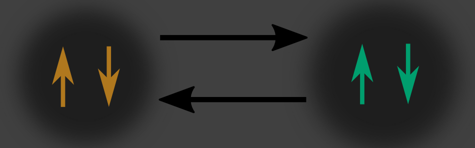
Unveiling the Kondo cloud: unitary RG study of the Kondo model



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

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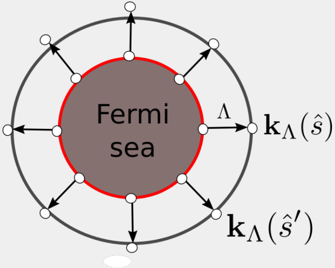
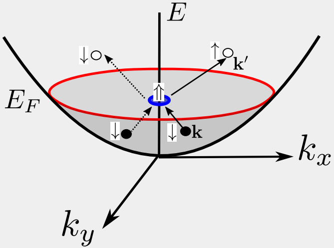
The Model

The Model

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + J\vec{S}_d \cdot \vec{s}, \qquad \vec{s} \equiv \sum_{kk',\alpha,\beta} \vec{\sigma}_{\alpha\beta} c^\dagger_{k\alpha} c_{k'\beta}$$

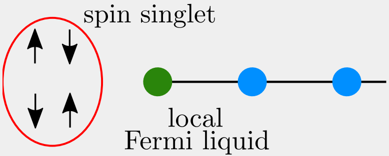


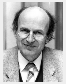


Kondo 1964; Schrieffer and Wolff 1966.

The Model

- Kondo coupling J renormalises to infinity

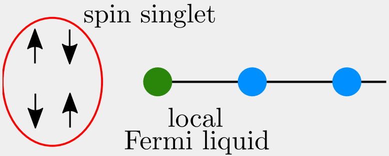


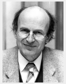


Anderson and Yuval 1969; Anderson 1970; Wilson 1975; Andrei, Furuya, and Lowenstein 1983a; Andrei, Furuya, and Lowenstein 1983b; Wiegmann 1981; Nozieres 1974.

The Model

- Kondo coupling J renormalises to infinity
- low energy phase of metal is local Fermi liquid





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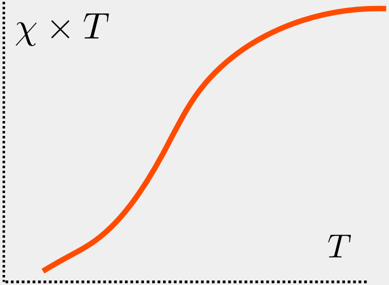



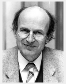

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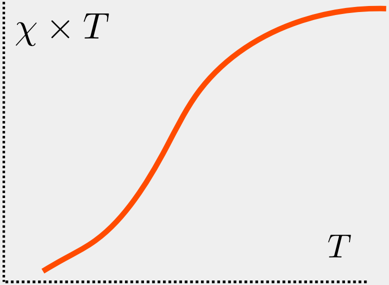
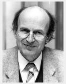
- χ constant at low temperatures, C_v linear
- thermal quantities functions of single scale T/T_K







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What's Left To Understand?

- Finite *J* effective Hamiltonian at fixed point
- Hamiltonian for the itinerant electrons forming the **macroscopic singlet**
- 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

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

Mukherjee and Lal 2020a; Mukherjee and Lal 2020b.

The General Idea

- Apply unitary many-body transformations to the Hamiltonian
- Successively decouple high energy states

$$H_j \xrightarrow{U_j} H_{j-1}$$

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The Unitary Renormalization Group Method

The General Idea

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

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

Mukherjee and Lal 2020a; Mukherjee and Lal 2020b.

Select a UV-IR Scheme

UV shell

$\vec{k}_N$ (zeroth RG step)

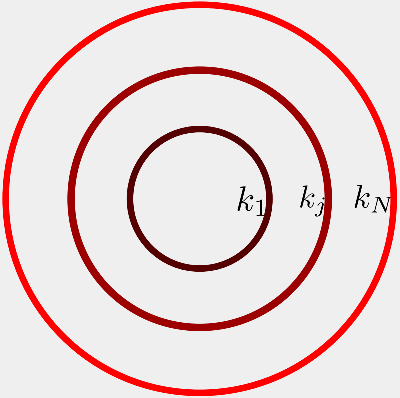
$\vdots$

$\vec{k}_j$ $\left(j^{\text{th}}\text{ RG step}\right)$

$\vdots$

$\vec{k}_1$ (Fermi surface)

IR shell

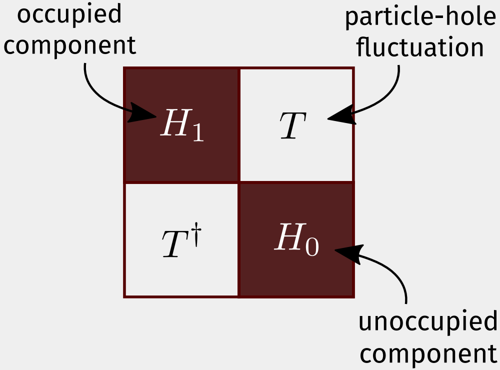


Mukherjee and Lal 2020a; Mukherjee and Lal 2020b.

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

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

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



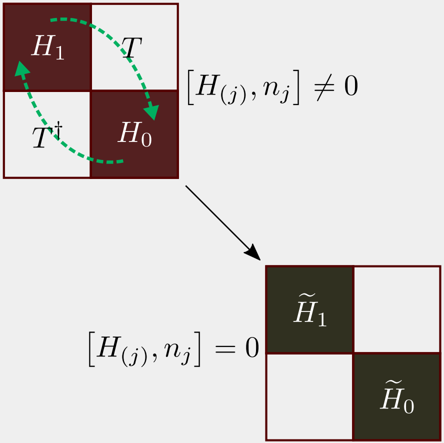
Mukherjee and Lal 2020a; Mukherjee and Lal 2020b.

Rotate Hamiltonian and kill off-diagonal blocks

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

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

$$\left.\eta^{\dagger}_{(j)} = \frac{1}{\hat{\omega}_{(j)} - H_D} c^{\dagger}_j T \right\} \rightarrow \text{many-particle rotation}$$

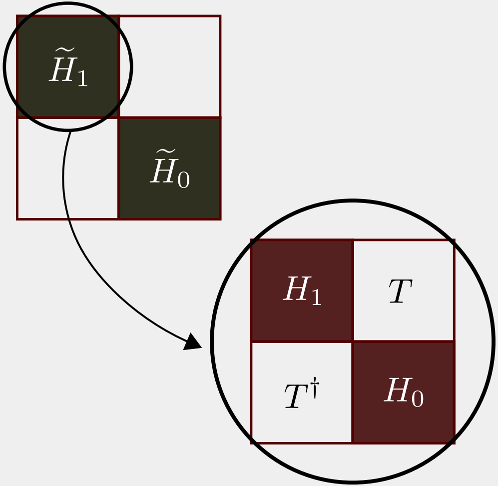


Mukherjee and Lal 2020a; Mukherjee and Lal 2020b.

Repeat with renormalised Hamiltonian

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

$$\widetilde{H}_1 = H_1 \hat{n}_{j-1} + H_0 \left(1 - \hat{n}_{j-1}\right) + c^\dagger_{j-1} T + T^\dagger c_{j-1}$$



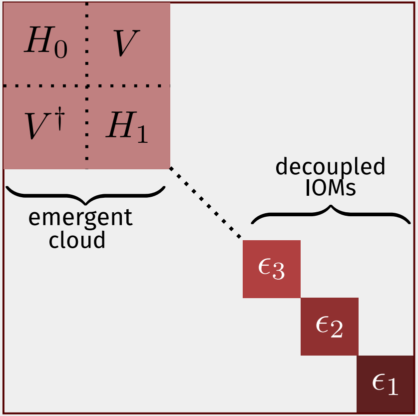
Mukherjee and Lal 2020a; Mukherjee and Lal 2020b.

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



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Novel Features of the Method

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

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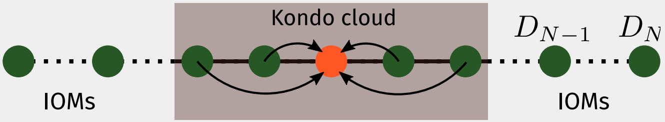
URG of the Kondo Model

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:

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

Anderson 1970; Sørensen and Affleck 1996.

RG flows and fixed points

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

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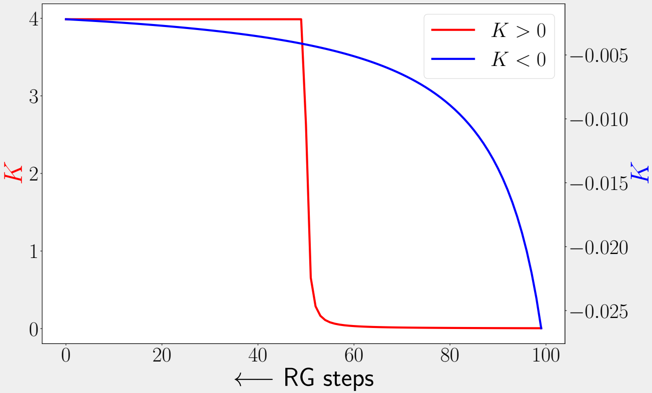

URG of the Kondo Model

Phase diagram

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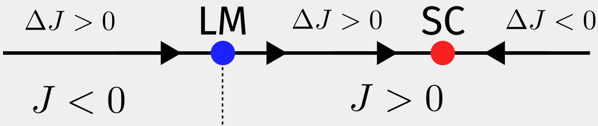

- Decay towards FM fixed point for $J < 0$
- Attractive flow towards AFM fixed point for $J > 0$

Kondo cloud length ξ_K

$$T_K = \frac{\hbar v_F \Lambda_0}{k_B} \exp\left(\frac{1}{2n(0)} - \frac{1}{n(0)K_0} - \frac{K_0}{n(0)16}\right), \quad \xi_K = \frac{h v_F}{k_B \xi_K}$$

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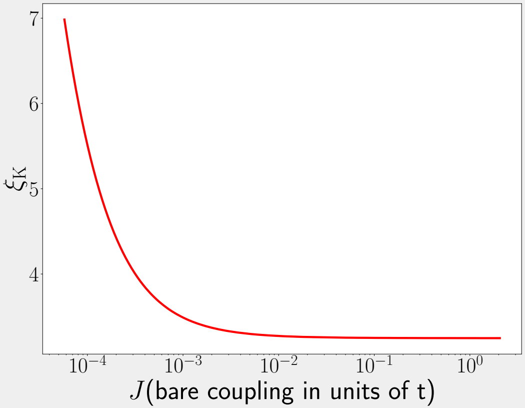

Fixed point Hamiltonian

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

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

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

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

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

$$s^z_q = \frac{1}{2}\left(\hat{n}_{q\uparrow} - \hat{n}_{q\downarrow}\right)$$

Wilson 1975.

Approach towards the continuum

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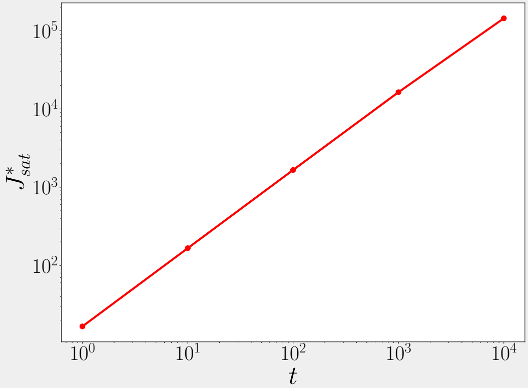
$J^* \to \infty$ in thermodynamic limit



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**

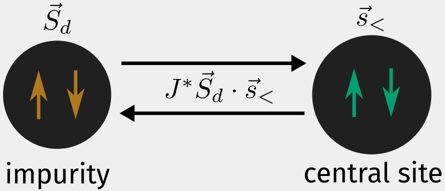
$$H^*_{\text{zero bw}} = J\vec{S}_d \cdot \vec{s}_< + (\epsilon_F - \mu)\,\hat{n}_{k_F} \quad \text{(center of motion)}$$

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

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

Effective two-site problem

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



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

Goldhaber-Gordon et al. 1998.

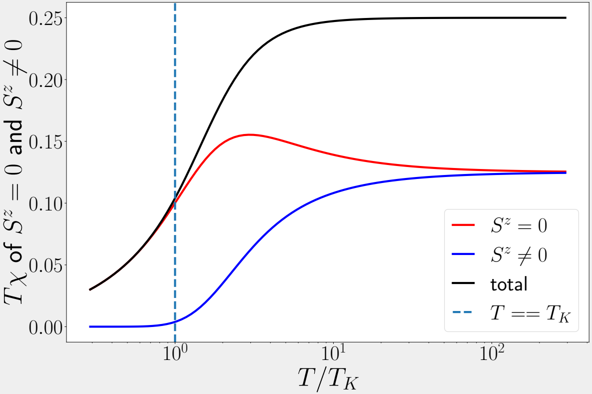
Impurity magnetic susceptibility

$$H^*_{\text{zero}}(B) = J^* \vec{S}_d \cdot \vec{s}_< + B S^z_d$$

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

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

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



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

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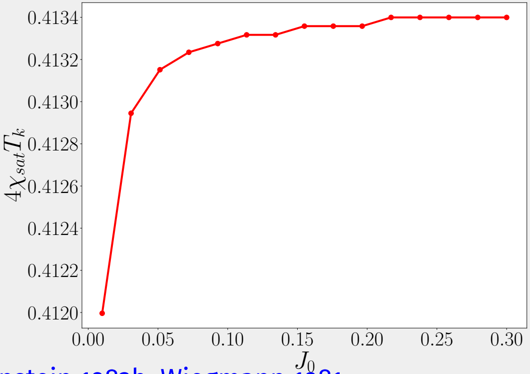
$$\chi(T\to 0) = \frac{1}{2J^*}, \quad 4T_K\chi(T\to 0) = W \sim 0.413$$

LM is screened W =Wilson number



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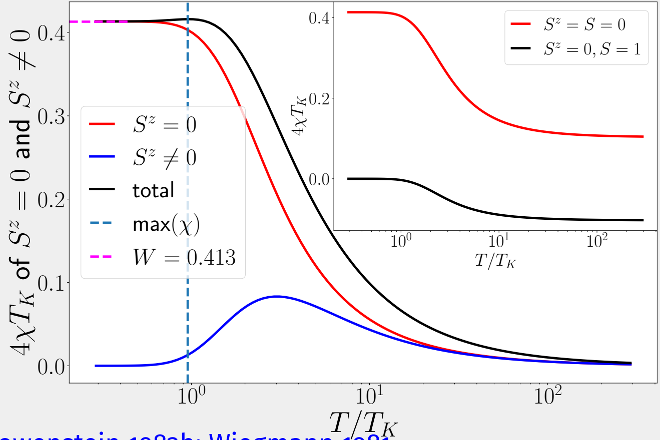
Maximum in χ at T_K

Contribution from polarised states vanish



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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:

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

Hewson 1993.

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- Resolve $k-$space part by expanding denominator in $\epsilon_k / E_{\text{gs}}$:

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

Hewson 1993.

Effective Hamiltonian for the Kondo Cloud

Form of Kondo cloud Hamiltonian

$$H_{\text{eff}} = 2H_0^* + \frac{2}{J^*}H_0^{*2} + \sum_{1234} V_{1234} c^\dagger_{k_4\uparrow} c^\dagger_{k_3\downarrow} c_{k_2\downarrow} c_{k_1\uparrow}$$

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

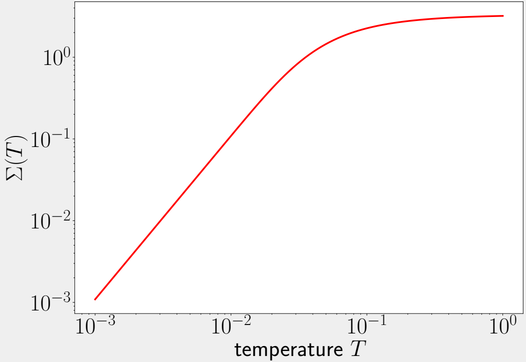
- Mixture of **Fermi liquid** and **two-particle off-diagonal scattering term**
- Fermi liquid part: **result of Ising scattering**
- 2P off-diagonal term: **Non-Fermi liquid** in character - **result of spin-flip scattering**
- NFL part **leads to screening** and formation of singlet

Impurity specific heat

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

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

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



Impurity specific heat

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

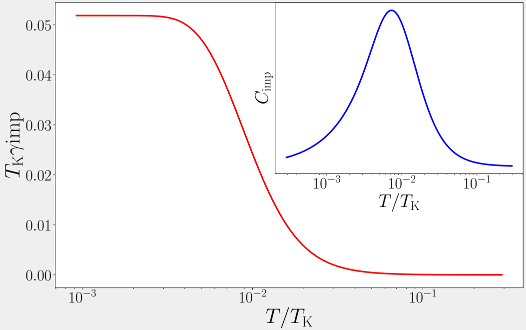
$$\bar{\epsilon}_k = \epsilon_k + \Sigma_k$$

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

- Compute renormalisation in C_V:

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

$$C_V = \gamma \times T$$



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

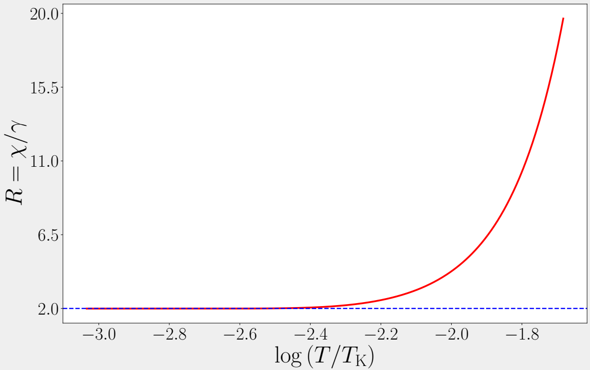
Wilson ratio

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

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

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

R saturates to 2 as $T \to 0$



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

(UV) Hamiltonian RG flow (IR)

$$\begin{tikzcd}
H_N \arrow[r, "U_N"] & H_{N-1} \arrow[r, "U_{N-1}"] & \cdots \arrow[r, "U_{j^*+1}"] & H_{j^*} \arrow[d, "\text{Eigenstate of fixed-point Hamiltonian}"'] \\
|\Psi_N\rangle & \cdots \arrow[l, "U_N^\dagger"'] & |\Psi_{j^*+1}\rangle \arrow[l, "U_{j^*}^\dagger"'] & |\Psi_{j^*}\rangle \arrow[l, "U_{j^*+1}^\dagger"']
\end{tikzcd}$$

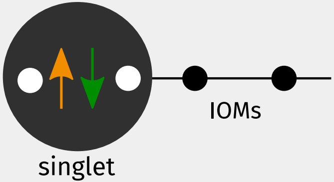
reconstruction of UV eigenstate by re-entangling decoupled qubits

Patra and Lal 2021; Anirban Mukherjee and Lal 2021.

Reverse RG: Algorithm

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

$$|\Psi\rangle_0 = |\text{singlet}\rangle \otimes |\text{IOMs}\rangle$$

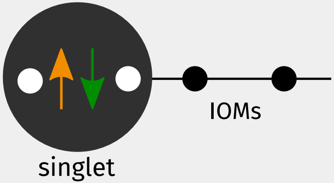


Patra and Lal 2021; Anirban Mukherjee and Lal 2021.

Reverse RG: Algorithm

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

$$|\Psi\rangle_0 = |\text{singlet}\rangle \otimes |\text{IOMs}\rangle$$

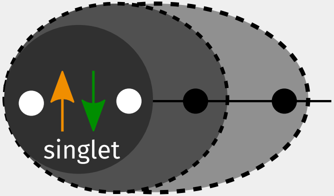


- **Re-entangle** $|\Psi\rangle_0$ with IOMs:

$$|\Psi\rangle_1 = U_0^\dagger |\Psi\rangle_0$$

$$U_{q\sigma}^{-1} = \frac{1}{\sqrt{2}}\left[1 - \frac{J^2}{2}\frac{1}{2\omega\tau_{q\sigma} - \epsilon_q\tau_{q\sigma} - JS^z s_q^z}\left(\hat{O} + \hat{O}^\dagger\right)\right]$$

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



Patra and Lal 2021; Anirban Mukherjee and Lal 2021.

Entanglement and Correlation along RG Flow

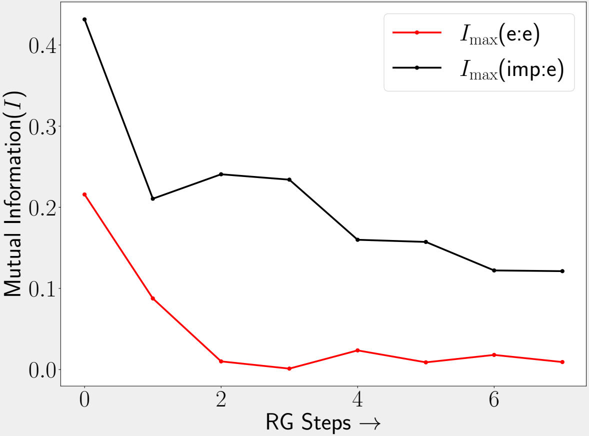
Mutual Information

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

$$S_i = \mathrm{Tr}\left(\rho_i \ln \rho_i\right), S_{ij} = \mathrm{Tr}\left(\rho_{ij} \ln \rho_{ij}\right)$$

- MI between imp. and a k-state
- MI between k-states

Both increase towards IR

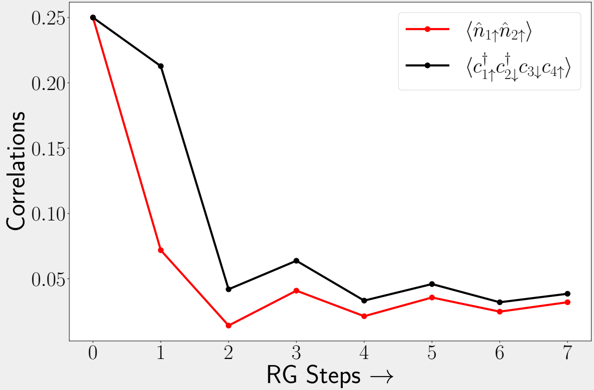


Entanglement and Correlation along RG Flow

Correlations

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

Both increase towards IR



Discussions & Conclusions

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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!

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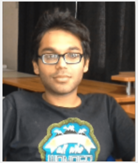



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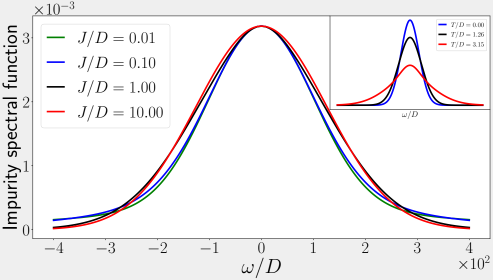
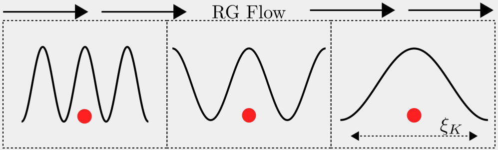
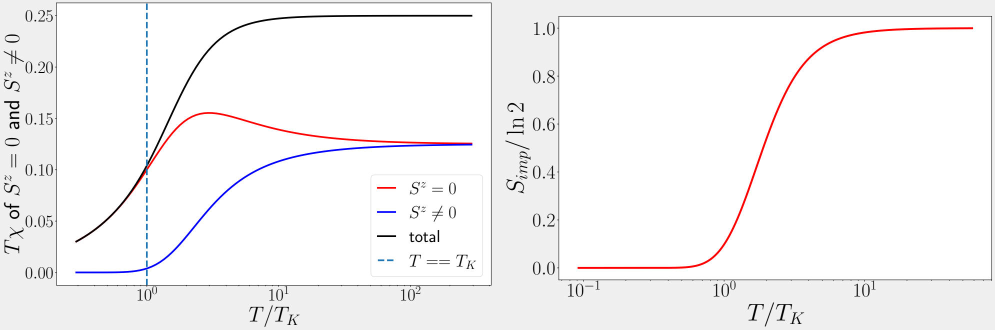
Spectral function

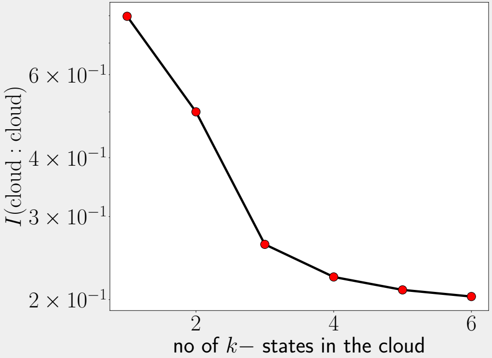


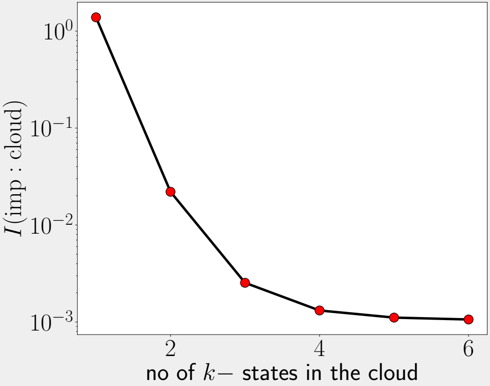


$\chi \times T$ and thermal entropy via zero-bandwidth model



Mutual Information





Many-body correlation