## 7.8 Calculation of Wilson ratio from effective local Fermi liquid

In this section, we will calculate the zero temperature Wilson ratio of the impurity in the Kondo regime of the SIAM. Since this is a low energy property, our starting point will be the fixed point Hamiltonian of eq. 6.4.3, after substituting $U^* = K^* = 0$ (because we are in the first quadrant):

$$\mathcal{H}^* = \sum_{\sigma,k} \epsilon_k \tau_{k\sigma} + \sum_{\sigma,k<\Lambda^*} \left( V^* c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right) + J^* \vec{S}_d \cdot \vec{s} \tag{7.8.1}$$

We also convert $\tau$ to $\hat{n}$, ignoring the constant part, and write the kinetic energy part as a nearest-neighbor hopping problem:

$$\mathcal{H}^* = t \sum_{\sigma\langle i,j\rangle} \left( c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} \right) + \sum_\sigma \left( V^* c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right) + J^* \vec{S}_d \cdot \vec{s} \tag{7.8.2}$$

We know that the ground state for the interacting part is predominantly the spin-singlet (it was shown while calculating the ground states of the effective zero-mode Hamiltonian that the ground state is a mixture of singlet and triplet, and the triplet part dies out at large system sizes, see eq. 6.4.40), so we will take that as our reference state and treat the hopping part that connects the origin to the first site,

$$V = t \sum_{\vec{r}_1,\sigma} c_{0\sigma}^\dagger c_{\vec{r}_1,\sigma} + \text{h.c.} \tag{7.8.3}$$

as a weak perturbation. $\vec{r}_1$ here sums over the sites that are nearest to the origin. Once that is taken care of, we will have a decoupled singlet formed by the impurity and the zeroth site, and the rest of the lattice formed by $N-1$ sites along with the interaction induced by the perturbation. The goal here is to see whether the effect of the perturbation is to lower the energy of the singly-occupied state $|\hat{n}_1 = 1\rangle$ compared to the doubly-occupied state $|\hat{n}_1 = 2\rangle$ or to raise it. If the perturbation shifts the energy of the singly-occupied state below the doubly-occupied state, then we can conclude that the effect of the perturbation is to raise the energy of the doubly-occupied state, which can then be modeled by a repulsive term $|U|\hat{n}_{1\uparrow}\hat{n}_{1\downarrow}$. If, on the other hand, the effect is to raise the energy of the singly-occupied state with respect to the $\hat{n}_1 = 2$ state, then that effect is equivalent to an attractive term $-|U|\hat{n}_{1\uparrow}\hat{n}_{1\downarrow}$.

To be precise, we will compare the energy shifts corresponding to the two states

$$|\phi_1^{(0)}\rangle = \underbrace{|\uparrow\rangle}_{\text{site 1}} \otimes \frac{1}{\sqrt{2}} \left( |\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle \right)$$

$$|\phi_2^{(0)}\rangle = \underbrace{|\uparrow,\downarrow\rangle}_{\text{site 1}} \otimes \frac{1}{\sqrt{2}} \left( |\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle \right) \tag{7.8.4}$$

In the singlet part, the first entry is the configuration of the zeroth site while the second entry is the configuration of the impurity site. Choosing the $\uparrow$ configuration for the site 1 is not a problem because both the non-perturbative and the perturbative interactions are SU(2)-symmetric. To demonstrate this, note that all energy shifts will depend on the unperturbed states $|\phi^{(0)}\rangle$ in two ways: through the energies in the denominator and through the matrix element in the numerator. The unperturbed energy goes not depend on the configuration of the $\vec{r}_1$ site, because the energy is dominated by the singlet. The matrix element is also independent of the sigma:

$$V |\sigma\rangle \otimes \frac{1}{\sqrt{2}} \left( |\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle \right) = \left( t \sum_{\vec{r}_1, \sigma} c_{0\sigma}^\dagger c_{\vec{r}_1, \sigma} + \text{h.c.} \right) |\sigma\rangle \otimes \frac{1}{\sqrt{2}} \sum_\alpha \alpha |\alpha, \bar{\alpha}\rangle$$

$$= t \frac{1}{\sqrt{2}} \left( |2\rangle |0, \bar{\sigma}\rangle - |0\rangle |2, \sigma\rangle \right)$$

(7.8.5)

The first order correction will be zero as we will see shortly, but the short version is that $V |\phi^{(0)}\rangle$ is obviously orthogonal to $|\phi^{(0)}\rangle$. All higher energy shifts can be represented as

$$\langle \phi^{(0)} | VXV | \phi^{(0)} \rangle$$

(7.8.6)

where $X$, for example, is

$$\sum_{m^{(0)}} \frac{|\langle m^{(0)} | |\phi^{(0)}\rangle|^2}{E_\phi^{(0)} - E_m^{(0)}}$$

(7.8.7)

for the second order shift, and does not operate on the impurity. Since $X$ does not operate on the impurity, the shift can be written as

$$\langle \phi^{(0)} | VXV | \phi^{(0)} \rangle = \frac{t^2}{2} \left( \langle 2| \langle 0, \bar{\sigma}| - \langle 0| \langle 2, \sigma| \right) X \left( |2\rangle |0, \bar{\sigma}\rangle - |0\rangle |2, \sigma\rangle \right)$$

$$= \frac{t^2}{2} \langle 2| \langle 0, \bar{\sigma}| X |2\rangle |0, \bar{\sigma}\rangle + \frac{t^2}{2} \langle 0| \langle 2, \sigma| X |0\rangle |2, \sigma\rangle$$

$$= \frac{t^2}{2} \langle 2| \langle 0| X |2\rangle |0\rangle \langle \bar{\sigma}| |\bar{\sigma}\rangle + \frac{t^2}{2} \langle 0| \langle 2| X |0\rangle |2\rangle \langle \sigma| |\sigma\rangle$$

$$= \frac{t^2}{2} \langle 2| \langle 0| X |2\rangle |0\rangle + \frac{t^2}{2} \langle 0| \langle 2| X |0\rangle |2\rangle$$

(7.8.8)

This proves that the shift is independent of $\sigma$. The reason we could shift the bra $\langle \sigma|$ across the $X$ without any sign change is that $X$ will have even number of operators in product, because it operates on 0 and 1.

The energy corresponding to this singlet state (for both $\hat{n}_1 = 1$ and $\hat{n}_1 = 2$) is

$$E_1^{(0)} = E_2^{(0)} = -\frac{3J^*}{4}$$

(7.8.9)

The full list of unperturbed eigenstates are

$$\left\{ |\hat{n}_1 = 0\rangle, |\hat{n}_1 = 1\rangle, |\hat{n}_1 = 2\rangle \right\} \otimes \left\{ |S = 0\rangle, |S = 1, S^z = -1, 0, 1\rangle, |S_0^z \times S_d^z = 0\rangle \right\}$$

(7.8.10)

Since $V$ takes $|\phi_{1,2}^{(0)}\rangle$ to completely orthogonal states, the first order corrections are 0:

$$E_1^{(1)} = \langle\phi_1^{(0)}|V|\phi_1^{(0)}\rangle = \langle\phi_1^{(0)}|\frac{t}{\sqrt{2}}\left(-|0,2,\uparrow\rangle - |2,0,\uparrow\rangle\right) = 0$$

$$E_2^{(1)} = \langle\phi_2^{(0)}|V|\phi_2^{(0)}\rangle = \langle\phi_1^{(0)}|\frac{t}{\sqrt{2}}\left(|\downarrow,2,\uparrow\rangle - |\uparrow,2,\downarrow\rangle\right) = 0 \tag{7.8.11}$$

The second order correction for a general unperturbed state $|\phi^{(0)}\rangle$ is given by the formula

$$E^{(2)} = \sum_{m^{(0)} \neq \phi^{(0)}} \frac{|\langle m^{(0)}|V|\phi^{(0)}\rangle|^2}{E_\phi^{(0)} - E_m^{(0)}} \tag{7.8.12}$$

The index m sums over all unperturbed eigenstates not equal to $|\phi^{(0)}\rangle$, and $E_\phi^{(0)}, E_m^{(0)}$ are the unperturbed energies for the states $|\phi^{(0)}\rangle$ and $|m^{(0)}\rangle$. If we look at the forms of $V|\phi_{1,2}^{(0)}\rangle$ that we calculated above, the only eigenstates $|m^{(0)}\rangle$ that give non-zero numerators are

$$\left\{|m^{(0)}\rangle\right\} = \begin{cases} |0,2,\uparrow\rangle, |2,0,\uparrow\rangle & \text{if } |\phi^{(0)}\rangle = |\phi_1^{(0)}\rangle \\ |\downarrow,2,\uparrow\rangle, |\uparrow,2,\downarrow\rangle & \text{if } |\phi^{(0)}\rangle = |\phi_2^{(0)}\rangle \end{cases} \tag{7.8.13}$$

which then means that the only non-zero value of the numerator is

$$\left(\pm\frac{t}{\sqrt{2}}\right)^2 = \frac{t^2}{2} \tag{7.8.14}$$

Also, because all the states in $\left\{|m^{(0)}\rangle\right\}$ involve $S_0^z = 0$, those states will have zero energy, so all the denominators will have the value

$$E_{\phi_{1,2}}^{(0)} - E_m^{(0)} = E_{\phi_{1,2}}^{(0)} = -\frac{3J^*}{4} \tag{7.8.15}$$

The upshot of all this is that the second order shift will be same for both the single and doubly-occupied states, so we will ignore that correction as it can be absorbed into the zero-point energy.

The third order correction is given by

$$E^{(3)} = \sum_{i^{(0)}, j^{(0)} \neq \phi} \frac{\langle\phi^{(0)}|V|j^{(0)}\rangle\langle j^{(0)}|V|i^{(0)}\rangle\langle i^{(0)}|V|\phi^{(0)}\rangle}{\left(E_\phi^{(0)} - E_i^{(0)}\right)\left(E_\phi^{(0)} - E_j^{(0)}\right)} - E_\phi^{(1)}\sum_{m^{(0)} \neq \phi} \frac{|\langle m^{(0)}|V|\phi^{(0)}\rangle|^2}{\left(E_\phi^{(0)} - E_m^{(0)}\right)^2} \tag{7.8.16}$$

This correction can also be argued to be zero, as follows. The second term is of course trivially zero because $E_\phi^{(1)}$ itself is 0. For the first term, note that $|i^{(0)}\rangle$ must have $\hat{n}_0 = 0, 2$ in order to give non-zero inner product with $V|\phi^{(0)}\rangle$. If we continue this, $V|i^{(0)}\rangle$ will have $\hat{n}_0 = 1$, so $|j^{(0)}\rangle$ must also have the same. Then, $V|j^{(0)}\rangle$ will have $\hat{n}_0 = 0, 2$ and hence the

inner product $\langle \phi^{(0)} | V | j^{(0)} \rangle$ will be 0. The third order corrections for both the single and doubly occupied states are thus 0.

We move on to the fourth order correction. The general formula is quite formidable, so we only write down the terms that aren't outright zero for this problem:

$$E^{(4)} = \sum_{i^{(0)}, j^{(0)}, k^{(0)} \neq \phi} \frac{\langle \phi^{(0)} | V | k^{(0)} \rangle \langle k^{(0)} | V | j^{(0)} \rangle \langle j^{(0)} | V | i^{(0)} \rangle \langle i^{(0)} | V | \phi^{(0)} \rangle}{\left( E_\phi^{(0)} - E_k^{(0)} \right) \left( E_\phi^{(0)} - E_j^{(0)} \right) \left( E_\phi^{(0)} - E_i^{(0)} \right)} - E_\phi^{(2)} \sum_{m^{(0)} \neq \phi} \frac{| \langle m^{(0)} | V | \phi^{(0)} \rangle |^2}{\left( E_\phi^{(0)} - E_m^{(0)} \right)^2}$$

(7.8.17)

For the singly-occupied state, the calculation pans out as follows:

$$\left\{ |i^{(0)}\rangle \right\} = \begin{cases} |0, 2, \uparrow\rangle \implies \left\{ |j^{(0)}\rangle \right\} = \begin{cases} |\uparrow\rangle \otimes |S = 1, S^z = 0\rangle & \implies \left\{ |k^{(0)}\rangle \right\} = \begin{cases} |0, 2, \uparrow\rangle \\ |2, 0, \uparrow\rangle \end{cases} \\ |\downarrow\rangle \otimes |\uparrow, \uparrow\rangle & \implies \left\{ |k^{(0)}\rangle \right\} = |0, 2, \uparrow\rangle \end{cases} \\ |2, 0, \uparrow\rangle \implies \left\{ |j^{(0)}\rangle \right\} = \begin{cases} |\uparrow\rangle \otimes |S = 1, S^z = 0\rangle & \implies \left\{ |k^{(0)}\rangle \right\} = \begin{cases} |0, 2, \uparrow\rangle \\ |2, 0, \uparrow\rangle \end{cases} \\ |\downarrow\rangle \otimes |\uparrow, \uparrow\rangle & \implies \left\{ |k^{(0)}\rangle \right\} = |0, 2, \uparrow\rangle \end{cases} \end{cases}$$

(7.8.18)

The inner products in the numerators can be calculated from these states. The energies of the intermediate states are

$$E_i^{(0)} = 0, \quad E_j^{(0)} = \frac{J^*}{4}, \quad E_k^{(0)} = 0$$

(7.8.19)

which allow calculating the denominators. The total fourth order change for the singly-occupied state is

$$E_1^{(4)} = -\frac{16t^4}{3J^{*3}}$$

(7.8.20)

Carrying out a similar calculation for the doubly-occupied state gives

$$E_2^{(4)} = -\frac{16t^4}{9J^{*3}}$$

(7.8.21)

The last two equations together mean that the effect of the perturbation is to raise the energy of the doubly-occupied state by an amount

$$u \sim \frac{t^4}{J^{*3}}$$

(7.8.22)

and we can replace the perturbative term $V$ by an effective repulsive term on the first site (a.k.a, the "local Fermi liquid", [8]):

$$u \hat{n}_{1\uparrow} \hat{n}_{1\downarrow}$$

(7.8.23)

The total system now consists of two decoupled parts - the singlet composed of the impurity and the zeroth site, and the remaining lattice composed of N-1 sites with a tight-binding dispersion and a local interaction at the 1-th site. The effective Hamiltonian for the remaining lattice is

$$\sum_{\substack{i=1 \\ \sigma}}^{\infty} t \left( c_{i\sigma}^{\dagger} c_{i+1\sigma} + c_{i+1\sigma}^{\dagger} c_{i\sigma} \right) + u \hat{n}_{1\uparrow} \hat{n}_{1\downarrow} \tag{7.8.24}$$

We will now invoke the mean-field approximation in simplifying this term. We will be
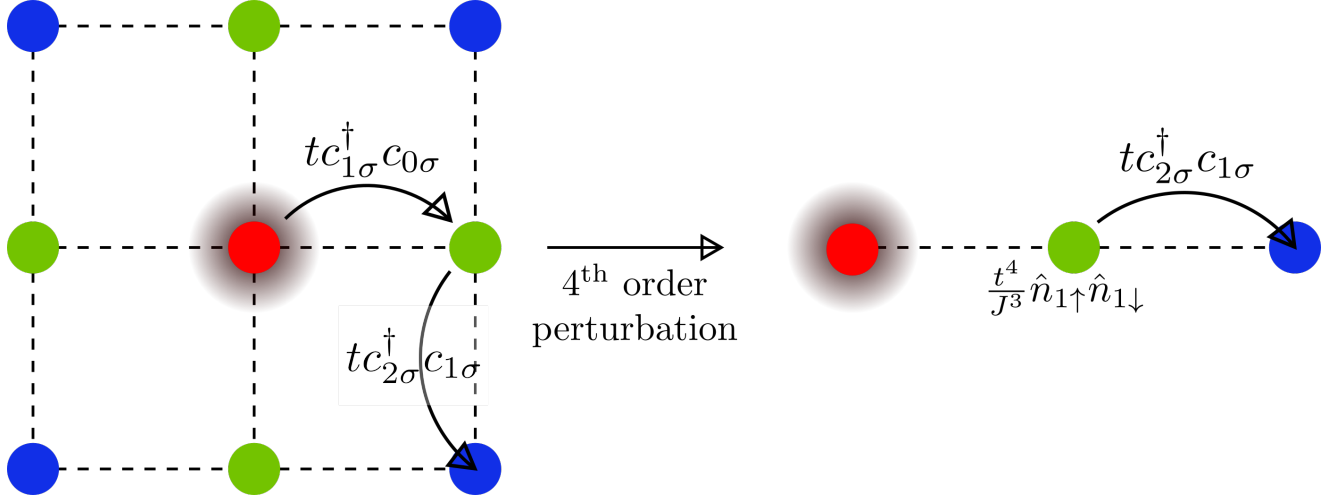


Figure 7.10: *Left*: The nearest-neighbor hopping described by the effective Hamiltonian. The red circle at the center is the impurity at the origin. The black cloud at the center demarcates the collection of electrons at the origin of the lattice (which couple to the impurity). The green circles represent lattice sites that are nearest to the origin. The blue circles represent next-nearest sites. *Right*: After treating the hopping between origin and its nearest neighbors as perturbation, we get a system consisting of two decoupled parts: one part is the impurity+cloud singlet, the other part is the rest of the lattice sites. The effect of the hopping between the origin and the green sites is a repulsion term on the green sites.

dealing with thermodynamic quantities soon, so the operators will be replaced by their thermodynamic values, that is, the values that minimize the free energy functional.

$$\hat{n}_{1\uparrow} \hat{n}_{1\downarrow} \rightarrow \langle \hat{n}_{1\uparrow} \hat{n}_{1\downarrow} \rangle = \langle \delta n_{1\uparrow} \delta n_{1\downarrow} \rangle + \langle n_{1\uparrow} \rangle \langle n_{1\downarrow} \rangle \tag{7.8.25}$$

where $\delta n_{1\sigma} \equiv n_{1\sigma} - \langle n_{1\sigma} \rangle$ is the fluctuation of the particle number above the ground state. The mean-field approximation then involves dropping the first term which is a quadratic fluctuation - since we are interested in values of quantities at $T \rightarrow 0$, this quadratic fluctuation is very small. The interaction we are left with is

$$u \langle n_{1\uparrow} \rangle \langle n_{1\downarrow} \rangle = \sum_{kq\sigma} f_{kq} \langle n_{k\sigma} \rangle \langle n_{q\bar{\sigma}} \rangle \tag{7.8.26}$$

This interaction converts the problem to that of a Landau Fermi liquid, with the quasi-particle energy functional being given by

$$\epsilon_{k\sigma} = \epsilon_k + \sum_q f_{kq} \left\langle \hat{n}_{q\bar{\sigma}} \right\rangle \tag{7.8.27}$$

From the form of the quasiparticle energy functional, we can see that there is no spin-parallel term, so we can write

$$f_{kk'\sigma\sigma} = 0, f_{kk'\sigma\bar{\sigma}} = f_{kk'} \tag{7.8.28}$$

We will now use this Fermi liquid form to extract the Wilson ratio. We will make use of the following definitions/results:

$$
\begin{aligned}
dn_{k\sigma} &= \frac{\partial n}{\partial \epsilon_{k\sigma}} \left(d\epsilon_{k\sigma} - d\mu\right) \quad \text{[follows from differentiating FD distribution]} \\
C_v &= \frac{d\epsilon}{dT} \\
\chi^{s,c} &= \frac{d}{d(B,\mu)} \left(n_\uparrow \mp n_\downarrow\right) \\
2f_0^{s,a} &= \sum_k \left(f_{kk'\uparrow\uparrow} \pm f_{kk'\uparrow\downarrow}\right) \\
F_0^{s,a} &= \rho(0) f_0^{s,a}
\end{aligned}
\tag{7.8.29}
$$

## 7.8.1 Low-$T$ Specific heat

$$
\begin{aligned}
C &= \frac{d}{dT} \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma} \\
&\approx \sum_{k\sigma} \epsilon_{k\sigma}^0 \frac{dn_{k\sigma}}{dT} \quad \text{[no quasiparticles at ground state]} \\
&\approx \sum_{k\sigma} \epsilon_{k\sigma}^0 \frac{dn_{k\sigma}}{dT} \quad \text{[same expression as Fermi gas but with modified distribution function]} \\
&= \rho(0)T
\end{aligned}
$$

$$\tag{7.8.30}$$

where $\rho$ is the total quasiparticle DOS with contributions from conduction bath and impurity.

$$\rho \sim \text{Im Trace}\,[G] = \text{Im} \sum_{d\sigma} G_{dd}^\sigma + \text{Im} \sum_{k\sigma} G_{kk}^\sigma = \rho_0 + \rho_{\text{imp}} \tag{7.8.31}$$

which gives

$$C_{imp} \equiv C - C_0 = \rho_{imp}(0)T \tag{7.8.32}$$

## 7.8.2 Low-$T$ Charge Susceptibility

$$\chi^c = \frac{dN}{d\mu} \tag{7.8.33}$$

Due to change in chemical potential, $\delta\epsilon_{k\sigma}$ is isotropic and SU(2)-symmetric. Hence

$$
\begin{aligned}
d\epsilon_{k\sigma} &= \sum_{k'\sigma'} f_{kk'\sigma\sigma'} dn_{k'\sigma'} \\
&= dn \sum_{k'} \left( f_{kk'\uparrow\uparrow} + f_{kk'\uparrow\downarrow} \right) \quad \left[ dn = dn_{k'\uparrow} = dn_{k\downarrow} \right] \\
&= 2dn f_0^s
\end{aligned}
\tag{7.8.34}
$$

Therefore,

$$
\begin{aligned}
dN &= \sum_{k\sigma} dn_{k\sigma} \\
&= \sum_{k\sigma} \frac{\partial n}{\partial \epsilon_{k\sigma}} \left( d\epsilon_{k\sigma} - d\mu \right) \\
&= \sum_{k\sigma} -\frac{1}{2}\rho \left( 2dn f_0^s - d\mu \right) \\
&= -\rho(0) dN f_0^s + d\mu\rho(0) \\
&\approx d\mu\rho(0) - \rho(0) f_0^s d\mu\rho(0) \ \left[\text{substitute } dN \text{ back into itself}\right] \\
\implies \frac{dN}{d\mu} &= \rho(0) \left( 1 - \rho(0) f_0^s \right) \\
\implies \chi^c_{imp} &= \rho(0)_{imp} - \rho(0) f_0^s
\end{aligned}
\tag{7.8.35}
$$

At an intermediate state, we substituted $dN$ back into itself and kept only the leading order term. This is justified because $f_{kk'}$ goes as $\frac{1}{NJ}$. At the fixed point and for a thermo-dynamically large system, both $J$ and $N$ are very large, so keeping only the leading order suffices.

From a previous calculation, we know that the charge susceptibility at $T = 0$ is zero, so we can write down the following relation:

$$f_0^s = \frac{\rho(0)_{imp}}{\rho(0)} \tag{7.8.36}$$

## 7.8.3 Low-$T$ Spin Susceptibility

$$\chi^s = \frac{dm}{d\mu} \tag{7.8.37}$$

Due to change in magnetic field, change in $\epsilon_{k\sigma}$ should be isotropic and SU(2)-antisymmetric. Hence

$$
\begin{aligned}
d\epsilon_{k\sigma} &= -\frac{1}{2} dB\sigma + \sum_{k'\sigma'} f_{kk'\sigma\sigma'} dn_{k'\sigma'} \\
&= -\frac{1}{2} dB\sigma + dn_\sigma \sum_{k'} \left( f_{kk'\uparrow\uparrow} - f_{kk'\uparrow\downarrow} \right) \quad \left[ dn_{k'\uparrow} = -dn_{k\downarrow} \right] \\
&= -\frac{1}{2} dB\sigma + 2dn_\sigma f_0^a
\end{aligned}
\tag{7.8.38}
$$

Since the total number remains constant, $\mu = 0$. Therefore,

$$
\begin{aligned}
dm &= \sum_k \left( dn_{k\uparrow} - dn_{k\downarrow} \right) \\
&= -\frac{1}{2} \sum_k \rho \left( d\epsilon_{k\uparrow} - d\epsilon_{k\downarrow} \right) \\
&= -\frac{1}{2} \sum_k \rho \left( -dB + 2f_0^a \left( dn_{k\uparrow} - dn_{k\downarrow} \right) \right) \\
&= dB\rho(0) - dm\rho(0) f_0^a \\
&\approx dB\rho(0) - \rho(0) f_0^a B\rho(0) \qquad \left[\text{substitute } dm \text{ back into itself}\right]
\end{aligned}
\tag{7.8.39}
$$

$$
\implies \frac{dm}{dB} = \rho(0) \left( 1 - \rho(0) f_0^a \right)
$$

$$
\implies \chi_{imp}^s = \rho(0)_{imp} - \rho(0) f_0^a
$$

### 7.8.4  Wilson ratio

The Wilson ratio for the impurity is defined as

$$
R = \frac{\chi_{imp}^s}{\frac{C_{imp}}{T}}
\tag{7.8.40}
$$

From eq. 7.8.28, we have $f_0^s = -f_0^a$, which, when combined with eq. 7.8.36, gives

$$
\chi_{imp}^s = 2\rho(0)_{imp}
\tag{7.8.41}
$$

The Wilson ratio becomes

$$
R = \frac{2\rho(0)_{imp}}{\rho(0)_{imp}} = 2
\tag{7.8.42}
$$

## 7.9  Luttinger's and Friedel's sum rules

The subsequent discussions are for the first quadrant where $U^* = 0$ and $J^* > K^*$. At high temperatures, we see that the impurity susceptibility attains the value of

$$
\frac{1}{8k_B T}
\tag{7.9.1}
$$

which implies that the impurity behaves as a free orbital in this limit, having no coupling with the bath. We can write down the following effective Hamiltonian for such a limit:

$$\mathcal{H}_{\text{high-T}} = \tilde{\epsilon}_d \hat{n}_d + \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} \tag{7.9.2}$$

Since the impurity is decoupled from the bath, we can immediately write down the Hamiltonian just for the impurity:

$$\mathcal{H}_{\text{high-T, imp}} = \tilde{\epsilon}_d \hat{n}_d \tag{7.9.3}$$

We consider the resonant-level model:

$$\mathcal{H}_{\text{res}} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d n_d + \sum_{k\sigma} \left( V_k c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right) \tag{7.9.4}$$

The total Green's function is

$$G(z) = \frac{1}{z - \mathcal{H}_{\text{res}}} \tag{7.9.5}$$

The impurity diagonal Green's function is

$$G_{dd}(z) = \frac{1}{z - \epsilon_d - \Sigma_d(z)}, \quad G_d(z) = G_{dd} \,|d\rangle\,\langle d| \tag{7.9.6}$$

where $\Sigma_d(z)$ is in general complex and is zero at the free orbital fixed point. The conduction electron Green's function is

$$G_{kk}(z) = G_k^0(z) + \left[ G_k^0(z) V_k \right]^2 G_{dd}(z), \quad G_c(z) \equiv \sum_k |k\rangle\,\langle k|\, G_{kk}(z), \quad G_{c0}(z) \equiv \sum_k G_{kk}^0(z)\, |k\rangle\,\langle k| \tag{7.9.7}$$

The total Green's function can be written as

$$\begin{aligned} G(z) &= \left( \sum_k |k\rangle\,\langle k| + |d\rangle\,\langle d| \right) G \left( \sum_k |k\rangle\,\langle k| + |d\rangle\,\langle d| \right) \\ &= \sum_k |k\rangle\,\langle k|\, G_{kk}(z) + G_{dd}(z)\,|d\rangle\,\langle d| + \text{off-diagonal terms} \\ &= G_c(z) + G_d(z) + \text{off-diagonal terms} \end{aligned} \tag{7.9.8}$$

The total number of electrons is given by

$$\begin{aligned} N &= \oint \frac{dz}{2\pi i} n_F(z) \text{Tr}\left[ G(z) \right] \\ &= \oint \frac{dz}{2\pi i} n_F(z) \text{Tr}\left[ G_d(z) + G_c(z) \right] \end{aligned} \tag{7.9.9}$$

The contour $\Gamma$ counts all the singularities of $\text{Tr} G(z)$, and thus encloses only the real axis of the complex plane (since $G(z)$ comes from a Hermitian matrix $\mathcal{H}_{\text{res}}$, all its singularities

are real). At this point, we can use an identity:

$$
\begin{aligned}
\mathrm{Tr}\left[G_d(z)\right] &= \mathrm{Tr}\left[\frac{|d\rangle\langle d|}{z-\epsilon_d-\Sigma_d(z)}\right] \\
&= \mathrm{Tr}\left[\frac{|d\rangle\langle d|}{z-\epsilon_d-\Sigma_d(z)}\frac{\partial(z-\epsilon_d)}{\partial z}\right] \\
&= \mathrm{Tr}\left[|d\rangle\langle d|\, G_{dd}\frac{\partial\left\{G_{dd}^{-1}(z)+\Sigma_d(z)\right\}}{\partial z}\right] \\
&= \mathrm{Tr}\left[G_d(z)\frac{\partial G_d^{-1}(z)}{\partial z}\right] + \mathrm{Tr}\left[G_d(z)\frac{\partial\Sigma_d(z)}{\partial z}\right] \\
&= \frac{\partial}{\partial z}\left[\ln\mathrm{Det}G_d^{-1}(z)\right] + \mathrm{Tr}\left[G_d(z)\frac{\partial\Sigma_d(z)}{\partial z}\right]
\end{aligned}
\tag{7.9.10}
$$

In the last step, we converted the trace to a determinant using

$$
\mathrm{Tr}\left[A\frac{\partial A^{-1}}{\partial z}\right] = \frac{\partial}{\partial z}\mathrm{Tr}\ln A^{-1} = \frac{\partial}{\partial z}\sum_i \ln\lambda_i = \frac{\partial}{\partial z}\ln\prod_i\lambda_i = \frac{\partial}{\partial z}\ln\mathrm{Det}A^{-1}
\tag{7.9.11}
$$

where $\lambda_i$ are the eigenvalues of $A^{-1}$. Substituting $\mathrm{Tr}\left[G_d(z)\right]$ into the total number of particles gives

$$
N = \oint\frac{dz}{2\pi i}n_F(z)\left[\frac{\partial}{\partial z}\ln\mathrm{Det}\left\{G_d^{-1}(z)\right\} + \mathrm{Tr}\left(G_d(z)\frac{\partial}{\partial z}\Sigma_d(z)\right) + \mathrm{Tr}G_c(z)\right]
\tag{7.9.12}
$$

The conduction electron part can also be simplified:

$$
\begin{aligned}
\mathrm{Tr}G_c(z) &= \mathrm{Tr}\left[G_{c0}(z) + \sum_k\left\{G_k^0(z)V_k\right\}^2 G_{dd}(z)\,|k\rangle\langle k|\right] \\
&= \mathrm{Tr}\left[G_{c0}(z)\right] + \sum_k\left[G_k^0(z)V_k\right]^2 G_{dd}(z)
\end{aligned}
\tag{7.9.13}
$$

Since $G_{c0}^{-1}(z) = z - \sum_k\epsilon_k\hat{n}_k$, we can write $\mathrm{Tr}\left[G_{c0}(z)\right] = \mathrm{Tr}\left[G_{c0}(z)\frac{\partial}{\partial z}G_{c0}^{-1}\right]$ and hence

$$
\mathrm{Tr}G_c(z) = \frac{\partial}{\partial z}\left[\ln\mathrm{Det}G_{c0}^{-1}(z)\right] + \sum_k\left[G_k^0(z)V_k\right]^2 G_{dd}(z)
\tag{7.9.14}
$$

Updating the total particles with this leads to

$$
\begin{aligned}
N = \oint\frac{dz}{2\pi i}n_F(z)\Bigg[&\frac{\partial}{\partial z}\ln\mathrm{Det}\left\{G_d^{-1}(z)\right\} + \frac{\partial}{\partial z}\ln\mathrm{Det}\left\{G_{c0}^{-1}(z)\right\} + \mathrm{Tr}\left(G_d(z)\frac{\partial}{\partial z}\Sigma_d(z)\right) \\
&+ \sum_k\left(V_kG_k^0\right)^2 G_{dd}(z)\Bigg]
\end{aligned}
\tag{7.9.15}
$$

For the resonant-level model, we have

$$\Sigma_d = \sum_k V_k^2 G_k^0 = \sum_k \frac{V_k^2}{z - \epsilon_k} \tag{7.9.16}$$

such that

$$\text{Tr}\left(G_d(z)\frac{\partial}{\partial z}\Sigma_d(z)\right) = -G_{dd}(z)\sum_k \left(V_k G_k^0\right)^2 \tag{7.9.17}$$

which allows us to write

$$N = \oint \frac{dz}{2\pi i}n_F(z)\left[\frac{\partial}{\partial z}\ln \text{Det}\left\{G_d^{-1}(z)\right\} + \frac{\partial}{\partial z}\ln \text{Det}\left\{G_{c0}^{-1}(z)\right\}\right] \tag{7.9.18}$$

At $T = 0$, $n_F$ is defined as 1 below the FS, $\frac{1}{2}$ at the FS and 0 above it.

$$N = \left[\oint_{\Gamma_<} + \frac{1}{2}\oint_{\Gamma_0}\right]\frac{dz}{2\pi i}\left[\frac{\partial}{\partial z}\ln \text{Det}\left\{G_d^{-1}(z)\right\} + \frac{\partial}{\partial z}\ln \text{Det}\left\{G_{c0}^{-1}(z)\right\}\right] \tag{7.9.19}$$

Following Seki and Yunoki, we can define a winding number for a Green's function $G(z)$:

$$n_{\text{Det}G^{-1}}(C) = \oint_C \frac{dz}{2\pi i}\frac{\partial\ln \text{Det}\,G^{-1}(z)}{\partial z} = \oint_{\text{Det}G^{-1}(C)}\frac{d\,\text{Det}\,G^{-1}}{\text{Det}\,G^{-1}} \tag{7.9.20}$$

Since $n_{\text{Det}\,G^{-1}(C)}$ counts the number of times the curve $\text{Det}\,G^{-1}(C)$ winds around the origin, it is integer-valued and topological. Seki and Yunoki also show that the this number is given by

$$n_{\text{Det}\,G^{-1}(C)} = P_{\text{Det}\,G}(C) - Z_{\text{Det}\,G}(C) \tag{7.9.21}$$

where $P_{f(z)}(C)$ is the number of poles of $f(z)$ enclosed by the contour $C$, and $Z$ is the corresponding number of zeros. The total number of particles in the resonant level model can thus be written as

$$\begin{aligned}
N = P_{\text{Det}\,G_d}(\Gamma_<) - Z_{\text{Det}\,G_d}(\Gamma_<) + \frac{1}{2}\left[P_{\text{Det}\,G_d}(\Gamma_0) - Z_{\text{Det}\,G_d}(\Gamma_0)\right]\\
+P_{\text{Det}\,G_{c0}}(\Gamma_<) - Z_{\text{Det}\,G_{c0}}(\Gamma_<) + \frac{1}{2}\left[P_{\text{Det}\,G_{c0}}(\Gamma_0) - Z_{\text{Det}\,G_{c0}}(\Gamma_0)\right]
\end{aligned} \tag{7.9.22}$$

The average number of particles can thus be expressed purely in terms of the number of poles and zeros of the impurity and the conduction electron Green's functions. As shown by Seki and Yunoki, the second line gives the Luttinger volume $V_L$:

$$N = P_{\text{Det}\,G_d}(\Gamma_<) - Z_{\text{Det}\,G_d}(\Gamma_<) + \frac{1}{2}\left[P_{\text{Det}\,G_d}(\Gamma_0) - Z_{\text{Det}\,G_d}(\Gamma_0)\right] + V_L \tag{7.9.23}$$

If we start from a non-interacting model ($V_k = 0$), we can write

$$N = \mathcal{N}_{imp}^0 + V_L^0 \tag{7.9.24}$$

where $\mathcal{N}_{imp}^0$ is simply the number of singularities of $G_d$ on the real axis, for the non-interacting case. We now turn up the interaction $V_k$, keeping the total number of particles conserved at $N$. With a non-zero $V_k$, the impurity self-energy can be written (assuming a constant density of states) as

$$\Sigma_d(z) = \Sigma_d^{\text{real}}(z) - i\Delta \tag{7.9.25}$$

so that the impurity Greens function becomes

$$G_d(z) = \frac{1}{z - \epsilon_d - \Sigma_d^{\text{real}}(z) + i\Delta} \tag{7.9.26}$$

We can see that the presence of an imaginary part lifts the pole of $G_d(z)$ off the real axis, and since the contour $\Gamma_0$ encloses only the real axis, this will count as a loss in the number of poles of $G_d(z)$. Also, if we specialize to the case where the renormalized impurity site energy $\epsilon_d^* = \epsilon_d + \Sigma_d^{\text{real}} = 0$, this loss will happen at the Fermi surface, and will hence be multiplied by a factor of half. We can therefore write

$$N = \mathcal{N}_{imp} + V_L = \mathcal{N}_{imp}^0 - \frac{1}{2} + V_L$$
$$\implies V_L = V_L^0 + \frac{1}{2} \tag{7.9.27}$$

If we take into account the spin-degeneracy and redefine $V_L$ to mean the Luttinger volume for both momentum and spin degrees of freedom, we get

$$V_L = V_L^0 + 1 \tag{7.9.28}$$

This is a specific case of the more general result for Kondo lattices obtained by Oshikawa
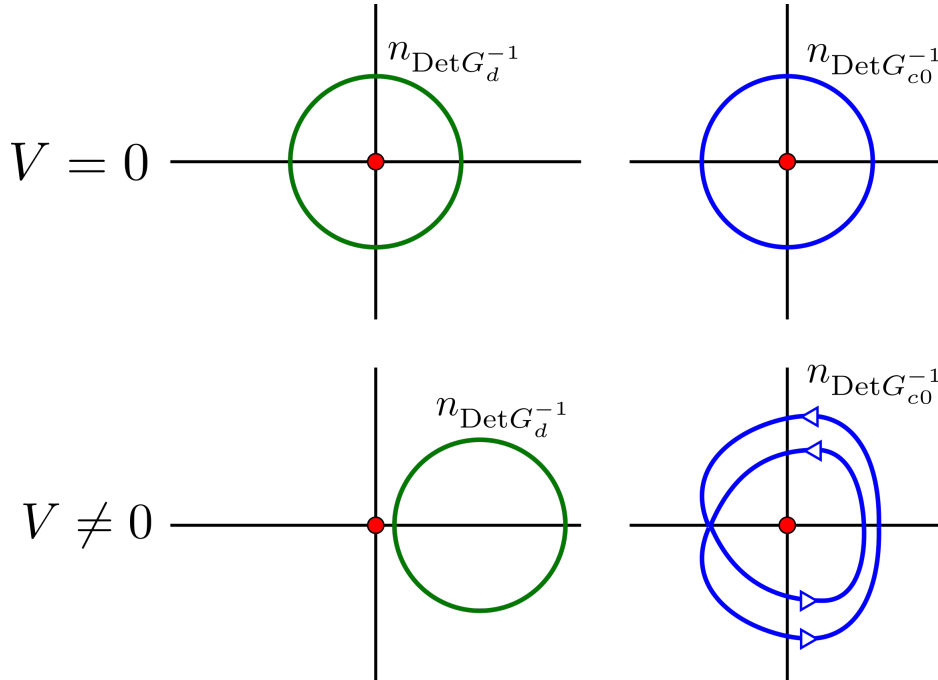
using flux-insertion arguments in [40]. One can now ask what happens to this result once we also incorporate the spin-exchange interaction $J\vec{S}_d \cdot \vec{s}$; we can expect that it will complicate the self-energy of the impurity. It cannot, however, preclude the loss of the real pole, nor can it create a new singularity - to do so would require the self-energy to diverge, and we are working with finite systems here. This suggests that the eq. 7.9.28 would still hold.

We have also not accounted for the RG flow from the local moment fixed point to the strong-coupling fixed point. The local moment fixed point is characterized by a decoupled quantum top:

$$\mathcal{H}_{\text{LM}} = \epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \tag{7.9.29}$$

It can be shown that the single-particle Green's function for this effective Hamiltonian is similar to the one at the free-orbital fixed point. We will use the equation of motion technique to solve for the Green's function. The time-domain retarded Green's function is defined as

$$G_{d\sigma}(t, t') = -i\theta(t - t') \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(t') \right\} \right\rangle \tag{7.9.30}$$

Since the Hamiltonian is time-translation invariant, we can drop one of the instants:

$$G_{d\sigma}(t, 0) = -i\theta(t) \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \tag{7.9.31}$$

The time derivative is

$$
\begin{aligned}
\partial_t G_{d\sigma} &= -i \left[ \partial_t \theta(t) \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle + \theta(t) \partial_t \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \right] \\
&= -i \left[ \delta(t) \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle + \theta(t) \left\langle \left\{ \partial_t c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \right] \\
&= -i\delta(t) - i\theta(t) \left\langle \left\{ \partial_t c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle
\end{aligned}
\tag{7.9.32}
$$

From the Heisenberg equations of motion, we get

$$i\partial_t c_{d\sigma}(t) = \left[ c_{d\sigma}(t), \mathcal{H}_{LM}(t) \right] = \left[ \epsilon_d + U\hat{n}_{d\bar{\sigma}}(t) \right] c_{d\sigma}(t) \tag{7.9.33}$$

Substituting this into the time-derivative gives

$$
\begin{aligned}
\partial_t G_{d\sigma} &= -i\delta(t) - i\theta(t) \left\langle \left\{ -i \left[ \epsilon_d + U\hat{n}_{d\bar{\sigma}}(t) \right] c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \\
&= -i\delta(t) - i\epsilon_d G_{d\sigma} - U\theta(t) \left\langle \hat{n}_{d\bar{\sigma}}(t) \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle
\end{aligned}
\tag{7.9.34}
$$

We define another Greens function

$$G' = -i\theta(t) \left\langle \hat{n}_{d\bar{\sigma}}(t) \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \tag{7.9.35}$$

which satisfies the equation of motion

$$\partial_t G' = -i\delta(t) - i\theta(t)\left\langle\left\{\partial_t \hat{n}_{d\bar{\sigma}}(t)c_{d\sigma}(t), c^{\dagger}_{d\sigma}(0)\right\}\right\rangle - i\theta(t)\left\langle\left\{\hat{n}_{d\bar{\sigma}}(t)\partial_t c_{d\sigma}(t), c^{\dagger}_{d\sigma}(0)\right\}\right\rangle \qquad (7.9.36)$$

The second term vanishes because $\left[\hat{n}_{d\bar{\sigma}}, \mathcal{H}_{LM}\right] = 0$ and hence $\partial_t \hat{n}_{d\bar{\sigma}} = 0$. Also,

$$\hat{n}_{d\bar{\sigma}}(t)\partial_t c_{d\sigma}(t) = -i\hat{n}_{d\bar{\sigma}}(t)\left[\epsilon_d + U\hat{n}_{d\bar{\sigma}}(t)\right]c_{d\sigma}(t) = -i\left[\epsilon_d + U\right]\hat{n}_{d\bar{\sigma}}(t)c_{d\sigma}(t) \qquad (7.9.37)$$

Therefore,

$$\partial_t G' = -i\delta(t)\left\langle\hat{n}_{d\bar{\sigma}}(0)\right\rangle - \left[\epsilon_d + U\right]\theta(t)\left\langle\left\{\hat{n}_{d\bar{\sigma}}(t)c_{d\sigma}(t), c^{\dagger}_{d\sigma}(0)\right\}\right\rangle = -i\delta(t) - i\left(\epsilon_d + U\right)G' \quad (7.9.38)$$

Changing all quantities to frequency-domain:

$$G'(t) = \int_{-\infty}^{\infty} d\omega e^{-i\omega t} G'(\omega)$$

$$\partial_t G'(t) = -\int_{-\infty}^{\infty} d\omega i\omega e^{-i\omega t} G'(\omega) \qquad (7.9.39)$$

$$\delta(t) = \int_{-\infty}^{\infty} d\omega e^{-i\omega t}$$

Substituting these forms in the equation and comparing the coefficients of $e^{i\omega t}$ gives

$$\omega G'(\omega) = \left\langle\hat{n}_{d\bar{\sigma}}(0)\right\rangle + \left(\epsilon_d + U\right)G'(\omega) \implies G'(\omega) = \frac{\left\langle\hat{n}_{d\bar{\sigma}}(0)\right\rangle}{\omega - \epsilon_d - U} \qquad (7.9.40)$$

The equation of motion $G_{d\sigma}$ can now be solved

$$\partial_t G_{d\sigma}(t) = -i\delta(t) - i\epsilon_d G_{d\sigma}(t) - iUG'_{d\sigma}(t)$$

$$\implies \omega G_{d\sigma}(\omega) = 1 + \epsilon_d G_{d\sigma}(\omega) + U\frac{\left\langle\hat{n}_{d\bar{\sigma}}(0)\right\rangle}{\omega - \epsilon_d - U} \qquad (7.9.41)$$

$$\implies G_{d\sigma}(\omega) = \frac{1}{\omega - \epsilon_d} + \frac{U\left\langle\hat{n}_{d\bar{\sigma}}(0)\right\rangle}{\left(\omega - \epsilon_d\right)\left(\omega - \epsilon_d - U\right)}$$

For a particle-hole symmetric system, we can substitute $\epsilon_d = -|\epsilon_d|$ and $\epsilon_d + U = |\epsilon_d|$.

$$G_{d\sigma}(\omega) = \frac{1}{\omega + |\epsilon_d|} + \frac{U\left\langle\hat{n}_{d\bar{\sigma}}(0)\right\rangle}{\left(\omega + |\epsilon_d|\right)\left(\omega - |\epsilon_d|\right)} \qquad (7.9.42)$$

which reveals two poles at $\pm|\epsilon_d|$, one above and one below the Fermi surface. Since the RHS of eq. 7.9.23 counts the number of poles on or below the FS, we will still count one pole for $G_{d\sigma}$. Thus, this Green's function is topological similar to the free-orbital one at $T = 0$.

The scattering phase shift suffered by the conduction electrons at the Fermi surface, off

the impurity, can be calculated from the impurity occupancy, using the Friedel sum rule. From the ground state wavefunction, we can calculate the average number of particles on the impurity:

$$\langle n_d \rangle = \langle GS | \sum_\sigma \hat{n}_{d\sigma} | GS \rangle \tag{7.9.43}$$

$|GS\rangle$ is the lower energy state in eq. 6.4.34. Performing the inner product gives

$$\langle n_d \rangle = \left( c_s^- \right)^2 + \left( c_c^- \right)^2 = 1 \tag{7.9.44}$$

The phase shift is thus

$$\frac{1}{\pi} \sum_\sigma \delta_\sigma(0) = \langle n_d \rangle \implies \delta_\sigma(0) = \frac{\pi}{2} \tag{7.9.45}$$

There we used $\delta_\uparrow = \delta_\downarrow$ because the model is SU(2)-symmetric. This line of arguments was first presented for the Kondo model in [24].

The change in Luttinger's number also allows us to calculate the Wilson ratio of the system, from eq. 2.7.7.

$$R = 1 + \sin^2 \left( \frac{\pi}{2} \Delta N_L \right) = 1 + \sin^2 \frac{\pi}{2} = 2 \tag{7.9.46}$$

## 7.10   Reverse RG analysis

The goal here is to chart the journey starting from the IR fixed point towards the UV regime, by following one particular wavefunction. We will start with a very simple IR ground state wavefunction, and then go back towards the UV ground state by applying the inverse unitary operator $U^\dagger$:

$$U: \quad \underbrace{|1, 2, ..., N\rangle}_{\text{UV ground state}} \rightarrow |1, 2, ..., N-1\rangle |N\rangle \rightarrow ... \rightarrow \underbrace{|1, 2, ..., N^*\rangle |N^* + 1\rangle ... |N\rangle}_{\text{IR ground state}}$$

$$U^\dagger: \underbrace{|1, 2, ..., N^*\rangle |N^* + 1\rangle ... |N\rangle}_{\text{IR ground state}} \rightarrow |1, 2, ..., N^* + 1\rangle |N^* + 2\rangle ... |N\rangle \rightarrow ... \rightarrow \underbrace{|1, , 2, ..., N\rangle}_{\text{UV ground state}}$$

The first process is the forward RG which we used to obtain the scaling equations. The second process is the reverse RG which we wil undertake now. *The IR ground state we will start with will consist of four momenta states, $k_{-2,-1,1,2}$. $k_{1,2}$ will be the states above the Fermi surface while $k_{-1,-2}$ will be the ones below it.* The algorithm of reverse RG is shown in fig. 7.11.

For the purpose of illustrating how we will construct the many-body ground state however, we will work with just two momenta states instead of four, one above and one below.

$$|\text{cloud}\rangle = c_-^s \left( |\uparrow^d, \downarrow\rangle - |\downarrow^d, \uparrow\rangle \right) + c_-^c \left( |\uparrow_c^d, \downarrow_c\rangle + |\downarrow_c^d, \uparrow_c\rangle \right) \tag{7.10.1}$$
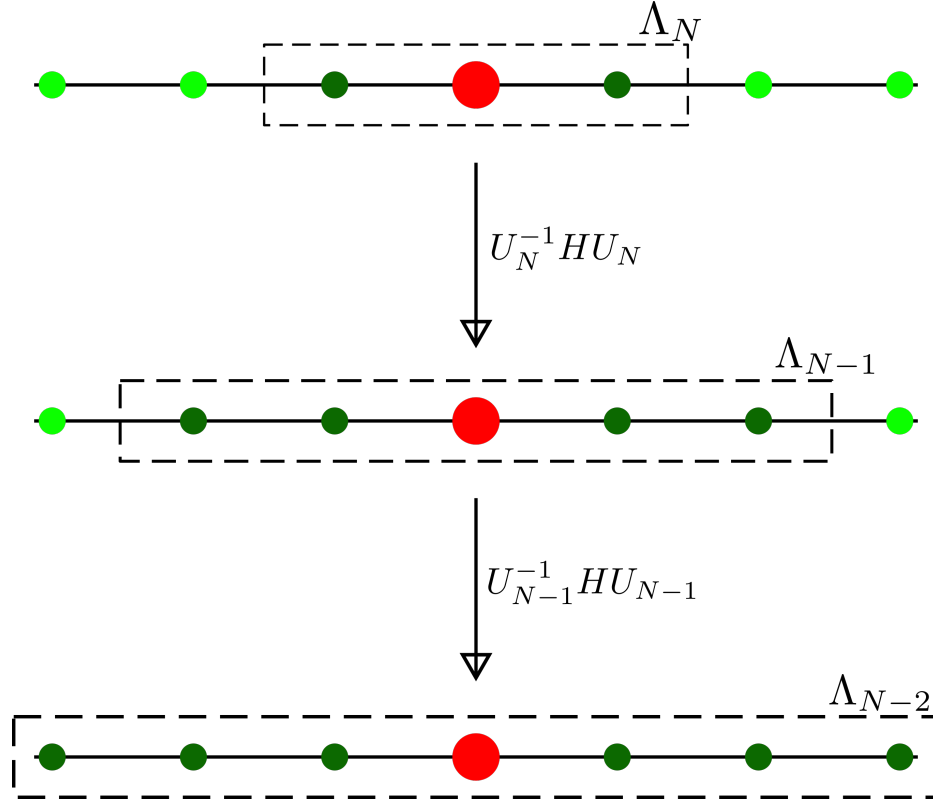
Figure 7.11: Algorithm of reverse RG. We start with a Hamiltonian with an impurity site (red) coupled with two conduction electrons (dark green), with four other decoupled electrons (bright green). The dotted rectangle represents the emergent window $\left(-\Lambda_j, \Lambda_j\right)$ at each step; the electrons inside that rectangle are still entangled with the impurity, while the ones inside have been decoupled. The next step of reverse RG involves applying the inverse transformation on the Hamiltonian, which will couple two more electrons from the IOMS (hence four dark green circles in the second step), leading to an enlargement of the emergent window. The unitary varies for each step, hence the notation $U_j$.
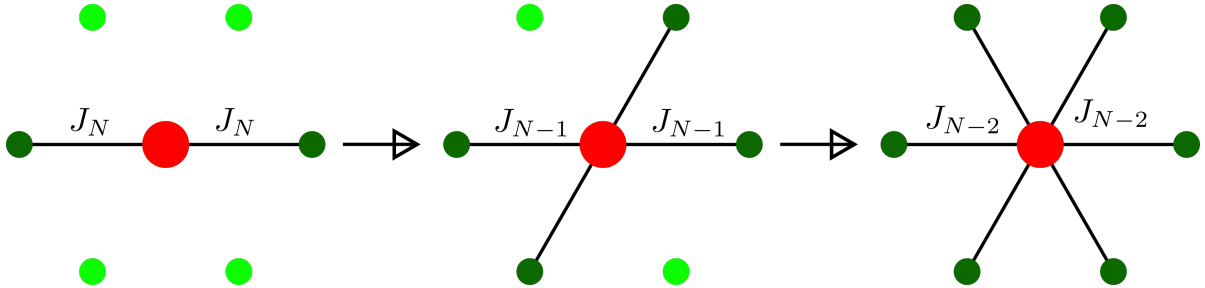


Figure 7.12: Increase in the number of coupled elements under reverse RG. We start with the impurity coupled with two electrons, which increases at each step of the reverse RG. The weight of the bonds changes at each step, and is described by the running couplings $V_j, J_j, K_j$. The onsite energy of the impurity itself also varies at each step, which is essentially the renormalization in $\epsilon_d$ and $U$.

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where $\uparrow_c$ represents a state with $C^z = \frac{1}{2}$ and the $d$ in the superscript indicates it is for the impurity. Cloud refers to the system of the still-entangled electrons and the impurity. To construct the states $|\uparrow\rangle, |\downarrow\rangle, |\uparrow_c\rangle$ and $|\downarrow_c\rangle$, we will look the two-site spin and charge operators. The impurity states are easy to construct. $\uparrow$ and $\downarrow$ consist of singly occupied impurities with the respective spins, while the charge versions involve double-occupied and vacant impurities respectively.

For the conduction electrons, we have

$$S_2^z = \frac{1}{2N^*} \sum_{kk'} \left( c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) \tag{7.10.2}$$

The eigenstate for this operator, with an eigenvalue of $+\frac{1}{2}$, is

$$|\uparrow\rangle \equiv \frac{1}{N^*} \sum_{k\in[-\Lambda^*,\Lambda^*]} |k \uparrow\rangle = \frac{1}{N^*} \sum_{k\in[-\Lambda^*,\Lambda^*]} |\hat{n}_{k\uparrow} = 1, \hat{n}_{q\sigma\neq k\uparrow} = 0\rangle \tag{7.10.3}$$

The state $|k \uparrow\rangle$ is formally $c_{k\uparrow}^\dagger |0\rangle$, $|0\rangle$ being the state with no particles. In other words, the state $|\uparrow\rangle$ is simply the equal superposition of all states with a single up electron.

To show that this is indeed the eigenstate of $S_2^z$, we compute the action of $S_2^z$ on this state:

$$S_2^z |\uparrow\rangle = \frac{1}{2N^{*2}} \sum_{kk'q} \left( c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) |q \uparrow\rangle \tag{7.10.4}$$

We have dropped the regime of the summation because it is understood that all momenta are summed inside the fixed point window. We can drop the second part $c_{k\downarrow}^\dagger c_{k'\downarrow}$ because there is no down spin electron to annihilate.

$$\begin{aligned}
S_2^z |\uparrow\rangle &= \frac{1}{2N^{*2}} \sum_{kk'q} c_{k\uparrow}^\dagger c_{k'\uparrow} |q \uparrow\rangle \\
&= \frac{1}{2N^{*2}} \sum_{kk'q} c_{k\uparrow}^\dagger c_{k'\uparrow} \delta_{k'q} |q \uparrow\rangle \\
&= \frac{1}{2N^{*2}} \sum_{kk'} c_{k\uparrow}^\dagger |0\rangle \qquad\qquad\qquad (7.10.5)\\
&= \frac{1}{2N^*} \sum_{k} c_{k\uparrow}^\dagger |0\rangle \qquad\qquad \left[\sum_{k'} = N^*\right] \\
&= \frac{1}{2} |\uparrow\rangle
\end{aligned}$$

We can find the other eigenstate by applying on this state with $S_2^-$:

$$S_2^- \left|\uparrow\right\rangle = \frac{1}{N^{*2}} \sum_{kk'q} c_{k\downarrow}^\dagger c_{k'\uparrow} \left|q \uparrow\right\rangle$$

$$= \frac{1}{N^*} \sum_{k} c_{k\downarrow}^\dagger \left|0\right\rangle \qquad (7.10.6)$$

$$= \frac{1}{N^*} \sum_{k} \left|k \downarrow\right\rangle$$

Thus, the eigenstate for $S_2^z = -\frac{1}{2}$ is

$$\left|\downarrow\right\rangle = \frac{1}{N^*} \sum_{k} \left|k \downarrow\right\rangle \qquad (7.10.7)$$

Now we turn to the eigenstates of $C_2^z$. That operator is defined as

$$C_2^z = \frac{1}{2N^*} \sum_{kk'} \left( c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k'\downarrow} c_{k\downarrow}^\dagger \right) \qquad (7.10.8)$$

The eigenstate for $C_2^z = +\frac{1}{2}$ will be

$$\left|\uparrow_c\right\rangle \equiv \frac{1}{N^{*2}} \sum_{kk'} \left|k \uparrow, k' \downarrow\right\rangle \qquad (7.10.9)$$

which means you consider all pairs of momenta and place an up electron on one of them and a down on the other. The action of $C_2^z$ on this state is

$$C_2^z \left|\uparrow_c\right\rangle = \frac{1}{2N^{*3}} \sum_{kk'qq'} \left( c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k'\downarrow} c_{k\downarrow}^\dagger \right) \left|q \uparrow, q' \downarrow\right\rangle$$

$$= \frac{1}{2N^{*3}} \sum_{kk'qq'} \left[ c_{k\uparrow}^\dagger c_{k'\uparrow} \left|q \uparrow, q' \downarrow\right\rangle - \left( \delta_{k'k} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) \left|q \uparrow, q' \downarrow\right\rangle \right] \qquad (7.10.10)$$

$$= \frac{1}{2N^{*3}} \sum_{kk'qq'} \left[ \delta_{k'q} \left|k \uparrow, q' \downarrow\right\rangle - \delta_{k'k} \left|q \uparrow, q' \downarrow\right\rangle + \delta_{k'q'} \left|q \uparrow, k \downarrow\right\rangle \right]$$

Since all the momenta labels are dummy indices, we exchange the labels $k$ and $q'$ in the third term. The second and third terms then cancel out, and we are left with

$$C_2^z \left|\uparrow_c\right\rangle = \frac{1}{2N^{*2}} \sum_{kk'qq'} \left|k \uparrow, q' \downarrow\right\rangle$$

$$= \frac{1}{2} \left|\uparrow_c\right\rangle \qquad (7.10.11)$$

The down eigenstate is

$$C_2^- \left|\uparrow_c\right\rangle = \frac{1}{N^{*3}} \sum_{kk'qq'} c_{k\downarrow} c_{k'\uparrow} \left|q \uparrow, q' \downarrow\right\rangle \qquad (7.10.12)$$

$$= \left|0\right\rangle$$

which is the state with all states empty. We can thus write down the still-entangled of the ground state wavefunction:

$$|\text{cloud}\rangle = c^s_- \left[ |\uparrow^d\rangle \frac{1}{\sqrt{2}} \left( |k_1 \downarrow\rangle + |k_{-1} \downarrow\rangle \right) - |\downarrow^d\rangle \frac{1}{\sqrt{2}} \left( |k_1 \uparrow\rangle + |k_{-1} \uparrow\rangle \right) \right] + c^c_- \left[ |2^d\rangle |0\rangle \right.$$

$$\left. + |0^d\rangle \frac{1}{N^*} \sum_{kk'} |k \uparrow, k' \downarrow\rangle \right] \tag{7.10.13}$$

This state will of course be in direct product with the disentangled electronic states (integrals of motions, IOMS) outside the emergent window. If we assume there are two such momenta (hence four momenta+spin) states on either side of the emergent window (which we label as $k_{\pm2}\sigma, k_{\pm3}\sigma$), and if we recall that we had used the configuration $\hat{n} = 0$ for the IOMS above the FS and $\hat{n} = 1$ for the ones below, the total state becomes

$$|\text{IR}\rangle \equiv |\Psi_0\rangle = |\hat{n}_{k_{-2}} = \hat{n}_{k_{-3}} = 2\rangle \otimes |\text{cloud}\rangle \otimes |\hat{n}_{k_2} = \hat{n}_{k_3} = 0\rangle \tag{7.10.14}$$

In order to allow a numerical implementation of the reverse RG, we need to write this wavefunction completely as sums of Fock states. We will use the following notation:

$$\left| \overbrace{n_{k_3\uparrow} n_{k_3\downarrow} n_{k_2\uparrow} n_{k_2\downarrow}}^{\text{unoccupied IOMS}} \quad \underbrace{n_{k_1\uparrow} n_{k_1\downarrow}}_{\text{cloud above FS}} \quad \overbrace{n_{d\uparrow} n_{d\downarrow}}^{\text{impurity}} \quad \underbrace{n_{k_{-1}\uparrow} n_{k_{-1}\downarrow}}_{\text{cloud below FS}} \quad \overbrace{n_{k_{-2}\uparrow} n_{k_{-2}\downarrow} n_{k_{-3}\uparrow} n_{k_{-3}\downarrow}}^{\text{occupied IOMS}} \right\rangle \tag{7.10.15}$$

$$|\Psi_0\rangle = \frac{c^s_-}{\sqrt{2}} |0000\rangle \otimes |\uparrow^d\rangle |k_1 \downarrow, k_{-1} \downarrow\rangle \otimes |1111\rangle - \frac{c^s_-}{\sqrt{2}} |0000\rangle \otimes |\downarrow^d\rangle |k_1 \uparrow, k_{-1} \uparrow\rangle \otimes |1111\rangle$$

$$\frac{c^c_-}{\sqrt{2}} |0000\rangle \otimes |2^d\rangle |0\rangle \otimes |1111\rangle + \frac{c^c_-}{\sqrt{2}} |0000\rangle \otimes |0^d\rangle |k_1 \uparrow, k_1 \downarrow, k_{-1} \uparrow, k_{-1} \downarrow\rangle \otimes |1111\rangle$$

$$= |0000\rangle \otimes \left[ \frac{c^s_-}{\sqrt{2}} |01\rangle \underbrace{|10\rangle}_{\text{imp}} |01\rangle - \frac{c^s_-}{\sqrt{2}} |10\rangle \underbrace{|01\rangle}_{\text{imp}} |10\rangle + \frac{c^c_-}{\sqrt{2}} |00\rangle \underbrace{|11\rangle}_{\text{imp}} |00\rangle \right.$$

$$\left. + \frac{c^c_-}{\sqrt{2}} |11\rangle \underbrace{|00\rangle}_{\text{imp}} |11\rangle \right] \otimes |1111\rangle$$

$$\tag{7.10.16}$$

The next step is to write down the unitaries that will take us from the IR ground state to the UV ground state. In the forward RG, we used the following unitaries for decoupling an electron $q\beta$:

$$U_{0\beta} = \frac{1}{\sqrt{2}} \left[ 1 - \eta^\dagger_{0\beta} + \eta_{0\beta} \right]$$

$$U_{1\beta} = \frac{1}{\sqrt{2}} \left[ 1 + \eta^\dagger_{1\beta} - \eta_{1\beta} \right] \tag{7.10.17}$$

where the subscripts 0 and 1 indicate it decouples an electron above and below the Fermi surface respectively, and the subscript $\beta$ indicates the spin of that electron. The total unitary is

$$U = \frac{1}{4}\left[1 + \eta^\dagger_{1\uparrow} + \eta_{0\uparrow} + \eta^\dagger_{1\downarrow} + \eta_{0\downarrow}\right] \tag{7.10.18}$$

The inverse transformation for re-entangling $q\beta$ is

$$U^\dagger = \frac{1}{2}\left[1 + \eta_{1\uparrow} + \eta^\dagger_{0\uparrow} + \eta_{1\downarrow} + \eta^\dagger_{0\downarrow}\right] \tag{7.10.19}$$

Here, $U^\dagger_{0\beta}$ re-couples an electron $q\beta$ above the Fermi surface. The $\eta$-s are

$$
\eta^\dagger_{0\beta} = V\left[\lambda_2 \hat{n}_{d\overline{\beta}} + \lambda_1\left(1 - \hat{n}_{d\overline{\beta}}\right)\right]c^\dagger_{q\beta}c_{d\beta} + \lambda_3\sum_k\left\{\frac{J}{2}\left(S^z_d\beta c^\dagger_{q\beta}c_{k\beta} + c^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{q\beta}c_{k\overline{\beta}}\right)\right.
$$
$$
\left. + \frac{K}{2}\left(C^z_d c^\dagger_{q\beta}c_{k\beta} + c^\dagger_{q\beta}c^\dagger_{k\overline{\beta}}c_{d\overline{\beta}}c_{d\beta}\right)\right\} \tag{7.10.20}
$$

$$
\eta_{1\beta} = V^*\left[\lambda_1 \hat{n}_{d\overline{\beta}} + \lambda_2\left(1 - \hat{n}_{d\overline{\beta}}\right)\right]c^\dagger_{d\beta}c_{q\beta} + \lambda_3\sum_k\left\{\frac{J}{2}\left(S^z_d\beta c^\dagger_{k\beta}c_{q\beta} + c^\dagger_{d\beta}c_{d\overline{\beta}}c^\dagger_{k\overline{\beta}}c_{q\beta}\right)\right.
$$
$$
\left. + \frac{K}{2}\left(C^z_d c^\dagger_{k\beta}c_{q\beta} + c^\dagger_{d\beta}c^\dagger_{d\overline{\beta}}c_{k\overline{\beta}}c_{q\beta}\right)\right\} \tag{7.10.21}
$$

with

$$\lambda_1 = \frac{1}{\omega - \frac{1}{2}D + \epsilon_d + \frac{1}{2}K}, \quad \lambda_2 = \frac{1}{\omega - \frac{1}{2}D - \epsilon_d + \frac{1}{2}J}, \quad \lambda_3 = \frac{1}{\omega - \frac{1}{2}D + \frac{1}{4}\left(J + K\right)} \tag{7.10.22}$$

The wavefunction after reversing one step of the RG will thus be

$$|\Psi_1\rangle = U^\dagger_{0\uparrow}U^\dagger_{0\downarrow}U^\dagger_{1\uparrow}U^\dagger_{1\downarrow}|\Psi_0\rangle \tag{7.10.23}$$

The results of the reverse RG study are depicted in the following plots. We have used two types of quantities in the process - mutual information and correlation functions. The mutual information between two subsystems $A$ and $B$ in a wavefunction with many subsystems is defined as

$$I(A : B) = S_A + S_B - S_{AB} \tag{7.10.24}$$

where $S_{ij..q}$ is the von-Neumann entropy of the reduced density matrix obtained after tracing out all degrees of freedom except those in the subscript of $S$.

The mutual information between two electrons inside the entangled cloud increases as we go towards the IR fixed point. This can be understood in the following manner; as the wavefunction flows towards a smaller sized emergent cloud, the entanglement between those electrons gets distilled out.

We have also computed some correlation functions. All of them increase towards the IR fixed point. The increase in the correlation function $\left\langle \hat{n}_{k_1\uparrow}\hat{n}_{k_2\downarrow}\right\rangle$ arises from the crystallization of the spin singlet at the fixed point. The increase in the correlation function $\left\langle \hat{n}_{k\uparrow}\hat{n}_{k\downarrow}\right\rangle$ arises from the charge triplet content of the wavefunction, showing the increase of the charge contribution on the momenta. The increase in the off-diagonal correlation function $\left\langle c_{k\uparrow}^{\dagger}c_{k'\downarrow}c_{q\downarrow}^{\dagger}c_{q'\uparrow}\right\rangle$ shows that the there is a large and non-trivial interaction between the electrons of the cloud that is being mediated by the impurity electron. This interaction is not of the Fermi liquid type, but instead was obtained in the effective Hamiltonian for the Kondo cloud.
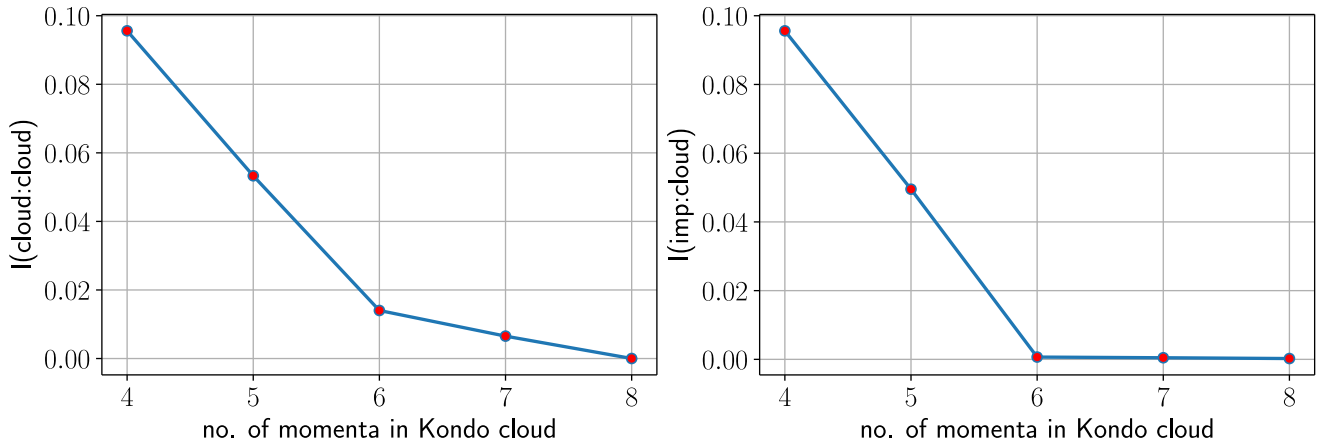


Figure 7.13: *Left*: Mutual information between two conduction electrons inside the cloud. *Right*: Mutual information between a conduction electron inside the cloud and an impurity electron.
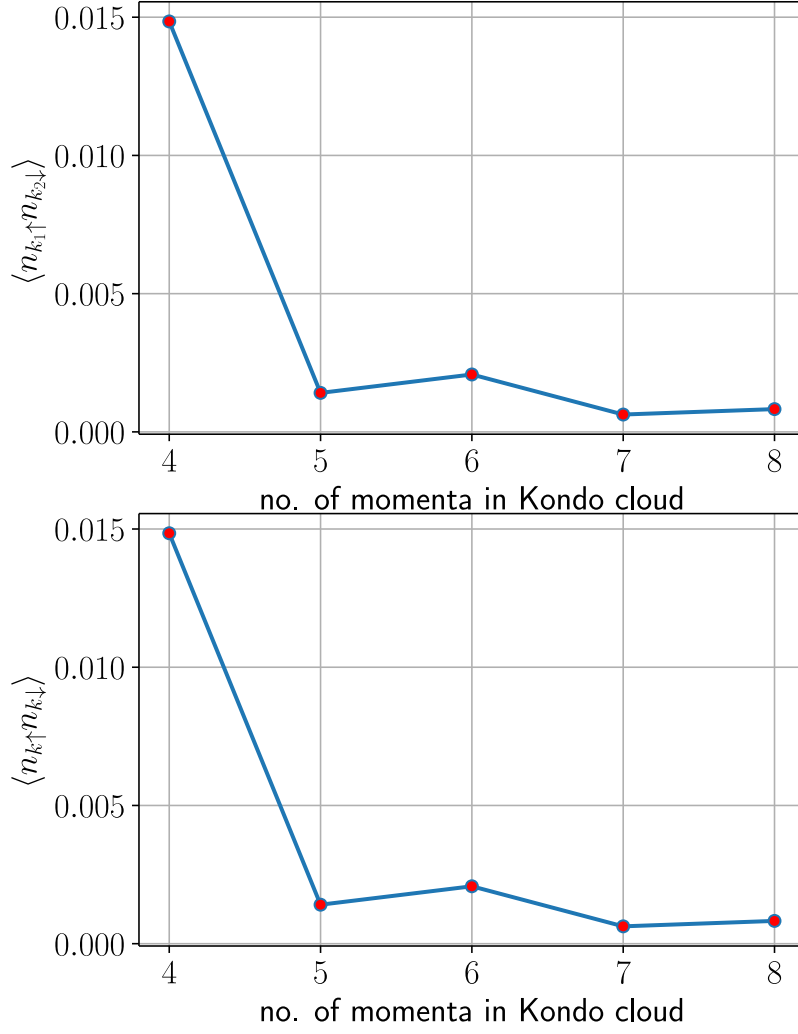
233

Figure 7.14: Diagonal correlation functions between cloud electrons
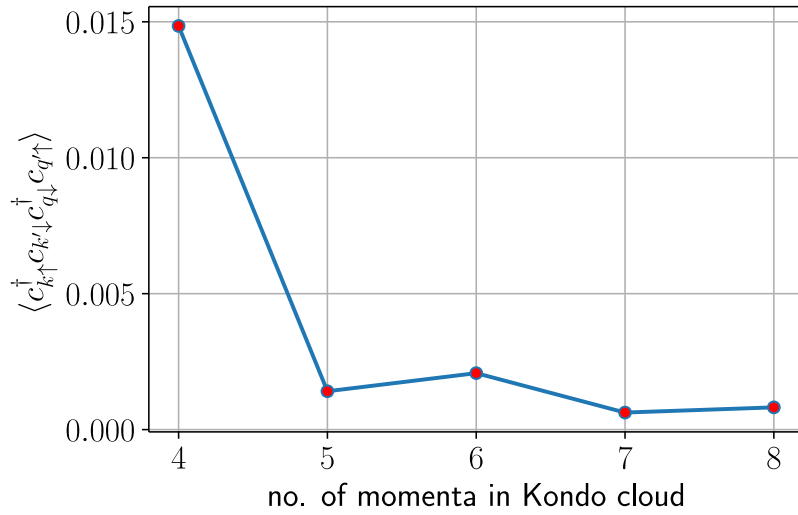


Figure 7.15: off-diagonal correlation function

# Chapter 8

# Conclusions and Future Directions

In this work, we have seen that the fate of the SIAM at low temperatures is a growth in the spin, charge and hybridisation couplings $J, K$ and $V$. This confirms the NRG and Bethe ansatz result that the low energy behavior is that of a screened impurity. We stress that the spin or the charge exchange coupling, $J$ or $K$, is necessary to screen the corresponding degree of freedom on the impurity. The ground state wavefunction for the low energy theory is primarily a spin-singlet with some charge-triplet content in the spin-Kondo regime. In the charge-Kondo regime, we find a charge-singlet instead. The susceptibility is seen to increase as we go to lower temperatures, signaling increased spin-flip scattering and providing a justification for the increase in resistivity after the Kondo temperature $T_K$. At high temperatures the susceptibility saturates to $\frac{1}{8}$, mimicking a four-fold degenerate object because at high temperatures, the impurity energy scales become blurred.

We also obtain a Hamiltonian for the Kondo cloud (the set of electrons which screen the impurity) - it has a Fermi liquid number diagonal term as well as an off-diagonal non-Fermi liquid piece. It is this off-diagonal piece that is responsible for the strong entanglement between the impurity and the conduction electrons. This contribution is found to increase as we move towards the infrared fixed point. Higher order scattering processes will give more complicated terms in the effective Hamiltonian. We also calculate information-theoretic quantities like mutual information between impurity and conduction electrons. They show that the conduction electrons become more strongly-entangled as we move towards the infrared fixed point. They also reveal an increase in off-diagonal correlations between conduction electrons which is indicative of an increase in the off-diagonal scattering content in the effective Hamiltonian of the Kondo cloud. We also find the value of the zero-temperature Wilson ratio to be 2 in the Kondo regime. Closely related to this is the result that the Luttinger's volume at the fixed point accommodates the impurity site into the Fermi volume such that Luttinger's count increases by 1 compared to the value at the free-orbital or local moment fixed points. The renormalization of the impurity spectral across the RG shows the emergence of the central resonance at the strong-coupling fixed point.

This work still leaves some problems untouched. Some new questions and interesting

prospects have also emerged. We discuss them now.

- Can we obtain an analytical expression for the finite temperature Wilson ratio? The zero temperature value was obtained using low temperature approximations, so a finite temperature calculation would need to be non-perturbative. In other words, the full effect of the conduction bath will most probably come into play.

- The spectral function of the impurity is another interesting quantity to explore. It is not yet completely certain which parts of the effective Hamiltonian for the cloud lead to which features of the spectral function. It would be interesting to check whether the Fermi liquid part gives the central peak and the non-Fermi liquid the side humps, or something else altogether. We also intend to explore the bath spectral function and its variation under the RG.

- In Chapter 4, we find that the URG renormalization in Hamiltonian has a form similar to that of URG - a generalized double-bracket form. This suggests that URG might have uses in linear algebra as well. It is well-known that transformations of the double-bracket form are unitary and can be used in minimization and sorting problems [10]. It has also been shown that the unitary flows correspond to motion along a geodesic if a suitable manifold is defined. This suggests that we can look for a quantity which is minimized by URG in the journey towards the fixed point and see if it can be used to provide a faster and more robust algorithm for optimization problems.

- One can also look into the lattice versions of these models - the Kondo lattice and the Anderson lattice problems which involve two interacting bands - one for the impurity and the other for the conduction electrons [41]. Since there is a macroscopic number of impurity electrons, such a model shows phase transitions. One big project for the future can be to look into such models, map the phase diagram and search for superconducting phases or non-Fermi liquid phases.

- We have seen that the zero-mode of the low-energy effective Hamiltonian is essentially a two-site Anderson model(a.k.a Anderson dimer), which can be solved exactly. An interesting endeavor in this context could be to see if there is a unitary transformation that converts the Anderson dimer to a two-site Hubbard model (Hubbard dimer). The point of this exercise would be to shed some light on the inner workings of DMFT. The imposition of the self-consistency requirement in DMFT introduces a translational invariance into the Anderson model and converts it into the Hubbard model. If we could figure out a transformation that does the same (albeit, between dimers and not the full-fledged models), it might lead to new insights into DMFT). This might allows us to see a metal-insulator phase transition, specially because of the impurity spectral function morphing that we saw from the effective Hamiltonian, shown again in fig. 8.1.

- It is known from DMFT calculations that the spectral function of the bath changes under a change of $U$, leading to a metal-insulator transition. An interesting project could be to redo the URG of the SIAM with more complicated baths (by inserting
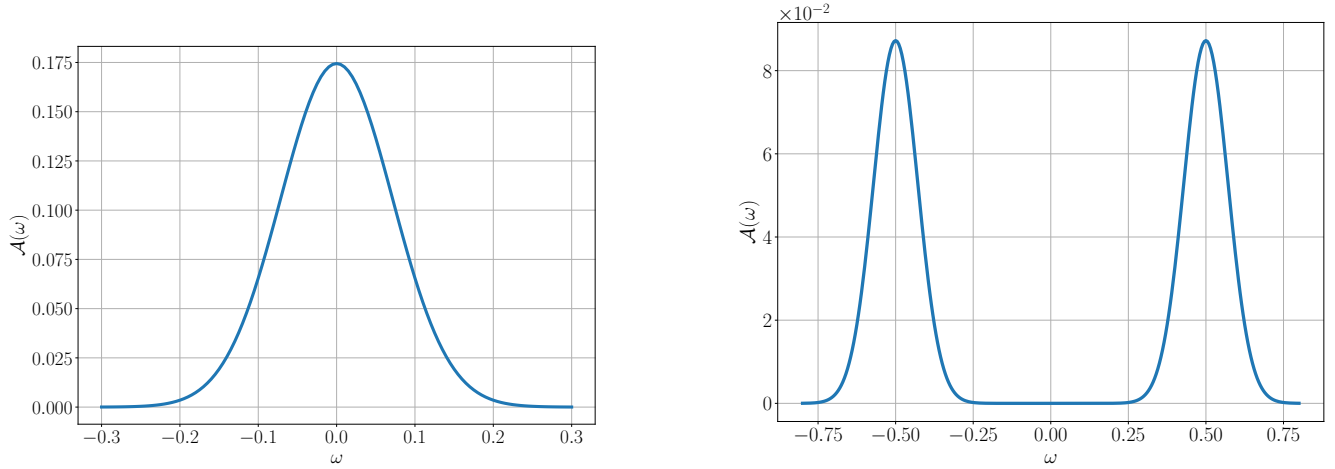
Figure 8.1: Change in the spectral function from single peak to double peak structure under increase of $U$. A similar change happens under DMFT for the bath spectral function of the Hubbard model.

non-trivial self-energies into the bath), and see if the phase-diagram changes. As it stands now, there is no provision for a phase transition in the SIAM because there is only one stable phase. If the inclusion of a non-trivial bath brings about a phase-transition in the impurity phase diagram, that is essentially a mirror of the phase transition happening in the Hubbard model. The importance of this potential discovery is that the self-energies that we wish to insert into the bath have been obtained from a URG treatment of the Hubbard model, and the appearance of the phase transition would then show that URG can be used to do much of the work that DMFT does, and it provides an avenue of improving/remodeling DMFT.

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