Numerical methods for quantum impurity models
DRSTP (9-20 March 2015. Doorn, Netherlands)
Lecturer: Andrew Mitchell

Exercise 3: NRG tutorial code

Try it yourself:
After downloading and compiling the code:

1. Run the NRG code for different impurity parameters. Try $\epsilon_d = -U/2$, with $U = 0, 0.1, 0.2, 0.3, 0.4, 0.5$. Try varying V. Try varying ϵ_d for a fixed U and V. Each time, save the output entropy.dat to a new file (with the parameters in the filename).

2. Define the Kondo temperature T_K through $S_{\rm imp}(T_K) = \frac{1}{2}\ln(2)$. Extract T_K from the data collected. How does the NRG Kondo scale vary with ϵ_d, U and V. Plot $\ln(T_K)$ against U/V^2 in the case $\epsilon_d = -U/2$. Plot $\ln(T_K)$ against ϵ_d for fixed U and V. How well do the perturbative scaling results agree with NRG? When do they work best?

3. Plot the entropy vs T/T_K, with T_K extracted for each curve. Confirm universal scaling collapse in the 'Kondo regime'.

4. Modify the NRG code to output the NRG many-particle energy levels at each iteration. Print them to a file (e.g. energies.dat), labeling each energy by its iteration number (l) and an index (r). Have a look at the energy levels resulting from a representative NRG calculation. Why are there degeneracies? Using graphing utility gnuplot, plot the energy of level with a given index r vs iteration number N to see the RG flow between fixed points. Try plotting the energies for just even or odd iteration numbers.

5. Modify the NRG code to include a (small) magnetic field hS_d^z acting *on the impurity site* (only). What happens to the entropy when a field acts? What if the field is on the order of, or smaller than, T_K?

6. Experiment with the number of kept states, rlim. When does the calculation break down?

Optional: for those interested, try this more advanced problem at home. Charge and spin are conserved quantities in the Anderson impurity model. All states at each iteration are therefore eigenstates of total charge, Q and total spin projection S^z. Labeling the states by Q and S^z means that the Hamiltonian becomes *block-diagonal*. Matrix diagonalization can therefore be done independently in each block. This drastically speeds up the calculation. Try implementing the quantum numbers in the tutorial NRG code. Having access to S^z for each state also allows you to calculate the thermodynamic magnetic susceptibility $T\chi_{\rm imp}(T) = \langle (S^z_{\rm tot})^2 \rangle$.