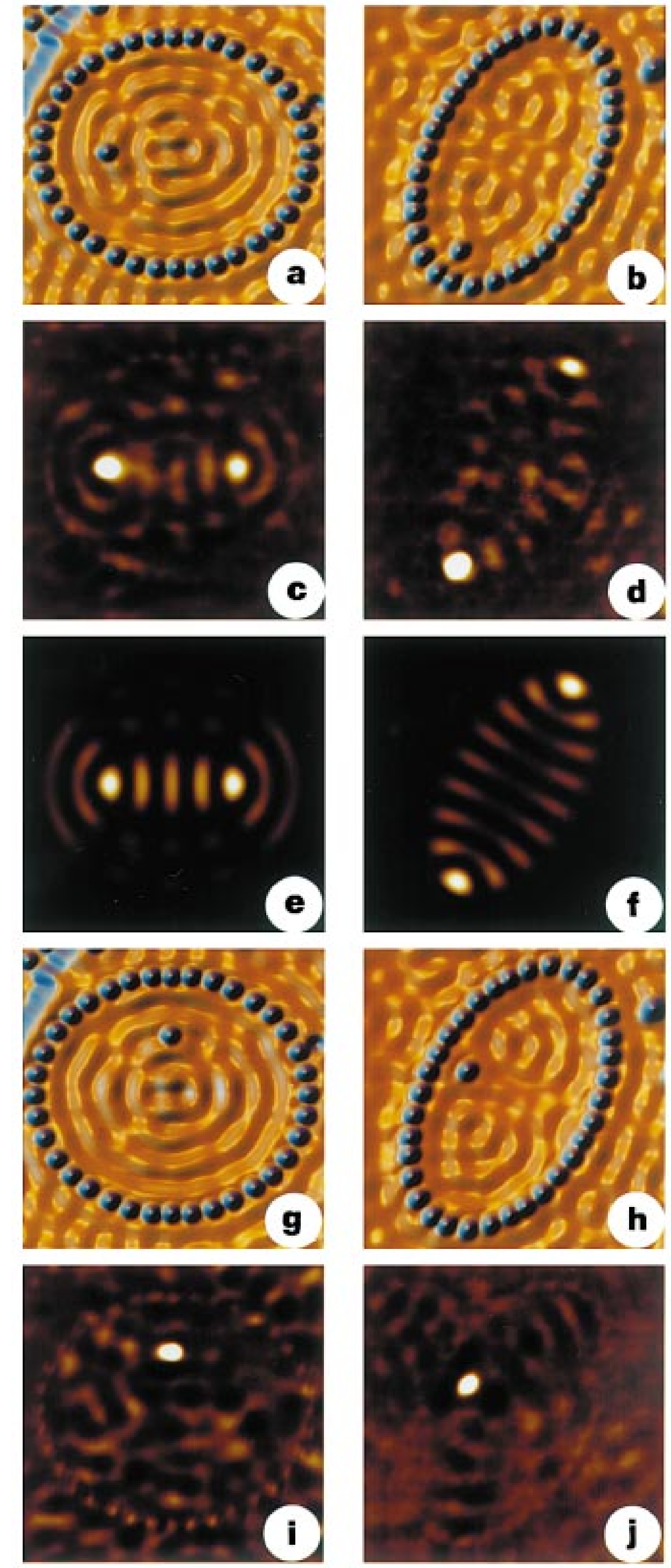
TABLE I. Mean Fano line shape parameters and Kondo temperatures T_K from fits of Eq. (1) to scanning tunneling spectra of ten different Co adatoms on Cu(100) and Cu(111). n is the number of nearest neighbor Cu atoms.

	Co/Cu(111)	Co/Cu(100)	Co in bulk
T_K [K]	54 ± 2 53 ± 5 [6]	88 ± 4	~ 500 [9]
n	3	4	12
q	0.18 ± 0.03	1.13 ± 0.06	
ΔE [meV]	1.8 ± 0.6	-1.3 ± 0.4	

Knorr et al., PRL 88, 096804 (2002)



Co/Cu(100), Co/Cu(111)

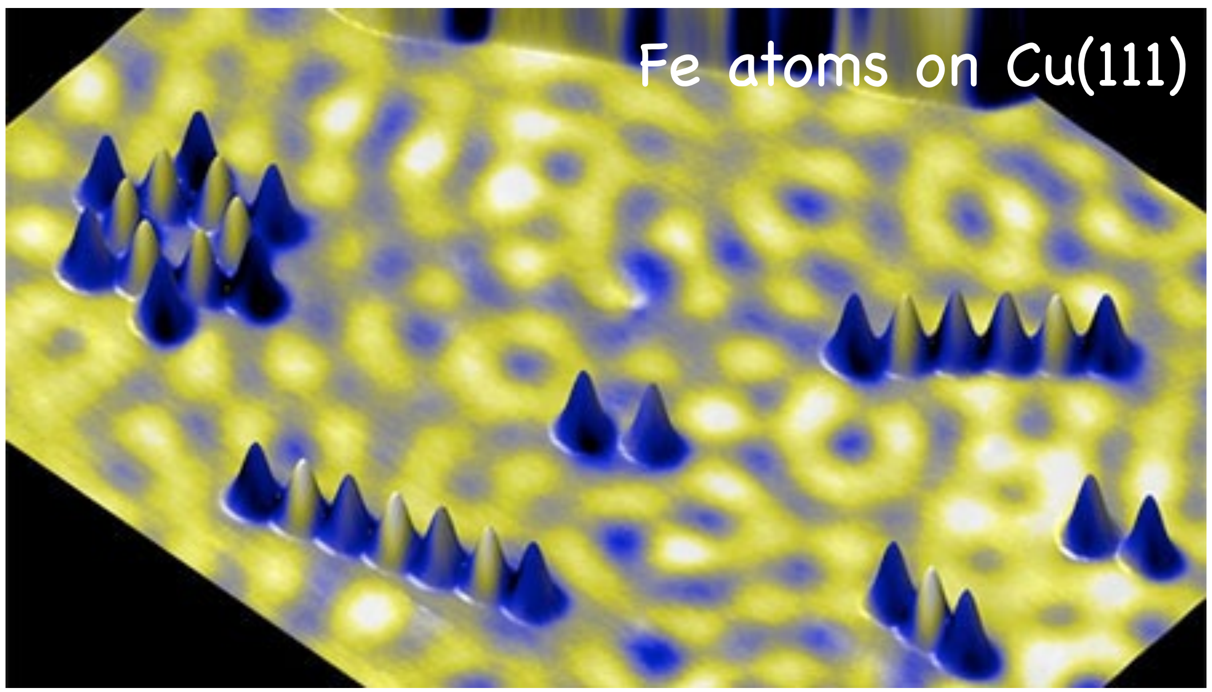


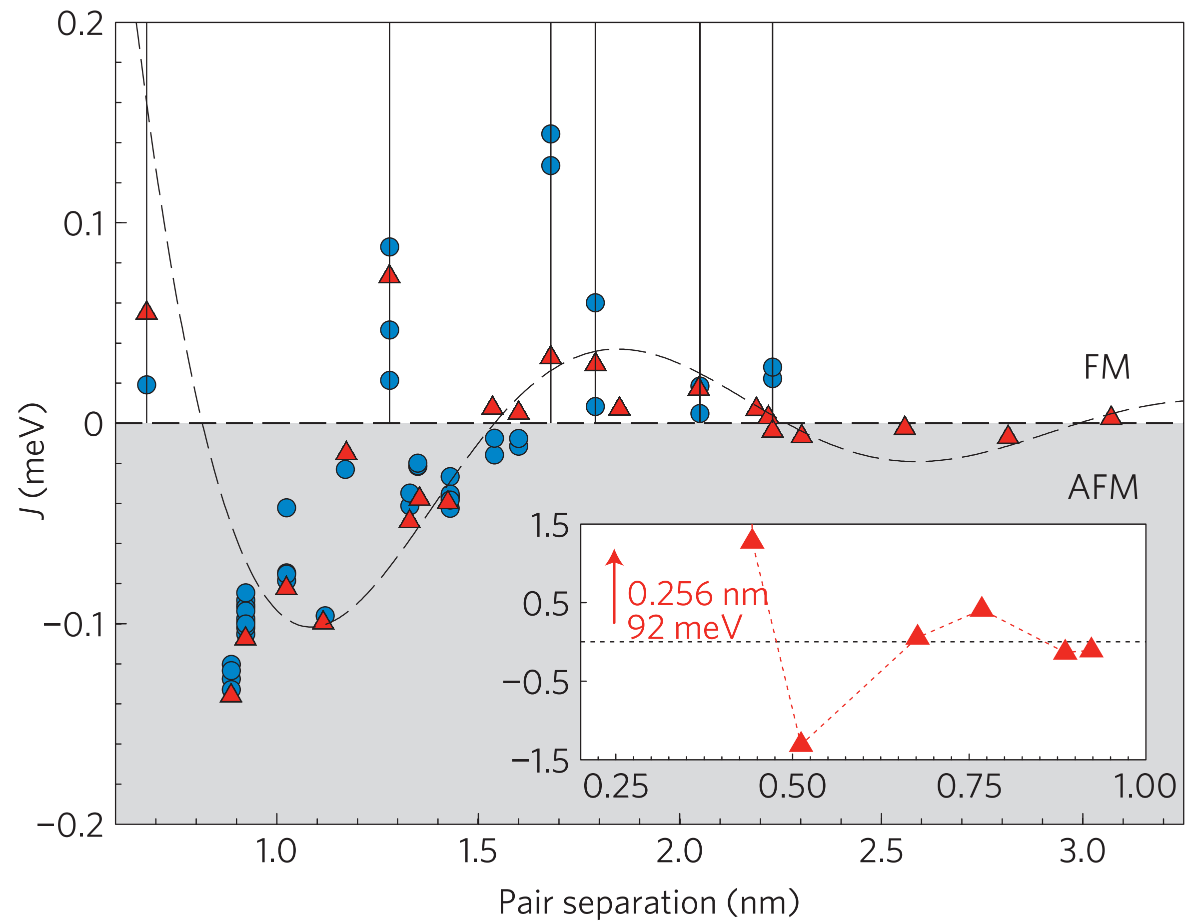
Manoharan et al., Nature 403, 512 (2000)

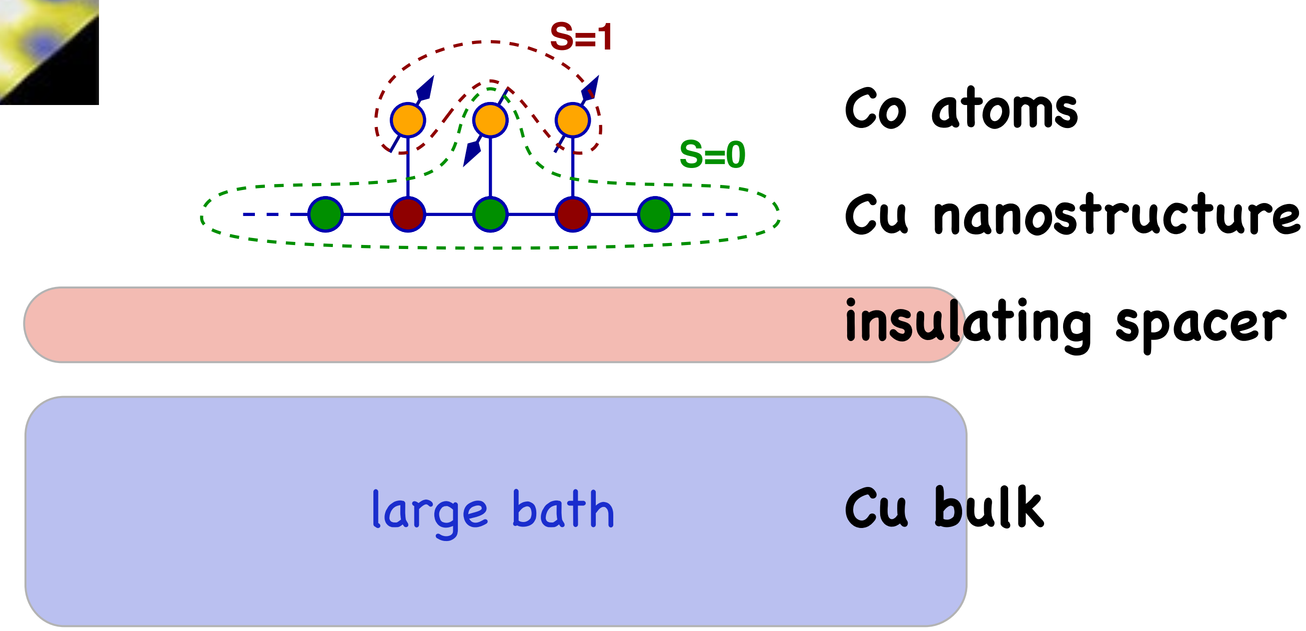
Co/Cu(111): quantum mirage effect in an elliptical quantum corral

RKKY interaction at metallic surfaces

Khajetoorians et al.,
Nat. Phys. 8, 497 (2012)



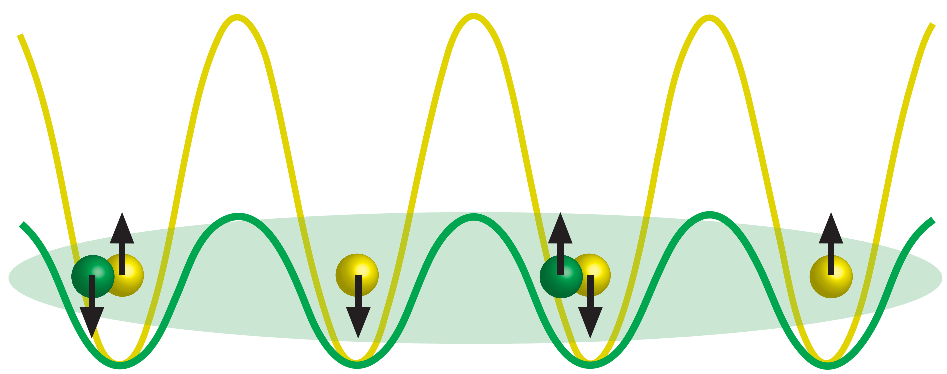




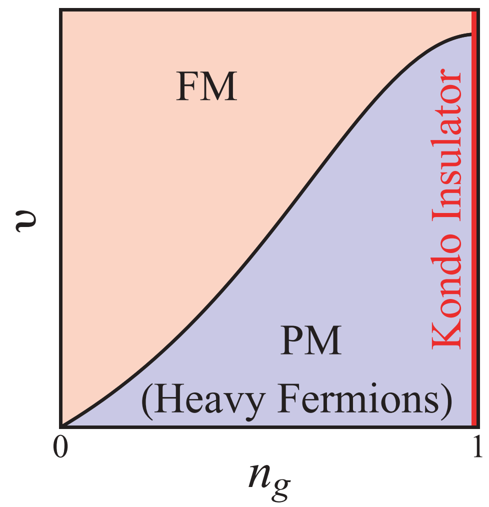
Ultracold atoms in optical lattices

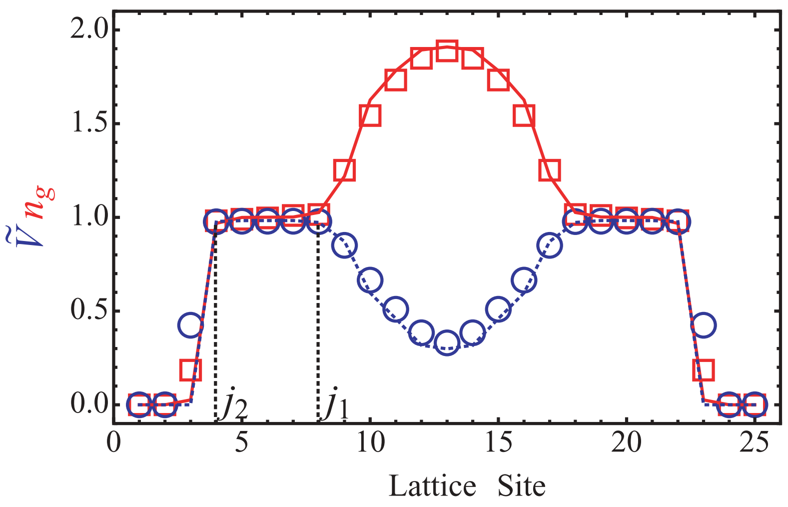
- Fermionic alkaline earth atoms
- simulation of the Kondo-lattice model

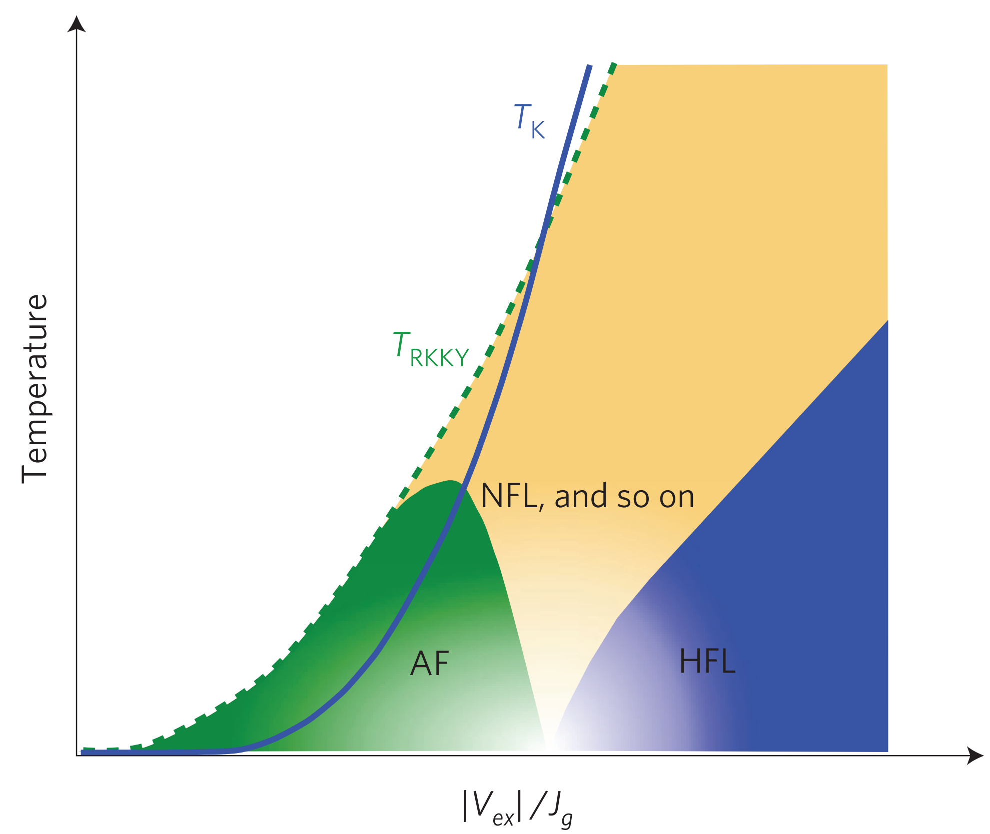
Gorshkov et al.,
Nat. Phys. 6, 289 (2010)



Foss-Feig, Hermele, Rey,
Phys. Rev. A 81, 051603(R) (2010)



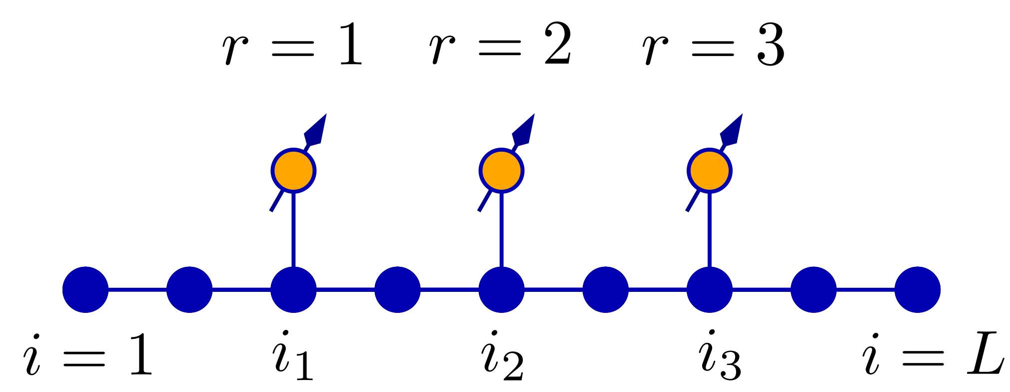




Multi-impurity Kondo model

Hamiltonian:

$$H = -t \sum_{\langle i,j \rangle, \sigma} c^\dagger_{i\sigma} c_{j\sigma} + J \sum_{r=1}^{R} \mathbf{s}_{i_r} \cdot \mathbf{S}_r$$



conduction electrons   cond.-el. spins   local spins (s=1/2)

energy scale: $t=1$

AF coupling: $J>0$

sites: L

spins: R

electrons: N

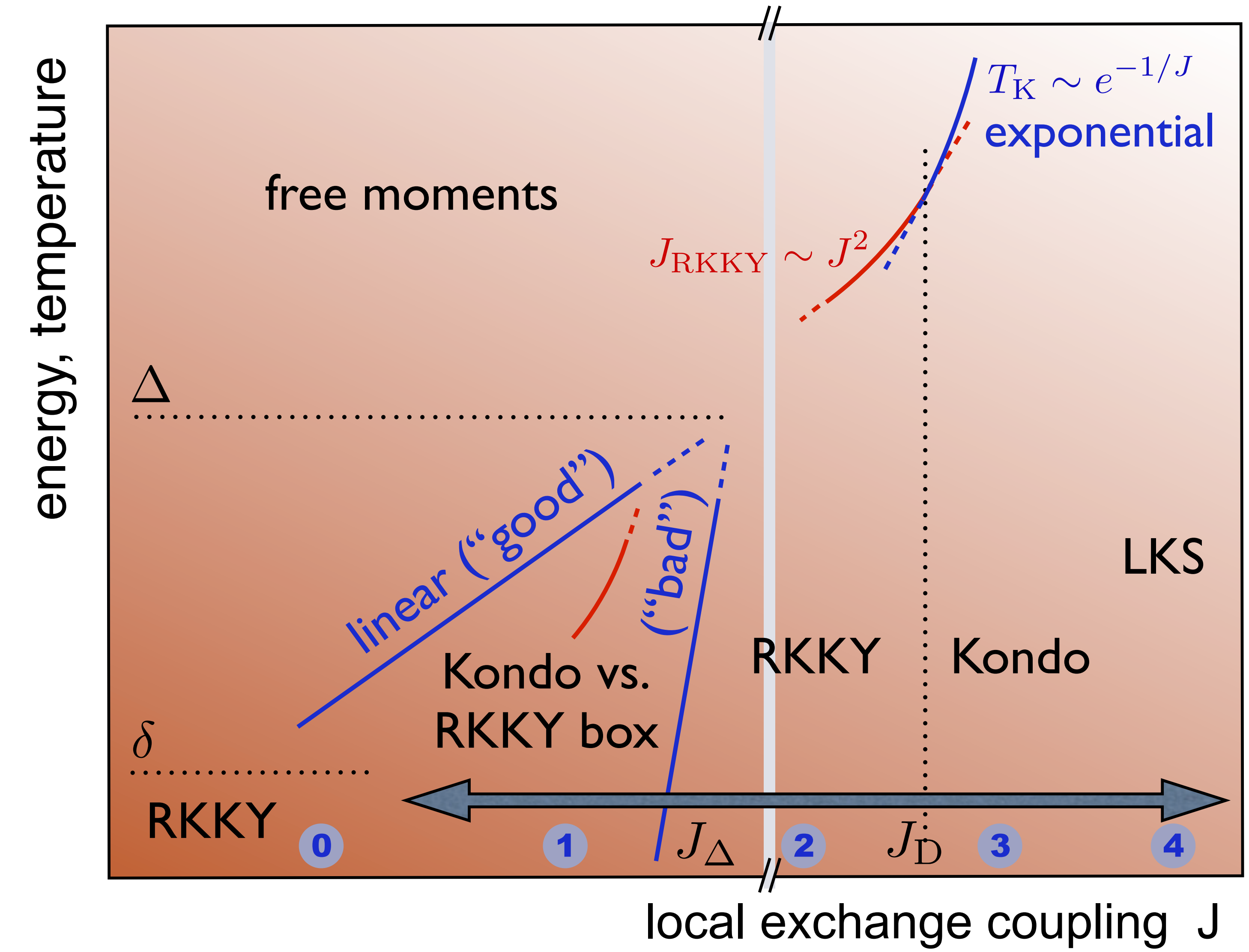
assume, e.g.:

half-filling: $N=L$

Fermi liquid state (large L): $N+R$ even

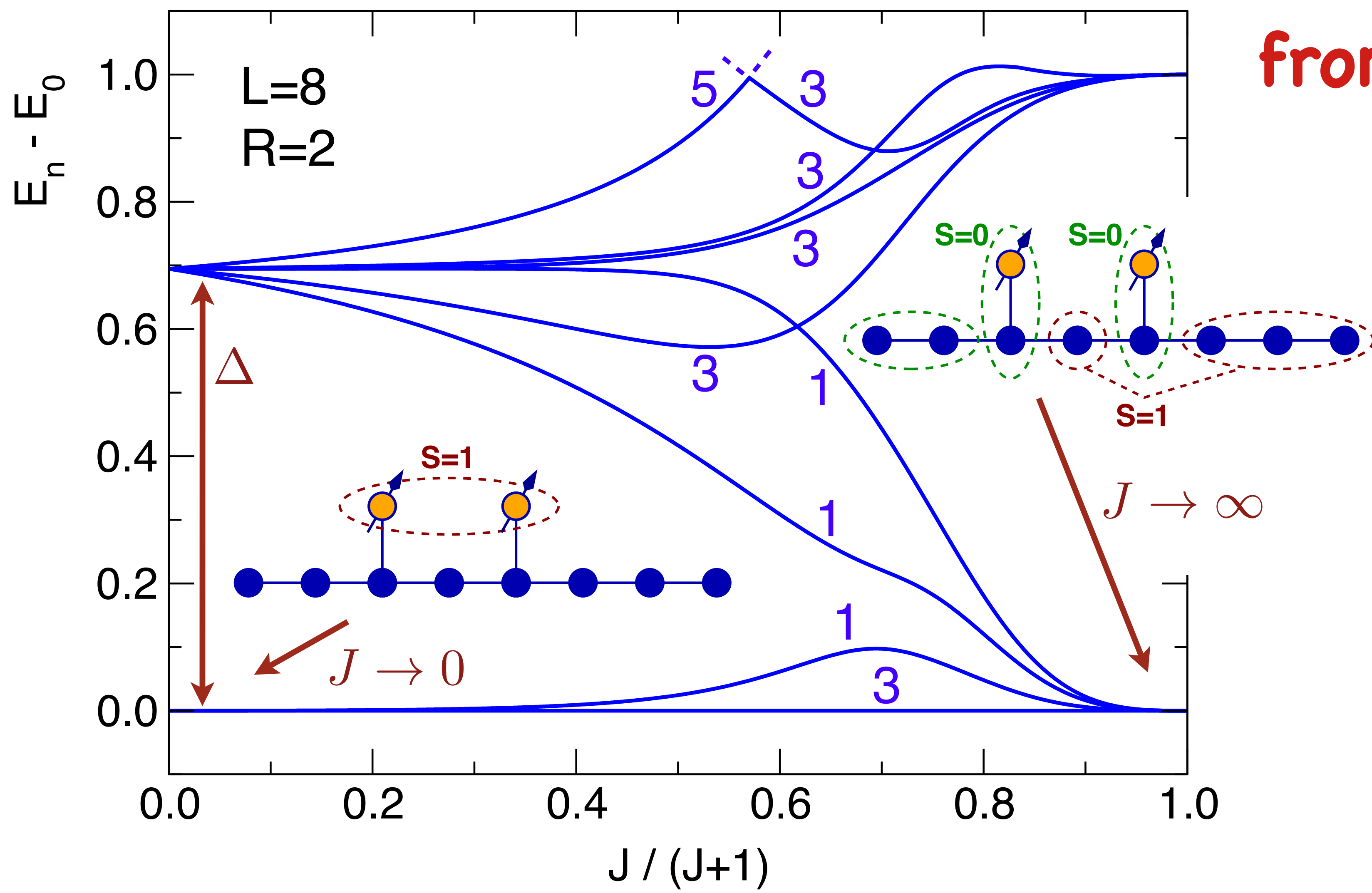
Kondo vs. RKKY in a quantum box

modified Doniach diagram:



A. Schwabe, D. Gütersloh, M.P., PRL 109, 257202 (2012)

"Inverse" indirect magnetic exchange



from weak to strong J

- unique ground state
- local Kondo singlets: magnetically inert
- confinement of conduction electrons
- local moment formation
- magnetic coupling: IIME
- IIME mediated by virtual excitations of local Kondo singlets
- Kondo effect "helps"

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Lieb-Mattis theorem

Lieb, Mattis (1962):
Heisenberg model on a bipartite lattice
antiferromagnetic coupling between A and B sites
arbitrary dimension

→ ground state is **non-degenerate** (apart from spin degeneracy)
$S_{tot}=0$ (singlet) if $N_A=N_B$, $S_{tot}=1/2(N_A-N_B)$ else

proof: "spin-reflection positivity" and Perron-Frobenius theorem

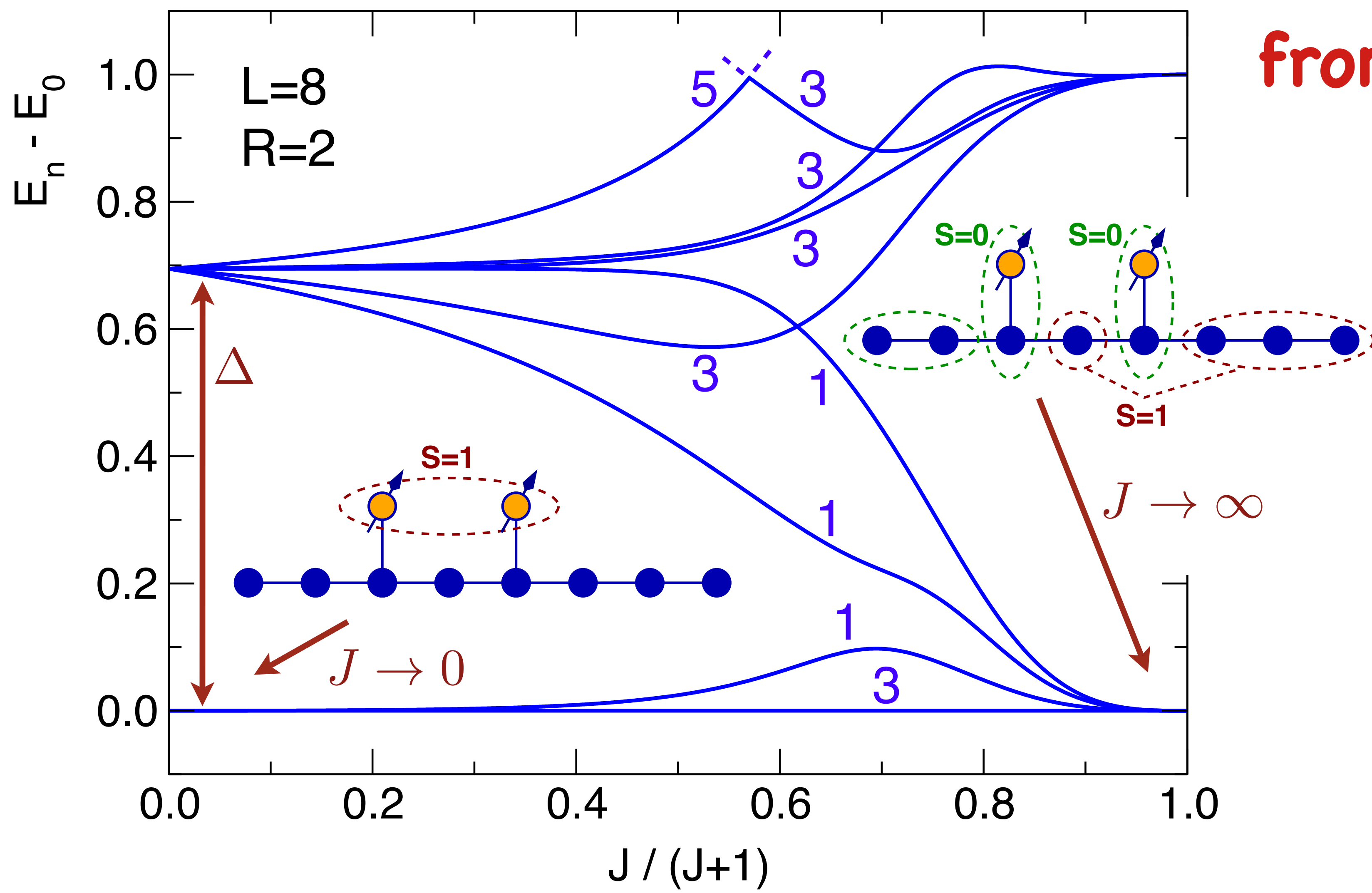
Lieb (1989):
generalization to the Hubbard model
(bipartite lattice, half-filling, arbitrary dimension)

Yanagisawa, Shimoi (1995), Shen (1996), Tsunetsugu (1997)
generalization to the correlated Kondo lattice model
(bipartite lattice, half-filling, arbitrary dimension)

→ unique ground state with $S_{tot}=1/2(N_A-N_B)$

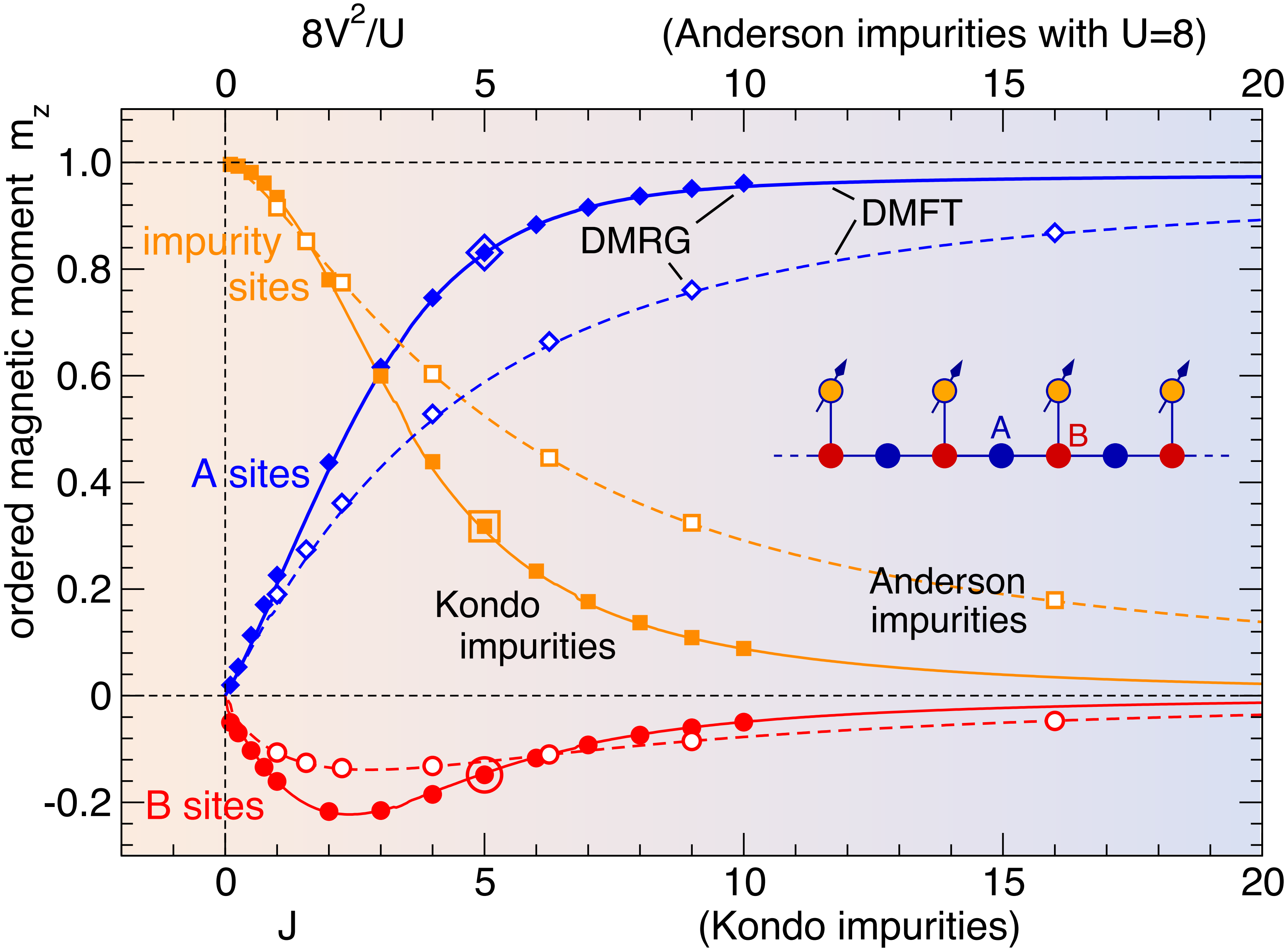
"Inverse" indirect magnetic exchange

from weak to strong J



- unique ground state
- local Kondo singlets: magnetically inert
- confinement of conduction electrons
- local moment formation
- magnetic coupling: IIME
- IIME mediated by virtual excitations of local Kondo singlets
- Kondo effect "helps"

Depleted Kondo lattice in D=1



RKKY limit ⟷ IIME limit

DMRG study:

- Kondo impurities and Anderson impurities
- L=49, R=25 spins commensurate with RKKY period
- convergence check: L=89, R=49
- $S_{tot}=(R-1)/2=\text{const.}$
- weak J: one spin is Kondo screened
- strong J: R-1 local moments coupled by IIME

A. Schwabe, I. Titvinidze, M.P., PRB 88, 121107(R) (2013)

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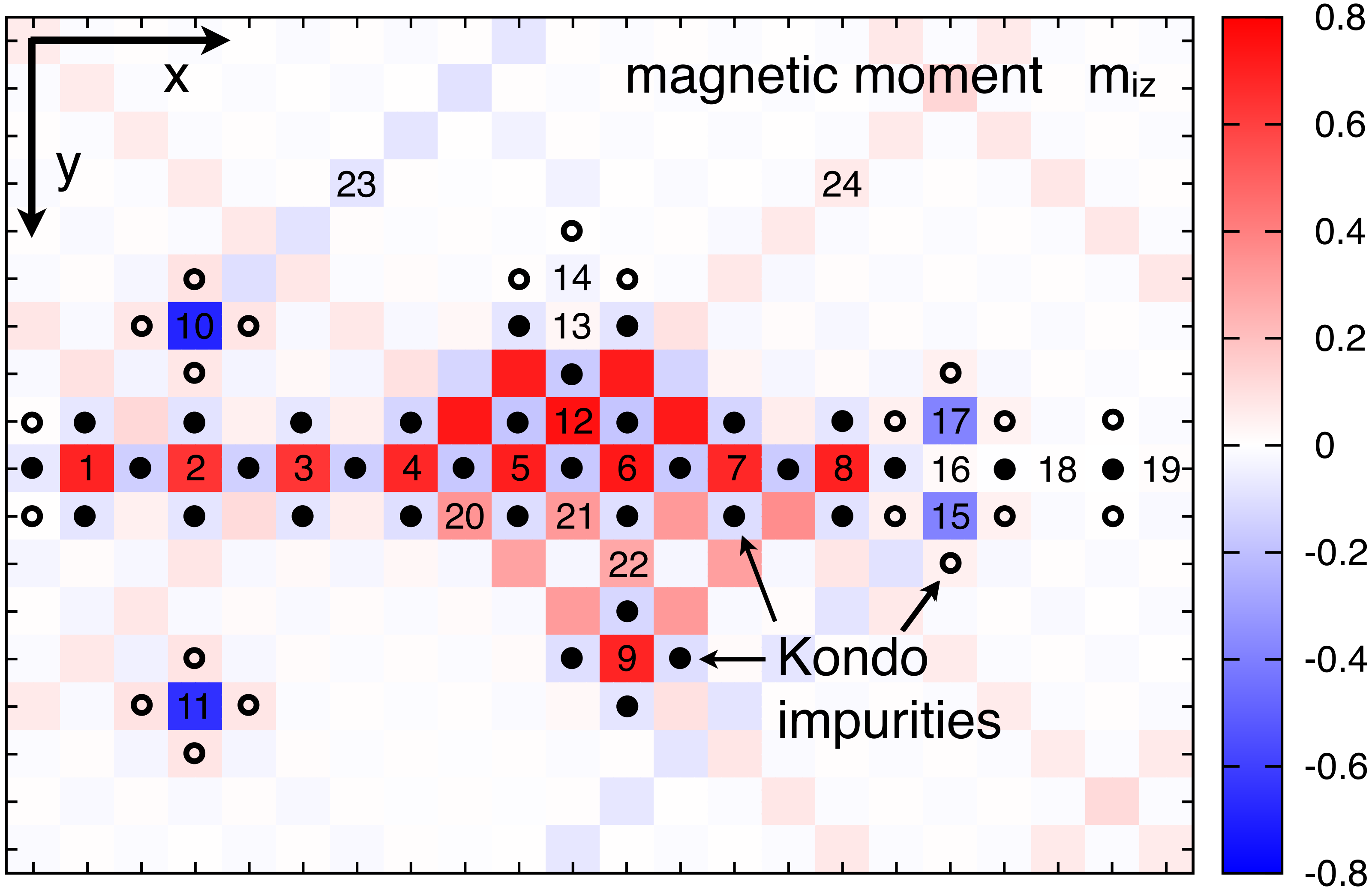
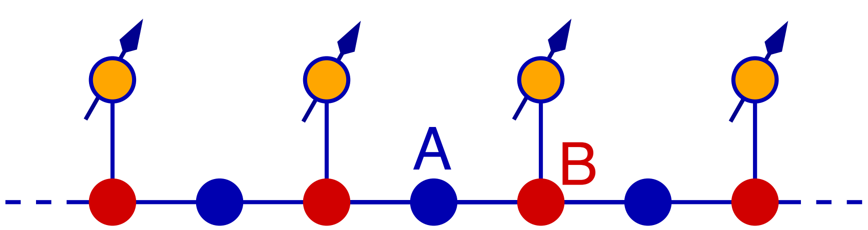
IIME in a 2D array



2D

1D



real-space DMFT:

magnetic adatoms on metal surface, strong J (J=5)

substrate: 18x22 array (PBC)

R=57 impurities

$N_A - N_B = 36-21=15$, $2S_{tot}=15.06$

IIME:

- ferromagnetic chain
- oscillatory distance dependence
- proximity effect
- confinement is essential
- odd-even effects
- interference pattern

"Inverse" indirect magnetic exchange

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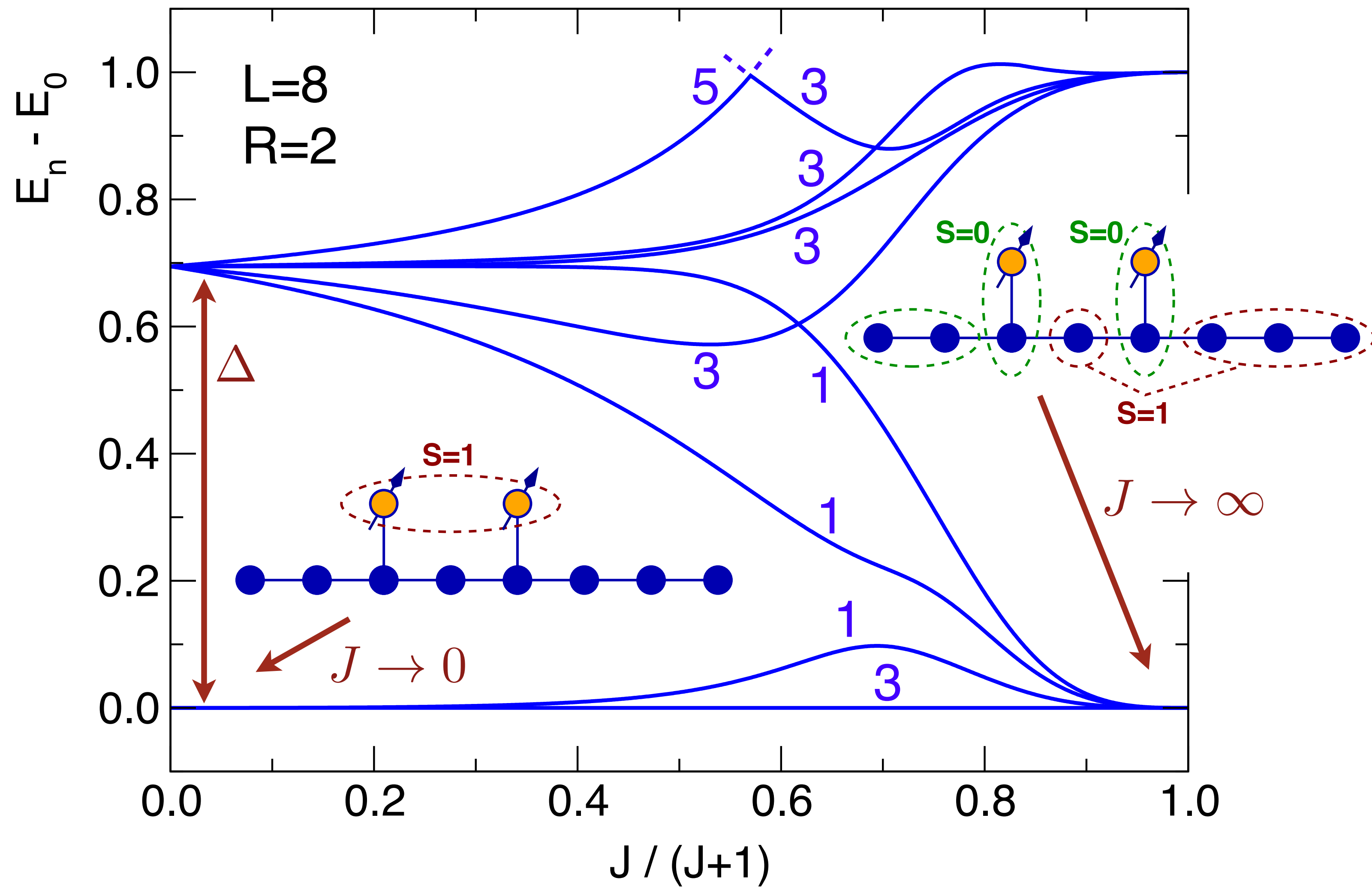

	weak J	strong J
effective low-energy theory:	$H_{\rm eff} = J_{\rm RKKY}\, \boldsymbol{S}_1 \boldsymbol{S}_2$	?

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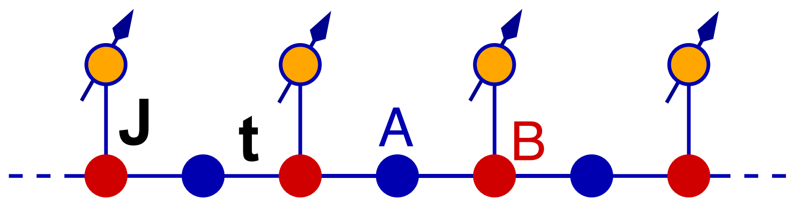
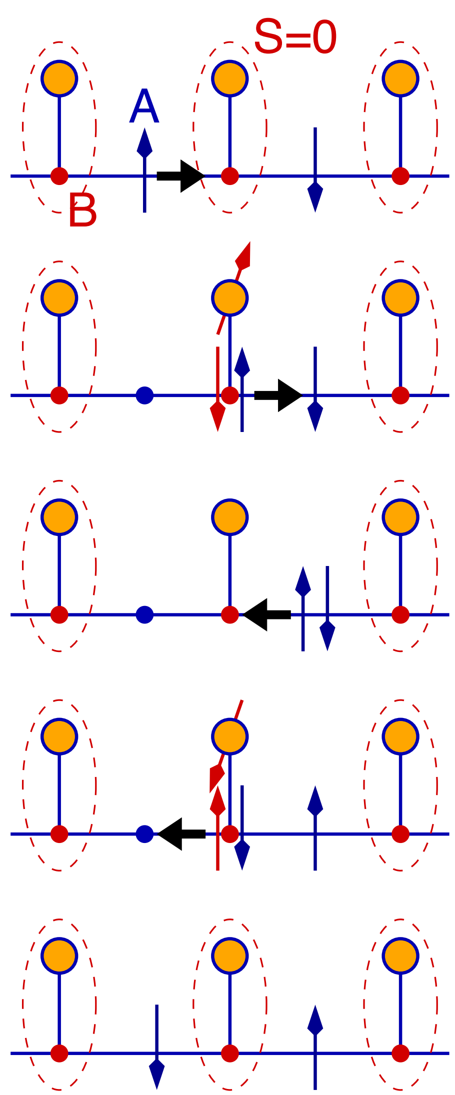
Strong-coupling perturbation theory

Kondo-lattice



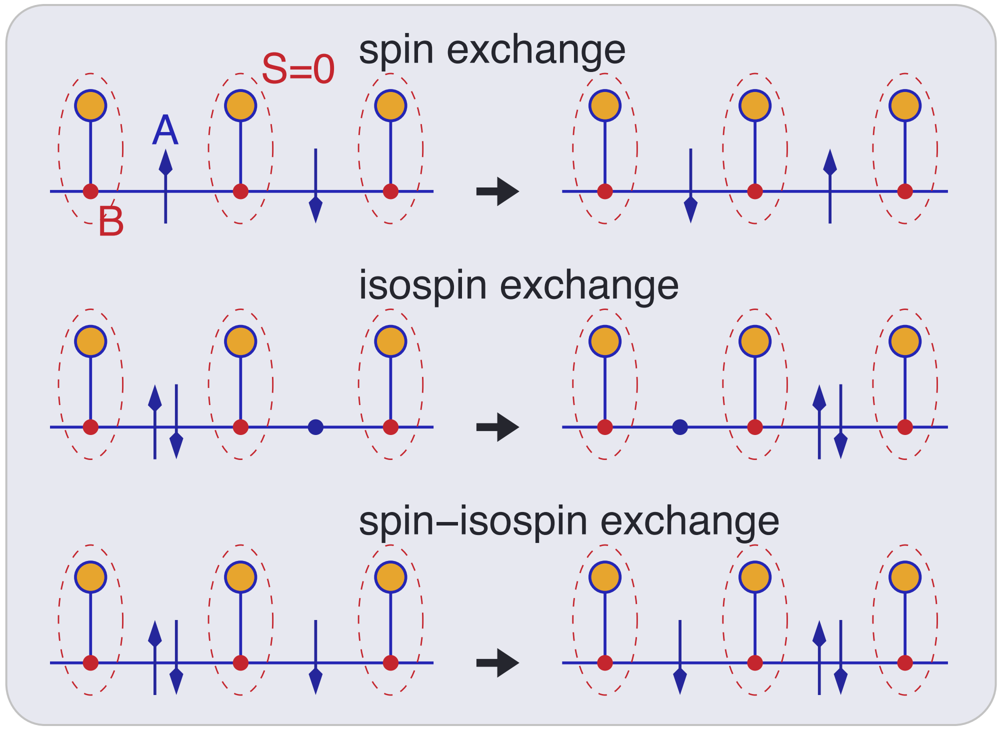
perturbation theory up to O(t/J)⁴



effective Hamiltonian

$$H_{\text{eff}}/\alpha = -\sum_{i<j\in A} (\mathbf{s}_i \mathbf{s}_j - \mathbf{t}_i \mathbf{t}_j) + \sum_{i\in A} (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2})$$

$$-\frac{1}{2} \sum_{i<j\in A} \sum_{\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + \text{H.c.})(1 - n_{i-\sigma} - n_{j-\sigma})$$



$$\alpha = \frac{64}{3}\frac{t^4}{J^3}$$

SO(4) = SU(2)xSU(2) symmetry

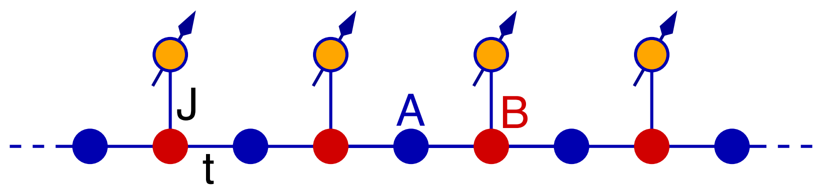
spin

$$\mathbf{s}_i = \frac{1}{2}(c^\dagger_{i\uparrow}, c^\dagger_{i\downarrow}) \cdot \boldsymbol{\sigma} \cdot \begin{pmatrix} c_{i\uparrow} \\ c_{i\downarrow} \end{pmatrix}$$

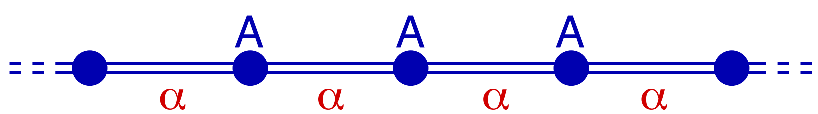
isospin

$$\mathbf{t}_i = \frac{1}{2}(c^\dagger_{i\uparrow}, (-1)^i c_{i\downarrow}) \cdot \boldsymbol{\sigma} \cdot \begin{pmatrix} c_{i\uparrow} \\ (-1)^i c^\dagger_{i\downarrow} \end{pmatrix}$$

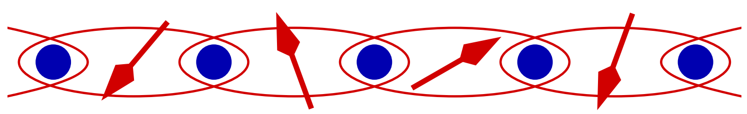
Effective Hamiltonian



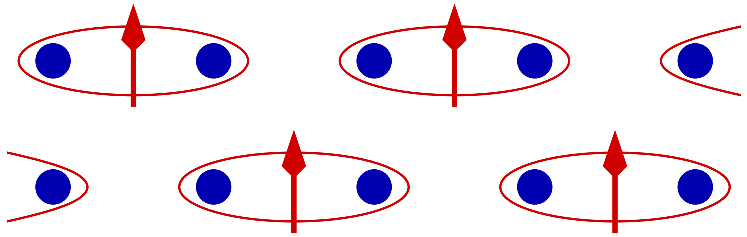
$$\mathcal{H} = -t \sum_{\langle i,j\rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} + J \sum_{r=1}^{R} \mathbf{s}_{i_r} \mathbf{S}_r \, .$$



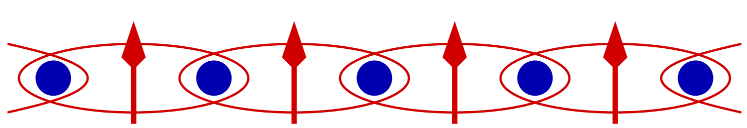
$$H_{\mathrm{eff}}/\alpha = -\sum_{i<j\in A} (\mathbf{s}_i \mathbf{s}_j - \mathbf{t}_i \mathbf{t}_j) + \sum_{i\in A} (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2})$$
$$-\frac{1}{2} \sum_{i<j\in A} \sum_{\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + \mathrm{H.c.})(1 - n_{i-\sigma} - n_{j-\sigma})$$



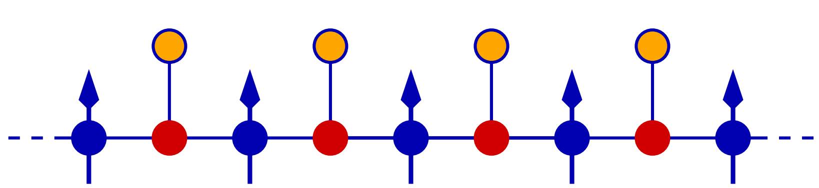
$$H_{\mathrm{eff}} = -\frac{4\alpha}{3} \sum_{\mathrm{bonds}} \mathbf{S}^2_{\mathrm{bond}}$$ bond-spin representation



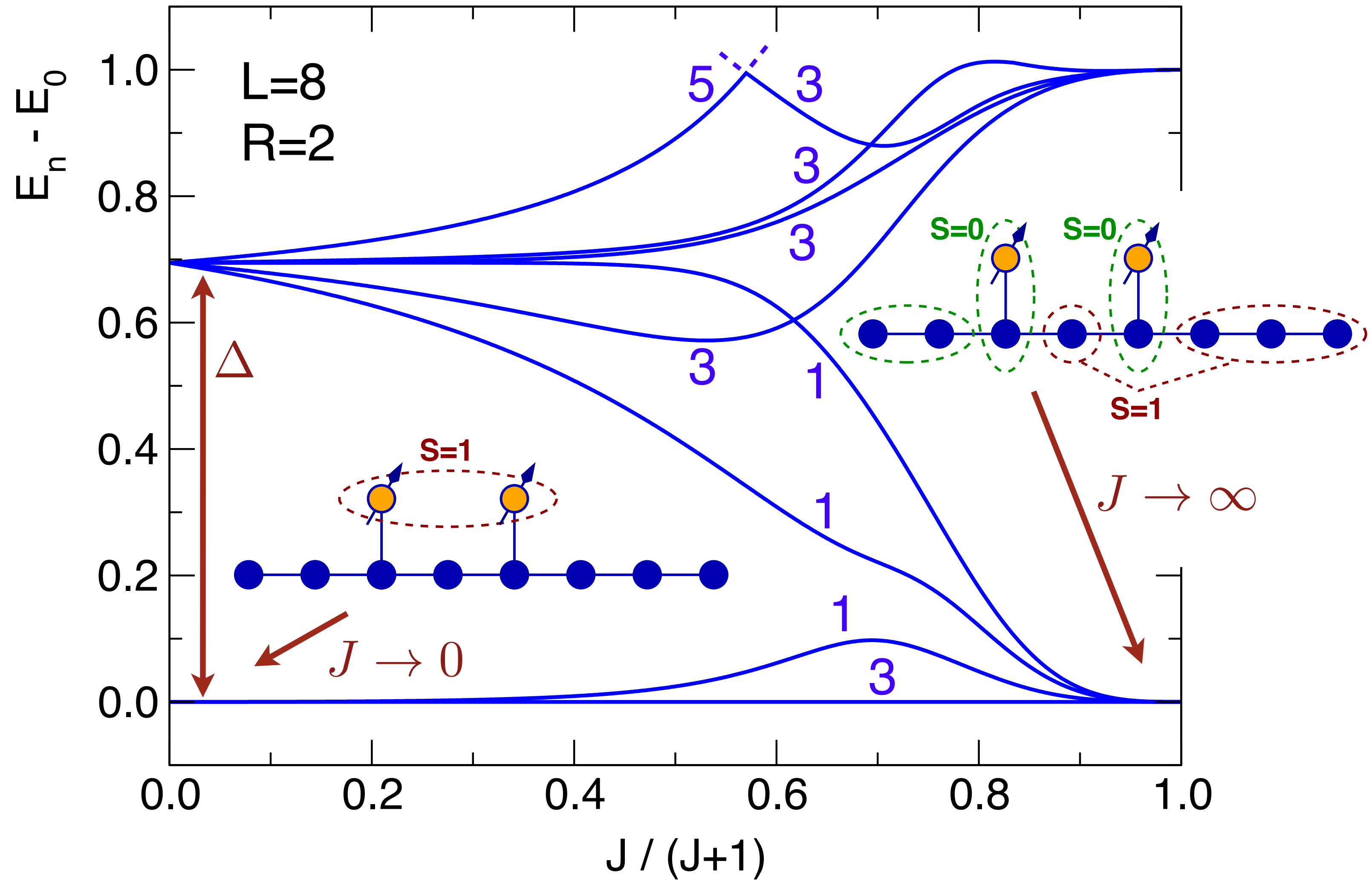
$$H_{\mathrm{eff}} = H_{\mathrm{A},1} + H_{\mathrm{A},2}$$



ferromagnetic ground state



Bond-spin representation



	weak J	strong J
effective low-energy theory:	$H_{\text{eff}} = J_{\text{RKKY}}\, \boldsymbol{S}_1 \boldsymbol{S}_2$	$H_{\text{eff}} = -\frac{4\alpha}{3} \sum_{\text{bonds}} \mathbf{S}^2_{\text{bond}}$

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Static mean-field theory for H_{eff} at T>0

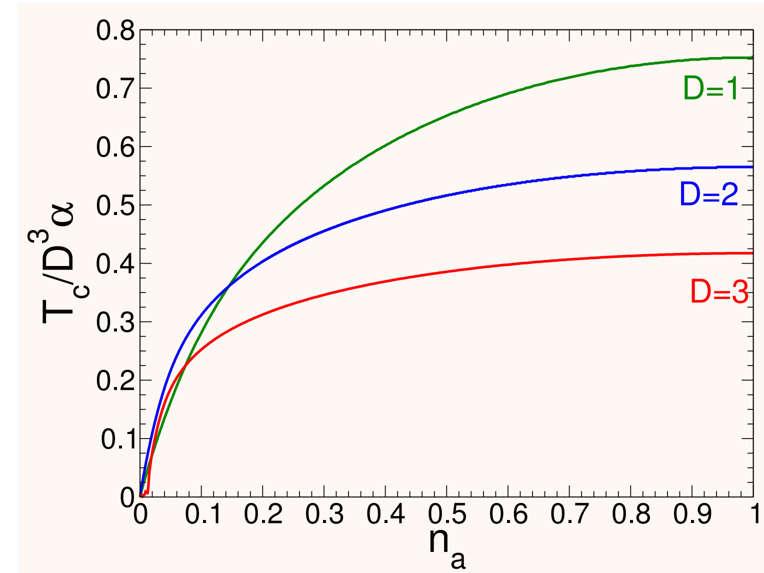
mean-field decoupling:

$$c^\dagger c^\dagger c c \longrightarrow \langle c^\dagger c\rangle c^\dagger c + c^\dagger c \langle c^\dagger c\rangle - \langle c^\dagger c\rangle\langle c^\dagger c\rangle$$

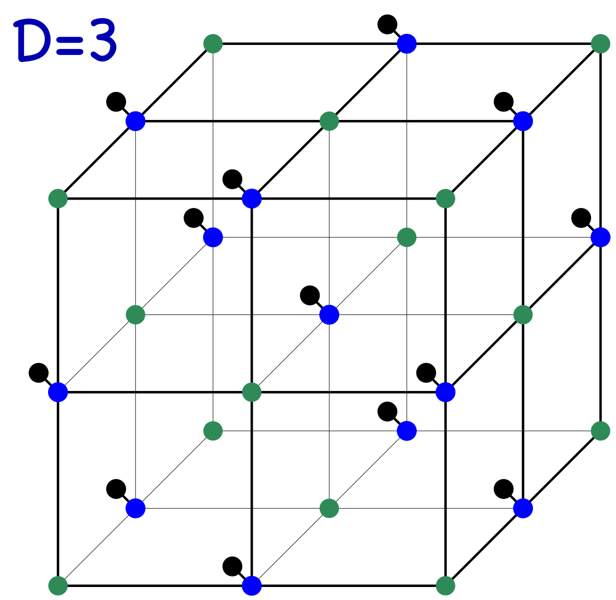
4-th order perturbation theory

$$H_{\mathrm{eff}} = -\frac{\alpha}{4}\sum_{i\in B}\left[2D \sum_{j_1,j_2\in A_i}\sum_{\sigma} c^\dagger_{j_1,\sigma}c_{j_2,\sigma} - 2\sum_{j_1,j_2,j_3,j_4\in A_i} c^\dagger_{j_1,\uparrow}c_{j_2,\uparrow}c^\dagger_{j_3,\downarrow}c_{j_4,\downarrow}\right]$$

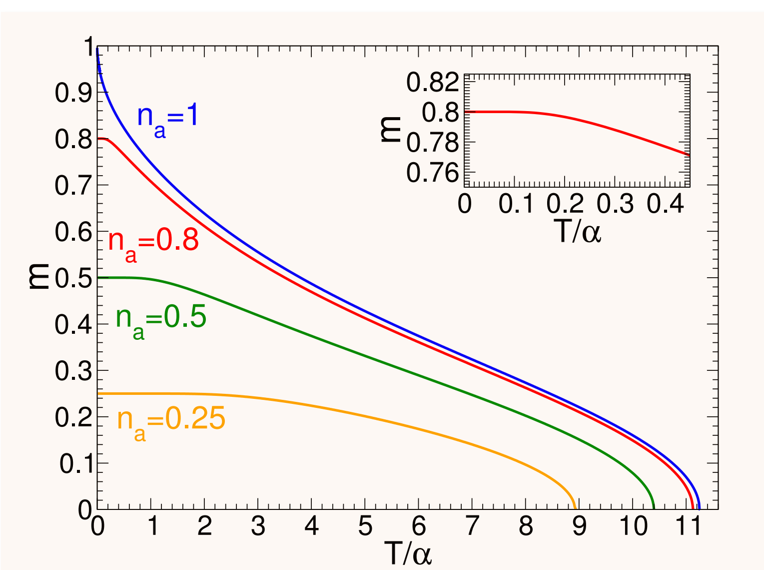
T_C >> coordination



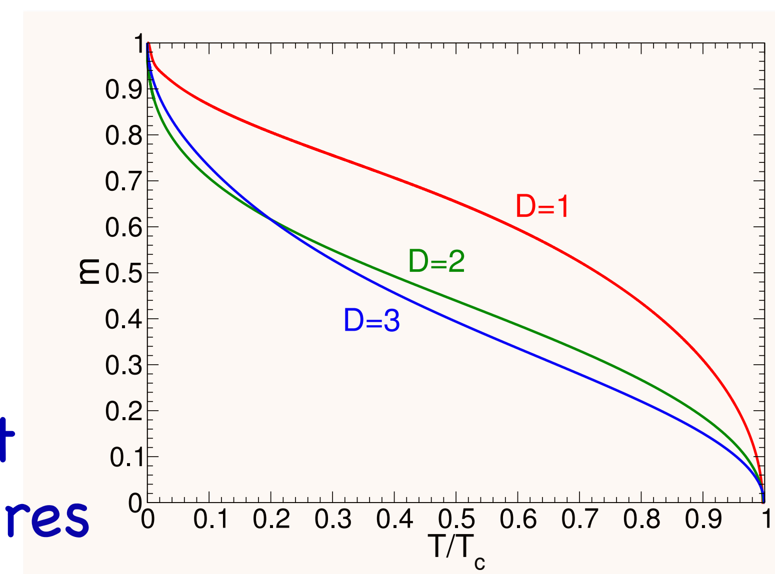
D=3



off half-filling:
fully polarized state at T=0
T_C decreases



half-filling:
upturn of m at low temperatures



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Static mean-field theory for H_{eff} at T>0

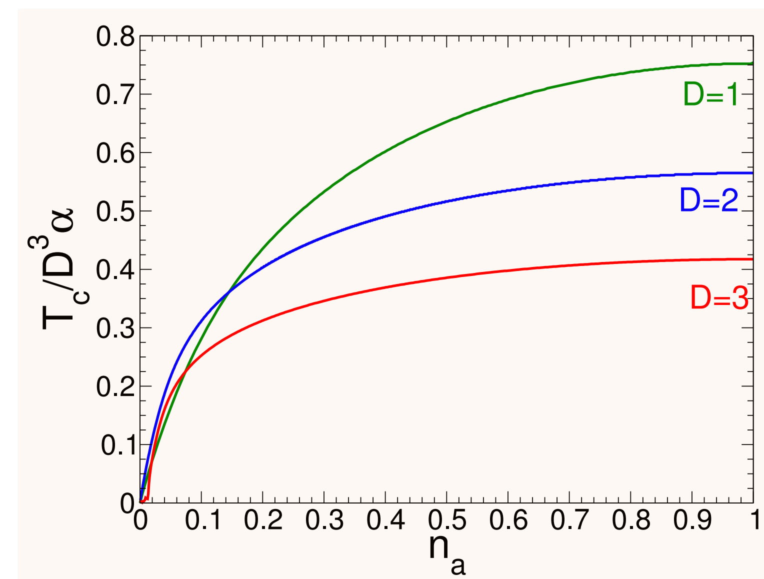
mean-field decoupling:

$$c^\dagger c^\dagger c c \longrightarrow \langle c^\dagger c \rangle c^\dagger c + c^\dagger c \langle c^\dagger c \rangle - \langle c^\dagger c \rangle \langle c^\dagger c \rangle$$

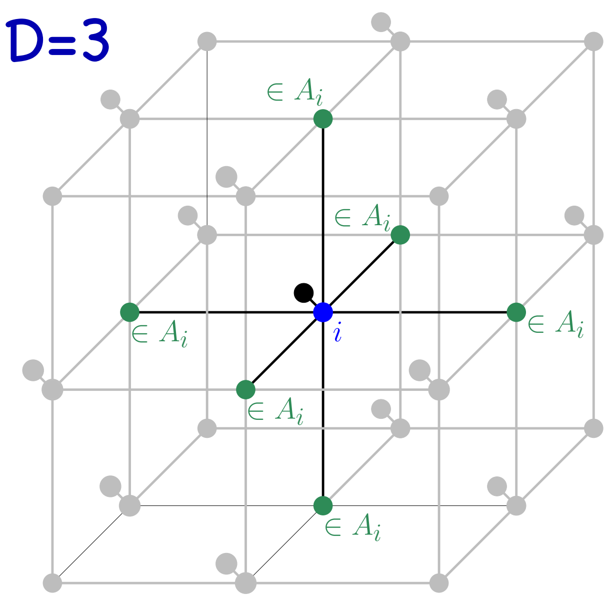
4-th order perturbation theory

$$H_{\rm eff} = -\frac{\alpha}{4} \sum_{i \in B} \left[2D \sum_{j_1, j_2 \in A_i} \sum_{\sigma} c^\dagger_{j_1,\sigma} c_{j_2,\sigma} - 2 \sum_{j_1,j_2,j_3,j_4 \in A_i} c^\dagger_{j_1,\uparrow} c_{j_2,\uparrow} c^\dagger_{j_3,\downarrow} c_{j_4,\downarrow} \right]$$

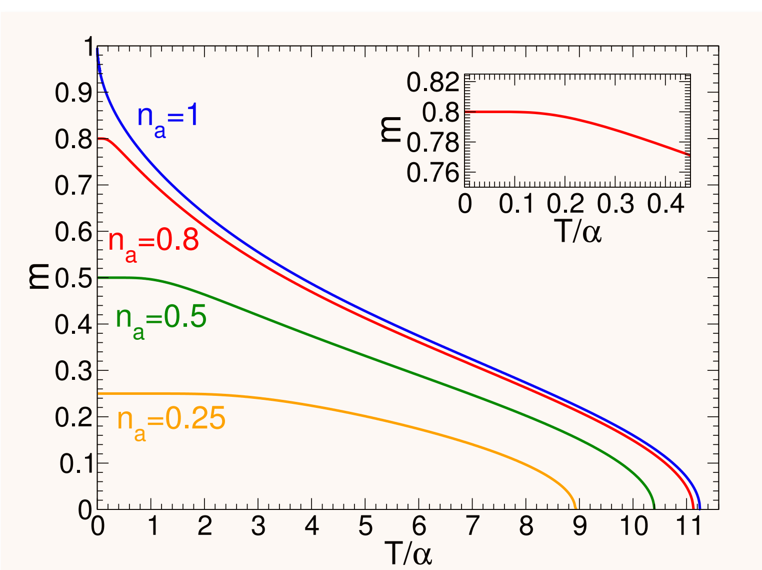
T_C >> coordination



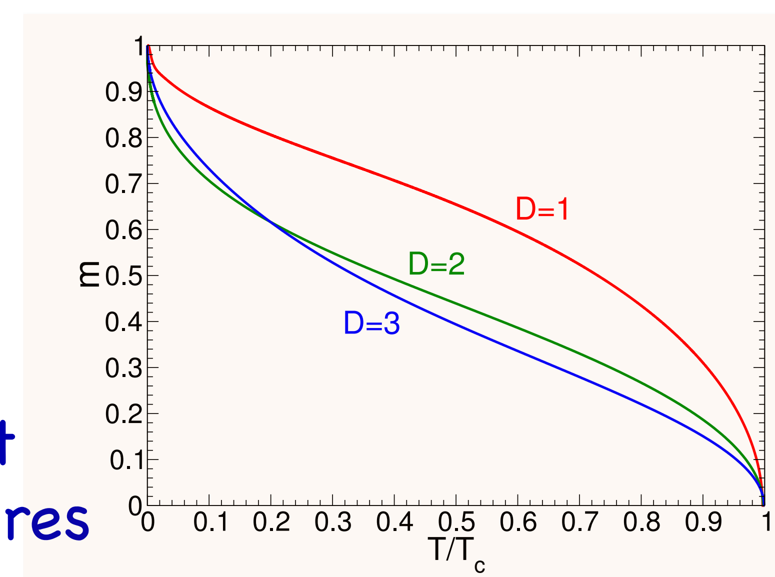
D=3



off half-filling:
fully polarized state at T=0
T_C decreases

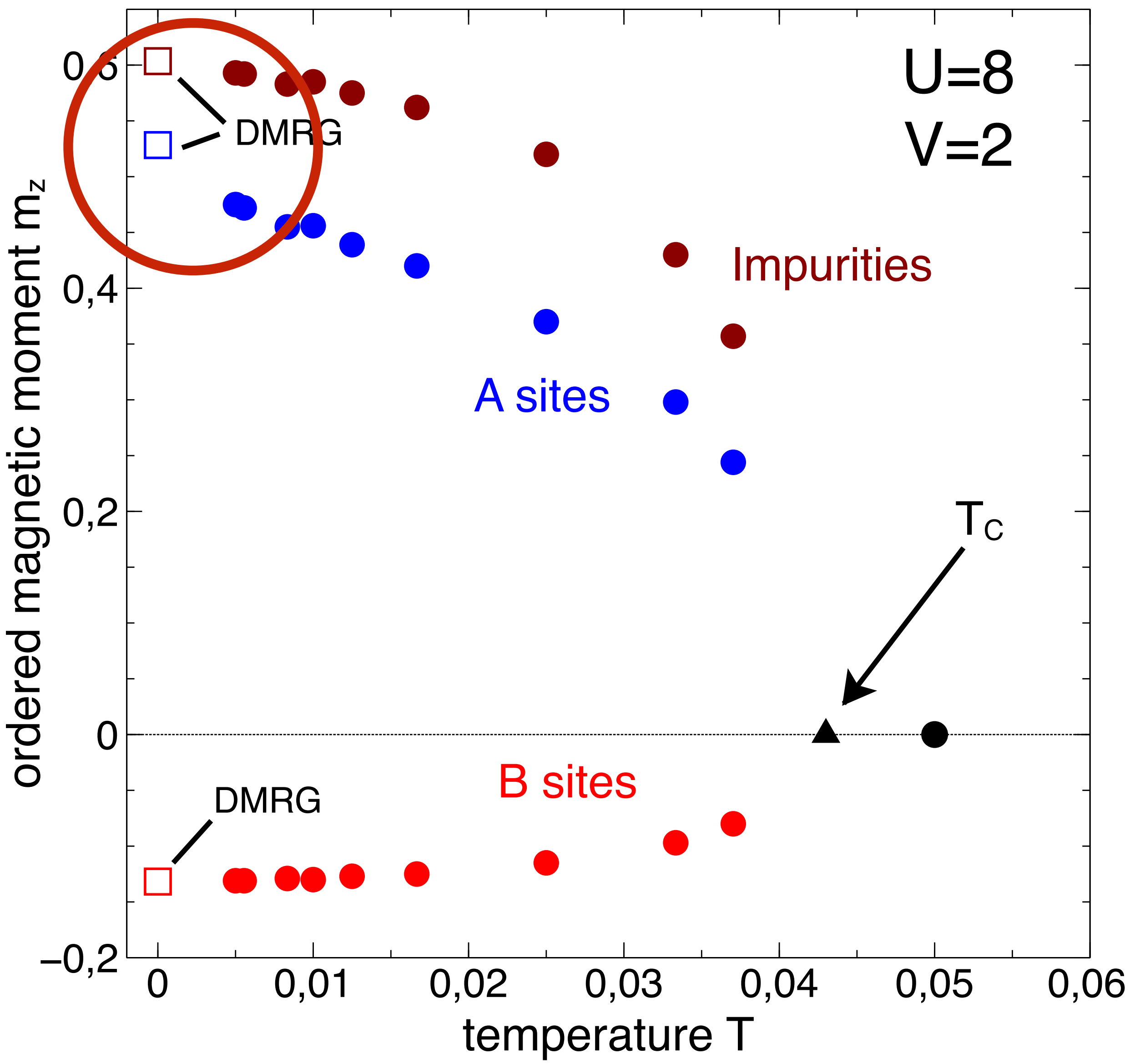


half-filling:
upturn of m at
low temperatures

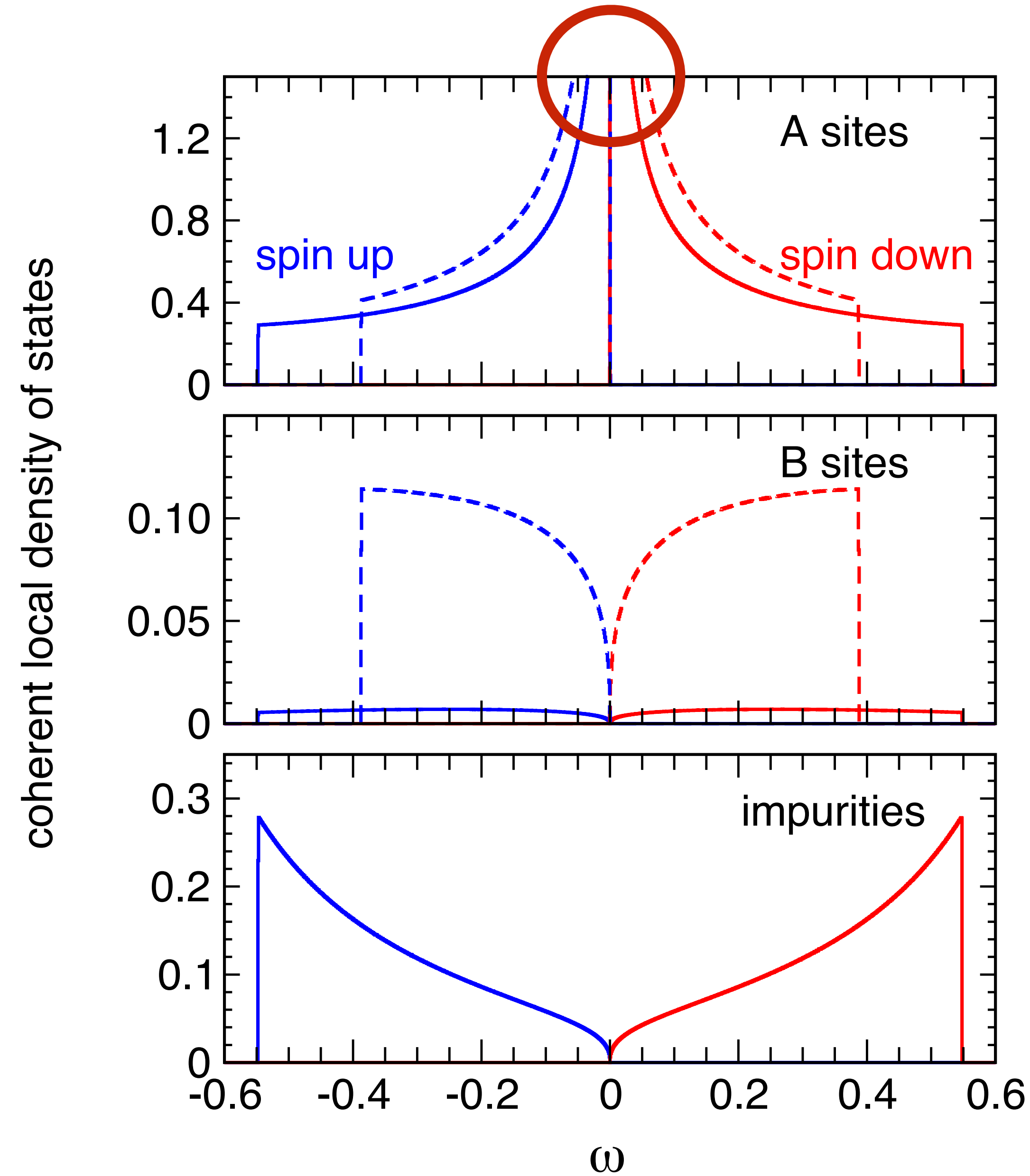


Depleted Anderson model: DMFT-QMC

full DMFT-CT-QMC-hyb-segment calculation for the depleted Anderson model



DMFT-ED at T=0: low-energy excitation spectrum



M. Aulbach, I. Titvinidze, M.P., t.b.p.

I. Titvinidze, A. Schwabe, M.P., arXiv:1402.6657

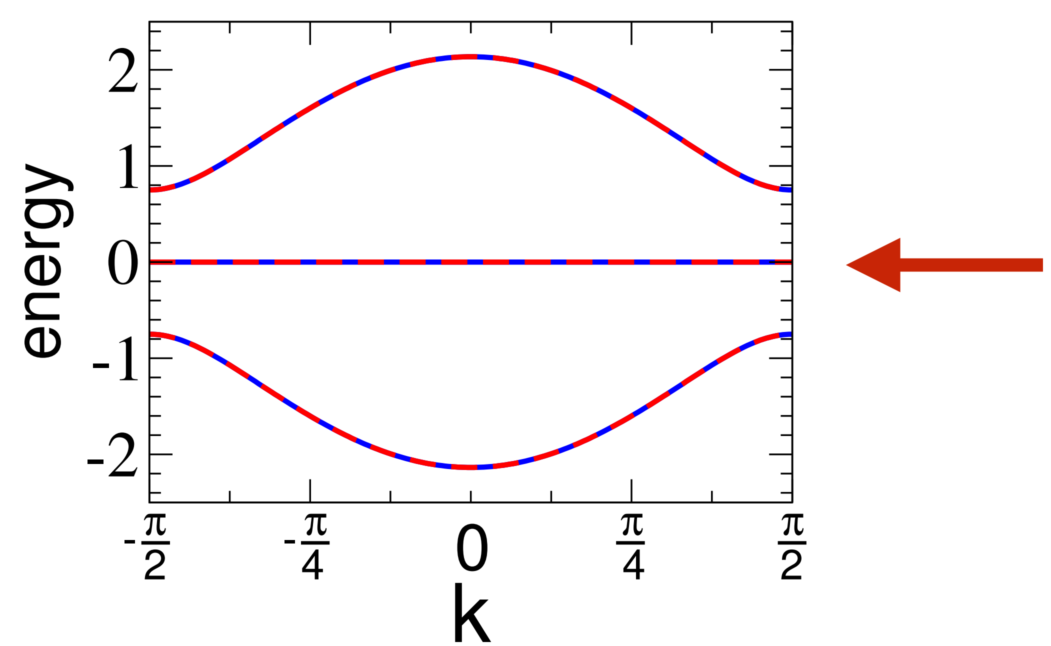
Flat band

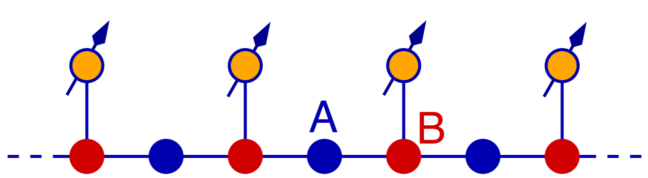
"flat-band ferromagnetism"

Mielke (1991), Tasaki (1992)

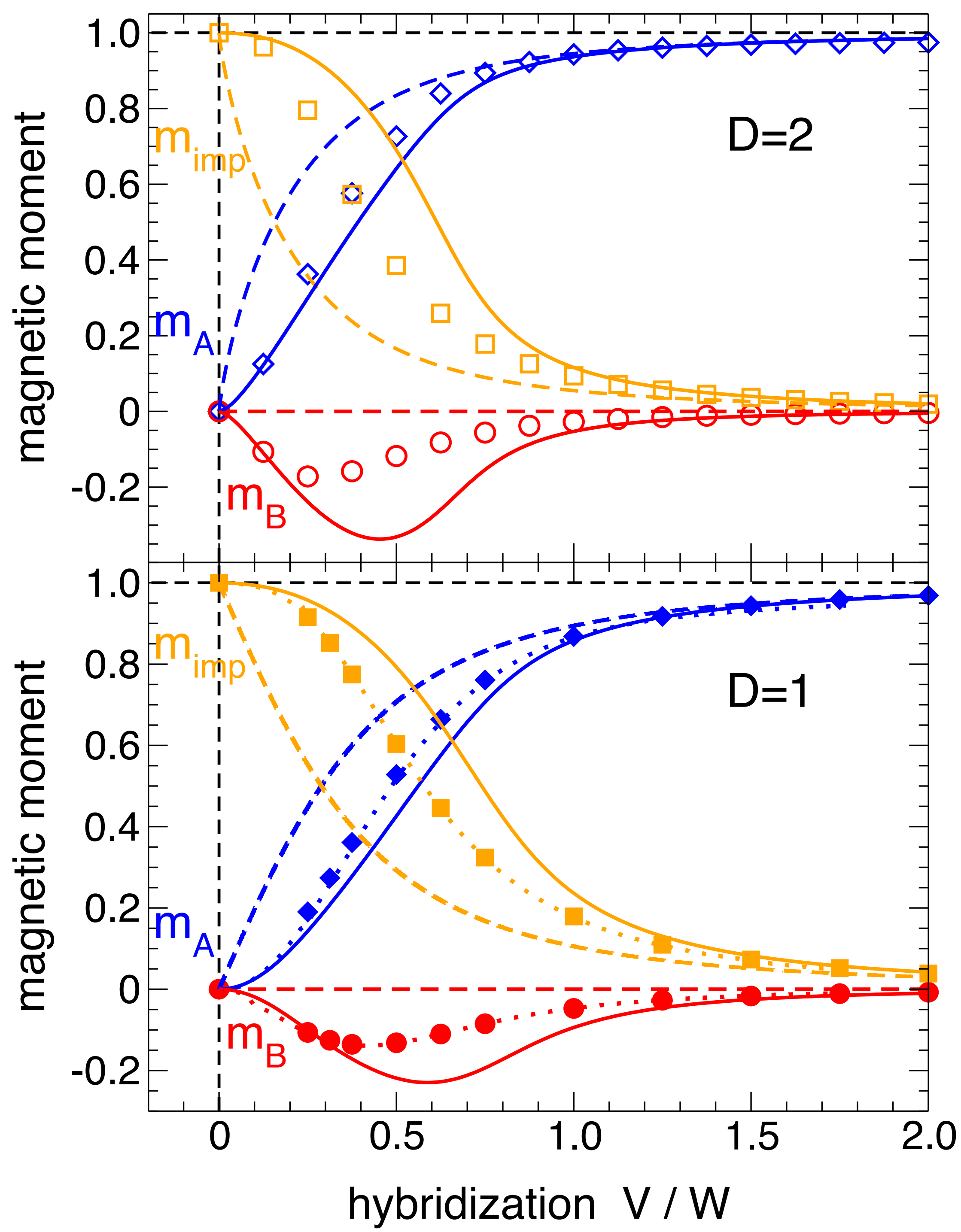
- in certain geometries, not necessarily bipartite lattices
- ground state is a polarized uncorrelated Fermi sea even at U>0

free band structure:





Hartree-Fock vs. DMRG/DMFT



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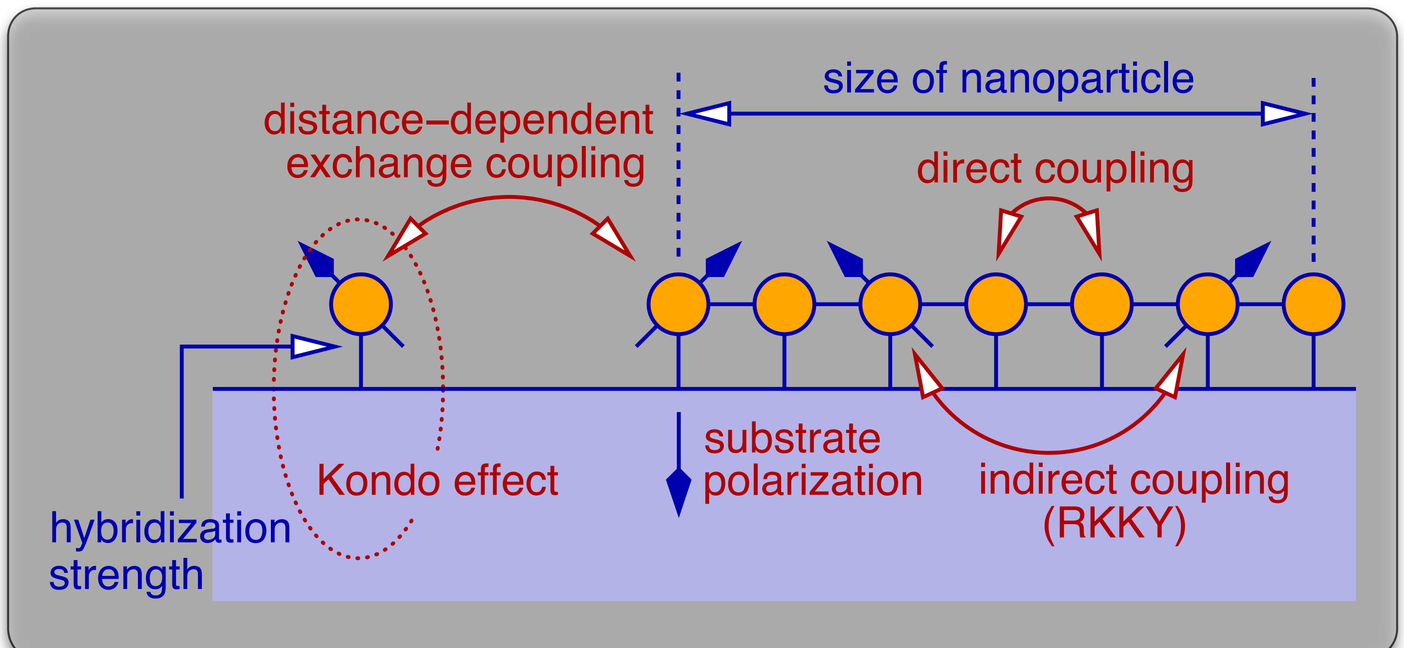
Inverse Indirect Magnetic Exchange



conclusions

- Kondo effect vs. indirect exchange: new phenomena due to confinement
- IIME: Kondo effect helps (rather than competes)
- effective Hamiltonian: spins on bonds, plaquettes, ...
- comprises the predictions of the Lieb-Mattis theorem
- different from flat-band ferromagnetism

$$H_{\rm eff} = -\frac{4\alpha}{3} \sum_{\rm bonds} \mathbf{S}^2_{\rm bond}$$