The full list of eigenstates is

Although E_-^2 is the ground state of this two-dimensional subspace, we haven't yet checked what is the true ground state of the full Hilbert space. The eigenstates eq. 6.4.28 through 6.4.30 are obviously higher than E_-^2, because of the presence of the singlet $-\frac{3}{4}j$ and the negative γ contribution in E_-^2 compared to the positive triplet contribution $\frac{1}{4}j$ in those equations. The only other competitors are the one in eq. 6.4.31 which we call E_c^2, and the low energy eigenstate in eq. 6.4.23, which we call E_-^1. We first shown that $E_-^1 > E_-^2$. The difference between E_-^2 and E_-^1 is

$$E_-^2 - E_-^1 = -\frac{3}{4}\left(j+k\right) - \sqrt{4v^2 + \frac{\epsilon_d^2}{4} + \frac{9}{64}\left(j-k\right)^2 - \frac{3}{8}\epsilon_d\left(j-k\right)} + \sqrt{\frac{1}{4}\epsilon_d^2 + v^2} \tag{6.4.41}$$

From the nature of the fixed point phases, we know that

$$J^* > K^* \implies \epsilon_d^* \leq 0 \tag{6.4.42}$$

and

$$J^* < K^* \implies \epsilon_d^* \geq 0 \tag{6.4.43}$$

such that

$$\epsilon_d\left(j-k\right) \leq 0 \tag{6.4.44}$$

This result then very easily implies that

$$4v^2 + \frac{\epsilon_d^2}{4} + \frac{9}{64}\left(j-k\right)^2 - \frac{3}{8}\epsilon_d\left(j-k\right) > \frac{1}{4}\epsilon_d^2 + v^2 \tag{6.4.45}$$

and we can apply this inequality to the difference between E_-^2 and E_-^1 to see that E_-^2 is greater that E_-^1.

We now compare E_-^2 and E_c^2:

$$\Delta E_g \equiv E_-^2 - E_c^2 = \frac{1}{2}\epsilon_d - \frac{3j+k}{8} + k - \sqrt{4v^2 + \left(\frac{3j+k}{8} - \frac{1}{2}\epsilon_d\right)^2} \tag{6.4.46}$$

Because of the presence of the large v in the first quadrant, this will necessarily be negative there. So, the true ground state in the first quadrant is E_-^2. In the third quadrant, the large value of k will make the difference positive and the true ground state will be the charge singlet.

These conclusions have been checked numerically and shown in fig. 6.15, where we have plotted the sign of ΔE_g as a function of $K_0 - J_0$. For positive values of $K_0 - J_0$, we are in the third quadrant, and the sign of ΔE_g being +1 implies that $E_-^2 > E_c^2$, and so the third quadrant ground state is the charge singlet (E_c^2). On the other hand, as $K_0 - J_0$ becomes negative, we move into the first quadrant, and the sign of ΔE_g also flips, implying that we have a transition from the charge singlet to the (mostly) spin-singlet ground state.

One of the most striking conclusions of this chapter is that the renormalized ground state of the SIAM in the Kondo regime is purely a singlet. The holon-doublon contributions of the ground state die out in the limit of large system size, and we are left purely with spin-sector contributions.

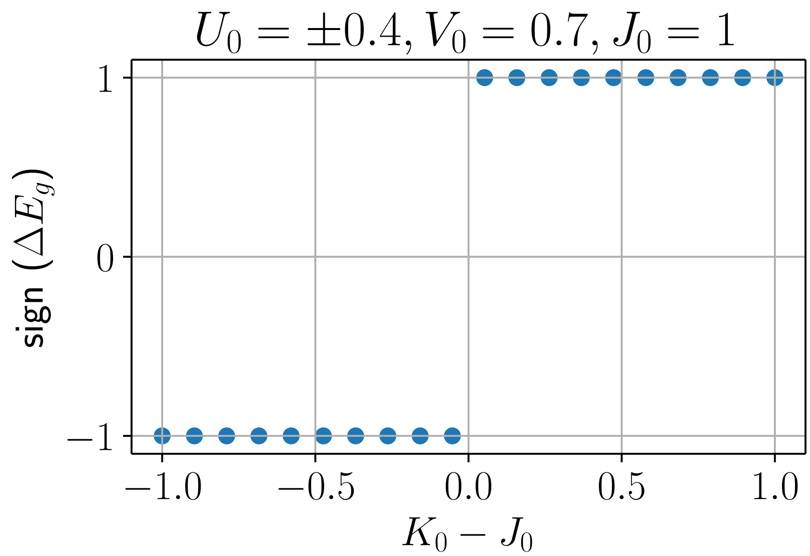

Figure 6.15: Shift in the ground state in going from the first to third quadrant, depicted via the switch in sign of ΔE_g.

Chapter 7

Results and Features of the Low-Energy Theory

7.1 Effective Kondo temperature

We now define an energy scale for the low energy fluctuations:

$$T_K \equiv \frac{2N^*}{\pi}\left(D^* - 2\omega\right) \tag{7.1.1}$$

The term in brackets, $D^* - 2\omega$, is the fluctuation energy at the fixed point. The factor of $2N^*$ is inserted to make the Kondo temperature intensive (we will see below that the N^* allows it to be written in terms of parameters of the two-site Hamiltonian) - $2N^*$ is the total number of momentum states in the fixed point theory. The factor of $\frac{1}{\pi}$ is for aesthetic reasons. From the fixed-point condition $\omega - \frac{D}{2} + \frac{J+K}{4} = 0$, the Kondo temperature can be written as

$$T_K = \frac{2N^*}{\pi}\frac{1}{2}\left(J^* + K^*\right) = \frac{1}{\pi}\left(j + k\right) \tag{7.1.2}$$

7.2 Magnetic susceptibility

The thermal susceptibility is defined as

$$\chi(\beta) = \beta\left(\left\langle\left(S_d^z\right)^2\right\rangle - \left\langle S_d^z\right\rangle^2\right) \tag{7.2.1}$$

There is an alternate way of calculating this. We insert a fictitious magnetic field that couples only to the impurity site. The Hamiltonian in the presence of this field is

$$\mathcal{H}'(B) = \mathcal{H} + BS_d^z \tag{7.2.2}$$

The susceptibility is then given by

$$\chi(\beta) = \lim_{B\to 0}\frac{1}{\beta}\left[\frac{1}{Z(B)}\frac{\partial^2 Z(B)}{\partial B^2} - \frac{1}{Z(B)^2}\left(\frac{\partial Z(B)}{\partial B}\right)^2\right] \tag{7.2.3}$$

where $Z(B)$ is the partition function of the Hamiltonian $\mathcal{H}'(B)$. The following is to prove that the RHS of eqs. 7.2.1 and 7.2.3 are the same. We start with 7.2.3. The first derivative can be written as

$$\frac{\partial Z(B)}{\partial B} = \text{Trace}\left[\frac{\partial}{\partial B}\exp\left\{-\beta\left(\mathcal{H} + BS_d^z\right)\right\}\right] = \text{Trace}\left[-\beta S_d^z \exp\left\{-\beta\left(\mathcal{H} + BS_d^z\right)\right\}\right] \tag{7.2.4}$$

which means the first term becomes

$$\lim_{B\to 0} -\frac{1}{Z(B)^2}\left(\frac{\partial Z(B)}{\partial B}\right)^2 = -\left(\beta\frac{1}{\text{Trace}\left[\exp\left\{-\beta\mathcal{H}\right\}\right]}\text{Trace}\left[S_d^z \exp\left\{-\beta\mathcal{H}\right\}\right]\right)^2 = -\beta^2\left\langle S_d^z\right\rangle^2 \tag{7.2.5}$$

The second derivative is

$$\frac{\partial^2 Z(B)}{\partial B^2} = \text{Trace}\left[-\beta S_d^z\frac{\partial}{\partial B}\exp\left\{-\beta\left(\mathcal{H} + BS_d^z\right)\right\}\right] = \text{Trace}\left[\beta^2\left(S_d^z\right)^2\exp\left\{-\beta\left(\mathcal{H} + BS_d^z\right)\right\}\right] \tag{7.2.6}$$

so the second term becomes

$$\lim_{B\to 0}\frac{1}{Z(B)}\frac{\partial^2 Z(B)}{\partial B^2} = \beta^2\frac{1}{\text{Trace}\left[\exp\left\{-\beta\mathcal{H}\right\}\right]}\text{Trace}\left[\left(S_d^z\right)^2\exp\left\{-\beta\mathcal{H}\right\}\right] = \beta^2\left\langle\left(S_d^z\right)^2\right\rangle \tag{7.2.7}$$

The full thing becomes

$$\begin{aligned}\lim_{B\to 0}\frac{1}{\beta}\left[\frac{1}{Z(B)}\frac{\partial^2 Z(B)}{\partial B^2} - \frac{1}{Z(B)^2}\left(\frac{\partial Z(B)}{\partial B}\right)^2\right] &= \frac{1}{\beta}\left(-\beta^2\left\langle S_d^z\right\rangle^2 + \beta^2\left\langle\left(S_d^z\right)^2\right\rangle\right)\\ &= \beta\left(\left\langle\left(S_d^z\right)^2\right\rangle - \left\langle S_d^z\right\rangle^2\right)\end{aligned} \tag{7.2.8}$$

This completes the proof.

7.2.1 For $v = 0$

In the presence of a magnetic field coupling term BS_1^z, the eigenvalues become (setting $v = 0$)

$$\begin{aligned}
\hat{n} = 0, 4 &\longrightarrow E^0 = \frac{1}{4}k \\
\hat{n} = 1, 3 &\longrightarrow \begin{cases} E^1_{\pm,\uparrow} = \frac{1}{2}\left(\epsilon_d + \frac{1}{2}B\right) \pm \frac{1}{2}\Delta\left(\epsilon_d + \frac{1}{2}B, v\right) = \epsilon_d + \frac{1}{2}B, 0 \\ E^1_{\pm,\downarrow} = \frac{1}{2}\left(\epsilon_d - \frac{1}{2}B\right) \pm \frac{1}{2}\Delta\left(\epsilon_d - \frac{1}{2}B, v\right) = \epsilon_d - \frac{1}{2}B, 0 \end{cases} \\
\hat{n} = 2 &\longrightarrow \begin{cases} \epsilon_d + \frac{1}{4}j + \frac{1}{2}B \\ \epsilon_d + \frac{1}{4}j - \frac{1}{2}B \\ \frac{1}{4}k \\ -\frac{3}{4}k \\ \epsilon_d - \frac{1}{4}j \pm \frac{1}{2}\Gamma \end{cases}
\end{aligned} \tag{7.2.9}$$

where we defined $\Gamma = \sqrt{B^2 + j^2}$. The eigenvalues in $\hat{n} = 2$ can be elaborated upon. The action of the total Hamiltonian $\mathcal{H}'$ (with $v = 0$) is

$$|\uparrow, \uparrow\rangle \mapsto \left(\epsilon_d + \frac{1}{4}j + \frac{1}{2}B\right)|\uparrow, \uparrow\rangle \tag{7.2.10}$$

$$|\downarrow, \downarrow\rangle \mapsto \left(\epsilon_d + \frac{1}{4}j - \frac{1}{2}B\right)|\downarrow, \downarrow\rangle \tag{7.2.11}$$

$$\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle\right) \mapsto \frac{1}{4}k\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle\right) \tag{7.2.12}$$

$$\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle\right) \mapsto -\frac{3}{4}k\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle\right) \tag{7.2.13}$$

$$\frac{1}{\sqrt{2}}\left(|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle\right) \mapsto \left(\epsilon_d + \frac{1}{4}j\right)\frac{1}{\sqrt{2}}\left(|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle\right) + \frac{1}{2}B\frac{1}{\sqrt{2}}\left(|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle\right) \tag{7.2.14}$$

$$\frac{1}{\sqrt{2}}\left(|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle\right) \mapsto \left(\epsilon_d - \frac{3}{4}j\right)\frac{1}{\sqrt{2}}\left(|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle\right) + \frac{1}{2}B\frac{1}{\sqrt{2}}\left(|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle\right) \tag{7.2.15}$$

$$\tag{7.2.16}$$

The first four states directly give the first four eigenvalues in $\hat{n} = 2$. The remaining two states form the matrix

$$\begin{pmatrix} \epsilon_d + \frac{1}{4}j & \frac{1}{2}B \\ \frac{1}{2}B & \epsilon_d - \frac{3}{4}j \end{pmatrix} \tag{7.2.17}$$

The eigenvalues satisfy the equation

$$0 = \left(E - \epsilon_d + \frac{3}{4}j\right)\left(E - \epsilon_d - \frac{1}{4}j\right) - \frac{1}{4}B^2 = \left(E - \epsilon_d - \frac{1}{4}j\right)^2 + j\left(E - \epsilon_d - \frac{1}{4}j\right) - \frac{1}{4}B^2 \tag{7.2.18}$$

The solutions are

$$E = \epsilon_d + \frac{1}{4}j + \frac{-j \pm \sqrt{j^2 + B^2}}{2} = \epsilon_d - \frac{1}{4}j \pm \frac{1}{2}\Gamma \tag{7.2.19}$$

which are the final two eigenvalues.

The partition function is

$$\begin{aligned}
Z(B) &= 2\exp\left\{-\beta\frac{k}{4}\right\} + 2\left(\exp\left\{-\beta\left(\epsilon_d + \frac{1}{2}B\right)\right\} + e^0\right) + 2\left(\exp\left\{-\beta\left(\epsilon_d - \frac{1}{2}B\right)\right\} + e^0\right) \\
&\quad + \exp\left\{-\beta\left(\epsilon_d + \frac{1}{4}j + \frac{1}{2}B\right)\right\} + \exp\left\{-\beta\left(\epsilon_d + \frac{1}{4}j - \frac{1}{2}B\right)\right\} \\
&\quad + \exp\left\{-\beta\frac{k}{4}\right\} + \exp\left\{\beta\frac{3k}{4}\right\} + \exp\left\{-\beta\left(\epsilon_d - \frac{1}{4}j + \frac{1}{2}\Gamma\right)\right\} + \exp\left\{-\beta\left(\epsilon_d - \frac{1}{4}j - \frac{1}{2}\Gamma\right)\right\} \\
&= 4 + 3\exp\left\{-\beta\frac{k}{4}\right\} + \exp\left\{\beta\frac{3k}{4}\right\} + 4e^{-\beta\epsilon_d}\cosh\beta\frac{B}{2} + 2e^{-\beta\left(\epsilon_d + \frac{j}{4}\right)}\cosh\beta\frac{B}{2} \\
&\quad + 2e^{-\beta\left(\epsilon_d - \frac{j}{4}\right)}\cosh\beta\frac{1}{2}\Gamma \\
&= 4 + 3\exp\left\{-\beta\frac{k}{4}\right\} + \exp\left\{\beta\frac{3k}{4}\right\} + \left[4e^{-\beta\epsilon_d} + 2e^{-\beta\left(\epsilon_d + \frac{j}{4}\right)}\right]\cosh\left(\beta\frac{B}{2}\right) \\
&\quad + 2e^{-\beta\left(\epsilon_d - \frac{j}{4}\right)}\cosh\left(\beta\frac{1}{2}\Gamma\right)
\end{aligned} \tag{7.2.20}$$

We can now compute the derivatives.

$$\begin{aligned}
Z' \equiv \frac{\partial Z}{\partial B} &= \left[4e^{-\beta\epsilon_d} + 2e^{-\beta\left(\epsilon_d + \frac{j}{4}\right)}\right]\frac{\beta}{2}\sinh\left(\beta\frac{B}{2}\right) + 2e^{-\beta\left(\epsilon_d - \frac{j}{4}\right)}\frac{1}{2}\beta\sinh\left(\frac{1}{2}\beta\Gamma\right)\frac{\partial\Gamma}{\partial B} \\
&= \left[4e^{-\beta\epsilon_d} + 2e^{-\beta\left(\epsilon_d + \frac{j}{4}\right)}\right]\frac{\beta}{2}\sinh\left(\beta\frac{B}{2}\right) + e^{-\beta\left(\epsilon_d - \frac{j}{4}\right)}\beta\sinh\left(\frac{1}{2}\beta\Gamma\right)\frac{B}{\Gamma} \\
Z'' \equiv \frac{\partial^2 Z}{\partial B^2} &= \left[4e^{-\beta\epsilon_d} + 2e^{-\beta\left(\epsilon_d + \frac{j}{4}\right)}\right]\left(\frac{\beta}{2}\right)^2\cosh\left(\beta\frac{B}{2}\right) \\
&\quad + e^{-\beta\left(\epsilon_d - \frac{j}{4}\right)}\beta\left[\cosh\left(\frac{1}{2}\beta\Gamma\right)\times\frac{1}{2}\beta\left(\frac{B}{\Gamma}\right)^2 + \sinh\left(\frac{1}{2}\beta\Gamma\right)\left(-\frac{B}{\Gamma^2}\times\frac{B}{\Gamma} + \frac{1}{\Gamma}\right)\right]
\end{aligned} \tag{7.2.21}$$

Taking the limit of $B \to 0$ gives

$$\begin{aligned}
Z|_{B=0} &= 4 + 3\exp\left\{-\beta\frac{k}{4}\right\} + \exp\left\{\beta\frac{3k}{4}\right\} + 4e^{-\beta\epsilon_d} + 2e^{-\beta\left(\epsilon_d + \frac{j}{4}\right)} + 2e^{-\beta\left(\epsilon_d - \frac{j}{4}\right)}\cosh\left(\beta\frac{j}{2}\right) \\
Z'|_{B=0} &= 0 \\
Z''|_{B=0} &= \left[4e^{-\beta\epsilon_d} + 2e^{-\beta\left(\epsilon_d + \frac{j}{4}\right)}\right]\left(\frac{\beta}{2}\right)^2 + e^{-\beta\left(\epsilon_d - \frac{j}{4}\right)}\beta\sinh\left(\beta\frac{j}{2}\right)\frac{1}{j}
\end{aligned} \tag{7.2.22}$$

The susceptibility is thus

$$\begin{aligned}\chi(\beta) &= \frac{1}{\beta}\frac{\left[4e^{-\beta\epsilon_d}+2e^{-\beta\left(\epsilon_d+\frac{j}{4}\right)}\right]\left(\frac{\beta}{2}\right)^2+e^{-\beta\left(\epsilon_d-\frac{j}{4}\right)}\beta\sinh\left(\beta\frac{j}{2}\right)\frac{1}{j}}{4+3\exp\left\{-\beta\frac{k}{4}\right\}+\exp\left\{\beta\frac{3k}{4}\right\}+4e^{-\beta\epsilon_d}+2e^{-\beta\left(\epsilon_d+\frac{j}{4}\right)}+2e^{-\beta\left(\epsilon_d-\frac{j}{4}\right)}\cosh\left(\beta\frac{j}{2}\right)} \\ &= \frac{\left[2e^{-\beta\epsilon_d}+e^{-\beta\left(\epsilon_d+\frac{j}{4}\right)}\right]\frac{1}{2}\beta+e^{-\beta\left(\epsilon_d-\frac{j}{4}\right)}\sinh\left(\beta\frac{j}{2}\right)\frac{1}{j}}{4+3\exp\left\{-\beta\frac{k}{4}\right\}+\exp\left\{\beta\frac{3k}{4}\right\}+4e^{-\beta\epsilon_d}+2e^{-\beta\left(\epsilon_d+\frac{j}{4}\right)}+2e^{-\beta\left(\epsilon_d-\frac{j}{4}\right)}\cosh\left(\beta\frac{j}{2}\right)}\end{aligned} \tag{7.2.23}$$

At high temperatures, we can write

$$\frac{\chi}{\beta}|_{\beta\to 0} = \frac{\left[4+2\right]\frac{1}{4}+\frac{1}{2}\lim_{\beta\to 0}\sinh\left(\beta\frac{j}{2}\right)\frac{2}{\beta j}}{4+3+1+\left[4+2\right]+2} = \frac{\frac{3}{2}+\frac{1}{2}}{16} = \frac{1}{8} \quad \left[\lim_{x\to 0}\frac{\sinh x}{x}=1\right] \tag{7.2.24}$$

At low temperatures,

$$\chi|_{\beta\to\infty} = \lim_{\beta\to\infty}\frac{e^{-\beta\left(\epsilon_d-\frac{j}{4}\right)}\sinh\left(\beta\frac{j}{2}\right)\frac{1}{j}}{\exp\left\{\beta\frac{3k}{4}\right\}+2e^{-\beta\left(\epsilon_d-\frac{j}{4}\right)}\cosh\left(\beta\frac{j}{2}\right)} = \frac{1}{2j}\lim_{\beta\to\infty}\frac{1}{\exp\left\{\beta\left(\frac{3k}{4}+\epsilon_d-\frac{3j}{4}\right)\right\}+1} \tag{7.2.25}$$

There we used $\sinh x \approx \cosh x \approx \frac{1}{2}e^x$ for $x \to \infty$. The exponential will take the following limiting values:

$$\exp\left\{\beta\left(\frac{3k}{4}+\epsilon_d-\frac{3j}{4}\right)\right\} \to \begin{cases}\infty, & \text{if } \frac{3k}{4}+\epsilon_d-\frac{3j}{4} > 0 \\ 1, & \text{if } \frac{3k}{4}+\epsilon_d-\frac{3j}{4} = 0 \\ 0, & \text{if } \frac{3k}{4}+\epsilon_d-\frac{3j}{4} < 0\end{cases} \tag{7.2.26}$$

which means

$$\left[\exp\left\{\beta\left(\frac{3k}{4}+\epsilon_d-\frac{3j}{4}\right)\right\}+1\right]^{-1} \to \begin{cases}0, & \text{if } \frac{3k}{4}+\epsilon_d-\frac{3j}{4} > 0 \\ \frac{1}{2}, & \text{if } \frac{3k}{4}+\epsilon_d-\frac{3j}{4} = 0 \\ 1, & \text{if } \frac{3k}{4}+\epsilon_d-\frac{3j}{4} < 0\end{cases} = \Theta\left(\frac{3j}{4}-\frac{3k}{4}-\epsilon_d\right) \tag{7.2.27}$$

where the theta function (Heaviside function) is defined as

$$\Theta(x) = \begin{cases}1, & \text{if } x > 0 \\ \frac{1}{2}, & \text{if } x = 0 \\ 0, & \text{if } x < 0\end{cases} \tag{7.2.28}$$

The thermal susceptibility at high temperatures is thus

$$\chi|_{\beta\to\infty} = \frac{1}{2j}\Theta\left(\frac{3j}{4}-\frac{3k}{4}-\epsilon_d\right) \tag{7.2.29}$$

If we are in the first quadrant, then the fixed point values are such that $\frac{3k}{4} + \epsilon_d - \frac{3j}{4} < 0$, so the theta function will evaluate to 1, and we can write

$$\chi|_{\beta\to\infty} = \frac{1}{2j} \tag{7.2.30}$$

For sufficiently large values of j compared to k, we can also approximate the Kondo temperature T_K as $T_K \approx \frac{j}{\pi}$. Then, the zero temperature value of χ deep in the first quadrant is

$$\chi(T=0) \approx \left(2\pi T_K\right)^{-1} \tag{7.2.31}$$

This is in accordance with the results obtained from Bethe ansatz in [38].

On the other hand, in the third quadrant, we have $\frac{3k}{4} + \epsilon_d - \frac{3j}{4} > 0$, and Θ gives

$$\chi|_{\beta\to\infty} = 0 \tag{7.2.32}$$

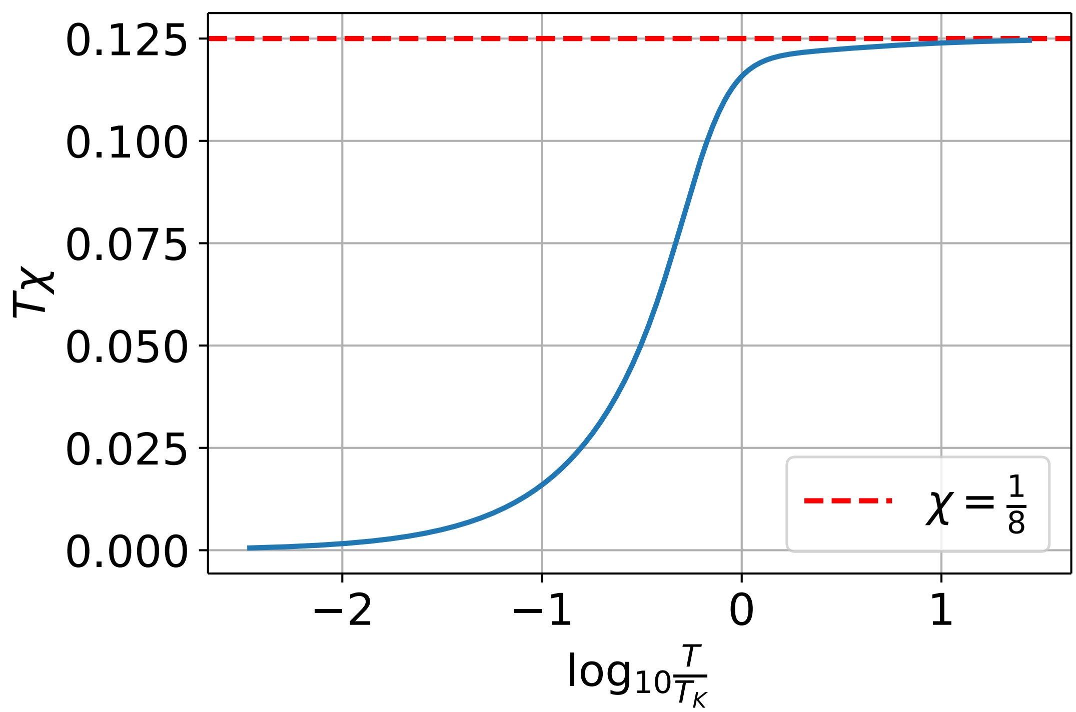

Figure 7.1: Variation of $\chi \times T$ over six decades of temperature. The low temperature behaviour is characteristic of a local Fermi liquid paramagnetic susceptibility, while at high temperatures we see the Curie-Weiss susceptibility resulting from the local moment.

7.3 Charge Susceptibility

We can also calculate the impurity contribution to the charge susceptibility of the system in a very similar fashion. We insert a magnetic field that couples to the impurity charge

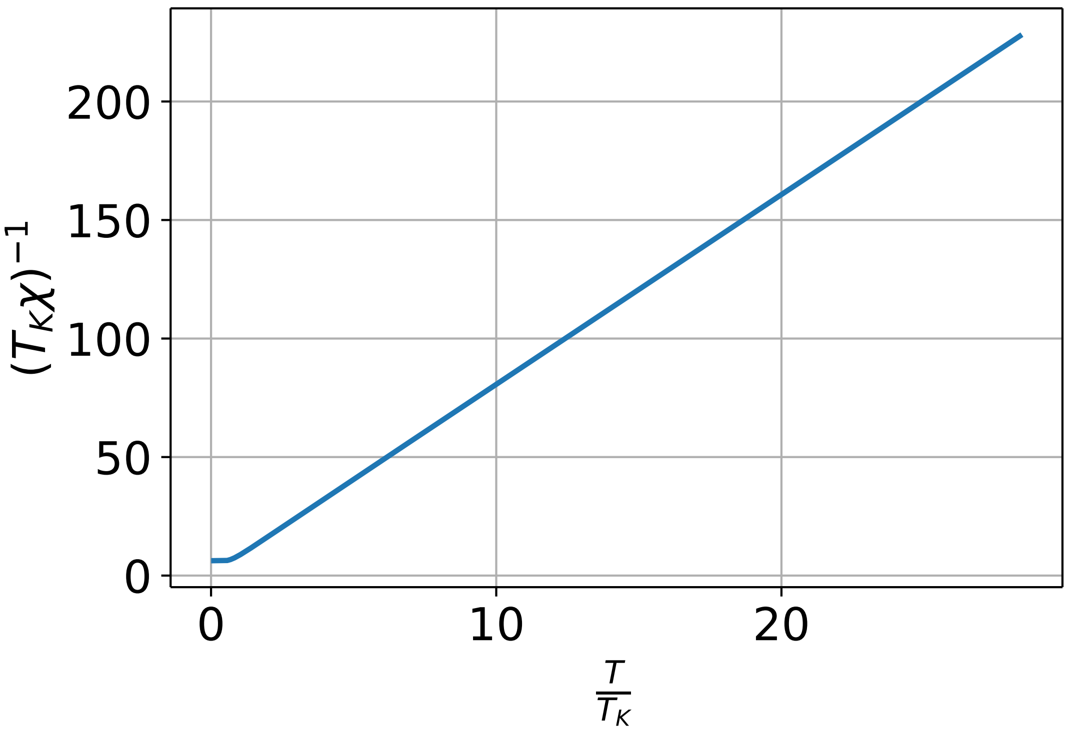

Figure 7.2: Variation of $(T_k \times \chi)^{-1}$ with temperature.

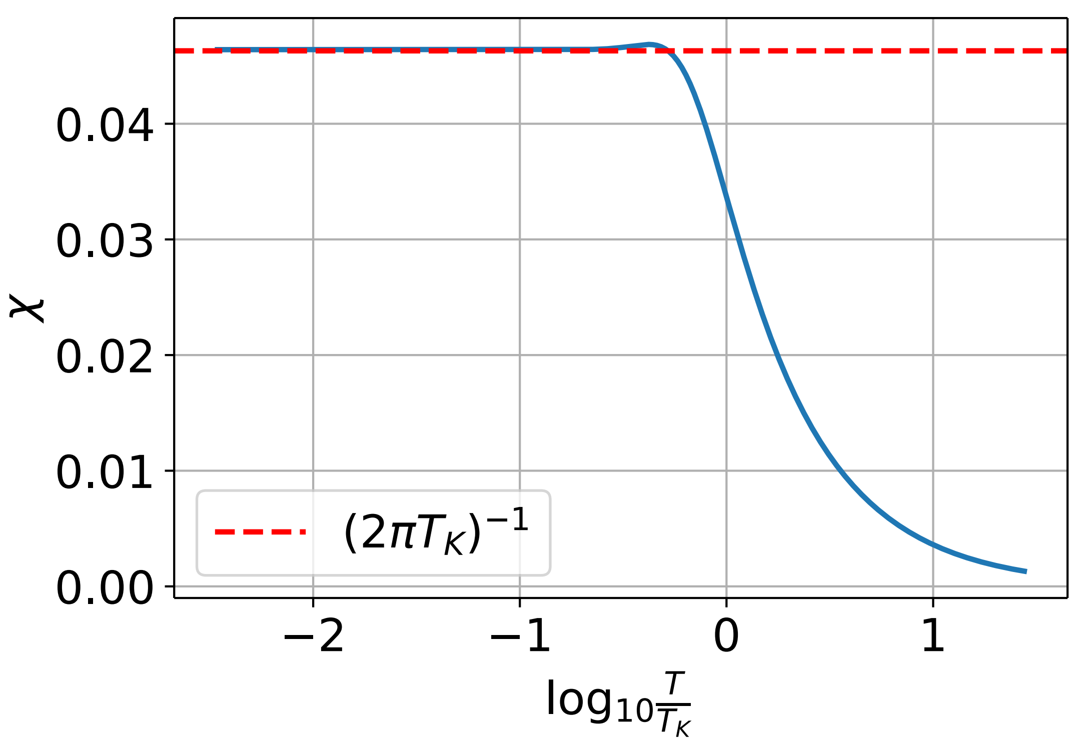

Figure 7.3: Variation of χ against temperature. It saturates to a value close to $(2\pi T_K)^{-1}$

isospin:

$$\mathcal{H}'(B) = \mathcal{H} + BC_d^z \tag{7.3.1}$$

We again work in the simpler case of $v = 0$. The energy eigenvalues for this Hamiltonian are

$$\begin{aligned}
\hat{n} = 0 &\longrightarrow \frac{1}{4}k - \frac{B}{2} \\
\hat{n} = 4 &\longrightarrow \frac{1}{4}k + \frac{B}{2} \\
\hat{n} = 1,3 &\longrightarrow \begin{cases} \epsilon_d - \frac{1}{2}B, 0 \\ \epsilon_d + \frac{1}{2}B, 0 \end{cases} \\
\hat{n} = 2 &\longrightarrow \begin{cases} \left.\epsilon_d + \frac{1}{4}j\right\} \times 3 \\ \epsilon_d - \frac{3}{4}j \\ \epsilon_d - \frac{1}{4}k \pm \frac{1}{2}\Gamma \end{cases}
\end{aligned} \tag{7.3.2}$$

where $\Gamma \equiv \sqrt{k^2 + B^2}$. We will again use eq. 7.2.3 to calculate the susceptibility. The partition function and its derivatives are

$$\begin{aligned}
\lim_{B\to 0} Z &= 2e^{-\beta\frac{k}{4}} + 4 + 4e^{-\beta\epsilon_d} + 3e^{-\beta\left(\epsilon_d + \frac{j}{4}\right)} + e^{\beta\left(3\frac{j}{4} - \epsilon_d\right)} + 2e^{\beta\left(\frac{k}{4} - \epsilon_d\right)} \cosh\beta\frac{k}{2} \\
\lim_{B\to 0} \frac{\partial Z}{\partial B} &= 0 \\
\lim_{B\to 0} \frac{\partial^2 Z}{\partial B^2} &= \frac{\beta^2}{2}\left[e^{-\beta\frac{k}{4}} + 2e^{-\beta\epsilon_d}\right] + \frac{\beta}{k}e^{\beta\left(\frac{k}{4} - \epsilon_d\right)} \sinh\beta\frac{k}{2}
\end{aligned} \tag{7.3.3}$$

The charge susceptibility is thus

$$\chi_c = \frac{1}{\beta}\frac{\frac{\beta^2}{2}\left[e^{-\beta\frac{k}{4}} + 2e^{-\beta\epsilon_d}\right] + \frac{\beta}{k}e^{\beta\left(\frac{k}{4} - \epsilon_d\right)} \sinh\beta\frac{k}{2}}{2e^{-\beta\frac{k}{4}} + 4 + 4e^{-\beta\epsilon_d} + 3e^{-\beta\left(\epsilon_d + \frac{j}{4}\right)} + e^{\beta\left(3\frac{j}{4} - \epsilon_d\right)} + 2e^{\beta\left(\frac{k}{4} - \epsilon_d\right)} \cosh\beta\frac{k}{2}} \tag{7.3.4}$$

An important result that we will use later is the value at $T = 0$.

$$\chi_c(T = 0) = \frac{1}{2k}\lim_{\beta\to\infty}\frac{1}{1 + e^{\frac{3\beta}{4}(j-k)}} \tag{7.3.5}$$

There we used the observation that near the fixed point, ϵ_d is either close to zero or large positive such that $e^{-\beta\epsilon_d}$ does not affect the value of χ_c at $T = 0$. In the Kondo regime of the SIAM ($j \gg k$), the denominator diverges and the charge susceptibility vanishes at $T = 0$.

$$\chi_c(T = 0)\Big|_{j\gg k} = 0 \tag{7.3.6}$$

The charge susceptibility at large temperatures becomes

$$\left(\chi_c \times T\right)(T \to \infty) = \frac{1}{8} \tag{7.3.7}$$

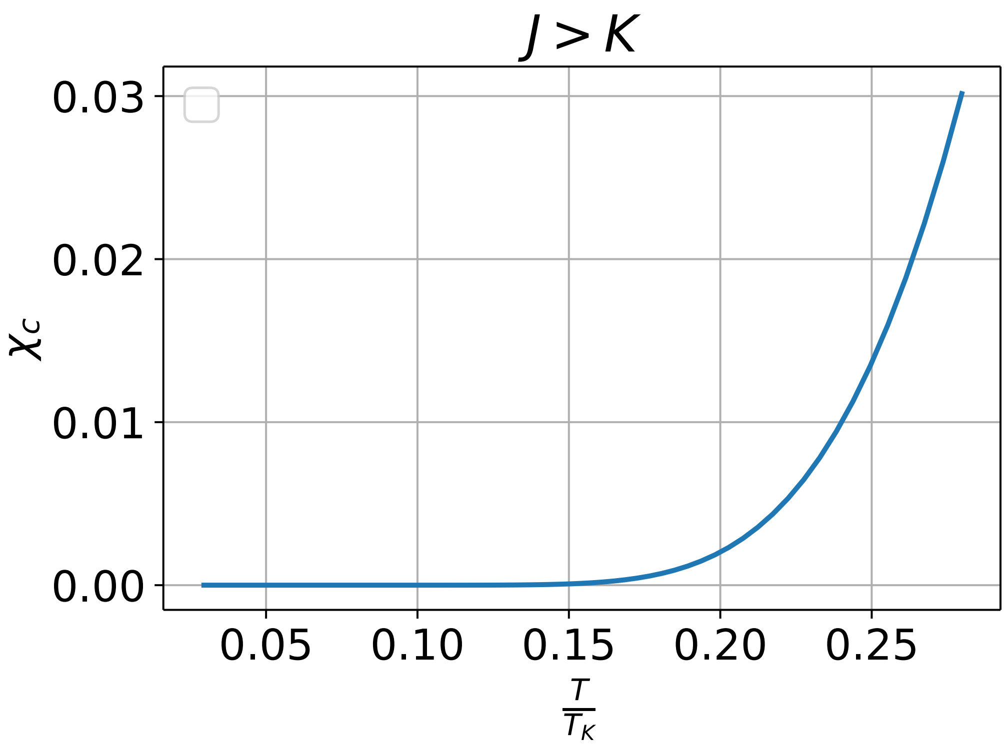

Figure 7.4: Flow of charge susceptibility to 0 at low temperatures for the spin-Kondo regime ($J > K$).

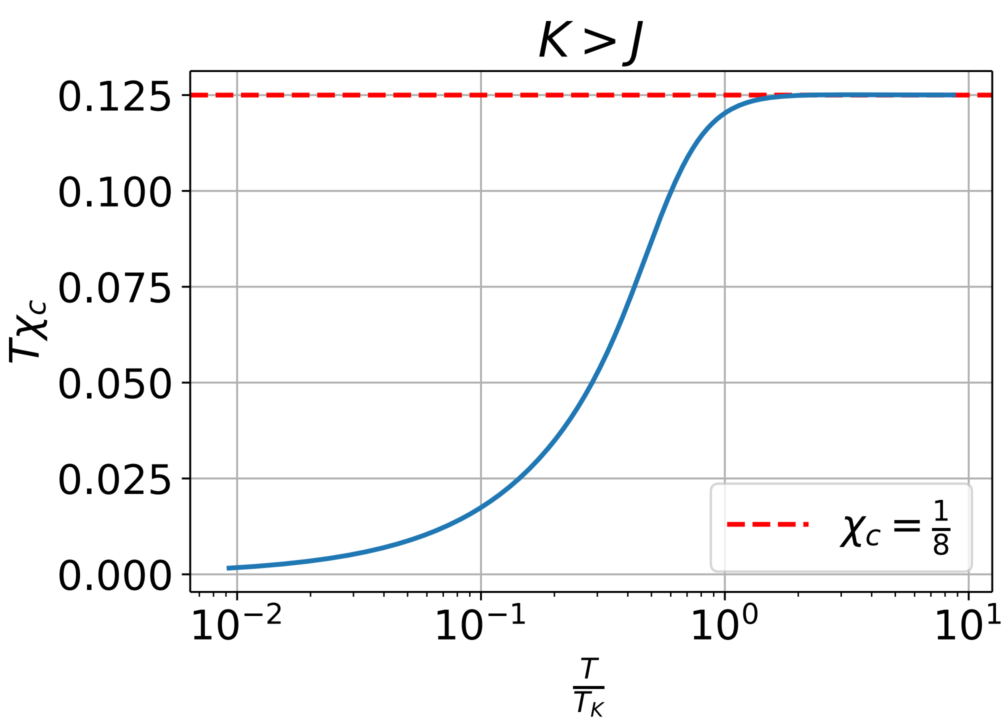

Figure 7.5: Behavior of $\chi_c \times T$ for the charge-Kondo regime. It is qualitatively very similar to the behavior of the magnetic susceptibility in the spin-Kondo regime.

7.4 Specific heat

The specific heat is calculated by diagonalizing the fixed point Hamiltonian, numerically. The obtained spectrum is denoted by $\{\mathcal{E}_i\}$. The total average energy of the impurity+cloud at temperature T is then

$$\langle \mathcal{E} \rangle = \frac{1}{Z} \sum_i \mathcal{E}_i e^{-\beta \mathcal{E}_i} \tag{7.4.1}$$

where $Z = \sum_i e^{-\beta E_i}$ is the partition function. The specific heat of this system is thus

$$\begin{aligned} C_v &= \frac{\partial \langle \mathcal{E} \rangle}{\partial T} \\ &= -\frac{1}{k_B T^2} \frac{\partial \langle \mathcal{E} \rangle}{\partial \beta} \\ &= \frac{1}{k_B T^2} \left[\frac{1}{Z} \sum_i \mathcal{E}_i^2 e^{-\beta \mathcal{E}_i} - \left(\frac{1}{Z} \sum_i \mathcal{E}_i e^{-\beta \mathcal{E}_i} \right)^2 \right] \end{aligned} \tag{7.4.2}$$

In the absence of impurity, the eigenvalues of the Hamiltonian are $\left\{\mathcal{E}_i^0\right\}$ with a partition function $Z^0 = \sum_i e^{-\beta E_i^0}$, so the bath specific heat is

$$C_v^0 = \frac{1}{k_B T^2} \left[\frac{1}{Z_0} \sum_i \mathcal{E}_i^2 e^{-\beta \mathcal{E}_i^0} - \left(\frac{1}{Z_0} \sum_i \mathcal{E}_i^0 e^{-\beta \mathcal{E}_i^0} \right)^2 \right] \tag{7.4.3}$$

The impurity specific heat is the difference.

$$C_v^{\text{imp}} = C_v - C_v^0 \tag{7.4.4}$$

These values were calculated numerically and plotted against temperature in fig. 7.6.

7.5 Impurity Spectral function

In this section we will obtain the impurity spectral function, which is defined in terms of the impurity Green's function as

$$\mathcal{A}(\omega) = -\frac{1}{\pi} \text{Im} \left[G_{dd}^{\sigma}(\omega) \right] \tag{7.5.1}$$

The impurity retarded Green's function (assuming the Hamiltonian to be time-independent, which it is) is defined as

$$G_{dd}^{\sigma}(t) = -i\theta(t) \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^{\dagger} \right\} \right\rangle \tag{7.5.2}$$

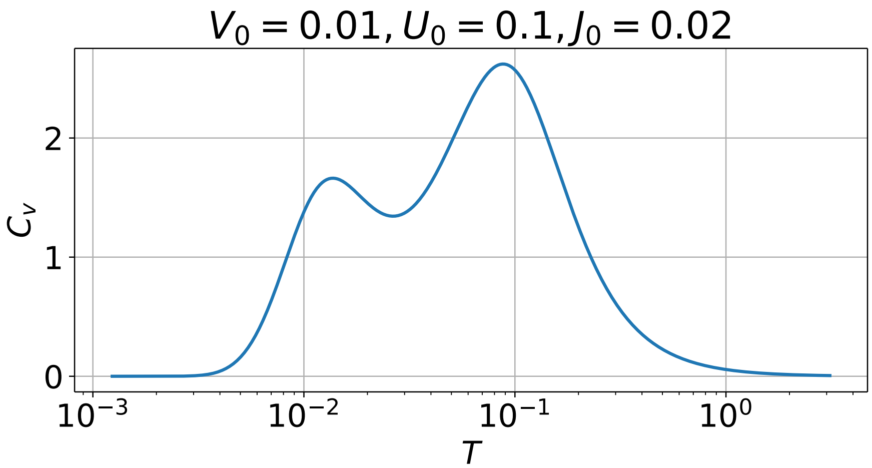

Figure 7.6: Impurity specific heat

where the average $\langle\rangle$ is over a canonical ensemble at temperature T. What follows is a standard calculation where we write the Green's function in the Lehmann representation. We will write the ensemble average in terms of the exact eigenstates of the fixed point Hamiltonian:

$$\begin{aligned} H^* \left|n\right\rangle &= E_n^* \left|n\right\rangle \\ \left\langle \hat{O} \right\rangle &\equiv \frac{1}{Z} \sum_n \left\langle n\right| \hat{O} \left|n\right\rangle e^{-\beta E_n^*} \end{aligned} \tag{7.5.3}$$

where $Z = \sum_n e^{-\beta E_n^*}$ is the fixed point partition function and $\left\{\left|n\right\rangle\right\}$ is the set of eigenfunctions of the fixed point Hamiltonian. We can therefore write

$$\begin{aligned} &\left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger \right\} \right\rangle \\ &= \sum_m e^{-\beta E_m} \left\langle m\right| \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger \right\} \left|m\right\rangle \\ &= \sum_{m,n} e^{-\beta E_m} \left\langle m\right| \left(c_{d\sigma}(t) \left|n\right\rangle \left\langle n\right| c_{d\sigma}^\dagger + c_{d\sigma}^\dagger \left|n\right\rangle \left\langle n\right| c_{d\sigma}(t) \right) \left|m\right\rangle & \left[\sum_n \left|n\right\rangle \left\langle n\right| = 1\right] \\ &= \sum_{m,n} e^{-\beta E_m} \left\langle m\right| \left(e^{iH^*t} c_{d\sigma} e^{-iH^*t} \left|n\right\rangle \left\langle n\right| c_{d\sigma}^\dagger + c_{d\sigma}^\dagger \left|n\right\rangle \left\langle n\right| e^{iH^*t} c_{d\sigma} e^{-iH^*t} \right) \left|m\right\rangle \\ &= \sum_{m,n} e^{-\beta E_m} \left(e^{i(E_m - E_n)t} \left\langle m\right| c_{d\sigma} \left|n\right\rangle \left\langle n\right| c_{d\sigma}^\dagger \left|m\right\rangle + e^{i(E_n - E_m)t} \left\langle m\right| c_{d\sigma}^\dagger \left|n\right\rangle \left\langle n\right| c_{d\sigma} \left|m\right\rangle \right) \\ &= \sum_{m,n} e^{i(E_m - E_n)t} || \left\langle m\right| c_{d\sigma} \left|n\right\rangle ||^2 \left(e^{-\beta E_m} + e^{-\beta E_n} \right) \end{aligned} \tag{7.5.4}$$

The time-domain impurity Green's function can thus be written as (this is the so-called Lehmann representation)

$$G_{dd}^\sigma = -i\theta(t) \sum_{m,n} e^{i(E_m - E_n)t} || \left\langle m\right| c_{d\sigma} \left|n\right\rangle ||^2 \left(e^{-\beta E_m} + e^{-\beta E_n} \right) \tag{7.5.5}$$

We are interested in the frequency domain form.

$$\begin{aligned} G^{\sigma}_{dd}(\omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t} G^{\sigma}_{dd}(t) \\ &= \sum_{m,n} || \langle m| c_{d\sigma} |n\rangle ||^2 \left(e^{-\beta E_m} + e^{-\beta E_n}\right) (-i) \int_{-\infty}^{\infty} dt \theta(t) e^{i\left(\omega + E_m - E_n\right)t} \end{aligned} \tag{7.5.6}$$

To evaluate the time-integral, we will use the integral representation of the Heaviside function:

$$\theta(t) = \frac{1}{2\pi i} \lim_{\eta \to 0^+} \int_{-\infty}^{\infty} \frac{1}{x - i\eta} e^{ixt} dx \tag{7.5.7}$$

With this definition, the integral in $G^{\sigma}_{dd}(\omega)$ becomes

$$\begin{aligned} (-i) \int_{-\infty}^{\infty} dt \theta(t) e^{i\left(\omega + E_m - E_n\right)t} &= (-i) \frac{1}{2\pi i} \lim_{\eta \to 0^+} \int_{-\infty}^{\infty} dx \frac{1}{x - i\eta} \int_{-\infty}^{\infty} dt e^{i\left(\omega + E_m - E_n + x\right)t} \\ &= (-i) \frac{1}{2\pi i} \lim_{\eta \to 0^+} \int_{-\infty}^{\infty} dx \frac{1}{x - i\eta} 2\pi \delta\left(\omega + E_m - E_n + x\right) \\ &= (-i) \frac{1}{i} \lim_{\eta \to 0^+} \frac{-1}{\omega + E_m - E_n - i\eta} \\ &= \frac{1}{\omega + E_m - E_n} \end{aligned} \tag{7.5.8}$$

The frequency-domain Green's function is thus

$$G^{\sigma}_{dd}(\omega) = \sum_{m,n} || \langle m| c_{d\sigma} |n\rangle ||^2 \left(e^{-\beta E_m} + e^{-\beta E_n}\right) \frac{1}{\omega + E_m - E_n} \tag{7.5.9}$$

The zero temperature Green's function is obtained by taking the limit of $\beta\ to \infty$:

$$\begin{aligned} G^{\sigma}_{dd}(\omega, \beta \to \infty) &= \sum_{m,n} || \langle m| c_{d\sigma} |n\rangle ||^2 \left(\delta(E_m) + \delta(E_n)\right) \frac{1}{\omega + E_m - E_n} \\ &= \sum_{m,0} \left[|| \langle 0| c_{d\sigma} |n\rangle ||^2 \frac{1}{\omega - E_n} + || \langle m| c_{d\sigma} |0\rangle ||^2 \frac{1}{\omega + E_m} \right] \end{aligned} \tag{7.5.10}$$

The label 0 sums over all states with zero energy eigenvalue. The spectral function is the imaginary part of this Green's function. To extract the imaginary part, we insert an infinitesimal imaginary part in the denominator:

$$G^{\sigma}_{dd}(\omega, T = 0, \eta) = \lim_{\eta \to 0^-} \sum_{m,0} \left[|| \langle 0| c_{d\sigma} |n\rangle ||^2 \frac{1}{\omega - E_n + i\eta} + || \langle m| c_{d\sigma} |0\rangle ||^2 \frac{1}{\omega + E_m + i\eta} \right] \tag{7.5.11}$$

The spectral function can then be written as

$$\begin{aligned}
\mathcal{A}(\omega) &= -\frac{1}{\pi}\,\mathrm{Im}\,\left[G^{\sigma}_{dd}\left(\omega\right)\right] \\
&= -\frac{1}{\pi}\,\mathrm{Im}\,\left[\lim_{\eta\to 0^-}\sum_{m,0}\left(||\left\langle 0\right| c_{d\sigma}\left|n\right\rangle||^2\frac{-i\eta}{\left(\omega-E_n\right)^2+\eta^2}+||\left\langle m\right| c_{d\sigma}\left|0\right\rangle||^2\frac{-i\eta}{\left(\omega+E_m\right)^2+\eta^2}\right)\right] \\
&= \frac{1}{\pi}\sum_{m,0}\left[||\left\langle 0\right| c_{d\sigma}\left|n\right\rangle||^2\pi\delta\left(\omega-E_n\right)+||\left\langle m\right| c_{d\sigma}\left|0\right\rangle||^2\pi\delta\left(\omega+E_m\right)\right] \\
&= \sum_{m,0}\left[||\left\langle 0\right| c_{d\sigma}\left|n\right\rangle||^2\delta\left(\omega-E_n\right)+||\left\langle m\right| c_{d\sigma}\left|0\right\rangle||^2\delta\left(\omega+E_m\right)\right]
\end{aligned} \tag{7.5.12}$$

Since this is in terms of the exact eigenstates, it is a discrete sum of delta-functions. In practice, we get a continuous distribution. To compare with experiment, we need to convert the discrete sum into a continuous function. Following [39], we replace the delta-functions by Gaussian functions:

$$\delta(\omega-E_n) \to \frac{1}{w\sqrt{\pi}}e^{-\frac{1}{w}\left(\omega-E_n\right)^2} \tag{7.5.13}$$

where the width w will be set to the fixed-point bandwidth: $w = D^*$. So the function that we will numerically compute and plot is

$$\mathcal{A}(\omega) = \sum_{m,0}\left[||\left\langle 0\right| c_{d\sigma}\left|n\right\rangle||^2\frac{1}{w\sqrt{\pi}}e^{-\frac{1}{w}\left(\omega-E_n\right)^2}+||\left\langle m\right| c_{d\sigma}\left|0\right\rangle||^2\frac{1}{w\sqrt{\pi}}e^{-\frac{1}{w}\left(\omega+E_m\right)^2}\right] \tag{7.5.14}$$

The fixed-point Hamiltonian H^* is diagonalized numerically to obtain $\left\{E_m, \left|m\right\rangle\right\}$. The spectral function is plotted for three sets of bare values in fig. 7.7. For low values of U, the profile is that of a single peak at zero frequency. As U increases, shoulder-like structures appear on either side of the peak, which finally, at larger U, develop into two side-peaks.

The physics of the three peaks can now be looked into. Since the central peak is at zero energy, it has to do with excitations that do not cost any energy. There are two such excitations: excitations within the spin sector and within the charge sector.

$$\left|\uparrow\right\rangle \underset{JS_d^+}{\overset{JS_d^-}{\rightleftarrows}} \left|\downarrow\right\rangle, \qquad \left|\Uparrow\right\rangle \underset{KC_d^+}{\overset{KC_d^-}{\rightleftarrows}} \left|\Downarrow\right\rangle \tag{7.5.15}$$

The thick arrow $\Uparrow$ represents the charge isospin. At particle-hole symmetry, both the spin configurations has energy of ϵ_d, while the charge configurations have energy of $2\epsilon_d + U = 0$ and 0. Hence, no energy is required for these excitations, which is why see a macroscopic number of cloud electrons resonating with the impurity at the Fermi surface. Also note that if $\hat{S}_i$ and $\hat{C}_j$ are two operators of the spin and charge sector ($i, j \in \left\{x, y, z\right\}$), then

$$\hat{S}_i\hat{C}_j = \hat{C}_j\hat{S}_i = 0 \tag{7.5.16}$$

We can see this by applying that operator on a basis state. Since the set of four states

$$|\hat{S}_i = \pm\frac{1}{2}, \hat{C}_j = 0\rangle, |\hat{S}_i = 0, \hat{C}_j = \pm\frac{1}{2}\rangle \tag{7.5.17}$$

are all independent, they form a basis. If we apply the operator on these states:

$$\begin{aligned} \hat{S}_i\hat{C}_j |\hat{S}_i\rangle = 0, \qquad \hat{C}_j\hat{S}_i |S_i\rangle = S_i\hat{C}_j |S_i\rangle = 0 \\ \hat{C}_j\hat{S}_i |C_j\rangle = 0, \qquad \hat{S}_i\hat{C}_j |\hat{C}_j\rangle = C_j\hat{S}_i |\hat{C}_j\rangle = 0 \end{aligned} \tag{7.5.18}$$

This shows that each operator acts only on its own subspace. S_i does not act on the charge sector, and vice-versa. There is no single-particle excitation here.

The physics of the side-peaks is that of single number fluctuations on the impurity. These are brought about by the term $Vc^\dagger_{0\sigma}c_{d\sigma}$ + h.c..

$$(\epsilon_d)\ |\sigma\rangle \underset{Vc_{d\overline{\sigma}}/Vc^\dagger_{d\sigma}}{\overset{Vc^\dagger_{d\overline{\sigma}}/Vc_{d\sigma}}{\rightleftarrows}} |n_d = 2, 0\rangle\ (0) \tag{7.5.19}$$

These transitions involve energy transfer of the order of ϵ_d. This is why, at very small U, they remain absorbed inside the central peak. These transitions do not involve any spin or charge-flip, rather they take the impurity between the spin and charge sectors.

7.6 Renormalization of impurity spectral function

Another interesting study that we conducted is the change in the spectral function under revere-RG. Doing the actual reverse RG would require diagonalizing a huge matrix. Instead, we mimic the reverse journey by starting from the fixed point and then increasing the U (it was irrelevant in the forward RG) and decreasing J (it was relevant in the forward RG). The spectral function is then calculated at these points. The result is shown in fig. 7.8. At the strong-coupling fixed-point, we have a screened-local moment which only has a zero-energy excitation at the Fermi energy. As we move away from the fixed-point, the resonance at the Fermi surface disappears, and is replaced by two side peaks which are indicative of the two orientations of a local moment.

7.7 Effective Hamiltonian for excitations of the Kondo cloud

To find an effective Hamiltonian for the excitations of the Kondo cloud, we will integrate out the impurity part of the wavefunction. The Schrodinger equation for the $J > K$

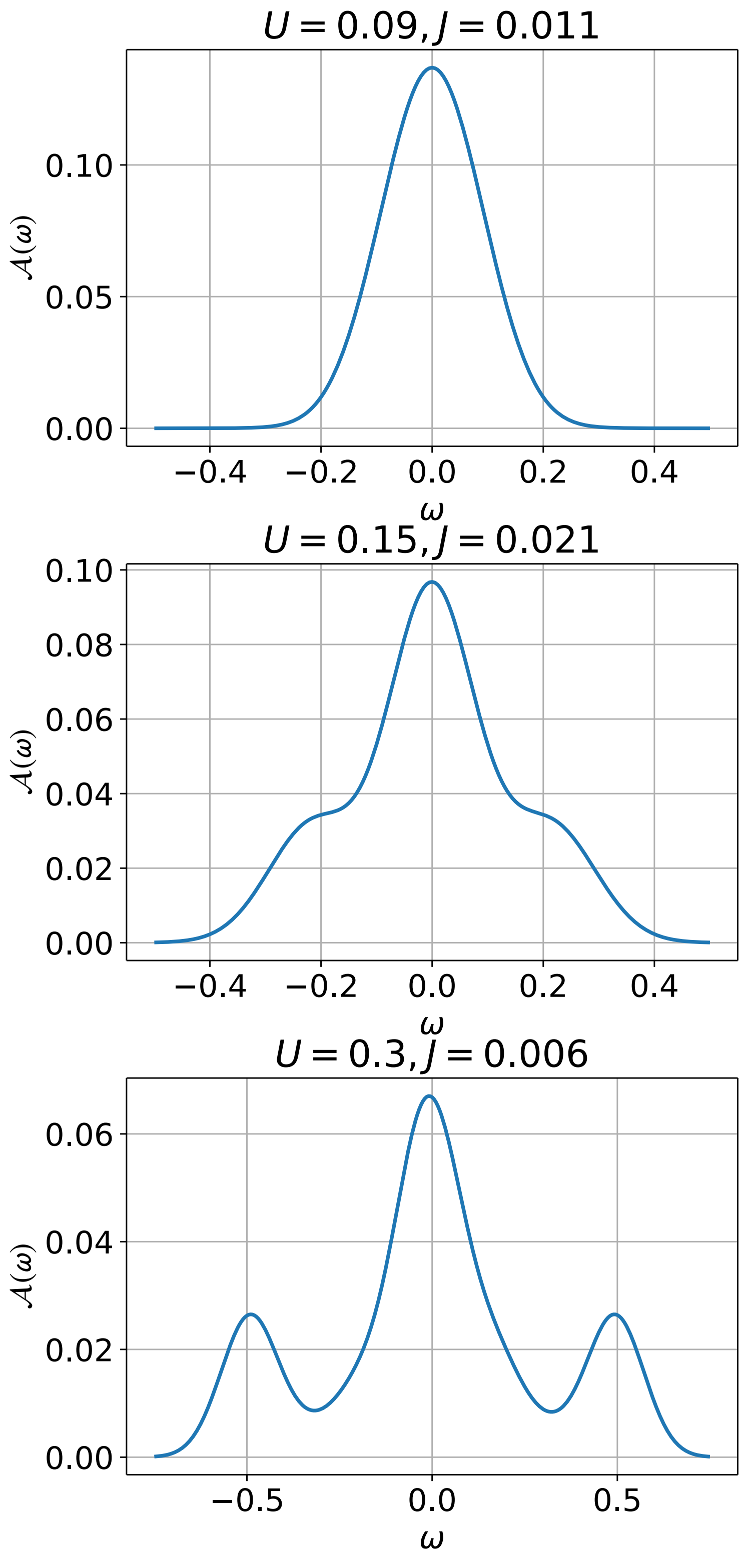

Figure 7.7: Impurity spectral function for three sets of bare values. The increase in value of U is accompanied by the appearance of the side-peaks. For all the plots, $V = 0.001$ and $D = 1$.

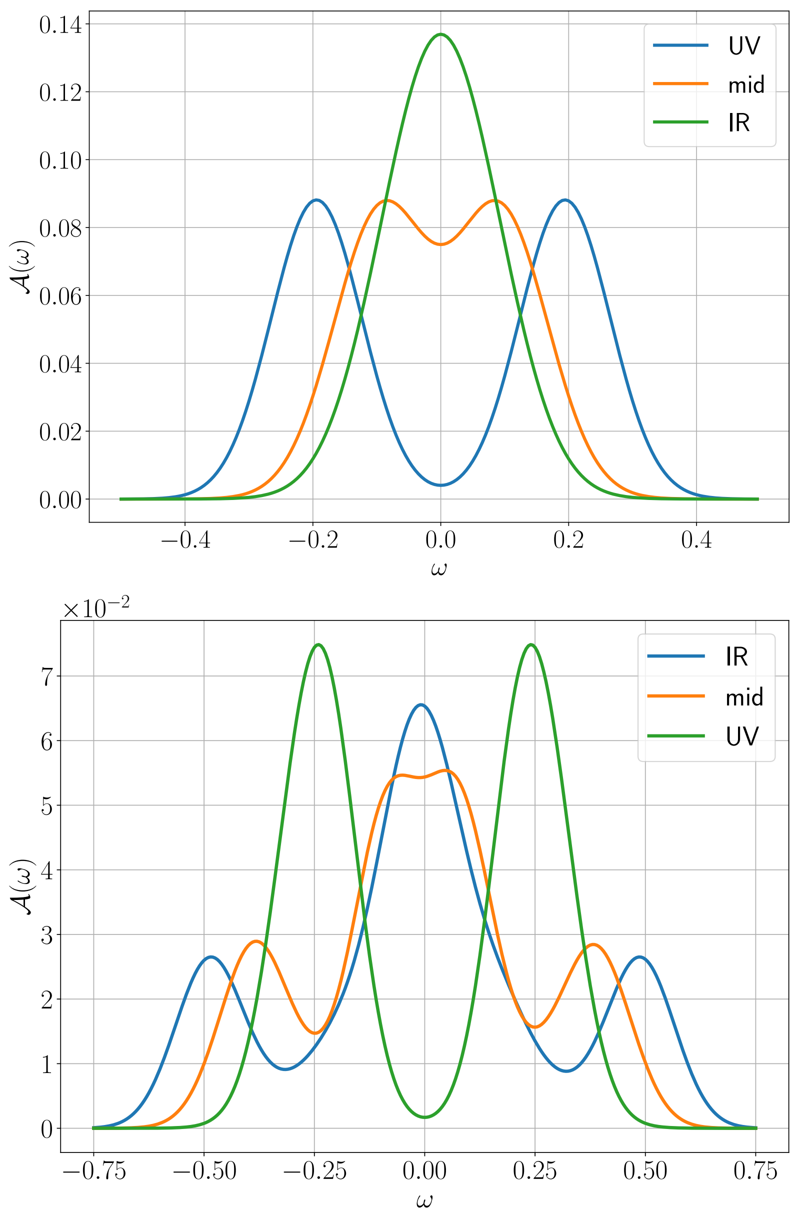

Figure 7.8: Variation of the spectral function as we move away from the strong-coupling fixed point (top) towards the local moment fixed point (bottom).

ground state is

$$\begin{aligned}
&E_g \left[c_-^s \left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right) + c_-^c \left(|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle\right)\right] \\
&\quad = \mathcal{H} \left[c_-^s \left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right) + c_-^c \left(|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle\right)\right] \\
&\quad = \mathcal{H}_0^* \left[c_-^s \left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right) + c_-^c \left(|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle\right)\right] \\
&\quad + V \sum_\beta \left[c_{2\beta}^\dagger c_{1\beta} - c_{2\beta} c_{1\beta}^\dagger\right] \left[c_-^s \left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right) + c_-^c \left(|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle\right)\right] \\
&\quad + J\vec{S}_d \cdot \vec{s} \left[c_-^s \left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right) + c_-^c \left(|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle\right)\right] \\
&\quad + K\vec{C}_d \cdot \vec{c} \left[c_-^s \left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right) + c_-^c \left(|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle\right)\right]
\end{aligned} \tag{7.7.1}$$

The last two lines gives

$$\begin{aligned}
\frac{1}{2}Jc_-^s \left[s^z \left(|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle\right) + s^+ |\downarrow,\downarrow\rangle - s^- |\uparrow,\uparrow\rangle\right] + \frac{1}{2}Kc_-^c \Big[c^z \left(|\uparrow\downarrow,0\rangle - |0,\uparrow\downarrow\rangle\right) + c^+ |0,0\rangle \\
+ c^- |2,2\rangle\Big]
\end{aligned} \tag{7.7.2}$$

The second line gives

$$\begin{aligned}
V c_{2\uparrow}^\dagger \left[c_-^s \left(|0,\downarrow\rangle\right) + c_-^c \left(|\downarrow,0\rangle\right)\right] + V c_{2\downarrow}^\dagger \left[c_-^s \left(-|0,\uparrow\rangle\right) + c_-^c \left(|\uparrow,0\rangle\right)\right] \\
-V c_{2\uparrow} \left[c_-^s \left(-|\uparrow\downarrow,\uparrow\rangle\right) + c_-^c \left(|\uparrow,\uparrow\downarrow\rangle\right)\right] - V c_{2\downarrow} \left[c_-^s \left(-|\uparrow\downarrow,\downarrow\rangle\right) + c_-^c \left(|\downarrow,\uparrow\downarrow\rangle\right)\right]
\end{aligned} \tag{7.7.3}$$

We will now write down four equations by comparing the coefficients of $|\uparrow\rangle$, $|\downarrow\rangle$, $|0\rangle$ and $|2\rangle$ of the impurity sector:

$$\begin{aligned}
\left(E_g - H_0^*\right) c_-^s |\downarrow\rangle &= V c_-^c \left(c_{2\downarrow}^\dagger |0\rangle - c_{2\uparrow} |2\rangle\right) + \frac{1}{2}Jc_-^s \left(s^z |\downarrow\rangle - s^- |\uparrow\rangle\right) && [\text{eq. from } |\uparrow\rangle] \\
\left(-E_g + H_0^*\right) c_-^s |\uparrow\rangle &= V c_-^c \left(c_{2\uparrow}^\dagger |0\rangle - c_{2\downarrow}^\dagger |2\rangle\right) + \frac{1}{2}Jc_-^s \left(s^z |\uparrow\rangle + s^+ |\downarrow\rangle\right) && [\text{eq. from } |\downarrow\rangle] \\
\left(E_g - H_0^*\right) c_-^c |2\rangle &= V c_-^s \left(c_{2\uparrow}^\dagger |\downarrow\rangle - c_{2\downarrow}^\dagger |\uparrow\rangle\right) + \frac{1}{2}Kc_-^c \left(-c^z |2\rangle + c^+ |0\rangle\right) && [\text{eq. from } |0\rangle] \\
\left(E_g - H_0^*\right) c_-^c |0\rangle &= V c_-^s \left(c_{2\uparrow} |\uparrow\rangle + c_{2\downarrow} |\downarrow\rangle\right) + \frac{1}{2}Kc_-^c \left(c^z |0\rangle + c^- |2\rangle\right) && [\text{eq. from } |2\rangle]
\end{aligned} \tag{7.7.4}$$

These can be rearranged into

$$\begin{aligned}
\left(E_g - H_0^* - \frac{1}{2}Js^z\right) |\downarrow\rangle &= V\lambda^{-1} \left(c_{2\downarrow}^\dagger |0\rangle - c_{2\uparrow} |2\rangle\right) - \frac{1}{2}Js^- |\uparrow\rangle \\
\left(E_g - H_0^* + \frac{1}{2}Js^z\right) |\uparrow\rangle &= V\lambda^{-1} \left(c_{2\downarrow} |2\rangle - c_{2\uparrow}^\dagger |0\rangle\right) - \frac{1}{2}Js^+ |\downarrow\rangle \\
\left(E_g - H_0^* + \frac{1}{2}Kc^z\right) |2\rangle &= V\lambda \left(c_{2\uparrow}^\dagger |\downarrow\rangle - c_{2\downarrow}^\dagger |\uparrow\rangle\right) + \frac{1}{2}Kc^+ |0\rangle \\
\left(E_g - H_0^* - \frac{1}{2}Kc^z\right) |0\rangle &= V\lambda \left(c_{2\uparrow} |\uparrow\rangle + c_{2\downarrow} |\downarrow\rangle\right) + \frac{1}{2}Kc^- |2\rangle
\end{aligned} \tag{7.7.5}$$

where $\lambda = \frac{c^s}{c^c_-}$. We want to find the effective Hamiltonian in the subspace of $|\downarrow\rangle$. We first eliminate the charge sector from these equations:

$$\begin{aligned}
|0\rangle =& V\lambda \left[\frac{1}{A^K_-} c_{2\uparrow} + \frac{K}{2} \frac{1}{A^K_-} c^- \frac{1}{A^K_+ - \left(\frac{K}{2}\right)^2 c^+ \frac{1}{A^K_-} c^-} \left(\frac{K}{2} c^+ \frac{1}{A^K_-} c_{2\uparrow} - c^\dagger_{2\downarrow} \right) \right] |\uparrow\rangle \\
&+ V\lambda \left[\frac{1}{A^K_-} c_{2\downarrow} + \frac{K}{2} \frac{1}{A^K_-} c^- \frac{1}{A^K_+ - \left(\frac{K}{2}\right)^2 c^+ \frac{1}{A^K_-} c^-} \left(c^\dagger_{2\uparrow} + \frac{K}{2} c^+ \frac{1}{A^K_-} c_{2\downarrow} \right) \right] |\downarrow\rangle \\
|2\rangle =& \frac{V\lambda}{A^K_+ - \left(\frac{K}{2}\right)^2 c^+ \frac{1}{A^K_-} c^-} \left[\left(c^\dagger_{2\uparrow} + \frac{K}{2} c^+ \frac{1}{A^K_-} c_{2\downarrow} \right) |\downarrow\rangle + \left(\frac{K}{2} c^+ \frac{1}{A^K_-} c_{2\uparrow} - c^\dagger_{2\downarrow} \right) |\uparrow\rangle \right]
\end{aligned} \tag{7.7.6}$$

where

$$A^K_\pm = E_g - H^*_0 \pm \frac{1}{2} K c^z \tag{7.7.7}$$

For ease of labeling, we will think of these equations as

$$|0\rangle = a^\uparrow_0 |\uparrow\rangle + a^\downarrow_0 |\downarrow\rangle, |2\rangle = a^\uparrow_2 |\uparrow\rangle + a^\downarrow_2 |\downarrow\rangle \tag{7.7.8}$$

The remaining two equations can then be written as

$$\begin{aligned}
A^J_- |\downarrow\rangle &= \frac{V}{\lambda} \left[c^\dagger_{2\downarrow} \left(a^\uparrow_0 |\uparrow\rangle + a^\downarrow_0 |\downarrow\rangle \right) - c_{2\uparrow} \left(a^\uparrow_2 |\uparrow\rangle + a^\downarrow_2 |\downarrow\rangle \right) \right] - \frac{J}{2} s^- |\uparrow\rangle \\
A^J_+ |\uparrow\rangle &= \frac{V}{\lambda} \left[c_{2\downarrow} \left(a^\uparrow_2 |\uparrow\rangle + a^\downarrow_2 |\downarrow\rangle \right) - c^\dagger_{2\uparrow} \left(a^\uparrow_0 |\uparrow\rangle + a^\downarrow_0 |\downarrow\rangle \right) \right] - \frac{J}{2} s^+ |\downarrow\rangle
\end{aligned} \tag{7.7.9}$$

where

$$A^J_\pm = E_g - H^*_0 \pm \frac{1}{2} J s^z \tag{7.7.10}$$

Eliminating $|\downarrow\rangle$ and solving for $|\uparrow\rangle$ gives

$$\begin{aligned}
A^J_+ |\uparrow\rangle =& \frac{V}{\lambda} \left(c_{2\downarrow} a^\uparrow_2 - c^\dagger_{2\uparrow} a^\uparrow_0 \right) |\uparrow\rangle + \left(\frac{V}{\lambda} c_{2\downarrow} a^\downarrow_2 - \frac{V}{\lambda} c^\dagger_{2\uparrow} a^\downarrow_0 - \frac{J}{2} s^+ \right) |\downarrow\rangle \\
=& \frac{V}{\lambda} \left(c_{2\downarrow} a^\uparrow_2 - c^\dagger_{2\uparrow} a^\uparrow_0 \right) |\uparrow\rangle \\
&+ \left[\frac{V}{\lambda} \left(c_{2\downarrow} a^\downarrow_2 - c^\dagger_{2\uparrow} a^\downarrow_0 \right) - \frac{J}{2} s^+ \right] \frac{1}{A^J_- - \frac{V}{\lambda} \left(c^\dagger_{2\downarrow} a^\downarrow_0 - c_{2\uparrow} a^\downarrow_2 \right)} \left[\frac{V}{\lambda} \left(c^\dagger_{2\downarrow} a^\uparrow_0 - c_{2\uparrow} a^\uparrow_2 \right) - \frac{J}{2} s^- \right] |\uparrow\rangle
\end{aligned} \tag{7.7.11}$$

The effective Hamiltonian for the $|\uparrow\rangle$ state is

$$\begin{aligned}
H^*_0 - \frac{J}{2} s^z + \frac{V}{\lambda} \left(c_{2\downarrow} a^\uparrow_2 - c^\dagger_{2\uparrow} a^\uparrow_0 \right) + \left[\frac{V}{\lambda} \left(c_{2\downarrow} a^\downarrow_2 - c^\dagger_{2\uparrow} a^\downarrow_0 \right) - \frac{J}{2} s^+ \right] \frac{1}{A^J_- - \frac{V}{\lambda} \left(c^\dagger_{2\downarrow} a^\downarrow_0 - c_{2\uparrow} a^\downarrow_2 \right)} \\
\times \left[\frac{V}{\lambda} \left(c^\dagger_{2\downarrow} a^\uparrow_0 - c_{2\uparrow} a^\uparrow_2 \right) - \frac{J}{2} s^- \right]
\end{aligned} \tag{7.7.12}$$

To get a clearer picture of this effective Hamiltonian, we will keep up to two-particle interactions. We first write down the full forms of $a^\sigma_{0,2}$:

$$\begin{aligned} a^\sigma_0 &= V\lambda\left[\frac{1}{A^K_-}c_{2\sigma} + \frac{K}{2}\frac{1}{A^K_-}c^- \frac{1}{A^K_+ - \left(\frac{K}{2}\right)^2 c^+ \frac{1}{A^K_-}c^-}\left(\frac{K}{2}c^+ \frac{1}{A^K_-}c_{2\sigma} - \sigma c^\dagger_{2\sigma}\right)\right] \\ a^\sigma_2 &= \frac{V\lambda}{A^K_+ - \left(\frac{K}{2}\right)^2 c^+ \frac{1}{A^K_-}c^-}\left(-\sigma c^\dagger_{2-\sigma} + \frac{K}{2}c^+ \frac{1}{A^K_-}c_{2\sigma}\right) \end{aligned} \tag{7.7.13}$$

We will first look at the special case of $K = 0$. There, the above expressions simplify to

$$\begin{aligned} a^\sigma_0 &= V\lambda\frac{1}{A^K_-}c_{2\sigma} = \frac{V\lambda}{E_g}\left[1 + \frac{1}{E_g}\left(H^*_0\right) + \frac{1}{E_g^2}\left(H^*_0\right)^2\right]c_{2\sigma} + \mathcal{O}({H^*_0}^3) \\ a^\sigma_2 &= -\sigma V\lambda\frac{1}{A^K_+}c^\dagger_{2-\sigma} = -\sigma\frac{V\lambda}{E_g}\left[1 + \frac{1}{E_g}\left(H^*_0\right) + \frac{1}{E_g^2}\left(H^*_0\right)^2\right]c^\dagger_{2-\sigma} + \mathcal{O}({H^*_0}^3) \end{aligned} \tag{7.7.14}$$

We will make use of the following commutators:

$$\begin{aligned} &\left[\left(H^*_0\right)^m, c_{2\sigma}\right] = -\sum_k \frac{\epsilon^m_k}{\sqrt{N^*}}c_{k\sigma}, && \left[\left(H^*_0\right)^m, c^\dagger_{2\sigma}\right] = \sum_k \frac{\epsilon^m_k}{\sqrt{N^*}}c^\dagger_{k\sigma}, && m = 1,2 \\ &\left[\left(H^*_0\right)^m, s^+\right] = \sum_{kk'}\left(\epsilon^m_k - \epsilon^m_{k'}\right)c^\dagger_{k\beta}c_{k'\overline{\beta}}, && && m = 1,2 \\ &\left[\left(s^z\right)^m, c_{2\sigma}\right] = -\left(\frac{\sigma}{2}\right)^m c_{2\sigma}, && \left[\left(s^z\right)^m, c^\dagger_{2\sigma}\right] = \left(\frac{\sigma}{2}\right)^m c^\dagger_{2\sigma}, && m = 1,2 \\ &\left[\left(c^z\right)^m, c_{2\sigma}\right] = -\left(\frac{1}{2}\right)^m c_{2\sigma}, && \left[\left(c^z\right)^m, c^\dagger_{2\sigma}\right] = \left(\frac{1}{2}\right)^m c^\dagger_{2\sigma}, && m = 1,2 \end{aligned} \tag{7.7.15}$$

Now we evaluate the various terms in the effective Hamiltonian.

$$\begin{aligned} \mathbf{c_{2\downarrow}a^\uparrow_2} &= -\frac{V\lambda}{E_g}c_{2\downarrow}\left[1 + \frac{1}{E_g}\left(H^*_0\right) + \frac{1}{E_g^2}\left(H^*_0\right)^2\right]c^\dagger_{2\downarrow} \\ &= -\frac{V\lambda}{E_g}\left[c_{2\downarrow} + \frac{1}{E_g}\left(H^*_0\right)c_{2\downarrow} + \sum_k \frac{\epsilon_k}{E_g\sqrt{N^*}}c_{k\downarrow} + \frac{1}{E_g^2}\left(H^*_0\right)^2 c_{2\downarrow} + \sum_k \frac{\epsilon^2_k}{E_g^2\sqrt{N^*}}c_{k\downarrow}\right]c^\dagger_{2\downarrow} \\ &= -\frac{V\lambda}{E_g}\left[1 + \frac{H^*_0}{E_g} + \left(\frac{H^*_0}{E_g}\right)^2\right]c_{2\downarrow}c^\dagger_{2\downarrow} - \frac{V\lambda}{E_g N^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g} + \frac{\epsilon^2_k}{E_g^2}\right)c_{k\downarrow}c^\dagger_{k'\downarrow} \\ \mathbf{c_{2\uparrow}a^\downarrow_2} &= -\frac{V\lambda}{E_g}\left[1 + \frac{H^*_0}{E_g} + \left(\frac{H^*_0}{E_g}\right)^2\right]c_{2\uparrow}c^\dagger_{2\uparrow} - \frac{V\lambda}{E_g N^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g} + \frac{\epsilon^2_k}{E_g^2}\right)c_{k\uparrow}c^\dagger_{k'\uparrow} \end{aligned}$$

$$
\begin{aligned}
\mathbf{c}^\dagger_{2\uparrow}\mathbf{a}^\uparrow_{\mathbf{0}} &= c^\dagger_{2\uparrow}\frac{V\lambda}{E_g}\left[1+\frac{1}{E_g}\left(H_0^*\right)+\frac{1}{E_g^2}\left(H_0^*\right)^2\right]c_{2\uparrow}\\
&= \frac{V\lambda}{E_g}\left[1+\frac{H_0^*}{E_g}+\left(\frac{H_0^*}{E_g}\right)^2\right]c^\dagger_{2\uparrow}c_{2\uparrow}-\frac{V\lambda}{E_gN^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g}+\frac{\epsilon_k^2}{E_g^2}\right)c^\dagger_{k\uparrow}c_{k'\uparrow}\\
\mathbf{c}^\dagger_{2\downarrow}\mathbf{a}^\downarrow_{\mathbf{0}} &= \frac{V\lambda}{E_g}\left[1+\frac{H_0^*}{E_g}+\left(\frac{H_0^*}{E_g}\right)^2\right]c^\dagger_{2\downarrow}c_{2\downarrow}-\frac{V\lambda}{E_gN^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g}+\frac{\epsilon_k^2}{E_g^2}\right)c^\dagger_{k\downarrow}c_{k'\downarrow}\\
\mathbf{c}_{2\downarrow}\mathbf{a}^\downarrow_{\mathbf{2}} &= \frac{V\lambda}{E_g}c_{2\downarrow}\left[1+\frac{1}{E_g}\left(H_0^*\right)+\frac{1}{E_g^2}\left(H_0^*\right)^2\right]c^\dagger_{2\uparrow}\\
&= \frac{V\lambda}{E_g}\left[1+\frac{1}{E_g}\left(H_0^*\right)\right]c_{2\downarrow}c^\dagger_{2\uparrow}+\frac{V\lambda}{E_gN^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g}+\frac{\epsilon_k^2}{E_g^2}\right)c_{k\downarrow}c^\dagger_{k'\uparrow}\\
\mathbf{c}_{2\uparrow}\mathbf{a}^\uparrow_{\mathbf{2}} &= -\frac{V\lambda}{E_g}\left[1+\frac{1}{E_g}\left(H_0^*\right)\right]c_{2\uparrow}c^\dagger_{2\downarrow}-\frac{V\lambda}{E_gN^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g}+\frac{\epsilon_k^2}{E_g^2}\right)c_{k\uparrow}c^\dagger_{k'\downarrow}\\
\mathbf{c}^\dagger_{2\uparrow}\mathbf{a}^\downarrow_{\mathbf{0}} &= \frac{V\lambda}{E_g}\left[1+\frac{H_0^*}{E_g}\right]c^\dagger_{2\uparrow}c_{2\downarrow}-\frac{V\lambda}{E_gN^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g}+\frac{\epsilon_k^2}{E_g^2}\right)c^\dagger_{k\uparrow}c_{k'\downarrow}\\
\mathbf{c}^\dagger_{2\downarrow}\mathbf{a}^\uparrow_{\mathbf{0}} &= \frac{V\lambda}{E_g}\left[1+\frac{H_0^*}{E_g}\right]c^\dagger_{2\downarrow}c_{2\uparrow}-\frac{V\lambda}{E_gN^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g}+\frac{\epsilon_k^2}{E_g^2}\right)c^\dagger_{k\downarrow}c_{k'\uparrow}\\
\mathbf{c}_{2\downarrow}\mathbf{a}^\uparrow_{\mathbf{2}}-\mathbf{c}^\dagger_{2\uparrow}\mathbf{a}^\uparrow_{\mathbf{0}} &= -\frac{V\lambda}{E_g}\left[1+\frac{H_0^*}{E_g}+\left(\frac{H_0^*}{E_g}\right)^2\right]\times 2+\frac{V\lambda}{E_gN^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g}+\frac{\epsilon_k^2}{E_g^2}\right)\left(c^\dagger_{k\uparrow}c_{k'\uparrow}-c_{k\downarrow}c^\dagger_{k'\downarrow}\right)\\
\mathbf{c}_{2\downarrow}\mathbf{a}^\downarrow_{\mathbf{2}}-\mathbf{c}^\dagger_{2\uparrow}\mathbf{a}^\downarrow_{\mathbf{0}} &= \frac{V\lambda}{E_g}\left[1+\frac{1}{E_g}\left(H_0^*\right)\right]c_{2\downarrow}c^\dagger_{2\uparrow}\times 2+\frac{V\lambda}{E_gN^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g}+\frac{\epsilon_k^2}{E_g^2}\right)\left(c_{k\downarrow}c^\dagger_{k'\uparrow}+c^\dagger_{k\uparrow}c_{k'\downarrow}\right)\\
\mathbf{c}^\dagger_{2\downarrow}\mathbf{a}^\downarrow_{\mathbf{0}}-\mathbf{c}_{2\uparrow}\mathbf{a}^\downarrow_{\mathbf{2}} &= \frac{V\lambda}{E_gN^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g}+\frac{\epsilon_k^2}{E_g^2}\right)\left(c_{k\uparrow}c^\dagger_{k'\uparrow}-c^\dagger_{k\downarrow}c_{k'\downarrow}\right)\\
\mathbf{c}^\dagger_{2\downarrow}\mathbf{a}^\uparrow_{\mathbf{0}}-\mathbf{c}_{2\uparrow}\mathbf{a}^\uparrow_{\mathbf{2}} &= \frac{V\lambda}{E_gN^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g}+\frac{\epsilon_k^2}{E_g^2}\right)\left(c_{k\uparrow}c^\dagger_{k'\downarrow}-c^\dagger_{k\downarrow}c_{k'\uparrow}\right)
\end{aligned}
$$

In all the expressions, we have dropped terms that have more than 4 operators in product. Also, in the last four equations, we have substituted $\hat{n}_{2\uparrow}-\hat{n}_{2\downarrow}=1$, because this is the effective Hamiltonian for the state with $s^z=\frac{1}{2}$. We now substitute these expressions into the effective Hamiltonian:

$$
\begin{aligned}
&H_0^* - \frac{J}{2}s^z - \frac{2V^2}{E_g}\left[1 + \frac{H_0^*}{E_g} + \left(\frac{H_0^*}{E_g}\right)^2\right] + \frac{V^2}{E_g N^*}\sum_{kk'} \xi_k \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow} c_{k'\downarrow}^\dagger\right) \\
&+ \left[\frac{V}{\lambda}\left(c_{2\downarrow} a_2^\downarrow - c_{2\uparrow}^\dagger a_0^\downarrow\right)\right] \frac{1}{A_-^J - \frac{V^2}{E_g N^*}\sum_{kk'} \xi_k \left(c_{k\uparrow} c_{k'\uparrow}^\dagger - c_{k\downarrow}^\dagger c_{k'\downarrow}\right)} \left[\frac{V}{\lambda}\left(c_{2\downarrow}^\dagger a_0^\uparrow - c_{2\uparrow} a_2^\uparrow\right)\right] \\
&+ \left[\frac{V}{\lambda}\left(c_{2\downarrow} a_2^\downarrow - c_{2\uparrow}^\dagger a_0^\downarrow\right)\right] \frac{1}{A_-^J - \frac{V^2}{E_g N^*}\sum_{kk'} \xi_k \left(c_{k\uparrow} c_{k'\uparrow}^\dagger - c_{k\downarrow}^\dagger c_{k'\downarrow}\right)} \left[-\frac{J}{2}s^-\right] \\
&+ \left[-\frac{J}{2}s^+\right] \frac{1}{A_-^J - \frac{V^2}{E_g N^*}\sum_{kk'} \xi_k \left(c_{k\uparrow} c_{k'\uparrow}^\dagger - c_{k\downarrow}^\dagger c_{k'\downarrow}\right)} \left[\frac{V}{\lambda}\left(c_{2\downarrow}^\dagger a_0^\uparrow - c_{2\uparrow} a_2^\uparrow\right)\right] \\
&+ \frac{J^2}{4}\left[s^+\right] \frac{1}{A_-^J - \frac{V^2}{E_g N^*}\sum_{kk'} \xi_k \left(c_{k\uparrow} c_{k'\uparrow}^\dagger - c_{k\downarrow}^\dagger c_{k'\downarrow}\right)} \left[s^-\right]
\end{aligned}
\tag{7.7.16}
$$

where $\xi_k = \frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2}$. We first consider only zeroth order terms of the central propagator.

$$
\begin{aligned}
&H_0^* - \frac{J}{2}\underbrace{s^z}_{\frac{1}{2}} - \frac{2V^2}{E_g}\left[1 + \frac{H_0^*}{E_g} + \left(\frac{H_0^*}{E_g}\right)^2\right] + \frac{V^2}{E_g N^*}\sum_{kk'} \left(\xi_k\right) \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow} c_{k'\downarrow}^\dagger\right) \\
&+ \frac{V^4}{E_g^2 N^{*2}\left(E_g + \frac{J}{4}\right)} \sum_{kk'} \left(\xi_{k'} + 2 - \xi_k\right) c_{k\uparrow}^\dagger c_{k'\downarrow} \sum_{kk'} \left(\xi_k + \xi_{k'}\right) c_{k\downarrow}^\dagger c_{k'\uparrow} \\
&+ \frac{V^2 J}{2E_g\left(E_g + \frac{J}{4}\right)N^*} \sum_{kk'} \left(\xi_{k'} + 2 - \xi_k\right) c_{k\uparrow}^\dagger c_{k'\downarrow} \sum_{kk'} c_{k\downarrow}^\dagger c_{k'\uparrow} \\
&+ \frac{JV^2}{2E_g\left(E_g + \frac{J}{4}\right)N^*} \sum_{kk'} c_{k\uparrow}^\dagger c_{k'\downarrow} \sum_{kk'} \left(\xi_k + \xi_{k'}\right) c_{k\downarrow}^\dagger c_{k'\uparrow} \\
&+ \frac{J^2}{4\left(E_g + \frac{J}{4}\right)} \underbrace{s^+ s^-}_{s^z + \frac{1}{2} = 1}
\end{aligned}
\tag{7.7.17}
$$

We have set $s^z = -\frac{1}{2}$ in the denominator, hence the $E_g = \frac{J}{4}$. If we also consider the first and second order terms from the central propagator, note that they will produce terms of more than quartic interactions in the first three terms. For the last term, we get

$$
\frac{J^2}{4\left(E_g + \frac{J}{4}\right)} s^+ \left[\frac{H_0^*}{E_g + \frac{J}{4}} + \left(\frac{H_0^*}{E_g + \frac{J}{4}}\right)^2\right] s^- \tag{7.7.18}
$$

Using the commutator of H_0^* with s^+ to bring H_0^* to the left, and using $s^+s^- = s^z + \frac{1}{2} = 1$, we get

$$\frac{J^2}{4\left(E_g + \frac{J}{4}\right)}\left[\frac{H_0^*}{E_g + \frac{J}{4}} + \left(\frac{H_0^*}{E_g + \frac{J}{4}}\right)^2 - \sum_{kk'qq'}\left(\xi_k^J - \xi_{k'}^J\right) c_{k\uparrow}^\dagger c_{k'\downarrow} c_{q\downarrow}^\dagger c_{q'\uparrow}\right] \tag{7.7.19}$$

where $\xi_k^J = \frac{\epsilon_k}{E_g + \frac{J}{4}} + \frac{\epsilon_k^2}{\left(E_g+\frac{J}{4}\right)^2}$. The full effective Hamiltonian, for $K = 0$, up to quartic interactions, is

$$\begin{aligned} &H_0^* + \frac{J}{4}\left(\frac{J}{E_g + \frac{J}{4}} - 1\right) - \frac{2V^2}{E_g} + \frac{V^2}{E_g N^*}\sum_{kk'}\left(\xi_k\right)\left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow} c_{k'\downarrow}^\dagger\right) - \frac{2V^2}{E_g}\left[\frac{H_0^*}{E_g} + \left(\frac{H_0^*}{E_g}\right)^2\right] \\ &\quad + \frac{J^2}{4\left(E_g + \frac{J}{4}\right)}\left[\frac{H_0^*}{E_g + \frac{J}{4}} + \left(\frac{H_0^*}{E_g + \frac{J}{4}}\right)^2\right] + \sum_{kk'qq'} F_{kk'qq'} c_{k\uparrow}^\dagger c_{k'\downarrow} c_{q\downarrow}^\dagger c_{q'\uparrow} \end{aligned} \tag{7.7.20}$$

The coefficient $F_{kk'qq'}$ is

$$\begin{aligned} F_{kk'qq'} = &\frac{V^2}{E_g N^*(E_g + \frac{J}{4})}\left[\frac{V^2}{E_g N^*}\left(\xi_{k'} + 2 - \xi_k\right)\left(\xi_q + \xi_{q'}\right) + \frac{J}{2}\left(\xi_{k'} + 2 - \xi_k + \xi_q + \xi_{q'}\right)\right] \\ &+ \frac{J^2}{4\left(E_g + \frac{J}{4}\right)}\left(\xi_{k'}^J - \xi_k^J\right) \end{aligned} \tag{7.7.21}$$

There are two main types of interactions that gets generated upon integrating out the impurity. One is the Fermi liquid type interactions arising from the H_0^{*2} terms. The Fermi liquid part of the Hamiltonian is

$$\begin{aligned} &\left[\frac{J^2}{4\left(E_g + \frac{J}{4}\right)^2} - \frac{2V^2}{E_g^2}\right] H_0^* + \left[\frac{J^2}{4\left(E_g + \frac{J}{4}\right)^2} - \frac{2V^2}{E_g^3}\right] H_0^{*2} \\ &= \left[\frac{J^2}{4\left(E_g + \frac{J}{4}\right)^2} - \frac{2V^2}{E_g^2}\right]\left[H_0^* + \sum_{kk'\sigma\sigma'} f_{kk'} \hat{n}_{k\sigma} \hat{n}_{k'\sigma'}\right] \end{aligned} \tag{7.7.22}$$

where the Landau parameter is given by

$$f_{kk'} = \left[\frac{J^2}{4\left(E_g + \frac{J}{4}\right)^2} - \frac{2V^2}{E_g^2}\right]^{-1}\left[\frac{J^2}{4\left(E_g + \frac{J}{4}\right)^3} - \frac{2V^2}{E_g^3}\right]\epsilon_k \epsilon_{k'} \tag{7.7.23}$$

The more interesting interaction is the off-diagonal term

$$\sum_{kk'qq'} F_{kk'qq'} c^\dagger_{k\uparrow} c_{k'\downarrow} c^\dagger_{q\downarrow} c_{q'\uparrow} \tag{7.7.24}$$

This interaction arises from the enhanced entanglement between the impurity and the conduction electrons; removing the impurity from the singlet and the triplet generates these off-diagonal scatterings. As such, this is an indicator of the macroscopic entanglement of the singlet formed at the IR fixed point, and plotted in fig. 7.13.

It is also very enlightening to note that this scattering is a signature of the change in Luttinger's count in going from the free orbital or local moment fixed point to the strong-coupling fixed point, as shown in eq. 7.9.28. Both this off-diagonal scattering as well as the change in Luttinger's count are a direct consequence of the non-number conserving term $V c^\dagger_k c_d$ in the full Hamiltonian. The topological change of Luttinger's count is concomitant with the presence of the off-diagonal scattering term in the effective Hamiltonian. *Just the Fermi liquid piece in eq. 7.7.23 will give neither the enhanced mutual information nor the change in Luttinger's count.*

We have shown the enhancement of this off-diagonal scattering during the flow towards the IR fixed point by computing it during the reverse RG program, in fig. 7.9. It is clear from this plot that the growth of this non-Fermi-liquid type interaction happens simultaneously with the formation of the singlet.

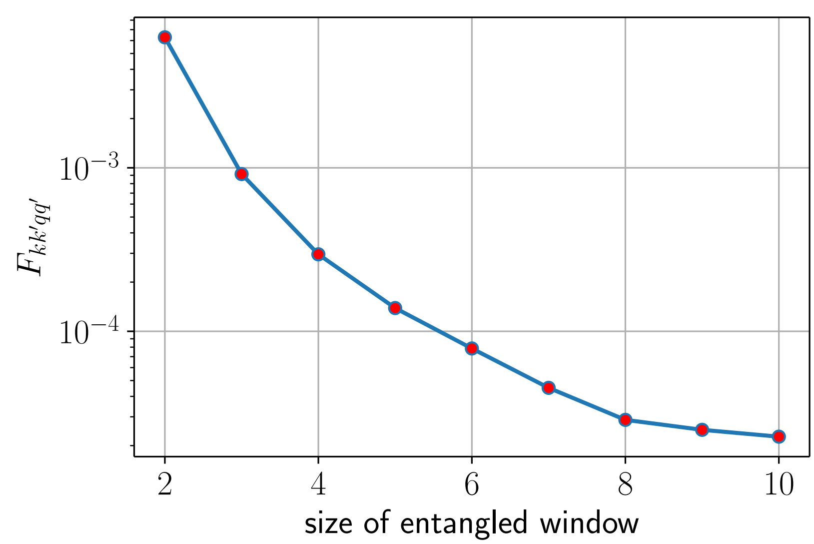

Figure 7.9: Variation of the coefficient of the two-particle off-diagonal scattering in the effective Hamiltonian, eq. 7.7.21 along the RG flow.

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):

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

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

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

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,

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

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

$$\begin{aligned} |\phi_1^{(0)}\rangle &= \underbrace{|\uparrow\rangle}_{\text{site 1}} \otimes \frac{1}{\sqrt{2}} \left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right) \\ |\phi_2^{(0)}\rangle &= \underbrace{|\uparrow,\downarrow\rangle}_{\text{site 1}} \otimes \frac{1}{\sqrt{2}} \left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right) \end{aligned} \tag{7.8.4}$$