

Title: Non-Fermi liquids and quantum criticality in multipolar Kondo systems

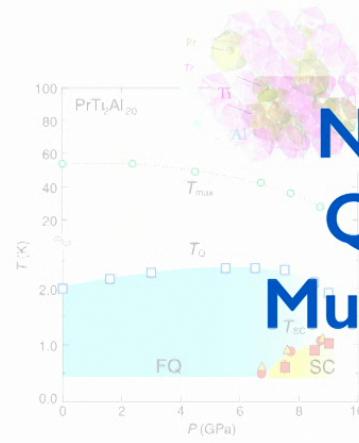
Speakers: Yong-Baek Kim

Collection: Quantum Matter Workshop

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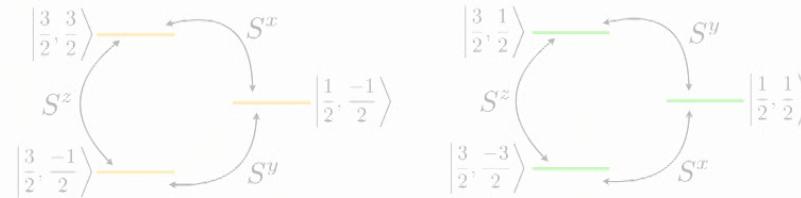
Abstract: We discuss emergent non-Fermi liquid behaviors in multipolar Kondo systems, where conduction electrons interact with the non-Kramers local moments carrying higher-rank multipolar moments such as quadrupolar and octupolar moments. We first show that unexpected non-Fermi liquid states arise in the single impurity multipolar Kondo system using the renormalization group and conformal field theory. Next, we study the competition between the Kondo and RKKY interactions in the Bose-Fermi Kondo systems, where the RKKY interaction between multipolar moments is represented by a bosonic degree of freedom. We present the renormalization group solution of this problem and describe the quantum critical behaviors. If time permits, we also discuss possible superconducting states arising from the multipolar Kondo interactions. We compare the theoretical results with existing experimental data on some cubic f-electron systems.



Non-Fermi Liquids and Quantum Criticality in Multipolar Kondo Systems

Yong Baek Kim
University of Toronto

Perimeter Institute
November 15, 2022



SIMONS FOUNDATION



John Simon
Guggenheim
Memorial Foundation

Outline

I. Non-Fermi liquids in multipolar Kondo systems

Single multipolar local moment coupled to
conduction electrons

(Focus on cubic Pr^{3+} systems)

RG and Conformal Field Theory

2. Competition with RKKY and quantum criticality

Bose-Fermi Kondo model and quantum criticality

3. Two-stage Kondo destruction and Fermi surface

reconstruction: cubic Ce^{3+} systems

Collaborators



Adarsh Patri
U of Toronto
=> MIT



SangEun Han
U of Toronto



Daniel Schulz
U of Toronto

A. Patri, YBK, PRX (2020), arXiv:2005.08973

A. Patri, I. Khait, YBK, PR Research (2020), arXiv:1904.02717

Kondo problem

S. Han, D. Schultz, YBK, arXiv:2206.02808 (2022)

S. Han, D. Schultz, YBK, arXiv:2207.07661 (2022)

Kondo + RKKY

Multipolar local moments

Many f-electron localized ions carry multipolar moments

Example:

Pr^{3+}

$4f^2$

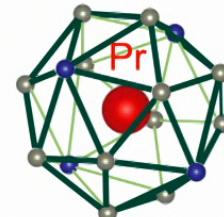


$J=4$

Crystal Electric Field
Splitting

Point Group Symmetry

T_d



$\text{PrV}_2\text{Al}_{20}$
(T_d)

$\text{PrTi}_2\text{Al}_{20}$
(T_d)

$\Gamma_1 \longrightarrow 156 \text{ K}$

$\Gamma_1 \longrightarrow ?$

$\Gamma_4 \equiv ?$

$\Gamma_5 \equiv 107 \text{ K}$

$\Gamma_5 \equiv \sim 40 \text{ K}$

$\Gamma_3 \equiv 0$

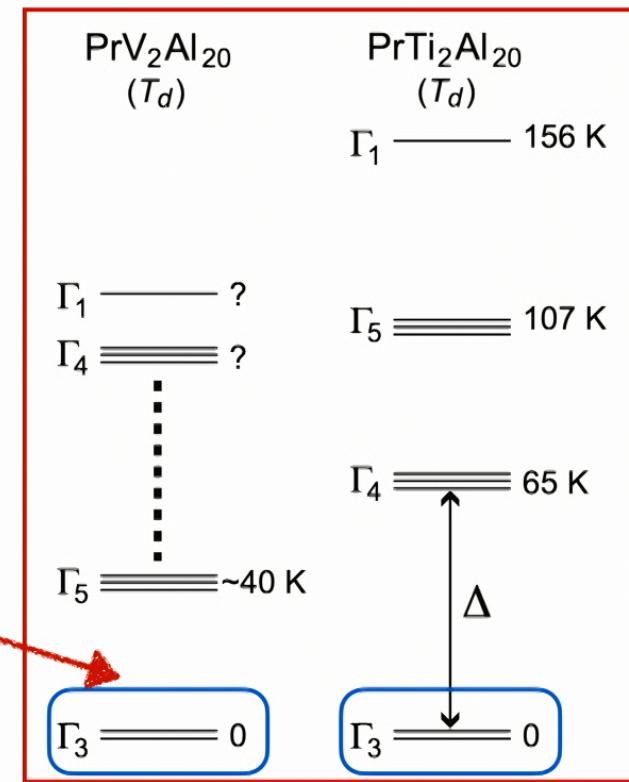
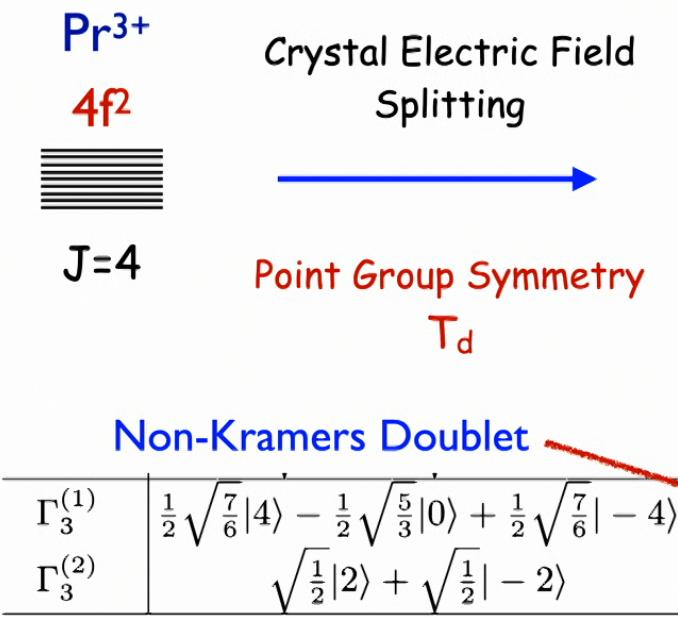
$\Gamma_4 \equiv 65 \text{ K}$

$\Gamma_3 \equiv 0$

Multipolar local moments

Many f-electron localized ions carry multipolar moments

Example:



Non-Kramers Doublet: Pr^{3+} $|+\rangle \equiv \Gamma_3^{(1)}$ $|-\rangle \equiv \Gamma_3^{(2)}$

$$\langle \pm | J_\alpha | \pm \rangle = 0 \quad \text{No dipole moment!}$$

But, finite matrix elements for

$$O_{22} = \frac{\sqrt{3}}{2}(J_x^2 - J_y^2) \quad O_{20} = \frac{1}{2}(3J_z^2 - J^2) \quad \text{Quadrupolar}$$

$$T_{xyz} = \frac{\sqrt{15}}{6} \overline{J_x J_y J_z} \quad \text{Octupolar}$$

Pseudo-spin basis

$$|\uparrow\rangle \equiv \frac{1}{\sqrt{2}}(|\Gamma_3^{(1)}\rangle + i|\Gamma_3^{(2)}\rangle)$$

$$|\downarrow\rangle \equiv \frac{1}{\sqrt{2}}(i|\Gamma_3^{(1)}\rangle + |\Gamma_3^{(2)}\rangle)$$

$$S^x = -\frac{1}{4}\mathcal{O}_{22}$$

$$S^y = -\frac{1}{4}\mathcal{O}_{20}$$

$$S^z = \frac{1}{3\sqrt{5}}\mathcal{T}_{xyz}$$

$$[S^\alpha, S^\beta] = i\epsilon_{\alpha\beta\gamma}S^\gamma$$

(S^x, S^y) Quadrupolar

time-reversal even

S^z Octupolar

time-reversal odd

Multipolar local moments with non-Kramers doublet

PrTi₂Al₂₀

PrV₂Al₂₀

PrIr₂Zn₂₀

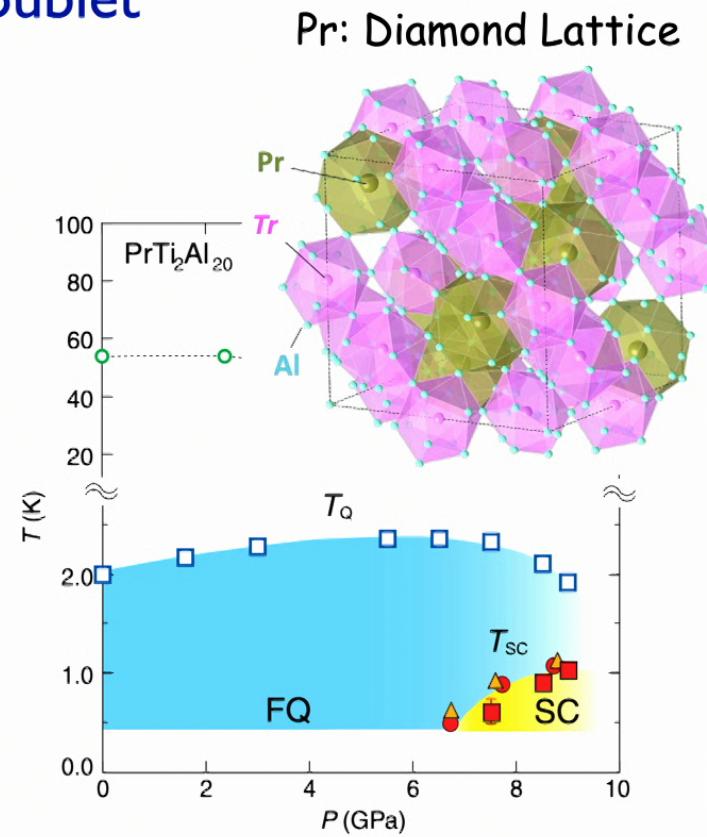
PrRh₂Zn₂₀

PrNi₂Cd₂₀

PrPd₂Cd₂₀

Pr³⁺ 4f²

S. Nakatsuji, A. Sakai,
P. Gegenwart,
T. Onimaru,
B. Maple, ...



Non-Kramers Doublet: Pr^{3+} $|+\rangle \equiv \Gamma_3^{(1)}$ $|-\rangle \equiv \Gamma_3^{(2)}$

Unusual forms of the Kondo and RKKY interaction

First, look at the single impurity Kondo problem !

Pseudo-spin basis

$$|\uparrow\rangle \equiv \frac{1}{\sqrt{2}}(|\Gamma_3^{(1)}\rangle + i|\Gamma_3^{(2)}\rangle)$$

$$|\downarrow\rangle \equiv \frac{1}{\sqrt{2}}(i|\Gamma_3^{(1)}\rangle + |\Gamma_3^{(2)}\rangle)$$

(S^x, S^y) **Quadrupolar**
time-reversal even

$$S^x = -\frac{1}{4}\mathcal{O}_{22}$$

$$S^y = -\frac{1}{4}\mathcal{O}_{20}$$

$$S^z = \frac{1}{3\sqrt{5}}\mathcal{T}_{xyz} \quad [S^\alpha, S^\beta] = i\epsilon_{\alpha\beta\gamma}S^\gamma$$

S^z **Octupolar**
time-reversal odd

PrIr₂Zn₂₀
Quadrupolar ordering

Dilution


Y_{1-x}Pr_xIr₂Zn₂₀
Non-Fermi liquid

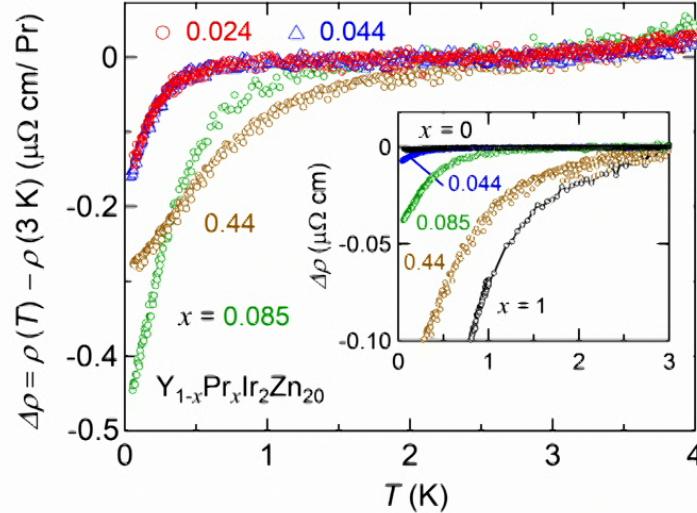
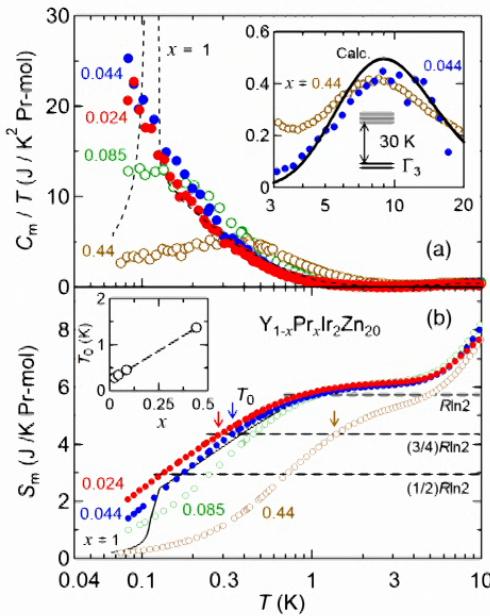
PHYSICAL REVIEW LETTERS 121, 077206 (2018)

Single-Site Non-Fermi-Liquid Behaviors in a Diluted 4f² System Y_{1-x}Pr_xIr₂Zn₂₀

Y. Yamane,¹ T. Onimaru,^{1,*} K. Wakiya,^{1,†} K. T. Matsumoto,^{1,‡} K. Umeo,² and T. Takabatake¹

¹Graduate School of Advanced Sciences of Matter, Hiroshima University, Higashi-Hiroshima 739-8530, Japan

²Cryogenic and Instrumental Analysis Division, N-BARD, Hiroshima University, Higashi-Hiroshima 739-8526, Japan



How to model conduction electrons ?

Local symmetry around Pr ion is T_d

Fermi pockets around
zone center

(quantum oscillations, S. Nagashima et al, 2014)

Conduction electron orbitals can be
classified in terms of
irreducible representation of T_d

A_1	$xyz, \quad x^4+y^4+z^4, \quad x^2y^2z^2$
A_2	$x^4(y^2-z^2)+y^4(z^2-x^2)+z^4(x^2-y^2)$
E	$\{x^2-y^2, \quad 2z^2-x^2-y^2\}$
T_1	$\{x(z^2-y^2), \quad y(z^2-x^2), \quad z(x^2-y^2)\}$
T_2	$\{x, \quad y, \quad z\}, \quad \{xy, \quad xz, \quad yz\},$

The “Kondo” model

S^x, S^y, S^z couple to fermion spin-orbital ‘currents’
that transform exactly in the same way

For example,

$$H_3 = K_3 S^z \left[\sigma_{\alpha\beta}^x (c_{p_y,\alpha}^\dagger c_{p_z,\beta} + h.c.) + \sigma_{\alpha\beta}^y (c_{p_z,\alpha}^\dagger c_{p_x,\beta} + h.c.) + \sigma_{\alpha\beta}^z (c_{p_x,\alpha}^\dagger c_{p_y,\beta} + h.c.) \right]$$

$\alpha, \beta = \uparrow, \downarrow$
 K_1, K_2, K_3 three independent couplings

Entangled fluctuations of both orbital and spin !

Perform RG computations up to 3rd order:
two stable fixed points

A. Patri, I. Khait, YBK, PR Research 2, 013257 (2020)

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$\alpha, \beta = \uparrow, \downarrow$
 K_1, K_2, K_3 three independent couplings

$L=1, S=1/2$  $|j, j_z\rangle = |j = 3/2, j_z\rangle, |j = 1/2, j_z\rangle$

$ p_x, \uparrow\rangle$	$ p_x, \downarrow\rangle$
$ p_y, \uparrow\rangle$	$ p_y, \downarrow\rangle$
$ p_z, \uparrow\rangle$	$ p_z, \downarrow\rangle$

Spin-orbital
entangled
basis

$ 3/2, 3/2\rangle$	$ 3/2, 1/2\rangle$
$ 3/2, -1/2\rangle$	$ 3/2, -3/2\rangle$
$ 1/2, 1/2\rangle$	$ 1/2, -1/2\rangle$

Fixed point I

Only $j=3/2$ electrons are involved

$$H_{\text{tot}} = S^x (\tau_A^x + \tau_B^x) - S^y (\tau_A^z + \tau_B^z) + S^z (\tau_A^y + \tau_B^y)$$

$$\left| \frac{3}{2}, \frac{3}{2} \right\rangle \quad \left| \frac{3}{2}, \frac{-1}{2} \right\rangle$$

$(\uparrow_A, \downarrow_A)$

conduction electron
pseudospin for
channel A

$$\vec{\tau}_A$$

$$\left| \frac{3}{2}, \frac{1}{2} \right\rangle \quad \left| \frac{3}{2}, \frac{-3}{2} \right\rangle$$

$(\uparrow_B, \downarrow_B)$

conduction electron
pseudospin for
channel B

$$\vec{\tau}_B$$

A. Patri, YBK, PRX, arXiv:2005.08973 (2020)

Fixed point ! Two channel Kondo model !

Only $j=3/2$ electrons are involved

$$H_{\text{tot}} = S^x (\tau_A^x + \tau_B^x) - S^y (\tau_A^z + \tau_B^z) + S^z (\tau_A^y + \tau_B^y)$$

$$\left| \frac{3}{2}, \frac{3}{2} \right\rangle \quad \left| \frac{3}{2}, -\frac{1}{2} \right\rangle$$

$(\uparrow_A, \downarrow_A)$

conduction electron
pseudospin for
channel A

$$\vec{\tau}_A$$

$$\left| \frac{3}{2}, \frac{1}{2} \right\rangle \quad \left| \frac{3}{2}, -\frac{3}{2} \right\rangle$$

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$$\left| \frac{3}{2}, \frac{3}{2} \right\rangle \quad \left| \frac{3}{2}, -\frac{1}{2} \right\rangle$$

$(\uparrow_A, \downarrow_A)$

conduction electron
pseudospin for
channel A

$$\vec{\tau}_A$$

$$C_v \propto T \ln T$$
$$\rho \propto \sqrt{T}$$

$$\left| \frac{3}{2}, \frac{1}{2} \right\rangle \quad \left| \frac{3}{2}, -\frac{3}{2} \right\rangle$$

$(\uparrow_B, \downarrow_B)$

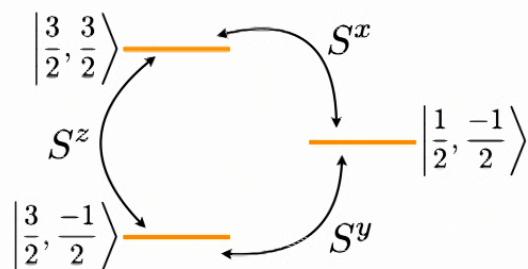
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A. Patri, YBK, PRX, arXiv:2005.08973 (2020)

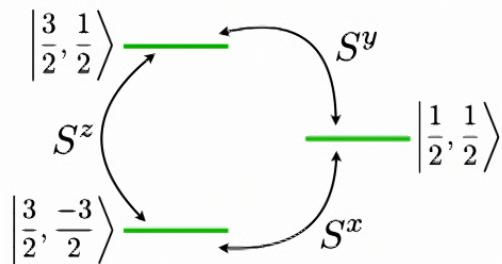
Fixed point II

All of $j=3/2$ and $j=1/2$ electrons are involved



Two channels

But each channel involves
three flavors of conduction
electrons - SU(3) 'current'



This is not the usual
Kondo problem

A. Patri, YBK, PRX, arXiv:2005.08973 (2020)

Fixed point II

From the perturbative RG

Approaching the fixed point by fixing the ratios of the couplings

$$K_1 = -\frac{1}{2\sqrt{6}}g_k, K_2 = -\frac{1}{12\sqrt{2}}g_k, K_3 = -\frac{1}{4\sqrt{3}}g_k$$

$$\begin{aligned} \frac{dg_k}{dl} &= \frac{g_k^2}{4} - \frac{g_k^3}{4} & g_k^* = 1 \text{ at the fixed point} \\ &\approx -\frac{1}{4}(g_k - g_k^*) \end{aligned}$$

$1 + \Delta$ dimension of the leading irrelevant operator

$$\Delta = 1/4 \quad C_v \propto T^{2\Delta} = T^{1/2} \quad \rho \propto T^\Delta = T^{1/4}$$

Fixed point II

True nature of this new fixed point ?

Rewriting the Kondo coupling

$$H_k = g_k \sum_{m=1,2} \vec{\psi}_m^\dagger(0) \left[\frac{S^x}{2} \frac{\lambda^4}{2} + \frac{S^y}{2} \frac{\lambda^6}{2} + \frac{S^z}{2} \frac{\lambda^2}{2} \right] \vec{\psi}_m(0)$$

$\lambda^a \quad a = 1, \dots, 8 \quad \text{3x3 SU(3) Gell-Mann matrices}$

$$\vec{\psi}_{m=1}^\dagger = \left(-c_{\frac{3}{2}, \frac{3}{2}}^\dagger, -c_{\frac{3}{2}, -\frac{1}{2}}^\dagger, c_{\frac{1}{2}, -\frac{1}{2}}^\dagger \right)$$

$$\vec{\psi}_{m=2}^\dagger = \left(c_{\frac{3}{2}, -\frac{3}{2}}^\dagger, c_{\frac{3}{2}, \frac{1}{2}}^\dagger, c_{\frac{1}{2}, \frac{1}{2}}^\dagger \right)$$

Fixed point II

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$\lambda^a \quad a = 1, \dots, 8 \quad 3 \times 3 \text{ SU}(3) \text{ Gell-Mann matrices}$

$$\vec{\psi}_{m=1}^\dagger = \left(-c_{\frac{3}{2}, \frac{3}{2}}^\dagger, -c_{\frac{3}{2}, -\frac{1}{2}}^\dagger, c_{\frac{1}{2}, -\frac{1}{2}}^\dagger \right)$$

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$$g_k^* = 1$$

at the perturbative
fixed point

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$$g_k^* = 1$$

at the perturbative
fixed point

This is not an SU(3) Kondo problem ...

Current Algebra and Conformal Field Theory (Results)

Useful to generalize this to k channels Here $k = 2$

$$g_k^* = \frac{2}{k+3} \quad \Delta = \frac{2}{4k+2}$$

$1 + \Delta$ dimension of the leading irrelevant operator

$$C_v \propto T^{2\Delta} \quad \rho \propto T^\Delta$$

Exact $k = 2$

$$g_k^* = 2/5$$

$$\Delta = 1/5$$

$$C_v/T \propto T^{-3/5}$$

$$\rho \propto T^{1/5}$$

A. Patri, YBK, PRX, arXiv:2005.08973 (2020)

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$1 + \Delta$ dimension of the leading irrelevant operator

$$C_v \propto T^{2\Delta} \quad \rho \propto T^\Delta$$

Perturbative regime $k \gg 1$

$$g_k^* \rightarrow 2/k \quad \Delta \rightarrow 1/2k$$

$$k = 2 \quad g_k^* \rightarrow 1 \quad \Delta \rightarrow 1/4$$

recover the perturbative results !

Exact $k = 2$

$$g_k^* = 2/5$$

$$\Delta = 1/5$$

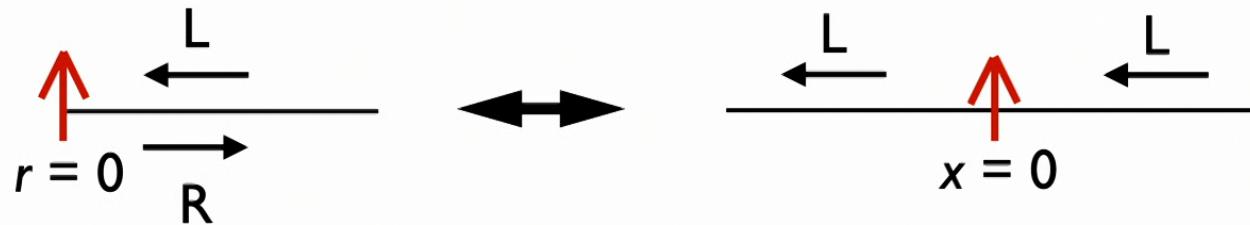
$$C_v/T \propto T^{-3/5}$$

$$\rho \propto T^{1/5}$$

A. Patri, YBK, PRX, arXiv:2005.08973 (2020)

Current Algebra and Conformal Field Theory Solution (Schematic)

Consider δ -function interaction and s-wave scattering
Mapping to 1+1 dimensional (chiral) model



$$\psi_L(x, \tau) = \psi_L(z = \tau + ix)$$

$$\psi_R(x, \tau) \equiv \psi_L(-x, \tau)$$

$$\psi_R(x, \tau) = \psi_R(z^* = \tau - ix)$$

$$\psi_L(0, \tau) = \psi_R(0, \tau)$$

Current Algebra and Conformal Field Theory Solution (Schematic)

Bulk free theory (before coupling to impurity)

Current algebra and conformal embedding

$$U(1) \times SU(3)_2 \times SU(2)_3$$

Charge Spin-Orbital Flavor(channel)

3 = three spin-orbital bands in each channel

2 = two channels

A. Patri, YBK, arXiv:2005.08973 (2020)

Current Algebra and Conformal Field Theory Solution (Schematic)

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Charge Spin-Orbital Flavor(channel)

3 = three spin-orbital bands in each channel

2 = two channels

$$H_0 = \frac{1}{12} : J J : (z) + \frac{1}{5} : J^a J^a : (z) + \frac{1}{5} : J^A J^A : (z)$$

Charge

Spin-Orbital

Flavor(channel)

$$a = 1, \dots, 8$$

$$A = 1, \dots, 3$$

A. Patri, YBK, arXiv:2005.08973 (2020)

Current Algebra and Conformal Field Theory Solution (Schematic)

Bulk free theory (before coupling to impurity)

Current algebra and conformal embedding

$$U(1) \times SU(3)_2 \times SU(2)_3$$

Charge Spin-Orbital Flavor(channel)

But only three of eight generators of $SU(3)$ are
coupled to the impurity

$$H_K = g_k \left(J^4(z) \frac{S^x}{2} + J^6(z) \frac{S^y}{2} + J^2(z) \frac{S^z}{2} \right) \text{ Kondo coupling}$$

We need a different conformal embedding ...

A. Patri, YBK, arXiv:2005.08973 (2020)

Current Algebra and Conformal Field Theory Solution (Schematic)

$U(1) \times SU(3)_2 \times SU(2)_3$

Charge Spin-Orbital Flavor(channel)

Bulk free theory

Conformal embedding

Coset construction

$$SU(3)_2 = [\text{3-state Potts model}] \times \widetilde{SU}(2)_8$$

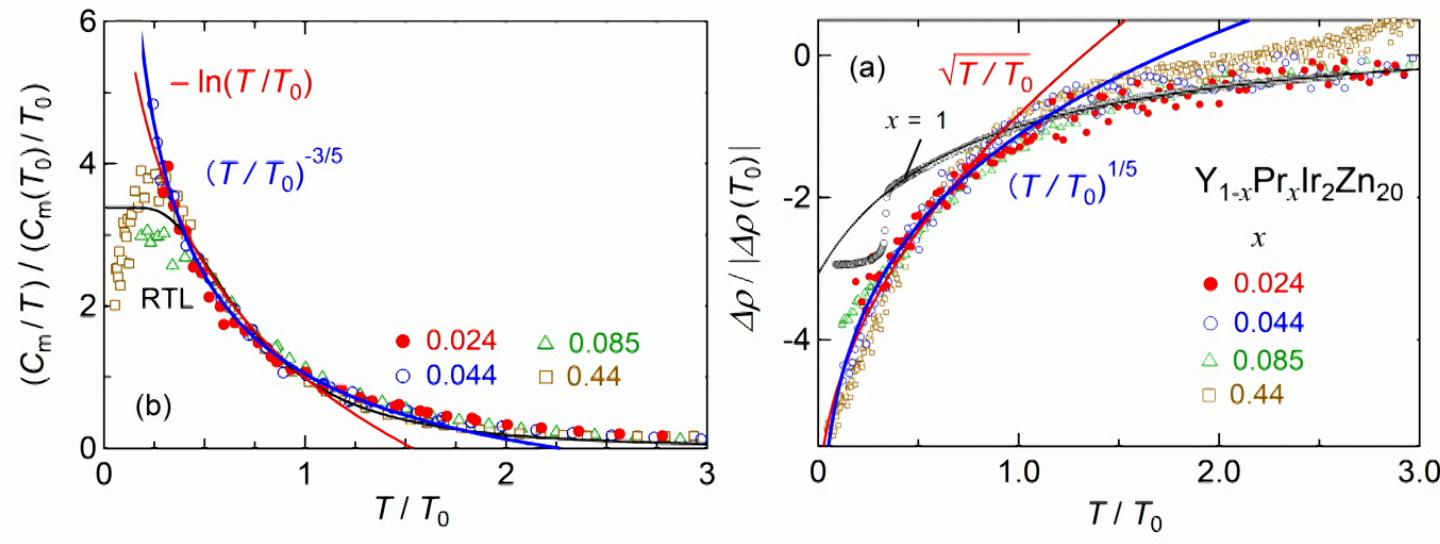
$$J^2, J^4, J^6 \in \widetilde{SU}(2)_8$$

Kondo coupling imposes (conformally invariant)
boundary conditions on the currents

↓
Boundary CFT (John Cardy)
Affleck + Ludwig (1991)

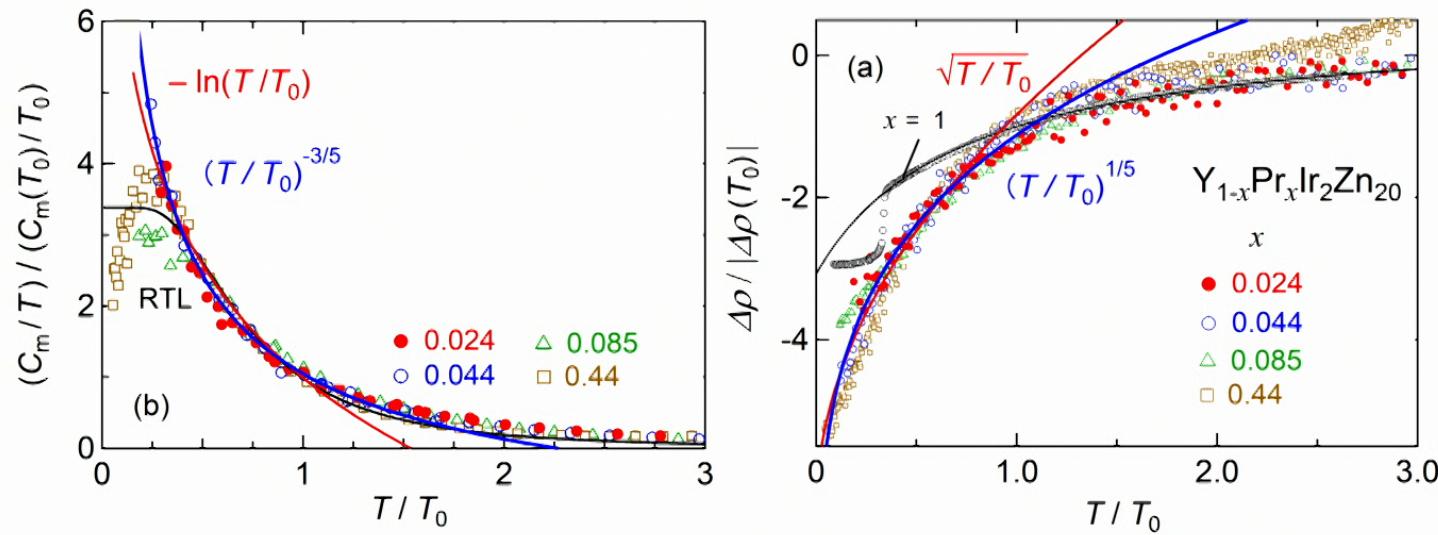
Rearrangement of the conformal towers

Experiments ?



Y.Yamane, T.Onimaru (2018, 2020)

Experiments ?



Y.Yamane, T. Onimaru (2018, 2020)

The fits are encouraging ! We need sharper predictions ...

Need more systematic understanding as to
Quadrupolar ordering (non-diluted) → “Kondo” regime (diluted)

Competition with RKKY: Bose-Fermi Kondo model

$$H = H_{\text{Fermi Kondo}} + H_{\text{Bose Kondo}}$$

$$H_{\text{RKKY}} = \sum_{ij} \left[J_{ij}^Q (S_i^x S_j^x + S_i^y S_j^y) + J_{ij}^O S_i^z S_j^z \right]$$

$$\begin{aligned} \rightarrow H_{\text{Bose Kondo}} = & g_Q (S^x \phi_0^x + S^y \phi_0^y) + g_O S^z \phi_0^z \\ & + \sum_{\mathbf{k}} \left[\Omega_{Q\mathbf{k}} (\phi_{\mathbf{k}}^{x\dagger} \phi_{\mathbf{k}}^x + \phi_{\mathbf{k}}^{y\dagger} \phi_{\mathbf{k}}^y) + \Omega_{O\mathbf{k}} \phi_{\mathbf{k}}^{z\dagger} \phi_{\mathbf{k}}^z \right] \end{aligned}$$

Boson density of states $D_i(\omega) = C_i |\omega|^{1-\epsilon_i} \text{sgn}(\omega) \quad i = Q, O$

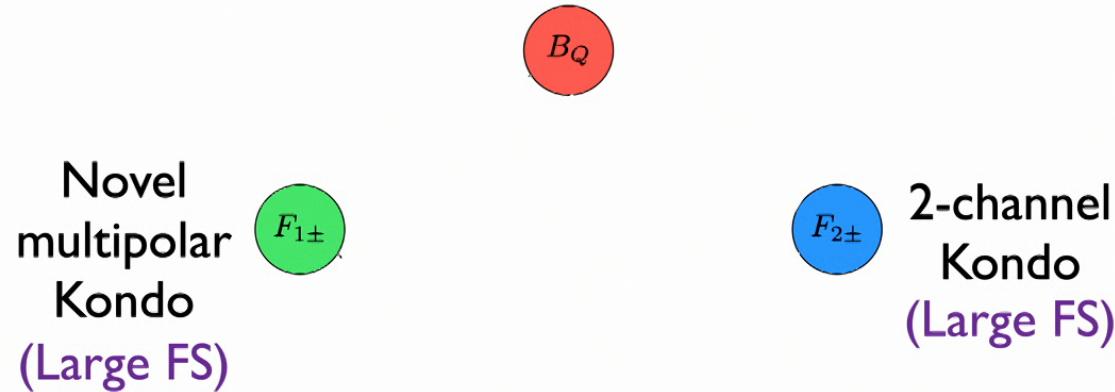
This is a local approximation of the RKKY interaction in the spirit of DMFT

J. L. Smith, Q. Si (96,97), A. M. Sengupta (97)

S. Han, D. Schultz, YBK, arXiv:2206.02808 (2022)

Renormalization Group Analysis

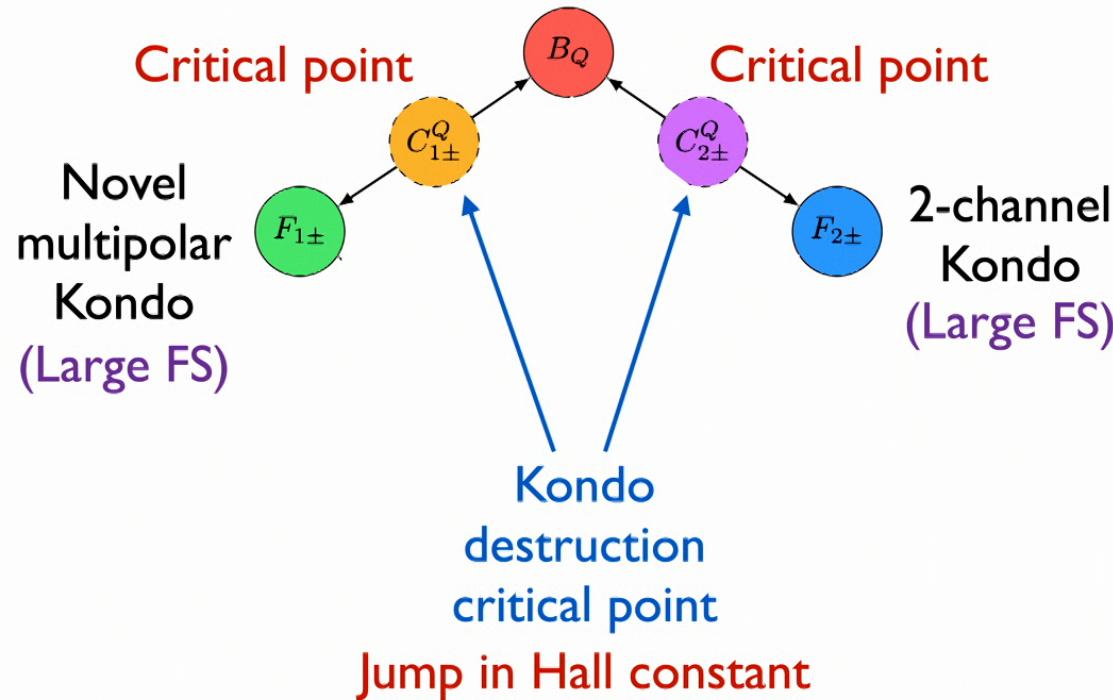
RKKY Quadrupolar Ordering (Small FS)



S. Han, D. Schultz, YBK, arXiv:2206.02808 (2022)

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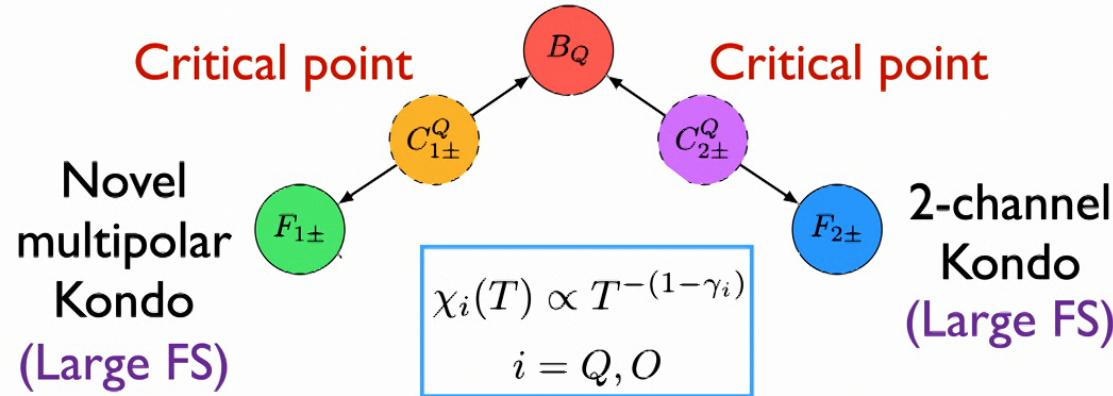
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Renormalization Group Analysis

RKKY Quadrupolar Ordering (Small FS)

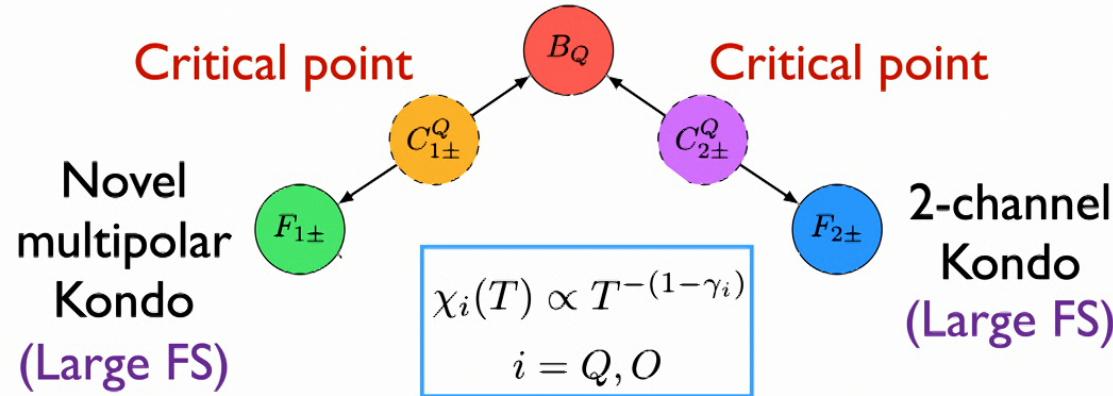


Quadrupolar susceptibility $\chi^Q(\tau) = \langle T_\tau S^{x,y}(\tau) S^{x,y}(0) \rangle \propto \left(\frac{\tau_0}{|\tau|} \right)^{\gamma_Q}$

Octupolar susceptibility $\chi^O(\tau) = \langle T_\tau S^z(\tau) S^z(0) \rangle \propto \left(\frac{\tau_0}{|\tau|} \right)^{\gamma_O}$

Renormalization Group Analysis

RKKY Quadrupolar Ordering (Small FS)

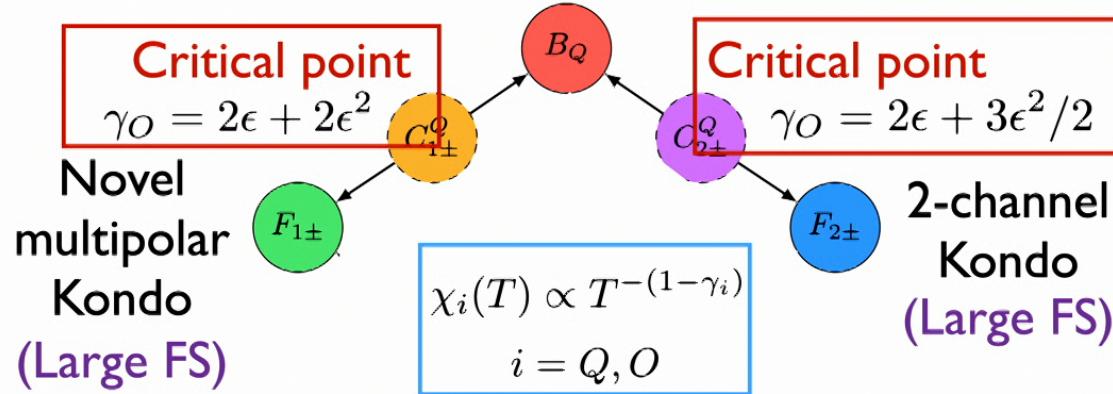


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Renormalization Group Analysis

RKKY Quadrupolar Ordering (Small FS)



Measurement via elastic constants (ultrasound)

$$(C_{11} - C_{12}) = (C_{11}^0 - C_{12}^0) - (s_Q^2) \chi'_Q,$$

$$C_{44} = C_{44}^0 - (s_O^2 h^2) \chi'_O,$$