Numerical methods for quantum impurity models
DRSTP (9-20 March 2015. Doorn, Netherlands)
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Exercise 2: Perturbative (Poor Man's) Scaling

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

$$H = \sum_{k,\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{k,k'} J_{kk'} \mathbf{S} \cdot \mathbf{s}_{kk'} \ , \tag{1}$$

where $\mathbf{S}$ is a spin-$\frac{1}{2}$ operator for the impurity and $\mathbf{s}_{kk'} = \sum_{\sigma,\sigma'} c^\dagger_{k\sigma} \vec{\sigma}_{\sigma\sigma'} c_{k'\sigma}$ is the conduction electron spin density (here $\vec{\boldsymbol{\sigma}}$ is a vector of Pauli matrices). For simplicity, we take a conduction band with constant density of states $\rho(\omega) = \rho_0 \theta(D - |\omega|)$ within a band of half-width D.

We imagine dividing up the conduction band as depicted in Fig. 1(a). It consists of a lower band edge (LBE), defined within $-D < \omega < -D + \delta D$; an upper band edge (UBE), defined within $D - \delta D < \omega < D$; and the bulk, defined for $-D + \delta D < \omega < D - \delta D$. The number of states in each band edge is therefore $\rho_0 \delta D$.

Just as with the Schrieffer-Wolff transformation, we can derive an effective low-energy model by perturbatively eliminating virtual excitations. Here, the excitations are to the band edges: the effective model then involves a reduced bandwidth, with $\tilde{D} = D - \delta D$, and a renormalized coupling $\tilde{J}_{kk'}$ that incorporates the effect of those excitations. The perturbative scaling technique then examines the *flow* of $\tilde{J}_{kk'}$ with $\tilde{D}$.

The part of the Hamiltonian describing scattering to the band edges is partitioned as $\delta H = H_0 + H_1$, where $H_0 = \sum_{k,\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma}$ is the full conduction electron Hamiltonian, and $H_1 = H_{1a} + H_{1b}$, with

$$H_{1a} = \sum_{k \in \text{bulk}} \sum_{q \in \text{BE}} \tfrac{1}{2} J_{qk} \left[S^+ c^\dagger_{q\downarrow} c_{k\uparrow} + S^- c^\dagger_{q\uparrow} c_{k\downarrow} + S^z \left(c^\dagger_{q\uparrow} c_{k\uparrow} - c^\dagger_{q\downarrow} c_{k\downarrow} \right) \right] \ , \tag{2a}$$

$$H_{1b} = \sum_{k \in \text{bulk}} \sum_{q \in \text{BE}} \tfrac{1}{2} J_{kq} \left[S^+ c^\dagger_{k\downarrow} c_{q\uparrow} + S^- c^\dagger_{k\uparrow} c_{q\downarrow} + S^z \left(c^\dagger_{k\uparrow} c_{q\uparrow} - c^\dagger_{k\downarrow} c_{q\downarrow} \right) \right] \ . \tag{2b}$$

We now define a projector, $\hat{1}_b = \sum_{\phi,\psi} |\phi\rangle|\psi\rangle\langle\psi|\langle\phi|$, for electronic states $|\psi\rangle = \prod_k |\psi_k\rangle \theta(\tilde{D} - |\epsilon_k|)$ in the bulk (and where $|\phi\rangle$ lives in the impurity subspace). At low temperatures, we assume that the LBE is completely filled, while the UBE is completely empty. This makes a connection between the temperature T and the reduced bandwidth $\tilde{D}$. The correction due to band-edge excitations is then given to second order in H_1 by,

$$\delta H_{\mathit{eff}} = \hat{1}_b \left[H_{1a} (E_0 - H_0)^{-1} H_{1b} + H_{1b} (E_0 - H_0)^{-1} H_{1a} \right] \hat{1}_b \tag{3}$$

Consider just the processes where the impurity spin is flipped from down to up (the amplitude of the other processes is the same by SU(2) spin symmetry), and evaluate Eq. 3. The structure of δH_{eff} should be the same as the bare Hamiltonian, Eq. 1. This allows you to identify the correction to the Kondo coupling, δJ. Express it in terms of δD.

Let $\delta D \to dD$ and $\delta J \to dJ$ and solve the resulting differential equation. What happens to the renormalized $\tilde{J}$ as the bandwidth $\tilde{D}$ is reduced (this corresponds to reducing the temperature)? Show that the Kondo temperature $T_K = D \exp(-1/\rho_0 J)$ is a scaling invariant of the RG trajectory.

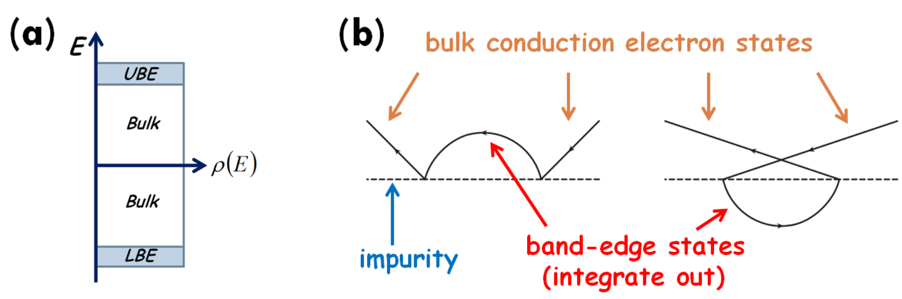

FIG. 1. (a) Conduction band divided into band edges and bulk. (b) Second-order diagrams eliminating band edge excitations.