Local magnetic field in a Kondo model leads to impurity phase transition

RPC Presentation 2022-23

Debraj Debata

Supervisor : Dr. Siddhartha Lal

July 14, 2023

Motivation for the project

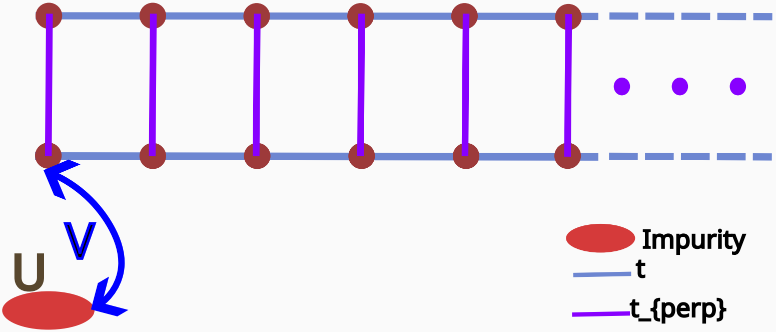
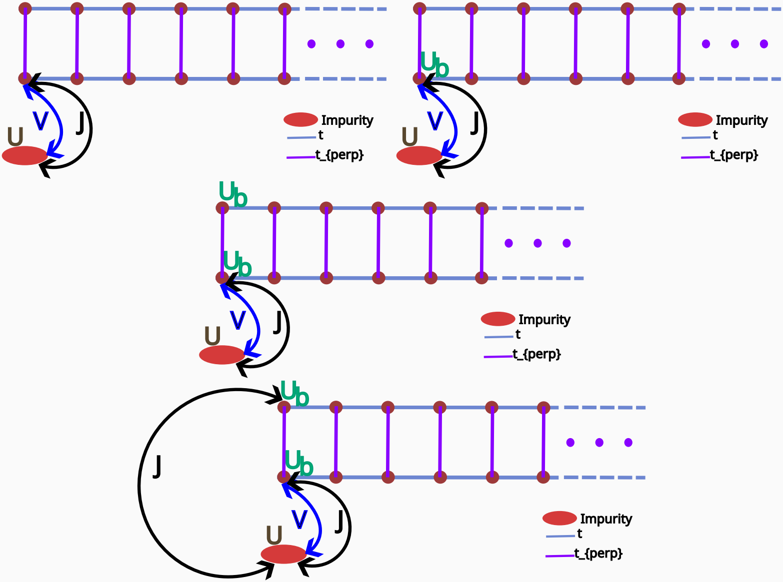
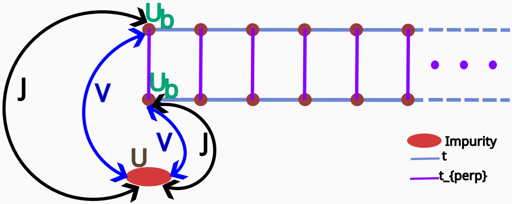


Figure 1: DMFT

Motivation for the project



Motivation for the project



Application of URG on Impurity Model

- It's interesting to understand the physics of Kondo Effect in the presence of magnetic field using non-perturbative Unitary Renormalisation Group(URG)
- This previously done by Costi. We reinvestigate the problem and try to not only reproduce old results but also produce some new results with the help of URG.

S2.png

Figure 2: Splitting of the Kondo resonance with increasing magnetic field at $T = 0$ and $T/T_K = 0.36$, T. A. Costi, PRL, 85, 1504 (2000)

Unitary Renormalisation Group(URG)

- RG scheme which proceeds by unitary transformations that decouple high-energy k-states
- Leads to fixed-point Hamiltonians that describe emergent IR physics

URG_transformation.pdf

Figure 3: Scaling concept: Low-energy model Hamiltonians are obtained from the detailed original model by integrating out the high-energy degrees of freedom.

Process of Unitary Renormalisation

URG_1.pdf

Figure 4: URG process

URG_2.pdf

Figure 5: URG emergent window and decoupled IOMs

$$U_{(j)} = \exp\{\tfrac{\pi}{4}(\eta^\dagger(j) - \eta(j))\}$$
$$\eta^\dagger(j) = \frac{1}{\hat{w}_{(j)} - Tr(H_{(j)}\hat{n}_j)} c_j^\dagger Tr(H_{(j)} c_j)$$

A. Mukherjee and S. Lal, Nuclear Physics B 960, 115170 & 115163 (2020)

Kondo Model in Local Magnetic Field

- The Kondo effect is an unusual mechanism of conduction electrons in a metal due to magnetic impurities
- It's one of the key concept in understanding the behavior of metallic systems with strongly interacting electrons.

Kondo.pdf

Figure 6: Kondo Effect

Kondo Effect in local magnetic field Hamiltonian is described by :
$H = \sum_{k,\sigma} \varepsilon_k n_{k\sigma} + J S_d . S_0 + B \mu_B S_d^z$.

RG Equations for Kondo in B-field

RG Equations calculated from URG:

$$\frac{\Delta J}{\Delta D} = -J^2 \frac{\tilde{w}}{\tilde{w}^2 - (\frac{\mu_B B}{2})^2}$$

$$\frac{\Delta B}{\Delta D} = -\frac{J^2}{4} \frac{B}{\tilde{w}^2 - (\frac{\mu_B B}{2})^2}$$

$\tilde{w}^2 = (\frac{\mu_B B}{2})^2$ is the fixed point condition where $\tilde{w} = w - \frac{\varepsilon_q}{2} + \frac{J}{4}$.

bitmap2.pdf

Figure 7: Graph when coupling J and B are relevent/irrelevant.

Graphical Nature of RG Equations

Two regions:

- Screened Kondo region where J is relevant and B is irrelevant
- Local moment region where B is relevant and J is irrelevant.

Figure 8: Initial magnetic field $B_0 = 2.5$ gives us the idea of Screened Kondo behaviour and $B_0 = 20$ for Local moment behaviour.

Impurity Phase Transition

QF_to_QPT.pdf

Quantum-classical transition.pdf

Figure 9: Singlet state becomes polarised state in the presence of B-field

Screened Kondo effective Hamiltonian is :

$H = \sum_{|k|<\Lambda,\sigma} \varepsilon_k n_{k\sigma} + J^* S_d \cdot S_0.$

Local moment effective Hamiltonian is :

$H = \sum \varepsilon_k n_{k\sigma} + B^* \mu_B S^z$

Zero-bandwidth Result

Zero-bandwidth Hamiltonian : $H = JS_d.S_0 + B\mu_B S_d^z$

- Zero-momentum model allows singlet and polarised states to becomes degenerate at $g_c \to \infty$.
- Becomes finite when dispersion taken into account.

KM_Zero-mode.pdf

Figure 11: Variation of four energies with dimensionless $g = \frac{\mu_B B}{J}$

QF_to_Frustration.pdf

Impurity Magnetization

Impurity magnetization : $\langle S_d^z \rangle = -\frac{1}{2}\frac{g^2+g\sqrt{1+g^2}}{1+g^2+g\sqrt{1+g^2}}$

For $g = 0$:

$\langle S_d^z \rangle$ is 0, matches with Kondo Effect singlet state.

For large g :

local moment state, $|\langle S_d^z \rangle| = \frac{1}{2}$

KM_Zero1-mode_slide_S_d_z_1.pdf

QF_to_Frustration.pd

Entanglement Entropy(EE)

Density Matrix :

$$\rho_d = \begin{bmatrix} \frac{1}{2} + \langle S_d^z \rangle & 0 \\ 0 & \frac{1}{2} - \langle S_d^z \rangle \end{bmatrix}$$

Entanglement Entropy

(EE)$= -\rho_d \ln \rho_d$

- Maximally entangled entropy($\ln 2$) for $g = 0$.

KM_Zero1-mode_slide_

Figure 13: EE varies with g

Nature of Gapless Excitation

Hamiltonian for gapless excitation :

$H = JS_d.S_0 + B\mu_B S_d^z - t\sum_\sigma(c_{0\sigma}^\dagger c_{1\sigma} + h.c.)$

At the Critical Point :

Non-Fermi liquid term, Fermi liquid term and local moment term observed.

Fermi-liquid term at the critical point nicely connected with Fermi-liquid side term. Same for at polarised state side.

4th_order.pdf

Figure 14: H_{FL}: effective Hamiltonian for Fermi-liquid region, H_{CP}: for Critical region and local moment region gives H_{LM}.

QF_to_Decoherence.pdf

Thermalisation at T=0

- This model shows a mechanism for thermalisation of pure impurity states into mixed states due to connection to the bath.
- An initial separable state $|{\uparrow_d}\rangle \otimes |\psi_{rest}\rangle$ ends up in an entangled state:

$$|{\uparrow_d \downarrow_0}\rangle = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{1+g^2+g\sqrt{1+g^2}}} \left[(g+\sqrt{1+g^2}) \left|\tilde{s} t_0\right\rangle - |\tilde{s} s\rangle \right]$$

QF_to_Decoherence.pd

Thermalisation at T=0

Thermalisation can be seen in the fact that both diagonal entries of impurity density matrix acquire non-vanishing values with time.

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \xrightarrow{\text{time dynamics of } \rho_d} \begin{pmatrix} A(t) & 0 \\ 0 & D(t) \end{pmatrix}$$

where $A(t) = P_+ + 4\langle S_d^z \rangle^2 P_-$ and $D(t) = (1 - 4\langle S_d^z \rangle^2)P_-$ and $P_\pm = \frac{1}{2}\left(1 \pm \cos wt\right)$.

QF_to_Decoherence.pdf

Thermalisation at T=0

- The rate of thermalisation ω can be controlled by tuning the magnetic field, as shown in Fig below

Figure 15: Time evolution of A and D for different $\langle S_d^z \rangle$: **Upper left** for $\langle S_d^z \rangle = 0$, **upper right** for $\langle S_d^z \rangle = 0.25$ and **below** for $\langle S_d^z \rangle = 0.5$.

Present Status & Future Plan

- implementing MERG, a wavefunction based renormalization group where for this project entangled state morphed into polarised state
- extending this project by adding bath(0-th site) magnetic field
- In the upcoming months, we will look into potential auxiliary models that can describe a QCP in the bulk

Acknowledgement and Thanks

- I would like to thank to my supervisor Dr. Siddhartha Lal for giving me this prototype toy problem which is connected to vast field of physics. Special thanks to him as I also gained various physics knowledge from him beyond my project.
- I am also greatful to my senior Abhirup da (collaborator of this project also) for a lot of scientific discussions and suggestions.

THANK_Y

Nature of Gapless Excitation(2nd order)

For 2nd Order

At second order, excitations are described by anisotropic Heisenberg model :

$$H^{eff} = \mathcal{J}^{\perp}(S_{gs}^{-}S_1^{+} + S_{gs}^{+}S_1^{-}) + \mathcal{J}^{z}S_{gs}^{z}S_1^{z} + \mathcal{H}_0^1 S_{gs}^{z} + \mathcal{H}_0^2 S_1^{z} + C$$

- In absence of B-field, impurity (d) and 0 site maximally entangled
- At critical point, due to degeneracy, entanglement gets shared between impurity, 0 and 1 sites.
- It tells us that Kondo cloud statrs destroying.

Nature of Gapless Excitation(4th Order)

4th order calculation at the critical point:

$$|\mathcal{A}\rangle\langle\mathcal{A}|\Bigg[Y_3+(N_1-Y_3)|\uparrow_1\rangle\langle\uparrow_1|-Y_3|\downarrow_1\rangle\langle\downarrow_1|\Bigg]$$

$$+|\mathcal{B}\rangle\langle\mathcal{B}|\Bigg[Y_5+(Y_4-Y_5)\Big(|0_1\rangle\langle 0_1|+|\uparrow_1\downarrow_1\rangle\langle\uparrow_1\downarrow_1|\Big)+(N_2-Y_5)|\downarrow_1\rangle\langle\downarrow_1|\Bigg]$$

$$+A_0^2 b_1\Big(Y_1(\lambda_+-a_1)+Y_2(\lambda_--a_1)\Big)\Big(|\mathcal{A}\rangle\langle\mathcal{B}|\uparrow_1\rangle\langle\downarrow_1|+|\mathcal{B}\rangle\langle\mathcal{A}|\downarrow_1\rangle\langle\uparrow_1|\Big)$$

where, $N_1=A_0^2 b_1^2(Y_1+Y_2)$ and $N_2=A_0^2 Y_1(\lambda_+-a_1)^2+A_0^2 Y_2(\lambda_--a_1)^2$.

4th order calculation at Fermi liquid side:

$$|\mathcal{B}\rangle\langle\mathcal{B}|\Big[Y_5+(Y_4-Y_5)(|0_1\rangle\langle 0_1|+|\uparrow_1\downarrow_1\rangle\langle\uparrow_1\downarrow_1|)+(Y_6-Y_5)|\downarrow_1\rangle\langle\downarrow_1|\Big]$$

4th order calculation at local moment side :

$$|\mathcal{A}\rangle\langle\mathcal{A}|\Big(Y_3+W_1|\uparrow_1\rangle\langle\uparrow_1|-Y_3|\downarrow_1\rangle\langle\downarrow_1|\Big)$$

$|\mathcal{A}\rangle=|\downarrow_d\downarrow_0\rangle$ and $|\mathcal{B}\rangle=-\frac{1}{\sqrt{2}}\frac{1}{\sqrt{1+g^2+g\sqrt{1+g^2}}}\Big[|\uparrow_d\downarrow_0\rangle-(g+\sqrt{1+g^2})|\downarrow_d\uparrow_0\rangle\Big]$

MERG

- Momentum-space Entanglement Renormalisation Group betterly known as MERG.
- It's a wavefunction based revese RG.
- We can go from initial entangled state wavefunction to polarised state wavefunction.

MERG.pdf

Figure 16: MERG Process