Title: DMRG Analysis of Mobile Impurities and Orbital-selective Mott Phases

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Abstract:

DMRG analysis of mobile impurities and orbital-selective Mott phases

Phys. Rev. B **88**, 140407(R) (2013)
Phys. Rev. Lett. (2014) - arXiv:1402.1689

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Outline

- *Mobile magnetic impurities.*
  - Kondo-type Model
  - Phase diagram
  - Quantum phase transition
- *Orbital-selective Mott phase.*
  - Phase diagram
  - Charge and magnetic order
  - Quantum phase transition?

Quantum phase transition in mobile Kondo impurity systems

Collaborators:

- ✓ D. Garcia, K. Hallberg (Balseiro Institute)
- ✓ M. Vojta (TU Dresden)

J. Rincón *et al*, Phys. Rev. B **88**, 140407(R) (2013)

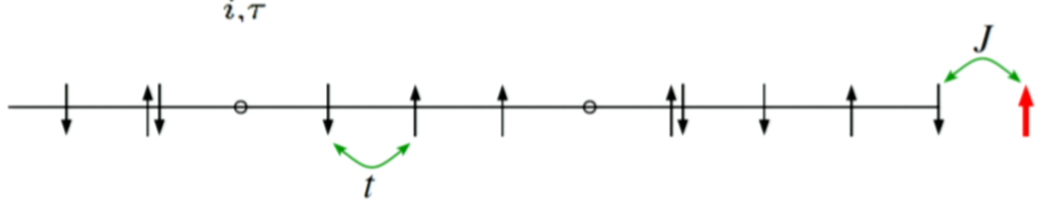
Motivation

- Dilute particles moving in quantum liquids: New physics?
- Charge carriers in weakly doped semiconductors or in Mott insulators.
- Ions in $^3\mathrm{He}$.
- Electrons in multi-band quantum wires.
- Multi-component ultracold gases with strong population imbalance.

A. Rosch, Adv. Phys. 48, 295 (1999)
I. Bloch et al., Rev. Mod. Phys. 80, 885 (2008)

Static Kondo model

$$H = -t\sum_{i,\tau}\left(c_{i\tau}^{\dagger}c_{i+1\tau} + \mathrm{H.c.}\right) + J\mathbf{S}_0\cdot\boldsymbol{\sigma} - H\sigma^z$$



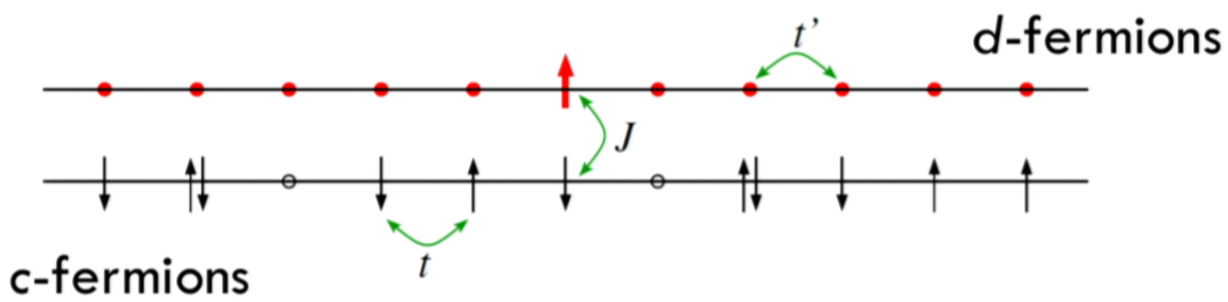
- (Non-)Fermi liquid physics (channel).
- (Un)Stable fixed point (RG).
- (In)Finite magnetic susceptibility (χ_0).

J. Kondo, Prog. Theor. Phys. 32, 37 (1964)
K. Wilson, Rev. Mod. Phys. 47, 773 (1975)

Mobile Kondo model

- Half-filled band. One "impurity."

$$H = -t\sum_{i,\tau}\left(c^\dagger_{i\tau}c_{i+1\tau} + \mathrm{H.c.}\right) + J\sum_i \mathbf{S}_i\cdot\boldsymbol{\sigma}_i + V\sum_i N_i n_i - t'\sum_{i,\tau}\left(d^\dagger_{i\tau}d_{i+1\tau} + \mathrm{H.c.}\right) - H\sum_i \sigma^z_i$$

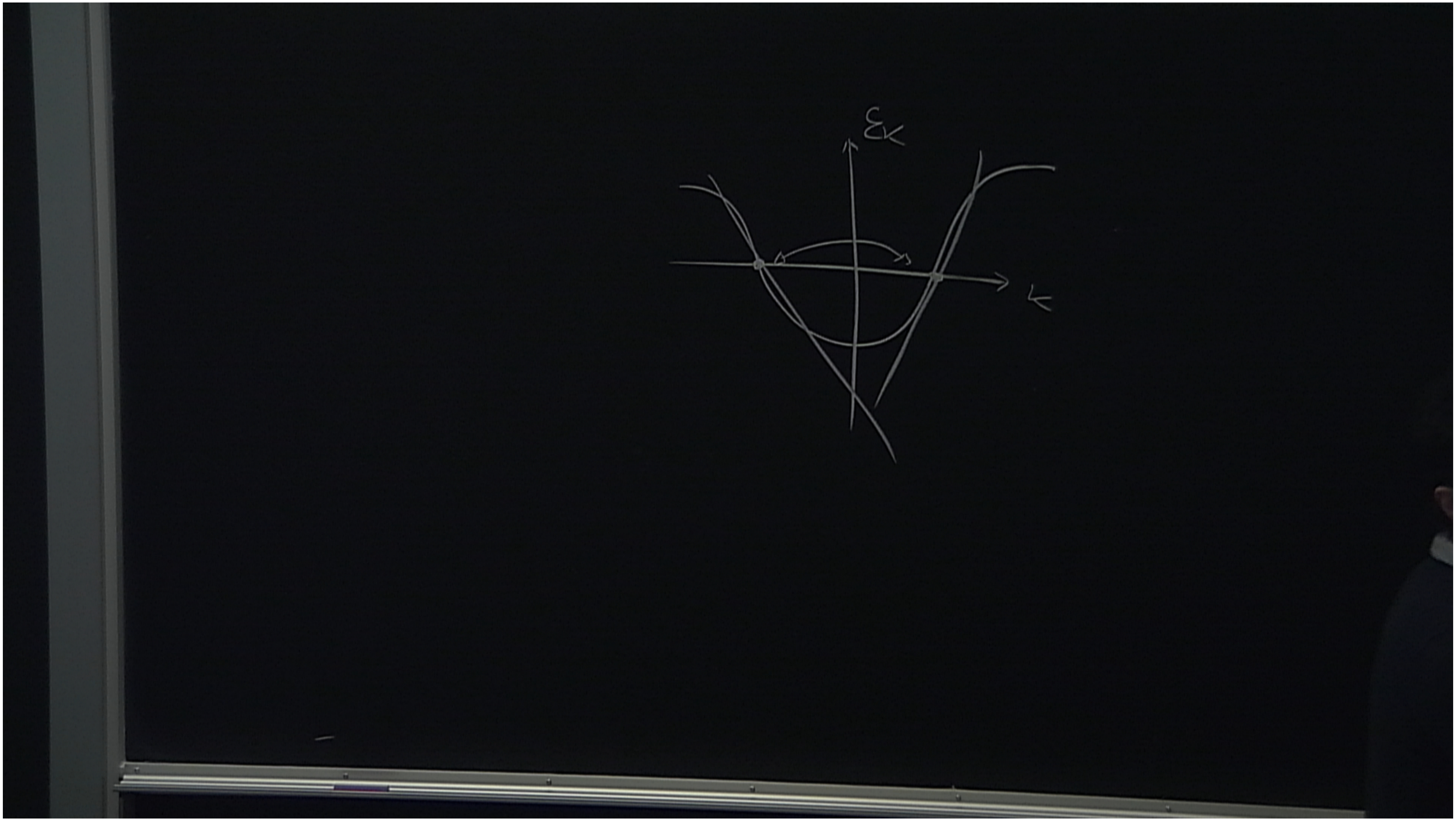


A. Lamacraft, Phys. Rev. Lett. 101, 225301 (2008)
J. Rincón *et al.*, Phys. Rev. B 88, 140407(R) (2013)

Mobile impurity model

- 2CK: left and right movers form two separate channels for screening (Lamacraft, PRL 2008).
  - Log. divergent χ_0 as $H \to 0, T \to 0.$
- 1CK: $J/t' \to \infty$, only even modes coupled.
  - Finite χ_0 as $H \to 0, T \to 0.$
- Technique: **DMRG** with PBC and OBC:
  - System sizes: from 2x11 to 2x101.
  - Numerical error: 10^{-4} (fittings).

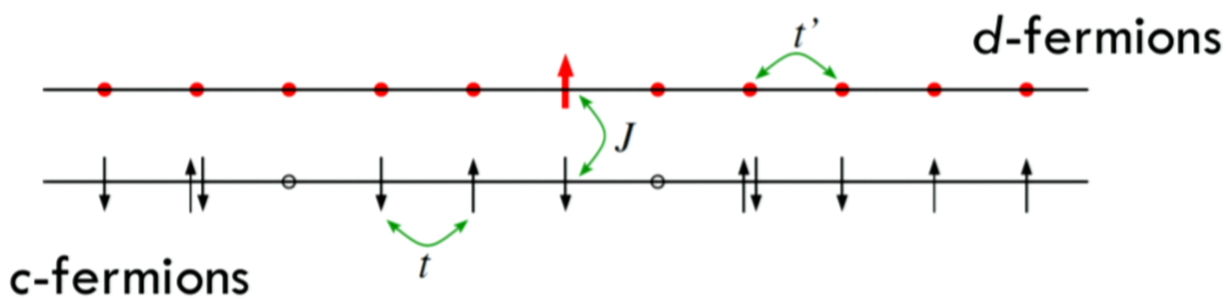
A. Lamacraft, Phys. Rev. Lett. 101, 225301 (2008)
S. White, Phys. Rev. Lett. 69, 2863 (1992)
K. Hallberg, Adv. Phys. 55, 477 (2006)


ε_k
k

Mobile Kondo model

- Half-filled band. One "impurity."

$$H = -t \sum_{i,\tau} \left(c^\dagger_{i\tau} c_{i+1\tau} + \mathrm{H.c.} \right) + J \sum_i \mathbf{S}_i \cdot \boldsymbol{\sigma}_i$$
$$+ V \sum_i N_i n_i - t' \sum_{i,\tau} \left(d^\dagger_{i\tau} d_{i+1\tau} + \mathrm{H.c.} \right) - H \sum_i \sigma^z_i$$



A. Lamacraft, Phys. Rev. Lett. 101, 225301 (2008)
J. Rincón *et al.*, Phys. Rev. B 88, 140407(R) (2013)

Finite-size scaling of χ_0

- For an immobile impurity:
- 2CK

$$\chi = \frac{1}{2(\Delta_L + 4\pi^2\Gamma)} \ln\left[1 + \frac{4\Gamma}{\Delta_L} + \left(\frac{2\pi\Gamma}{\Delta_L}\right)^2\right]$$

$$\approx \frac{1}{4\pi^2\Gamma} \ln\left(\frac{4\pi\Gamma}{\Delta_L}\right)$$

$$T_K \gg \Delta_L$$

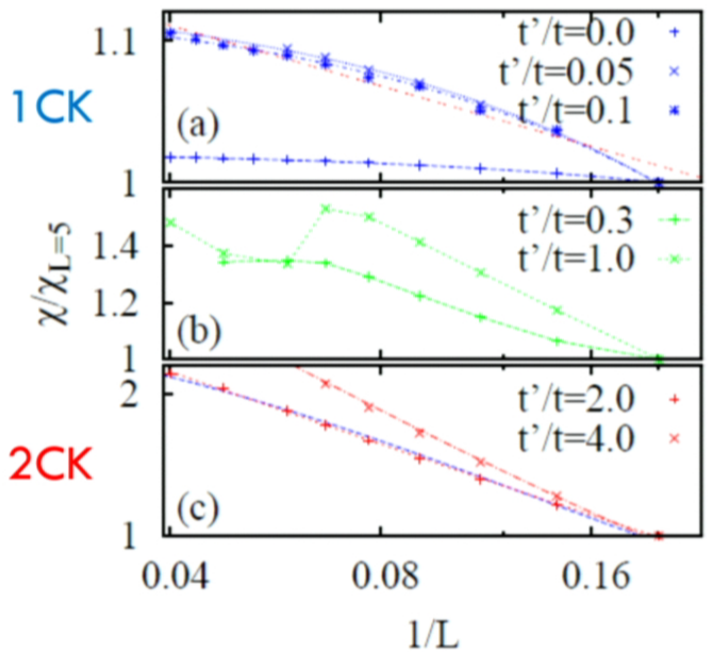
- 1CK

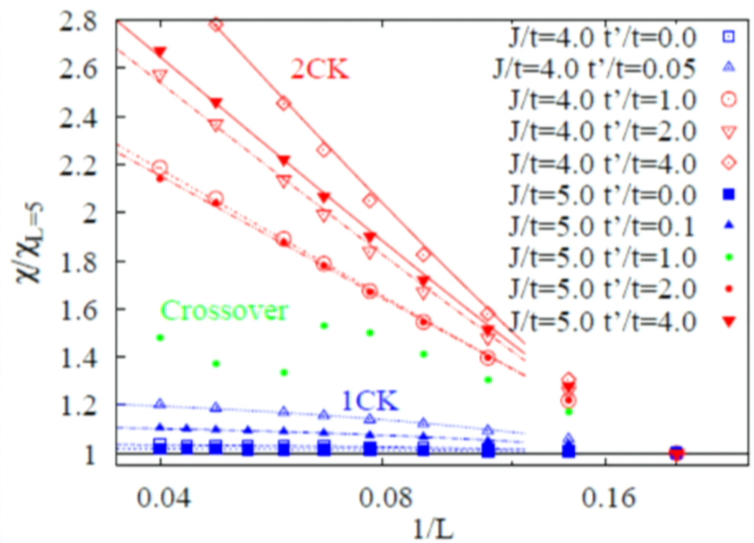
$$\chi = \frac{2\pi^2\Gamma + \Delta_L}{2(\pi^2\Gamma + \Delta_L)^2} \approx \frac{1}{\pi^2\Gamma} - \frac{3}{2}\frac{\Delta_L}{(\pi^2\Gamma)^2}$$

G. Zarand, J. von Delft, Phys. Rev. B 61, 6918 (2000)
D. Cox, A. Zawadowski, Adv. Phys. 47, 599 (1998)

Signaling the transition

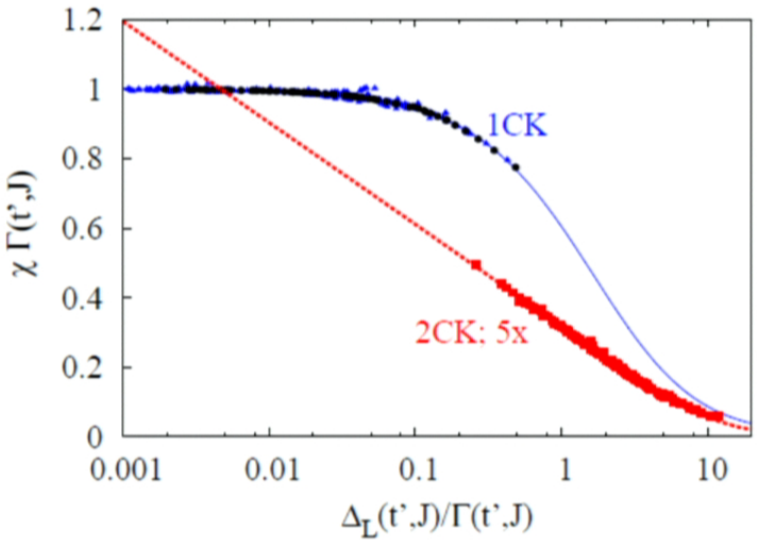
$J/t = 5$	**Several couplings**



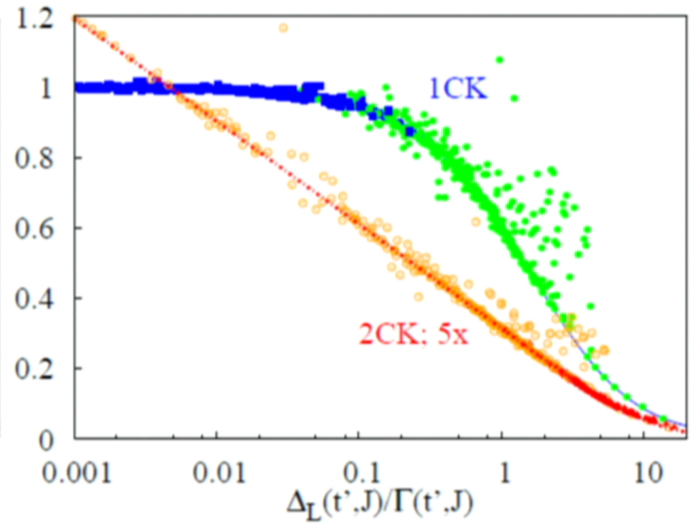


Scaled susceptibility (2CK/1CK)

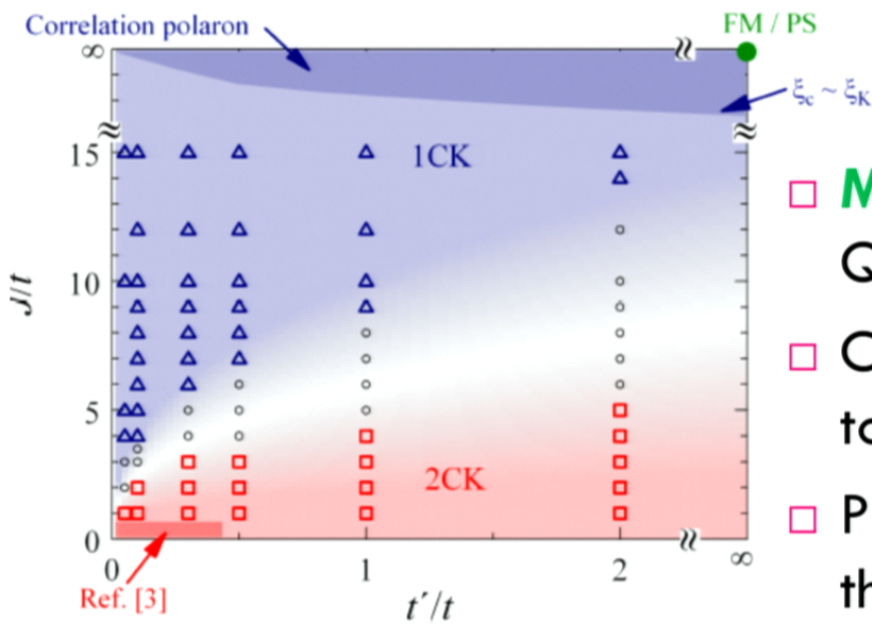
- Full scaling



- Crossover



GS phase diagram



- **Main result**: QPT 2CK-1CK.
- Crossover region due to finite-size effects.
- Present in the thermodynamic limit?

Magnetic field

- Same as temperature and length.
- It destroys NFL recovering FL physics.
- 2CK

$$M \propto (H/T_K)\ln(H/T_K),$$
$$\chi \propto \ln(H/T_K),$$

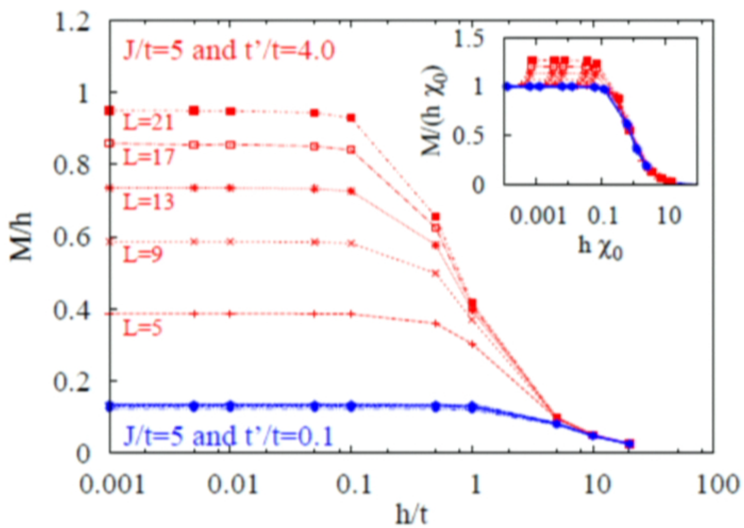
- 1CK

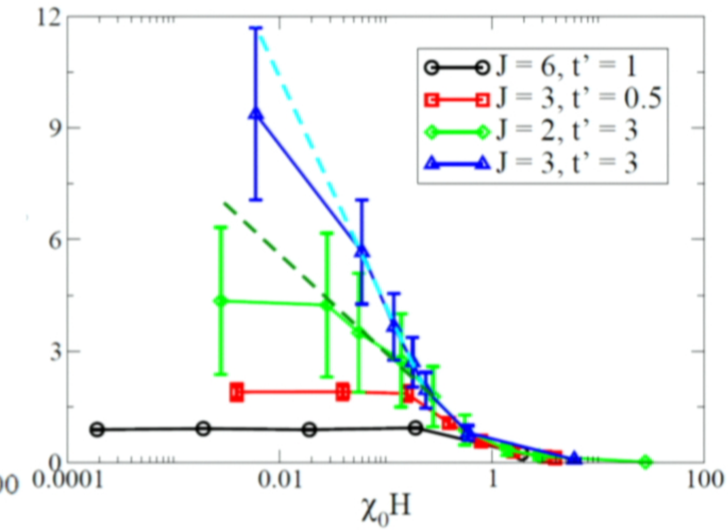
$$M \propto H/T_K,$$
$$\chi \propto 1/T_K,$$

P. D. Sacramento, P. Schlottmann, Phys. Rev. B 43, 13294 (1991)
D. Cox, A. Zawadowski, Adv. Phys. 47, 599 (1998)

Magnetic field

$$M(h) = \frac{\chi_0 h}{\sqrt{1 + 4(\chi_0 h)^2}}$$





Summary

- By using DMRG, we have constructed the ground state phase diagram for the mobile impurity model.
- A magnetic impurity moving in an electron bath displays a novel **quantum phase transition between one-channel** and **two-channel** Kondo polarons.
- We have verified and extended field theoretical results beyond the low-energy limit.
- Field-theory for crossover region.

Spin order in the orbital-selective Mott phase of multiorbital systems

Collaborators:

- ✓ G. Alvarez (CNMS - ORNL)
- ✓ A. Moreo, E. Dagotto (UTK, MST - ORNL)

J. Rincón *et al*, Phys. Rev. Lett. - arXiv:1402.1689

Orbital-selective Mottness

- Several orbitals stabilize diff phases: BI, M, MI.
- OSMP: state with Mott insulator (MI) physics restricted to a subset of active orbitals.
- OSMP: has narrow-band localized electrons (MI), coexisting with wide-band itinerant ones.
- Robust magnetic moment.
- It has an associate OSMP transition.
- Stable by strong *J* and small *V*.

V. Anisimov *et al.*, Eur. Phys. J. B **25**, 191 (2002)
M. Vojta, J. Low. Temp. Phys. **161**, 203 (2010)
A. Georges *et al.*, Annu. Rev. Cond. Mat. Phys. **4**, 137 (2013)

Motivation

- Iron-based superconductors.
  - Non-Fermi liquid near a Mott insulator.
  - Block states in FeSe materials (Caron, PRB 2012).
- Analogies with Kondo models (Vojta, JLTP 2010).
- Techniques applied thus far:
  - DMFT (S. Biermann, PRL 2005; de' Medici, PRL 2009).
  - Slave-spins (Yu, PRL 2012).
  - Hartree-Fock (Bascones, PRB 2012).
- Many-body technique: **DMRG** (White, PRL 1992).
  - $L \simeq 50$ sites, 1200 states, 19 sweeps $\rightarrow$ $\varepsilon \sim 10^{-5}$.

Multiorbital model Hamiltonian

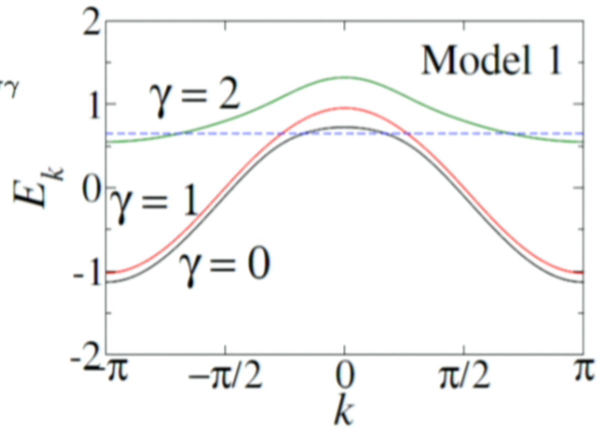
- Three orbital model. Filling $n = 4/3$.
- Analogy with selenides/pnictides.

$$H = H_K + H_{\text{int}}$$

$$H_K = -\sum_{i\sigma\gamma\gamma'} t_{\gamma\gamma'}(c^+_{i\sigma\gamma} c_{i+1\sigma\gamma'} + \text{H.c.}) + \sum_{i\sigma\gamma} \Delta_\gamma n_{i\sigma\gamma}$$

$$H_{\text{int}} = U \sum_{i\gamma} n_{i\uparrow\gamma} n_{i\downarrow\gamma} + (U' - J/2) \sum_{i\gamma<\gamma'} n_{i\gamma} n_{i\gamma'}$$
$$- 2J \sum_{i\gamma<\gamma'} \mathbf{S}_{i\gamma} \cdot \mathbf{S}_{i\gamma'} + J \sum_{i\gamma<\gamma'} (P^+_{i\gamma} P_{i\gamma'} + \text{H.c.})$$

$$U' = U - 2J \qquad P_{i\gamma} = c_{i\downarrow\gamma} c_{i\uparrow\gamma}$$

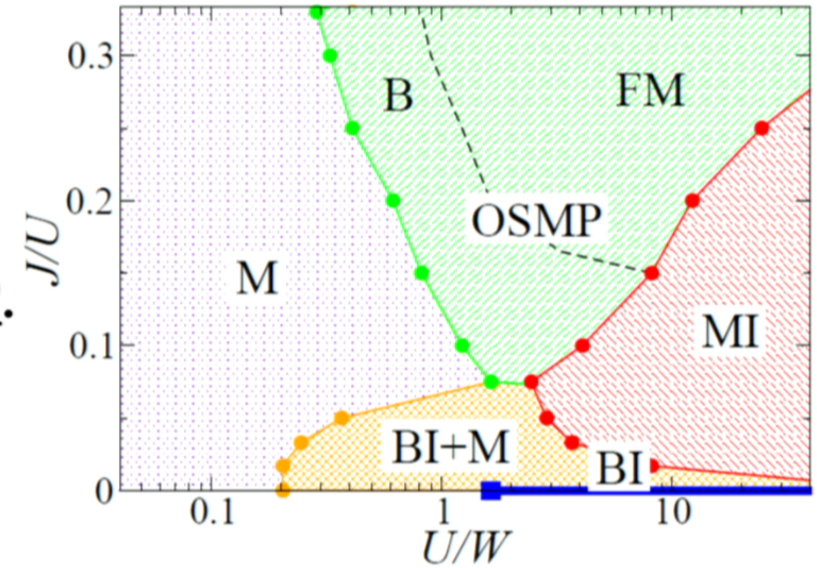


E. Dagotto *et al.*, Phys. Rep. **44**, 1 (2001)
E. Dagotto, Rev. Mod. Phys. **85**, 849 (2013)
M. Daghofer, Phys. Rev. B **81**, 014511 (2010)

Phase diagram

J. Rincon *et al.*, Phys. Rev. Lett. (2014)
arXiv:1402.1689

- Metal.
- "Correlated" band insulator.
- Slightly doped BI.
- Mott insulator.
- **Main result:**
  presence of **OSMP**.
  - *Block states.*
  - (Full) FM.



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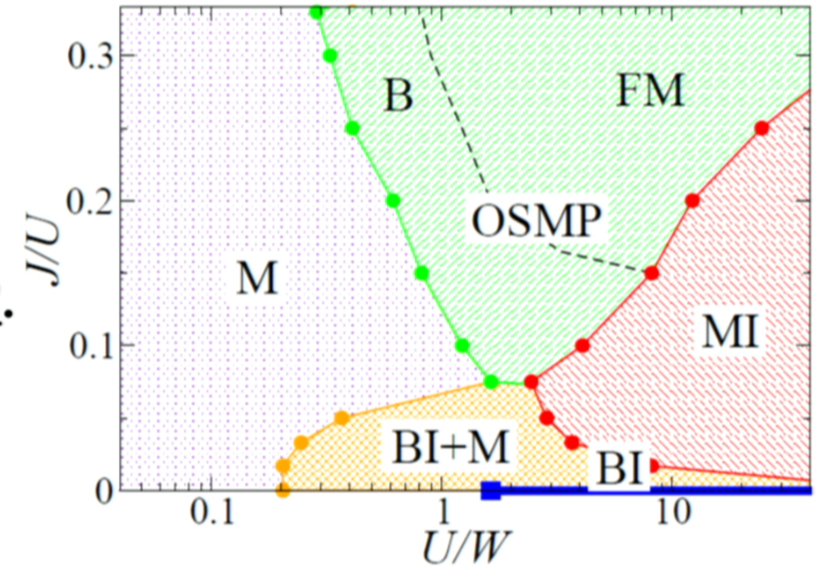
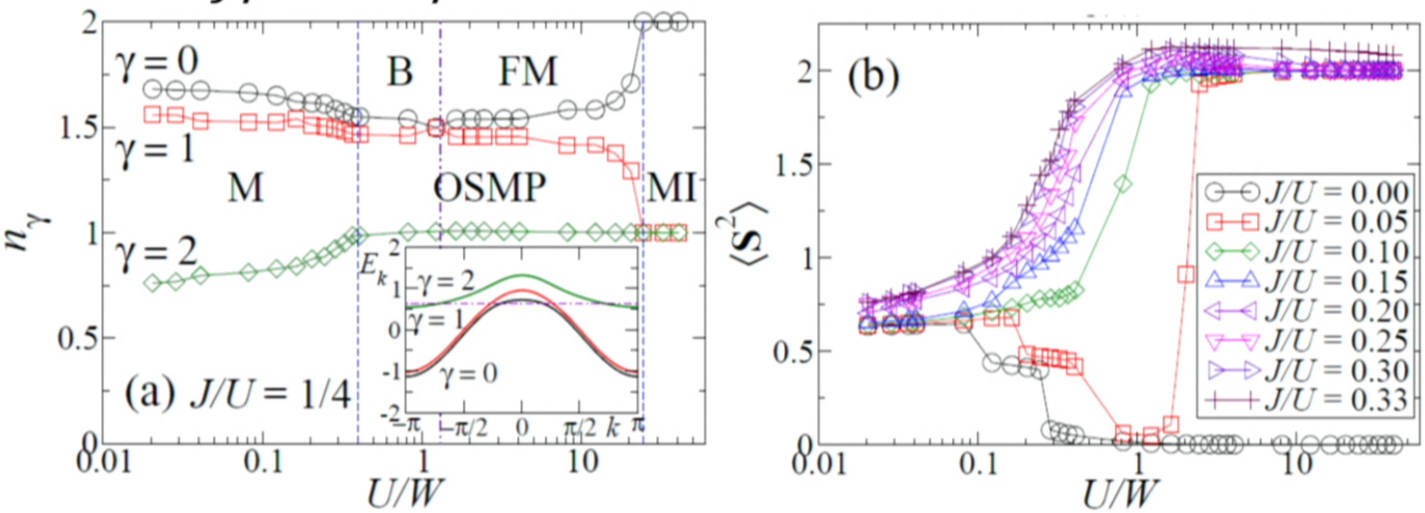


Orbital occupation and spin

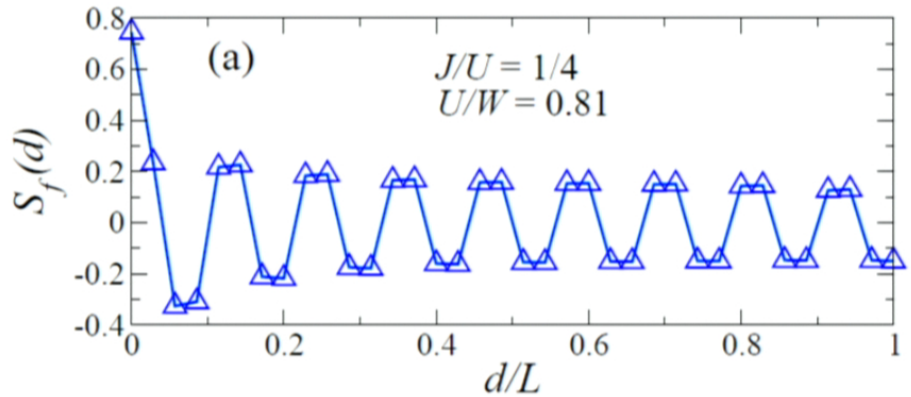
- OSMP $U \sim W$ (intermediate coupling).
- Robust moment.

$J/U = 1/4$

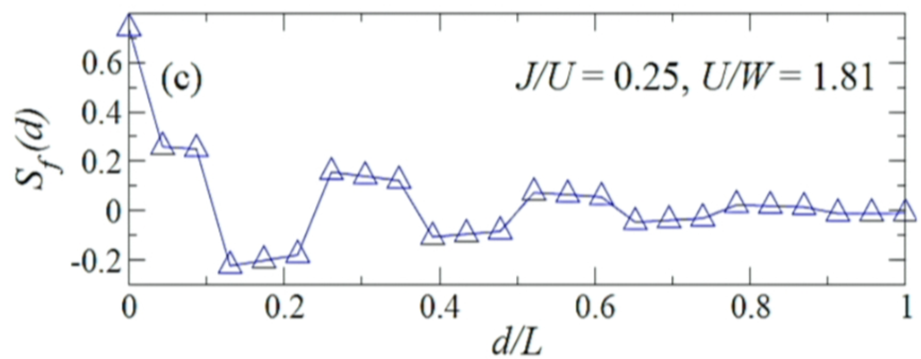


Magnetic order

- Model 1:
- ...↓↓↑↑...



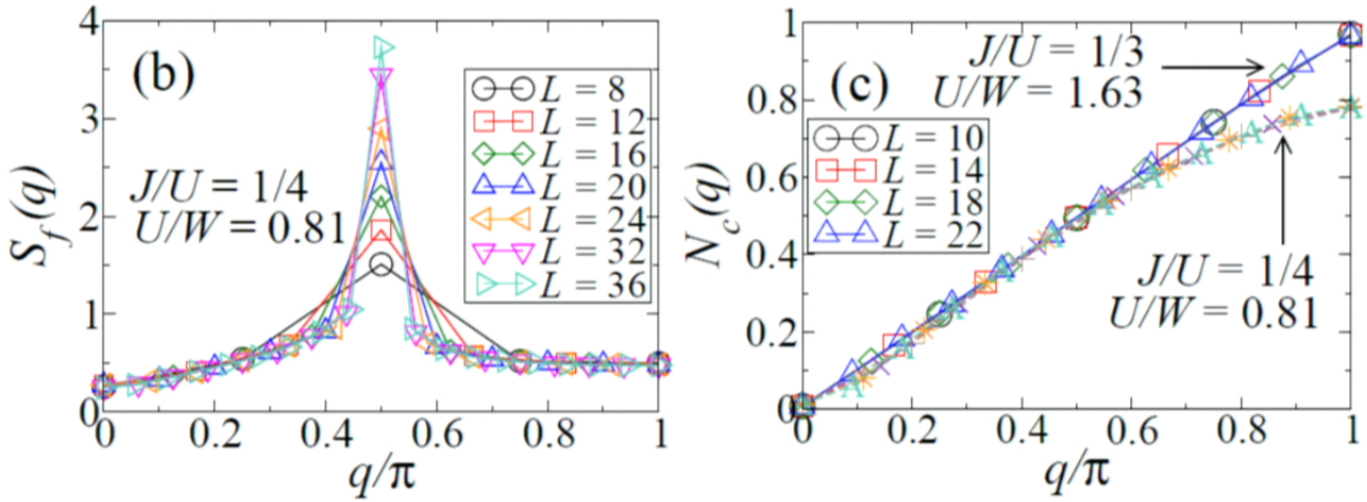
- Model 2:
- ...↓↓↓↑↑↑...



$$S(d) = \frac{1}{L-d} \sum_{j=1}^{L-d} \langle \mathbf{S}_j \cdot \mathbf{S}_{j+d} \rangle$$

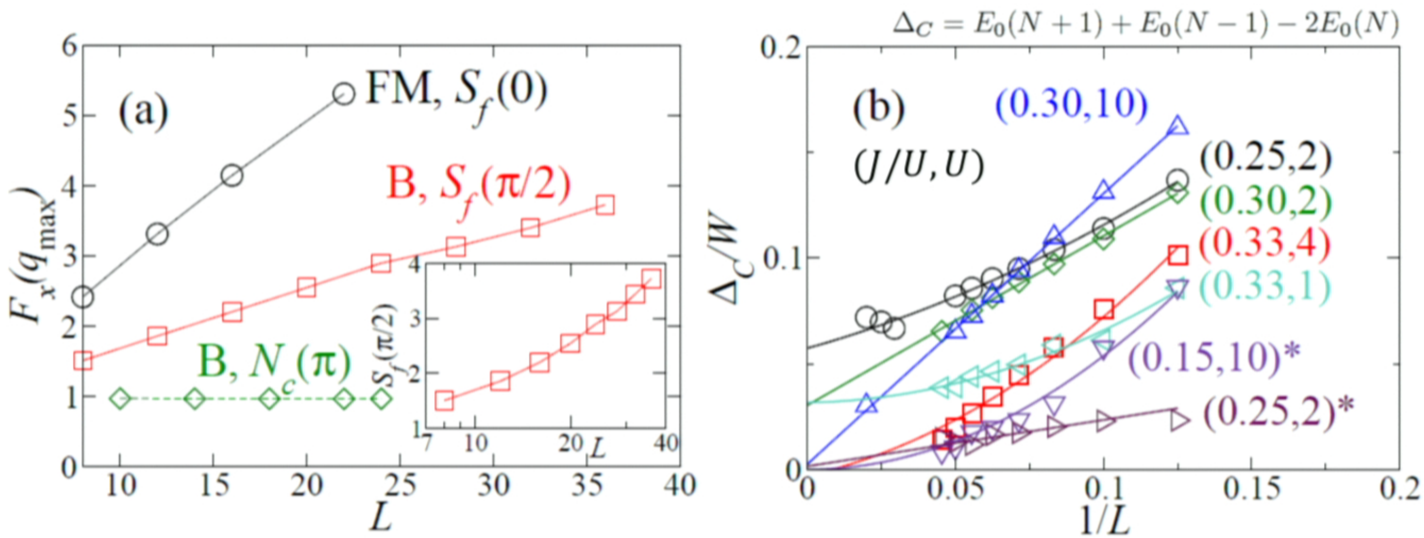
Magnetic order

- "Long-range" magnetic order.
- Short range charge order.
- (Broadened) spinless behavior.



Finite-size behavior

- "Long-range" (Block and FM) magnetic order.
- Instability towards metallic state as doped.
  - 2D analogue expected to be metallic.



Origin of block phase

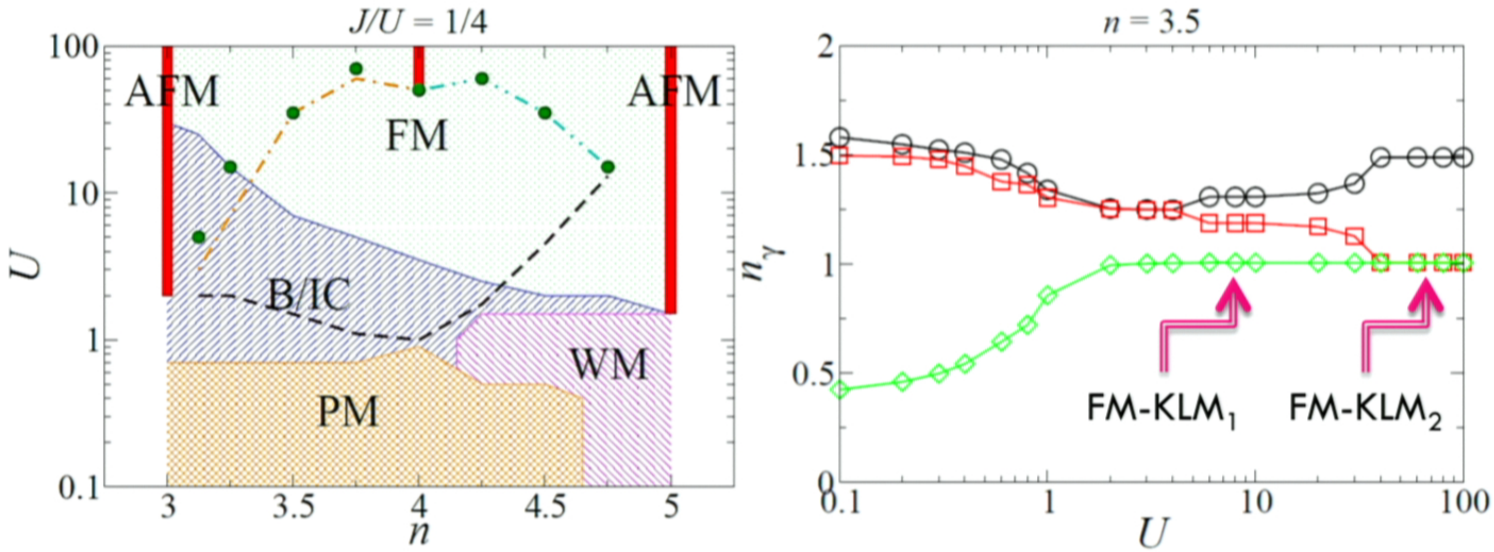
- Low-energy properties are governed by a *correlated* FM Kondo lattice. Non-Fermi liquid physics.
- Two orbitals

$$H_{\rm eff} = -t \sum_{ij\sigma} c^{+}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - 2J \sum_{i} \mathbf{S}_i \cdot \mathbf{s}_i$$

- Typical magnetic phases (1D and 2D):
  - B: …↓↓↑↑…
  - FM: …↑↑↑↑…
  - AFM: …↑↓↑↓…

OSMP$_1$-OSMP$_2$ transition

- Exotic transition between different OSMPs upon doping and/or varying interaction parameters.



Conclusions

- Using DMRG for a 3-orbital model, we found a stable OSMP robust to full many-body fluctuations.
- Within the OSMP there exists magnetic order (B and FM) and short-range charge order.
- Block states arise from frustration generated by competing FM/AFM tendencies.
- Results relevant to quasi-1D, and maybe 2D, compounds: Selenides, heavy fermions, etc.
- Quantum phase transition.