Goethe-Universität Frankfurt
Fachbereich Physik

Institut für Theoretische Physik
Dr. Harald O. Jeschke
Daniel Guterding

GOETHE UNIVERSITÄT FRANKFURT AM MAIN

Frankfurt, May 19, 2015

Exercises for Computational Methods in Solid State Theory
SS 2015

Exercise Set 4
(Due date: Monday, June 8, 2015)

Exercise 4 (**Hubbard I approximation of the Anderson impurity model**) (10 points)

We use equations of motion within a mean-field decoupling scheme 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 $\hat{n}_\sigma = d^\dagger_\sigma d_\sigma$.

a) Use the general equation of motion for the Greens function

(2)
$$\omega \langle\langle A; B \rangle\rangle = \left\langle [A, B]_+ \right\rangle + \langle\langle [A, \hat{H}]_-; B \rangle\rangle$$

to derive the following three equations:

(3)
$$(\omega - \epsilon_d) \langle\langle d_\sigma; d^\dagger_\sigma \rangle\rangle = 1 + U \langle\langle d_\sigma \hat{n}_{\bar{\sigma}}; d^\dagger_\sigma \rangle\rangle + \sum_k V_{k\sigma} \langle\langle c_{k\sigma}; d^\dagger_\sigma \rangle\rangle$$

(4)
$$(\omega - \epsilon_k) \langle\langle c_{k\sigma}; d^\dagger_\sigma \rangle\rangle = V^*_{k\sigma} \langle\langle d_\sigma; d^\dagger_\sigma \rangle\rangle$$

(5)
$$\begin{aligned}(\omega - \epsilon_d - U) \langle\langle d_\sigma \hat{n}_{\bar{\sigma}}; d^\dagger_\sigma \rangle\rangle \quad = \quad & \langle \hat{n}_{\bar{\sigma}} \rangle + \sum_k V^*_{k\bar{\sigma}} \langle\langle c^\dagger_{k\bar{\sigma}} d_\sigma d_{\bar{\sigma}}; d^\dagger_\sigma \rangle\rangle + \sum_k V_{k\sigma} \langle\langle c_{k\sigma} \hat{n}_{\bar{\sigma}}; d^\dagger_\sigma \rangle\rangle \\ & - \sum_k V_{k\bar{\sigma}} \langle\langle c_{k\bar{\sigma}} d^\dagger_{\bar{\sigma}} d_\sigma; d^\dagger_\sigma \rangle\rangle\end{aligned}$$

b) Use the equations of motion derived in a) to show that the d electron Greens function can be written as

(6)
$$\langle\langle d_\sigma; d^\dagger_\sigma \rangle\rangle = \frac{1 + \frac{U \langle \hat{n}_{\bar{\sigma}} \rangle}{\omega - \varepsilon_d - U - \Delta(\omega)}}{\omega - \varepsilon_d - \Delta(\omega)}$$

where the hybridization function $\Delta(\omega)$ is given as:

(7) $$\Delta(\omega) = \sum_k \frac{V^2}{\omega - \varepsilon_k}$$

For some of the four operator terms a mean-field decoupling is necessary to close the set of equations, e.g.

(8) $$\langle\langle c_{k\sigma} d^\dagger_{\bar{\sigma}} d_{\bar{\sigma}}; d^\dagger_\sigma \rangle\rangle \approx \left\langle d^\dagger_{\bar{\sigma}} d_{\bar{\sigma}} \right\rangle \langle\langle c_{k\sigma}; d^\dagger_\sigma \rangle\rangle$$

Exercise 5 (**Anderson impurity model and Hubbard model on the Bethe lattice**) (10 points)

We use the Hubbard I impurity solver derived in Exercise 4b) to solve the Anderson impurity model and dynamical mean-field theory (DMFT) for the Hubbard model on the Bethe lattice. All calculations should be done in the paramagnetic phase, where $\langle n_\sigma \rangle = \langle n_{\bar{\sigma}} \rangle$.

The Hubbard I solver can be used on the imaginary frequency axis by replacing $\omega \to i\omega_n$. For the calculation of occupation numbers on the Matsubara axis the high-frequency tails of the Greens function must be taken into account analytically.

Set the parameter ϵ_d to $-\frac{U}{2}$ to make the impurity solver symmetric with respect to the Fermi energy. Mind that the lattice only enters through the density of states, which is semicircular for the Bethe lattice.

a) Use expression (6) for the d electron Greens function to solve the Anderson impurity model on the Bethe lattice with a band width of $W = 4$ eV. Consider an energy independent hybridization of $V = \sqrt{0.4}$ eV and a temperature $T = 0.1$ eV. Plot the density of states of the d electrons.

b) Use the impurity solver of b) to solve the Hubbard model with dynamical mean field theory on the Bethe lattice (W, T as in a)). Find the critical interaction U_c for the metal to insulator transition at half filling. Plot the converged interacting density of states.

Exercise 6 (**DMFT solution of the one-band Hubbard model for a cuprate**) (10 points)

Use dynamical mean field theory with the Hubbard I impurity solver to solve the one-band Hubbard model for the cuprate of Exercises 2 and 3. Here, U and T are $U = 6$ eV and $T = 0.1$ eV, respectively. Consider only the paramagnetic phase.

The parameter ϵ_d must be adjusted in order to conserve the initial filling of the tight binding model.

Plot the converged interacting density of states.