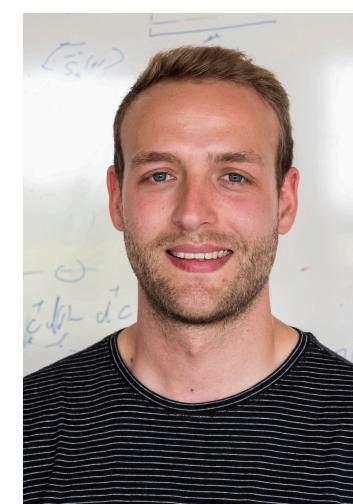


Strongly correlated multi-impurity models: The crossover from a single-impurity problem to lattice models

Frithjof B. Anders

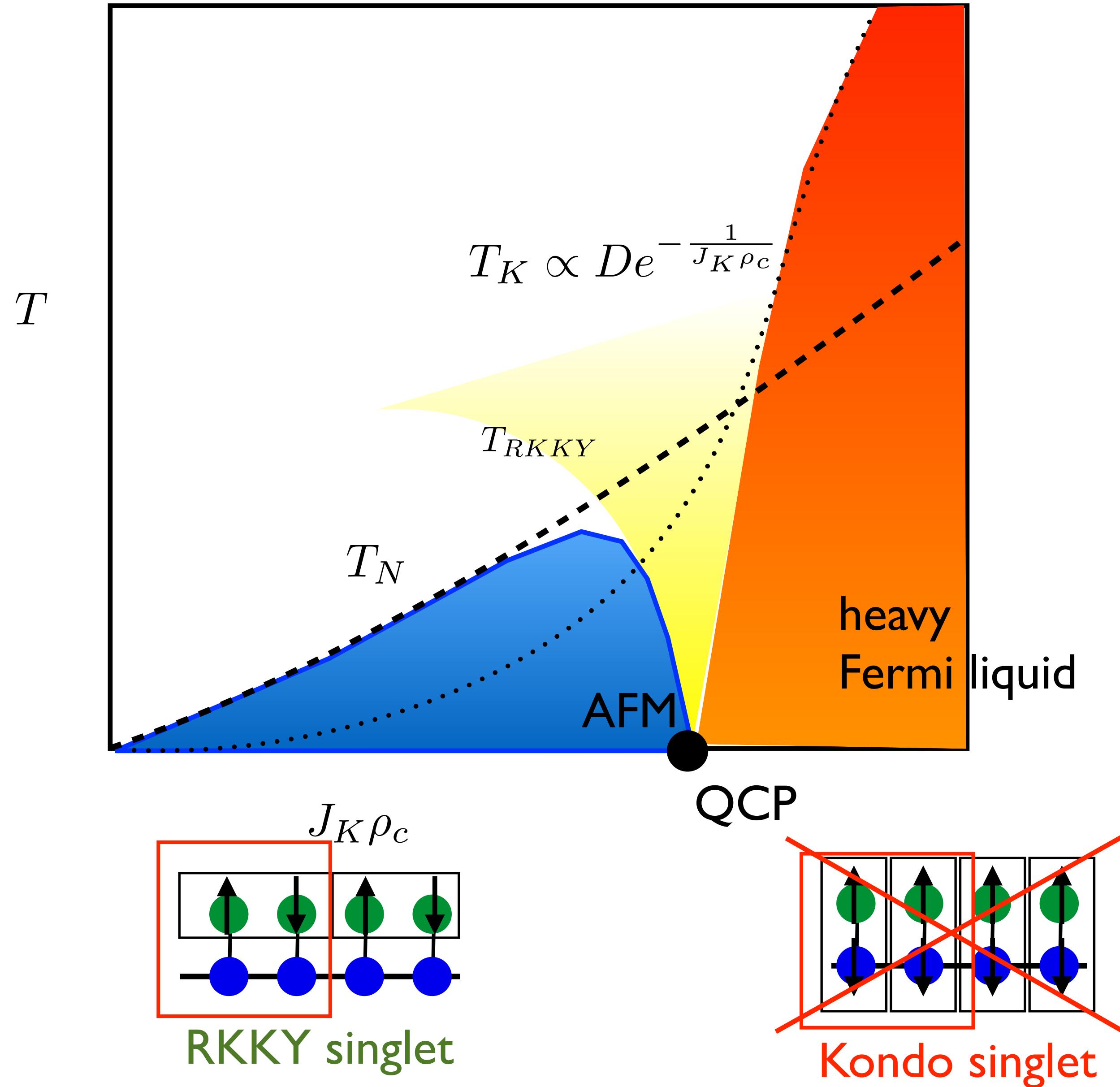
Condensed Matter Theory - Technische Universität Dortmund

Collaborator: Fabian Eickhoff

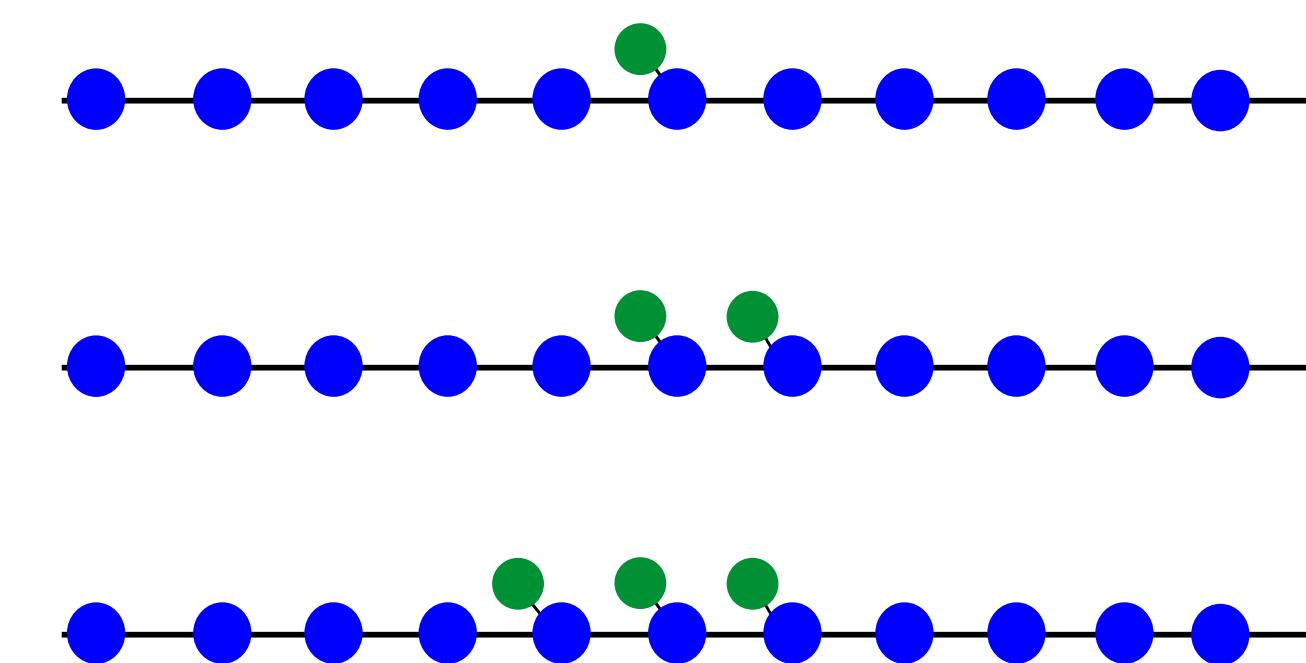
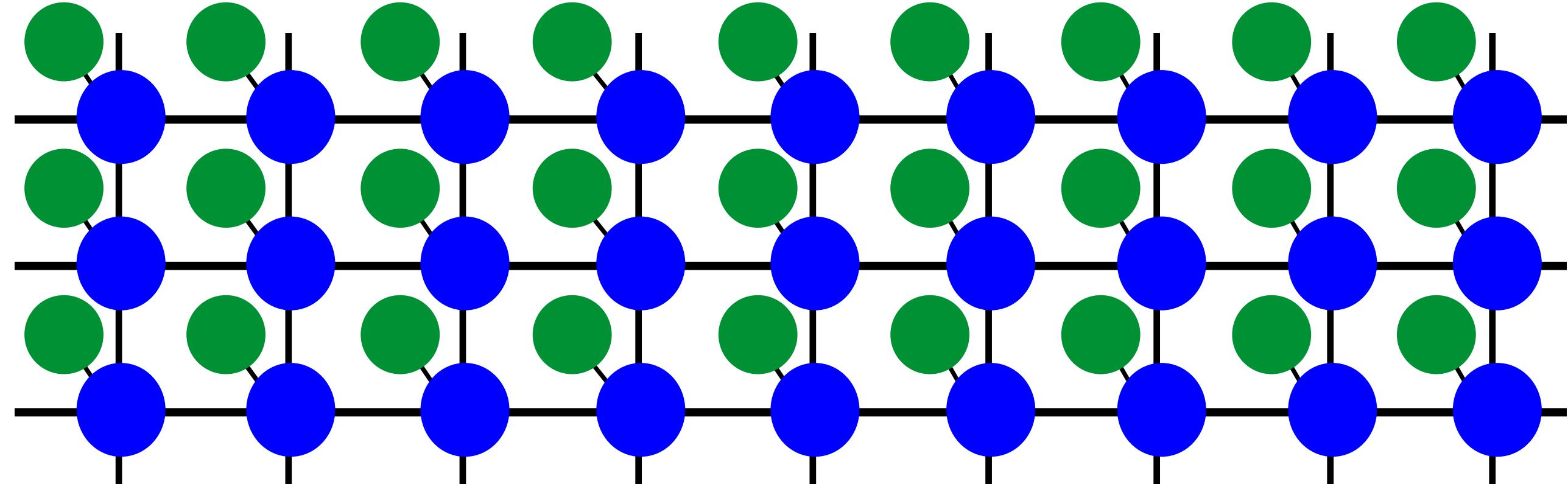


F. Eickhoff and F.B. Anders,
PRB **98**, 115103 (2018)
PRB 102, 205132 (2020)
PRB **104**, 045115 (2021)
PRB 104, 165105 (2021)

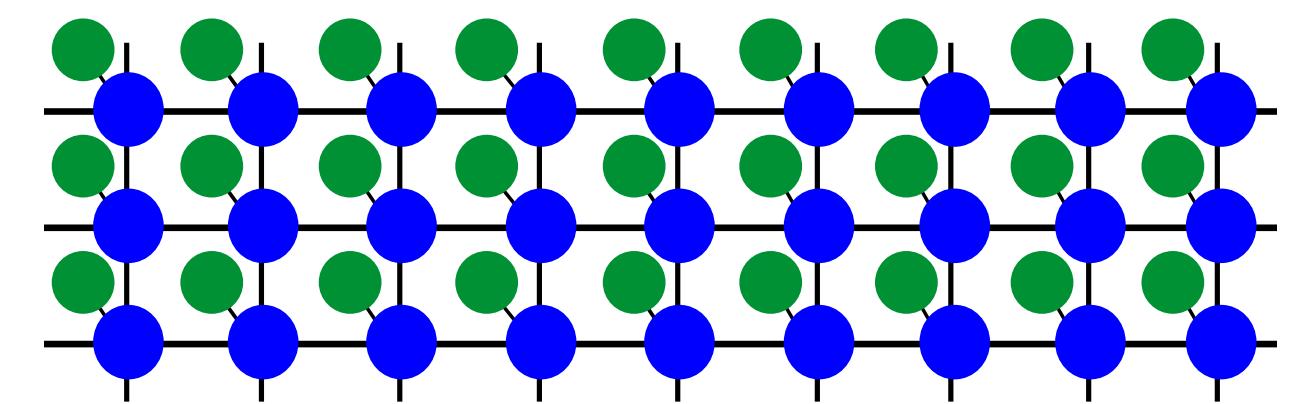
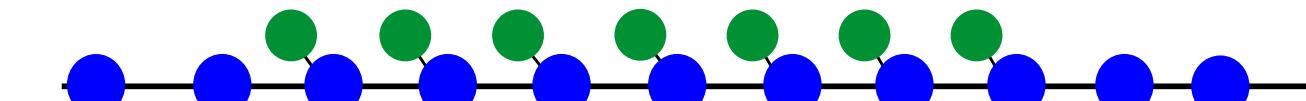
Heavy Fermions: Doniach phase diagram (1977)



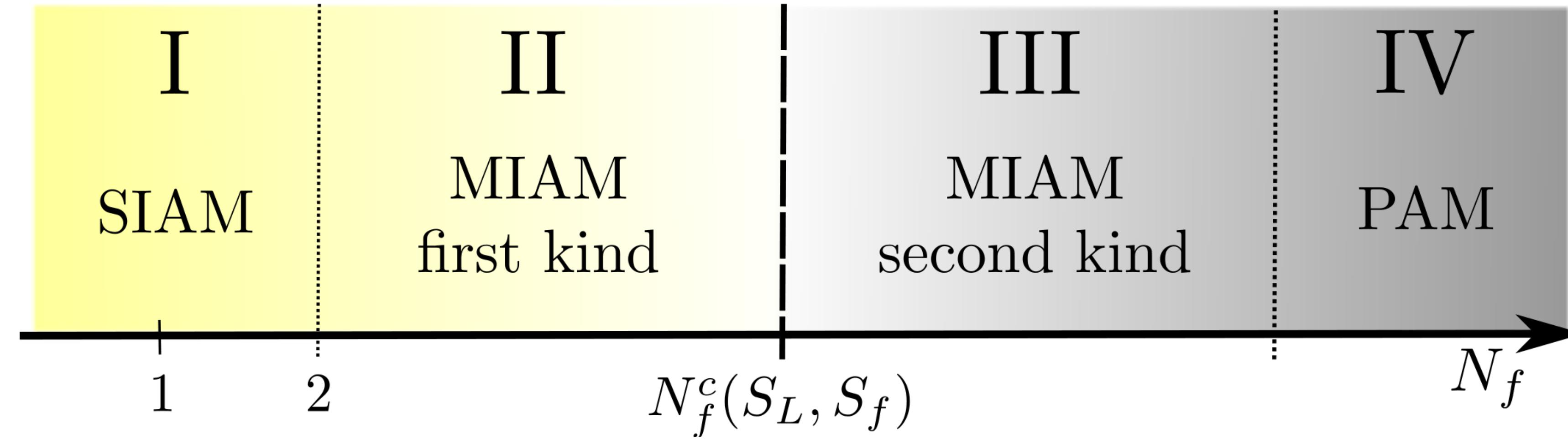
- simplified picture:
 - AFM: singlet formation via RKKY
 - HFL: itinerant Kondo screening?
- minimal model: two impurity Kondo model (1980s)
 - particle-hole asymmetry destroys the QCP (Affleck, Jones et al, 1995)
- Nozières: how does the Kondo screening work in the lattice, not enough electron?
- claim: no single impurity Kondo screening in a lattice model with N_f screening channels!



- Uncorrelated tight binding lattice with N_c lattice sites
- N_f correlated orbitals
$$H_l^f = \sum_{\sigma} \epsilon_l^f f_{l,\sigma}^\dagger f_{l,\sigma} + U n_{l\uparrow} n_{l\downarrow}$$
- $N_f \leq N_c$
- $N_f=1$: Single impurity Anderson model (SIAM)
- $N_f=N_c$: periodical Anderson model (PAM)



N_f



Criterium: adding a strong FM Heisenberg interaction between the correlated orbitals:

- Kondo screening possible: singlet ground state
- always enough screening channels $K=N_f$

- local moment ground state
- not enough screening channels available: $K < N_f$

$$H_{FM} = -J \sum_{\langle ij \rangle} \vec{S}_i \vec{S}_j$$

Exact Green's function

$$\underline{\underline{G}}_{\sigma}^f(z) = [z - \underline{\underline{E}}_{\sigma} - \underline{\underline{\Delta}}_{\sigma}(z) - \underline{\underline{\Sigma}}_{\sigma}(z)]^{-1},$$

Hybridization matrix encodes the geometry

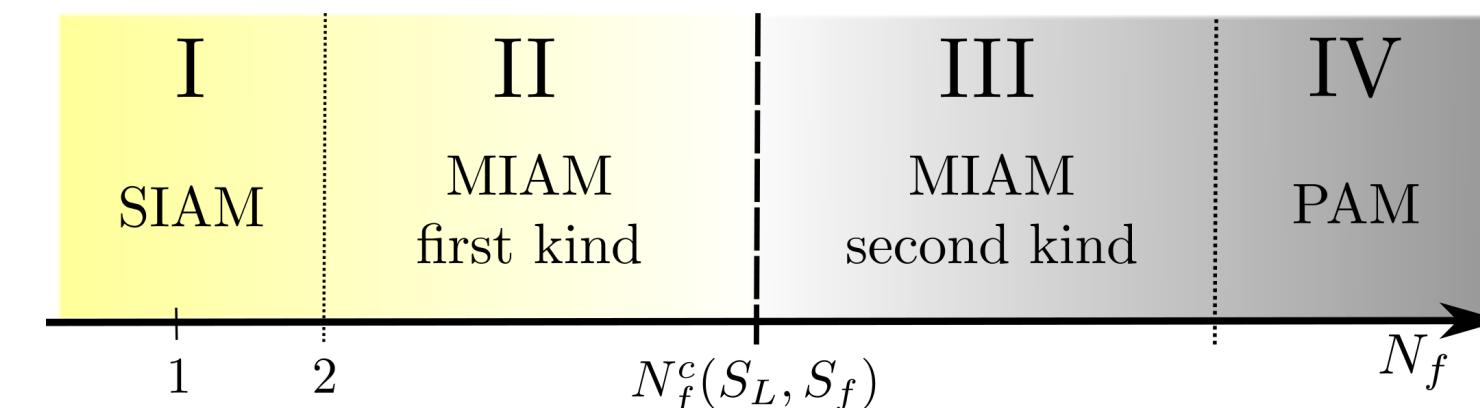
$$\Delta_{l,l',\sigma}(z) = \frac{V_l V_{l'}^*}{N} \sum_{\vec{k}} \frac{e^{i\vec{k}(\vec{R}_l - \vec{R}_{l'})}}{z - \varepsilon_{\vec{k}\sigma}}.$$

Wide band limit: V/D small

$$\Delta_{l,l',\sigma}(z) \approx \Delta_{l,l',\sigma}(0) = \Re[\Delta_{l,l',\sigma}(0)] + i\Gamma_{l,l',\sigma}(0)$$

effective hopping between the f-orbitals

hybridization strength to effective conduction bands



Two step mapping

I. diagonalize $\underline{\underline{\Gamma}}$

$$\text{diag}(\Gamma_n) = \underline{\underline{U}}^\dagger \underline{\underline{\Gamma}}(0) \underline{\underline{U}}$$

$$K = \text{rank}[\underline{\underline{\Gamma}}]$$

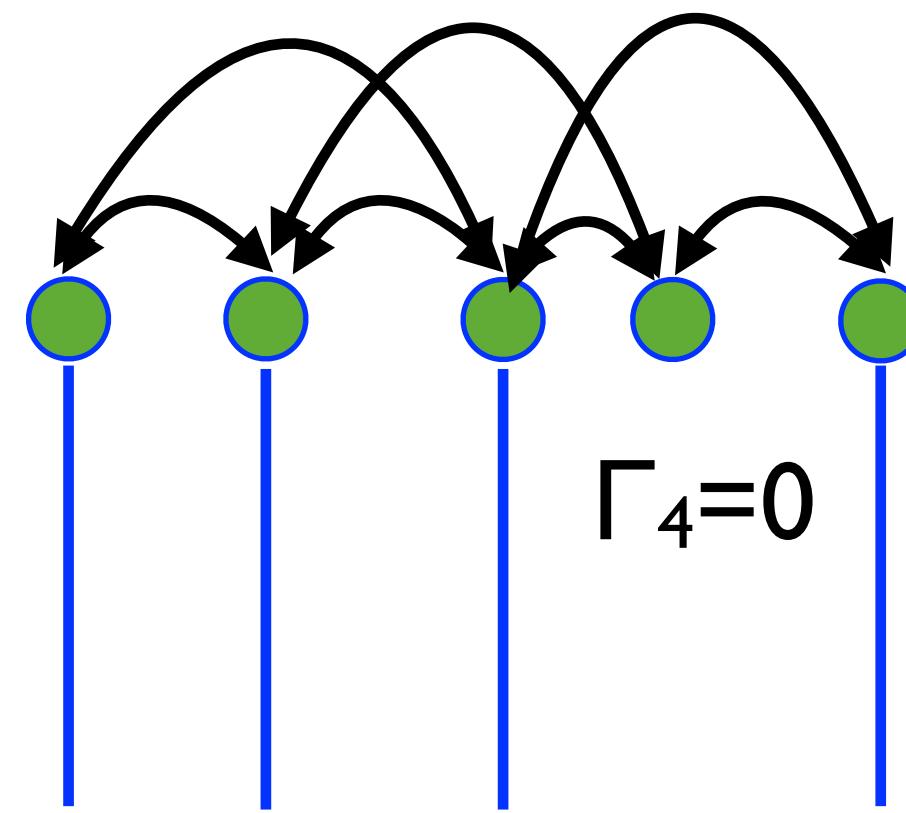
→ number of effective screening channels

2. rotate hopping matrix

$$\underline{\underline{T}} = \underline{\underline{U}}^\dagger \Re[\underline{\underline{E}} + \underline{\underline{\Delta}}(0)] \underline{\underline{U}}$$

→ effective TB model

Result: Hubbard-cluster coupled to K bands

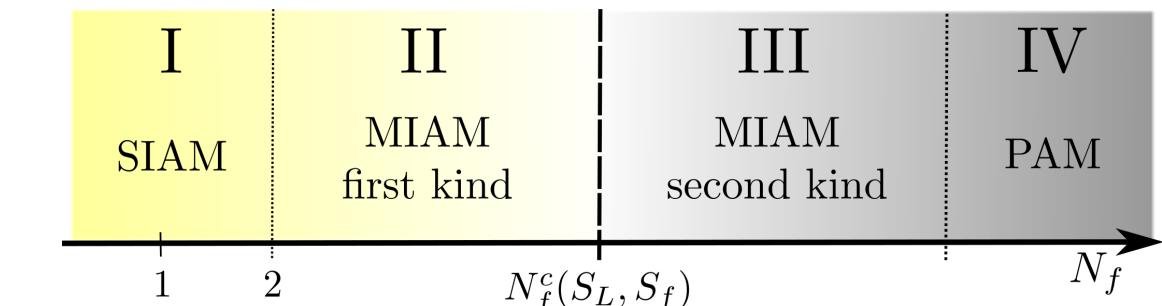


PAM:

- Δ diagonal in k-space $\Delta_{\vec{k}}(z) = \frac{|V_{\vec{k}}|^2}{z - \varepsilon_{\vec{k}\sigma}}$
- $K = \text{rank}(\Gamma) = \#\text{k points on the Fermi surface}$

- not enough screening channels for Kondo screening each local spin in the PAM
- PAM: self-screening via AF RKKY interaction

- Hopping generates AF part of the RKKY
- hybridization matrix Γ : FM RKKY
- Upper limit of $K = \text{rank}(\Gamma)$?



Eickhoff and FBA, PRB **102**, 205132 (2020)

Kondo Insulator regime: Extended Lieb-Mattis theorem

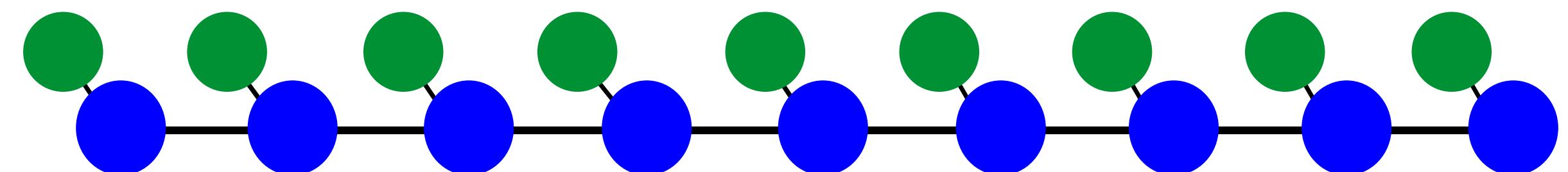
Shen PRB 53, 14252 (1996)

- bipartite Kondo lattice $N_f \leq N_c$
- ground state spin:

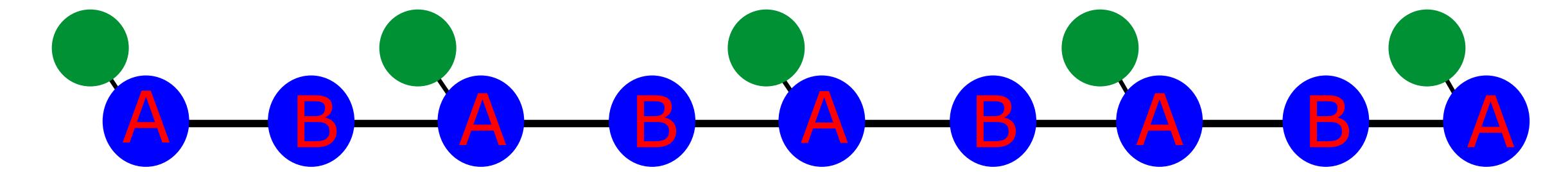
$$2J_z = |N_{c,A} - N_{c,B} - N_{f,A} + N_{f,B}|$$

Extension of the theorem to a finite size cluster coupled to a continuum.
PRB 104, 045115 (2021)

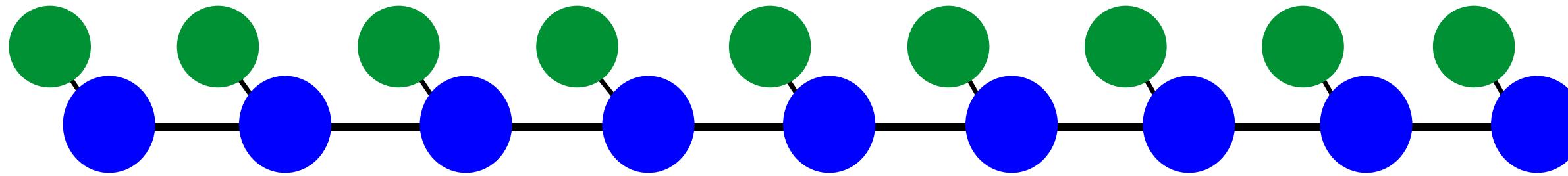
1. M. Sigrist et al PRL 1991: Periodic Anderson model (PAM) in 1d with one electron in the conduction band ($\mu \rightarrow 0$): ground state $J_z = (N_f - 1)/2$



2. Titvinidze et al, PRB (2015): Depleted PAM at half filling:
ground state $J_z = (N_f - 1)/2$



3. Held and Bulla (2000): PAM in large d with nearest neighbor hybridization: Mott-Hubbard physics

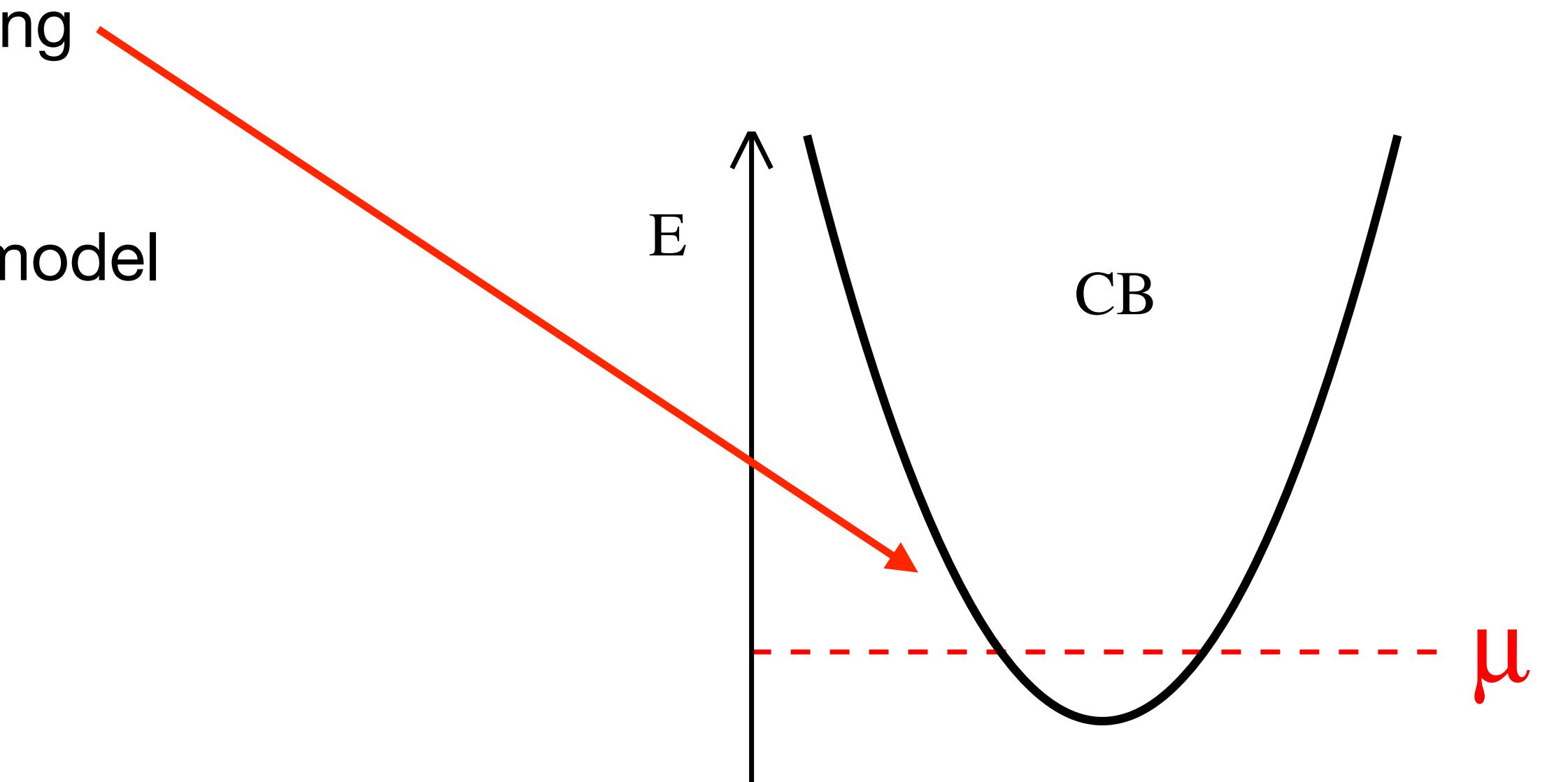


M. Sigrist et al PRL 1991: conduction band is filled with a single electron, while the correlated orbital remains at half filling

- μ approaches the lower band edge in a continuum model
- exact statement: ground state $J_z = (N_f - 1)/2$

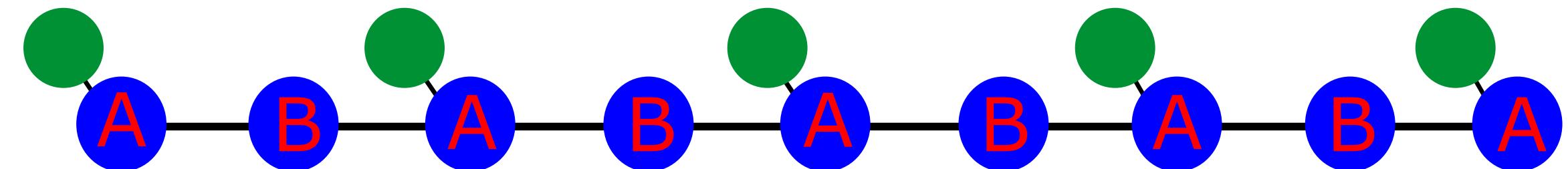
Our mapped MIAM:

- $\Gamma_{\text{Im}} = \Gamma$: $K = \text{rank}(\Gamma) = 1$: only one Kondo screening channel
- hopping vanishes due to van Hove singularity:
- ground state $J_z = (N_f - 1)/2$: FM alignment and 1 screening channel



$$\Delta_{l,l',\sigma}(z) = \frac{V_l V_{l'}^*}{N} \sum_{\vec{k}} \frac{e^{i\vec{k}(\vec{R}_l - \vec{R}_{l'})}}{z - \varepsilon_{\vec{k}\sigma}}.$$

2. Depleted PAM at half filling



- A/B bipartite 1D lattice
- DMRG results: ground state: $J_z = (N_f - 1)/2$

Titvinidze et al, PRB (2015)

$$\Delta_{l,l',\sigma}(z) = \frac{V_l V_{l'}^*}{N} \sum_{\vec{k}} \frac{e^{i\vec{k}(\vec{R}_l - \vec{R}_{l'})}}{z - \varepsilon_{\vec{k}\sigma}}.$$

Predictions from the mapped MIAM:

- $K = \text{rank}(\Gamma) = 1$: one Kondo screening channel
- no effective hopping between orbitals on the same sublattice + 1 screening channel
- ground state: $J_z = (N_f - 1)/2$
- consistent with the extended Lieb-Mattis theorem

**Kondo Insulator regime:
Extended Lieb-Mattis theorem**

Shen PRB 53, 14252 (1996)

- bipartite Kondo lattice $N_f \leq N_c$
- ground state spin:

$$2J_z = |N_{c,A} - N_{c,B} - N_{f,A} + N_{f,B}|$$

Take home message: mapped MIAM also fulfills the extended Lieb-Mattis theorem

3. Large D PAM with nearest neighbor hybridization

Rapid Note

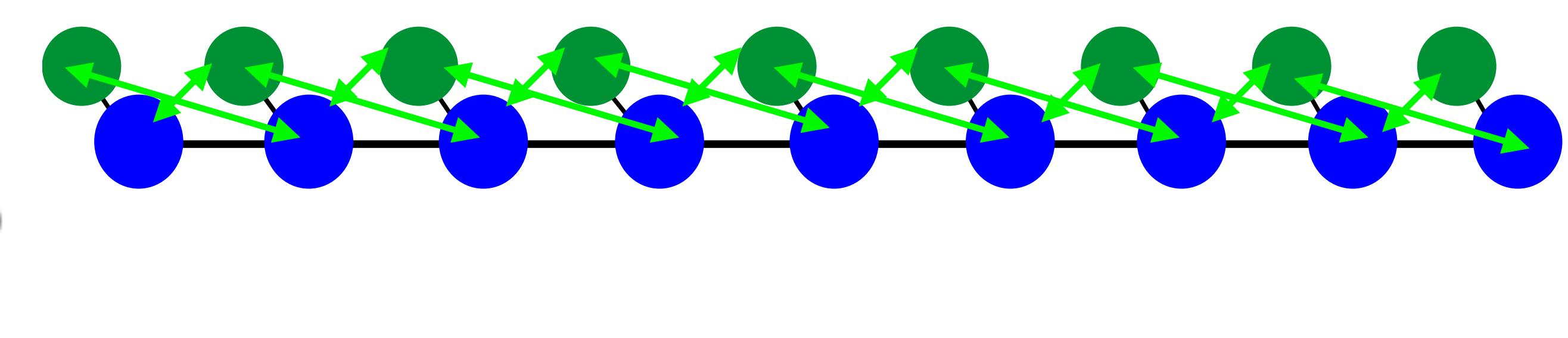
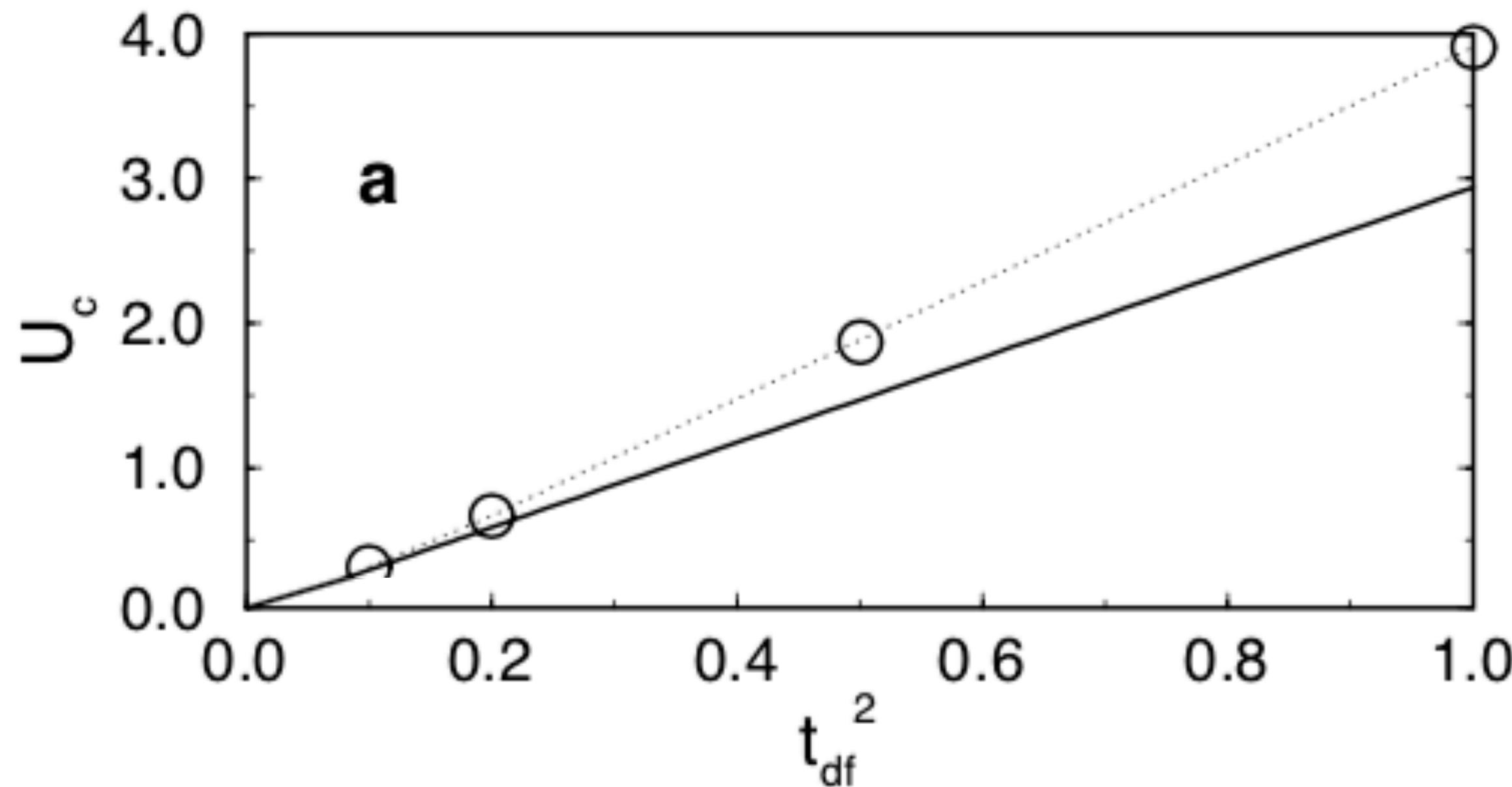
**Mott transition of the f-electron system in the periodic
Anderson model with nearest neighbor hybridization**

Held, Bulla Eur. Phys. J. B 17, 7 (2000)

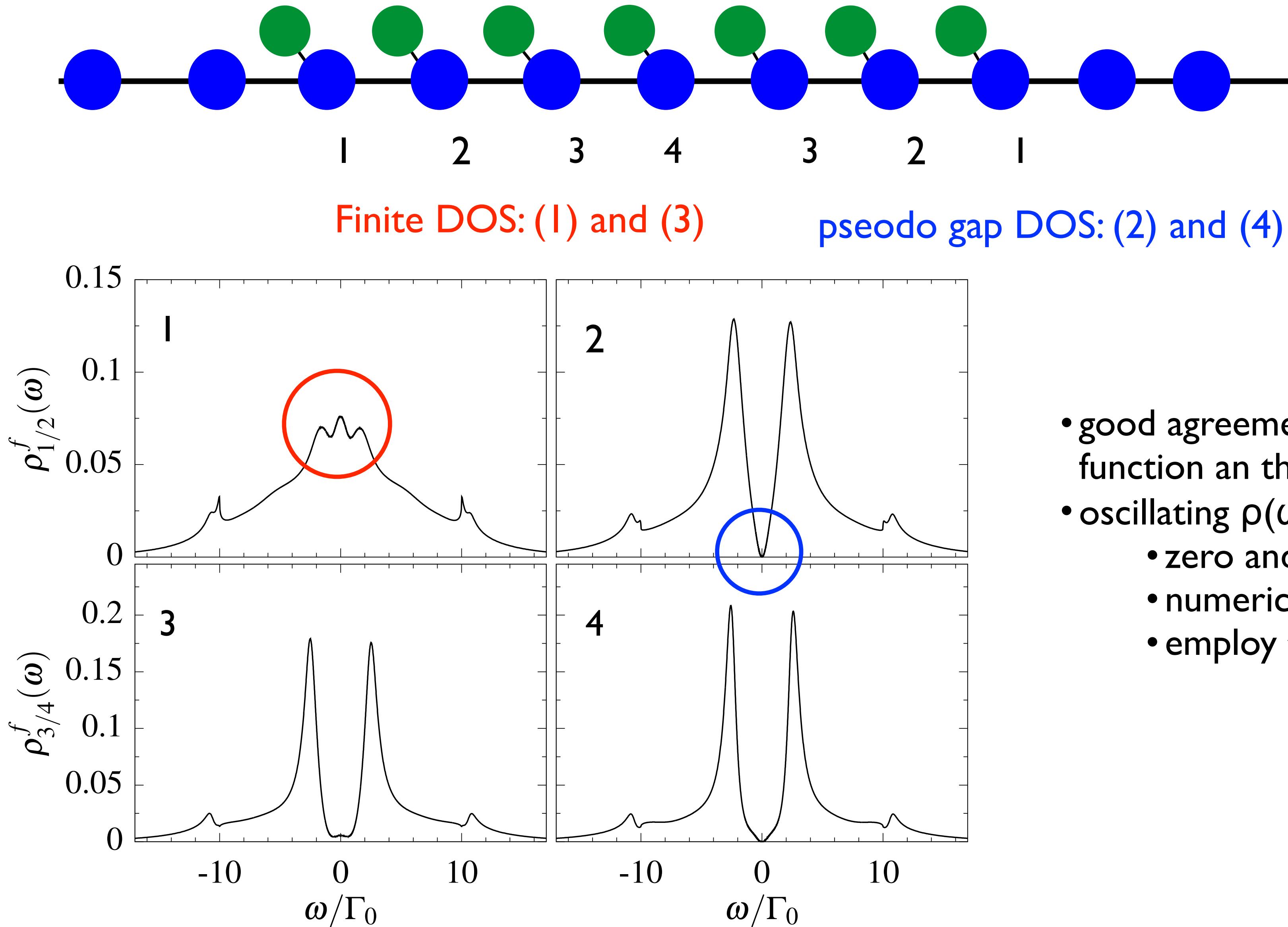
K. Held^a and R. Bulla

Theoretische Physik III, Elektronische Korrelationen und Magnetismus, Universität Augsburg, 86135 Augsburg, Germany

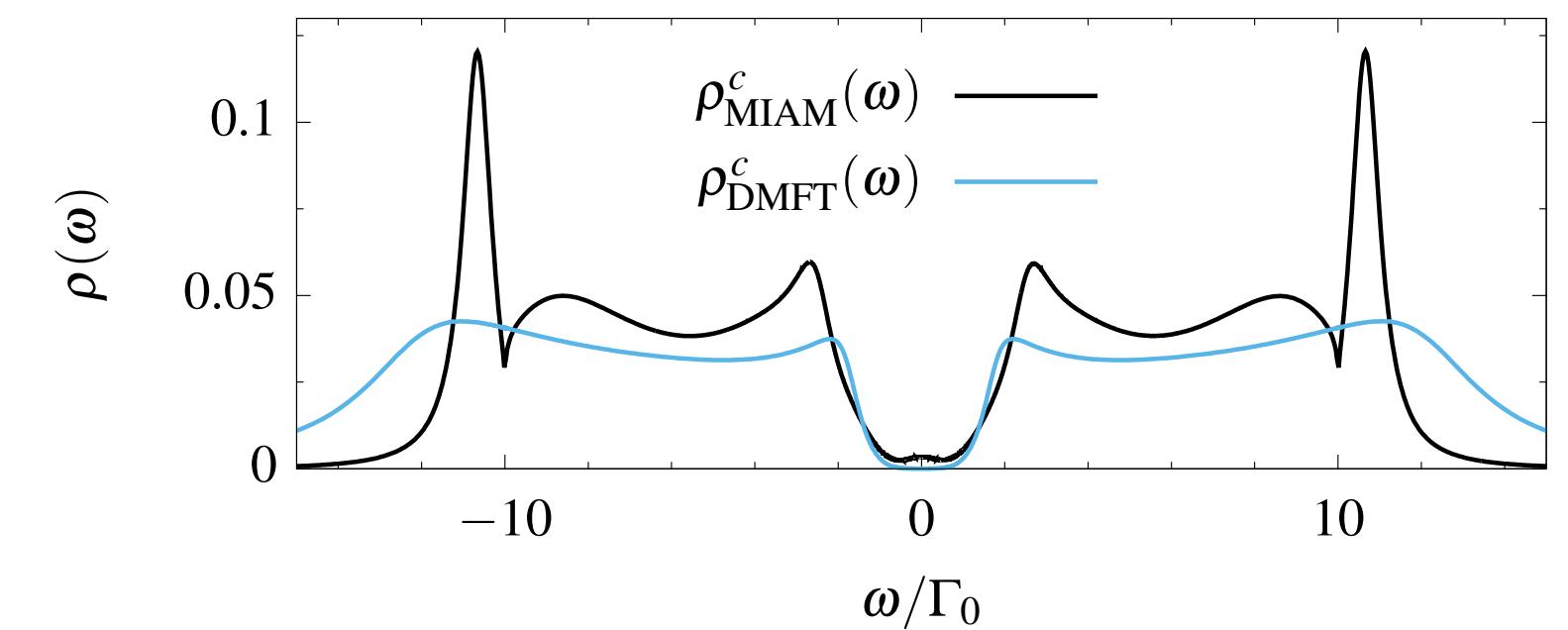
- $K = \text{rank}(\Gamma) = 0$ at half-filling: no Kondo screening channel
- Prediction: Equivalent to a Hubbard model with Mott-Hubbard insulator transition with a renormalized hopping



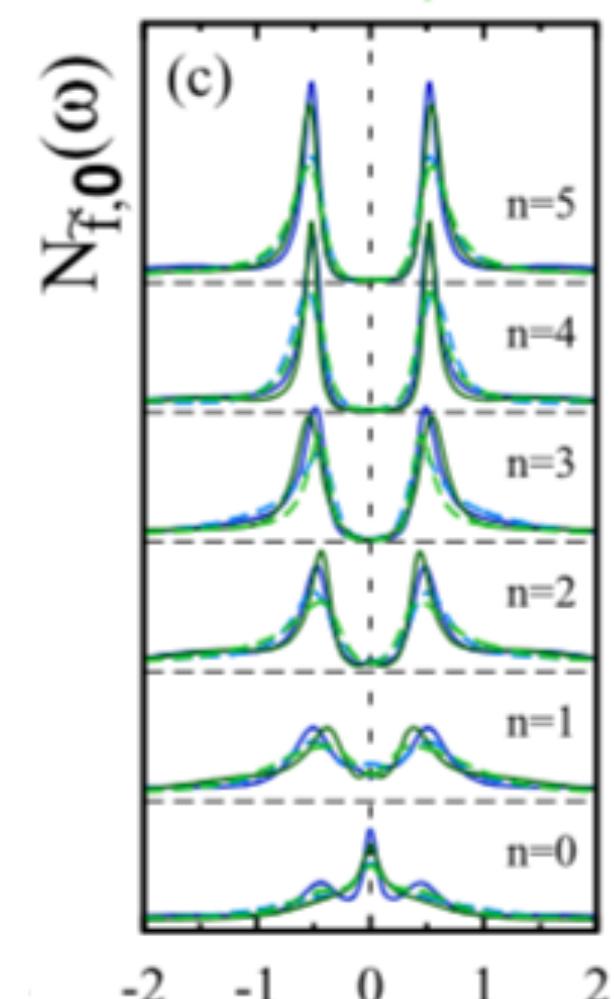
Eickhoff and FBA, PRB **104**, 165105 (2021)



DMFT vs central cluster position



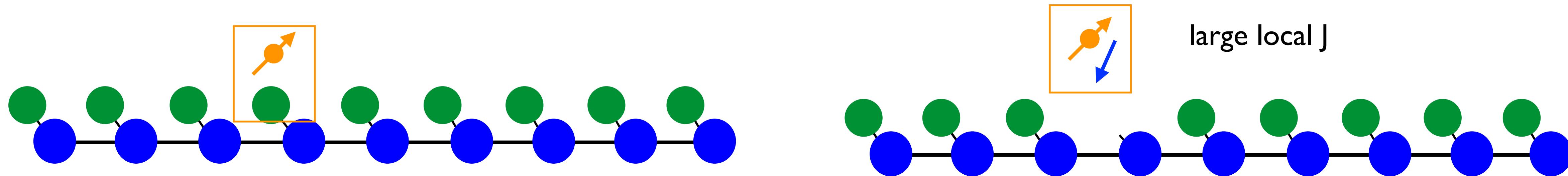
- good agreement between DMFT Kondo lattice spectral function an the “bulk” site of a $N_f=7$ cluster model
- oscillating $\rho(\omega=0)$:
 - zero and non zero NRG results
 - numerical artifacts?
 - employ the Lieb Mattis theorem



Raczkowski and Assaad, PRL 2019

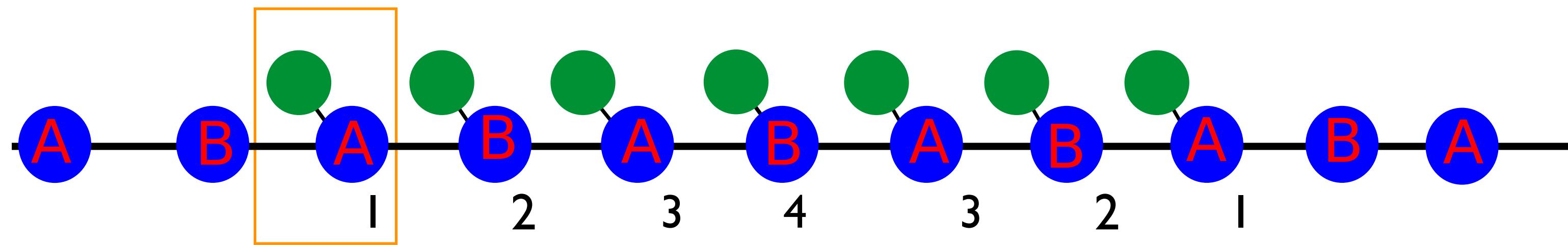
Q: Can we use the extended Lieb-Mattis theorem to predict a gap or a finite DOS in the local spectral function?

probe spin+ AF Kondo coupling



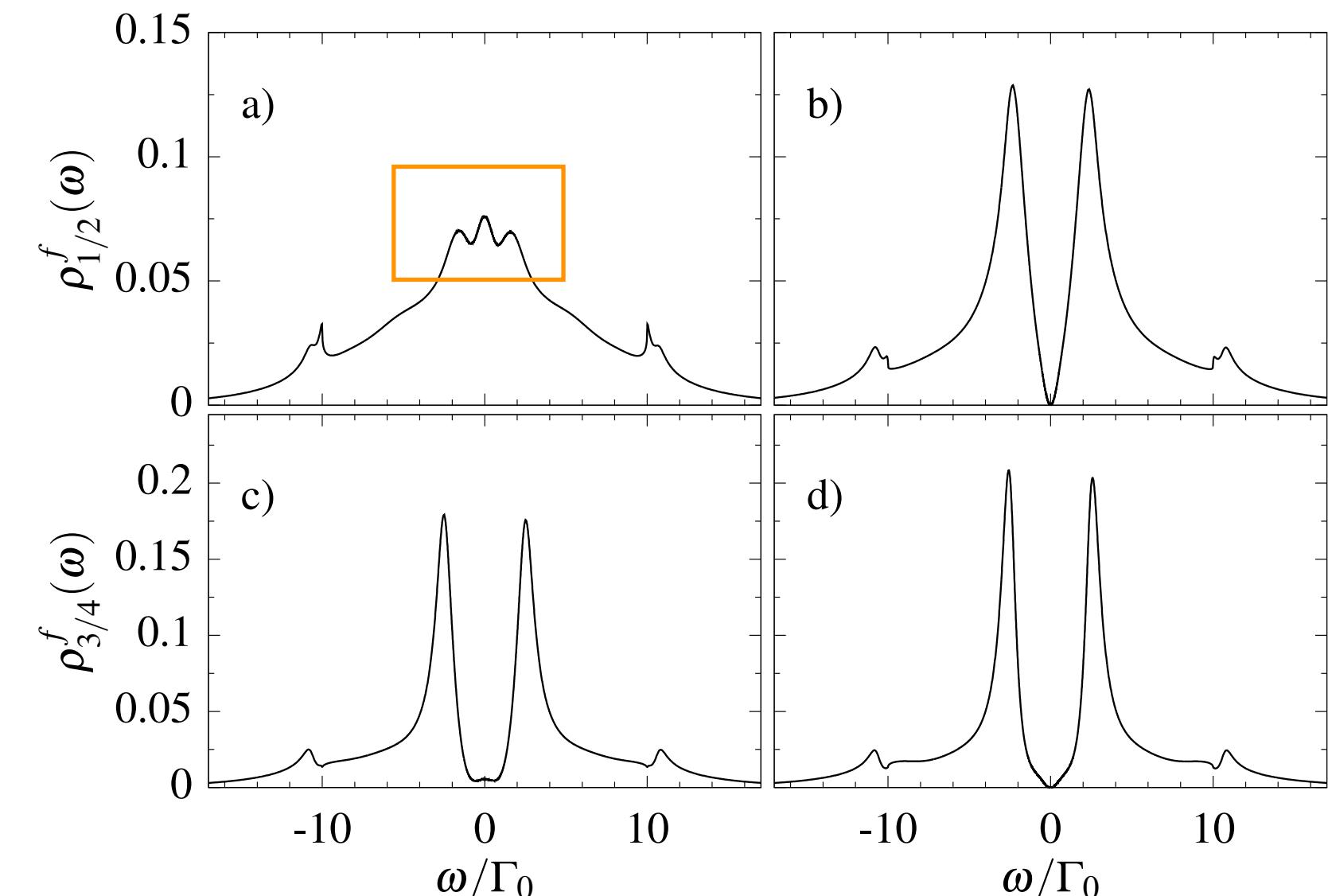
Ground state:

- local moment: pseudo gap DOS
- singlet: finite DOS at $\omega=0$
- extend Lieb Mattis theorem: the coupling strength does not enter!
- Lieb Mattis theorem to determine the ground state of the corresponding Kondo hole problem



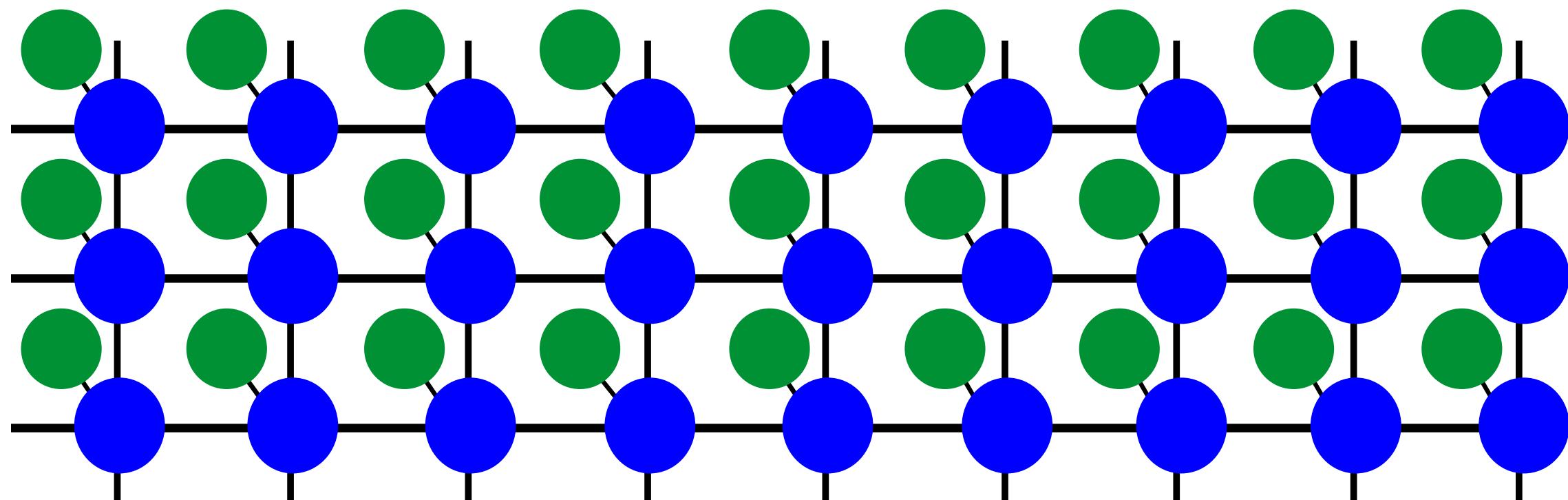
Eickhoff, FBA, PRB **104**, 165105 (2021)

1. Elimination of the first correlated orbital: singlet \Rightarrow finite DOS
2. Kondo hole on **same** sublattice as the two outside orbitals: local moment formation \Rightarrow pseudo gap DOS
3. Kondo hole on a **different** sublattice as the two outside orbitals: singlet formation \Rightarrow finite DOS
4. Kondo hole on **same** sublattice as the two outside orbitals: local moment formation \Rightarrow pseudo gap DOS



Note:

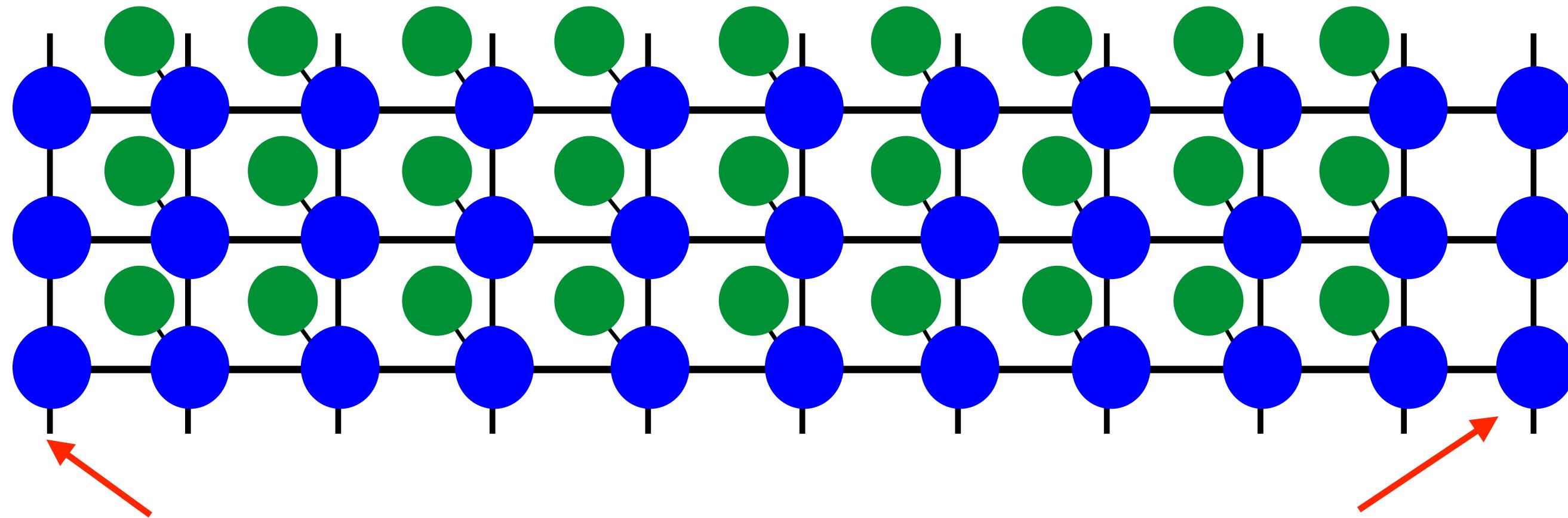
- extended Lieb-Mattis-theorem does not predict the magnitude of the finite DOS:
- consistent with approaching the bulk limit
- also the spatial dimension of the problem does not enter: applicable to 3D!



Eickhoff, FBA, PRB **104**, 165105 (2021)

PAM: $N_f = N_c$
DOS: Shen Lieb-Mattis theorem
predicts a gap in the DOS for all
c- and f-orbital spectra

Q: What is the minimal extension of the PAM to generate a metallic surface state?

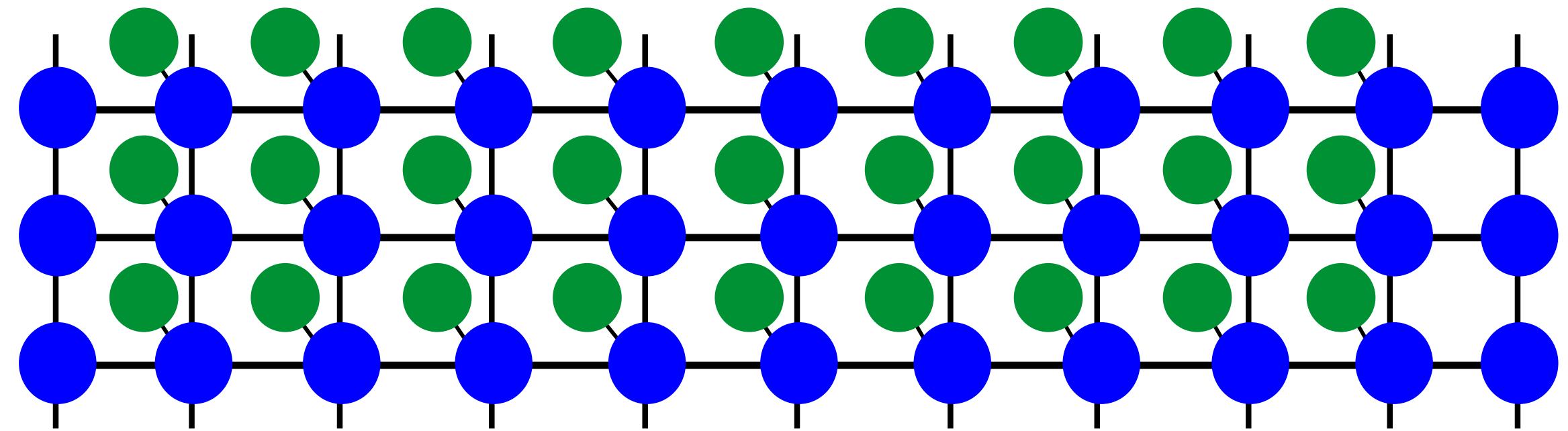


Adding an uncorrelated half-filled edge orbital:

- screening of the edge local moment
- extended Lieb-Mattis theorem: singlet GS, finite DOS at the edge of 2d/3D Kondo insulator

Q: What is the minimal extension of the PAM to generate a metallic surface state?

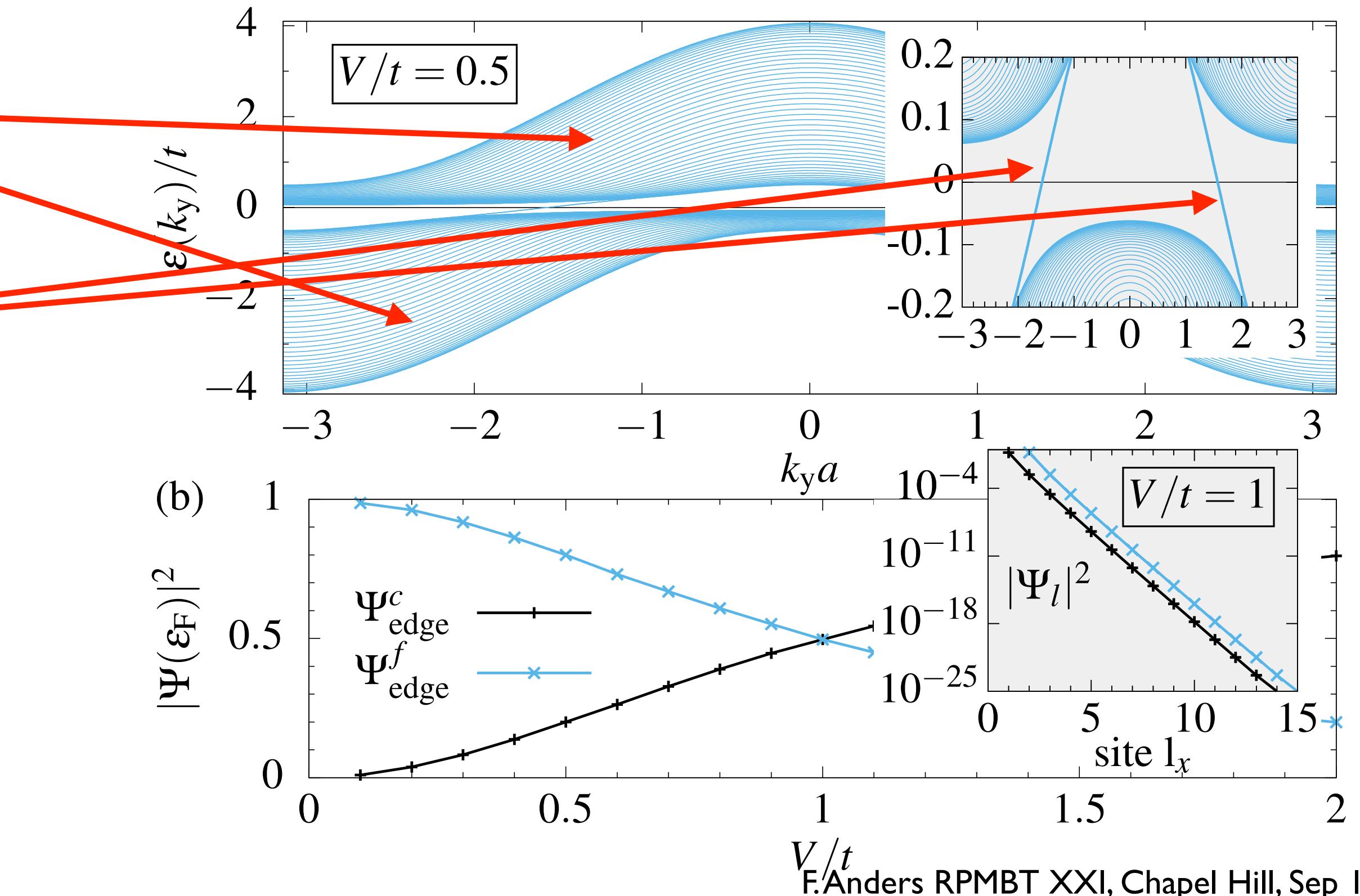
PRB **104**, 165105 (2021)



Kondo insulator bulk states: gapped

- two metallic edge band:
- exponentially localized
- small V: mainly f-character
- large V: mainly c-character

Trivial insulator with metallic surface state:
prevails at finite U (extended Lieb-Mattis theorem)



- Mapping of MIAM onto effective models
 - ◆ identifying the **number of screening channels K** : MIAM of first or second kind
 - ◆ separating AF and FM parts of the RKKY interaction
 - ◆ correlated PAM and Kondo lattices are MIAM of the second kind: singlet via self-screening and not a Kondo singlet!
- **Application of the extended Lieb Mattis theorem:**
 - identifying the ground state spin configuration, particularly for Kondo hole problems
 - prediction of pseudo gap or finite spectrum on a bipartite lattice with half-filling
- **PAM plus uncorrelated surface orbital layer: A metallic surface band emerges which has mainly f-electron character**

Eickhoff and FBA,
PRB **102**, 205132 (2020),
PRB **104**, 045115 (2021)
PRB **104**, 165105 (2021)