

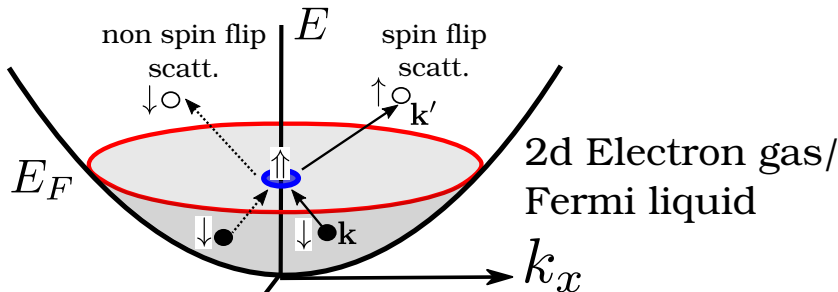
# Entanglement properties in the Kondo Model

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# Kondo Model



Kondo coupling

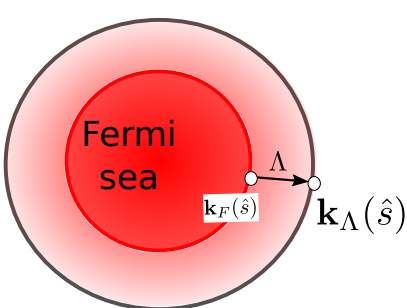
$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} \hat{n}_{\mathbf{k}\sigma} + \frac{J}{2} \sum_{\mathbf{k}\mathbf{k}'} \mathbf{S} \cdot c_{\mathbf{k}\alpha} \boldsymbol{\sigma}_{\alpha\beta} c_{\mathbf{k}'\beta}$$

# Motivation for the work

In the antiferromagnetic side a Kondo cloud is formed via the entanglement between the impurity spin and conduction electrons. On the otherhand in the ferromagnetic side the impurity spin disentangles from the conduction electrons.

- How does electronic correlation in the Fermi surface neighbourhood of the impurity spin and fermion exchange signs interplay in shaping the entanglement properties of the Kondo model?
- How does the around the impurity entanglement physics differ across the critical point? Can we understand the distinction on the basis of entanglement based witness and green function based measures?

# Unitary RG Algorithm



$$\mathbf{k}_\Lambda(\hat{s}) = \mathbf{k}_F(\hat{s}) + \Lambda \hat{s}$$



1. Effective H's are generated from UV to IR.

2. At each step a shell in UV at distance  $\Lambda$  is disentangled by the unitary map  $U$ .

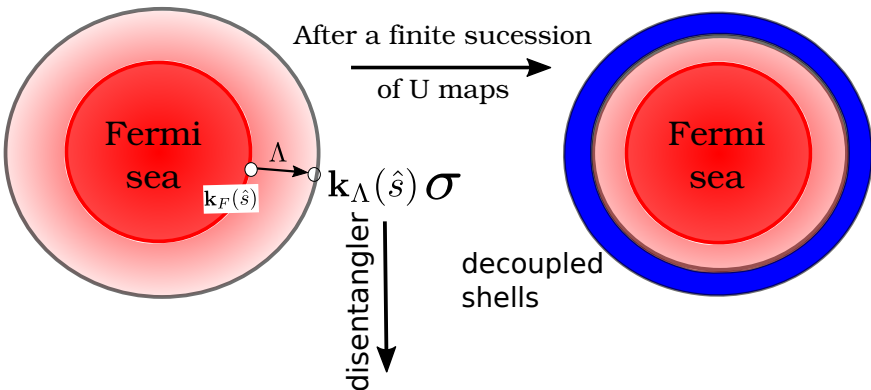
$$\hat{H}$$

$$H' = U_1 H U_1^\dagger, [H', \hat{n}_1] = 0$$

$$H \rightarrow H', \hat{n}_1 \rightarrow \hat{n}_2, U_1 \rightarrow U_2$$

RG algorithm

# Unitary RG Algorithm



$$U_\Lambda = \prod_{\hat{s}, \sigma} U_{\Lambda, \hat{s}, \sigma}$$

This disentangles all electronic states  $|\mathbf{k}_{\Lambda \hat{s} \sigma}\rangle$  on shell  $\Lambda$

# Hamiltonian RG flow equation

Hamiltonian flow  $H_{(j)} \xrightarrow{U_{(j)}} H_{(j-1)}$

Structure of the unitary disentangler  $U_{(j)} = \prod_{j,l} U_{j,l}$  disentangles electronic state

$$U_{j,l} = \frac{1}{\sqrt{2}} \left[ 1 + \eta_{j,l} - \eta_{j,l}^\dagger \right]$$
$$= \exp \frac{\pi}{4} (\eta_{j,l} - \eta_{j,l}^\dagger)$$

$|\mathbf{k}_{\Lambda_j}(\hat{s}), \sigma\rangle = |j, l\rangle$   
where  $l = \hat{s}, \sigma$

$$\{\eta_{j,l}, \eta_{j,l}^\dagger\} = 1, [\eta_{j,l}, \eta_{j,l}^\dagger] = 1 - 2\hat{n}_{j,l} \quad \text{algebra of the operators}$$

$\eta_{j,l}$ : many body electron-hole transition operator

# Hamiltonian RG flow equation

Definition of electron-hole transition operator

$$\eta_{j,l} = Tr(c_{j,l}^\dagger H_{j,l}) c_{j,l} \frac{1}{\hat{\omega}_{j,l} - Tr_{j,l}(H_{j,l}^D \hat{n}_{j,l}) \hat{n}_{j,l}}$$

off-diagonal scattering operation between e-h configuration

Quantum fluctuation operator

diag. part of H

$$\hat{\omega}_{j,l} = \boxed{H_{j,l}^D} + \boxed{H_{j,l}^X - H_{j,l-1}^X}$$

renormalized off diag. part of H

$$H_{j,l}^D = \sum_{\Lambda \hat{s}, \sigma} \epsilon_{\mathbf{k}_{\Lambda \hat{s}}}^{j,l} \hat{n}_{\mathbf{k}_{\Lambda \hat{s}}, \sigma} + \sum_{\alpha} \Gamma_{\alpha}^{4, (j,l)} \hat{n}_{\mathbf{k} \sigma} \hat{n}_{\mathbf{k}' \sigma'} + \dots$$

Number diagonal Hamiltonian composed of  
1-p self energy and higher order diagonal terms

# Hamiltonian RG flow equation

Definition of electron-hole transition operator

$$\eta_{j,l} = Tr(c_{j,l}^\dagger H_{j,l}) c_{j,l} \frac{1}{\hat{\omega}_{j,l} - Tr_{j,l}(H_{j,l}^D \hat{n}_{j,l}) \hat{n}_{j,l}}$$

off-diagonal scattering operation between e-h configuration

Quantum fluctuation operator

diag. part of H

$$\hat{\omega}_{j,l} = H_{j,l}^D + [H_{j,l}^X - H_{j,l-1}^X]$$

renormalized off diag. part of H

$$H_{j,l}^X = \sum_{\alpha} \Gamma_{\alpha}^2 c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}'\sigma'} + \sum_{\beta} \Gamma_{\beta}^2 c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}'\sigma'}^{\dagger} c_{\mathbf{k}'_1\sigma'_1} c_{\mathbf{k}_1\sigma_1} + \dots$$

Number off-diagonal Hamiltonian composed of 1-p scattering vertex and higher order terms.



# Hamiltonian RG flow equation

H flow eqn.

$$\Delta H_{(j)} = \sum_{l=1}^{2n_j} \{c_{j,l}^\dagger T r_{j,l}(H_{(j)} c_{j,l}), \eta_{j,l}\}$$

ignored higher order correlated tangential scattering

Kondo coupling flow

**Assumption**

$$\frac{\Delta J^{(j)}(\omega)}{\Delta \log \frac{\Lambda_j}{\Lambda_0}} = \frac{n_j (J^{(j)})^2 \left[ \left( \omega - \frac{\hbar v_F \Lambda_j}{2} \right) \right]}{\left( \omega - \frac{\hbar v_F \Lambda_j}{2} \right)^2 - \frac{(J^{(j)})^2}{16}}$$

Circular Fermi surface( at low filling in 2d TB model).

Note the nontrivial appearance of coupling J in the denominator. This is a nonperturbative effect.

# Hamiltonian RG flow equation

H flow eqn.

$$\Delta H_{(j)} = \sum_{l=1}^{2n_j} \{c_{j,l}^\dagger T r_{j,l}(H_{(j)} c_{j,l}), \eta_{j,l}\}$$

ignored higher order correlated tangential scattering

Kondo coupling flow

no. of states on F  
(n(0))

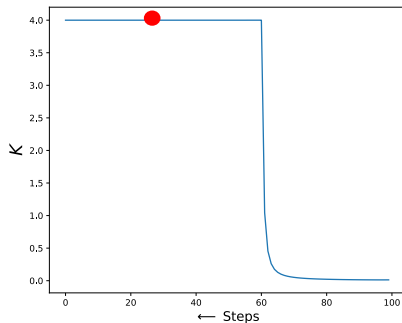
$$\frac{\Delta J^{(j)}(\omega)}{\Delta \log \frac{\Lambda_j}{\Lambda_0}} \bigg|_{\substack{\text{no. of e states} \\ \text{on the shell}}} = \frac{n_j (J^{(j)})^2 \left[ \left( \omega - \frac{\hbar v_F \Lambda_j}{2} \right) \right]}{\left( \omega - \frac{\hbar v_F \Lambda_j}{2} \right)^2 - \frac{(J^{(j)})^2}{16}} \Rightarrow \frac{dK}{d \log \frac{\Lambda}{\Lambda_0}} = \frac{n(0) K^2}{1 - \frac{K^2}{16}}$$

continuum RG  
flow eqn.

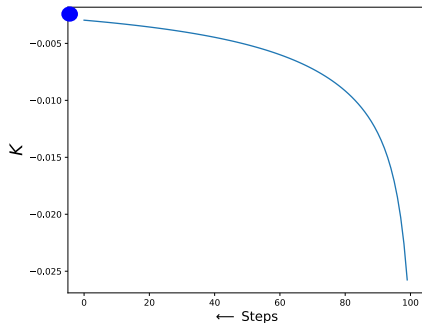
$$K^{(j)} = \frac{J^{(j)}}{\omega - \frac{\hbar v_F}{2} \Lambda_j} \text{ (dimensionless coupling)}$$

condition:  $\omega > \frac{\hbar v_F}{2} \Lambda_0$

# Coupling RG phase diagram



$J_0 > 0$

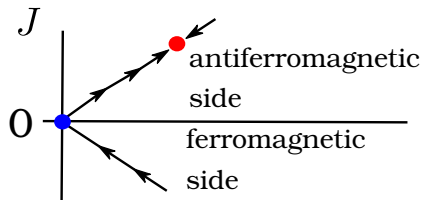


$J_0 < 0$

$$\frac{dK}{d \log \frac{\Lambda}{\Lambda_0}} = \frac{n(0)K^2}{1 - \frac{K^2}{16}} = n(0)K^2 \quad \text{for } K \ll 1,$$

● intermediate coupling fixed point

● critical fixed point



# IR fixed point theory

Low energy fixed point Hamiltonian for  $J_0 > 0$

$$H^*(\omega) = \sum_{|\Lambda| < \Lambda^*} \hbar v_F \Lambda \hat{n}_{\Lambda, \hat{s}, \sigma} + \frac{J^*(\omega)}{2} \sum_{\Lambda, \Lambda' < \Lambda^*, \hat{s} \hat{s}'} \mathbf{S} \cdot c_{\mathbf{k}_{\Lambda \hat{s}}, \alpha}^\dagger \boldsymbol{\sigma}_{\alpha \beta} c_{\mathbf{k}_{\Lambda' \hat{s}'}, \alpha}^\dagger$$

Hamiltonian containing only zero mode

$$H_0^*(\omega) = \boxed{\frac{\hbar v_F}{N(\Lambda^*)} \sum_{|\Lambda| < \Lambda^*, \hat{s}} \Lambda \sum_{\Lambda, \hat{s}} \hat{n}_{\mathbf{k}_{\Lambda \hat{s}} \sigma}} + \frac{J^*(\omega)}{2} \sum_{\Lambda, \Lambda' < \Lambda^*, \hat{s} \hat{s}'} \mathbf{S} \cdot c_{\mathbf{k}_{\Lambda \hat{s}}, \alpha}^\dagger \boldsymbol{\sigma}_{\alpha \beta} c_{\mathbf{k}_{\Lambda' \hat{s}'}, \alpha}^\dagger$$

This term is zero, due to equal and opposite energy contribution from between inside and outside of FS.

# IR fixed point theory

Low energy fixed point Hamiltonian for  $J_0 > 0$

$$H^*(\omega) = \sum_{|\Lambda| < \Lambda^*} \hbar v_F \Lambda \hat{n}_{\Lambda, \hat{s}, \sigma} + \frac{J^*(\omega)}{2} \sum_{\Lambda, \Lambda' < \Lambda^*, \hat{s} \hat{s}'} \mathbf{S} \cdot c_{\mathbf{k}_{\Lambda \hat{s}}, \alpha}^\dagger \boldsymbol{\sigma}_{\alpha \beta} c_{\mathbf{k}_{\Lambda' \hat{s}'}, \alpha}^\dagger$$

Hamiltonian containing only zero mode  $J_0 > 0$

$$H_0^*(\omega) = \boxed{\frac{\hbar v_F}{N(\Lambda^*)} \sum_{|\Lambda| < \Lambda^*, \hat{s}} \Lambda \sum_{\Lambda, \hat{s}} \hat{n}_{\mathbf{k}_{\Lambda \hat{s}} \sigma}} + \frac{J^*(\omega)}{2} \sum_{\Lambda, \Lambda' < \Lambda^*, \hat{s} \hat{s}'} \mathbf{S} \cdot c_{\mathbf{k}_{\Lambda \hat{s}}, \alpha}^\dagger \boldsymbol{\sigma}_{\alpha \beta} c_{\mathbf{k}_{\Lambda' \hat{s}'}, \alpha}^\dagger$$

- Zero mode accounts for the low energy physics near FS, and is responsible for the singlet ground state.
- The other non-zero mode are sources of excitation around the ground state.

# Singlet ground state in the AF regime

$$H_0^*(\omega) = \frac{J^*(\omega)}{2} \sum_{\Lambda, \Lambda' < \Lambda^*, \hat{s}\hat{s}'} \mathbf{S} \cdot c_{\mathbf{k}_{\Lambda\hat{s}}, \alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} c_{\mathbf{k}_{\Lambda'\hat{s}'}, \alpha}^\dagger$$

zero mode IR theory

$$|\Psi\rangle = \frac{1}{\sqrt{2}} \left[ |\uparrow\rangle \sum_{\Lambda\hat{s}} |1_{\mathbf{k}_{\Lambda\hat{s},\downarrow}}\rangle \otimes_{\Lambda' \neq \Lambda, \hat{s}' \neq \hat{s}} |\Lambda'\hat{s}', \sigma\rangle - |\downarrow\rangle \sum_{\Lambda\hat{s}} |1_{\mathbf{k}_{\Lambda\hat{s},\uparrow}}\rangle \otimes_{\Lambda' \neq \Lambda, \hat{s}' \neq \hat{s}} |\Lambda'\hat{s}', \sigma\rangle \right]$$

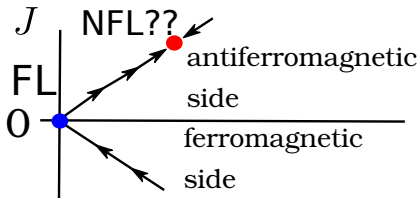
ground state wavefunction

A electronic local quantum liquid couples with the impurity spin in AF side

Note: in Ferromagnetic side the electronic state is a Fermi liquid

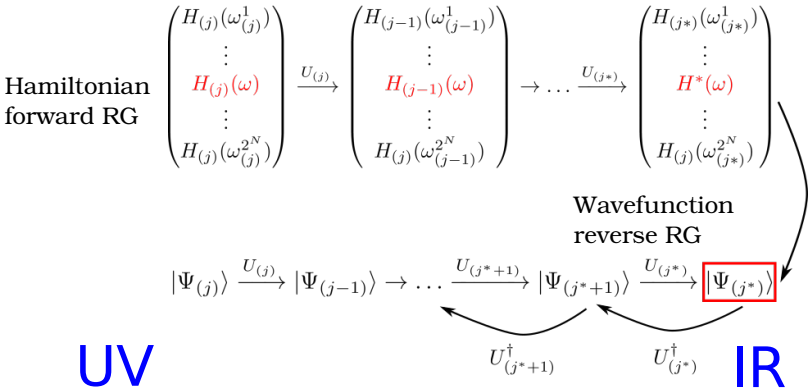
Could this be a local non Fermi Liquid?

Note: not not to be confused with Nozieres local Fermi liquid obtained by tracing out Kondo singlet



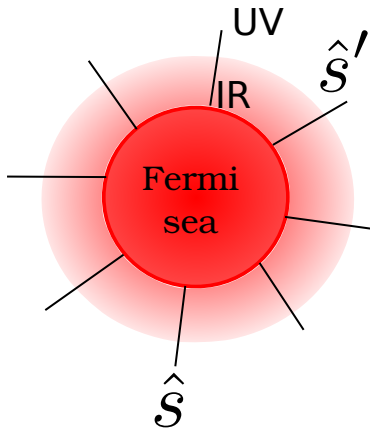
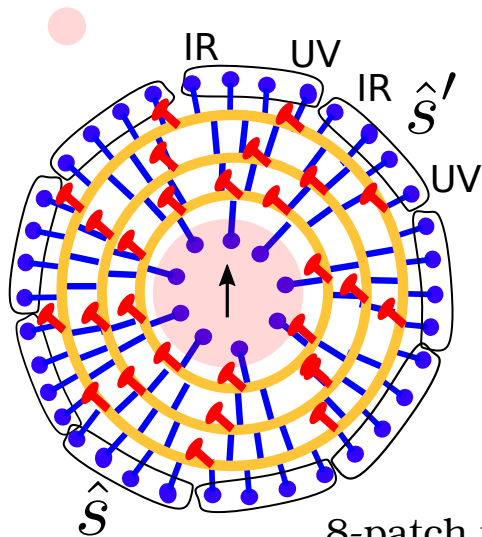
# Studying the electronic quantum liquid in AF Kondo regime

In order to study its properties we reverse the RG procedure, thus generating states at UV from IR fixed point.



# Tensor network (TN) representation of the Kondo URG program

Kondo cloud



red arrow disentangled nodes

blue dot entangled e states

8-patch model for circular FS



# Studying EQL using TN

## Properties of TN

### Green Function based

$$c_{\mathbf{k}\sigma}(\tau) = U^\dagger(\tau) c_{\mathbf{k}\sigma} U(\tau)$$

equivalent RG time evolution

$$U(\tau) = \prod_{j=N}^l U_{(j)}, \tau = \frac{1}{v_F \Lambda_l}$$

$$G(\mathbf{k}\sigma, \tau) = \langle c_{\mathbf{k}\sigma}(\tau) c_{\mathbf{k}\sigma}^\dagger(\tau) \rangle,$$

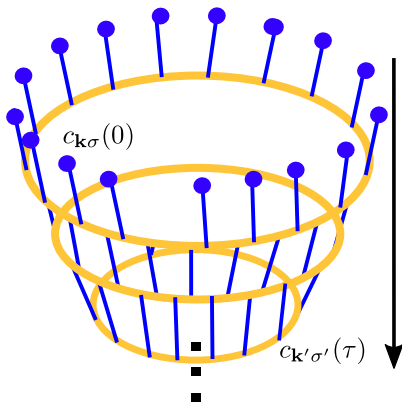
$U(\tau)$  1 electron green func.

### Entanglement based

$$S_{\mathbf{k}\sigma}(\tau) = -\text{Tr}(\rho_{\mathbf{k}\sigma}(\tau) \ln \rho_{\mathbf{k}\sigma}(\tau)),$$

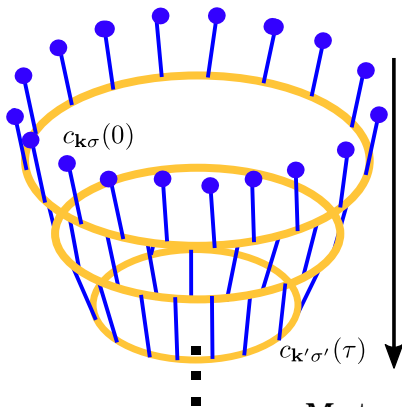
$$\rho_{\mathbf{k}\sigma} = \text{Tr}_{\bar{\mathbf{k}}\sigma}(|\Psi(\tau)\rangle \langle \Psi(\tau)|)$$

Entanglement entropy



# Studying EQL using TN

## Properties of TN



Green Function based

$$G(\mathbf{k}\sigma, \tau; \mathbf{k}'\sigma', \tau') = \langle c_{\mathbf{k}\sigma}(\tau) c_{\mathbf{k}'\sigma'}^\dagger(\tau') \rangle$$

off diagonal green function

Entanglement based

$$I(\mathbf{k}\sigma : \mathbf{k}'\sigma', \tau) = S(\rho_{\mathbf{k}\sigma}) + S(\rho_{\mathbf{k}'\sigma'}) - S(\rho_{\mathbf{k}\sigma, \mathbf{k}'\sigma'})$$

Mutual Information = entangledness between pair of electron states

$$I(\mathbf{k}\sigma : \mathbf{k}'\sigma') \geq \frac{C(\hat{O}_{\mathbf{k}\sigma}, \hat{O}_{\mathbf{k}'\sigma'})}{|\hat{O}_{\mathbf{k}\sigma}| |\hat{O}_{\mathbf{k}'\sigma'}|} \text{Hastings 2008}$$

# A dual probe for the EQL

From the organization of eigenstates in the TN from UV to IR we can obtain the complete 1e Greens function

$$G(\tau) = \begin{pmatrix} G(k\sigma) & G(k\sigma, k'\sigma') & \dots \\ G(k\sigma, k'\sigma') & G(k'\sigma') & \dots \\ \vdots & \ddots & \end{pmatrix}$$

And therefore obtain  
the Self energy matrix

$$\Sigma(\tau) = G^{-1}(\tau) - G_0^{-1}(\tau)$$

$$|\Psi(\tau)\rangle = \sum_{\phi} \lambda_{\phi} |a_{\phi}\rangle |b_{\phi}\rangle$$

From the Schmidt decomposition of the TN states we can obtain the entanglement features

# Looking forward...

1. Computing the self energy operator can allow us to compute many body properties like lifetime, spectral function, quasiparticle residue, etc.
2. What kind of experimental signatures can be proposed to measure entanglement based witnesses of Kondo cloud?
3. We can decouple the impurity spin to obtain a effective Hamiltonian for the electronic cloud.
4. Can we use the Kondo problem as a RG cluster embedding in momentum space, this can allow to treat the electronic correlation for various many body Hamiltonians?

# References

1. Coleman, Piers. Introduction to many-body physics. Cambridge University Press, 2015.
2. Mukherjee, Anirban, and Siddhartha Lal. arXiv:2004.06897 (2020).
3. Anderson, P. W. Journal of Physics C: Solid State Physics 3.12 (1970): 2436

# Thank you