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Exercises for Computational Methods in Solid State Theory SS 2015

Exercise Set 6

(Due date: Monday, July 13, 2015)

Exercise 9 (Continuous-time auxiliary-field Monte Carlo method for quantum impurity models) (30 points)

We use a numerically exact Monte Carlo method to solve the Anderson impurity model.

(1)

$$\mathcal{H} = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_\sigma \varepsilon_d d^\dagger_\sigma d_\sigma + \frac{U}{2} \sum_\sigma \hat{n}_\sigma \hat{n}_{\bar{\sigma}} + \sum_{k\sigma} \left(V^*_{k\sigma} c^\dagger_{k\sigma} d_\sigma + V_{k\sigma} d^\dagger_\sigma c_{k\sigma} \right)$$

where $\hat{n}_\sigma = d^\dagger_\sigma d_\sigma$.

The impurity solver is employed together with the previously developed DMFT routines to solve the dynamical mean field approximation for the Hubbard model on the Bethe lattice.

a) Implement routines that transform a Greens function from Matsubara frequencies ($i\omega_n$) to imaginary time (τ) and vice versa.

(2)
$$G(i\omega_n) = \int_0^\beta d\tau \; e^{i\omega_n \tau} G(\tau)$$

The transformation from imaginary time to Matsubara frequencies can be done using trapezoidal integration.

(3)
$$G(\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} e^{-i\omega_n \tau} G(i\omega_n)$$

When going from Matsubara frequencies to imaginary time, the high-frequency tail of the Greens function must be taken into account analytically. Using the first order high-frequency correction in ω_n, this can be written as:

$$(4)\quad G(\tau) \approx \frac{2}{\beta}\sum_{n=0}^{N}\left[\mathrm{Re}G(\omega_n)\cos(\omega_n\tau) + \left(\mathrm{Im}G(\omega_n) + \frac{1}{\omega_n}\right)\sin(\omega_n\tau)\right] - \frac{1}{2}$$

N is the number of Matsubara frequencies for which data are available.

b) Implement the continuous-time auxiliary field Monte Carlo (CTAUX) method to solve the Anderson impurity model.

c) Use the DMFT routines developed on Sheet 4 to solve the Hubbard model on the Bethe lattice at half filling. Consider a temperature $T = 0.1$ eV and use a Hubbard interaction of about $U = 1.2W$, where W is the bandwidth. Plot the interacting density of states.