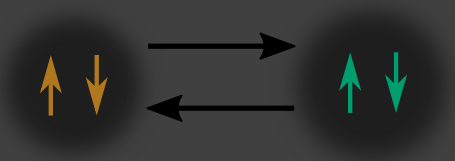


UNVEILING THE KONDO CLOUD: UNITARY RG STUDY OF THE KONDO MODEL

arXiv:2111.10580v2[cond-mat.str-el]



ANIRBAN MUKHERJEE ¹, ABHIRUP MUKHERJEE ¹, N. S. VIDHYADHIRAJA ²,
A. TARAPHDER ³, SIDDHARTHA LAL ¹

¹DEPARTMENT OF PHYSICAL SCIENCES, IISER KOLKATA,

²THEORETICAL SCIENCES UNIT, JNCASR,

³DEPARTMENT OF PHYSICS, IIT KHARAGPUR

FEBRUARY 4, 2022

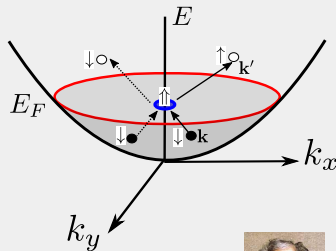
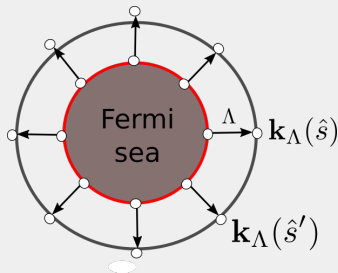


THE MODEL

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$$H = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + J \vec{S}_d \cdot \vec{S}, \quad \vec{S} \equiv \sum_{kk',\alpha,\beta} \vec{\sigma}_{\alpha\beta} c_{k\alpha}^\dagger c_{k'\beta}, \quad \vec{S}_d \longrightarrow \text{impurity spin}$$

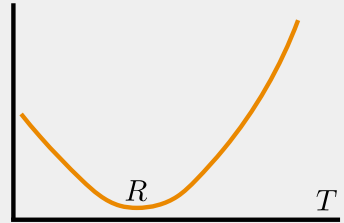
local s-wave interaction between impurity spin \vec{S}_d and conduction electrons \vec{S}



Kondo 1964; Schrieffer and Wolff 1966.

THE MODEL

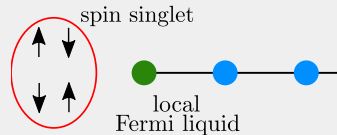
- Resistance of metal **reveals a minimum** at low T - possibly due to **spin-flip scattering**



Anderson and Yuval 1969; Anderson 1970; Wilson 1975; Andrei, Furuya, and Lowenstein 1983a; Andrei, Furuya, and Lowenstein 1983b; Wiegmann 1981; Nozieres 1974.

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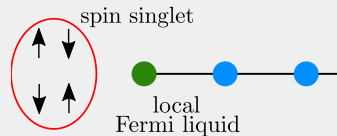
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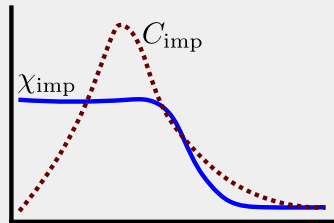
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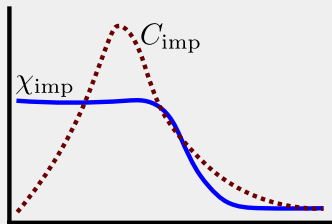
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- χ_{imp} becomes constant at low temperatures - C_{imp} becomes linear - total resistance R rises after going through a minimum



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- **thermal quantities functions of single scale T/T_K**



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- Finite J effective Hamiltonian at fixed point
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- Nature of correlations inside the Kondo cloud: **Fermi liquid vs off-diagonal** - what leads to the maximally entangled singlet?
- Behaviour of **many-particle entanglement** and many-body correlation under RG flow

THE UNITARY RENORMALIZATION GROUP METHOD

The General Idea

- Apply unitary many-body transformations to the Hamiltonian

$$\begin{array}{c} H_j \\ \downarrow U_j \\ H_{j-1} \end{array}$$

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- Apply unitary many-body transformations to the Hamiltonian
- Successively decouple high energy states
- Obtain sequence of Hamiltonians and hence scaling equations

$$\begin{array}{c} H_j \\ \downarrow U_j \\ H_{j-1} \end{array}$$

THE UNITARY RENORMALIZATION GROUP METHOD

Select a UV-IR Scheme

UV shell

\vec{k}_N (zeroth RG step)

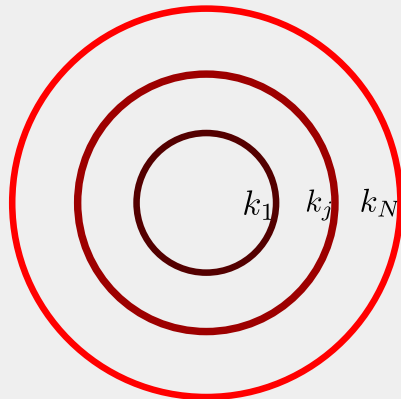
\vdots

\vec{k}_j (j^{th} RG step)

\vdots

\vec{k}_1 (Fermi surface)

IR shell

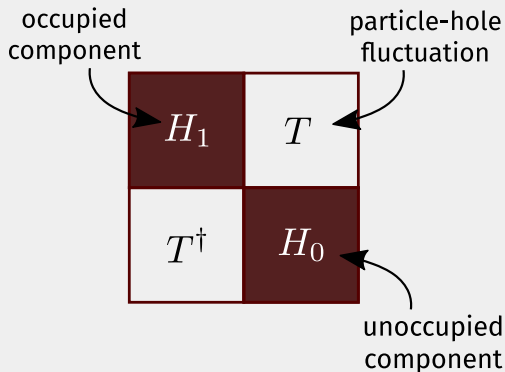


THE UNITARY RENORMALIZATION GROUP METHOD

Write Hamiltonian in the basis of \vec{k}_j

$$H_{(j)} = H_1 \hat{n}_j + H_0 (1 - \hat{n}_j) + c_j^\dagger T + T^\dagger c_j$$

$$2^{j-1}\text{-dim.} \longrightarrow \begin{cases} H_1, H_0 \longrightarrow \text{diagonal parts} \\ T \longrightarrow \text{off-diagonal part} \end{cases}$$



THE UNITARY RENORMALIZATION GROUP METHOD

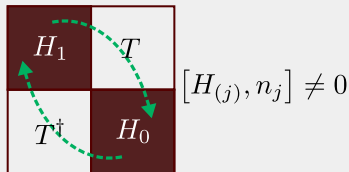
Rotate Hamiltonian and kill off-diagonal blocks

$$H_{(j-1)} = U_{(j)} H_{(j)} U_{(j)}^\dagger$$

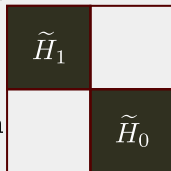
$$U_{(j)} = \frac{1}{\sqrt{2}} \left(1 - \eta_{(j)} + \eta_{(j)}^\dagger \right)$$

$$\eta_{(j)}^\dagger = \frac{1}{\hat{\omega}_{(j)} - H_D} c_j^\dagger T \left\} \rightarrow \text{many-particle rotation}$$

$$\left\{ \eta_{(j)}, \eta_{(j)}^\dagger \right\} = 1$$



$[H_{(j)}, n_j] = 0$
 n_j becomes an
integral of motion
(IOM)

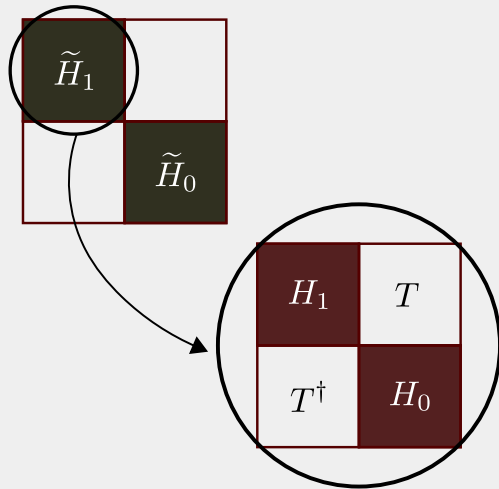


THE UNITARY RENORMALIZATION GROUP METHOD

Repeat with renormalised Hamiltonian

$$H_{(j-1)} = \tilde{H}_1 \hat{n}_j + \tilde{H}_0 (1 - \hat{n}_j)$$

$$\tilde{H}_1 = H_1 \hat{n}_{j-1} + H_0 (1 - \hat{n}_{j-1}) + c_{j-1}^\dagger T + T^\dagger c_{j-1}$$



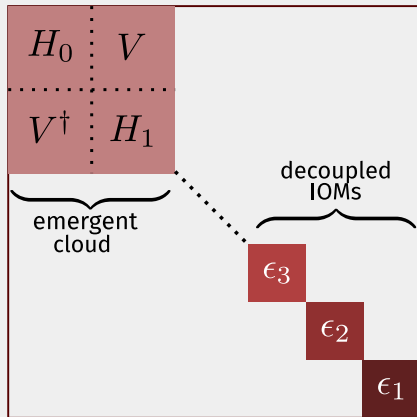
THE UNITARY RENORMALIZATION GROUP METHOD

RG Equations and Denominator Fixed Point

$$\Delta H_{(j)} = \left(\hat{n}_j - \frac{1}{2} \right) \left\{ c_j^\dagger T, \eta_{(j)} \right\}$$

$$\eta_{(j)}^\dagger = \frac{1}{\hat{\omega}_{(j)} - H_D} c_j^\dagger T$$

Fixed point: $\hat{\omega}_{(j^*)} - (H_D)^* = 0$



THE UNITARY RENORMALIZATION GROUP METHOD

Novel Features of the Method

- **Quantum fluctuation scale $\hat{\omega}$ that tracks all orders of renormalisation**

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- Finite-valued fixed points for finite systems - leads to **emergent degrees of freedom**
- **Spectrum-preserving** unitary transformations - partition function does not change
- **Tractable low-energy effective Hamiltonians** - allows **renormalised perturbation theory** around them

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URG OF THE KONDO MODEL

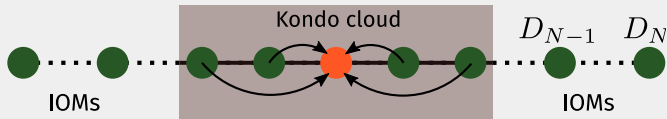
URG OF THE KONDO MODEL

RG Equation

$$\Delta J_{(j)} = \frac{n_j J_{(j)}^2 \left(\omega_{(j)} - \frac{D_j}{2} \right)}{\left(\omega_{(j)} - \frac{D_j}{2} \right)^2 - \frac{1}{16} J_{(j)}^2}$$

$$J^* = 4 \left(\omega^* - \frac{1}{2} D^* \right)$$

$D^* \longrightarrow$ emergent window



For $J_{(j)} \ll D_j$, we recover weak-coupling form:

$$\frac{\Delta J_{(j)}}{\Delta \ln D_j} \sim n_j J_{(j)}^2$$

URG OF THE KONDO MODEL

RG flows and fixed points

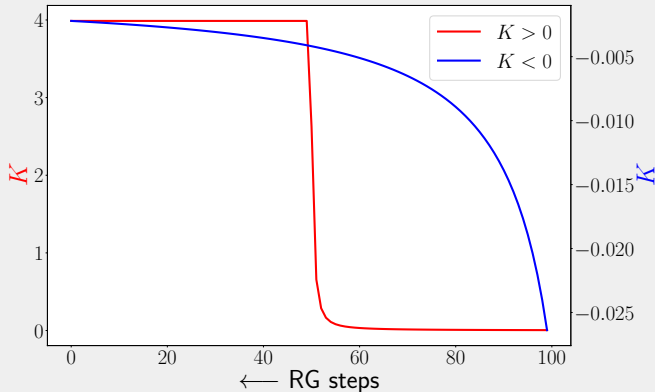
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$$\omega_{(j)} > \frac{D_j}{2}$$

$$K_{(j)} = J_{(j)} \left(\omega^* - \frac{1}{2} D^* \right)^{-1}, \quad K^* = 4$$



URG OF THE KONDO MODEL

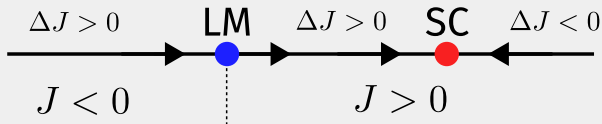
Phase diagram

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■ Decay towards FM fixed point for $J < 0$

■ Attractive flow towards AFM fixed point for $J > 0$

URG OF THE KONDO MODEL

Kondo cloud length ξ_K

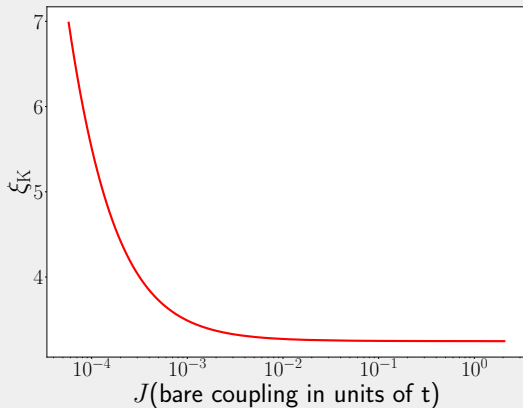
$$T_K = \frac{\hbar v_F \Lambda_0}{k_B} \exp \left(\frac{1}{2n(o)} - \frac{1}{n(o)K_0} - \frac{K_0}{n(o)16} \right), \quad \xi_K = \frac{\hbar v_F}{k_B T_K}$$

$$\Delta J_{(j)} = \frac{n_j J_{(j)}^2 \left(\omega_{(j)} - \frac{D_j}{2} \right)}{\left(\omega_{(j)} - \frac{D_j}{2} \right)^2 - \frac{1}{16} J_{(j)}^2}$$

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URG OF THE KONDO MODEL

Fixed point Hamiltonian

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$$J^* = 4 \left(\omega^* - \frac{1}{2} D^* \right)$$

$D^* \longrightarrow$ emergent window

$$\omega_{(j)} > \frac{D_j}{2}$$

$$H^* = \underbrace{\sum_{k < k^*, \sigma} \epsilon_k \hat{n}_{k\sigma}}_{\text{emergent window}} + J^* \vec{S}_d \cdot \vec{S}_{<} + \underbrace{\sum_{j=j^*}^N J^j S_d^z \sum_{|q|=q_j} S_{q_j}^z}_{\text{integrals of motion}}$$

$$\vec{S}_{<} = \frac{1}{2} \sum_{k, k' < k^*} c_{k\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{k',\beta}$$

$$S_q^z = \frac{1}{2} (\hat{n}_{q\uparrow} - \hat{n}_{q\downarrow})$$

URG OF THE KONDO MODEL

Approach towards the continuum

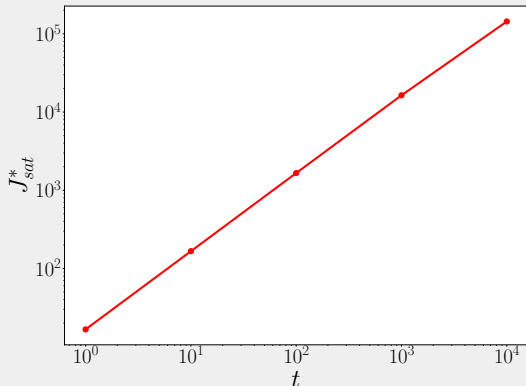
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$D^* \longrightarrow$ emergent window

$$\omega_{(j)} > \frac{D_j}{2}$$

$J^* \rightarrow \infty$ in thermodynamic limit



ZERO-BANDWIDTH LIMIT OF FIXED POINT HAMILTONIAN

Route to the zero-bandwidth model

At strong-coupling fixed point,

- kinetic energy acts as a perturbation
- **compress the bandwidth to just the Fermi surface**

$$H_{\text{zero bw}}^* = J \vec{S}_d \cdot \vec{S}_{<} + (\epsilon_F - \mu) \hat{n}_{k_F} \quad (\text{center of motion})$$

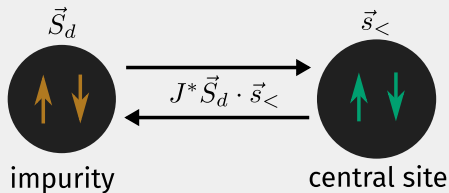
- Setting $\mu = \epsilon_F$ gives a **two-spin Heisenberg model**

$$H_{\text{zero}}^* = J^* \vec{S}_d \cdot \vec{S}_{<}$$

ZERO-BANDWIDTH LIMIT OF FIXED POINT HAMILTONIAN

Effective two-site problem

$$H_{\text{zero}}^* = J^* \vec{S}_d \cdot \vec{s}_{<} + H_{\text{IOMS}}^*$$



Singlet ground state: $|\Psi\rangle_{\text{gs}} = \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) \otimes_{j=j^*}^N |n_j\rangle$

ZERO-BANDWIDTH LIMIT OF FIXED POINT HAMILTONIAN

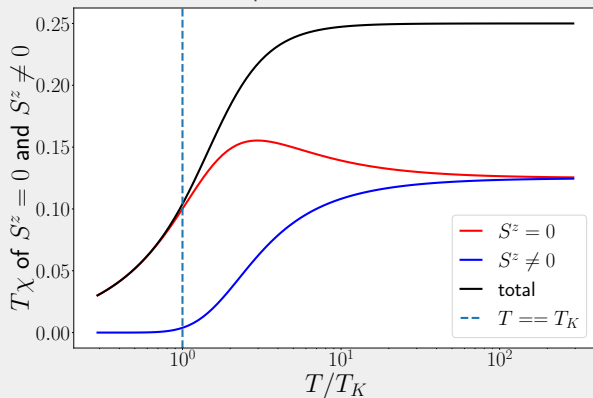
Impurity magnetic susceptibility

$$H_{\text{zero}}^*(B) = J^* \vec{S}_d \cdot \vec{S}_< + B S_d^z$$

$$\chi = \lim_{B \rightarrow 0} \frac{d}{dB} \left(\frac{k_B T}{Z(B)} \frac{dZ(B)}{dB} \right)$$

$$\chi = \frac{\frac{\beta}{4} + \frac{1}{2J^*} e^{\beta \frac{J^*}{2}} \sinh(\frac{\beta}{2} J^*)}{1 + e^{\beta \frac{J^*}{2}} \cosh(\frac{\beta}{2} J^*)}$$

$\chi \times T(T \rightarrow \infty) = \frac{1}{4}$, **Curie paramagnetism**



Wilson 1975; Andrei, Furuya, and Lowenstein 1983b; Wiegmann 1981.

ZERO-BANDWIDTH LIMIT OF FIXED POINT HAMILTONIAN

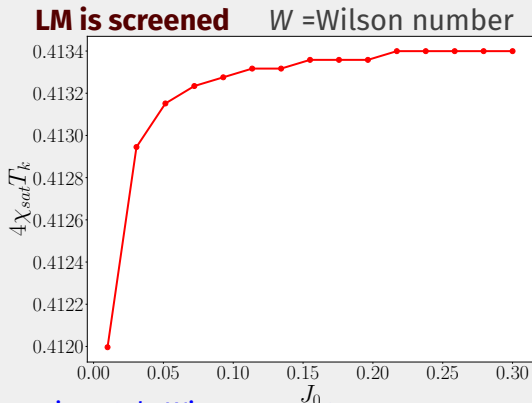
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$$\chi(T \rightarrow 0) = \frac{1}{2J^*}, \quad 4T_K \chi(T \rightarrow 0) = W \sim 0.413$$



Wilson 1975; Andrei, Furuya, and Lowenstein 1983b; Wiegmann 1981.

ZERO-BANDWIDTH LIMIT OF FIXED POINT HAMILTONIAN

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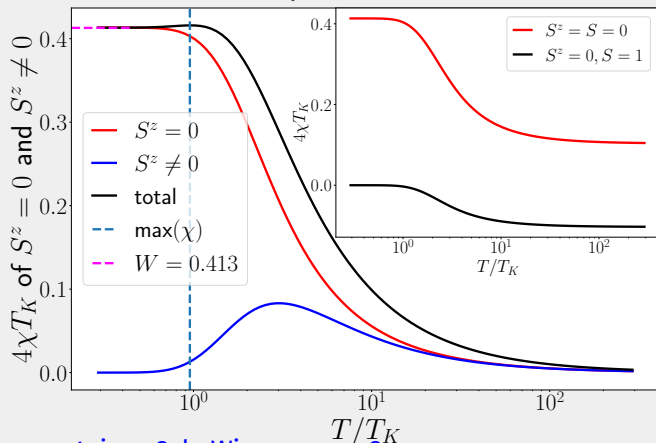
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Maximum in χ at T_K

Contribution from polarised states vanish



Wilson 1975; Andrei, Furuya, and Lowenstein 1983b; Wiegmann 1981.

EFFECTIVE HAMILTONIAN FOR THE KONDO CLOUD

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- Restore the kinetic energy part:

$$H^* = \sum_{k < k^*, \sigma} \epsilon_k \hat{n}_{k\sigma} + J^* \vec{S}_d \cdot \vec{S}_< = \underbrace{\sum_{k < k^*, \sigma} \epsilon_k \hat{n}_{k\sigma} + J^* S_d^z S_{<}^z}_{H_D} + \underbrace{J^* S_d^+ S_{<}^- + \text{h.c.}}_{V + V^\dagger}$$

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- Freeze impurity dynamics by integrating out V :

$$H_{\text{eff}} = H_D + V \frac{1}{E_{\text{gs}} - H_D} V^\dagger + V^\dagger \frac{1}{E_{\text{gs}} - H_D} V$$



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- Resolve k -space part by expanding denominator in ϵ_k/E_{gs} :

$$V \frac{1}{E_{\text{gs}} - H_D} V^\dagger = V \left(\frac{1}{E_{\text{gs}}} + \frac{H_D}{E_{\text{gs}}^2} + \dots \right)$$



Form of Kondo cloud Hamiltonian

$$H_{\text{eff}} = 2H_{\text{O}}^* + \frac{2}{J^*} H_{\text{O}}^{*2} + \sum_{1234} V_{1234} c_{k_4\uparrow}^\dagger c_{k_3\downarrow}^\dagger c_{k_2\downarrow} c_{k_1\uparrow}$$

$$V_{1234} = (\epsilon_{k_1} - \epsilon_{k_3}) \left[1 - \frac{2}{J^*} (\epsilon_{k_3} - \epsilon_{k_1} + \epsilon_{k_2} + \epsilon_{k_4}) \right]$$

- Mixture of **Fermi liquid** and **two-particle off-diagonal scattering term**
- Fermi liquid part: **result of Ising scattering**
- 2P off-diagonal term: **Non-Fermi liquid** in character - **result of spin-flip scattering**
- NFL part **leads to screening** and formation of singlet

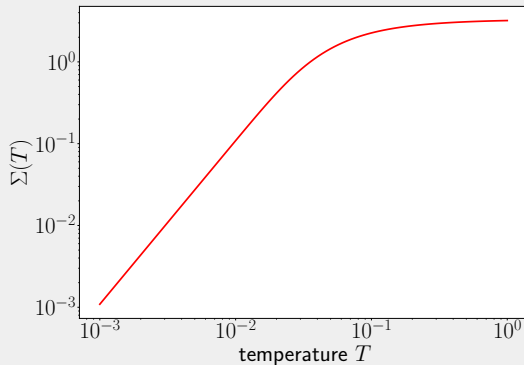
EFFECTIVE HAMILTONIAN FOR THE KONDO CLOUD

Impurity specific heat

- Fermi-liquid part renormalises one-particle **self-energy**

$$\bar{\epsilon}_k = \epsilon_k + \Sigma_k$$

$$\Sigma_k = \sum_{k'\sigma'} \frac{\epsilon_{k'} \epsilon_k}{J^*} \delta n_{k',\sigma'}$$



EFFECTIVE HAMILTONIAN FOR THE KONDO CLOUD

Impurity specific heat

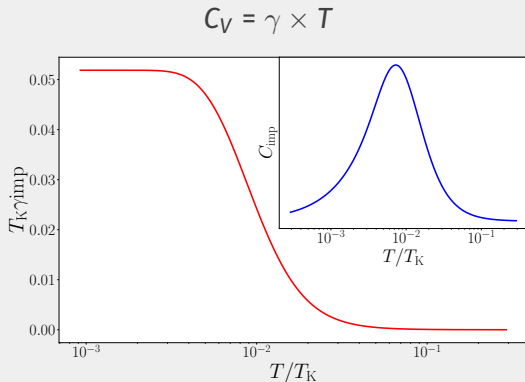
- Fermi-liquid part renormalises one-particle **self-energy**

$$\bar{\epsilon}_k = \epsilon_k + \Sigma_k$$

$$\Sigma_k = \sum_{k'\sigma'} \frac{\epsilon_{k'} \epsilon_k}{J^*} \delta n_{k',\sigma'}$$

- Compute renormalisation in C_V :

$$C_{\text{imp}} = \sum_{k,\sigma} \frac{1}{T^2} \left[\frac{(\bar{\epsilon}_k)^2 e^{\beta \bar{\epsilon}_k}}{(e^{\beta \bar{\epsilon}_k} + 1)^2} - \frac{(\epsilon_k)^2 e^{\beta \epsilon_k}}{(e^{\beta \epsilon_k} + 1)^2} \right]$$



EFFECTIVE HAMILTONIAN FOR THE KONDO CLOUD

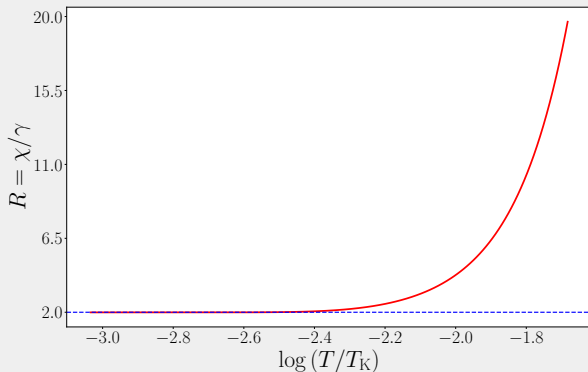
Wilson ratio

$$R = \frac{\chi}{\gamma}$$

$$\chi(T \rightarrow 0) = \frac{1}{2J^*}$$

$$\gamma(T \rightarrow 0) = \frac{1}{4J^*}$$

R saturates to 2 as $T \rightarrow 0$

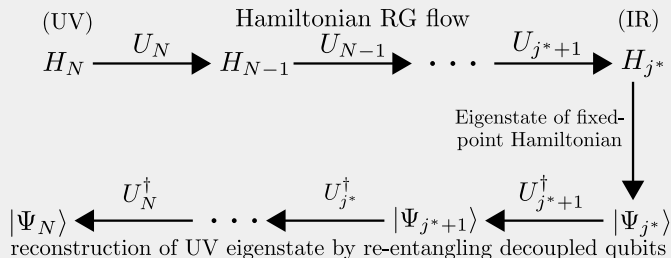


Wilson 1975; Andrei, Furuya, and Lowenstein 1983b; Wiegmann 1981.

MANY-PARTICLE ENTANGLEMENT & MANY-BODY CORRELATION

Reverse RG: What does it mean?

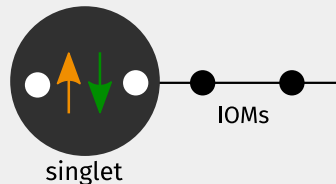
- **retrace RG flow** by applying **inverse unitary transformations** on ground state



Reverse RG: Algorithm

- Start with **minimal IR ground state**:

$$|\Psi\rangle_o = |\text{singlet}\rangle \otimes |\text{IOMs}\rangle$$



Reverse RG: Algorithm

- Start with **minimal IR ground state**:

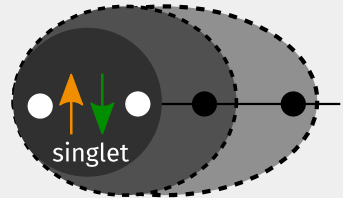
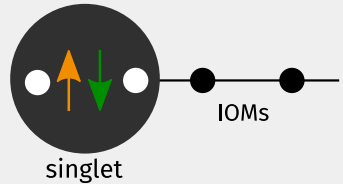
$$|\Psi\rangle_o = |\text{singlet}\rangle \otimes |\text{IOMs}\rangle$$

- Re-entangle** $|\Psi\rangle_o$ with IOMs:

$$|\Psi\rangle_1 = U_o^\dagger |\Psi\rangle_o$$

$$U_{q\sigma}^{-1} = \frac{1}{\sqrt{2}} \left[1 - \frac{J^2}{2} \frac{1}{2\omega_{Tq\sigma} - \epsilon_{qTq\sigma} - JS^Z S_q^Z} (\hat{O} + \hat{O}^\dagger) \right]$$

$$\hat{O} = \sum_{k < \Lambda^*} \sum_{\alpha=\uparrow,\downarrow} \sum_{a=x,y,z} S^a \sigma_{\alpha\sigma}^a c_{k\alpha}^\dagger c_{q\sigma}$$



Entanglement and Correlation along RG Flow

Mutual Information

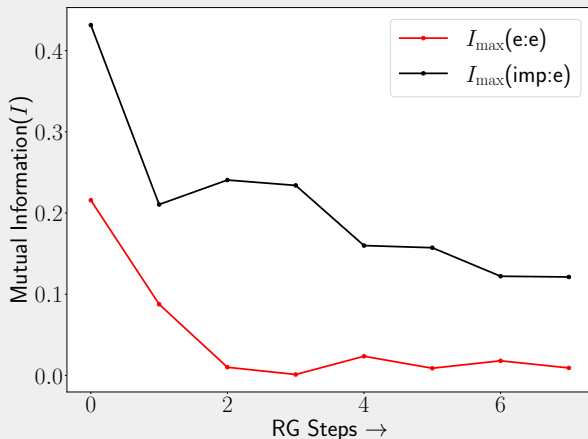
$$I(i : j) = S_i + S_j - S_{ij}$$

$$S_i = \text{Tr}(\rho_i \ln \rho_i), S_{ij} = \text{Tr}(\rho_{ij} \ln \rho_{ij})$$

■ MI between imp. and a k -state

■ MI between k -states

Both increase towards IR

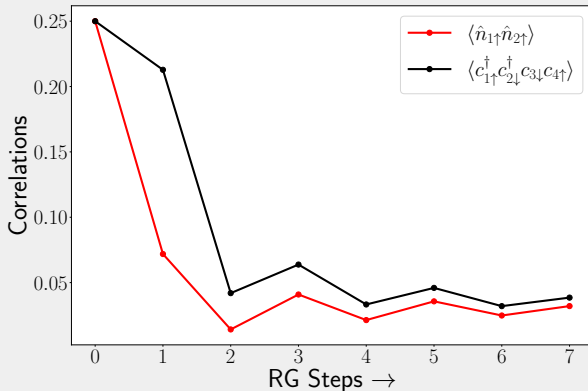


Entanglement and Correlation along RG Flow

Correlations

- Diagonal correlation $\langle \hat{n}_{1\uparrow} \hat{n}_{2\uparrow} \rangle$
- 2-particle off-diagonal correlation $\langle c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger c_{3\downarrow} c_{1\uparrow} \rangle$

Both increase towards IR



DISCUSSIONS & CONCLUSIONS

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DISCUSSIONS & CONCLUSIONS

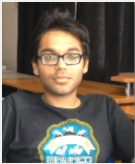
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- Consistent with **growth of entanglement and off-diagonal correlation near strong-coupling**

DISCUSSIONS & CONCLUSIONS

- **Zero-bandwidth model explains the singlet** state and magnetic susceptibility - acts as a zeroth-level Hamiltonian for studying excitations
- Both diagonal and off-diagonal components in Kondo cloud - off-diagonal component is **responsible for screening**
- Consistent with **growth of entanglement and off-diagonal correlation** near strong-coupling
- Possible extensions include a similar analysis for Kondo lattice models: should yield **far richer phase diagram**

That's all. Thank you!

Anirban Mukherjee thanks the CSIR, Govt. of India and IISER Kolkata for funding through a research fellowship. Abhirup Mukherjee thanks IISER Kolkata for funding through a research fellowship. AM and SL thank JNCASR, Bangalore for hospitality at the inception of this work. SL acknowledges funding from a SERB grant. NSV acknowledges funding from JNCASR and a SERB grant (EMR/2017/005398)



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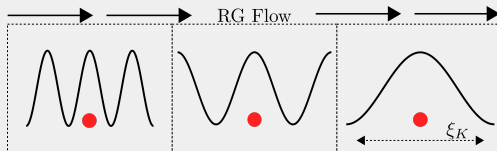
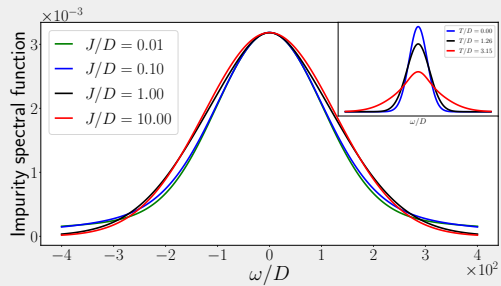
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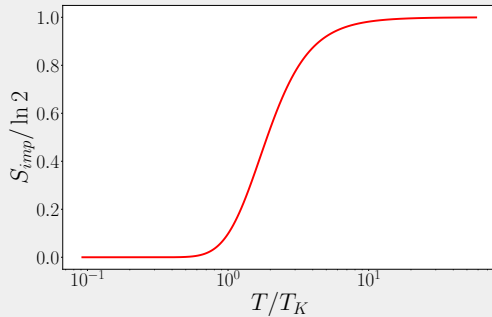
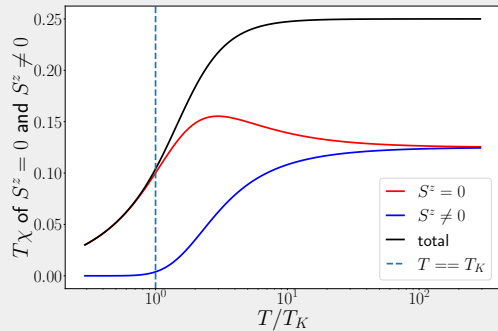
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OTHER RESULTS

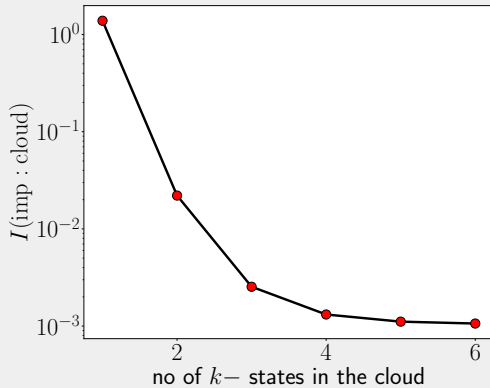
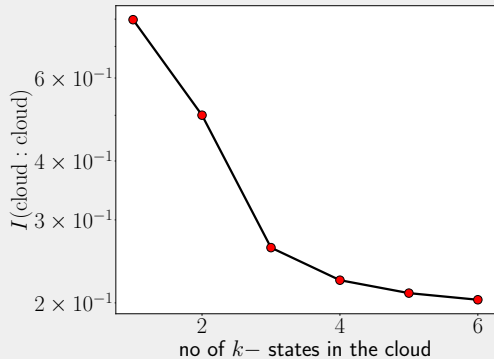
SPECTRAL FUNCTION



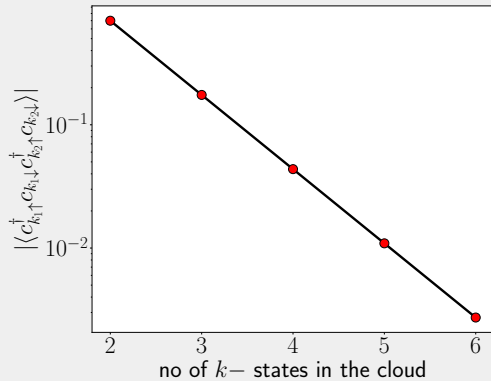
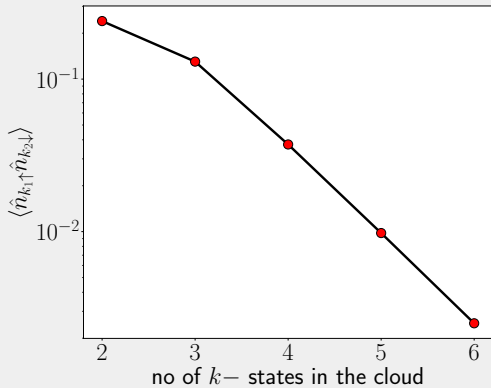
$\chi \times T$ AND THERMAL ENTROPY VIA ZERO-BANDWIDTH MODEL



MUTUAL INFORMATION (KONDO REGIME OF SIAM)



MANY-BODY CORRELATION (KONDO REGIME OF SIAM)

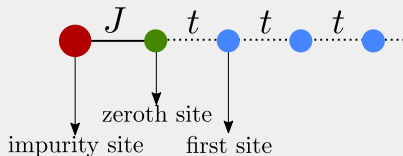


LOCAL FERMI LIQUID EXCITATIONS

Effective Hamiltonian in singlet subspace

We approximate the dispersion as a **real-space nearest neighbour hopping**:

$$H^* = J^* \vec{S}_d \cdot \vec{S}_< - t \sum_{i\sigma} \left(c_{i\sigma}^\dagger c_{i+1,\sigma} + \text{h.c.} \right)$$
$$t \ll J$$



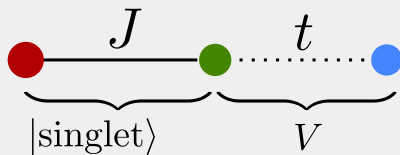
LOCAL FERMI LIQUID EXCITATIONS

Effective Hamiltonian in singlet subspace

Initially consider **just the first site**. Treat **hopping as perturbation**:

$$|\Psi\rangle_0^* = \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle)$$

$$V = -t \sum_{\sigma} (c_{0\sigma}^{\dagger} c_{1,\sigma} + \text{h.c.})$$



Effective Hamiltonian in singlet subspace

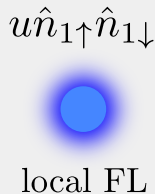
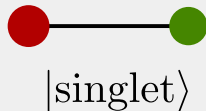
At **fourth order**, effective Hamiltonian is

$$H_{\text{eff}}^* = -\frac{16\alpha t^4}{3J^{*3}} \mathcal{P}_{\text{spin}} + \frac{32\alpha t^4}{3J^{*3}} \mathcal{P}_{\text{charge}}$$

$\mathcal{P}_{\text{spin}} \longrightarrow$ projector onto $\hat{n}_1 = 1$

$\mathcal{P}_{\text{charge}} \longrightarrow$ projector onto $\hat{n}_1 \neq 1$

- charge sector has a **repulsive term**
- so, first site harbours a local FL



LOCAL FERMI LIQUID EXCITATIONS

Effective Hamiltonian in singlet subspace

On reinstating the **rest of the sites**, the complete effective Hamiltonian is

$$H_{\text{eff}}^* = |\mathcal{C}_{\text{LFL}}| \mathcal{P}_{\text{charge}} - t \sum_{i>0, \sigma} \left(c_{i\sigma}^\dagger c_{i+1, \sigma} + \text{h.c.} \right)$$

