Numerical methods for quantum impurity models
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Exercise 1: Schrieffer-Wolff transformation

The Anderson impurity model (AIM) describes a single interacting quantum level, locally tunnel-coupled to non-interacting conduction electrons of a continuum bath. Its Hamiltonian, in second-quantized notation, is given by $H_{\rm AIM} = H_{\rm bath} + H_{\rm imp} + H_{\rm hyb}$, where,

$$H_{\rm bath} = \sum_{\sigma,k} \epsilon_k c^\dagger_{\sigma k} c_{\sigma k} \ , \tag{1a}$$

$$H_{\rm imp} = \epsilon_d \left(d^\dagger_\uparrow d_\uparrow + d^\dagger_\downarrow d_\downarrow \right) + U \left(d^\dagger_\uparrow d_\uparrow d^\dagger_\downarrow d_\downarrow \right) \ , \tag{1b}$$

$$H_{\rm hyb} = \sum_{\sigma,k} \left(V_k d^\dagger_\sigma c_{\sigma k} + {\rm H.c.} \right) \ , \tag{1c}$$

where $c^\dagger_{\sigma k}$ creates a conduction electron with spin $\sigma =\uparrow$ or $\downarrow$ and momentum k; while $d^\dagger_\sigma$ creates a spin-σ electron on the *impurity* site.

The Kondo model (KM) describes a single spin-$\frac{1}{2}$ impurity, exchange coupled locally to conduction electrons. Its Hamiltonian is given by,

$$H_{\rm KM} = H_{\rm bath} + \sum_{k,k'} \left[J_{kk'} \mathbf{S} \cdot \mathbf{s}_{kk'} + K_{kk'} \sum_\sigma c^\dagger_{\sigma k} c_{\sigma k'} \right] \ , \tag{2}$$

where $\mathbf{S}$ is a spin-$\frac{1}{2}$ operator for the impurity and $\mathbf{s}_{kk'} = \sum_{\sigma,\sigma'} c^\dagger_{\sigma k} \vec{\sigma}_{\sigma\sigma'} c_{\sigma k'}$ is the conduction electron spin density (here $\vec{\boldsymbol{\sigma}}$ is a vector of Pauli matrices).

The Kondo model can be derived perturbatively from the Anderson model in a regime where the impurity is *singly-occupied*, and therefore hosts a spin-$\frac{1}{2}$ local moment corresponding to an electron with either up or down spin. When $V_k = 0$ (the 'atomic limit' of an isolated impurity), the impurity is single-occupied for $-U < \epsilon_d < 0$. When $\sum_k |V_k|^2/U \ll 1$, we may project onto the singly-occupied manifold of AIM impurity states, eliminating perturbatively virtual excitations to empty or doubly-occupied impurity states to second-order in $H_{\rm hyb}$. This is the Schrieffer-Wolff transformation.

The Brillouin-Wigner perturbation expansion,

$$H_{\rm eff} = \hat{1}_{so} H_0 \hat{1}_{so} + \hat{1}_{so} H_1 \hat{1}_{so} + \hat{1}_{so} \left[H_1 \left(E_0 - H_0 \right)^{-1} \hat{P}_{ex} H_1 \right] \hat{1}_{so} + ... \tag{3}$$

can be used to find the low-energy effective Kondo Hamiltonian by setting $H_0 = H_{\rm bath} + H_{\rm imp}$ and $H_1 = H_{\rm hyb}$. Here, $\hat{1}_{so}$ is a projector onto the singly-occupied impurity manifold, while $\hat{P}_{ex} = \hat{1}_{tot} - \hat{1}_{so}$ projects onto the excited impurity manifold (empty or doubly-occupied). E_0 is the energy of states of H_0, i.e., $H_0|\Psi_0\rangle = E_0|\Psi_0\rangle$. Ultimately we can assume that $U + \epsilon_d$ and $-\epsilon_d$ are $\gg |\epsilon_k - \epsilon_{k'}|$ at low temperatures/energies.

Find expressions for $J_{kk'}$ and $K_{kk'}$ appearing in Eq. 2, in terms of ϵ_d, U, and V_k appearing in Eq. 1.

From Eq. 1c, it can be seen that the impurity couples to a single localized bath orbital, $f_\sigma \propto \sum_k V_k c_{\sigma k}$. Express the Kondo model, Eq. 2, in terms of this localized orbital.