Numerical methods for quantum impurity models
DRSTP (9-20 March 2015. Doorn, Netherlands)
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Exercise 3: NRG tutorial code

Installation instructions (Windows):

- Download the file 'nrg_tutorial.zip' from
`http://www.staff.science.uu.nl/~mitch003/nrg_tutorial.zip`
- Unzip 'nrg_tutorial.zip' to create the directory 'nrg_tutorial' in your chosen location, <path>.
- From the directory 'nrg_tutorial', run the file 'mingw-get-setup.exe'. Follow the installation instructions.
- Run the program 'MinGW Installer' (if it does not start automatically). In the 'Basic Setup' tab, select the boxes for 'mingw32-base' and 'mingw32-gcc-fortran' (mark for installation). Select 'Apply Changes' from the 'Installation' menu dropdown. Click 'Apply'. Close the dialogue box and MinGW program when complete.
- Right click on your computer icon, go to properties → advanced system settings → Environment Variables. Look for the 'Path' variable in the 'system variables' box. Click on it and click the 'edit' button. At the start of 'Variable value:' write 'C:\MinGW\bin;' (including the semicolon, without the quotemarks, and before the text of the current value). Leave the remainder of the current value unchanged. Click 'OK' and close the dialogue boxes.
- From the directory 'nrg_tutorial', execute the file 'Force209GFortranSetup.exe', and follow the installation instructions.
- From the directory 'nrg_tutorial', execute the file 'gp500-win64-mingw.exe', and follow the installation instructions.
- From the directory 'nrg_tutorial', double-click to execute the file 'nrg_tut.f90', which should now automatically open in the Windows fortran code-editor 'Force 2.0'.
- From the 'Run' dropdown menu, select 'Compilation Options'. Under the 'Run' tab, in the 'Additional Parameters' → 'Compiler' → 'Options', type: "-L<path>\nrg_tutorial", where <path> is the full path of the directory 'nrg_tutorial'. In the 'Libraries' box, type "-llapack -lblas". Click 'Apply' and 'OK'.
- To run the NRG code, click 'Run' from the 'Run' dropdown menu (or hit the F9 key). Close the program Force when the NRG code has finished running. To run the compiled NRG code in future, the executable 'nrg_tut.exe' can be run directly (outside of Force). The code itself can be edited and/or compiled in Force.
- Run the graphing utility 'Gnuplot' (an icon may have been placed on your desktop). Change directories by selecting 'Change Directory...' from the 'File' dropdown menu. View the entopy plot by typing "plot 'entropy.dat' w lp". See it on a logscale by typing "set logscale x; set format x "\%G"; replot". See the fixed point values by typing "replot log(2)" and "replot log(4)".

Try it yourself:

Having downloaded, compiled and run the code, try the following:

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 $T\chi_{\rm imp}(T) = \langle (S^z_{\rm tot})^2 \rangle$.