

Title: Research Talk

Speakers: Fakher Assaad

Collection: Quantum Criticality: Gauge Fields and Matter

Date: May 16, 2022 - 2:00 PM

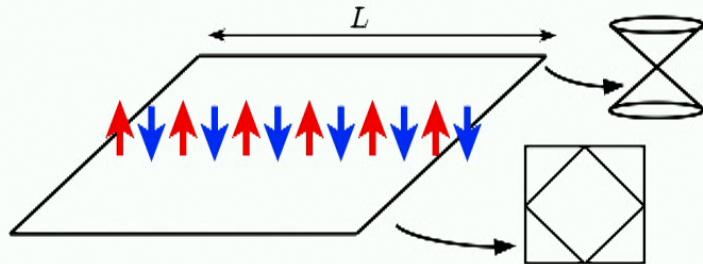
URL: <https://pirsa.org/22050029>

# Spin chains on metallic surfaces: Kondo destruction and magnetic order-disorder transitions

Fakher F. Assaad, Quantum Criticality: Gauge Fields and Matter, Perimeter ITP, 16<sup>th</sup> May 2022

**Introduction** Kondo systems. From experiments to models to field theories and quantum Monte Carlo simulations.

**Topics**



Kondo breakdown transitions and phases

Dissipation induced magnetic order-disorder transitions

**Conclusions**



SFB1170  
ToCoTronics



Leibniz-Rechenzentrum  
der Bayerischen Akademie der Wissenschaften



Gauss Centre for Supercomputing



# Spin chains on metallic surfaces: Kondo destruction and magnetic order-disorder transitions

Fakher F. Assaad, Quantum Criticality: Gauge Fields and Matter, Perimeter ITP, 16<sup>th</sup> May 2022

Many thanks to



M. Raczkowski



T. Sato



J. S.E. Portela



A. Götz



G. Rein



T. Grover



M. Vojta



M. Ulybyshev



F. Parisen Toldin



J. Schwab



B. Danu



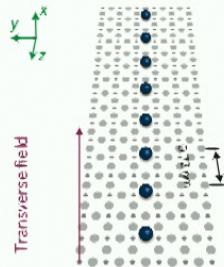
Z. Liu



M. Weber



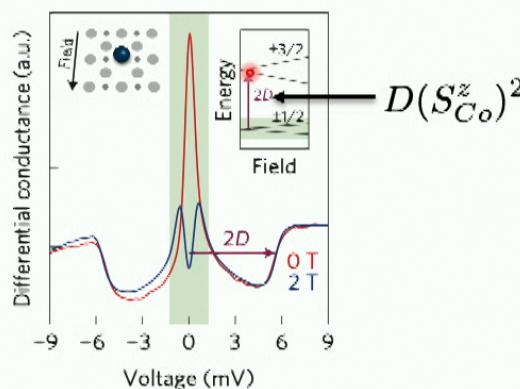
D. Luitz



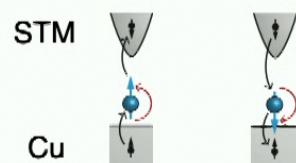
Co atoms on Cu<sub>2</sub>N/Cu(100) in magnetic field.

R. Toskovic, R. van den Berg, A. Spinelli, I. S. Eliens, B. van den Toorn, B. Bryant, J. S. Caux, and A. F. Otte, Nature Physics 12 (2016), 656

Single impurity limit

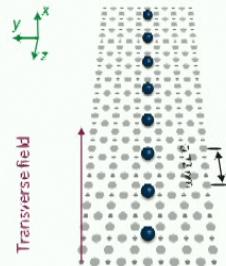


Cu<sub>2</sub>N decoupling layer, co-tunneling through Co-d orbital.



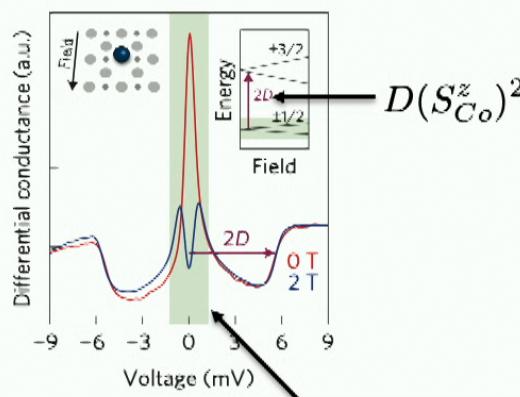
# Kondo systems

Experiments and models

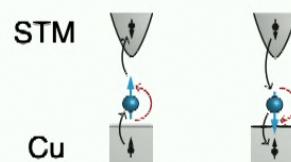


Co atoms on Cu<sub>2</sub>N/Cu(100) in magnetic field.

Single impurity limit



Cu<sub>2</sub>N decoupling layer, co-tunneling through Co-d orbital.



$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{c}_i^\dagger \hat{c}_j + h.c) + \frac{J_k}{2} \hat{c}_{r=0}^\dagger \boldsymbol{\sigma} \hat{c}_{r=0} \cdot \hat{\mathbf{S}} - g\mu_B h^z \hat{S}^z$$

$$\hat{c}_i^\dagger = (\hat{c}_{i,\uparrow}^\dagger, \hat{c}_{i,\downarrow}^\dagger)$$

T<sub>k</sub> ~ 0.2 meV

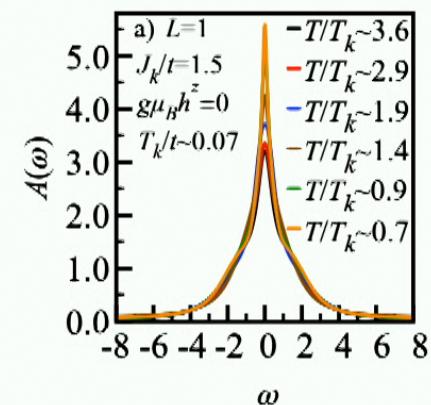
$\mu_B \sim 0.06 \text{ meV/T}$

$$A(\omega) = -\text{Im}G^{\text{ret}}(\omega), \quad G^{\text{ret}}(\omega) = -i \int_0^\infty dt e^{i\omega t} \sum_\sigma \langle \{\hat{\psi}_\sigma(t), \hat{\psi}_\sigma^\dagger(0)\} \rangle$$

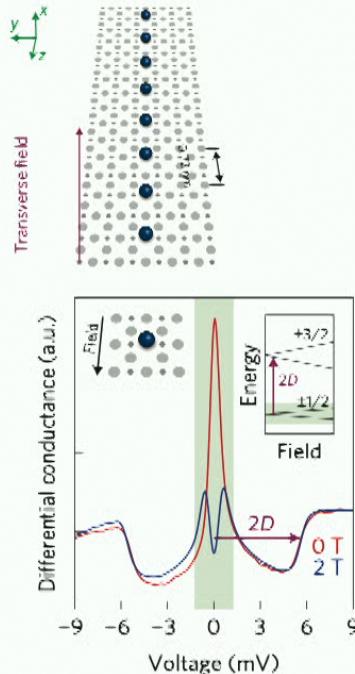
$$\hat{\psi}^\dagger = e^{-S} \hat{d}^\dagger e^S = \hat{c}_{r=0}^\dagger \boldsymbol{\sigma} \cdot \hat{\mathbf{S}}$$

(S: Schrieffer Wolff transformation)

T.A. Costi, Phys. Rev. Lett. 85, 1504 (2000).

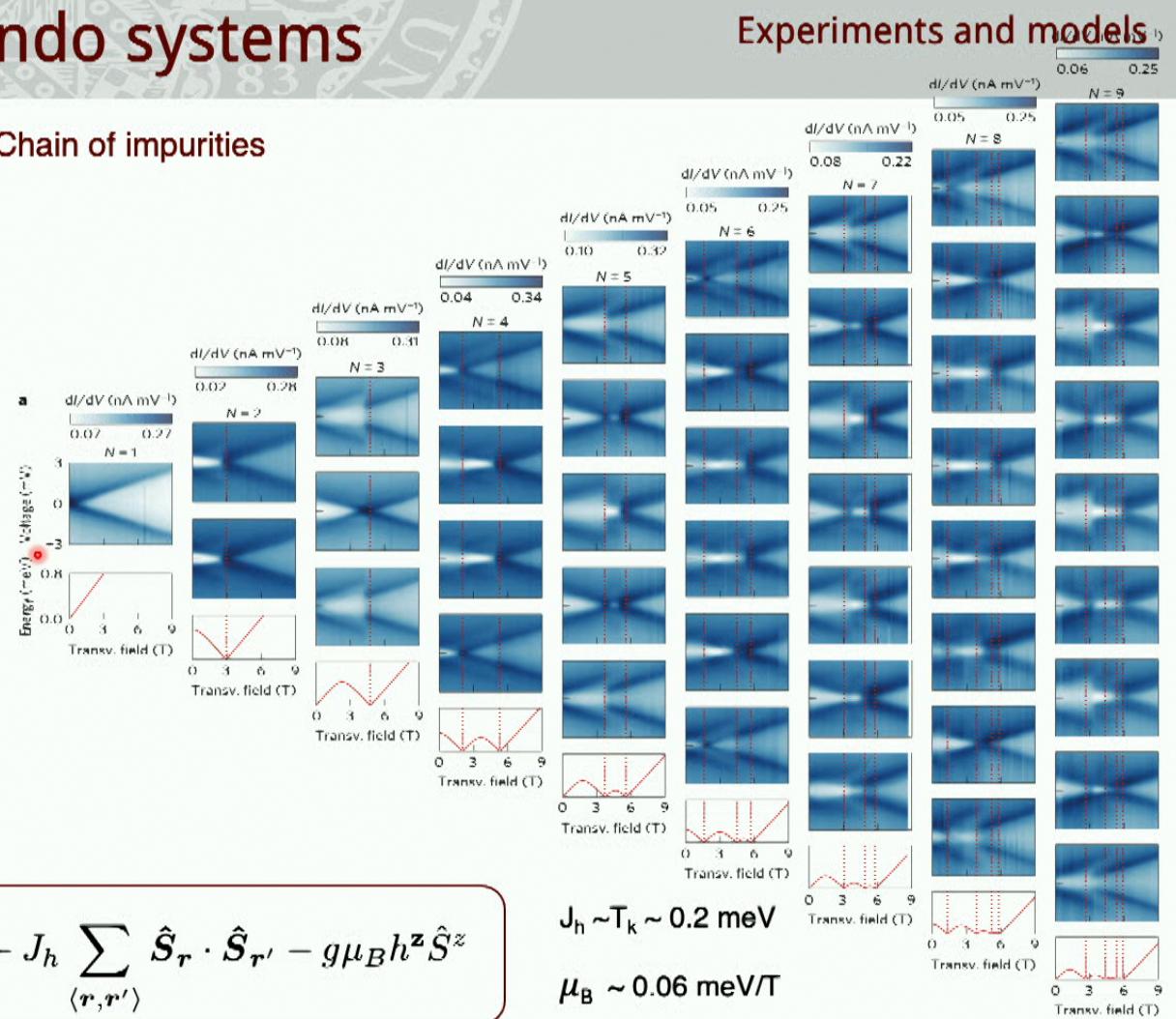


# Kondo systems



Site dependent  
field induced  
“Kondo resonance”

## Chain of impurities



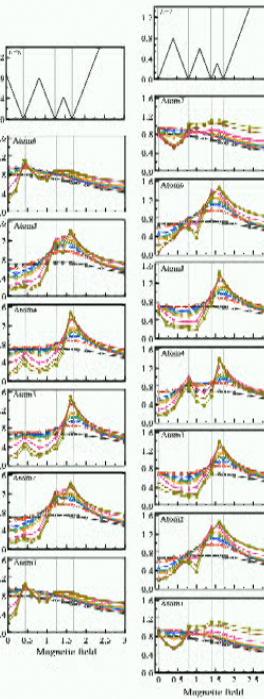
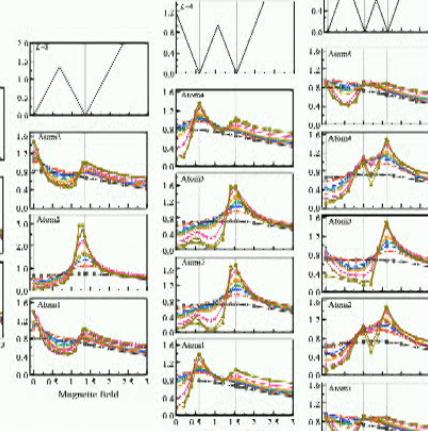
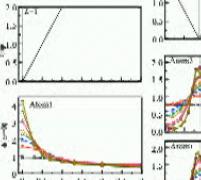
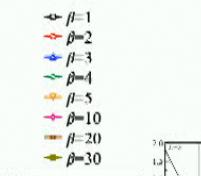
$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{c}_i^\dagger \hat{c}_j + h.c.) + \frac{J_k}{2} \sum_{\mathbf{r}} \hat{c}_{\mathbf{r}}^\dagger \boldsymbol{\sigma} \hat{c}_{\mathbf{r}} \cdot \hat{\mathbf{S}}_{\mathbf{r}} + J_h \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \hat{\mathbf{S}}_{\mathbf{r}} \cdot \hat{\mathbf{S}}_{\mathbf{r}'} - g\mu_B h^z \hat{S}^z$$

$$J_h \sim T_k \sim 0.2 \text{ meV}$$

$$\mu_B \sim 0.06 \text{ meV/T}$$

# Kondo systems

Experiments and models

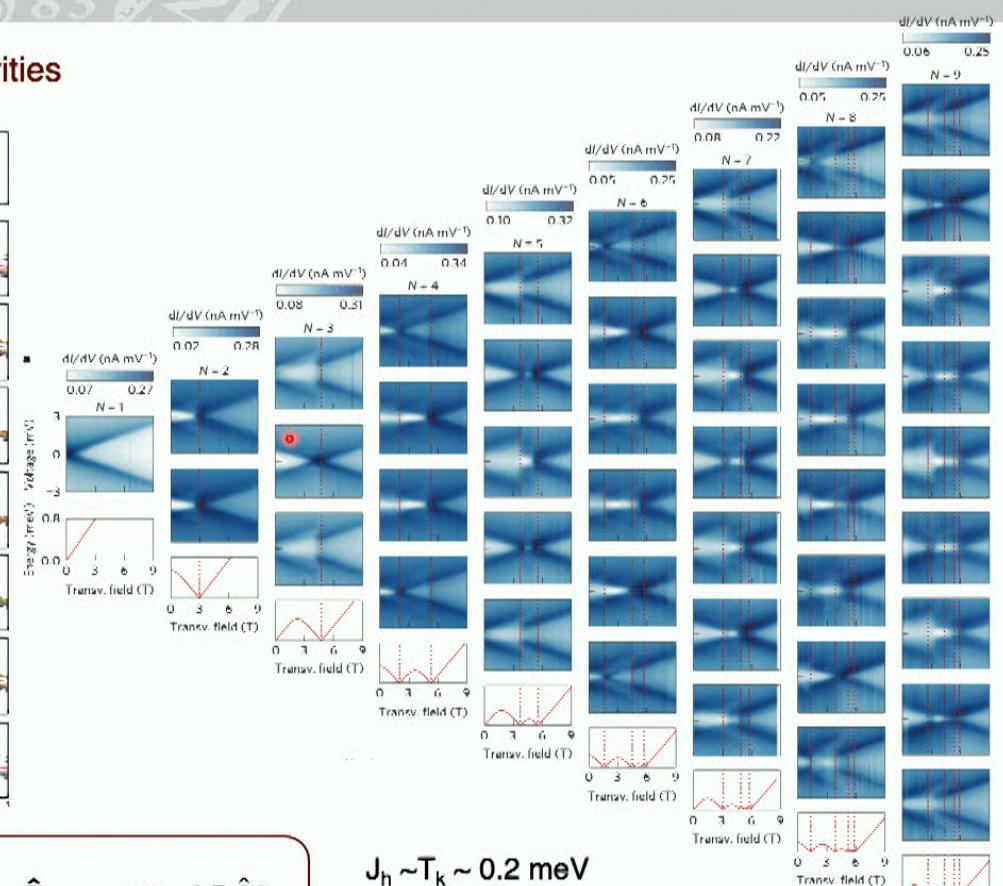


Chain of impurities

$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{c}_i^\dagger \hat{c}_j + h.c.) + \frac{J_k}{2} \sum_{\mathbf{r}} \hat{c}_{\mathbf{r}}^\dagger \boldsymbol{\sigma} \hat{c}_{\mathbf{r}} \cdot \hat{\mathbf{S}}_{\mathbf{r}} + J_h \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \hat{\mathbf{S}}_{\mathbf{r}} \cdot \hat{\mathbf{S}}_{\mathbf{r}'} - g\mu_B h^z \hat{S}^z$$

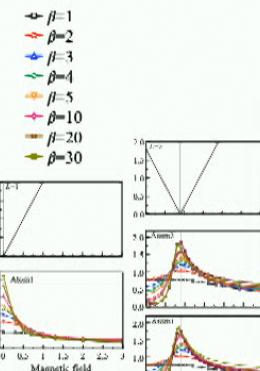
$J_h \sim T_k \sim 0.2 \text{ meV}$

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# Kondo systems

## Experiments and models



### Chain of impurities

PHYSICAL REVIEW LETTERS 123, 176601 (2019)

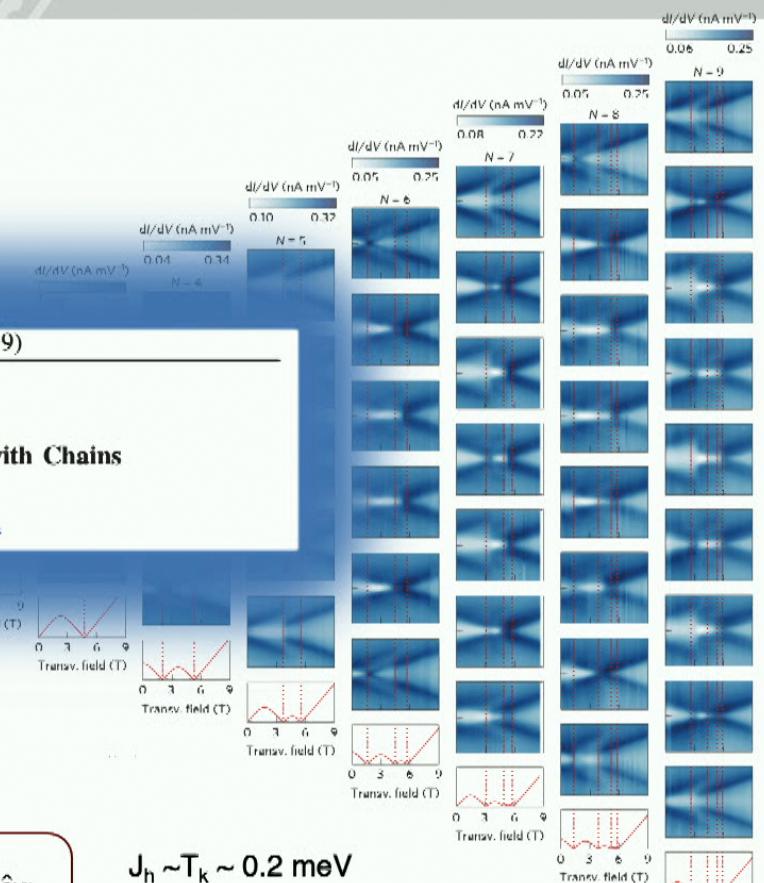
#### Exploring the Kondo Effect of an Extended Impurity with Chains of Co Adatoms in a Magnetic Field

Bimla Danu,<sup>1,\*</sup> Fakher F. Assaad,<sup>2,3,†</sup> and Frédéric Mila<sup>1,‡</sup>

$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{c}_i^\dagger \hat{c}_j + h.c.) + \frac{J_k}{2} \sum_{\mathbf{r}} \hat{c}_{\mathbf{r}}^\dagger \boldsymbol{\sigma} \hat{c}_{\mathbf{r}} \cdot \hat{\mathbf{S}}_{\mathbf{r}} + J_h \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \hat{\mathbf{S}}_{\mathbf{r}} \cdot \hat{\mathbf{S}}_{\mathbf{r}'} - g\mu_B h^z \hat{S}^z$$

$J_h \sim T_k \sim 0.2 \text{ meV}$

$\mu_B \sim 0.06 \text{ meV/T}$



$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{c}_i^\dagger \hat{c}_j + h.c) + \frac{J_k}{2} \sum_r \hat{c}_r^\dagger \boldsymbol{\sigma} \hat{c}_r \cdot \hat{\mathbf{S}}_r + J_h \sum_{\langle r,r' \rangle} \hat{\mathbf{S}}_r \cdot \hat{\mathbf{S}}_{r'}$$

Question:

Field theory for

- i) Numerical simulations
- ii) Classification of phases

$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{c}_i^\dagger \hat{c}_j + h.c) + \frac{J_k}{2} \sum_{\mathbf{r}} \hat{c}_{\mathbf{r}}^\dagger \boldsymbol{\sigma} \hat{c}_{\mathbf{r}} \cdot \hat{\mathbf{S}}_{\mathbf{r}} + J_h \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \hat{\mathbf{S}}_{\mathbf{r}} \cdot \hat{\mathbf{S}}_{\mathbf{r}'} \quad \bullet$$

Field theory:

$$\hat{\mathbf{S}}_{\mathbf{r}} = \frac{1}{2} \hat{\mathbf{f}}_{\mathbf{r}}^\dagger \boldsymbol{\sigma} \hat{\mathbf{f}}_{\mathbf{r}} \quad \text{with constraint} \quad \hat{\mathbf{f}}_{\mathbf{r}}^\dagger \hat{\mathbf{f}}_{\mathbf{r}} = 1 \quad \text{Def} \quad \hat{\mathbf{f}}_{\mathbf{r}}^\dagger = (\hat{f}_{\mathbf{r},\uparrow}^\dagger, \hat{f}_{\mathbf{r},\downarrow}^\dagger)$$

$$\begin{aligned} \hat{H} = & -t \sum_{\langle i,j \rangle} (\hat{c}_i^\dagger \hat{c}_j + h.c) - \frac{J_k}{8} \sum_{\mathbf{r}} \left[ (\hat{V}_{\mathbf{r}} + \hat{V}_{\mathbf{r}}^\dagger)^2 + (i\hat{V}_{\mathbf{r}} - i\hat{V}_{\mathbf{r}}^\dagger)^2 \right] \\ & - \frac{J_h}{8} \sum_{b=\langle \mathbf{r}, \mathbf{r}' \rangle} \left[ (\hat{D}_b + \hat{D}_b^\dagger)^2 + (i\hat{D}_b - i\hat{D}_b^\dagger)^2 \right] + U \underbrace{\sum_{\mathbf{r}} (\hat{\mathbf{f}}_{\mathbf{r}}^\dagger \hat{\mathbf{f}}_{\mathbf{r}} - 1)^2}_{= \hat{H}_U} \\ \hat{D}_b = & \hat{\mathbf{f}}_{\mathbf{r}}^\dagger \hat{\mathbf{f}}_{\mathbf{r}'}, \quad \hat{V}_{\mathbf{r}} = \hat{\mathbf{f}}_{\mathbf{r}}^\dagger \hat{c}_{\mathbf{r}} \end{aligned}$$

Exact in the limit  $U \rightarrow \infty$ . But since  $[\hat{H}_U, \hat{H}] = 0$  the constraint is imposed very efficiently.

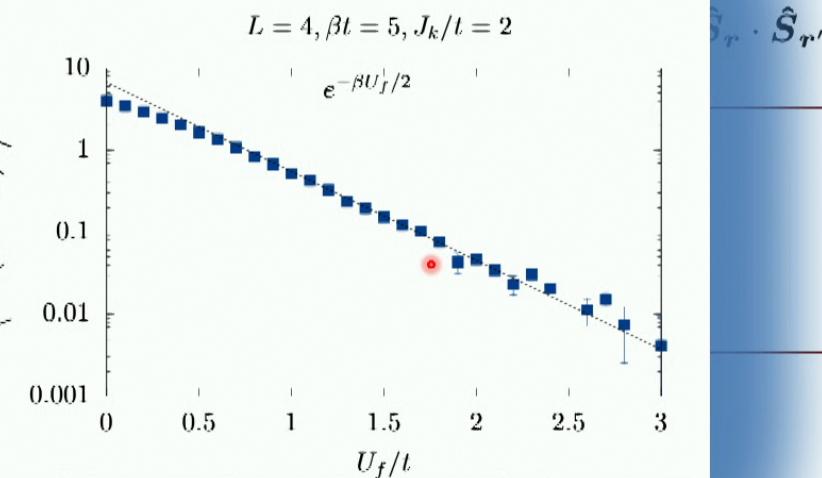
Field theory:

$$\hat{H} = -t \sum_{\langle i,j \rangle}$$

$$\hat{S}_r = \frac{1}{2} \hat{f}_r^\dagger \sigma^z \left( \hat{n}_r^{\downarrow} \right)^{\frac{N}{2}}$$

$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{c}_i^\dagger \hat{c}_j + h.c) - \frac{J}{8} \sum_{\langle r,r' \rangle} \left[ \left( \hat{D}_b + \hat{D}_b^\dagger \right)^2 + \left( i\hat{D}_b - i\hat{D}_b^\dagger \right)^2 \right] + U \underbrace{\sum_r \left( \hat{f}_r^\dagger \hat{f}_r - 1 \right)^2}_{= \hat{H}_U}$$

$$\hat{D}_b = \hat{f}_r^\dagger \hat{f}_{r'}, \quad \hat{V}_r = \hat{f}_r^\dagger \hat{c}_r$$



Def  $\hat{f}_r^\dagger = (\hat{f}_{r,\uparrow}^\dagger, \hat{f}_{r,\downarrow}^\dagger)$

Exact in the limit  $U \rightarrow \infty$ . But since  $[\hat{H}_U, \hat{H}] = 0$  the constraint is imposed very efficiently.

$$\hat{H} = -t \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} (\hat{c}_{\mathbf{i}}^\dagger \hat{c}_{\mathbf{j}} + h.c.) - \frac{J_k}{8} \sum_{\mathbf{r}} \left[ (\hat{V}_{\mathbf{r}} + \hat{V}_{\mathbf{r}}^\dagger)^2 + (i\hat{V}_{\mathbf{r}} - i\hat{V}_{\mathbf{r}}^\dagger)^2 \right] - \frac{J_h}{8} \sum_{b=\langle \mathbf{r}, \mathbf{r}' \rangle} \left[ (\hat{D}_b + \hat{D}_b^\dagger)^2 + (i\hat{D}_b - i\hat{D}_b^\dagger)^2 \right] + U \sum_{\mathbf{r}} (\hat{\mathbf{f}}_{\mathbf{r}}^\dagger \hat{\mathbf{f}}_{\mathbf{r}} - 1)^2$$

$$\hat{D}_b = \hat{\mathbf{f}}_{\mathbf{r}}^\dagger \hat{\mathbf{f}}_{\mathbf{r}'}, \quad \hat{V}_{\mathbf{r}} = \hat{\mathbf{f}}_{\mathbf{r}}^\dagger \hat{c}_{\mathbf{r}}$$

$$b_{\mathbf{r}} = |b_{\mathbf{r}}| e^{i\varphi_{\mathbf{r}}} \quad \chi_b = |\chi_b| e^{i \int_{\mathbf{r}}^{\mathbf{r}'} \mathbf{a} \cdot d\mathbf{l}}$$

$$a_0$$

Partition function,  $Z \equiv \text{Tr } e^{-\beta \hat{H}} = \int D\{f^\dagger f\} D\{c^\dagger c\} D\{z_b\} D\{b_{\mathbf{r}}\} D\{a_{0,\mathbf{r}}\} e^{-S}$  with, for  $U \rightarrow \infty$

$$S = \int_0^\beta d\tau \left\{ \frac{2}{J_h} \sum_b |\chi_b(\tau)|^2 + \frac{2}{J_k} \sum_{\mathbf{r}} |b_{\mathbf{r}}(\tau)|^2 + \sum_{\mathbf{i}, \mathbf{j}} \mathbf{c}_{\mathbf{i}}^\dagger(\tau) [\partial_\tau \delta_{\mathbf{i}, \mathbf{j}} - T_{\mathbf{i}, \mathbf{j}}] \mathbf{c}_{\mathbf{j}}(\tau) + \sum_{\mathbf{r}} |b_{\mathbf{r}}(\tau)| \left[ e^{i\varphi_{\mathbf{r}}(\tau)} \mathbf{f}_{\mathbf{r}}^\dagger(\tau) \mathbf{c}_{\mathbf{r}}(\tau) + h.c. \right] + \sum_{\mathbf{r}} \mathbf{f}_{\mathbf{r}}^\dagger(\tau) [\partial_\tau - ia_{0,\mathbf{r}}(\tau)] \mathbf{f}_{\mathbf{r}}(\tau) + ia_{0,\mathbf{r}}(\tau) + \sum_{b=\langle \mathbf{r}, \mathbf{r}' \rangle} |\chi_b(\tau)| \left[ \mathbf{f}_{\mathbf{r}}^\dagger(\tau) e^{-i \int_{\mathbf{r}}^{\mathbf{r}'} \mathbf{a}(\mathbf{l}, \tau) d\mathbf{l}} \mathbf{f}_{\mathbf{r}'}(\tau) + h.c. \right] \right\}$$

$$S = \int_0^\beta d\tau \left\{ \frac{2}{J_h} \sum_b |\chi_b(\tau)|^2 + \frac{2}{J_k} \sum_{\mathbf{r}} |b_{\mathbf{r}}(\tau)|^2 + \sum_{\mathbf{i}, \mathbf{j}} \mathbf{c}_{\mathbf{i}}^\dagger(\tau) [\partial_\tau \delta_{\mathbf{i}, \mathbf{j}} - T_{\mathbf{i}, \mathbf{j}}] \mathbf{c}_{\mathbf{j}}(\tau) \right. \\ \left. + \sum_{\mathbf{r}} |b_{\mathbf{r}}(\tau)| \left[ e^{i\varphi_{\mathbf{r}}(\tau)} \mathbf{f}_{\mathbf{r}}^\dagger(\tau) \mathbf{c}_{\mathbf{r}}(\tau) + h.c. \right] \right. \\ \left. + \sum_{\mathbf{r}} \mathbf{f}_{\mathbf{r}}^\dagger(\tau) [\partial_\tau - ia_{0, \mathbf{r}}(\tau)] \mathbf{f}_{\mathbf{r}}(\tau) + ia_{0, \mathbf{r}}(\tau) + \sum_{b=\langle \mathbf{r}, \mathbf{r}' \rangle} |\chi_b(\tau)| \left[ \mathbf{f}_{\mathbf{r}}^\dagger(\tau) e^{-i \int_{\mathbf{r}}^{\mathbf{r}'} \mathbf{a}(l, \tau) dl} \mathbf{f}_{\mathbf{r}'}(\tau) + h.c. \right] \right).$$

•

Local U(1) gauge invariance:  $\mathbf{f}_{\mathbf{r}}^\dagger(\tau) \rightarrow \mathbf{f}_{\mathbf{r}}^\dagger(\tau) e^{i\eta_{\mathbf{r}}(\tau)}$

$$\begin{bmatrix} a_{0, \mathbf{r}}(\tau) & \rightarrow a_{0, \mathbf{r}}(\tau) + \partial_\tau \eta_{\mathbf{r}}(\tau) \\ \mathbf{a}_{\mathbf{r}}(\tau) & \rightarrow \mathbf{a}_{\mathbf{r}}(\tau) + \nabla_{\mathbf{r}} \eta_{\mathbf{r}}(\tau) \\ \varphi_{\mathbf{r}}(\tau) & \rightarrow \varphi_{\mathbf{r}}(\tau) + \eta_{\mathbf{r}}(\tau) \end{bmatrix}$$

Other symmetry allowed terms, such as U(1) flux, and dynamics of the b-field, will be dynamically generated.

$$S = \int_0^\beta d\tau \left\{ \frac{2}{J_h} \sum_b |\chi_b(\tau)|^2 + \frac{2}{J_k} \sum_{\mathbf{r}} |b_{\mathbf{r}}(\tau)|^2 + \sum_{\mathbf{i}, \mathbf{j}} \mathbf{c}_{\mathbf{i}}^\dagger(\tau) [\partial_\tau \delta_{\mathbf{i}, \mathbf{j}} - T_{\mathbf{i}, \mathbf{j}}] \mathbf{c}_{\mathbf{j}}(\tau) \right. \\ \left. + \sum_{\mathbf{r}} |b_{\mathbf{r}}(\tau)| \left[ e^{i\varphi_{\mathbf{r}}(\tau)} \mathbf{f}_{\mathbf{r}}^\dagger(\tau) \mathbf{c}_{\mathbf{r}}(\tau) + h.c. \right] \right. \\ \left. + \sum_{\mathbf{r}} \mathbf{f}_{\mathbf{r}}^\dagger(\tau) [\partial_\tau - ia_{0, \mathbf{r}}(\tau)] \mathbf{f}_{\mathbf{r}}(\tau) + ia_{0, \mathbf{r}}(\tau) + \sum_{b=\langle \mathbf{r}, \mathbf{r}' \rangle} |\chi_b(\tau)| \left[ \mathbf{f}_{\mathbf{r}}^\dagger(\tau) e^{-i \int_{\mathbf{r}}^{\mathbf{r}'} \mathbf{a}(l, \tau) dl} \mathbf{f}_{\mathbf{r}'}(\tau) + h.c. \right] \right).$$

Numerical simulations

$$Z \equiv \text{Tr } e^{-\beta \hat{H}} = \int D\{f^\dagger f\} D\{c^\dagger c\} D\{z_b\} D\{b_{\mathbf{r}}\} D\{a_0\} e^{-S} = \int D\{z_b, b_{\mathbf{r}}, a_0\} e^{-(S_0 - \log \det M)}$$

For our specific case, the action is real!  $\rightarrow$  No sign problem. Absence of sign problem is shown on the basis of symmetry arguments.  
(T. Sato, FFA, and T. Grover, Phys. Rev. Lett. 120 (2018), 107201)

The integration over the fields is carried out with Monte Carlo importance sampling.

## Kinetic

$$\hat{H} = \sum_{k=1}^{M_T} \sum_{\sigma=1}^{N_{\text{col}}} \sum_{s=1}^{N_{\text{fl}}} \sum_{x,y} \hat{c}_{x\sigma s}^\dagger T_{xy}^{(ks)} \hat{c}_{y\sigma s} + \sum_{k=1}^{M_V} U_k \left\{ \sum_{\sigma=1}^{N_{\text{col}}} \sum_{s=1}^{N_{\text{fl}}} \left[ \left( \sum_{x,y} \hat{c}_{x\sigma s}^\dagger V_{xy}^{(ks)} \hat{c}_{y\sigma s} \right) + \alpha_{ks} \right]^2 \right\}$$

## Potential (sum of perfect squares)

- Block diagonal in flavors,  $N_{\text{fl}}$
- $SU(N_{\text{col}})$  symmetric in colors  $N_{\text{col}}$
- Arbitrary Bravais lattice for  $d=1,2$
- Model can be specified at minimal programming cost
- Fortran 2003 standard
- MPI implementation
- Global and local moves, Parallel tempering, Langevin
- Projective and finite  $T$  approaches
- pyALF: easy access python interface
- Predefined models

## Coupling of fermions to bosonic fields with predefined dynamics

$$+ \sum_{k=1}^{M_I} \hat{Z}_k \left( \sum_{\sigma=1}^{N_{\text{col}}} \sum_{s=1}^{N_{\text{fl}}} \sum_{x,y} \hat{c}_{x\sigma s}^\dagger I_{xy}^{(ks)} \hat{c}_{y\sigma s} \right) + \hat{H}_{\text{Ising}}$$



F. Goth



M. Bercx



J. Hoffmann



J. S.E. Portela J. Schwab



Z. Liu



E. Huffman



A. Götz



F. Parisen Toldin



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Literaturversorgungs  
und Informationssysteme (LIS)



$$\begin{aligned}
 S = \int_0^\beta d\tau & \left\{ \frac{2}{J_h} \sum_b |\chi_b(\tau)|^2 + \frac{2}{J_k} \sum_r |b_r(\tau)|^2 + \sum_{i,j} c_i^\dagger(\tau) [\partial_\tau \delta_{i,j} - T_{i,j}] c_j(\tau) \right. \\
 & + \sum_r |b_r(\tau)| \left[ e^{i\varphi_r(\tau)} f_r^\dagger(\tau) c_r(\tau) + h.c. \right] \\
 & + \sum_r f_r^\dagger(\tau) [\partial_\tau - ia_{0,r}(\tau)] f_r(\tau) + ia_{0,r}(\tau) + \sum_{b=\langle r, r' \rangle} |\chi_b(\tau)| \left[ f_r^\dagger(\tau) e^{-i \int_{r'}^{r'} \mathbf{a}(l, \tau) dl} f_{r'}(\tau) + h.c. \right]
 \end{aligned}$$

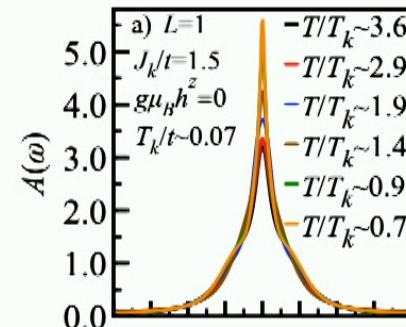
Classification of Phases	$\langle f_r^\dagger \sigma f_r \rangle \neq 0$	$\langle b_r \rangle \neq 0$	Gauge field
Kondo	✗	✓	confined
SDW	✓	✗	confined
Kondo + SDW	✓	✓	confined
FL*	✗	✗	De-confined
SDW*	✓	✗	De-confined

$$S = \int_0^\beta d\tau \left\{ \frac{2}{J_h} \sum_b |\chi_b(\tau)|^2 + \frac{2}{J_k} \sum_{\mathbf{r}} |b_{\mathbf{r}}(\tau)|^2 + \sum_{\mathbf{i}, \mathbf{j}} \mathbf{c}_{\mathbf{i}}^\dagger(\tau) [\partial_\tau \delta_{\mathbf{i}, \mathbf{j}} - T_{\mathbf{i}, \mathbf{j}}] \mathbf{c}_{\mathbf{j}}(\tau) \right. \\ \left. + \sum_{\mathbf{r}} |b_{\mathbf{r}}(\tau)| \left[ e^{i\varphi_{\mathbf{r}}(\tau)} \mathbf{f}_{\mathbf{r}}^\dagger(\tau) \mathbf{c}_{\mathbf{r}}(\tau) + h.c. \right] \right. \\ \left. + \sum_{\mathbf{r}} \mathbf{f}_{\mathbf{r}}^\dagger(\tau) [\partial_\tau - ia_{0, \mathbf{r}}(\tau)] \mathbf{f}_{\mathbf{r}}(\tau) + ia_{0, \mathbf{r}}(\tau) + \sum_{b=\langle \mathbf{r}, \mathbf{r}' \rangle} |\chi_b(\tau)| \left[ \mathbf{f}_{\mathbf{r}}^\dagger(\tau) e^{-i \int_{\mathbf{r}}^{\mathbf{r}'} \mathbf{a}(l, \tau) dl} \mathbf{f}_{\mathbf{r}'}(\tau) + h.c. \right] \right. \\ \left. , \right.$$

Kondo: composite fermion  $e^{i\varphi_{\mathbf{i}}(\tau)} \mathbf{f}_{\mathbf{i}}(\tau) \propto \psi_i = \mathbf{S}_{\mathbf{i}} \cdot \boldsymbol{\sigma} \mathbf{c}_{\mathbf{i}}$ .

Single impurity.

$$A(\omega) = -\text{Im}G^{\text{ret}}(\omega), \quad G^{\text{ret}}(\omega) = -i \int_0^\infty dt e^{i\omega t} \sum_{\sigma} \langle \{\hat{\psi}_{\sigma}(t), \hat{\psi}_{\sigma}^\dagger(0)\} \rangle$$

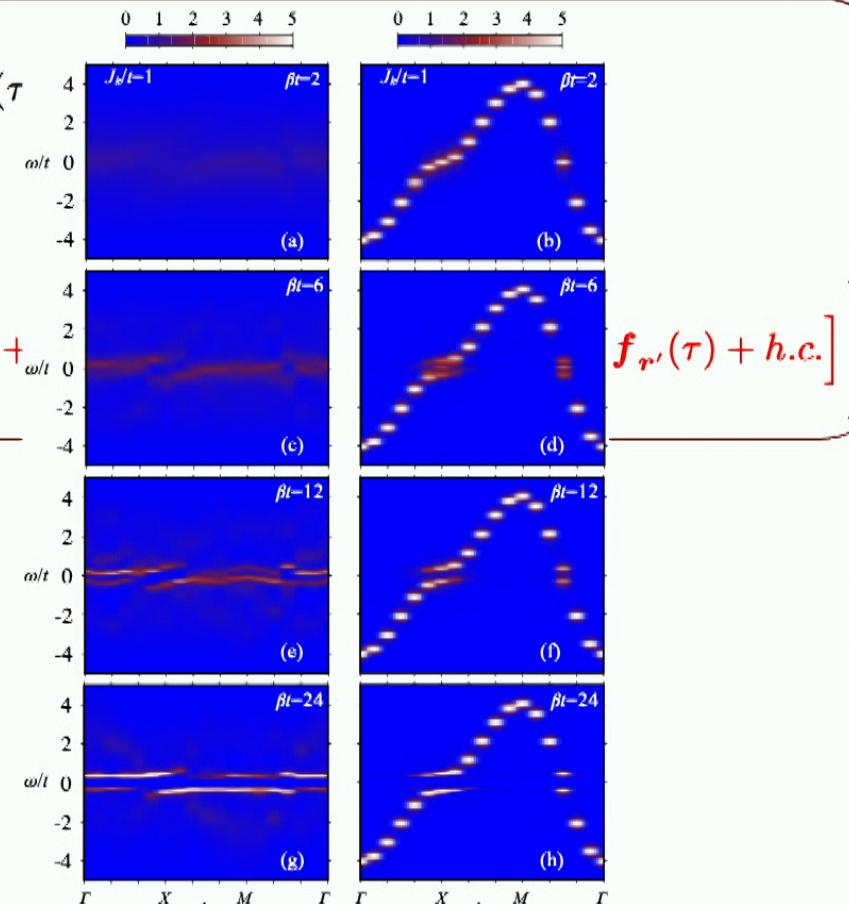


B. Danu, FFA, and F. Mila, Phys. Rev. Lett. 123 (2019), 176601.

# Kondo systems

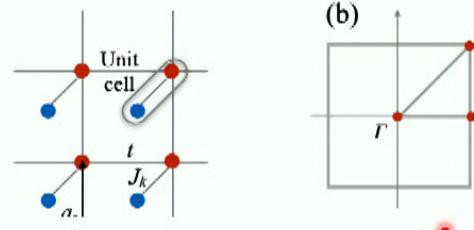
Phases

$$S = \int_0^\beta d\tau \left\{ \frac{2}{J_h} \sum_b |\chi_b(\tau)|^2 + \frac{2}{J_k} \sum_{\mathbf{r}} |b_{\mathbf{r}}(\tau)|^2 + \sum_{\mathbf{i}, \mathbf{j}} \mathbf{c}_{\mathbf{i}}^\dagger(\tau) \right. \\ \left. + \sum_{\mathbf{r}} |b_{\mathbf{r}}(\tau)| \left[ e^{i\varphi_{\mathbf{r}}(\tau)} \mathbf{f}_{\mathbf{r}}^\dagger(\tau) \mathbf{c}_{\mathbf{r}}(\tau) + h.c. \right] \right. \\ \left. + \sum_{\mathbf{r}} \mathbf{f}_{\mathbf{r}}^\dagger(\tau) [\partial_\tau - ia_{0,\mathbf{r}}(\tau)] \mathbf{f}_{\mathbf{r}}(\tau) + ia_{0,\mathbf{r}}(\tau) + \mathbf{f}_{\mathbf{r}'}^\dagger(\tau) + h.c. \right]$$



Kondo: composite fermion  $e^{i\varphi_i(\tau)} \mathbf{f}_i(\tau) \propto \psi_i = \mathbf{S}_i \cdot \boldsymbol{\sigma} \mathbf{c}_i$ .

Square Lattice



$$A_\psi(\mathbf{k}, \omega) = -\frac{1}{\pi} \text{Im} G_\psi^{ret}(\mathbf{k}, \omega) \quad G_\psi^{ret}(\mathbf{k}, \omega) = -i \int_0^\infty dt e^{i\omega t} \sum_\sigma \langle \{ \hat{\psi}_{\mathbf{k},\sigma}(t), \hat{\psi}_{\mathbf{k},\sigma}^\dagger(0) \} \rangle$$

B. Danu, Z. Liu, FFA, and M. Raczkowski, Phys. Rev. B 104 (2021), 155128.

# Spin chains on metallic surfaces: Kondo destruction and magnetic order-disorder transitions

Fakher F. Assaad, Quantum Criticality: Gauge Fields and Matter, Perimeter ITP, 16<sup>th</sup> May 2022

Topics      Kondo breakdown transitions and phases

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PHYSICAL REVIEW LETTERS **125**, 206602 (2020)

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## Kondo Breakdown in a Spin-1/2 Chain of Adatoms on a Dirac Semimetal

Bimla Danu,<sup>1,\*</sup> Matthias Vojta,<sup>2,†</sup> Fakher F. Assaad,<sup>1,‡</sup> and Tarun Grover<sup>3,§</sup>



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Leibniz-Rechenzentrum  
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Gauss Centre for Supercomputing

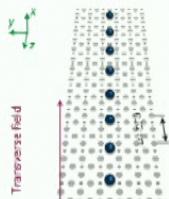


Center of excellence – complexity and  
topology in quantum matter

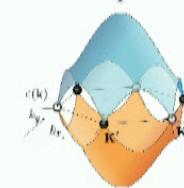


# Spin chain on semi-metal

Lattice model



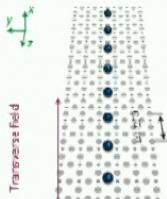
$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} (e^{\frac{2\pi i}{\Phi_0} J_i^j \mathbf{A} dl} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + h.c.) + J_k \sum_{l=1}^L \hat{\mathbf{S}}_l^c \cdot \hat{\mathbf{S}}_l + J_h \sum_{l=1}^L \hat{\mathbf{S}}_l \cdot \hat{\mathbf{S}}_{l+\Delta l}$$



# Spin chain on semi-metal

Lattice model

$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} (e^{\frac{2\pi i}{\Phi_0} \int_i^j A dl} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + h.c) + J_k \sum_{l=1}^L \hat{\mathbf{S}}_l^c \cdot \hat{\mathbf{S}}_l + J_h \sum_{l=1}^L \hat{\mathbf{S}}_l \cdot \hat{\mathbf{S}}_{l+\Delta l}$$



## Weak Coupling

Scaling dimensions of fermion and spin:  $\Delta_\psi = \frac{d}{2}$        $\Delta_s = \frac{1}{2}$

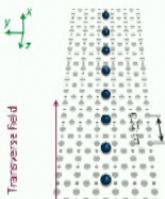
→ Kondo term has scaling dimension,  $2 - 2\Delta_\psi - \Delta_s = -1/2$

→ Irrelevant



# Spin chain on semi-metal

Lattice model



$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} (e^{\frac{2\pi i}{\Phi_0} \int_i^j \mathbf{A} dl} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + h.c) + J_k \sum_{l=1}^L \hat{\mathbf{S}}_l^c \cdot \hat{\mathbf{S}}_l + J_h \sum_{l=1}^L \hat{\mathbf{S}}_l \cdot \hat{\mathbf{S}}_{l+\Delta l}$$

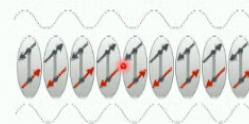
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→ Irrelevant

## Strong coupling



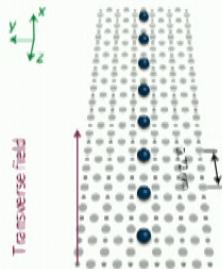
Each spin captures a conduction electron and forms a singlet.



# Spin chain on semi-metal

Lattice model

$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} (e^{\frac{2\pi i}{\Phi_0} \int_i^j \mathbf{A} dl} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + h.c) + J_k \sum_{l=1}^L \hat{\mathbf{S}}_l^c \cdot \hat{\mathbf{S}}_l + J_h \sum_{l=1}^L \hat{\mathbf{S}}_l \cdot \hat{\mathbf{S}}_{l+\Delta l}$$



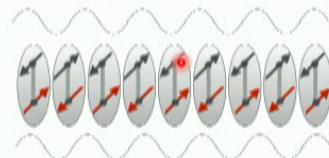
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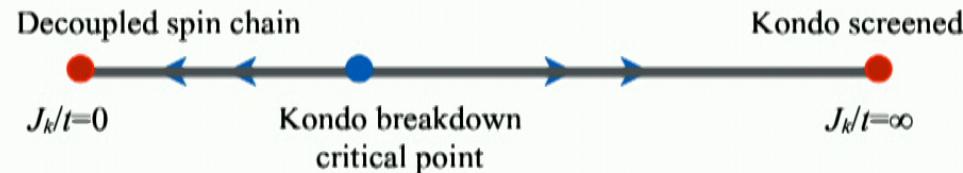
→ Irrelevant

## Strong coupling



Each spin captures a conduction electron and forms a singlet.

## $\epsilon$ -expansion

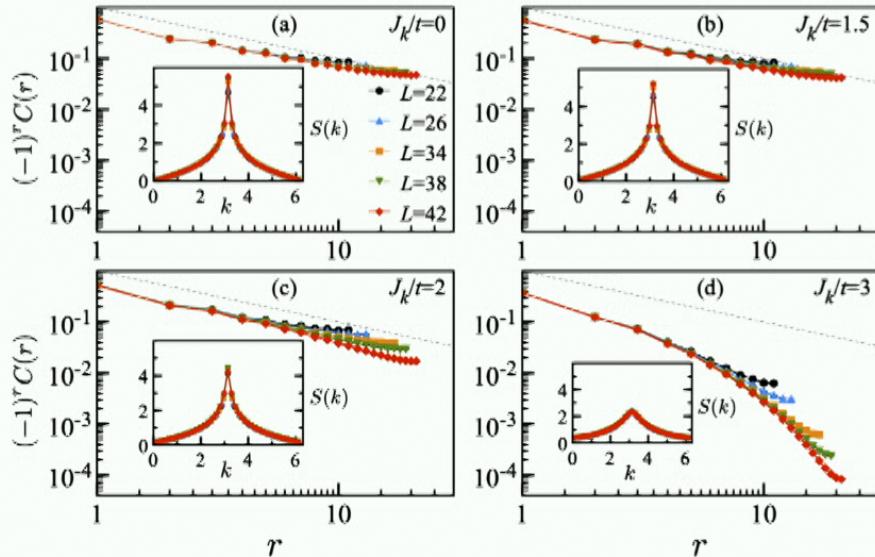


$$\frac{dj_k}{d \ln \Lambda} = \epsilon j_k - \frac{j_k^2}{2}$$

Spin-spin correlations along the Heisenberg chain

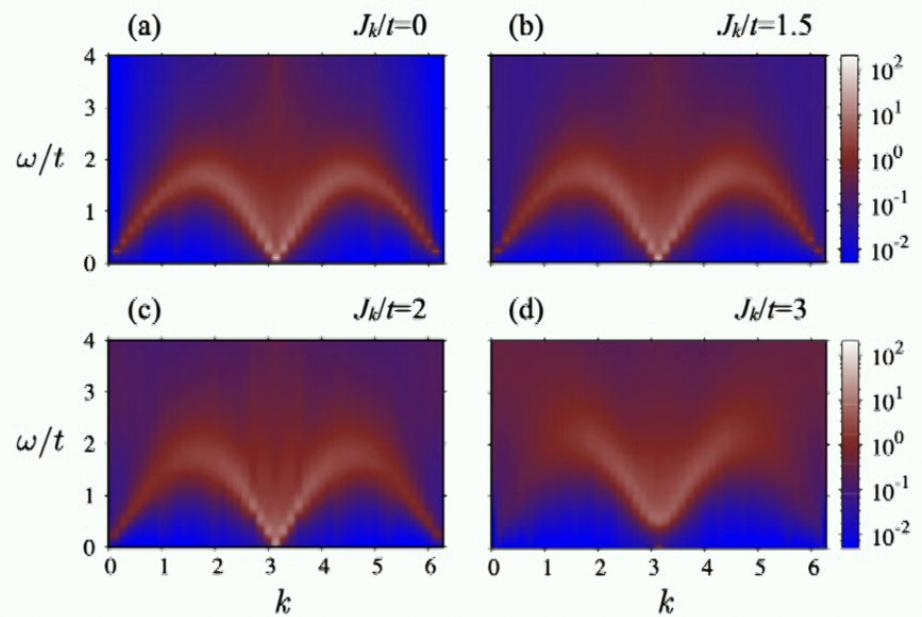
For isolated chain, SU(2) spin symmetry enforces

$$C(r) = \langle \hat{S}_l \hat{S}_{l+r} \rangle \simeq (-1)^{|r|} / |r|$$



Two spinon continuum

$$S(\mathbf{q}, \omega) = \frac{\chi''(\mathbf{q}, \omega)}{1 - e^{-\beta\omega}}$$



# Spin chain on semi-metal

## Interpretation

Gapping out of two-spinon continuum

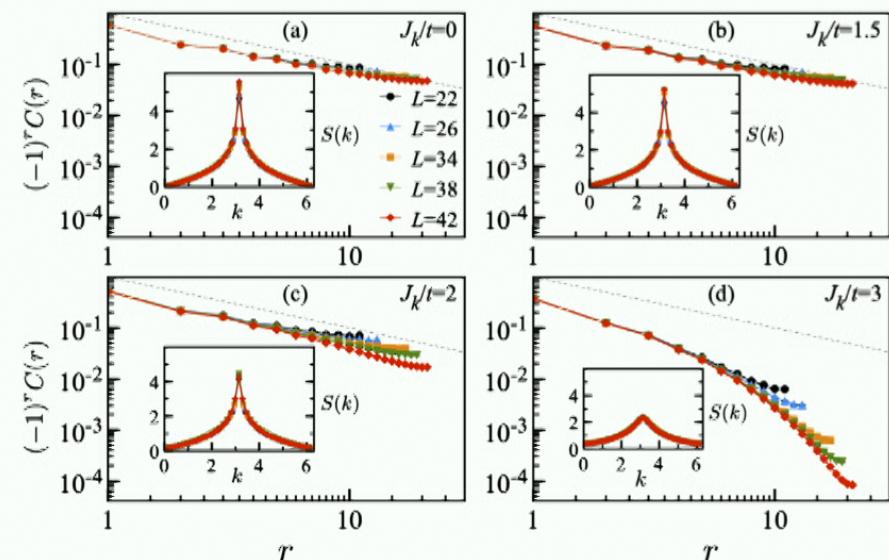
corresponds to confinement transition.

$$\langle f_{\mathbf{r}}^\dagger e^{i \int_{\mathbf{r}}^{\mathbf{r}'} \mathbf{a}(\mathbf{l}) \cdot d\mathbf{l}} f_{\mathbf{r}'} \rangle \propto \begin{cases} \frac{1}{|\mathbf{r}-\mathbf{r}'|^\alpha} & J_k < J_k^c \\ e^{-|\mathbf{r}-\mathbf{r}'|/\xi} & J_k > J_k^c \end{cases}$$

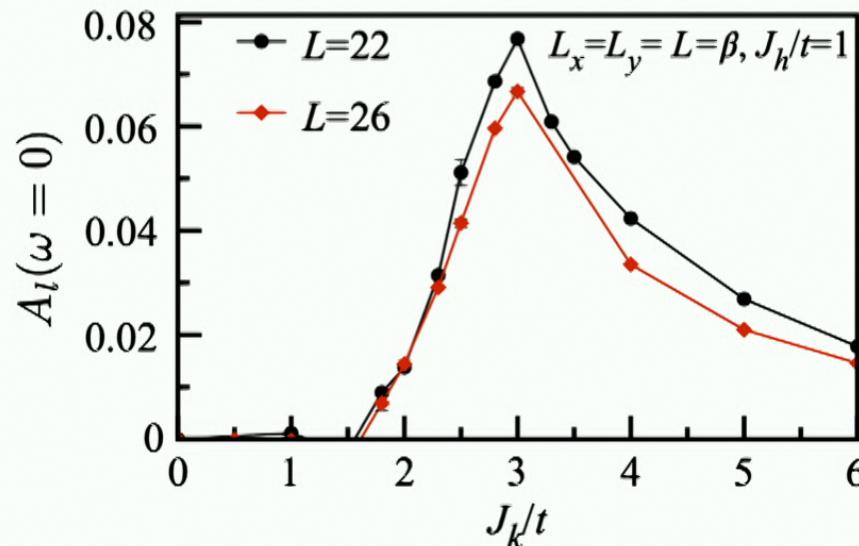
At large Kondo coupling, the spins  $\bullet$   
inherit the low energy properties of the  
conduction electrons.

$$\begin{aligned} \langle b_{\mathbf{r}} \rangle &= 0 & J_k < J_k^c \\ \langle b_{\mathbf{r}} \rangle &\neq 0 & J_k > J_k^c \end{aligned}$$

$$C(\mathbf{r}) = \langle \hat{S}_l \hat{S}_{l+r} \rangle \simeq (-1)^{|\mathbf{r}|} / |\mathbf{r}|$$



Zero bias tunneling through the magnetic adatom as a measure of the Higgs condensate.



$$A(\omega) = -\text{Im} G^{\text{ret}}(\omega), \quad G^{\text{ret}}(\omega) = -i \int_0^\infty dt e^{i\omega t} \sum_\sigma \langle \{\hat{\psi}_\sigma(t), \hat{\psi}_\sigma^\dagger(0)\} \rangle$$

$$\hat{\psi}^\dagger = e^{-S} \hat{\mathbf{d}}^\dagger e^S = \hat{\mathbf{c}}_{r=0}^\dagger \boldsymbol{\sigma} \cdot \hat{\mathbf{S}}$$

(S: Schrieffer Wolff transformation)

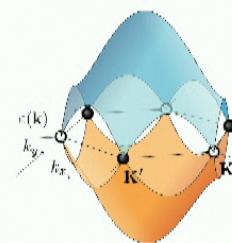
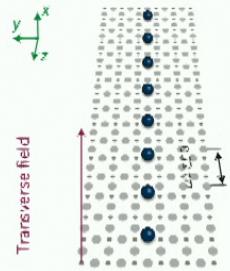
T.A. Costi, Phys. Rev. Lett. 85, 1504 (2000).

In the large-N limit:  $\hat{\psi}_r^\dagger \propto \hat{f}_r^\dagger b_r$

# Spin chain on semi-metal

Lattice model

$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} (e^{\frac{2\pi i}{\Phi_0} \int_i^j A dl} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + h.c) + J_k \sum_{l=1}^L \hat{\mathbf{S}}_l^c \cdot \hat{\mathbf{S}}_l + J_h \sum_{l=1}^L \hat{\mathbf{S}}_l \cdot \hat{\mathbf{S}}_{l+\Delta l}$$



Decoupled spin chain

$J_k/t=0$

FL\* phase

Spinons are deconfined

No Higgs condensate

Kondo screened

$J_k/t=\infty$

Kondo phase

Spinons are confined

Higgs condensate

# Spin chains on metallic surfaces: Kondo destruction and magnetic order-disorder transitions

Fakher F. Assaad, Quantum Criticality: Gauge Fields and Matter, Perimeter ITP, 16<sup>th</sup> May 2022

## Topics

### Spin chain on a metallic surface: Dissipation-induced order vs. Kondo entanglement

Bimla Danu,<sup>1</sup> Matthias Vojta,<sup>2</sup> Tarun Grover,<sup>3</sup> and Fakher F. Assaad<sup>1</sup>

arXiv:2204.00029v1

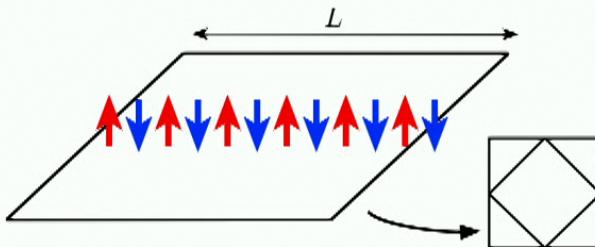


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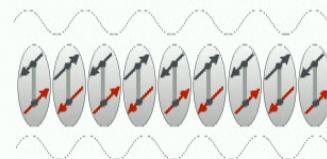


GCS  
Gauss Centre for Supercomputing  
TGCC  
Très Grand Centre de Calcul de l'INRA





Strong coupling



$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{c}_i^\dagger \hat{c}_j + h.c) + \frac{J_k}{2} \sum_r \hat{c}_r^\dagger \boldsymbol{\sigma} \hat{c}_r \cdot \hat{\mathbf{S}}_r + J_h \sum_{\langle r,r' \rangle} \hat{\mathbf{S}}_r \cdot \hat{\mathbf{S}}_{r'}$$

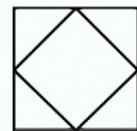
Spins are screened by conduction electrons and inherit the properties of the metal. → Heavy fermion metal.

Weak coupling

Integrate out electrons à la Hertz-Millis

$$\mathcal{S}(\mathbf{n}) = \mathcal{S}_{\text{chain}}(\mathbf{n}) + \mathcal{S}_{\text{diss}}(\mathbf{n})$$

$$\mathcal{S}_{\text{diss}}(\mathbf{n}) = \frac{J_k^2}{8} \int d\tau d\tau' \sum_{\mathbf{r}, \mathbf{r}'} \mathbf{n}_{\mathbf{r}}(\tau) \chi^0(\mathbf{r} - \mathbf{r}', \tau - \tau') \mathbf{n}_{\mathbf{r}'}(\tau').$$



$$\chi^0(\mathbf{0}, \tau - \tau') \propto \frac{1}{v_F^2 (\tau - \tau')^2}$$

$$\chi^0(r \mathbf{e}_x, 0) \propto \frac{1}{r^4}$$

At Heisenberg critical point ( $\Delta_n = \frac{1}{2}$ ) the coupling to electron in the temporal direction is marginal!



$$\mathcal{S}(\mathbf{n}) = \mathcal{S}_{\text{chain}}(\mathbf{n}) + \mathcal{S}_{\text{diss}}(\mathbf{n})$$

$$\mathcal{S}_{\text{diss}}(\mathbf{n}) = \alpha \int d\tau d\tau' \sum_{\mathbf{r}} \frac{\mathbf{n}_{\mathbf{r}}(\tau) \mathbf{n}_{\mathbf{r}}(\tau')}{(\tau - \tau')^2}.$$

arXiv:2112.02124v1

Dissipation-induced order: the  $S = 1/2$  quantum spin chain coupled to an ohmic bath

Manuel Weber,<sup>1</sup> David J. Luitz,<sup>1</sup> and Fakher F. Assaad<sup>2,3</sup>

Hamiltonian

$$\hat{H} = J \sum_i \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+1} + \sum_{i,q} \omega_q \hat{\mathbf{a}}_{i,q}^\dagger \hat{\mathbf{a}}_{i,q} + \sum_{i,q} \lambda_q \left( \hat{\mathbf{a}}_{i,q}^\dagger + \hat{\mathbf{a}}_{i,q} \right) \cdot \hat{\mathbf{S}}_i \quad J(\omega) = \pi \sum_q \lambda_q \delta(\omega - \omega_q) = 2\pi\alpha\omega$$

Conservation law

$$\hat{\mathbf{J}}_{tot} = \sum_{iq} \hat{\mathbf{Q}}_{iq} \times \hat{\mathbf{P}}_{iq} + \sum_i \hat{\mathbf{S}}_i$$

$$\hat{\mathbf{P}}_{iq} = \frac{1}{\sqrt{2}} \left( \hat{\mathbf{a}}_{iq}^\dagger - \hat{\mathbf{a}}_{iq} \right)$$

$$\hat{\mathbf{Q}}_{iq} = \frac{1}{\sqrt{2}} \left( \hat{\mathbf{a}}_{iq}^\dagger + \hat{\mathbf{a}}_{iq} \right)$$

A bath cannot screen



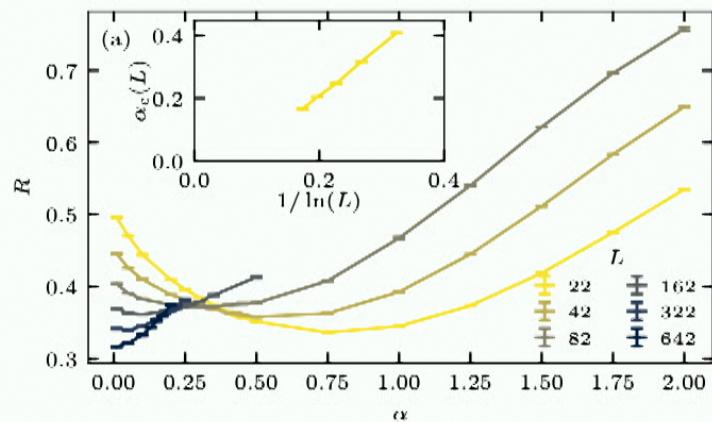
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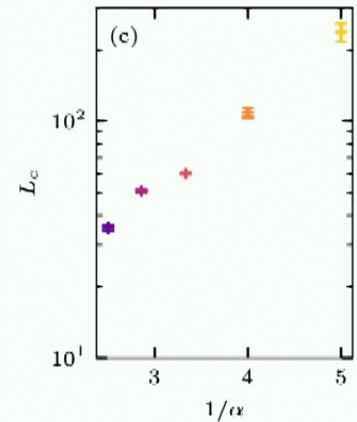
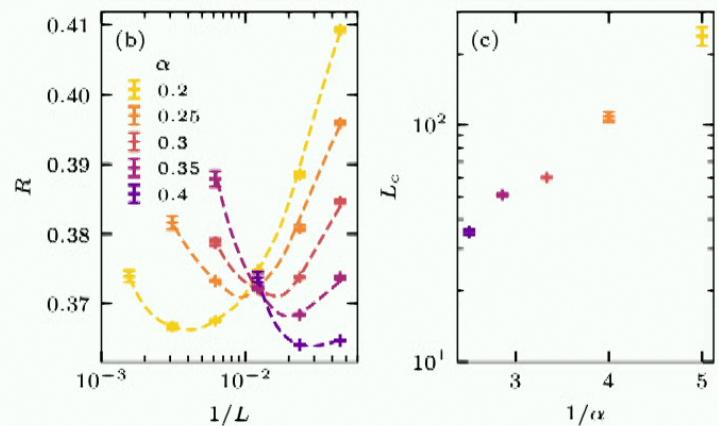
Dissipation-induced order: the  $S = 1/2$  quantum spin chain coupled to an ohmic bath

Manuel Weber,<sup>1</sup> David J. Luitz,<sup>1</sup> and Fakher F. Assaad<sup>2,3</sup>



$$S(\mathbf{q}) = \sum_{\mathbf{r}} e^{i\mathbf{q} \cdot \mathbf{r}} \langle \hat{\mathbf{S}}_{\mathbf{r}} \cdot \hat{\mathbf{S}}_{\mathbf{0}} \rangle$$

$$R = 1 - \frac{S(\mathbf{Q} + \delta\mathbf{q})}{S(\mathbf{Q})}$$



Long ranged interaction along the imaginary time invalidates Mermin-Wagner theorem and triggers long-ranged order.  
(Dissipation is marginally relevant)



$$\mathcal{S}(\mathbf{n}) = \mathcal{S}_{\text{chain}}(\mathbf{n}) + \mathcal{S}_{\text{diss}}(\mathbf{n})$$

$$\mathcal{S}_{\text{diss}}(\mathbf{n}) = \alpha \int d\tau d\tau' \sum_{\mathbf{r}} \frac{\mathbf{n}_{\mathbf{r}}(\tau) \mathbf{n}_{\mathbf{r}}(\tau')}{(\tau - \tau')^2}.$$

arXiv:2112.02124v1

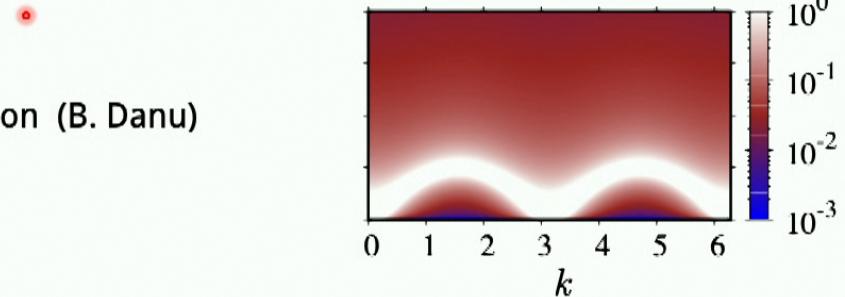
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Spin structure factor: Landau damped Goldstone modes (z=2).

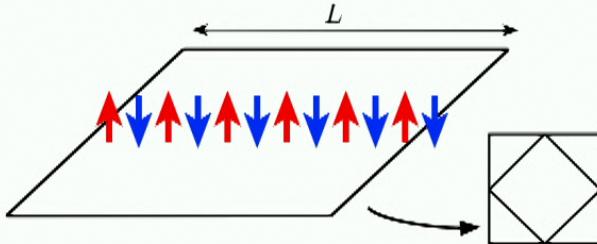
$$S(\mathbf{k}, \omega) = \frac{\text{Im}\chi(\mathbf{k}, \omega + i0^+)}{1 - e^{-\beta\omega}}$$

Spin-wave calculation (B. Danu)



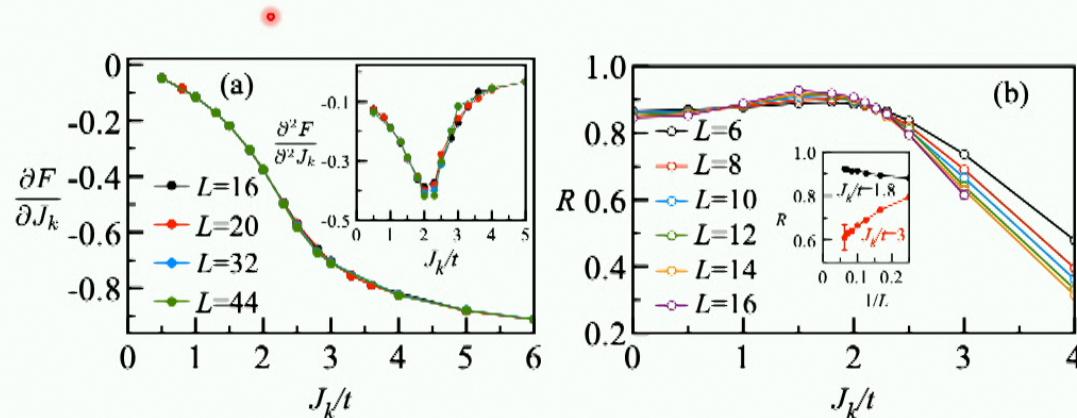
Long ranged interaction along the imaginary time invalidates Mermin-Wagner theorem and triggers long-ranged order.  
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## Spin chain on metallic surface



$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{c}_i^\dagger \hat{c}_j + h.c) + \frac{J_k}{2} \sum_{\mathbf{r}} \hat{c}_{\mathbf{r}}^\dagger \boldsymbol{\sigma} \hat{c}_{\mathbf{r}} \cdot \hat{\mathbf{S}}_{\mathbf{r}} + J_h \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \hat{\mathbf{S}}_{\mathbf{r}} \cdot \hat{\mathbf{S}}_{\mathbf{r}'}$$

Dissipation and Kondo singlet formation compete and trigger an order-disorder transition.



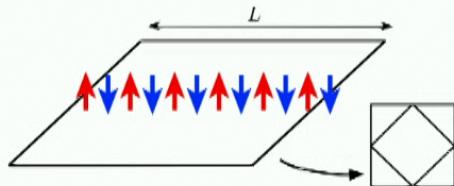
Numerics suggest a  $z=2$  QCP such that we adopt a  $\beta = L^2$  scaling.

$$\chi(\mathbf{k}, i\Omega_m) = \int_0^\beta d\tau \sum_{\mathbf{r}} e^{i(\Omega_m \tau - \mathbf{k} \cdot \mathbf{r})} \langle \hat{S}_{\mathbf{r}}^z(\tau) \hat{S}_{\mathbf{0}}^z(0) \rangle$$

$$R = 1 - \frac{\chi(\mathbf{Q} - \delta\mathbf{k}, 0)}{\chi(\mathbf{Q}, 0)}$$

$$R = f([J_k - J_k^c] L^{1/\nu}, \tilde{L}^z / \tilde{\beta}, L^{-\omega})$$

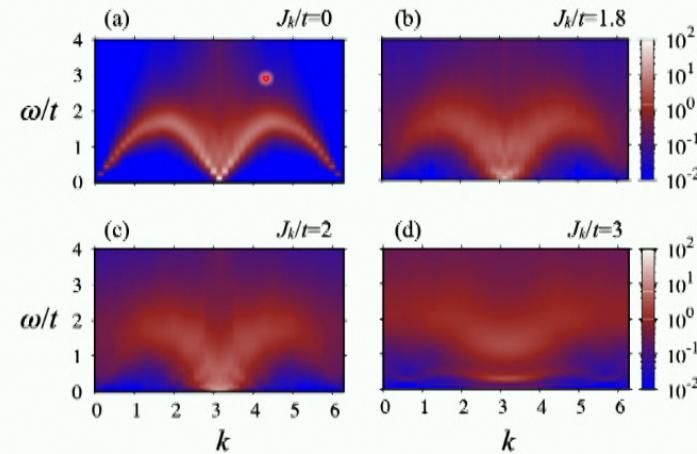
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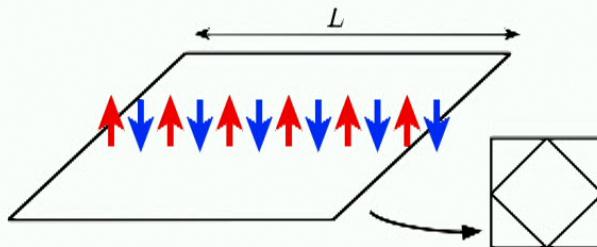


$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{c}_i^\dagger \hat{c}_j + h.c.) + \frac{J_k}{2} \sum_r \hat{c}_r^\dagger \boldsymbol{\sigma} \hat{c}_r \cdot \hat{\mathbf{S}}_r + J_h \sum_{\langle r,r' \rangle} \hat{\mathbf{S}}_r \cdot \hat{\mathbf{S}}_{r'}$$

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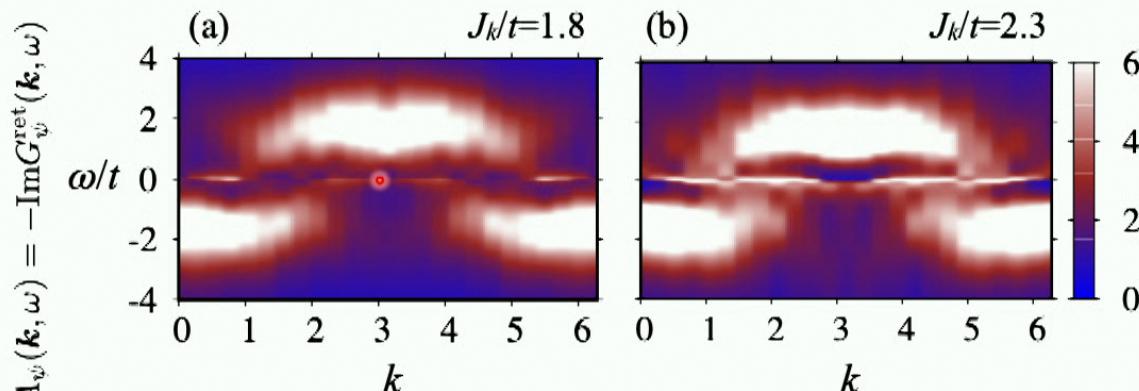
$$S(\mathbf{k}, \omega) = \frac{\text{Im}\chi(\mathbf{k}, \omega + i0^+)}{1 - e^{-\beta\omega}}$$





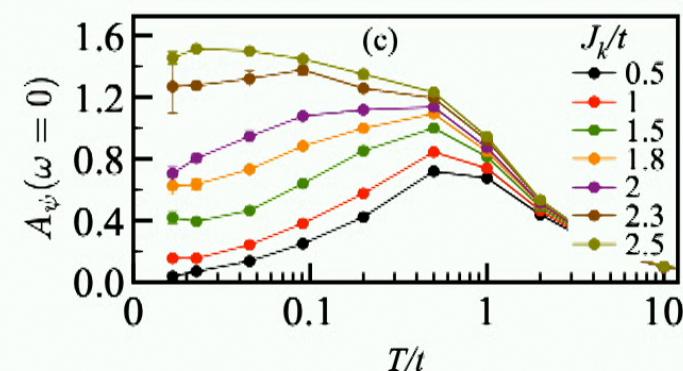
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Single particle spectral function shows heavy bands in both phases.



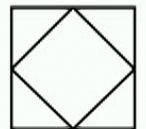
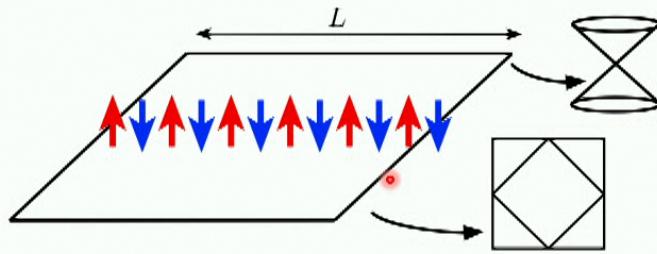
$$G_\psi^{\text{ret}}(\mathbf{k}, \omega) = -i \int_0^\infty dt e^{i\omega t} \sum_\sigma \langle \{\hat{\psi}_{\mathbf{k},\sigma}(t), \hat{\psi}_{\mathbf{k},\sigma}^\dagger(0)\} \rangle \quad \hat{\psi}_{r,\sigma}^\dagger = 2 \sum_{\sigma'} \hat{c}_{r,\sigma'}^\dagger \boldsymbol{\sigma}_{\sigma',\sigma} \cdot \hat{\mathbf{S}}_r$$

Consistent with the absence of Kondo breakdown.



# Spin chains on metallic surfaces: Kondo destruction and magnetic order-disorder transitions

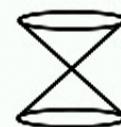
## Conclusions



AFM metal  
 $\langle \mathbf{n} \rangle \neq 0, \langle b \rangle \neq 0$



Heavy fermion metal  
 $\langle \mathbf{n} \rangle = 0, \langle b \rangle \neq 0$



FL\*

$\langle b \rangle = 0, \langle \mathbf{n} \rangle = 0$

Heavy fermion metal  
 $\langle b \rangle \neq 0, \langle \mathbf{n} \rangle = 0$



Dissipation versus Kondo screening.

Anti-ferromagnetic metal to heavy fermion metal QCP.

Spinons are deconfined  
Kondo Breakdown phase

Heavy-fermion phase  
Kondo screen

$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{c}_i^\dagger \hat{c}_j + h.c.) + \frac{J_k}{2} \sum_{\mathbf{r}} \hat{c}_{\mathbf{r}}^\dagger \boldsymbol{\sigma} \hat{c}_{\mathbf{r}} \cdot \hat{\mathbf{S}}_{\mathbf{r}} + J_h \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \hat{\mathbf{S}}_{\mathbf{r}} \cdot \hat{\mathbf{S}}_{\mathbf{r}'}$$

$$\text{U(1) gauge theory} \quad S = \int_0^T dt \left\{ \frac{2}{J_h} \sum_b |\chi_b(\tau)|^2 + \frac{2}{J_k} \sum_{\mathbf{r}} |b_{\mathbf{r}}(\tau)|^2 + \sum_{i,j} c_i^\dagger(\tau) [\partial_i \delta_{i,j} - T_{i,j}] c_j(\tau) \right. \\ \left. + \sum_{\mathbf{r}} |b_{\mathbf{r}}(\tau)| [e^{i\varphi_{\mathbf{r}}(\tau)} f_{\mathbf{r}}^\dagger(\tau) c_{\mathbf{r}}(\tau) + h.c.] \right. \\ \left. + \sum_{\mathbf{r}} f_{\mathbf{r}}^\dagger(\tau) [\partial_{\mathbf{r}} - ia_{0,\mathbf{r}}(\tau)] f_{\mathbf{r}}(\tau) + ia_{0,\mathbf{r}}(\tau) + \sum_{b \neq (\mathbf{r}, \mathbf{r}')} |\chi_b(\tau)| [f_{\mathbf{r}}^\dagger(\tau) e^{-i \int_{\mathbf{r}}^{\mathbf{r}'} \mathbf{a}(t, \tau) dt} f_{\mathbf{r}'}(\tau) + h.c.] \right\}$$