SIAM and SIKM using NRG

The NRG code distributed allows to do calculations for the Anderson model (SIAM) and the Kondo model (SIKM). To this end one needs to modify the corresponding input files. For the SIAM, it looks like the example below:

```
//NRG Parameterfile

name = "SIAM.cfg";

NRG =
{
        OUTPUT="Output_SIAM/";
        SAVEDIR="savedir_SIAM";

        PARAMETER={
                Lambda     = 3;
                Sites           = 201;
                States         = 1000;
                MinStates   = 900;
                Cutoff          = 10;
        };

        Temperature = -1e-40;
        Gamma       = 0.01;
        DOS = ("const","myhybrid1.inp");

        INTERACTION={
                U=0.08;
                E=-0.04;
                B=0;
        };
        EXPECTATION=(  {Operator=0; Name="n";},

                       {Operator=1; Name="m";}
        );

        SYMMETRIES=("ph","su2");
};
```

Note the negative sign in the temperature specification. It means that the code does produce a series of temperatures, while a positive value here will produce a single result for the given temperature. The parameter file for the SIKM looks very similar:

```
//NRG Parameterfile

name = "SIKM.cfg";

NRG =
{
        OUTPUT="Output_SIKM/";
        SAVEDIR="savedir_SIKM";

        PARAMETER={
                Lambda          = 3;
                Sites           = 201;
                States          = 1000;
                MinStates       = 900;
                Cutoff          = 10;
        };

        Temperature = -1e-40;
        Gamma       = 1.0;
        DOS = ("const","myhybrid1.inp");

        SPIN={  S_1=1; S_2=2; };

        INTERACTION={
                JK=(-0.05,-0.05);
                E=0.0;
                B=0.0;
        };
        EXPECTATION=(  {Operator=0; Name="nu";},
                                        {Operator=1; Name="nd";}
        );

        SYMMETRIES=("ph","su2");

};
```

For the SIKM, the value of Γ_0 does not play a role, but there are two new parameters, namely the spin of the impurity and the exchange interaction. The two values in the exchange interaction denote the Ising respectively spin-flip part. For the present purpose one should choose them to be identical, i.e. work with the isotropic interaction.

The output file `thermo.dat` contains the thermodynamic quantities as function of temperature on a logarithmically decreasing temperature scale. The columns are as follows: Temperature T, entropy $S(T)$, specific heat $c_V(T)$, effective local moment $\mu^2 := T \cdot \chi_I(T)$, double occupancy (SIAM only), local magnetization (SIAM only) and local occupancy (SIAM only). In the output of the Kondo model, the last three columns are meaningless. The quantity $\chi_I(T)$ denotes the magnetic susceptibility of the impurity.

(a) Solve the SIAM using NRG for $\Gamma_0 = 0.01$ and $U = 0$, 0.01, 0.0314, 0.0952 and $U = 3.14$. Choose for the local energy $E = -U/2$ to ensure a local occupancy $\langle n_f \rangle = 1$. Plot the resulting entropy (second column in the output file thermo.dat) as function of temperature for the different values of U. What happens? For the larger values of U, try to find a temperature scale $T_{\mathrm{K}}(U)$ such that when plotting $S(T/T_{\mathrm{K}}(U))$ the curves collapse onto a single *scaling curve* for low temperatures.

(b) Repeat the calculations for the Kondo model choosing $J = -8\Gamma_0/(\pi U)$ for $U > 0$. Can you also find corresponding Kondo scales? How are they related to the corresponding scales for the SIAM?

c) Play with the code, in particular reduce the number of states kept, increase Λ. Do you obtain reliable results for entropy and other quantities with small number of states kept?