Entanglement features in the Kondo Model

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Abstract

To be written...

INTRODUCTION

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. In the present work we want to study the interplay between electronic correlation in the Fermi surface neighbourhood and fermion exchange signs in shaping the entanglement between the Kondo cloud and the impurity spin. This will help in advancing our understanding of the quantum liquid composing the Kondo cloud. We will usa combination of entangled based and Green function based measures to unravel the various features of the quantum liquid.

THE MODEL

The Kondo model[1, 2] describes the coupling between a magnetic quantum impurity localized in real space with a conduction electron bath,

$$\hat{H} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} \hat{n}_{\mathbf{k}\sigma} + \frac{J}{2} \sum_{\mathbf{k},\mathbf{k}'} \mathbf{S} \cdot c^{\dagger}_{\mathbf{k}\alpha} \boldsymbol{\sigma}_{\alpha\beta} c_{\mathbf{k}'\beta} \ . \tag{1}$$

Here we consider a 2d electronic bath $\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y)$ with the Fermi energy $E_F = \mu$. J is the Kondo scattering coupling between the impurity and the conduction electrons. An important feature of the Kondo coupling is the two different classes of scattering processes, one involving spin flip $c^{\dagger}_{\mathbf{k}\uparrow} c_{\mathbf{k}'\downarrow} + h.c.$ another not involving spin flip. In the antiferromagnetic regime $J > 0$ the spin flip scattering processes generates quantum entanglement between the impurity spin and the Kondo cloud resultingly screening the impurity.

METHOD

We construct a unitary RG theory for the Kondo model, electronic states from the bath are stepwise disentangled starting with the highest energy electrons eventually scaling towards the Fermi surface. The electronic states are labelled in terms of the normal distance Λ

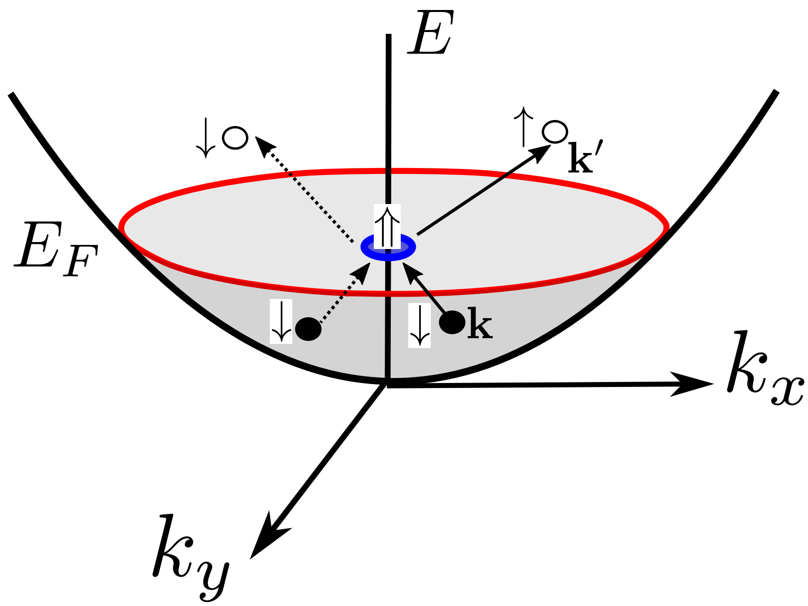

FIG. 1. The Kondo model is composed of a two dimensional conduction electron bath (Fermi liquid) coupled to a magnetic impurity via a spin flip(solid)/non spin flip(dashed) scattering coupling.

from the Fermi surface and the orientation unit vectors (Fig.2)$\hat{s}$: $\mathbf{k}_{\Lambda\hat{s}} = \mathbf{k}_F(\hat{s}) + \Lambda\hat{s}$ where $\hat{s} = \frac{\nabla\epsilon_{\mathbf{k}}}{|\nabla\epsilon_{\mathbf{k}}|}|_{\epsilon_{\mathbf{k}}=E_F}$. The states are labelled as $|j,l,\sigma\rangle = |\mathbf{k}_{\Lambda_j\hat{s}},\sigma\rangle, l := (\hat{s}_m,\sigma)$.

The Λ's are arranged as follows: $\Lambda_N > \Lambda_{N-1} > \ldots > 0$, where the electronic states farthest from Fermi surface Λ_N is disentangled first, eventually scaling towards the Fermi surface. This leads to the Hamiltonian flow equation,

$$H_{(j-1)} = U_{(j)}H_{(j)}U^{\dagger}_{(j)}\ . \tag{2}$$

where the unitary operation $U_{(j)}$ is the unitary map. $U_{(j)}$ disentangles all the electronic states $\mathbf{k}_{\Lambda_j\hat{s}_m},\sigma$ on the isogeometric curve and has the form[3],

$$U_{(j)} = \prod_l U_{j,l}, U_{j,l} = \frac{1}{\sqrt{2}}[1+\eta_{j,l}-\eta^{\dagger}_{j,l}], \tag{3}$$

where $\eta_{j,l}$ are electron hole transition operators following the algebra,

$$\{\eta_{j,l},\eta^{\dagger}_{j,l}\} = 1, \left[\eta_{j,l},\eta^{\dagger}_{j,l}\right] = 1\ . \tag{4}$$

The transition operator in terms of the diagonal H^D and off-diagonal parts of the Hamiltonian H^X has the form,

$$\eta_{j,l} = Tr_{j,l}(c^{\dagger}_{j,l}H_{j,l})c_{j,l}\frac{1}{\hat{\omega}_{j,l} - Tr_{j,l}(H^D_{j,l}\hat{n}_{j,l})\hat{n}_{j,l}}. \tag{5}$$

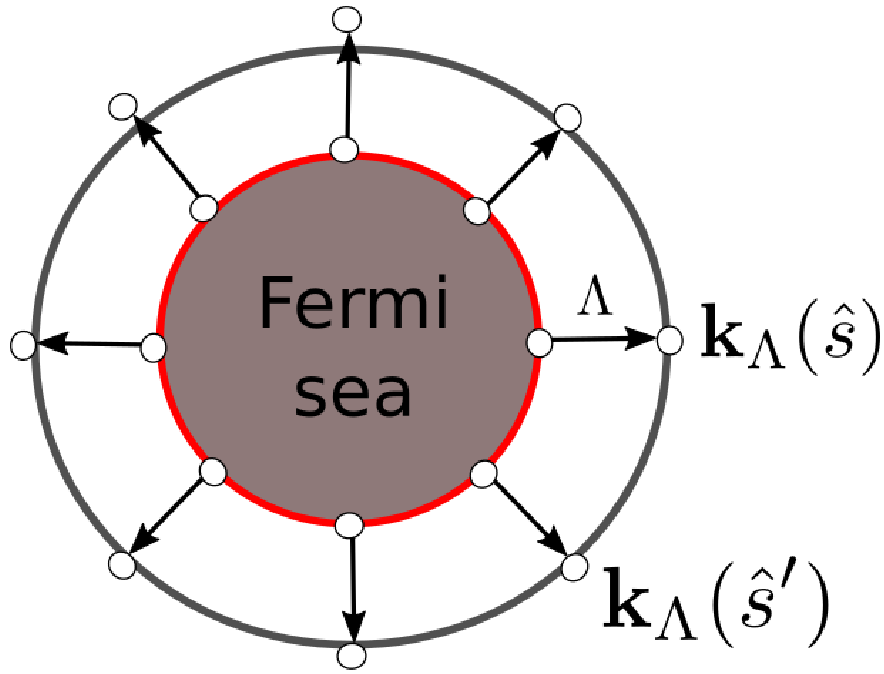

FIG. 2. Figure represents the circular Fermi sea of the conduction electron bath. Here the arrows represents the different normal directions of the FS(red circle). Thw white circles are electronic states on the curves isogeometric to FS.

In the numerator the operator $Tr_{j,l}(c^\dagger_{j,l}H_{j,l})c_{j,l} + h.c.$ is composed of all possible scattering vertices that modify the configuration of the electronic state $|j,l\rangle$. The generic forms of $H^D_{j,l}$, $H^X_{j,l}$ are as follows,

$$\begin{aligned} H^D_{j,l} &= \sum_{\Lambda\hat{s},\sigma} \epsilon^{j,l}\hat{n}_{\mathbf{k}_{\Lambda\hat{s}},\sigma} + \sum_\alpha \Gamma^{4,(j,l)}_\alpha \hat{n}_{\mathbf{k}\sigma}\hat{n}_{\mathbf{k}'\sigma'} + \sum_\beta \Gamma^{8,(j,l)}_\beta \hat{n}_{\mathbf{k}\sigma}\hat{n}_{\mathbf{k}'\sigma'}(1-\hat{n}_{\mathbf{k}''\sigma''}) + \dots \\ H^X_{j,l} &= \sum_\alpha \Gamma^2_\alpha c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}'\sigma'} + \sum_\beta \Gamma^2_\beta c^\dagger_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}'\sigma'}c_{\mathbf{k}'_1\sigma'_1}c_{\mathbf{k}_1\sigma_1} + \dots \end{aligned} \tag{6}$$

The operator $\hat{\omega}_{j,l}$ accounts for the quantum fluctuation arising from the non commutivity between different parts of the renormalized Hamiltonian and has the form,[4]

$$\hat{\omega}_{j,l} = H^D_{j,l} + H^X_{j,l} - H^X_{j,l-1} \ . \tag{7}$$

Upon disentangling electronic states $\hat{s},\sigma$ along a isogeometric curve at distance Λ_j the effective Hamiltonians $H_{j,l}$ are generated,

$$H_{j,l} = \prod_{m=1}^{l} U_{j,m}H_{(j)}[\prod_{m=1}^{l} U_{j,l}]^\dagger \ . \tag{8}$$

After having disentangled all the electronic states $2n_j$ on the isogeometric curve the effective Hamiltonian $H_{j,2n_j+1} = H_{(j-1)}$ for the next RG step is obtained. Disentangling multiple qubits succesively in a given momentum shell at distance Λ_j from FS leads to renormalized contribution from one and higher particle correlated tangential scattering process. Accounting for the leading tangential scattering processes and other momentum transfer processes along normal $\hat{s}$ the renormalized Hamiltonian has the form,

$$H_{(j-1)} = Tr_{j,(1,\dots,2n_j)}(H_{(j)}) + \sum_{l=1}^{2n_j}\{c^{\dagger}_{j,l}Tr_{j,l}(H_{(j)}c_{j,l}), \eta_{j,l}\}\tau_{j,l} \ . \tag{9}$$

Here $2n_j$ are the number of electronic states on the curve at distance Λ_j.

RESULTS

The unitary RG process generates the effective Hamiltonian $\hat{H}_{(j-1)}(\omega_{(j)})$ across the various eigen directions $|\Phi(\omega_{(j)})\rangle$ of the $\hat{\omega}_{(j)}$ operator. Note the associated eigenvalue $\omega_{(j)}$ identifies a subspectrum in the interacting many body eigenspace. The form of $\hat{H}_{(j-1)}(\omega_{(j)})$ is given by,

$$\begin{aligned}\hat{H}_{(j-1)}(\omega_{(j)}) = \sum_{j,l,\sigma}\epsilon_{j,l}\hat{n}_{j,l} + \frac{J^{(j)}(\omega_{(j)})}{2}\sum_{\substack{j_1,j_2<j-1,\\ m,m'}}\mathbf{S}\cdot c^{\dagger}_{j_1,\hat{s}_m,\alpha}\boldsymbol{\sigma}_{\alpha\beta}c_{j_2,\hat{s}_{m'},\beta} \\ (1+\sum_{j'=N,l=1}^{j,2n_j}\tau_{j',l} + \sum_{j',j''=N,l}^{j}\tau_{j',l}\tau_{j'',l} + \dots) \ . \end{aligned} \tag{10}$$

The renormalization of the effective Hamiltonian within the entangled subspace $\Lambda < \Lambda_j$ can be defined as,

$$\Delta H_{(j)}(\omega_{(j)}) = Tr_{N,\dots,j}(H_{(j-1)}(\omega_{(j-1)})) - Tr_{N,\dots,j}(H_{(j)}(\omega_{(j)})) = \sum_{l=1}^{2n_j}\{c^{\dagger}_{j,l}Tr_{j,l}(H_{(j)}c_{j,l}), \eta_{j,l}\} \tag{11}$$

The Hamiltonian renormalization group generates coupling RG flow as follows,

$$\begin{aligned}
\Delta H_{(j)}(\omega) &= \sum_{\substack{m=1,\\ \beta=\uparrow/\downarrow}}^{n_j} \frac{(J^{(j)})^2\tau_{j,\hat{s}_m,\beta}}{2(2\omega\tau_{j,\hat{s}_m,\beta}-\epsilon_{j,l}\tau_{j,\hat{s}_m,\beta}-\frac{J^{(j)}}{2}S^z(\tau_{j,\hat{s}_m,\uparrow}-\tau_{j,\hat{s}_m,\downarrow}))} S^aS^b\sigma^a_{\alpha\beta}\sigma^b_{\beta\gamma}c^\dagger_{j_1,\hat{s}_m,\alpha}c_{j_2,\hat{s}_m,\gamma}\ , \\
&= \sum_{\substack{m=1,\\ \beta=\uparrow/\downarrow}}^{n_j} \frac{(J^{(j)})^2\tau_{j,\hat{s}_m,\beta}}{2(\omega\tau_{j,\hat{s}_m,\beta}-\epsilon_{j,l}\tau_{j,\hat{s}_m,\beta}-\frac{J^{(j)}}{2}S^z(\tau_{j,\hat{s}_m,\uparrow}-\tau_{j,\hat{s}_m,\downarrow}))}(\frac{3}{4}\delta_{\alpha\gamma}+S^c\sigma^c_{\alpha\gamma})c^\dagger_{j_1,\hat{s}_m,\alpha}c_{j_2,\hat{s}_m,\gamma} \\
&= \sum_{\substack{m=1,\\ \beta=\uparrow/\downarrow}}^{n_j} \frac{(J^{(j)})^2\tau_{j,\hat{s}_m,\beta}}{2(2\omega\tau_{j,\hat{s}_m,\beta}-\epsilon_{j,l}\tau_{j,\hat{s}_m,\beta}-\frac{J^{(j)}}{2}S^z(\tau_{j,\hat{s}_m,\uparrow}-\tau_{j,\hat{s}_m,\downarrow}))} \\
&\times\left(\mathbf{S}\cdot c^\dagger_{j_1,\hat{s}_m,\alpha}\boldsymbol{\sigma}_{\alpha\gamma}c_{j_2,\hat{s}_m,\gamma}+\frac{3}{4}c^\dagger_{j_1,\hat{s}_m,\alpha}c_{j_2,\hat{s}_m,\alpha}\right) \\
&= \frac{1}{2}\sum_{\substack{m=1,\\ \beta=\uparrow/\downarrow}}^{n_j} \frac{(J^{(j)})^2\left[(\frac{\omega}{2}-\frac{\epsilon_{j,l}}{4})+\frac{J^{(j)}}{2}S^z\tau_{j,\hat{s}_m,\beta}(\tau_{j,\hat{s}_m,\uparrow}-\tau_{j,\hat{s}_m,\downarrow}))\right]}{(\omega-\frac{\epsilon_{j,l}}{2})^2-\frac{\left(J^{(j)}\right)^2}{16}} \\
&\times\left(\mathbf{S}\cdot c^\dagger_{j_1,\hat{s}_m,\alpha}\boldsymbol{\sigma}_{\alpha\gamma}c_{j_2,\hat{s}_m,\gamma}+\frac{3}{4}c^\dagger_{j_1,\hat{s}_m,\alpha}c_{j_2,\hat{s}_m,\alpha}\right) \\
&= \frac{1}{2}\sum_{m=1}^{n_j} \frac{(J^{(j)})^2\left[(\omega-\frac{\epsilon_{j,l}}{2})\right]}{(\omega-\frac{\epsilon_{j,l}}{2})^2-\frac{\left(J^{(j)}\right)^2}{16}}\left(\mathbf{S}\cdot c^\dagger_{j_1,\hat{s}_m,\alpha}\boldsymbol{\sigma}_{\alpha\gamma}c_{j_2,\hat{s}_m,\gamma}+\frac{3}{4}c^\dagger_{j_1,\hat{s}_m,\alpha}c_{j_2,\hat{s}_m,\alpha}+h.c.\right)
\end{aligned} \tag{12}$$

In obtaining the above RG equation we have replaced $\hat{\omega}_{(j)} = 2\omega\tau_{j,\hat{s}_m,\beta}$. We set the electronic configuration $\tau_{j,\hat{s}_m,\uparrow} = -\tau_{j,\hat{s}_m,\downarrow} = \frac{1}{2}$ to account for the spin scattering between the Kondo impurity and the fermionic bath. The operator $\hat{\omega}_{(j)}$ (eq.(7)) for RG step j is determined by the occupation number diagonal piece of the Hamiltonian $H^D_{(j-1)}$ attained at the next RG step $j-1$, this demands a self consistents treatment of the RG equation to determine the ω. In this fashion two particle and higher order quantum fluctuations autamatically get encoded into the RG dynamics of $\hat{\omega}$. In the present work we restrict our study by ignoring the RG contribution in ω. The electron/hole configuration $(|1_{j,\hat{s}_m,\beta}\rangle/|0_{j,\hat{s}_m,\beta}\rangle)$ of the disentangled electronic state and associated with $\pm\epsilon_{j,l}$ energy is accounted by $\pm\omega$ fluctuation energy scales. To proceed further we assume a circular Fermi surface such that $\epsilon_{j,l} = \epsilon_j - E_F \approx \hbar v_F\Lambda_j$ for $0 \leq \Lambda_j \leq \Lambda_0$. This leads to the RG equation,

$$\frac{\Delta J^{(j)}(\omega)}{\Delta\log\frac{\Lambda j}{\Lambda_0}} = \frac{n_j(J^{(j)})^2\left[(\omega-\frac{\hbar v_F\Lambda_j}{2})\right]}{(\omega-\frac{\hbar v_F\Lambda_j}{2})^2-\frac{\left(J^{(j)}\right)^2}{16}} \tag{13}$$

Note the denominator $\Delta \log \frac{\Lambda j}{\Lambda_0} = 1$ for the RG scale parameterization $\Lambda_j = \Lambda_0 \exp(-j)$. We redefine Kondo coupling as a dimensionless parameter,

$$K^{(j)} = \frac{J^{(j)}}{\omega - \frac{\hbar v_F}{2}\Lambda_j} \ , \tag{14}$$

We operate in the regime $\omega > \frac{\hbar v_F}{2}\Lambda_j$. With the above parametrization eq.(14) we can convert the difference RG eq.(13) to continuum RG equation,

$$\frac{dK}{d\log\frac{\Lambda}{\Lambda_0}} = \left(1 - \frac{\omega}{\omega - \hbar v_F \Lambda}\right) K + \frac{n(\Lambda)K^2}{1 - \frac{K^2}{16}} \tag{15}$$

Upon approaching the Ferm surface $\Lambda_j \to 0$ therefore $\left(1 - \frac{\omega}{\omega - \hbar v_F \Lambda}\right) \to 0$ and $n(\Lambda)$ can be replaced by no. of states on the Fermi surface $n(0)$.

$$\frac{dK}{d\log\frac{\Lambda}{\Lambda_0}} = \frac{n(0)K^2}{1 - \frac{K^2}{16}} \tag{16}$$

We observe two important aspects of the RG equation: for $K << 1$ the RG equation

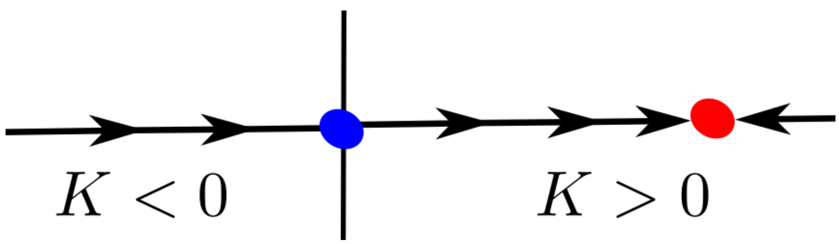

FIG. 3. Schematic RG phase diagram. Red dot represents intermediate coupling fixed point. Blue dot is the critical fixed point.

reduces to the one loop form, $\frac{dK}{d\log\frac{\Lambda}{\Lambda_0}} = K^2$[2]. On the otherhand the nonperturbative form of flow equations shows the presence of intermediate coupling fixed points $K^* = 4$ in the antiferromagnetic regime $K > 0$.

At the IR fixed point in the AF regime the effective Hamiltonian is given by,

$$H^* = \sum_{|\Lambda|<\Lambda^*} \hbar v_F \Lambda \hat{n}_{\Lambda,\hat{s},\sigma} + \frac{J^*(\omega)}{2} \sum_{\substack{j_1,j_2<j^*,\\ m,m'}} \mathbf{S}\cdot c^{\dagger}_{j_1,\hat{s}_m,\alpha} \boldsymbol{\sigma}_{\alpha\beta} c_{j_2,\hat{s}_{m'},\beta} \tag{17}$$

We can now extract a zero mode from the above Hamiltonian that captures the low energy theory near the Fermi surface,

$$\begin{aligned} H_{coll} &= \frac{1}{N}\sum_{|\Lambda|<\Lambda^*} \hbar v_F \Lambda \sum_{|\Lambda|<\Lambda^*} \hat{n}_{\Lambda,\hat{s},\sigma} + \frac{J^*(\omega)}{2} \sum_{\substack{j_1,j_2<j^*,\\ m,m'}} \mathbf{S}\cdot c^{\dagger}_{j_1,\hat{s}_m,\alpha} \boldsymbol{\sigma}_{\alpha\beta} c_{j_2,\hat{s}_{m'},\beta} \\ &= \frac{J^*(\omega)}{2} \sum_{\substack{j_1,j_2<j^*,\\ m,m'}} \mathbf{S}\cdot c^{\dagger}_{j_1,\hat{s}_m,\alpha} \boldsymbol{\sigma}_{\alpha\beta} c_{j_2,\hat{s}_{m'},\beta} \end{aligned} \tag{18}$$

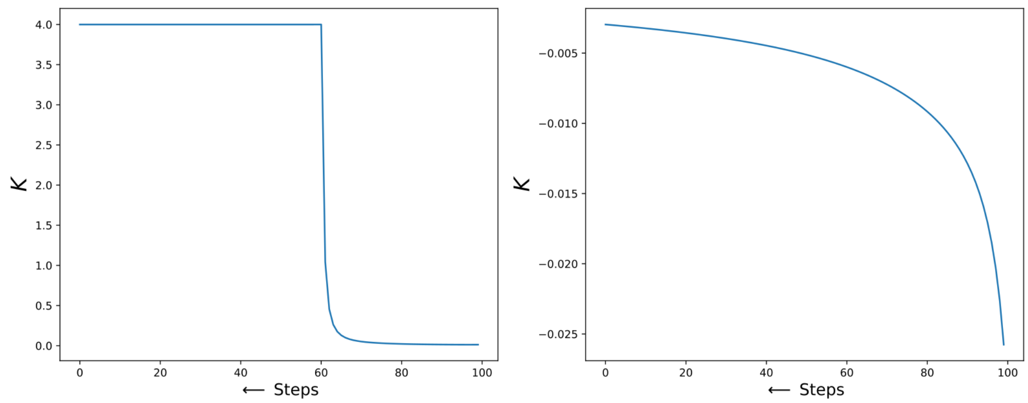

FIG. 4. Renormalized dimensionless Kondo coupling K with RG steps ($\log \Lambda_j/\Lambda_0$), left panel:$K > 0$, right panel: $K < 0$.

Indeed we observe that the zero mode Hamiltonian at the IR fixed point is responsible for the formation of the singlet ground state.

$$|\Psi*\rangle = \frac{1}{\sqrt{2}}\left[|\uparrow\rangle \sum_{\Lambda,\hat{s}} |1_{\Lambda,\hat{s},\downarrow}\rangle \otimes_{\Lambda'\neq\Lambda,\hat{s}'\neq\hat{s}} |\Lambda',\hat{s}'\rangle - |\downarrow\rangle \sum_{\Lambda,\hat{s}} |1_{\Lambda,\hat{s},\uparrow}\rangle \otimes_{\Lambda'\neq\Lambda,\hat{s}'\neq\hat{s}} |\Lambda',\hat{s}'\rangle\right] \tag{19}$$

TENSOR NETWORK REPRESENTATION OF THE KONDO URG PROGRAM

In this section we present the tensor network representation of the URG program[4, 5]. The yellow blocks represent the complete U transformation $U_{(j)}$ for a given RG step that is composed of $U_{j,l}$ here individual $U_{j,l}$ disentangles one electronic state $\mathbf{k}_{\Lambda\hat{s}},\sigma$. The wavefunction $|\Psi^*\rangle$ comprises the IR bulk of the tensor network. The yellow layers are arranged along the RG direction.

The tensor network Fig.5 is composed of yellow layers that lead to a holographic arrangement of eigenstates from UV to IR. From the singlet state obtained at RG fixed point we can perform the inverse unitary map to regenerate the entanglement with UV degrees of freedom Fig.(6). This enables udsd to obtain the complete form of the two point retarded green function along the RG flow direction (RG time)$\tau_j = 1/v_F\Lambda_j$,

$$G(\mathbf{k}\sigma,\tau;\mathbf{k}'\sigma',\tau') = \Theta(\tau-\tau')\langle\Psi_0|\{c_{\mathbf{k}\sigma}(\tau)c^\dagger_{\mathbf{k}'\sigma'}(\tau')\}|\Psi_0\rangle \tag{20}$$

where $|\Psi_0\rangle = U_N^\dagger \ldots U_{j^*}^\dagger|\Psi_{(j^*)}\rangle$ is the many body state residing at the UV boumdary of the

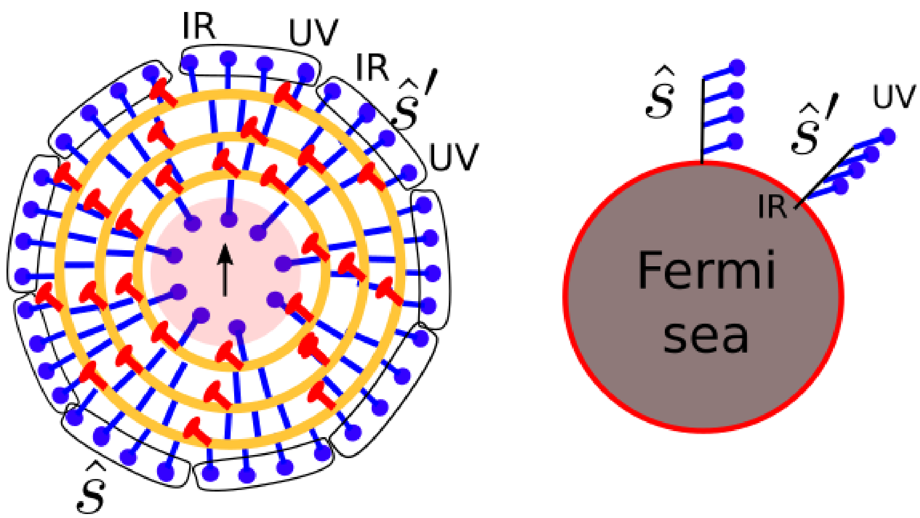

FIG. 5. Figure in the left shows a tensor network representation of the Kondo RG with 8 Fermi surface patches. The 32 blue nodes represents the 8 (for 8 $\hat{s}$) sets of 4(along a given normal $\hat{s}$) electronic states (qubits). arranged from UV to IR (see figure in the right). The yellow circular block represents the unitary gate that disentangles at each RG step 8 electronic qubits at UV. The red nodes represents the disentangled qubits comprising the bulk of the tensor network. At the IR bulk of the tensor network the pink circle represents the Kondo cloud coupling with the spin vector (up arrow).

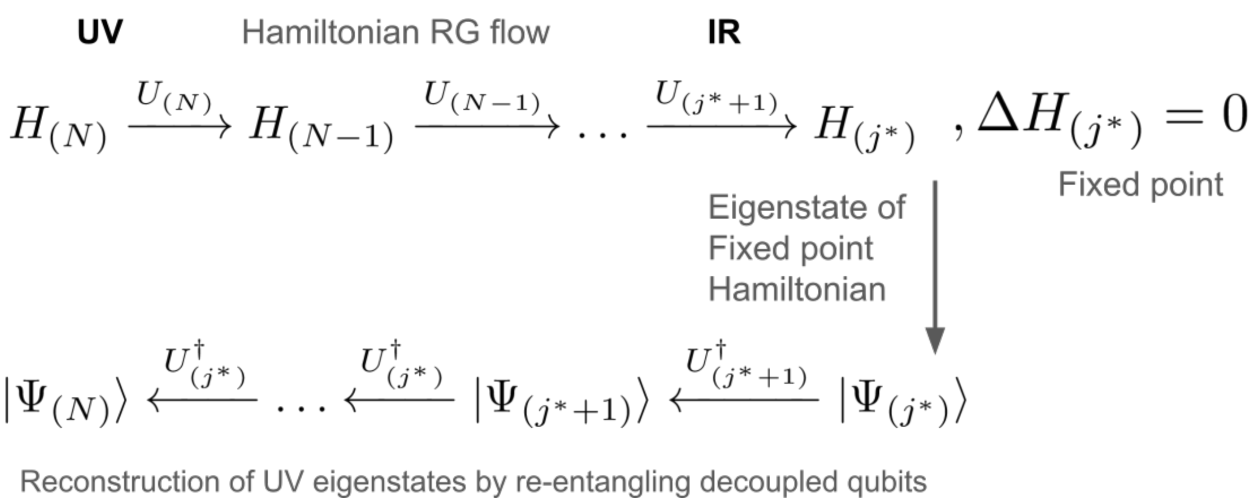

FIG. 6. The first line represent the Hamiltonian RG flow via the unitary maps. Upon reaching the Kondo IR fixed point, reverse RG will re-entangled decoupled electronic states with the Kondo singlet. This will result in generation of the many body eigenstates at UV.

tensor network. The many body rotated $c^\dagger$, c operators are given by,

$$c^\dagger_{\mathbf{k}'\sigma'}(\tau') = [U_j \dots U_N] c^\dagger_{\mathbf{k}'\sigma'} [U_j \dots U_N]^\dagger \tag{21}$$

From equal time green function $G(\mathbf{k}\sigma, \tau; \mathbf{k}'\sigma', \tau)$ we can obtain the complete one particle self energy and compute the spectral function, lifetime, quasoparticle residue. On the otherhand this quantity is related to mutual information or entanglement content between pair of electronic states. This quantity will enable a dual probe study of the quantum liquid composing the Kondo cloud.

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