Guide to the use and compilation of the MAS-SEOM code

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I. SINGLE-LEVEL ANDERSON IMPURITY MODEL

The total Hamiltonian of a single-level AIM consists of three parts:

$$H_{\rm T} = H_{\rm S} + H_{\rm B} + H_{\rm SB}. \tag{1}$$

Each part is defined as ($e = \hbar \equiv 1$ and $k_{\rm B} \equiv 1$):

$$\begin{aligned} H_{\rm S} &= \epsilon_\uparrow \hat{n}_\uparrow + \epsilon_\downarrow \hat{n}_\downarrow + U \hat{n}_\uparrow \hat{n}_\downarrow, \\ H_{\rm B} &= \sum_{\alpha k} \sum_{s} \epsilon_{\alpha k}\, \hat{d}^\dagger_{\alpha k s} \hat{d}_{\alpha k s}, \\ H_{\rm SB} &= \sum_{\alpha} \sum_{s} \hat{c}^\dagger_s\, \hat{F}_{\alpha s} + \hat{F}^\dagger_{\alpha s}\, \hat{c}_s. \end{aligned} \tag{2}$$

As shown in Fig. 1, the impurity is coupled to two spin-unpolarized electron reservoirs ($\alpha = L, R$). Both reservoirs have a spectral function of a Lorentz form, i.e.,

$$J_\alpha(\omega) \equiv \pi \sum_k |t_{\alpha k}|^2 \delta(\omega - \epsilon_{\alpha k}) = \frac{\Gamma_\alpha}{2} \frac{W_\alpha^2}{(\omega - \Omega_\alpha)^2 + W_\alpha^2}, \tag{3}$$

II. COMPILATION OF THE CODE

- The compiler is INTEL FORTRAN with MKL library.
- OpenMP parallelization is utilized.
- In Makefile, NAME: define the directory where the complied HEOM executable file (i.e., seom.x) will appear; e.g. NAME=/home/home/aa/seom.x
- "make clean" delete objects/*.o, objmod/*.o
- "make" obtains the MAS-SEOM executable file; can be of any name, e.g. seom

III. INPUT FILE

- e1u ≡ energy of spin-up electron, e1d ≡ energy of spin-down electron, u1 ≡ electron-electron coulomb interaction energy.
- dt ≡ timestep, ntime ≡ number of timestep
- ntraj ≡ number of trajectories, dref ≡ λ
- nstate ≡ number of pseudo states
- Vlt1, Vlt2 ≡ bias voltage
- nlead ≡ number of leads

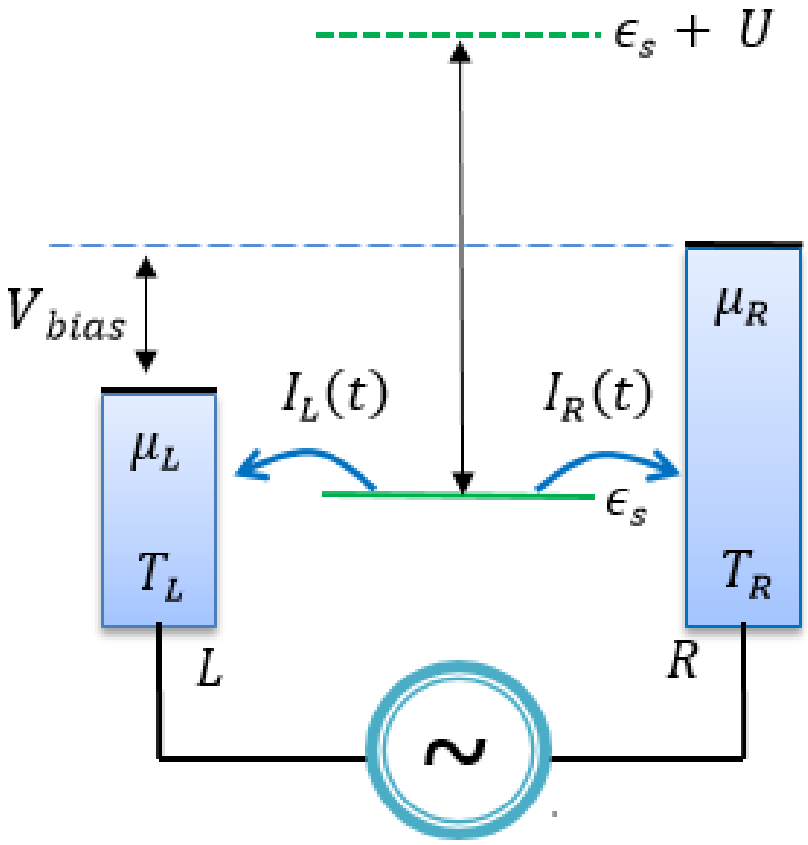

FIG. 1. Schematic diagram of a single-level impurity coupled with two electron reservoirs ($\alpha = L, R$). ϵ_s is the level energy for a spin-s electron, U is the electron-electron Coulomb interaction energy, and μ_α and T_α are the chemical potential and temperature of the α-reservoir. $I_\alpha(t)$ represents the current flow between the impurity and the α-reservoir when a bias voltage $V_{\rm bias}$ is applied across the two reservoirs.

IV. OUTPUT FILES

run SEOM $\rightarrow$ *./seom.x < input > output*

- population.dat, 2nd column $\rightarrow$ population of spin-up, 3rd column $\rightarrow$ population of spin-down
- 1current.dat, data for current using Eq.(36) [1], the 6th column is I_L while the 7th column is I_R.
- 2current.dat, data for current using Eq.(37) [1], the 2nd column is I_L while the 3rd column is I_R.

V. EXAMPLES

We have provided input files for the user to test the code

- by using the input file provided in "example-1" folder, user can generate the high temperature results of Fig.2,
- by using the input file provided in "example-2" folder, user can generate the low temperature results of Fig.2,
- by using the input file provided in "example-3" folder, user can generate Fig.3 results.

References

[1] arXiv:1912.05271