KONDO BREAKDOWN AND MAGNETIC MOMENT REVIVAL IN MULTI-ORBITAL ANDERSON LATTICES

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- **motivation - towards a unified understanding of strange metals**
- **Kondo lattice and Kondo breakdown**
- **local moment revival in dilute Kondo lattices (preliminary results)**

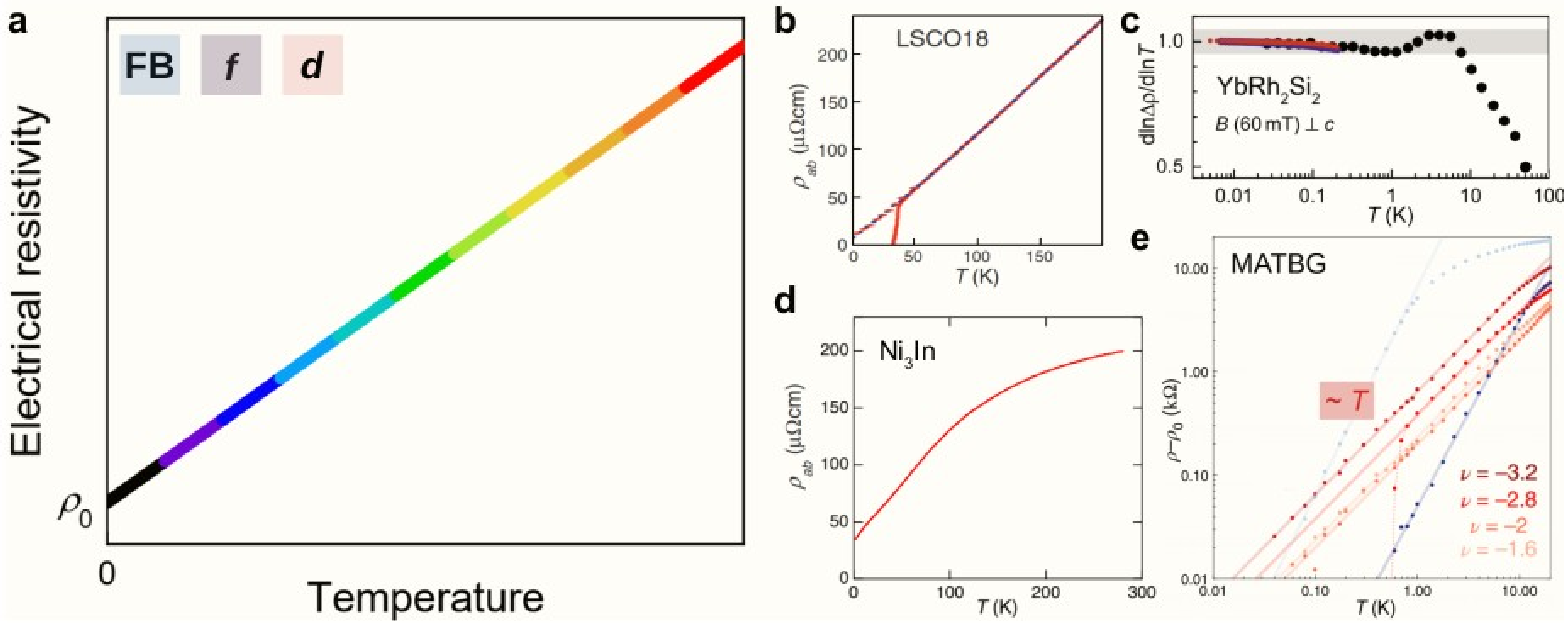
DLR

Towards a unified understanding of strange metals

strange metal phenomena are observed across different material platforms

- linear-in-temperature electrical resistivity

flat band systems
transition metal compounds
f-based compounds



Joseph G. Checkelsky, B. Andrei Bernevig, Piers Coleman, Qimiao Si, Silke Paschen, **arXiv:2312.10659**

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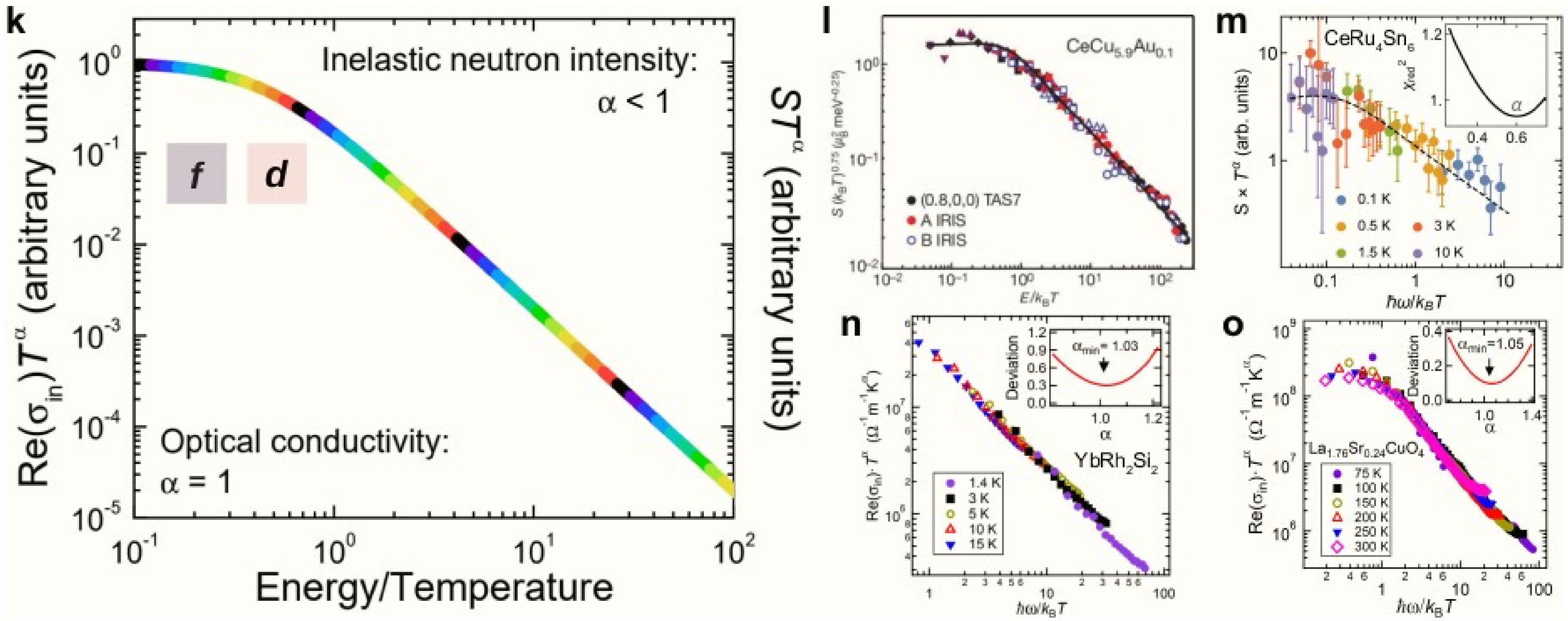

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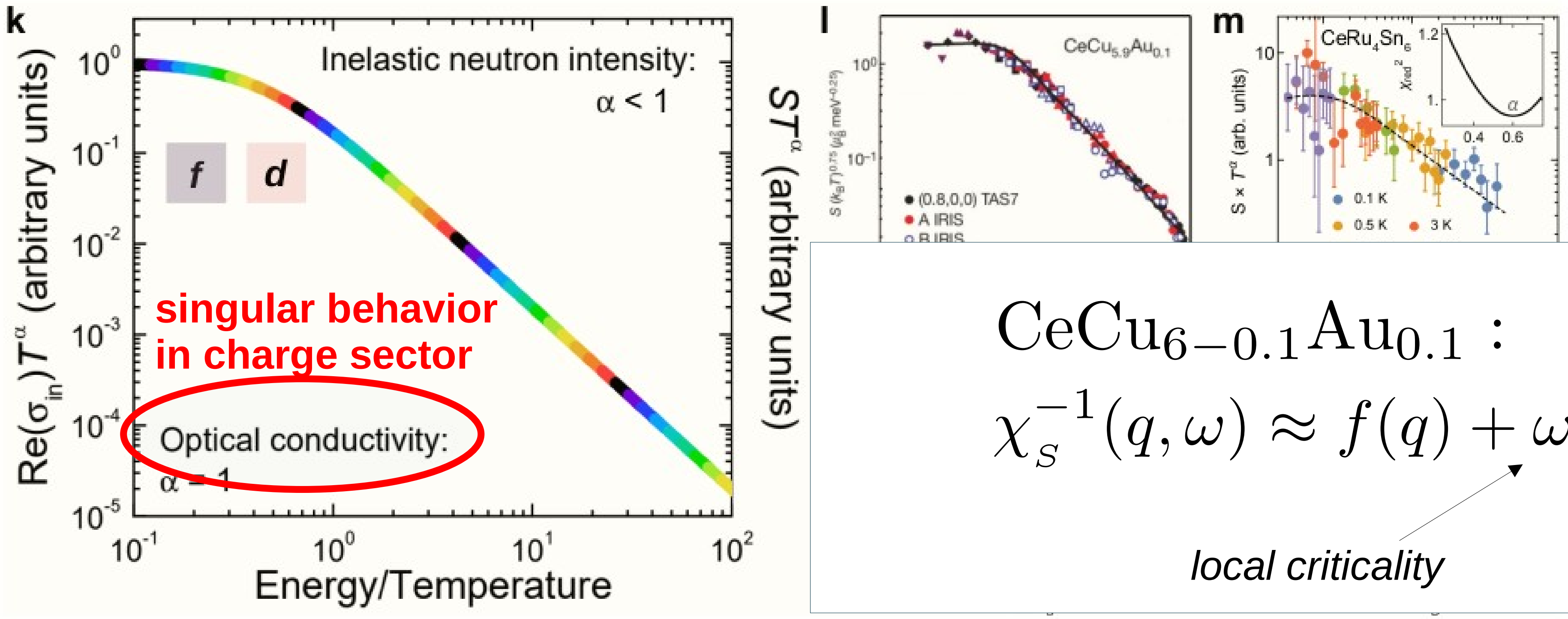

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local criticality

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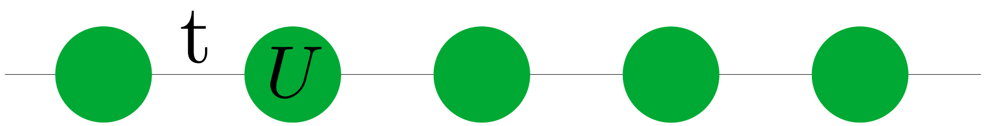
recap: Mott transition and DMFT



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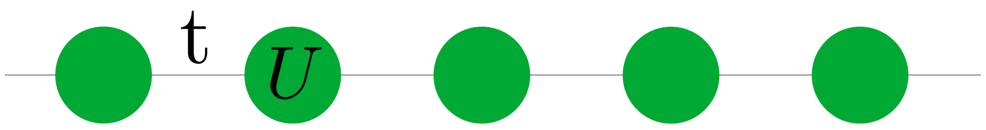

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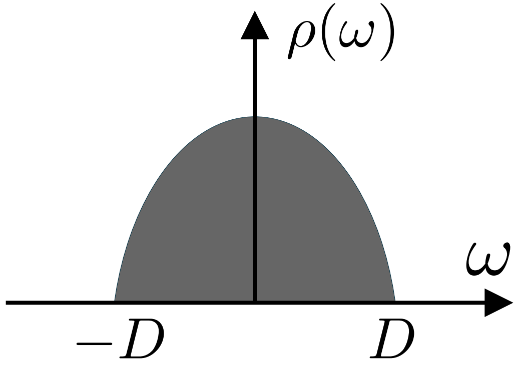
How to connect these limits?

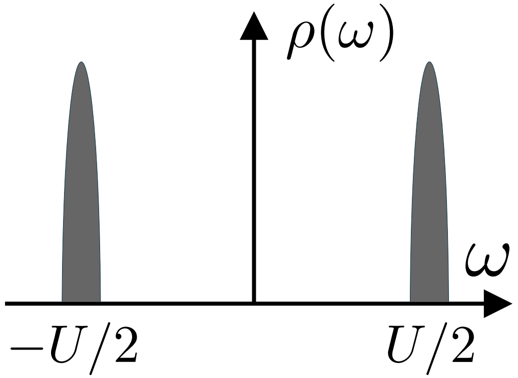
$$D/U \gg 1$$

metal



$$D/U \ll 1$$

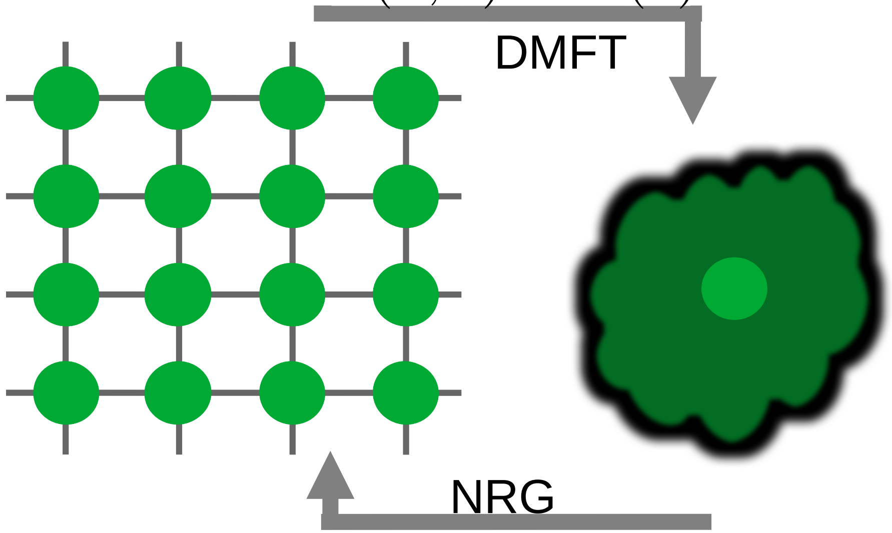
insulator



recap: Mott transition and DMFT

$\Sigma(k,z) \approx \Sigma(z)$ - exact on Bethe lattice or infinite dimensionality

$$\mathcal{G}^{\mathrm{lat}}(z) = \int \frac{d\vec{k}}{z - \epsilon_{\vec{k}} - \Sigma(k,z)}$$



$$\mathcal{G}^{\mathrm{imp}}(z) = \frac{1}{z - \Delta(z) - \Sigma(z)}$$

DMFT self consistency condition

$$\mathcal{G}^{\mathrm{lat}}(z) = \mathcal{G}^{\mathrm{imp}}(z)$$

$$\Delta(z) = z - \Sigma(z) - [\mathcal{G}^{\mathrm{lat}}(z)]^{-1}$$

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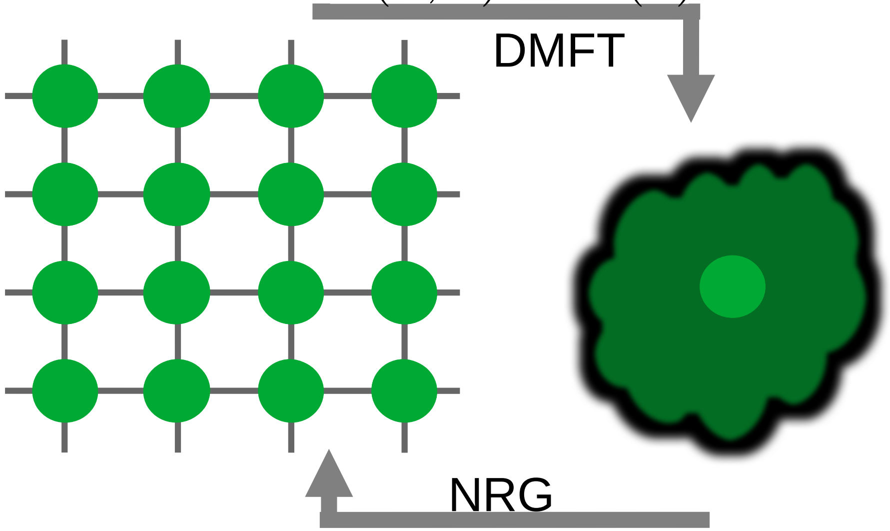

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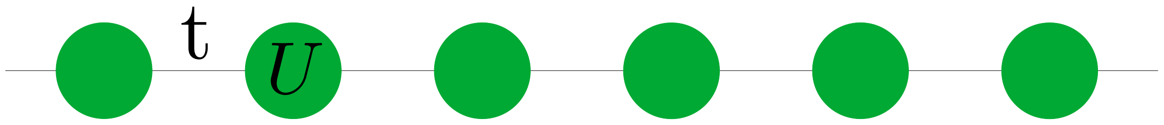
DMFT removes magnetism from phase diagram

recap: Mott transition and DMFT



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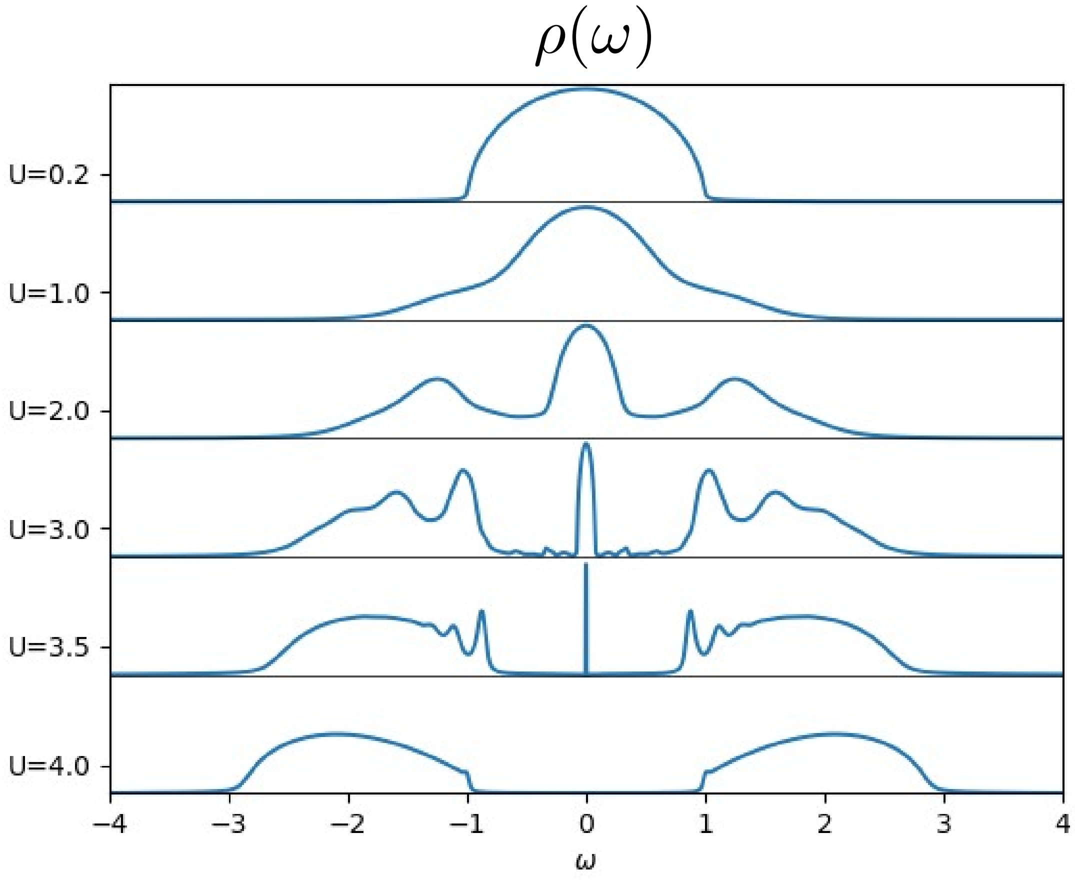
Hubbard model – Mott transition:

- U=0 ⟶ metal
- U>>t ⟶ insulator

localization due to strong interactions!
without the need of magnetic order!!



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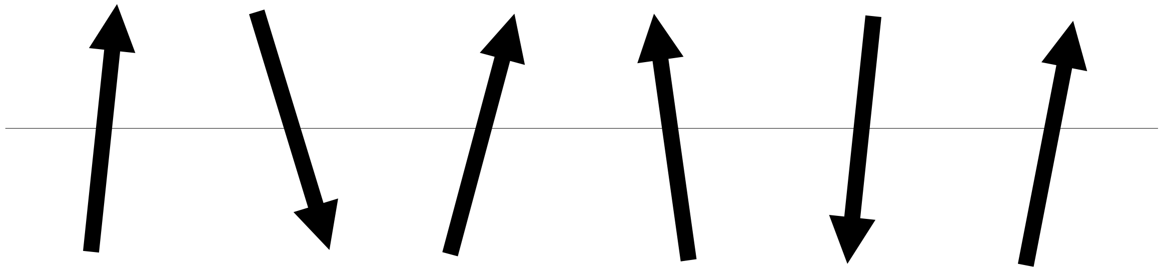

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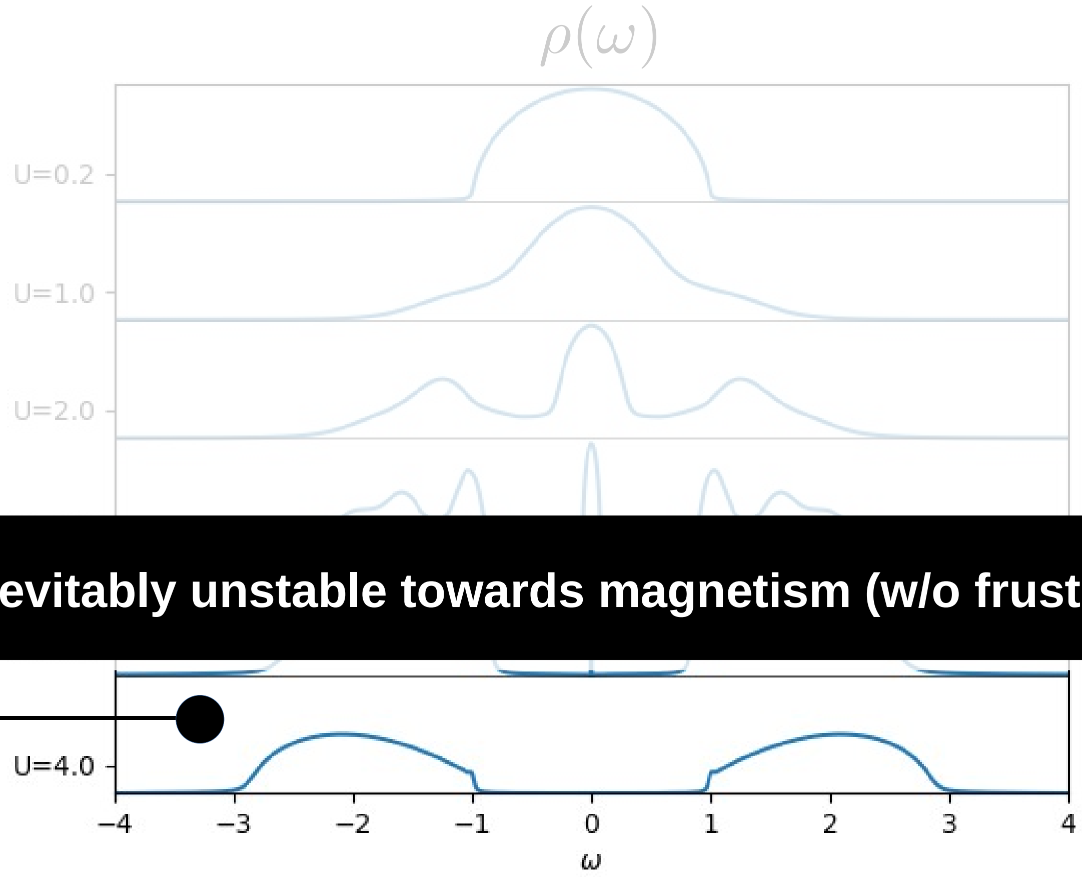
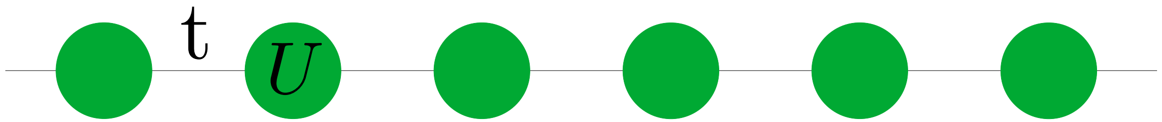


inevitably unstable towards magnetism (w/o frustration)

localization due to strong interactions!
without the need of magnetic order!!

recap: Mott transition and DMFT



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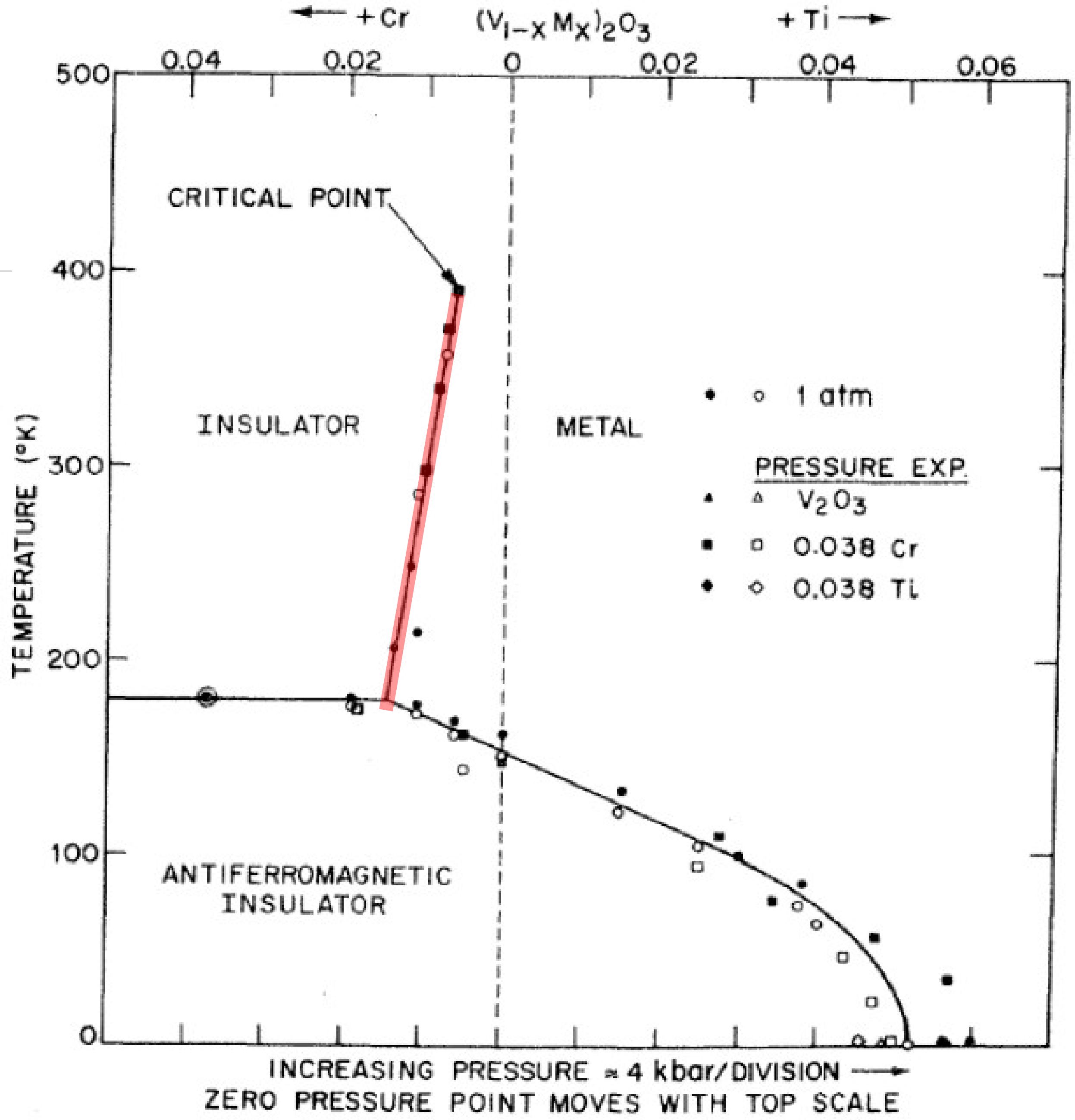

from McWhan *et al.*, Phys. Rev. B (1973)

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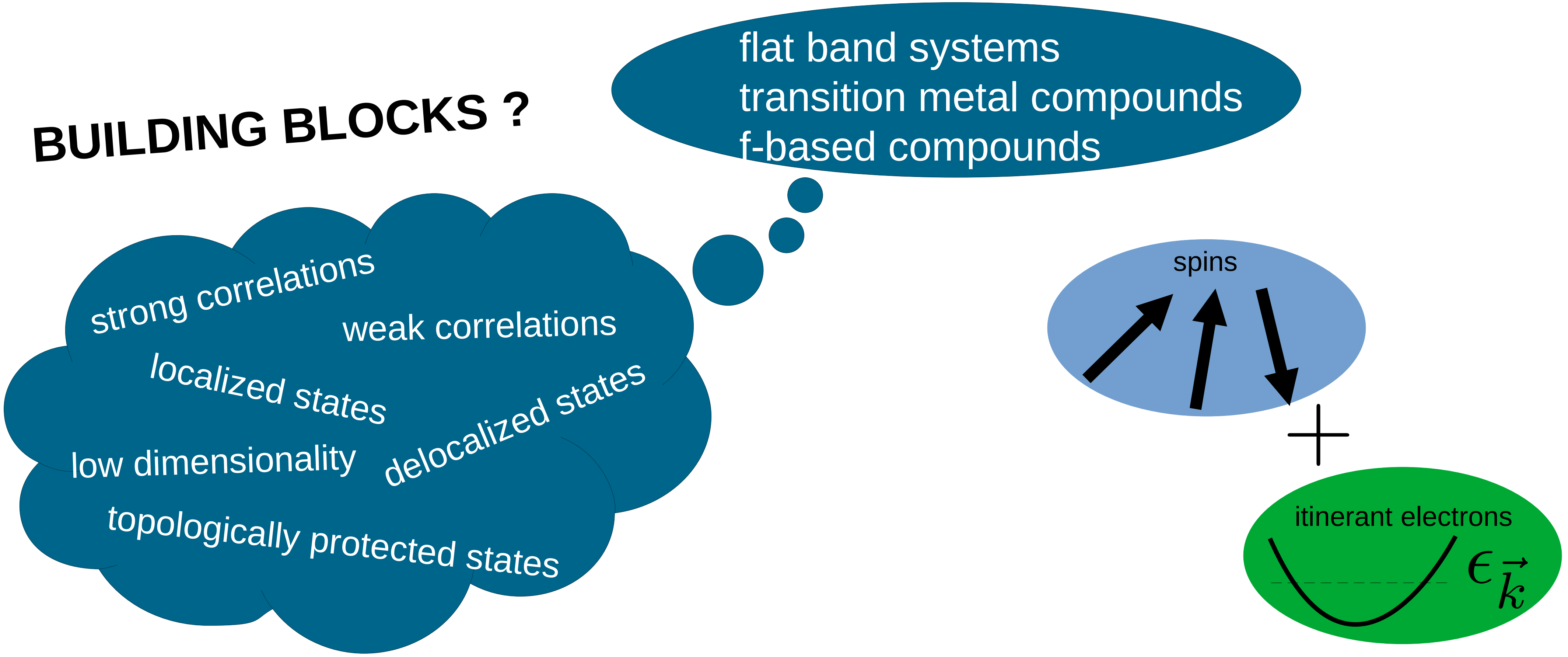
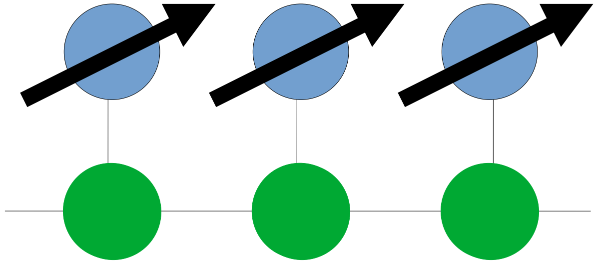


Lets put that on a lattice: PAM / KL



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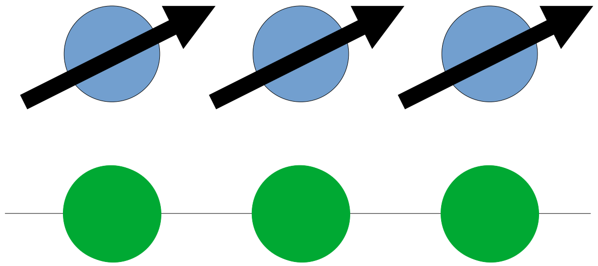
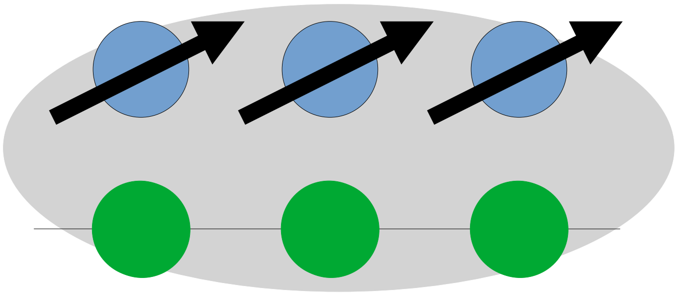


$T > T_0$

strong coupling →



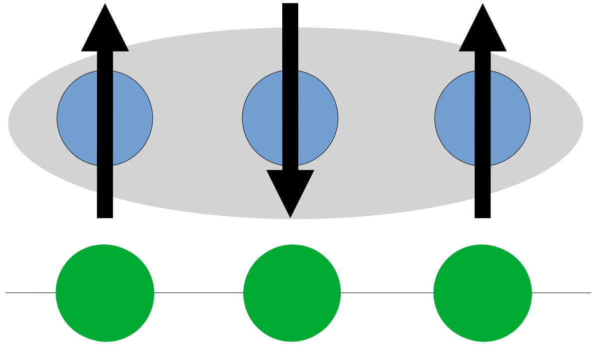
$T < T_0$

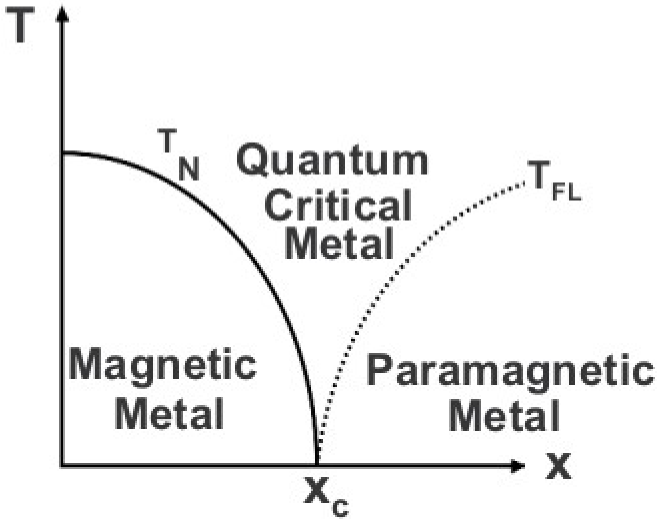
spins get eaten up by conduction band electrons

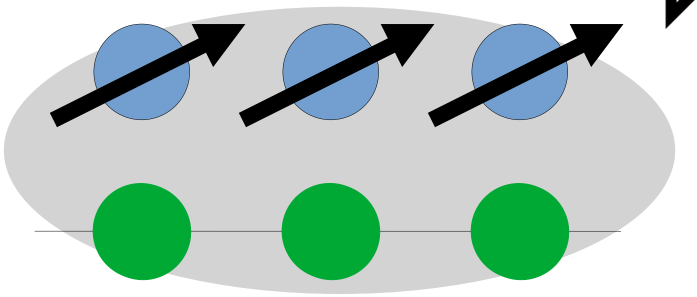
Kondo effect / emergence of heavy quasiparticles

can we break up these new quasiparticles ?

Kondo breakdown / orbital-selective Mott transition







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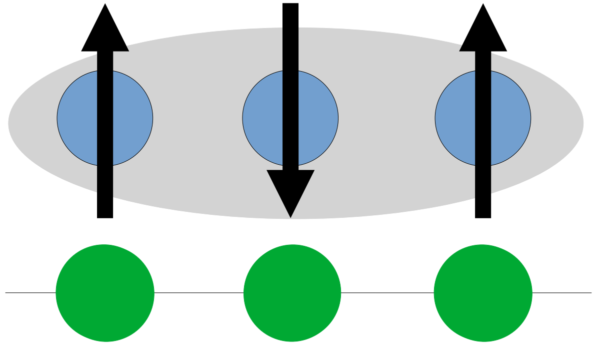
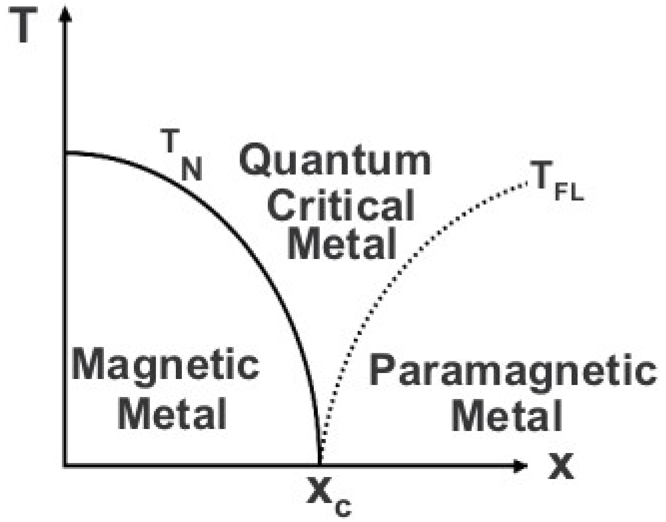
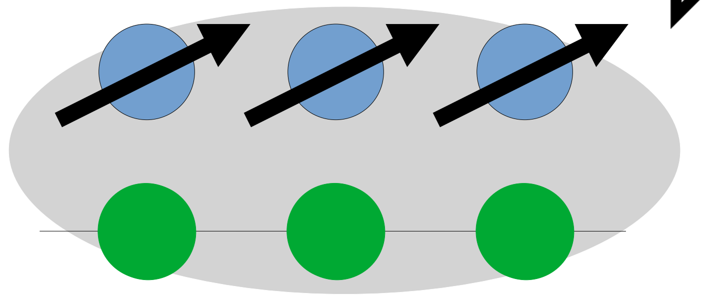


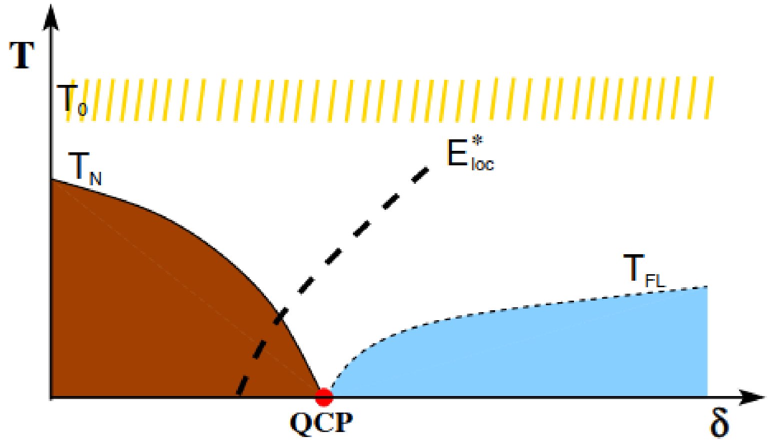
Doniach scenario





SDW – critical order parameter
magnetism enforced transition

OSM – critical fermions
magnetism as a byproduct



J. Phys. Soc. Jpn. 81 011001

what becomes critical at QCP?

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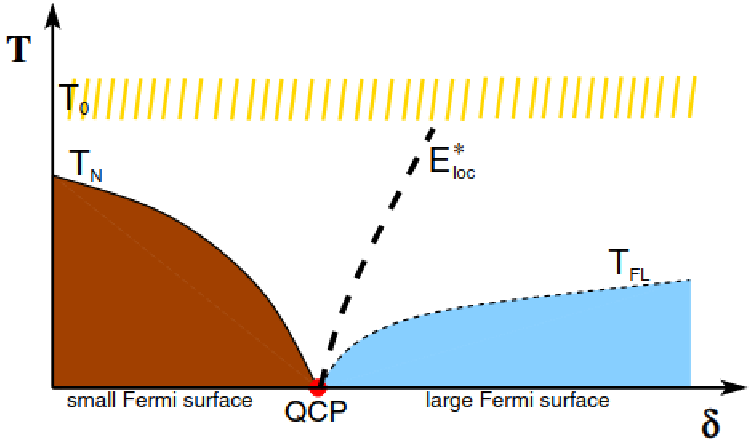
local criticality



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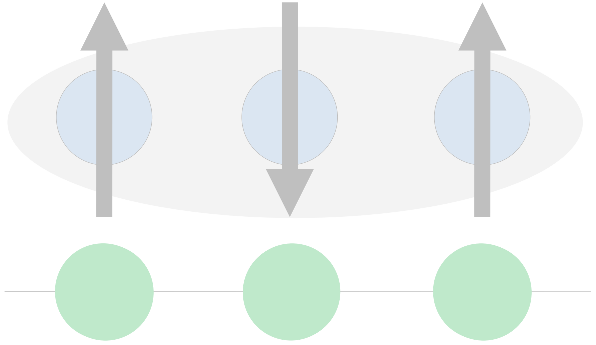

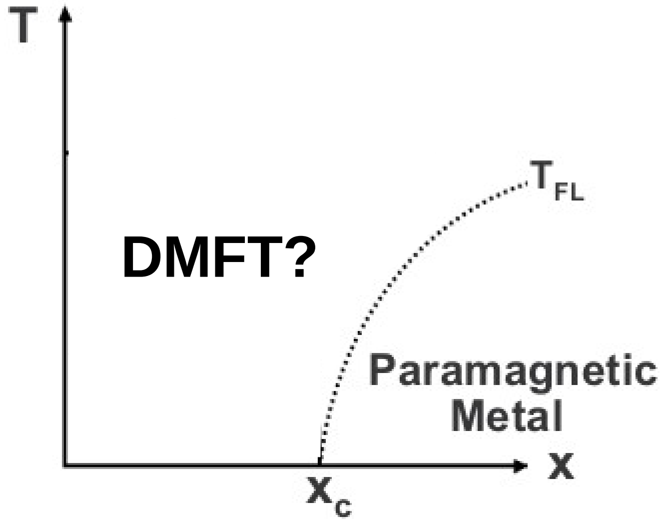

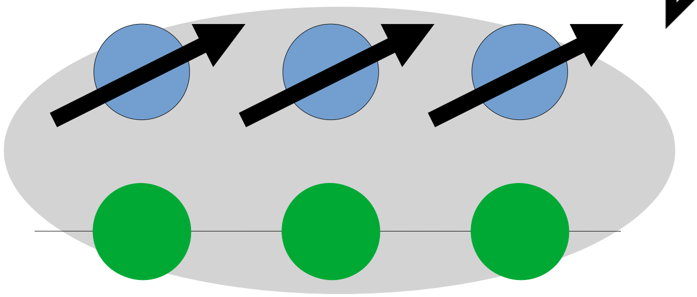

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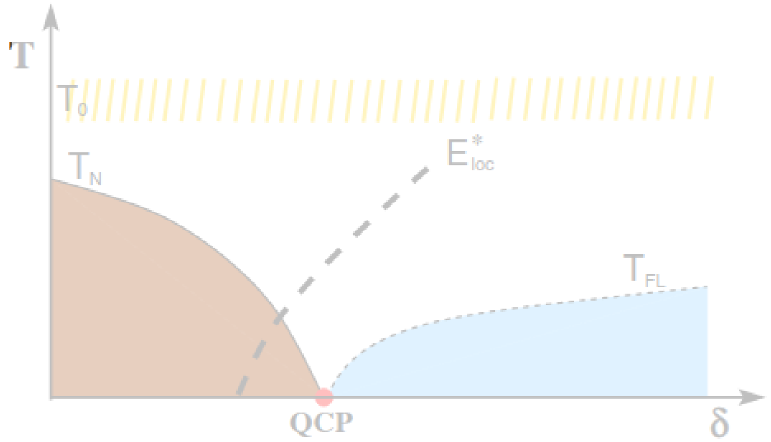

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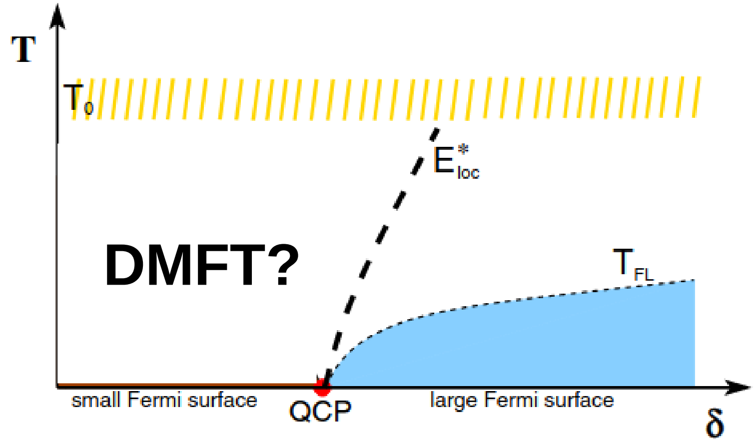

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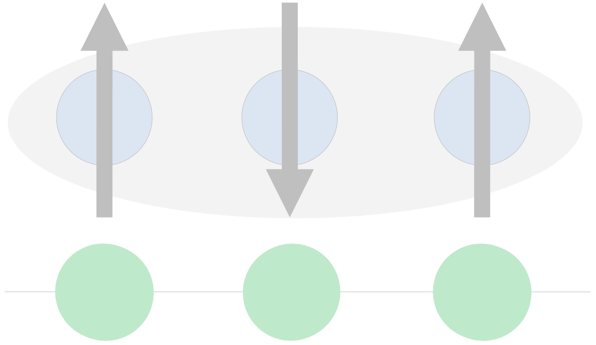
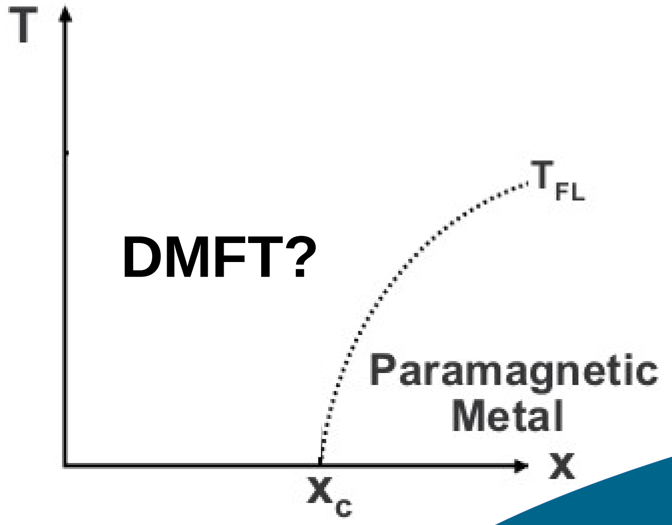
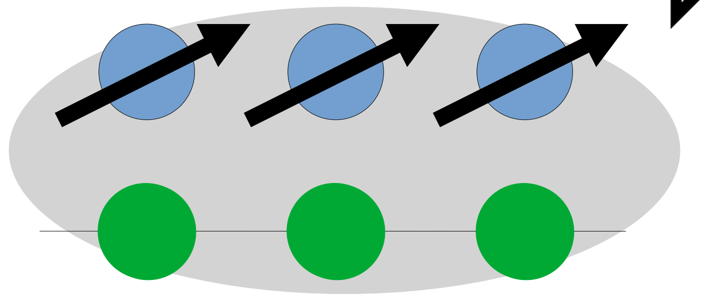




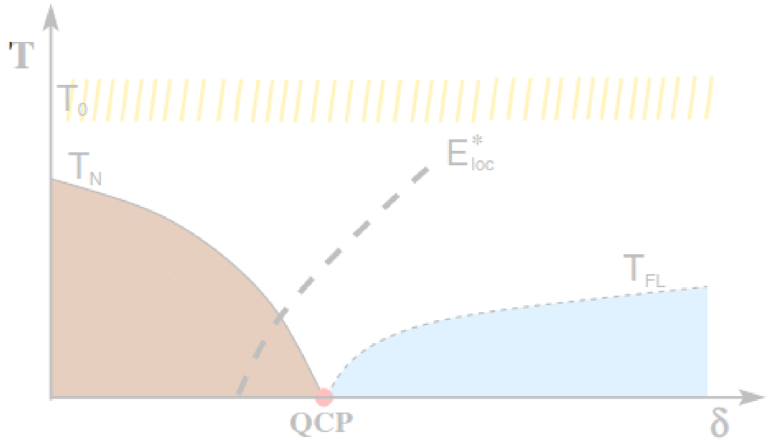


Doniach scenario

SDW – critical order parameter
magnetism enforced transition

how to get rid of the Kondo effect without magnetism?

…ermions
…gnetism as a byproduct



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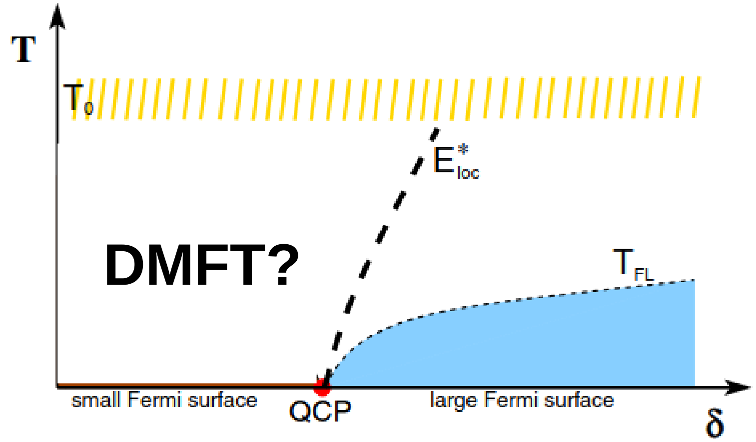
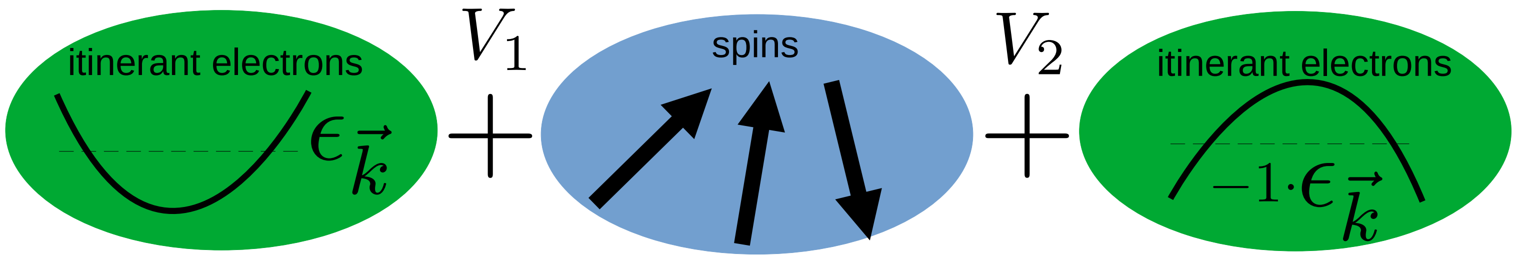


Kondo breakdown in multi-orbital extensions



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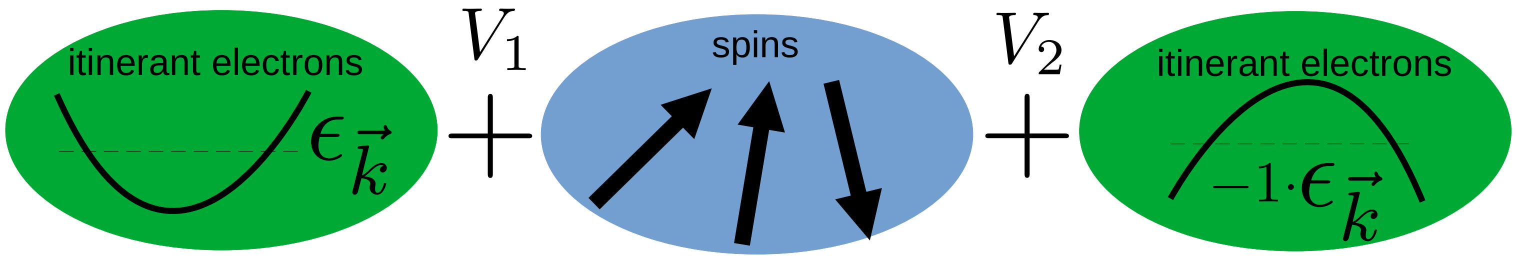

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why on earth…?

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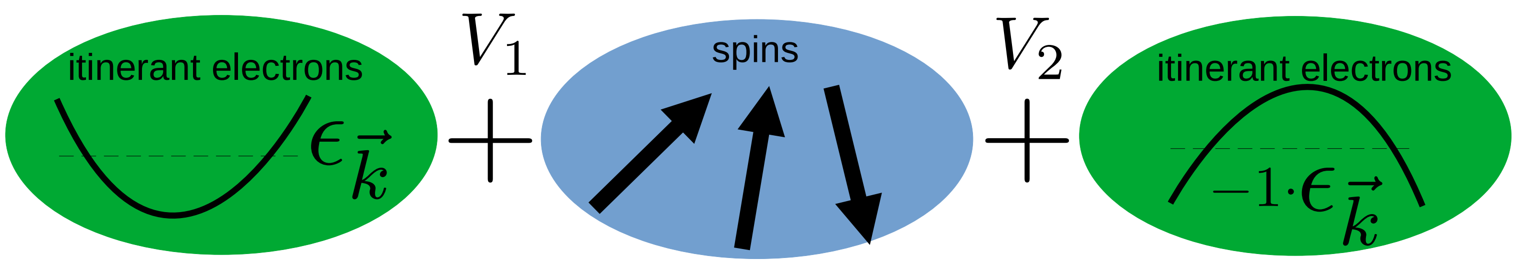

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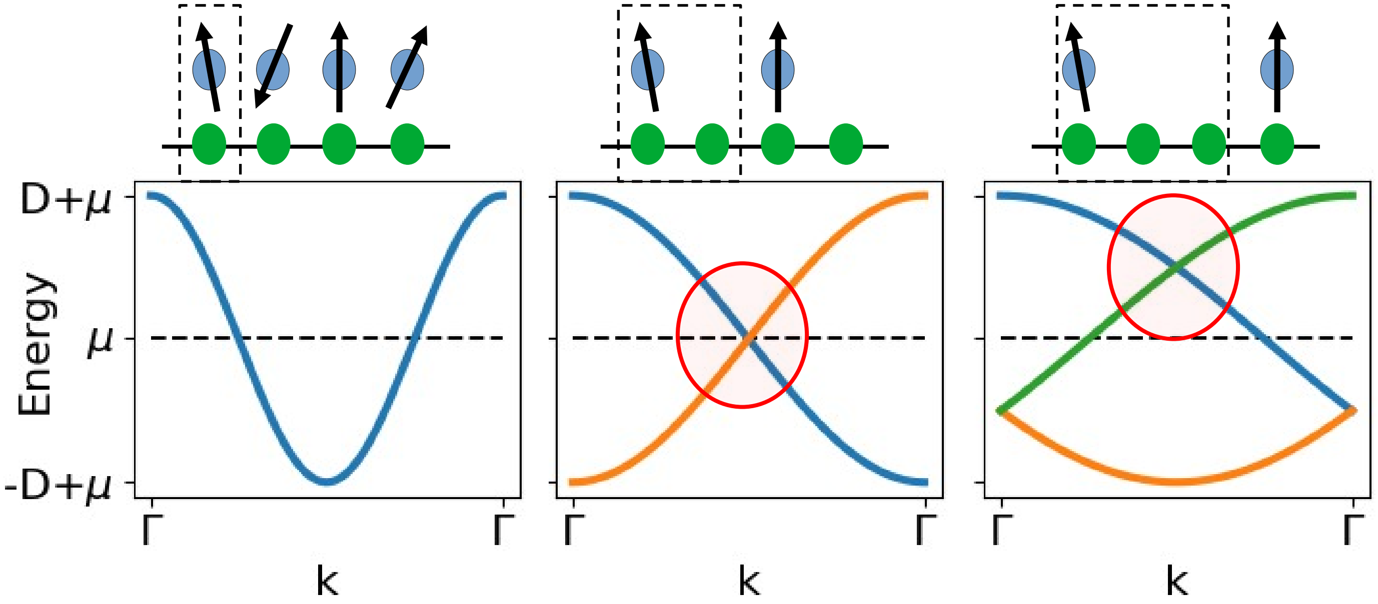
why on earth…?

I. band folding due to larger unit cell



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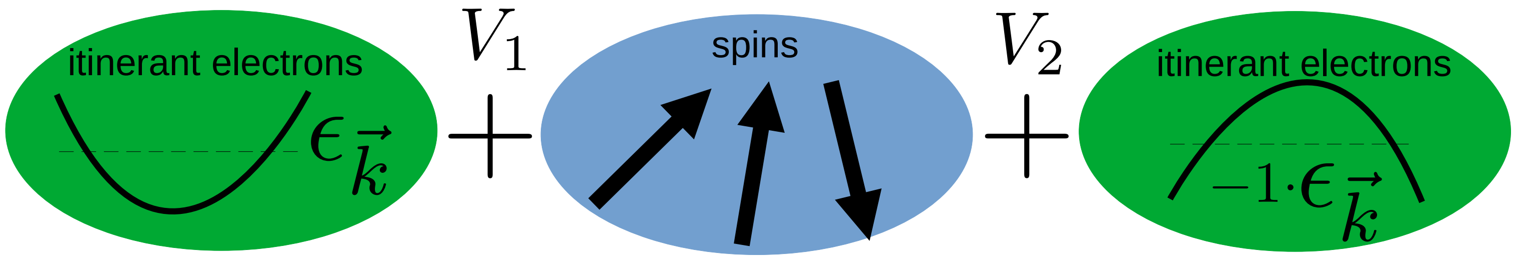

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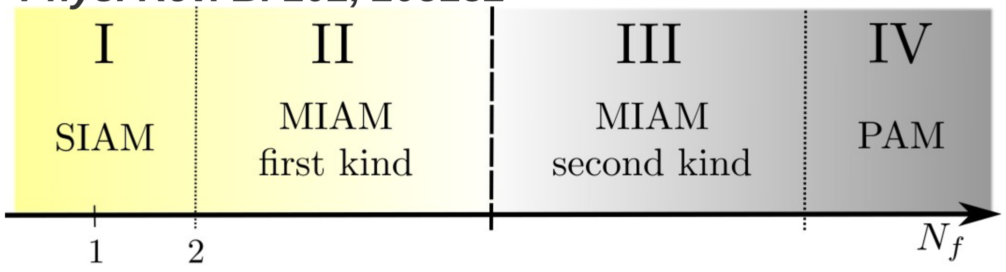
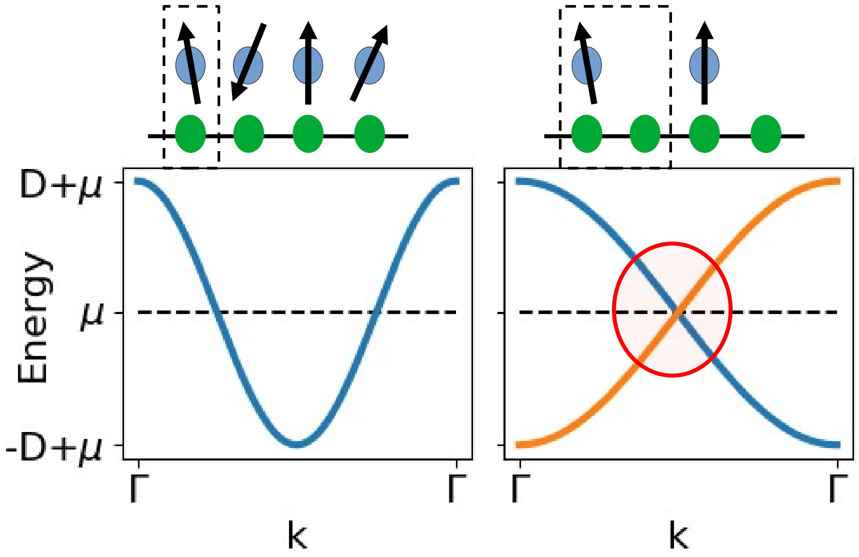
I. band folding due to larger unit cell

II. destructive hybridization interference?

Phys. Rev. B. 102, 205132





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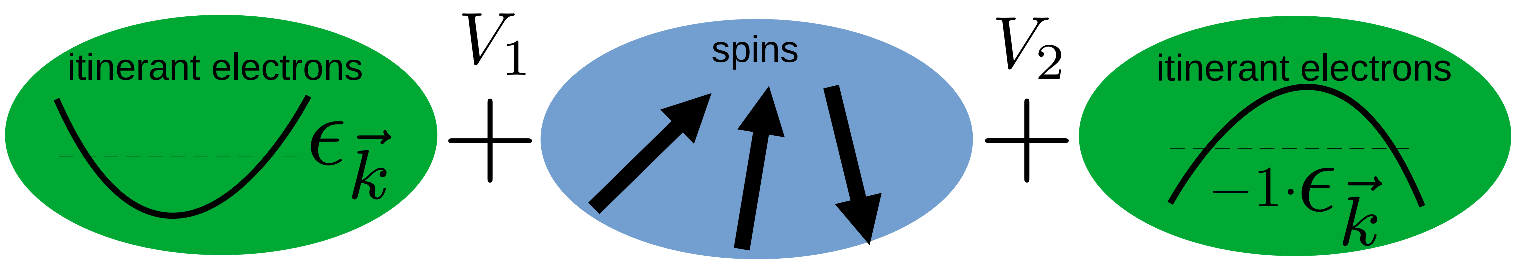

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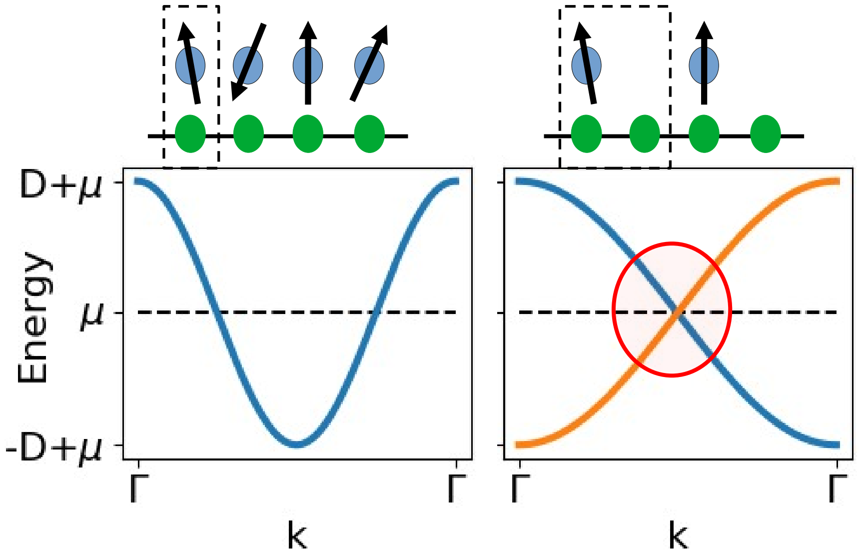

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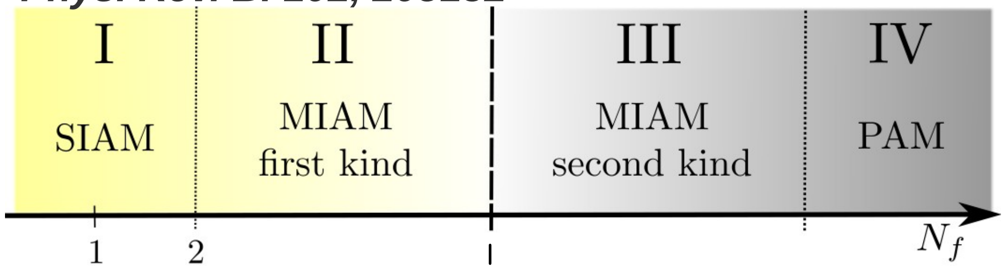


eff. hybridization

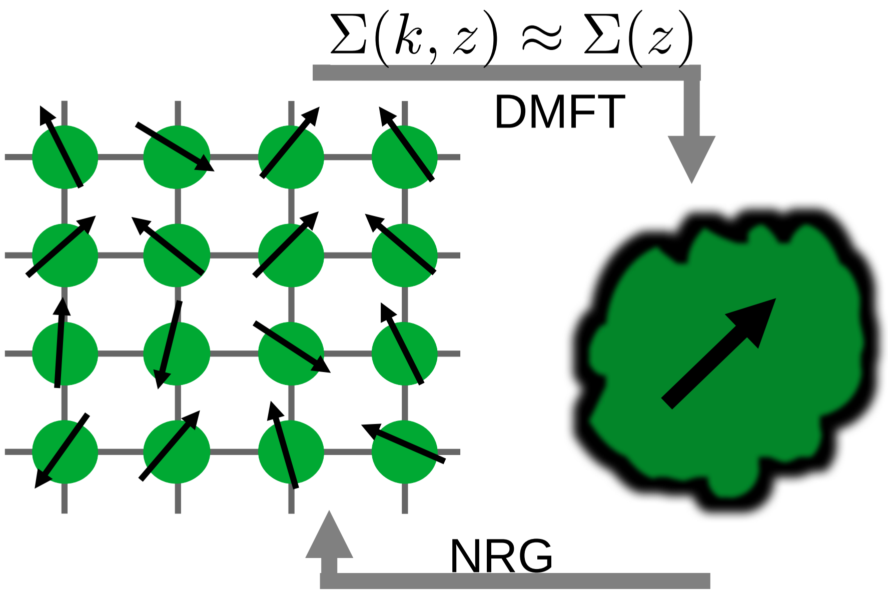
$$\tilde{\Delta} \propto \sum V_i^2 \Im\left[\mathcal{G}_k^i(0)\right] \qquad \sum V_i^2 \Re\left[\mathcal{G}_k^i(0)\right]$$

$$= \sum V_i^2 / \epsilon_k^i$$

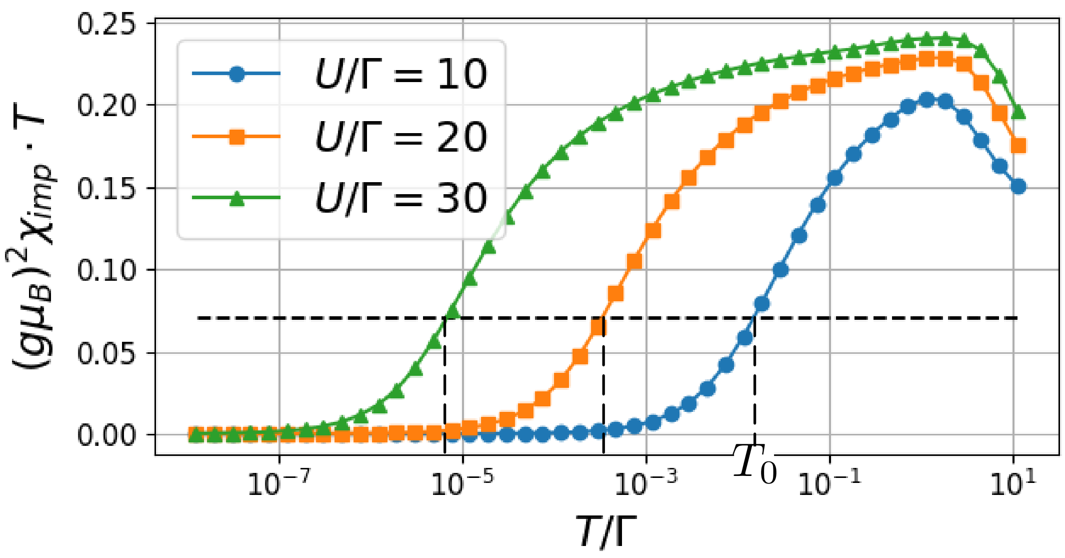
fixed sign	
constructive	constructive / **destructive**

Kondo breakdown – DMFT(NRG)

results arXiv:2401.04540



definition of low energy scale



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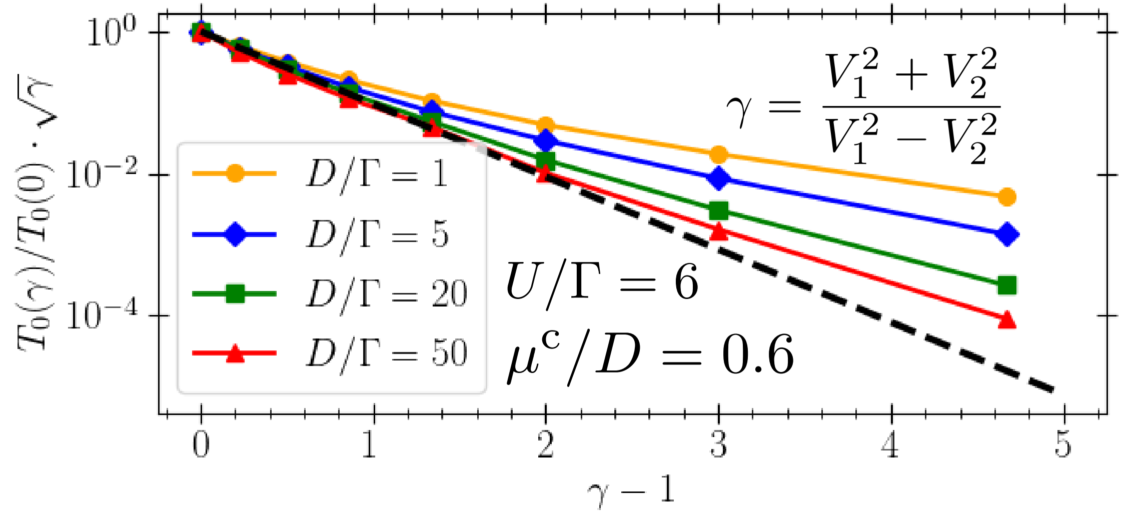
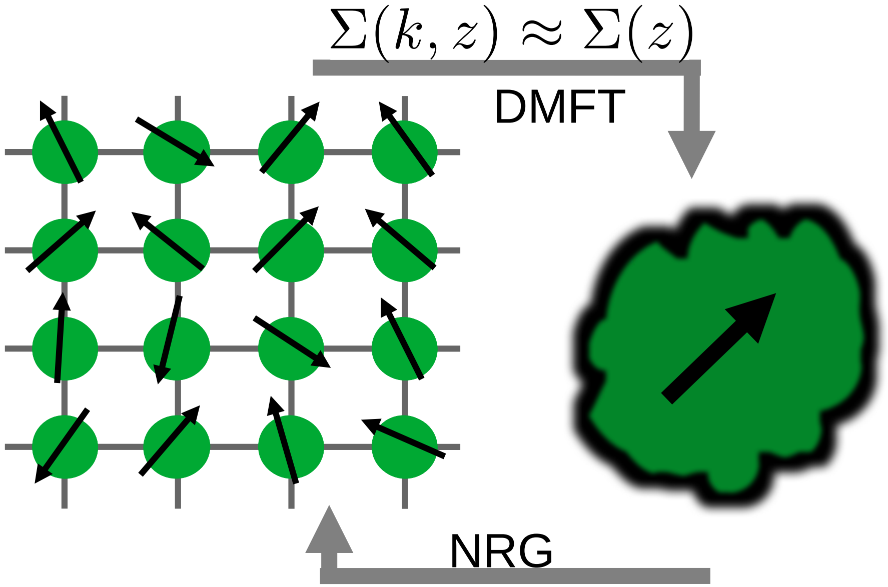
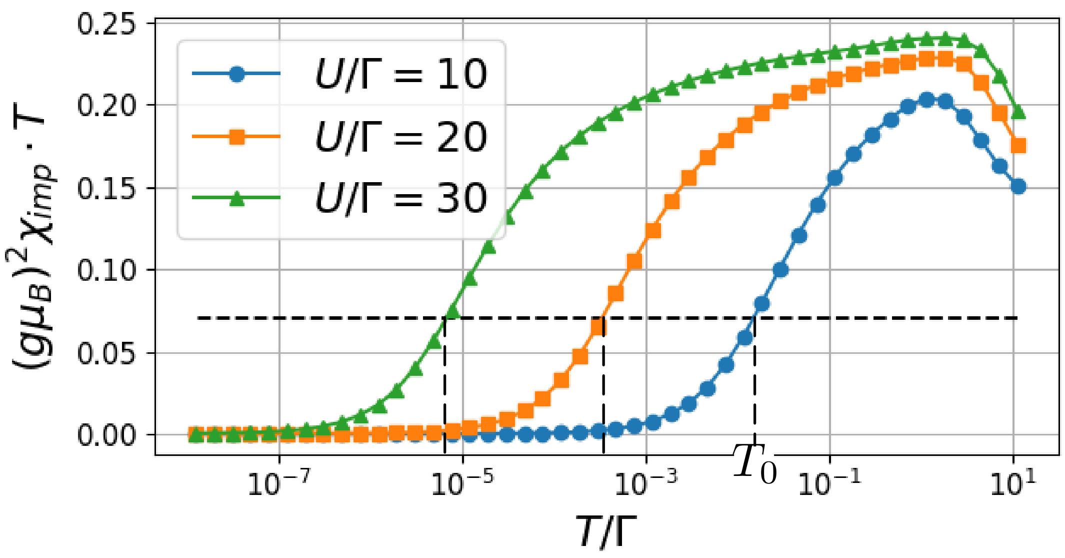
- exponentially suppressed T_0 due to destructive interference
- → generic effect in multi-orbital Kondo systems







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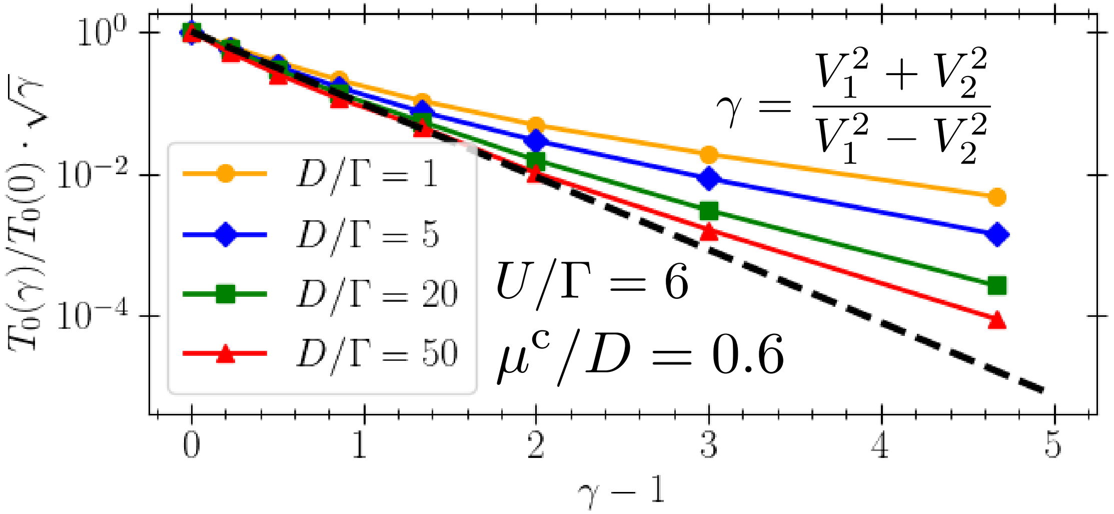
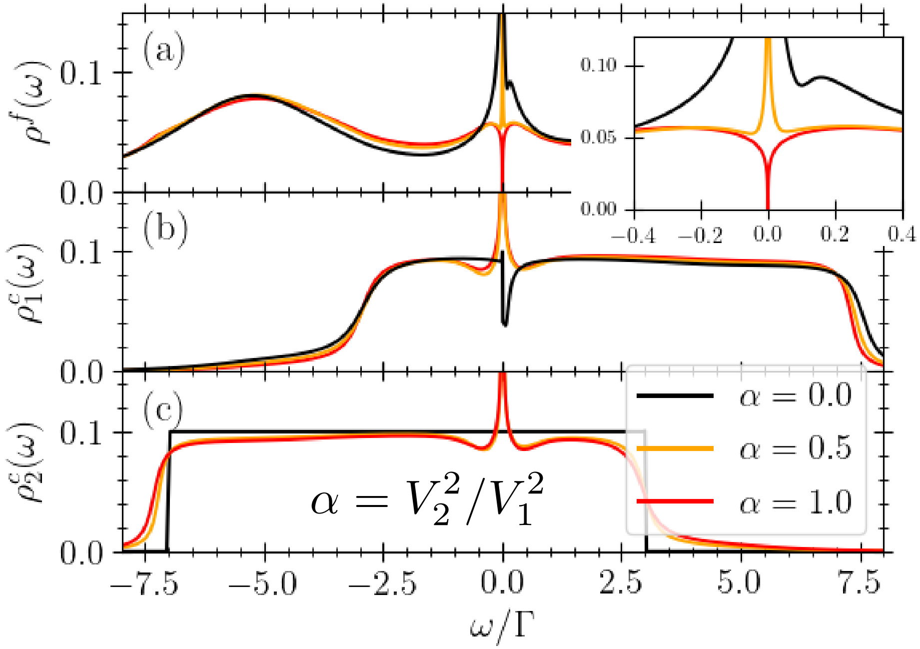
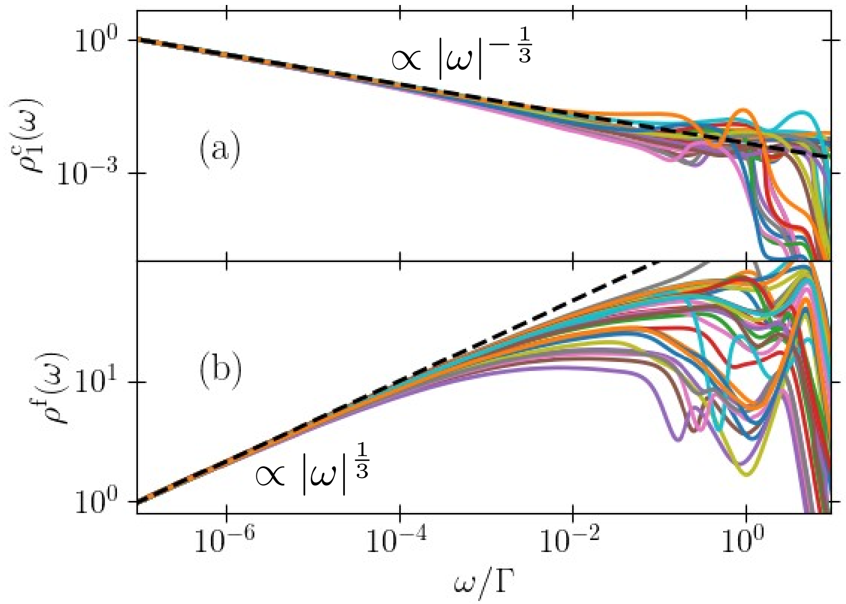
- exponentially suppressed T_0 due to destructive interference
  → generic effect in multi-orbital Kondo systems
- Kondo breakdown! - w/o the need of magnetism
  → non trivial pseudo-gap SIAM due to self consistency
- local PH symmetry: universal power law scaling



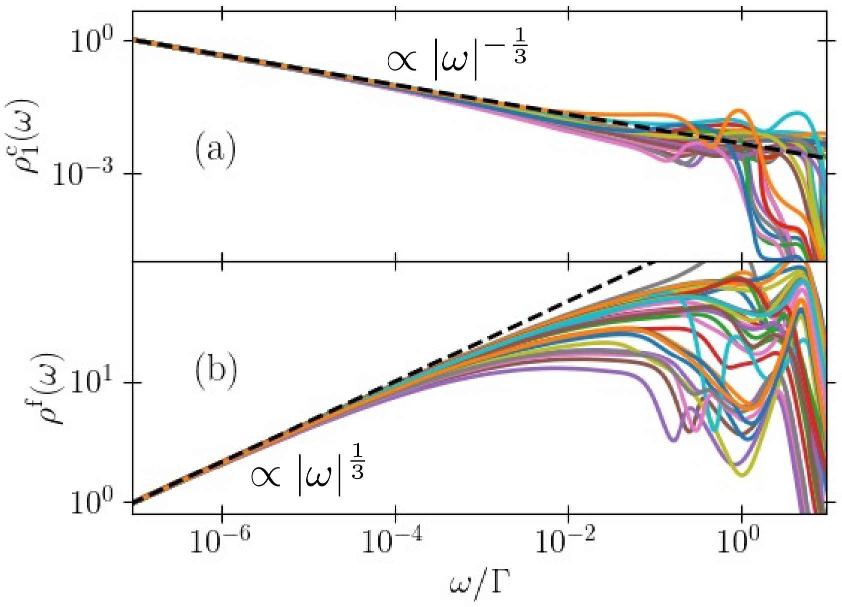




Kondo breakdown – DMFT(NRG)

to do

- calculate thermodynamic and transport properties
- analytical insight? (large N mean filed, …)
- distance to interacting non-Fermi-liquid fixed point?



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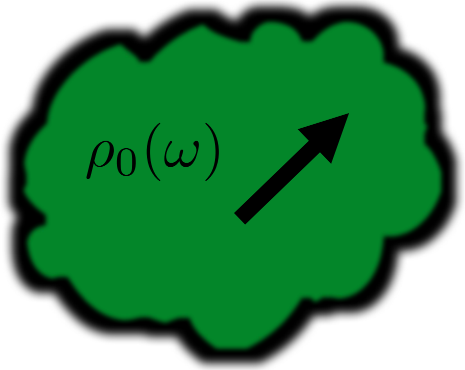
effective SIAM at KB point :

$$\rho_0(\omega) \propto |\omega|^r \quad r < 0.5$$



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Phys. Rev. B, 70, 214427

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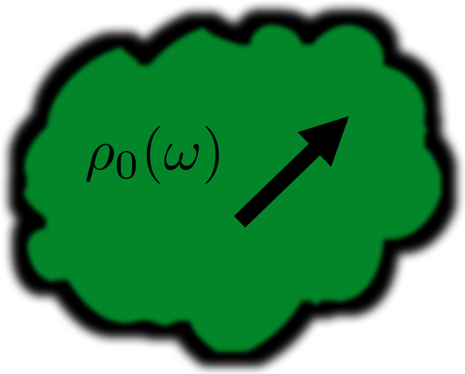

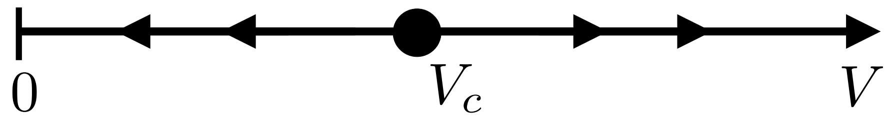

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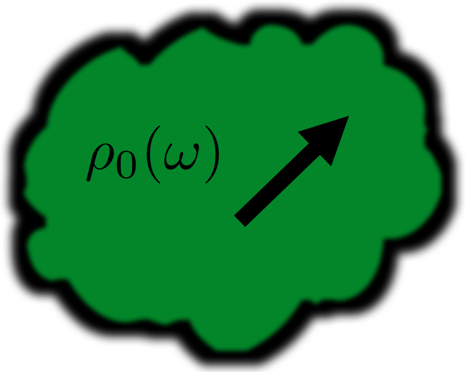

Phys. Rev. B, 70, 214427
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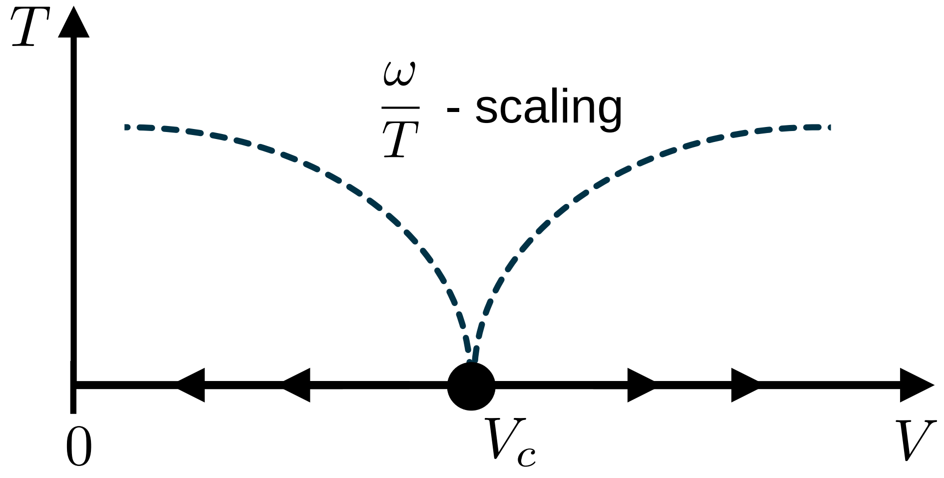

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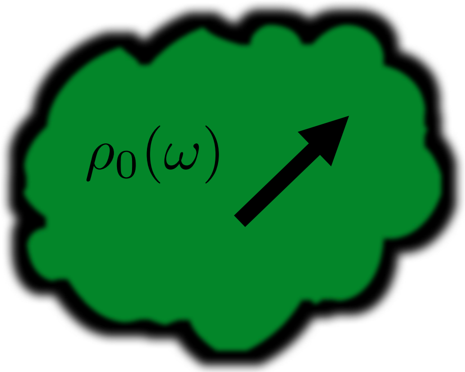

DMFT self-consistency:

$$V_{\mathrm{DMFT}} < V_c$$

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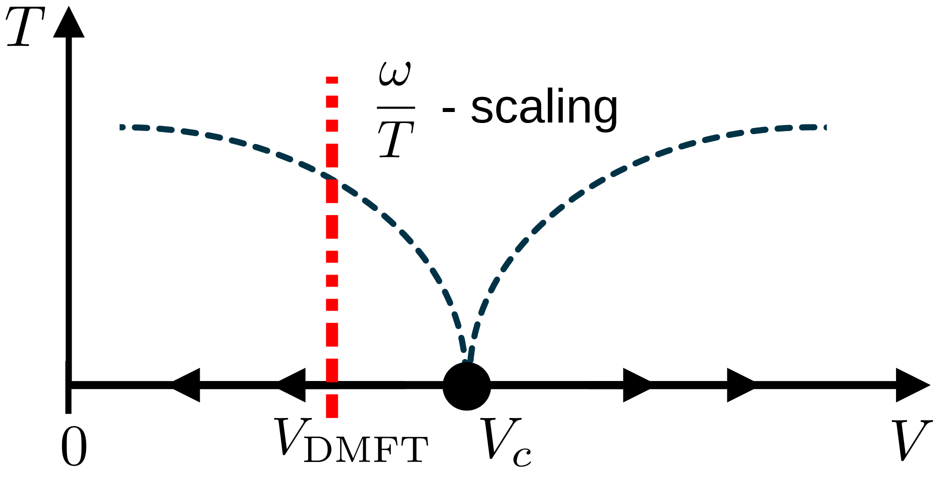
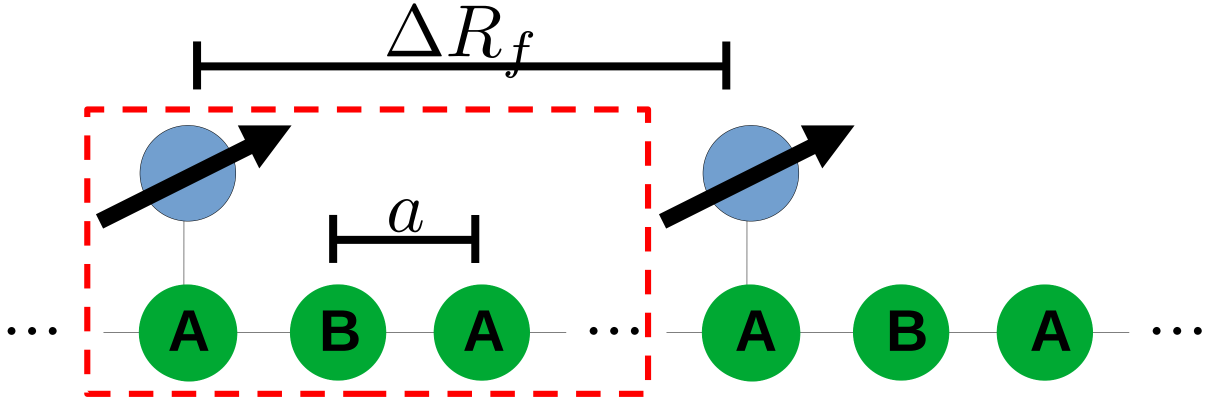
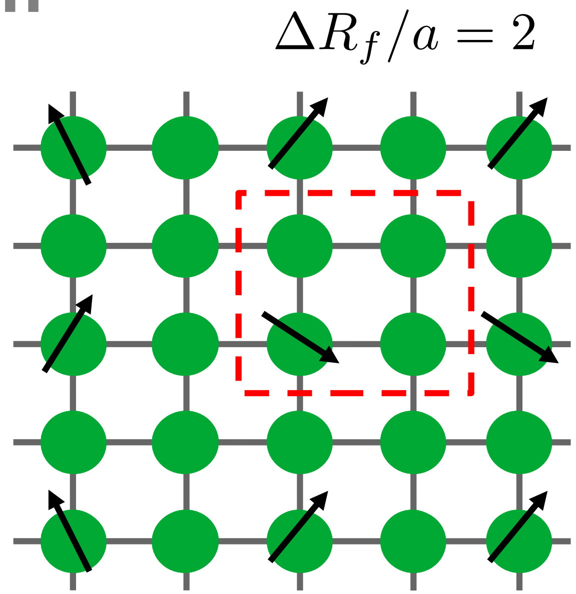


premilinary results:
local moment revival in dilute periodic Anderson models

PAM: dilute limit vs Lieb Mattis theorem





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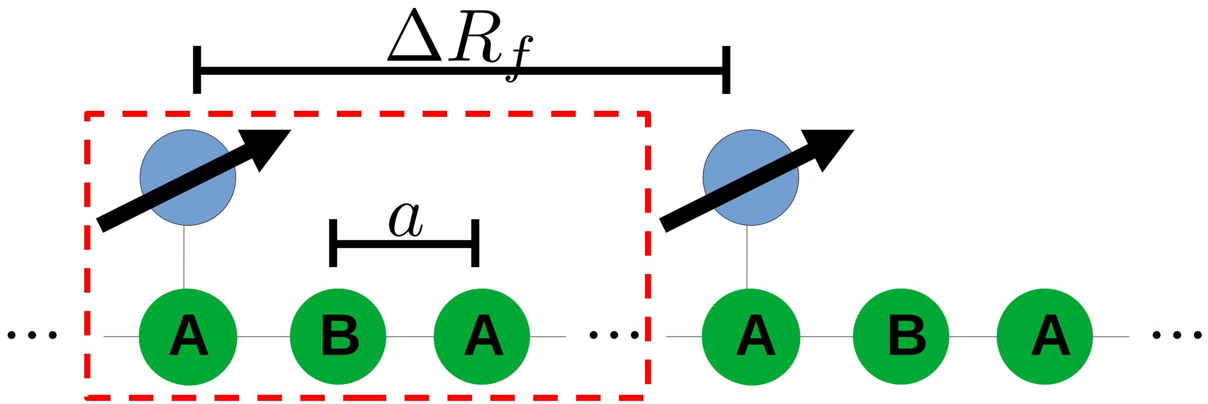
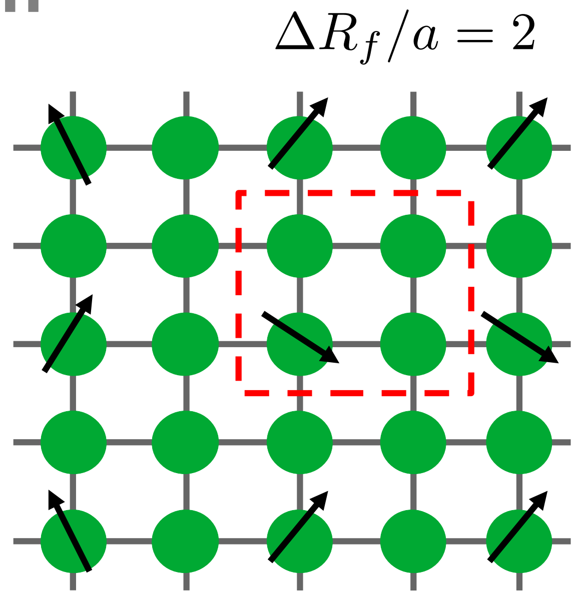




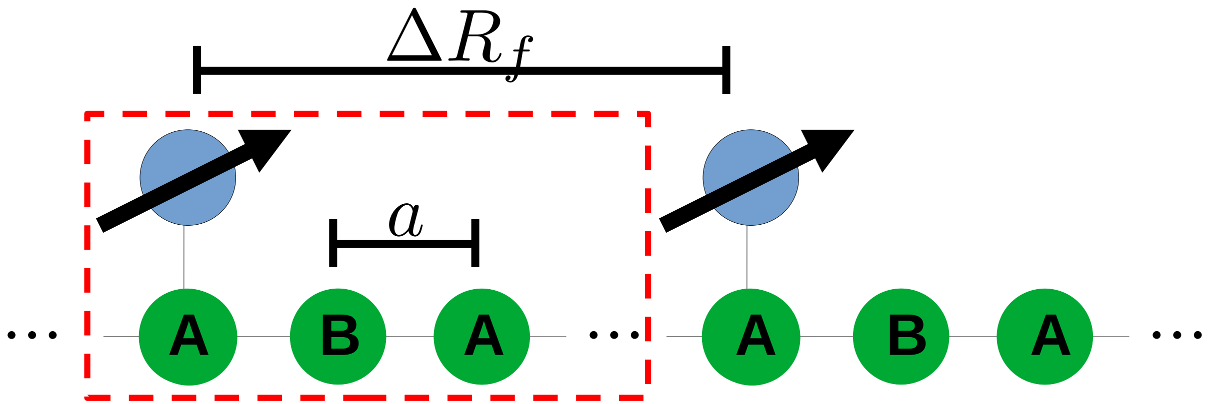
$$\Delta R_f/a = 1$$

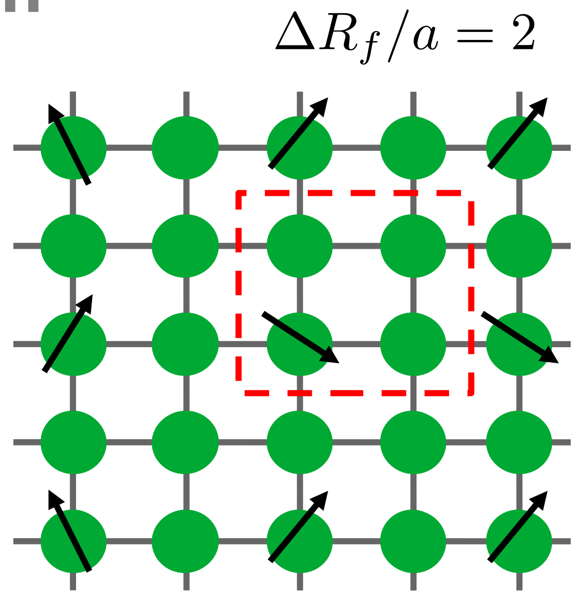
standard Kondo lattice / periodic Anderson model

$$\Delta R_f/a \gg 1$$

single impurity limit (SIAM)

PAM: dilute limit vs Lieb Mattis theorem





$$\Delta R_f / a = 1$$

standard Kondo lattice / periodic Anderson model

$$\Delta R_f / a \gg 1$$

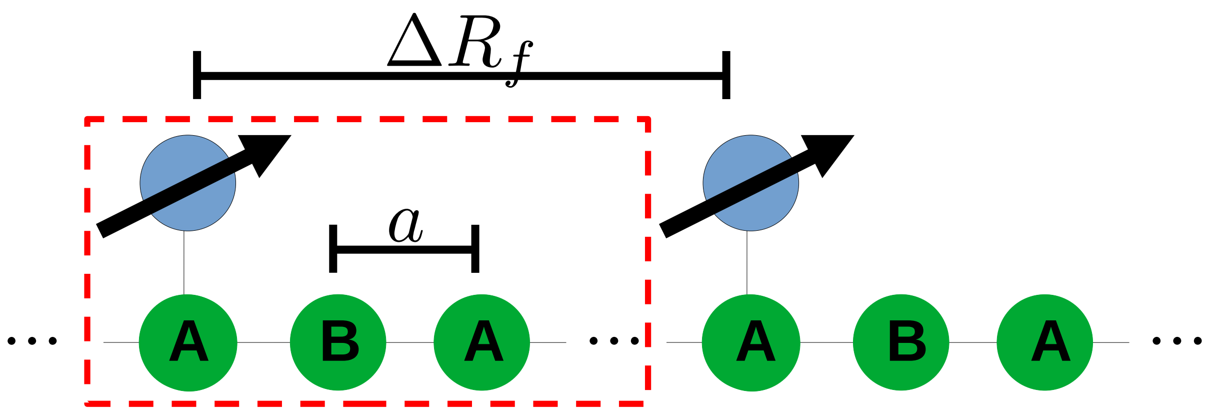
single impurity limit (SIAM): $\langle S_z \rangle = 0$

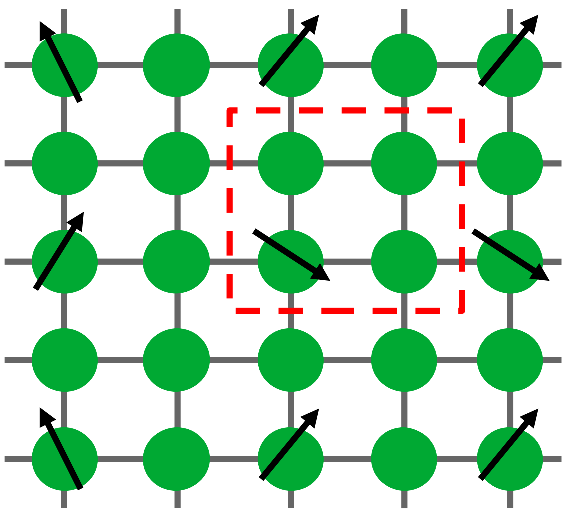
Lieb Mattis theorem:
(spins on A-site only + PH symmetry)

$$\langle S_z \rangle = \frac{\mathrm{N^u} - 1}{2}$$

$\mathrm{N^u} =$ number of unit cells

PAM: dilute limit vs Lieb Mattis theorem





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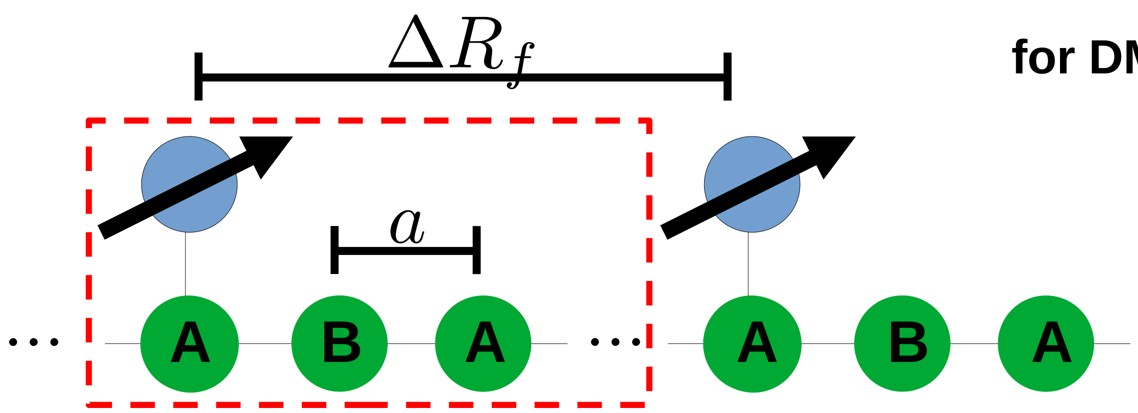
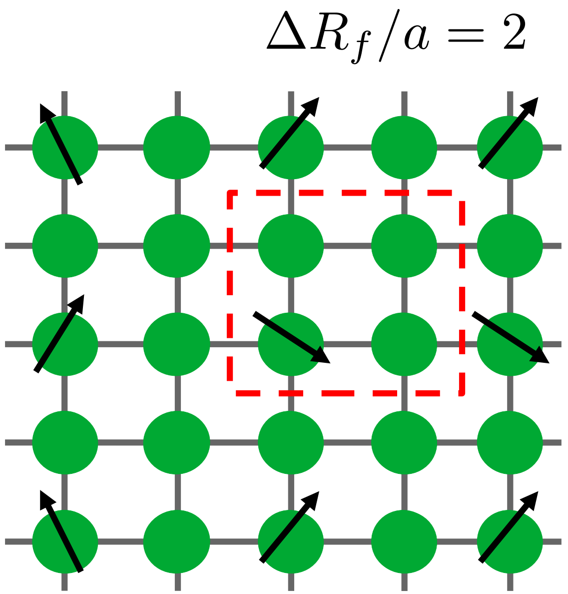
How to combine the SIAM limit with LM theorem ?

correlations should be local in the dilute limit
DMFT is well suited

PAM: dilute limit vs Lieb Mattis theorem





for DMFT we need to integrate Greens functions...

$$G_0^{-1}(k) = \begin{bmatrix} i\omega - V_i & -t & -t & 0 & \dots \\ -t & i\omega - V_i & -t & -t & \dots \\ -t & -t & i\omega - V_i & -t & \dots \\ 0 & -t & -t & i\omega & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}, \qquad (2)$$

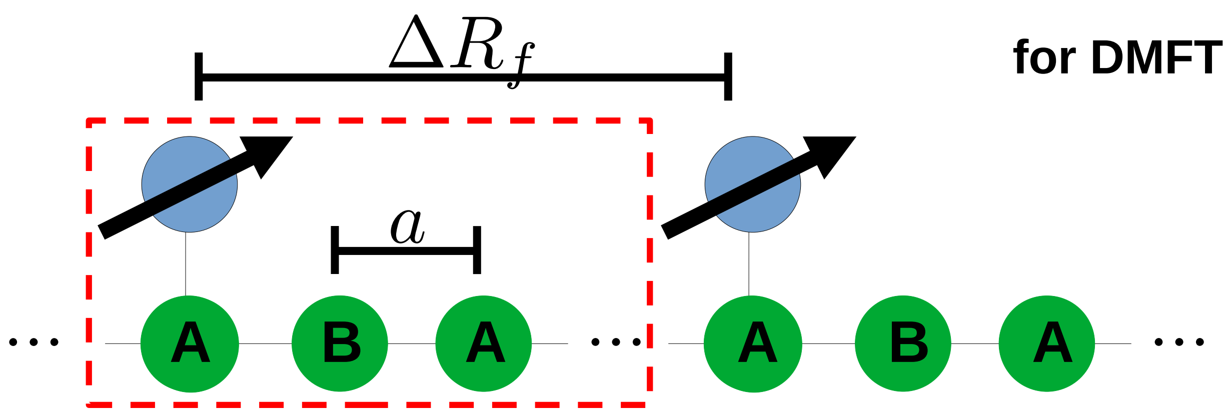
$$G^{-1}(k) = \left[\begin{array}{cccc|c} & & & & V_{if} \\ & & & & V_{if} \\ & G_0^{-1}(k) & & & V_{if} \\ & & & & 0 \\ & & & & \vdots \\ \hline V_{if} \; V_{if} & V_{if} & 0 & \dots & \epsilon_f - \Sigma \end{array}\right]. \qquad (3)$$

Here V_{if}, ϵ_f, t, and V_i are defined in (1), $i\omega_n$ is the n's Matsubara frequency, while the substrate sites are ordered in such a way that the three sites connected to the adatom are listed first.

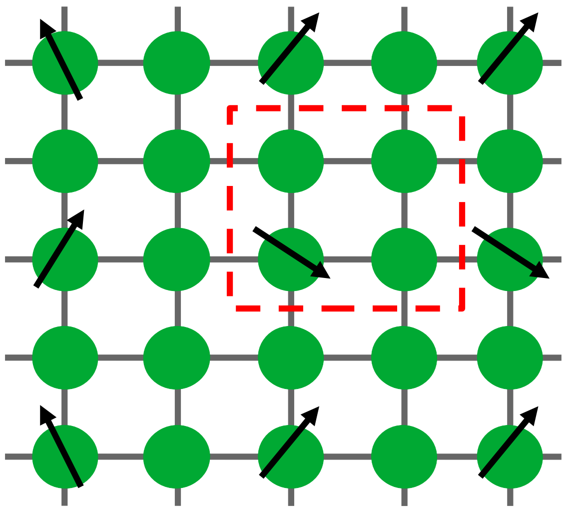
G_0 is obtained via matrix products for all n_{freq} (N^2 operations), G is then updated from G_0. Since only three substrate sites hybridizes with the adatom, the updating process scales linearly with N.

Lee et al. ***Commun Phys 2, 49 (2019)***

PAM: dilute limit vs Lieb Mattis theorem



$\Delta R_f / a = 2$



for DMFT we need to integrate Greens functions...

Sherman–Morrison formula

$$\mathcal{G}^f(z) = \sum_q \left(z - \epsilon^f - \Sigma(z) - \frac{V^2}{\mathrm{N^u}} \sum_r \mathcal{G}^{0c}_{\vec{q}+\vec{P}_r} \right)^{-1}$$

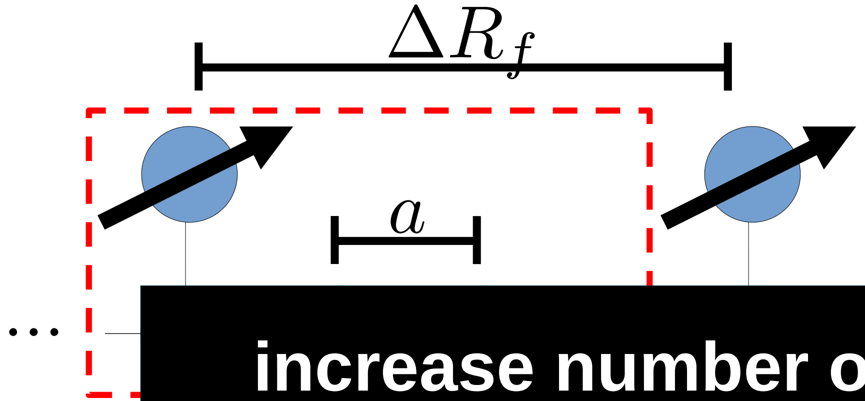
$$\mathcal{G}^{0c}_{\vec{q}+\vec{P}_l} = \left(z - \epsilon_{\vec{q}+\vec{P}_l} \right)^{-1}$$

$$\mathcal{G}^{\mathrm{c}}_i(z) = \sum_q \sum_{lm} e^{i(\vec{P}_l - \vec{P}_m)\vec{R}_i} \left[\mathcal{G}^{0c}_{\vec{q}+\vec{P}_l} \delta_{lm} + G^f \frac{\mathcal{G}^{0c}_{\vec{q}+\vec{P}_l} \mathcal{G}^{0c}_{\vec{q}+\vec{P}_m}}{1 - \frac{G^f}{\mathrm{N^u}} \sum_r \mathcal{G}^{0c}_{\vec{q}+\vec{P}_r}} \right]$$

$$G^f = \frac{V^2}{z - \epsilon^f - \Sigma(z)}$$

$$\vec{P}_i \in \mathrm{Bz}^c \wedge \vec{P}_i \cdot \Delta\vec{R}_f = 2n\pi$$

PAM: dilute limit vs Lieb Mattis theorem



for DMFT we need to integrate Greens functions...

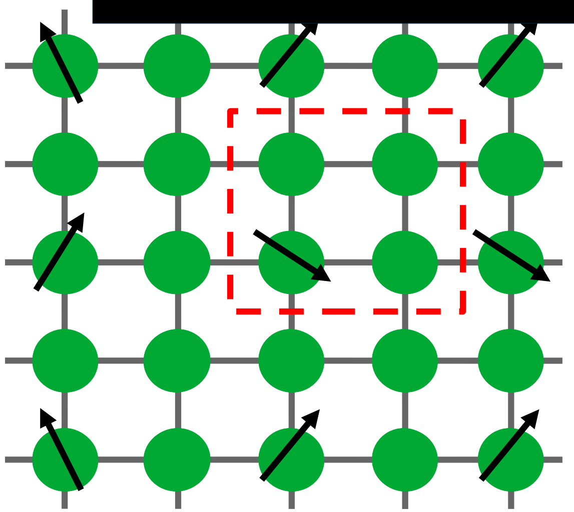
Sherman–Morrison formula

increase number of Brillouin zone sampling points by factor

$$\mathcal{O}(10^4)$$

$$\left(z - \epsilon^f - \Sigma(z) - \frac{V^2}{\mathrm{N^u}}\sum_r \mathcal{G}^{0c}_{\vec{q}+\vec{P}_r}\right)^{-1}$$

$$\mathcal{G}_{\vec{q}+\vec{P}_l} = \left(z - \epsilon_{\vec{q}+\vec{P}_l}\right)^{-1}$$



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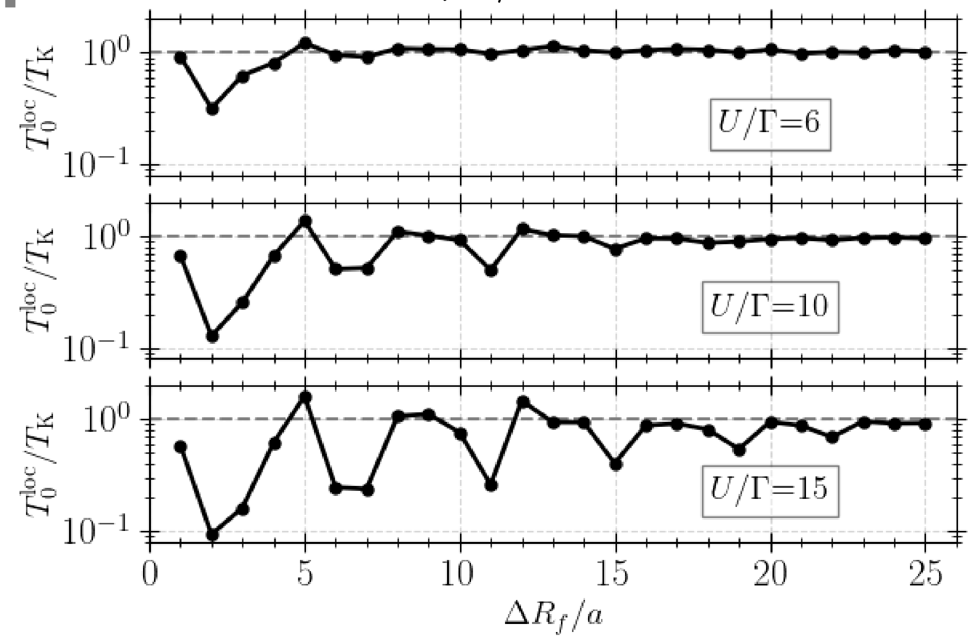
PAM: dilute limit vs Lieb Mattis theorem

$$\chi_{\rm loc} \propto \frac{\partial \langle S_{\rm z}^{\rm imp} \rangle}{\partial H_{\rm z}^{\rm imp}}$$

$T_0^{\rm loc}$

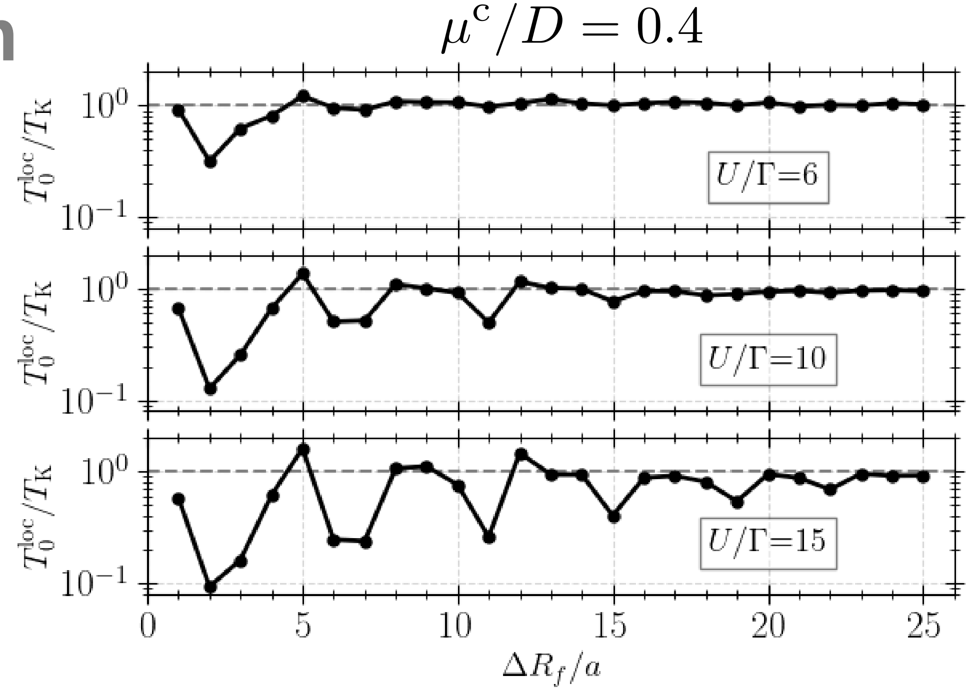
$\mu^{\rm c}/D = 0.4$

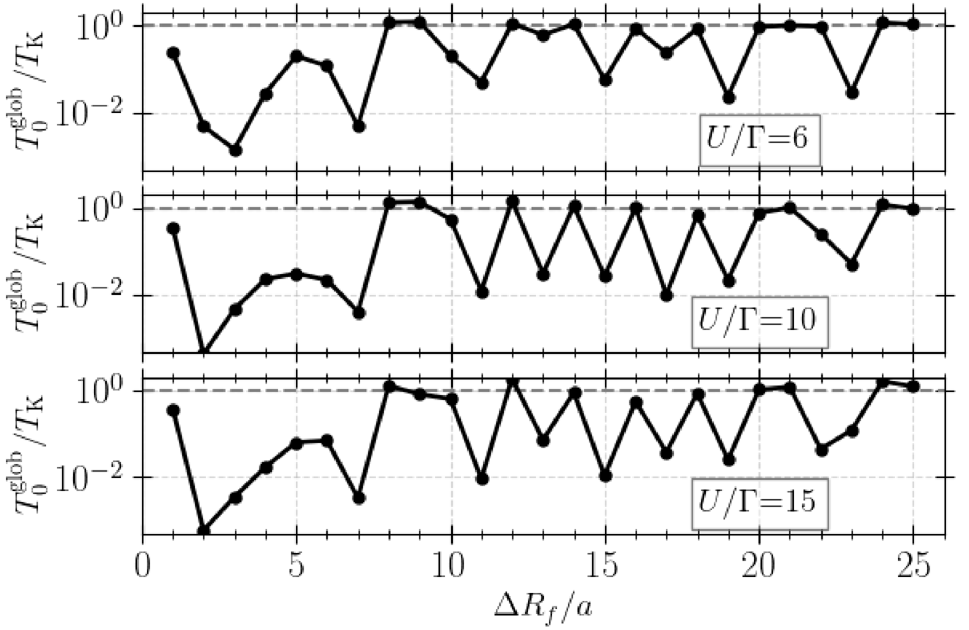


PAM: dilute limit vs Lieb Mattis theorem

$$\chi_{\rm loc} \propto \frac{\partial \langle S_{\rm z}^{\rm imp} \rangle}{\partial H_{\rm z}^{\rm imp}} \qquad \chi_{\rm glob} \propto \frac{\langle [S_{\rm z}^{\rm tot}]^2 \rangle}{T}$$

$T_0^{\rm loc}$ $\qquad$ $T_0^{\rm glob}$





PAM: dilute limit vs Lieb Mattis theorem

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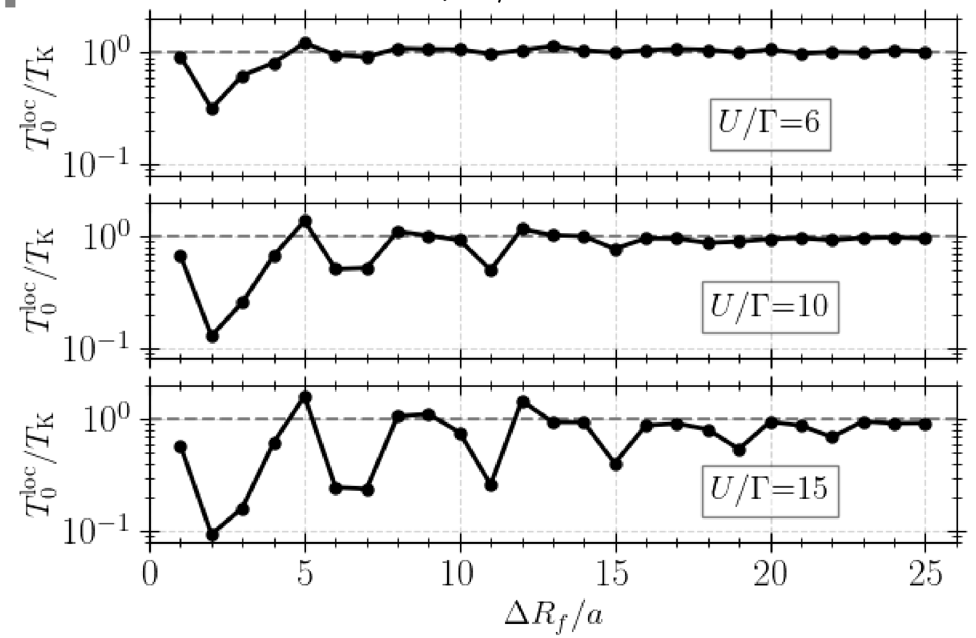

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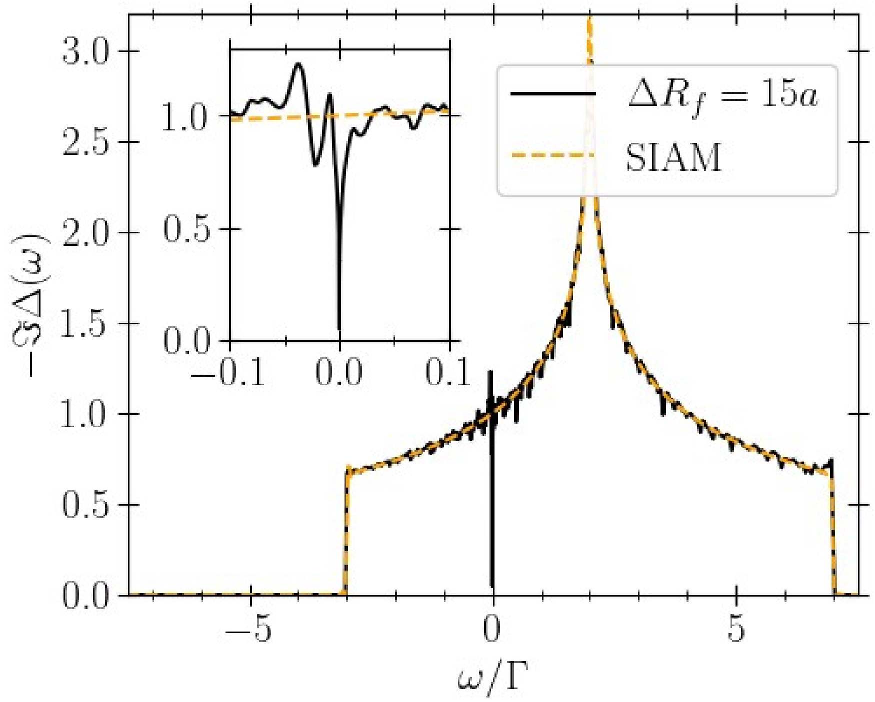
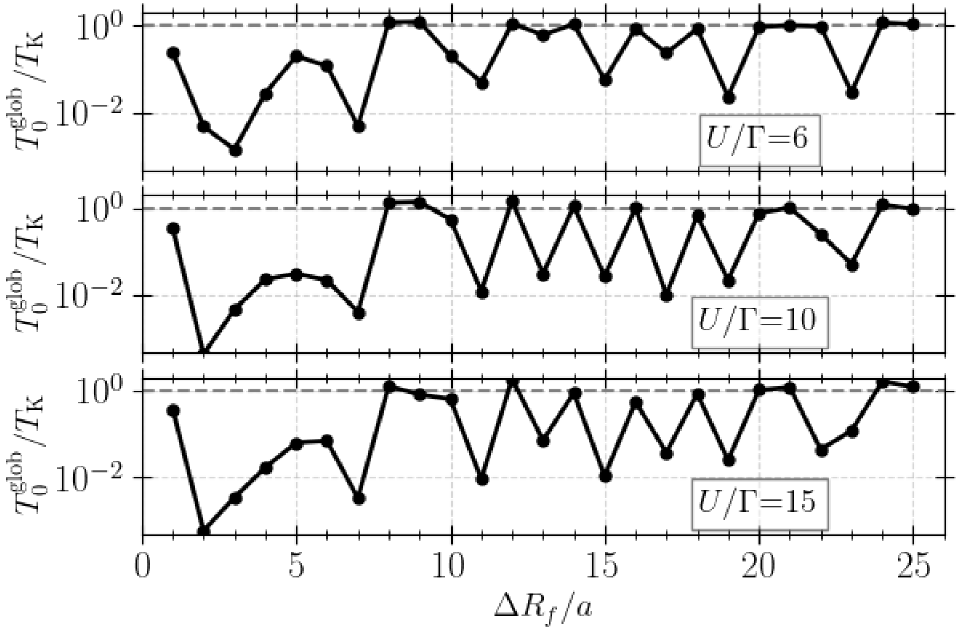
$$T_0^{\mathrm{loc}} \qquad T_0^{\mathrm{glob}}$$

what happens to the local momet?

$$T_0^{\mathrm{loc}}/T_{\mathrm{K}} \approx 1 \qquad T_0^{\mathrm{glob}}/T_{\mathrm{K}} \ll 1$$

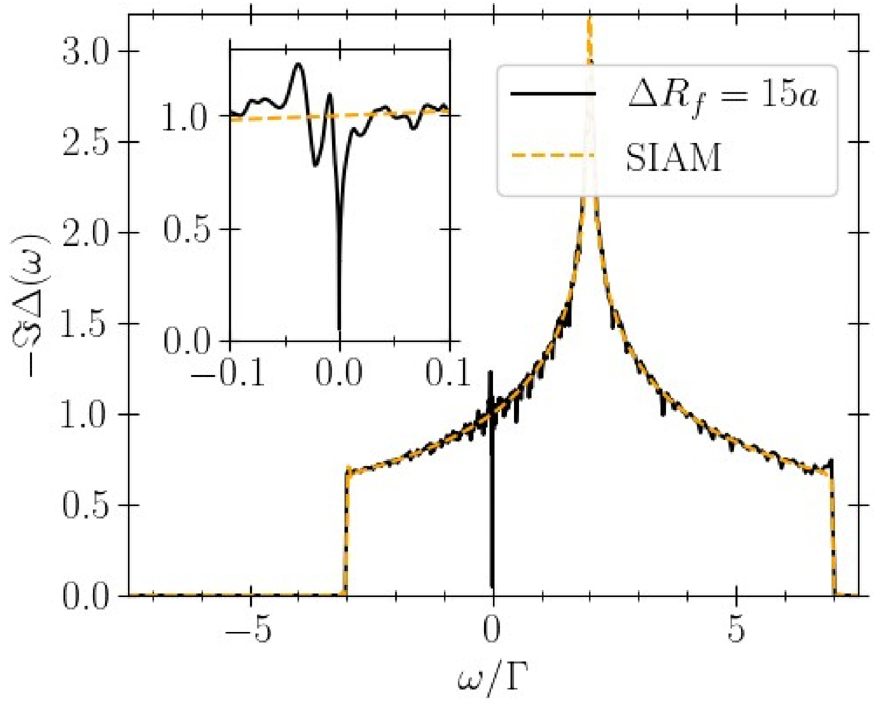




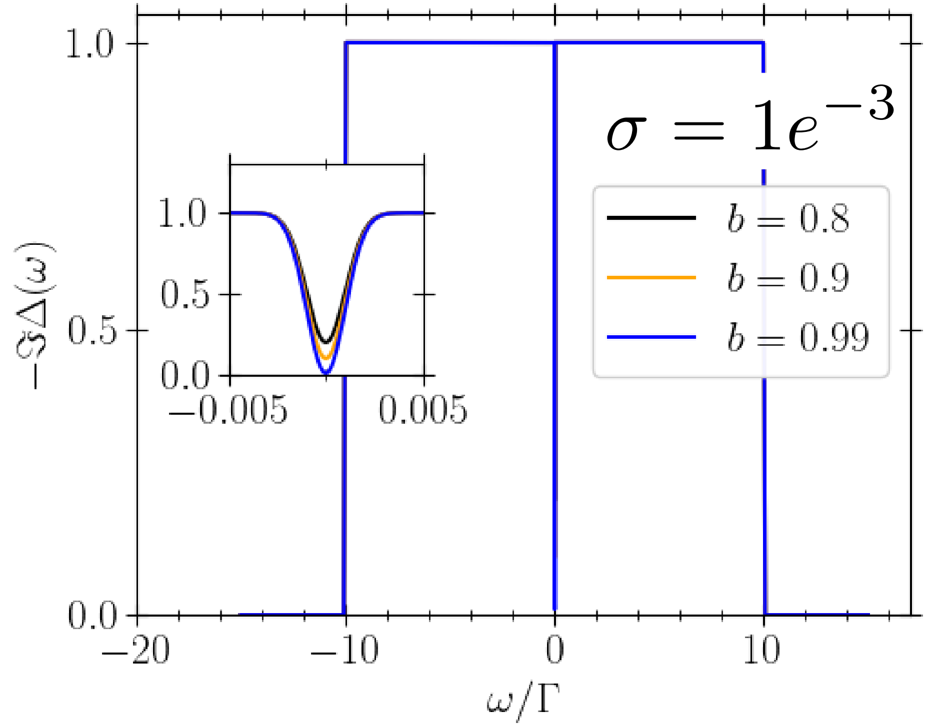
PAM: dilute limit vs Lieb Mattis theorem

Common feature: emergence of sharp dip in effective medium due to self consistency condition

- ➔ explore SIAM toy-model to gain better understanding



$$\Delta(\omega) \rightarrow \Delta(\omega)\left[1 - b \cdot e^{-\frac{1}{2}\frac{\omega^2}{\sigma^2}}\right]$$



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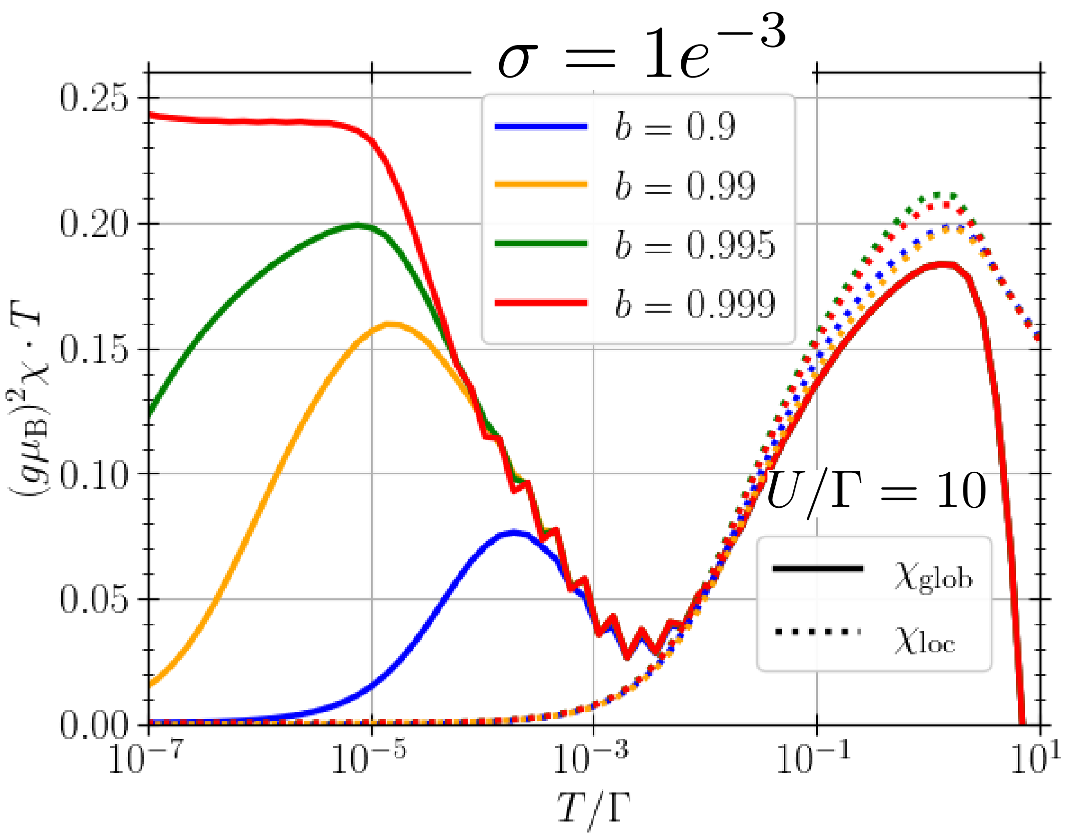

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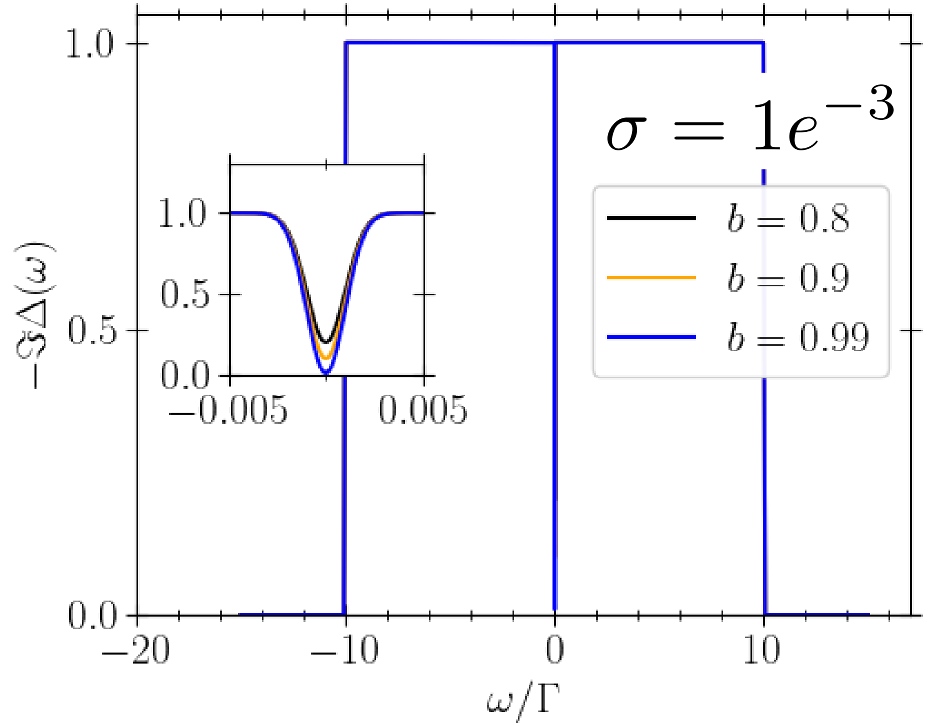

PAM: dilute limit vs Lieb Mattis theorem

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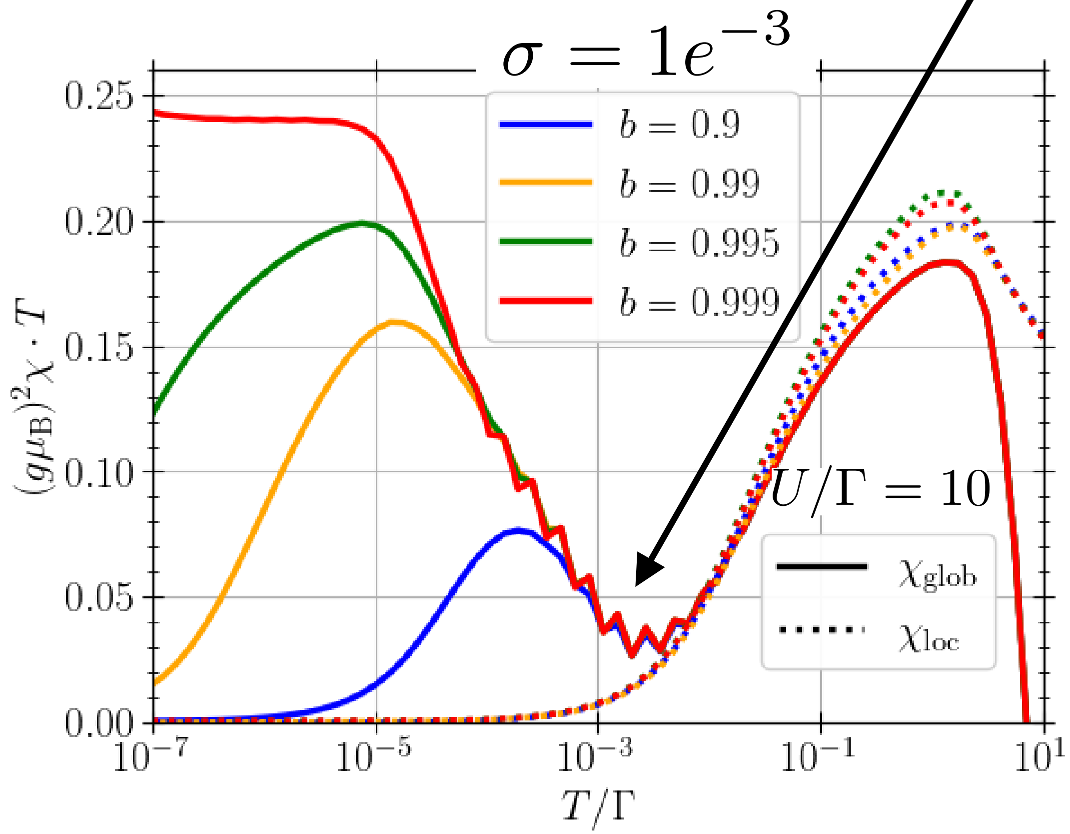
revival of magnetic moment

$\sigma \lesssim T_K$



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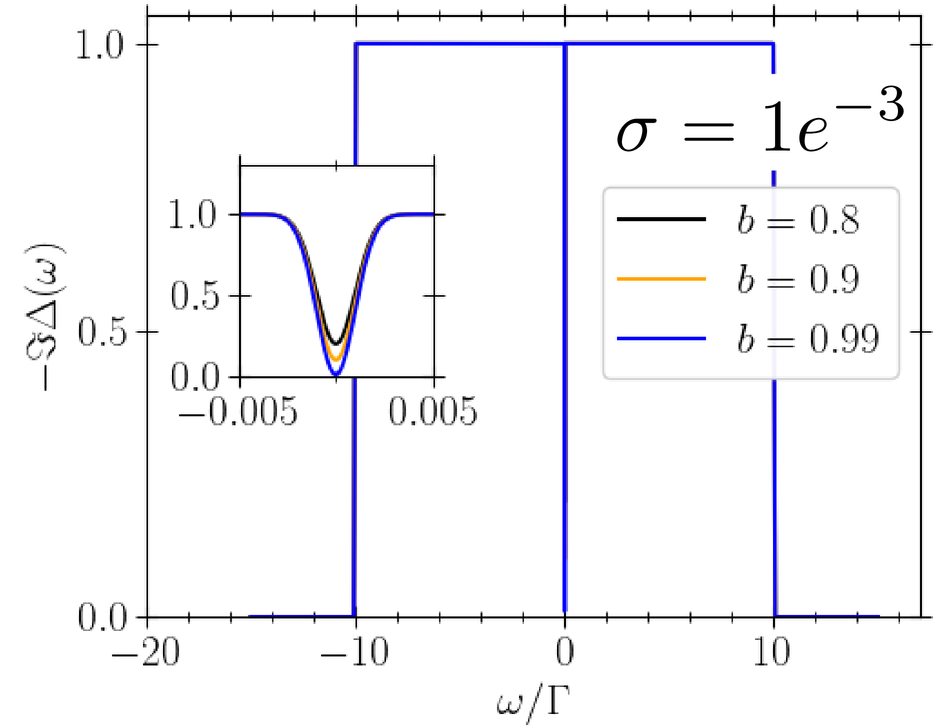


PAM: dilute limit vs Lieb Mattis theorem

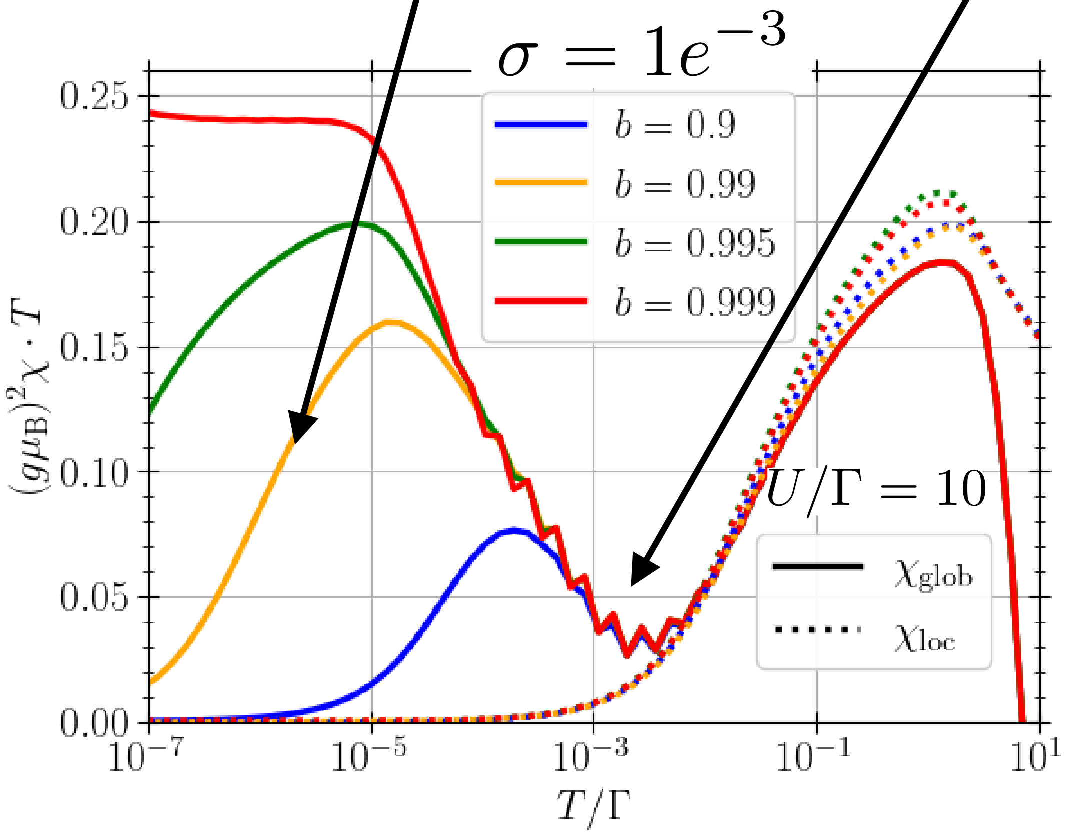
Common feature: emergence of sharp dip in effective medium due to self consistency condition

- ➔ explore SIAM toy-model to gain better understanding

second Kondo scale

revival of magnetic moment

$\sigma \lessapprox T_{\mathrm{K}}$



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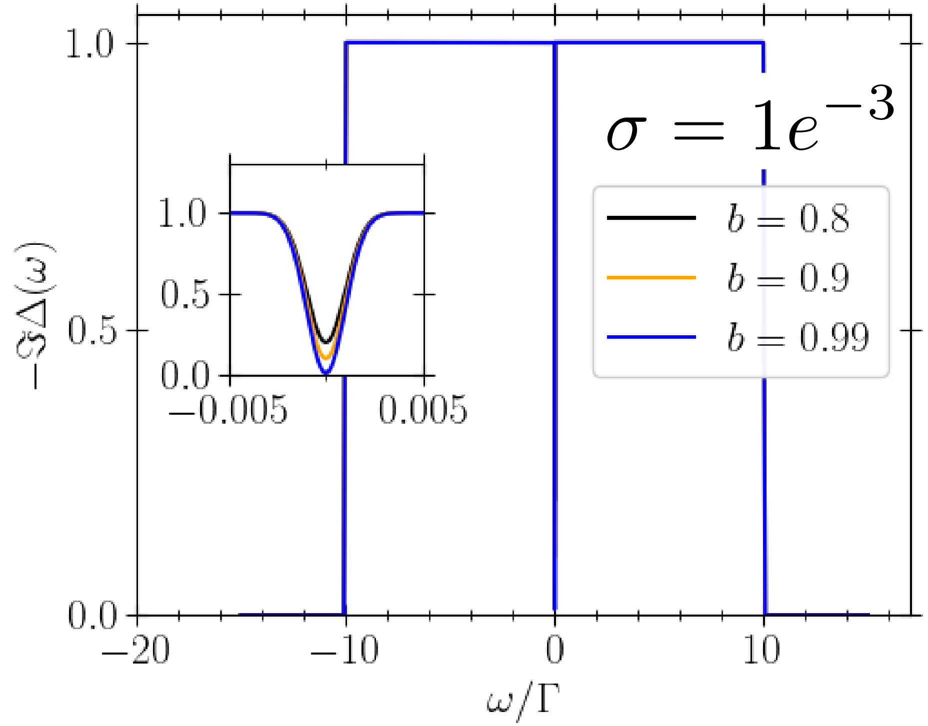

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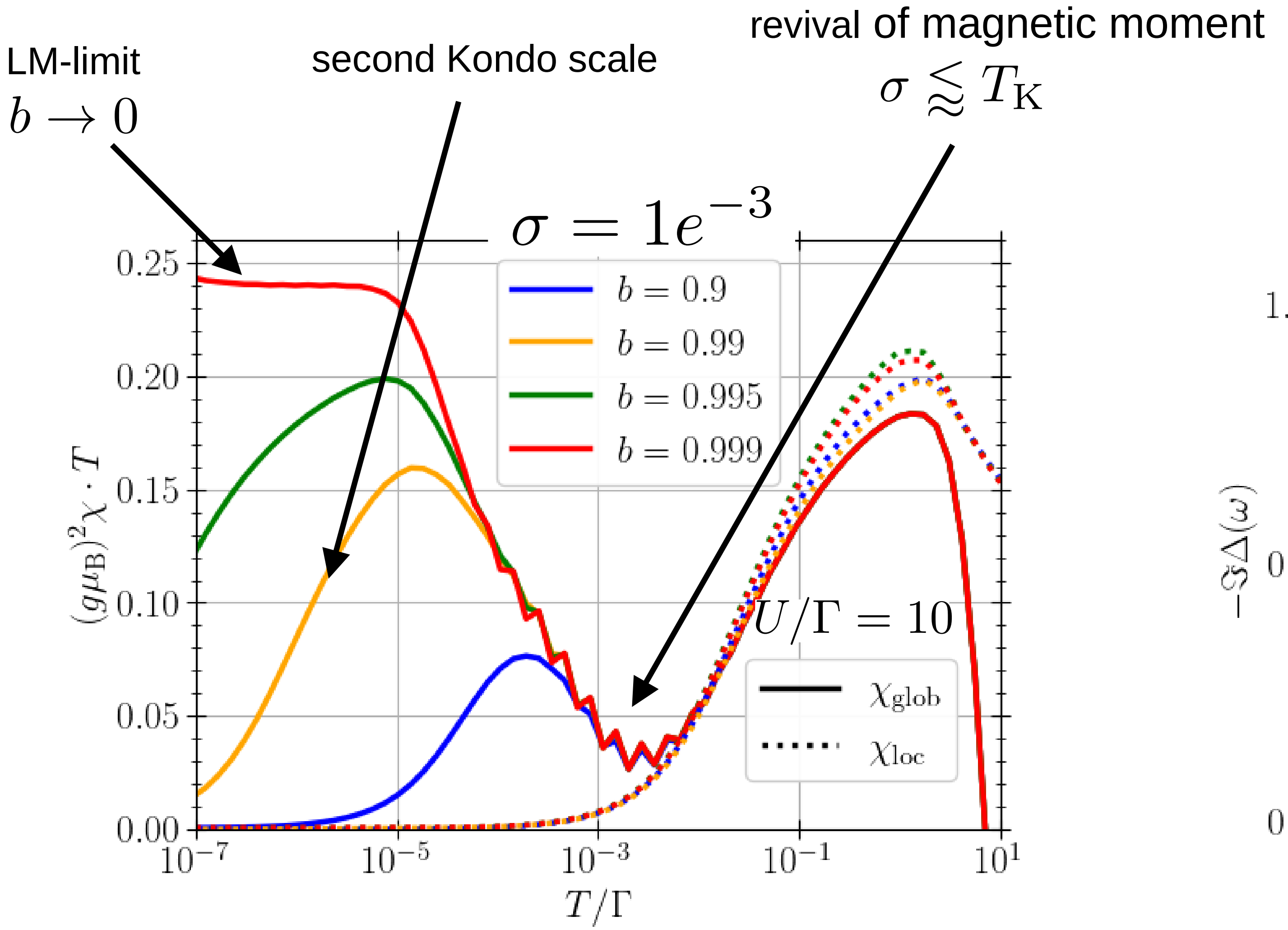

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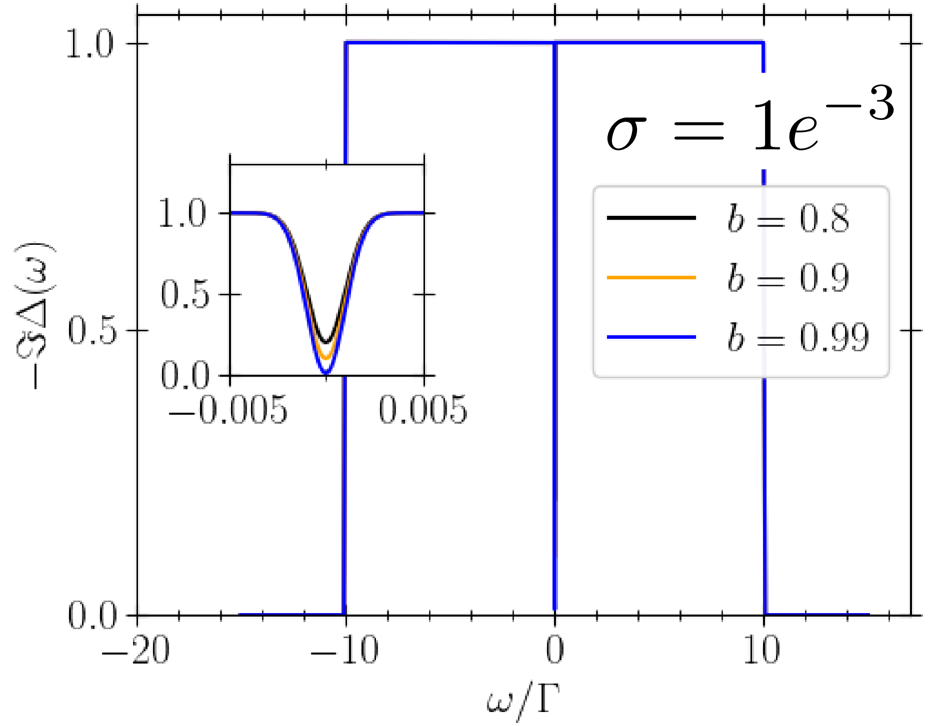

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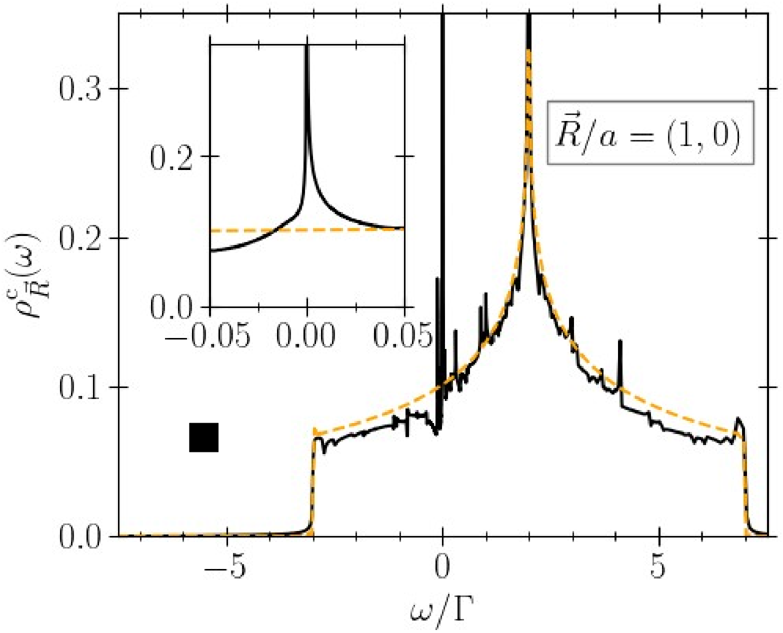

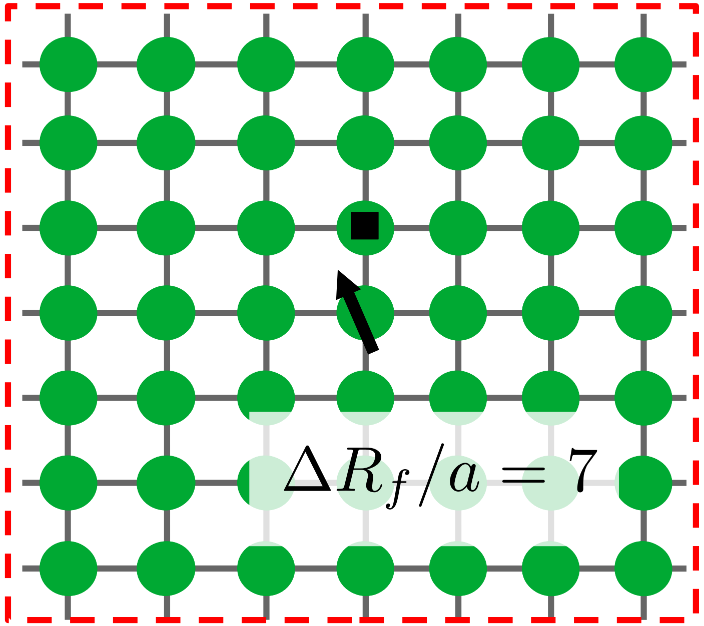

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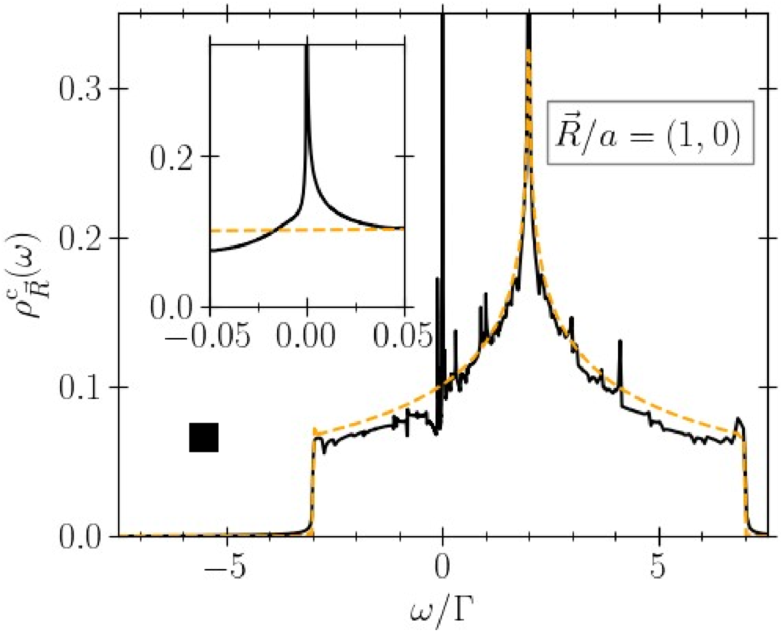

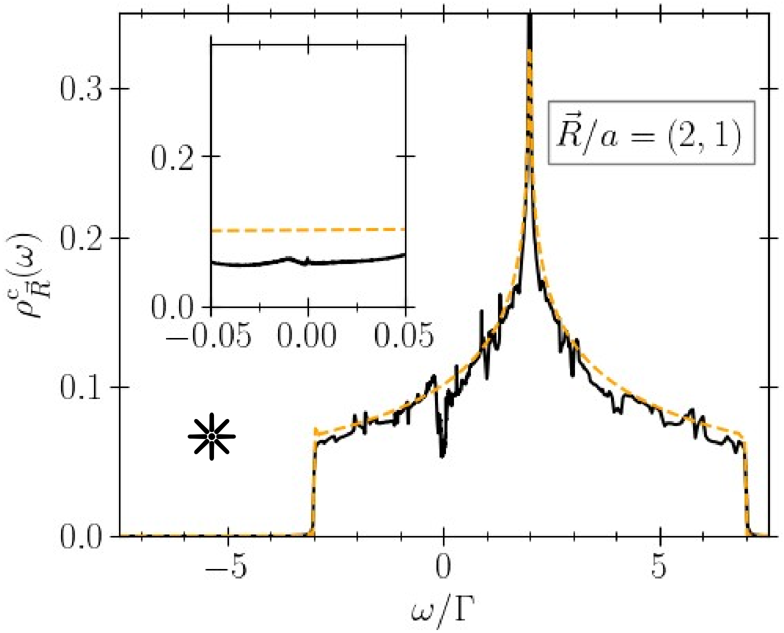

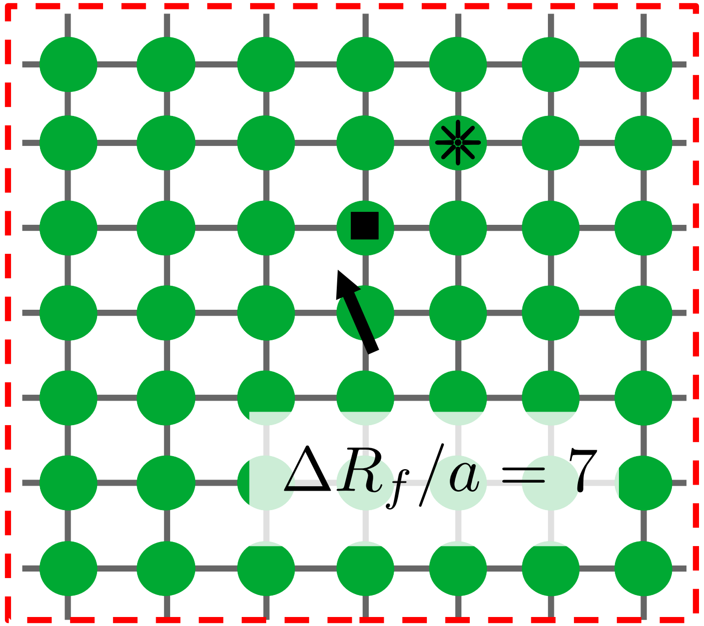

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