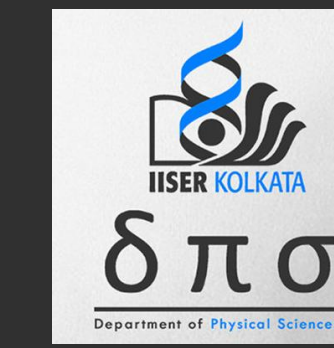


# Unitary RG Approach to Quantum Impurity Problems

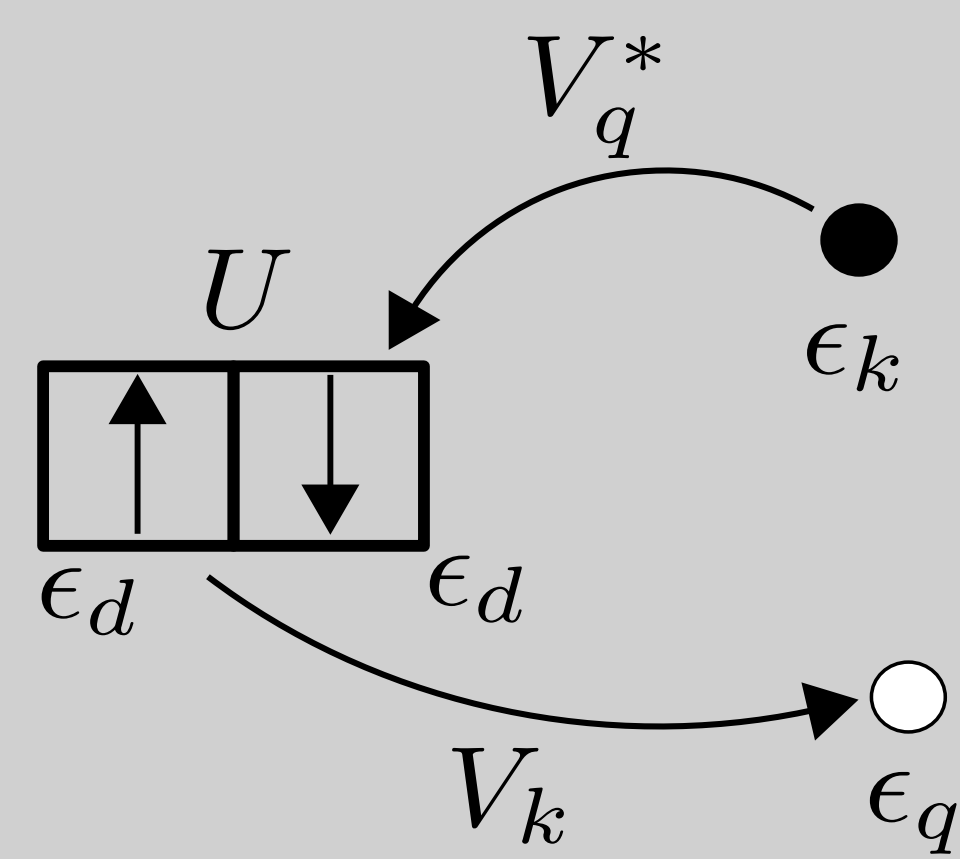
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Phys. Rev. B 105, 085119 Anirban Mukherjee<sup>[1]</sup>, Abhirup Mukherjee<sup>[1]</sup>, N.S. Vidhyadhiraja<sup>[2]</sup>, A. Taraphder<sup>[3]</sup>, Siddhartha Lal<sup>[1]</sup>

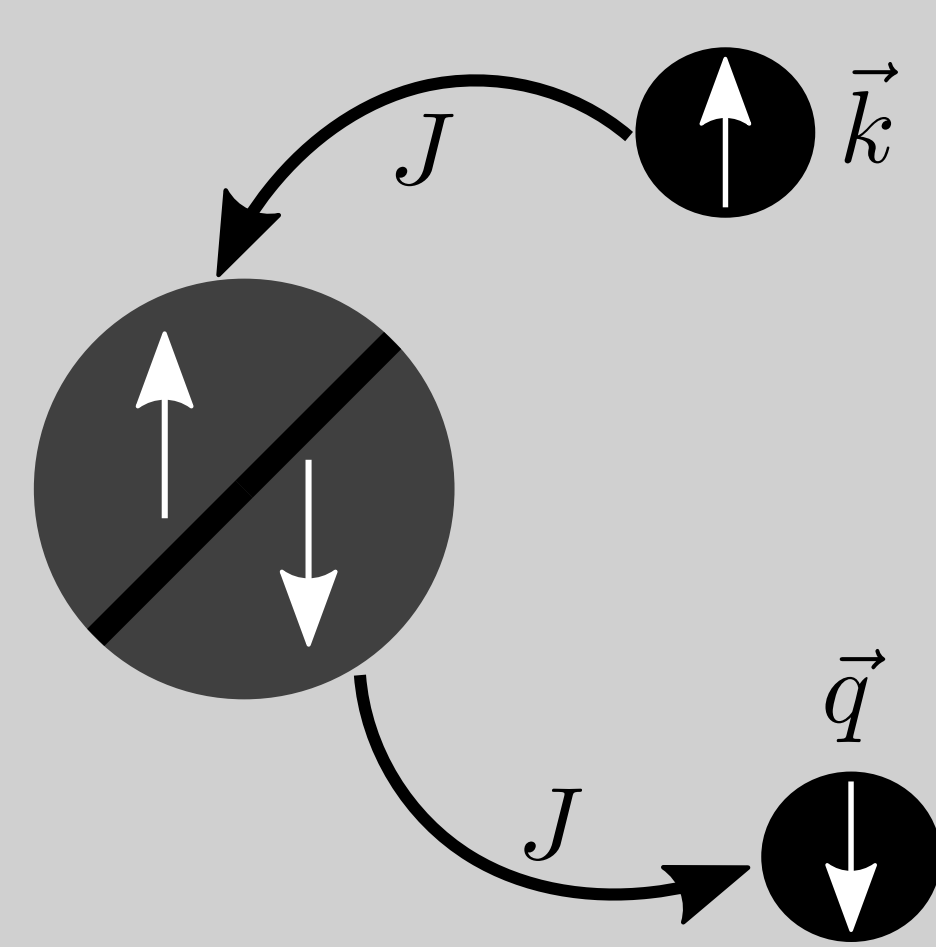
[2] Theoretical Sciences Unit, JNCASR [3] Department of Physics, IIT Kharagpur

## The Anderson impurity model (SIAM)



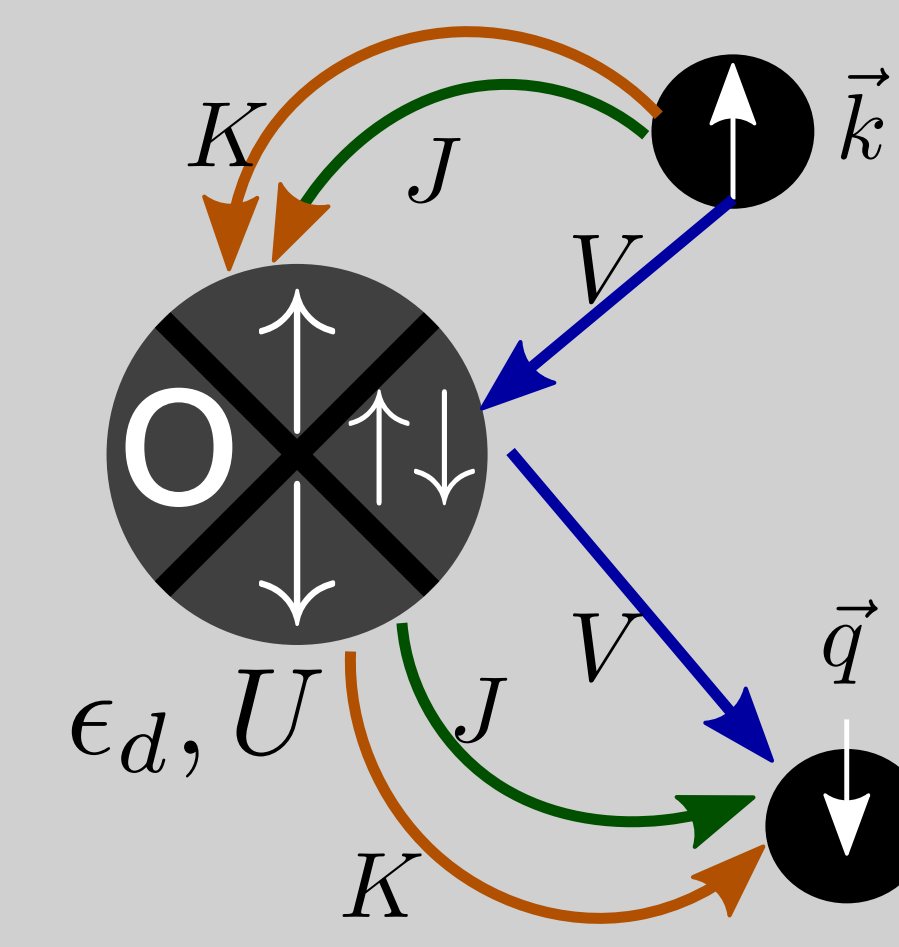
- Local impurity interacting with bath:  $H_{\text{bath}} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma}$
  - Hubbard repulsion  $U$  on impurity and 1-particle hybridisation  $V$  with bath
  - Microscopic origin of local moments in metals
- $$H = H_{\text{bath}} + \epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + V \sum_{k\sigma} (c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.})$$

## The Kondo model



- Impurity projected to spin-half Hilbert space
  - Spin-exchange coupling with conduction bath spin
  - Ground state is a **macroscopic singlet** formed by the impurity and the conduction bath
  - Charge variant involves **isospin exchange**
- $$H = H_{\text{bath}} + J \vec{S}_d \cdot \vec{s}$$

## Generalised Kondo-SIAM model

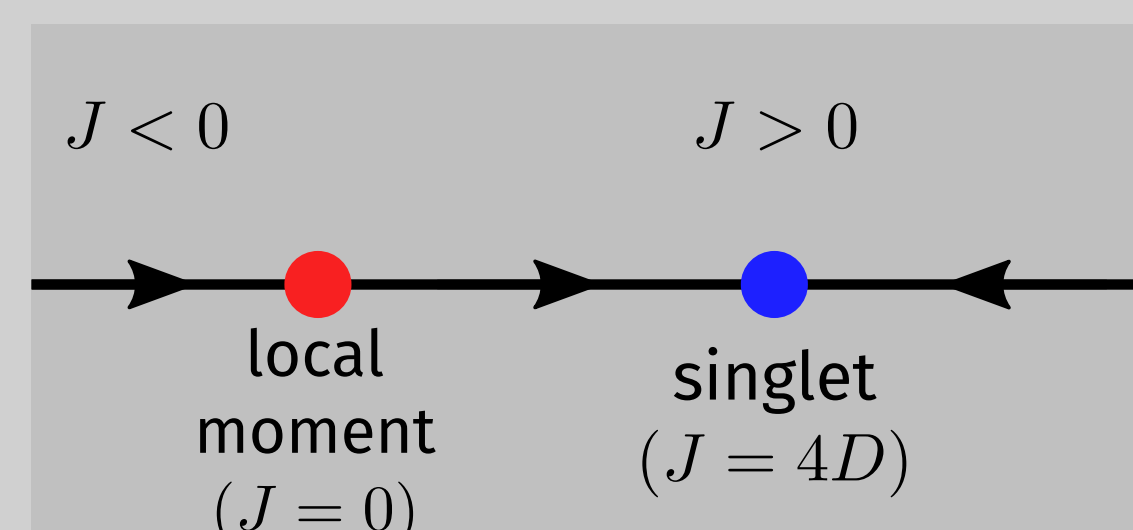


- Add spin and isospin exchange  $J$  and  $K$  to SIAM
- Exchange couplings are **dynamically generated under RG**, simpler to keep them at the start
- $V$  renormalises at lowest order
- Describes **both spin and charge screening** in one model

## Outstanding Questions

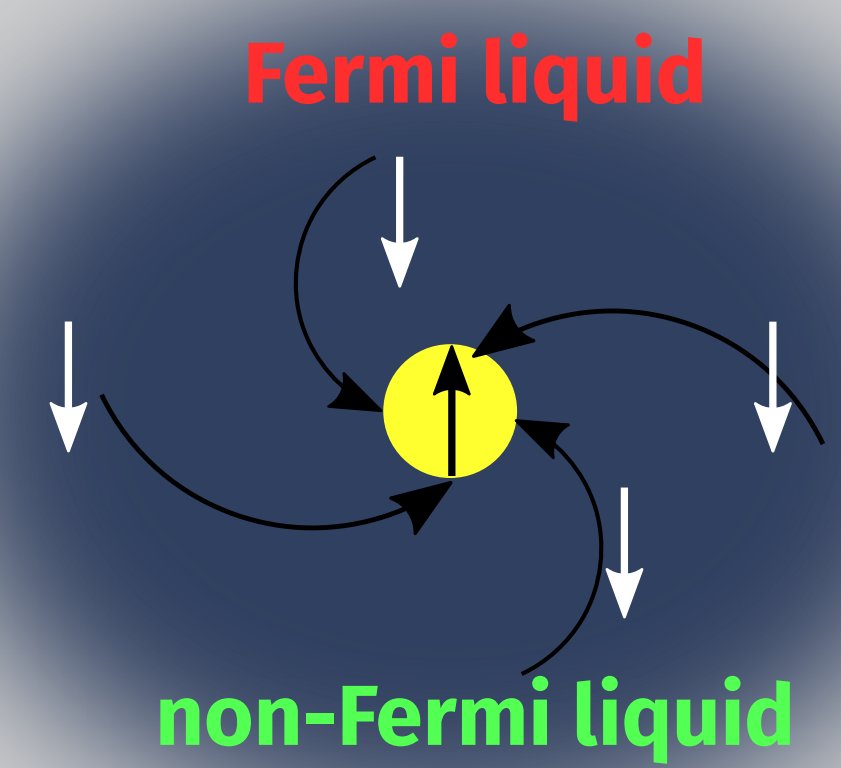
- What's the **effective Hamiltonian** for the conduction electrons that screen the impurity?
- Does the interplay of  $V$ ,  $J$  and  $K$  change the phase diagram in the generalised SIAM?
- What is the **nature of the metal** responsible for this screening?
- Is there any **topological quantity** that changes in the process of screening?
- Quantitative insight into **many-particle entanglement** at and near the fixed point
- Can we track the **evolution of the impurity spectral function** along the RG flow?

## URG Flows of the Kondo Model: Phase Diagram



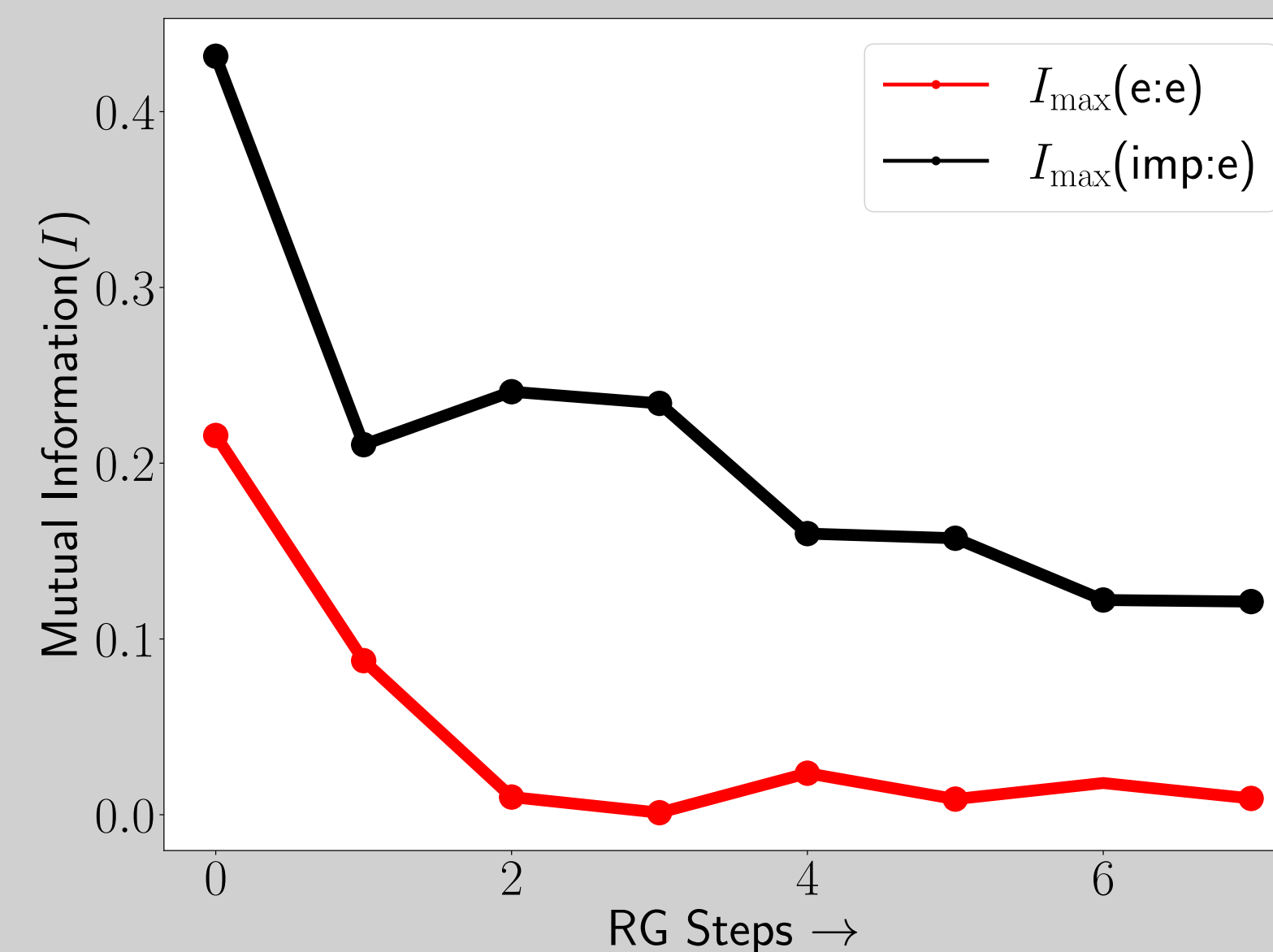
- $J = 0$  is stable for  $J \leq 0$ : **local moment** fixed point
- $J = 2D$  is globally stable: **strong-coupling** fixed point

## Effective Hamiltonian for Kondo Cloud



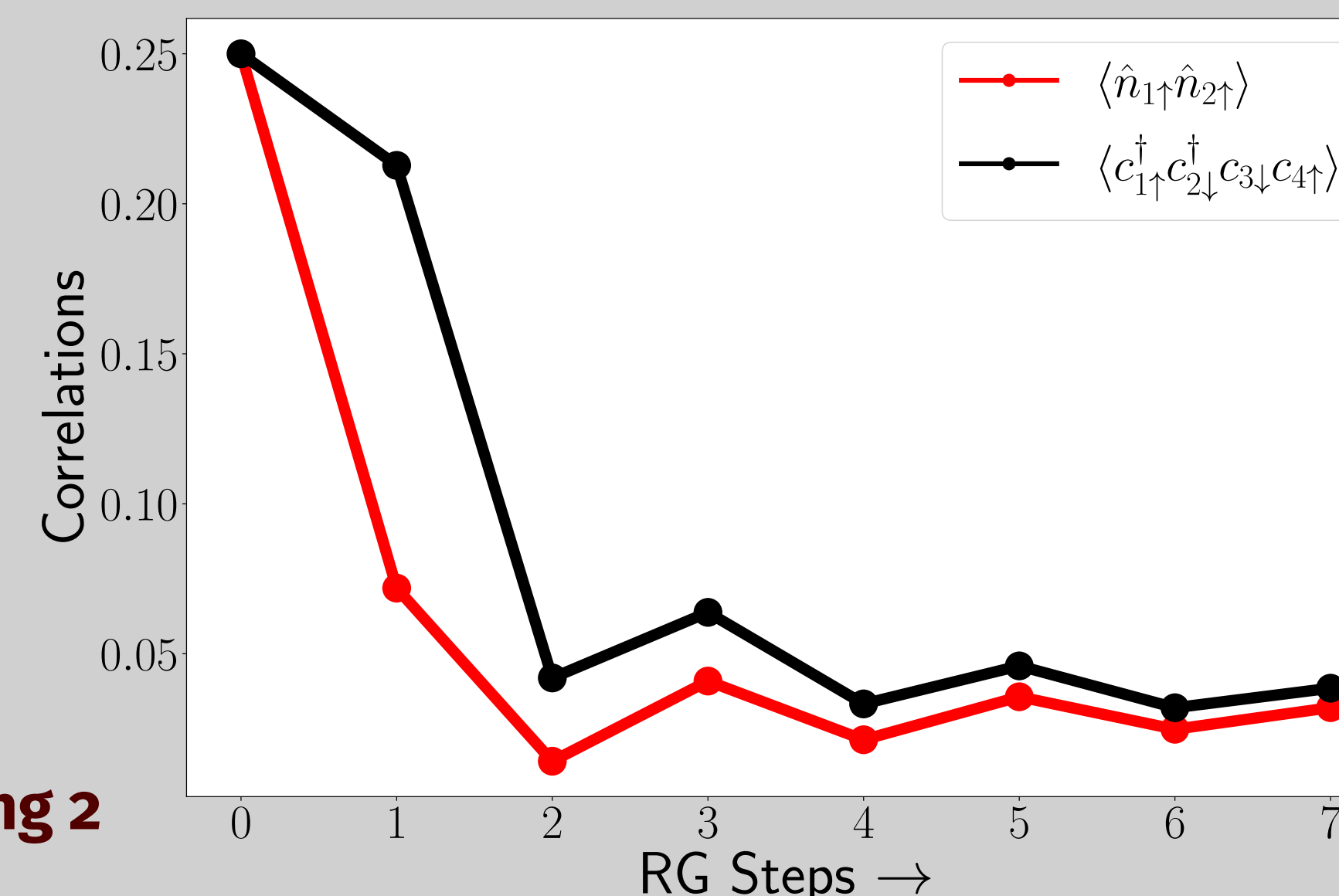
- Treat kinetic energy as perturbation above singlet ground state
- Integrate out impurity dynamics** via Schrieffer-Wolff transformation
- Resultant effective Hamiltonian has diagonal Fermi liquid piece:  $\sum \epsilon_k \hat{n}_{k\sigma} + \sum f_{kk'} \hat{n}_{k\sigma} \hat{n}_{k'\sigma'}$
- More importantly, it has **off-diagonal non-Fermi** liquid terms:  $\sum_{k_1, k_2, k_3, k_4} \mathcal{F} c_{k_1\uparrow}^\dagger c_{k_2\downarrow}^\dagger c_{k_3\downarrow} c_{k_4\uparrow}$

## RG Evolution of Entanglement in Kondo cloud



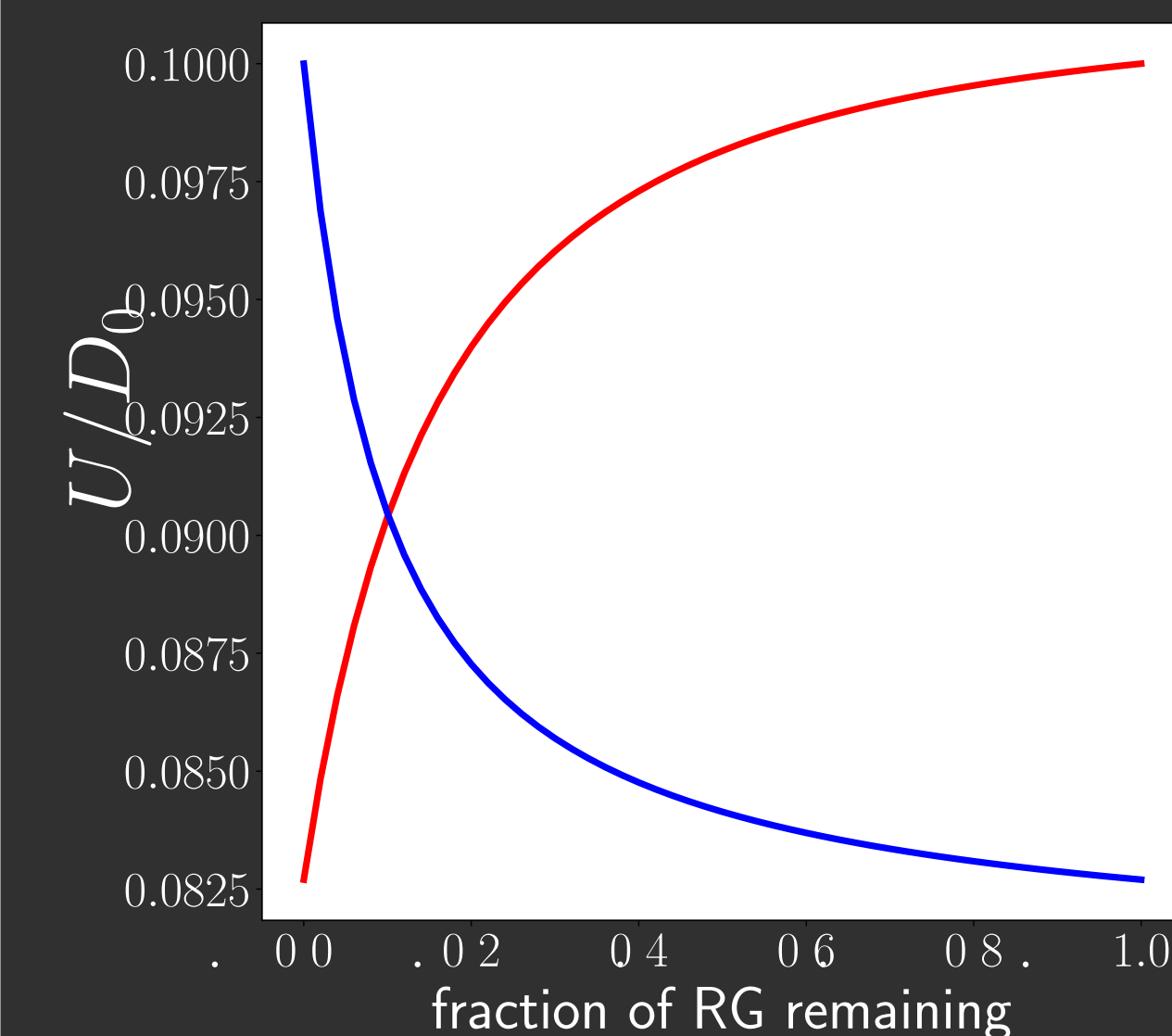
Mutual Information:  
 $I(1:2) = S(1) + S(2) - S(1,2)$   
 $S(1)$  - entanglement entropy of 1

Information obtained about 1, on measuring 2



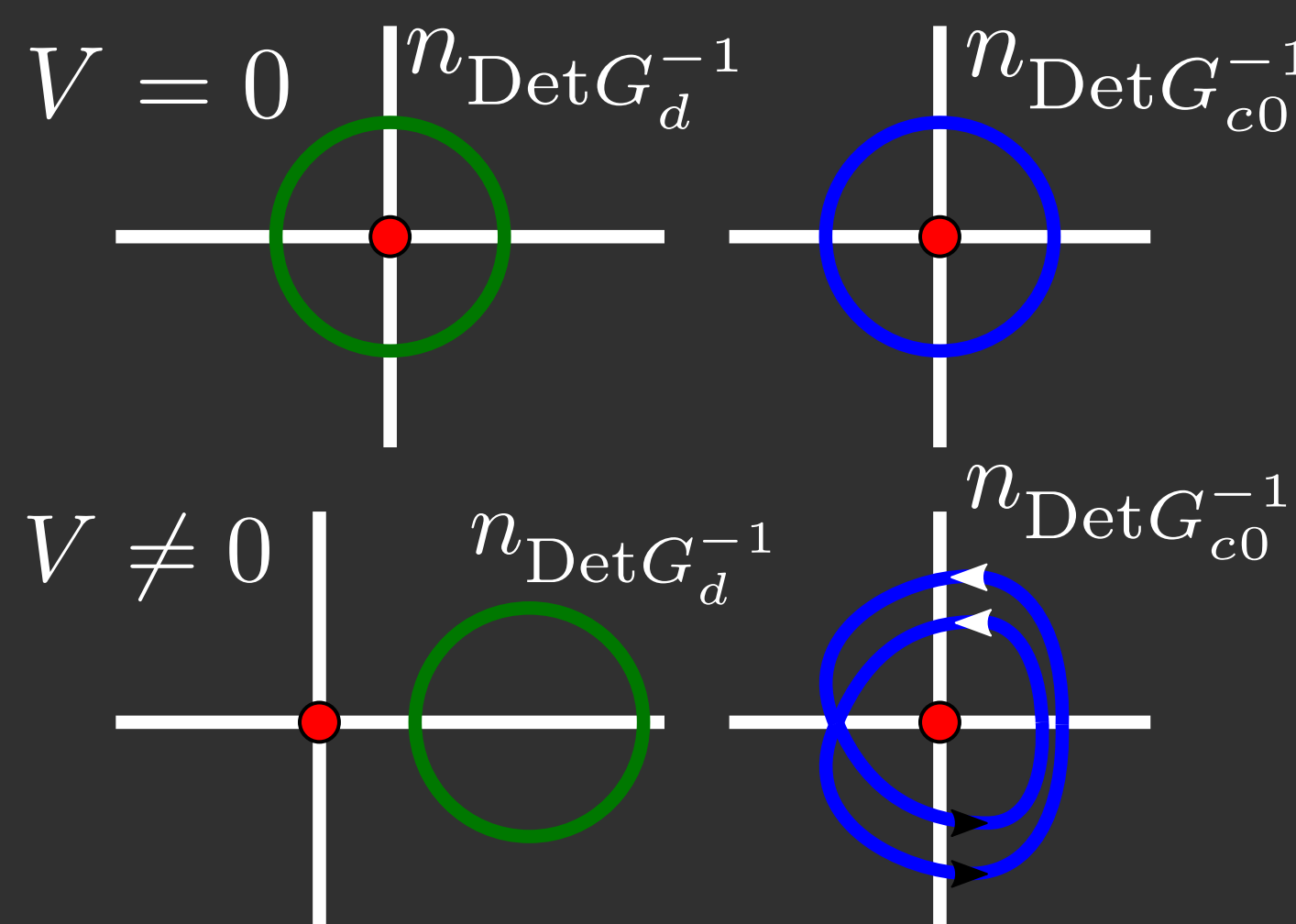
- Mut. Info. and correlations grow** towards strong-coupling IR fixed point
- Demonstrates the screening of impurity and formation of the singlet
- Consistent with the **presence of non-FL terms** in Kondo cloud Hamiltonian

## RG Flows of the Gen. SIAM, Effective Hamiltonian



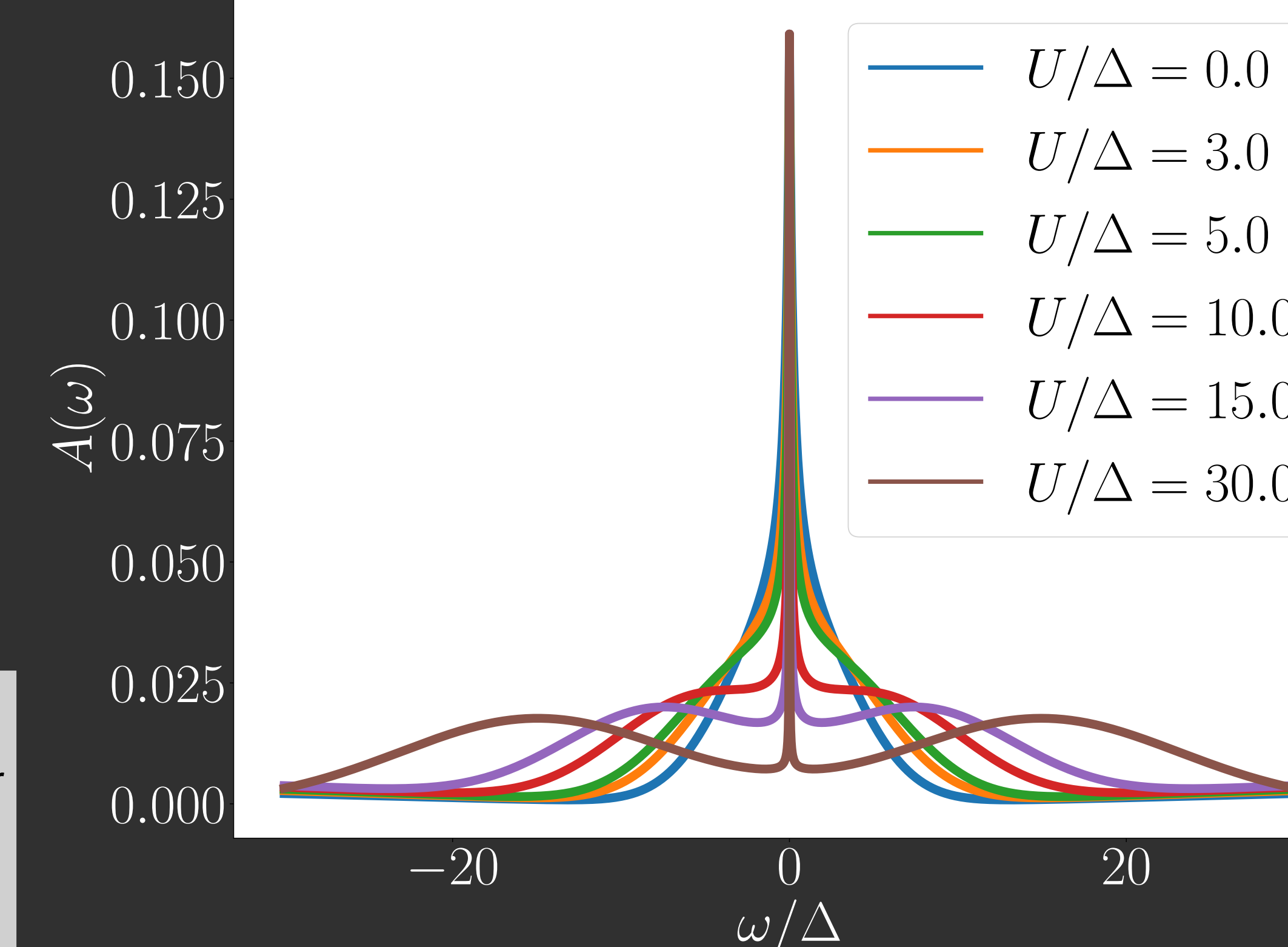
- $J, V$  flow to strong-coupling,  $U$  may be relevant if  $J > V$
- Ground state is **mixture** of spin-singlet and charge-triplet-zero
- Effective Hamiltonian of Kondo again features **non-Fermi liquid** terms
- Quantities computed from fixed point Hamiltonian **agree quantitatively** with the literature

## Topological change: Increase in Luttinger's volume



- Total number of electrons is given by **Luttinger's volume** (LV)
- At strong-coupling fixed point, impurity hybridises with the impurity
- This leads to an **increase in the topological quantity** LV by 1
- A **pole is transferred** from the impurity Greens function to the bath Greens function

## Evolution of Impurity Spectral Function



- Impurity spectral function obtained from effective Hamiltonian
- Single broad central peak at  $J, V \gg U \rightarrow$  low-energy scattering
- Side peaks appear at  $J, V \ll U$ , representative of local moment

## Future Directions

- Self-energy calculation of the complete cloud should reveal the type of non-Fermi liquid
- Enhance gen. SIAM to stabilise local moment - **metal-insulator transition** of DMFT
- More rich physics can be obtained from the lattice versions of the models

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