DMFT+HF-QMC Tutorial

Task: Find and explore MIT (Bethe lattice, paramagnetic case)

0. In your home directory create a symbolic link to the **bin** folder containing all the executables and scripts for this Tutorial:
   ln -s /home/bluemer/bin

1. Perform DMFT calculations for T = 0.04, fixed value of $\Delta\tau = 0.2$, and U = 3.5, 4, 4.5, 4.7, 4.8, 5, 5.5
   - in a series with increasing interaction values
   - in a series with decreasing interaction values

2. Extract observables:
   i. double occupancy D(U)
   ii. quasiparticle weight $Z(U) = (1-Im\Sigma(\omega_1)/\omega_1)^{-1}$

3. Check convergency with D and/or Z

4. Compute spectra (using MaxEnt)

5. Explore the dependence of the results on the imaginary time discretization $\Delta\tau$:
   i. For one of the U values perform calculations for a set of $\Delta\tau$ values.
   ii. Plot double occupancy as a function of $\Delta\tau^2$
   iii. Perform $\Delta\tau \to 0$ extrapolation

Hint: you may use the provided scripts to create input files and extract observables.

Top | Back to TOC

Workflow: Preparing and Performing DMFT calculations

1. Prepare input file for the first run.
   To scan the parameter region starting from the metal solution choose U = 3.5 and default initial guess for the self-energy:

   B250U035dt020_m0.in

```
B250U035dt020_m0
(beta=25, U=3.5, dt=0.2 on Bethe lattice)
Nwu 200, Nmc 10000, Nme 0
beta 25.0
U 3.5
dt 0.2
dos Bethe
NIter 10
```

Important! Do not use default parameters (Nwu, Nmc, Nme) for QMC calculation! They are chosen for production runs, not for tutorial purposes!

Hint: starting from U = 3.5 and going downgrade will lead to the insulating solution within the (co)existence region.

2. Run DMFT job using
DMFT_serial < B250U035dt020_m0.in > B250U035dt020_m0.out &

   Hint: you can trace the computational progress with
tail -f B250U035dt020_m0.out

3. After this run is finished you may proceed either with the same U to get better convergency, or with a slightly different U using the obtained pre-converged solution as an initial guess:

   i. Prepare corresponding input file, e.g.

   B250U040dt020_m1.in

```
B250U040dt020_m1
(beta=25, U=4, dt=0.2 on Bethe lattice, SE from U=3.5)
Nwu 200, Nmc 10000, Nme 0
beta 25.0
U 4.0
dt 0.2
dos Bethe
ReadSE
NIter 10
```

   Keyword ReadSE forces reading of the initial self-energy from the corresponding external file, in this case from the file B250U040dt020_m1.self.in

   ii. Create a symbolic link to the self-energy file from the previous calculation:
ln -s B250U035dt020_m0.self.sec B250U040dt020_m1.self.in

   iii. Run DMFT job:
DMFT_serial < B250U040dt020_m1.in > B250U040dt020_m1.out &

Top | Back to TOC

Observables

- Double occupancy for each DMFT iteration is written in the 5th colomn of the corresponding .mag file
- Quasiparticle weight can be calculated with the self-energy at first Matsubara frequency $\Sigma(\omega_1)$ known:
$Z = (1-Im\Sigma(\omega_1)/\omega_1)^{-1}$

Frequency-dependent self-energy $\Sigma(\omega)$ from the final DMFT iteration is written in the corresponding .self.sec file, whereas .self file contains the same information for each of the DMFT iterations.

Top | Back to TOC
