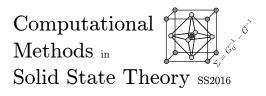
Goethe-Universität Frankfurt Fachbereich Physik

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



Frankfurt, July 8, 2016

Exercise Set 6

(Due date: Friday, July 15, 2016)

Exercise 6 (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

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k c_{k\sigma}^{\dagger} c_{k\sigma} + \sum_{\sigma} \epsilon_d d_{\sigma}^{\dagger} d_{\sigma} + \frac{U}{2} \sum_{\sigma} \hat{n}_{\sigma} \hat{n}_{\bar{\sigma}} + \sum_{k\sigma} \left(V_{k\sigma}^* c_{k\sigma}^{\dagger} d_{\sigma} + V_{k\sigma} d_{\sigma}^{\dagger} c_{k\sigma} \right)$$

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

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

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

to derive the following three equations:

$$(3) \qquad (\omega - \varepsilon_{\rm d}) \langle \! \langle d_{\sigma}; d_{\sigma}^{\dagger} \rangle \! \rangle = 1 + U \langle \! \langle d_{\sigma} \hat{n}_{\bar{\sigma}}; d_{\sigma}^{\dagger} \rangle \! \rangle + \sum_{\rm k} V_{\rm k\sigma} \langle \! \langle c_{\rm k\sigma}; d_{\sigma}^{\dagger} \rangle \! \rangle$$

(4)
$$(\omega - \epsilon_{\mathbf{k}}) \langle \langle c_{\mathbf{k}\sigma}; d_{\sigma}^{\dagger} \rangle \rangle = V_{\mathbf{k}\sigma}^* \langle \langle d_{\sigma}; d_{\sigma}^{\dagger} \rangle \rangle$$

$$\begin{array}{lll} (5) \\ (\omega - \varepsilon_{d} - U) \langle \! \langle d_{\sigma} \hat{n}_{\bar{\sigma}} ; d_{\sigma}^{\dagger} \rangle \! \rangle & = & \langle \hat{n}_{\bar{\sigma}} \rangle + \sum\limits_{k} V_{k\bar{\sigma}}^{*} \langle \! \langle c_{k\bar{\sigma}}^{\dagger} d_{\sigma} d_{\bar{\sigma}} ; d_{\sigma}^{\dagger} \rangle \! \rangle + \sum\limits_{k} V_{k\sigma} \langle \! \langle c_{k\sigma} \hat{n}_{\bar{\sigma}} ; d_{\sigma}^{\dagger} \rangle \! \rangle \\ & & - \sum\limits_{k} V_{k\bar{\sigma}} \langle \! \langle c_{k\bar{\sigma}} d_{\bar{\sigma}}^{\dagger} d_{\sigma} ; d_{\bar{\sigma}}^{\dagger} \rangle \! \rangle \end{array}$$

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

(6)
$$\langle\!\langle \mathbf{d}_{\sigma}; \mathbf{d}_{\sigma}^{\dagger} \rangle\!\rangle = \frac{1 + \frac{\mathbf{U}\langle \hat{\mathbf{n}}_{\sigma} \rangle}{\omega - \varepsilon_{d} - \mathbf{U} - \Delta(\omega)}}{\omega - \varepsilon_{d} - \Delta(\omega)}$$

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)
$$\langle \langle c_{k\sigma} d_{\bar{\sigma}}^{\dagger} d_{\bar{\sigma}}; d_{\sigma}^{\dagger} \rangle \rangle \approx \langle d_{\bar{\sigma}}^{\dagger} d_{\bar{\sigma}} \rangle \langle \langle c_{k\sigma}; d_{\sigma}^{\dagger} \rangle \rangle$$

Exercise 7 (Anderson impurity and Hubbard model on the Bethe lattice) (10 points)

We use the Hubbard I impurity solver derived in Exercise 5b) 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 $\langle \mathbf{n}_{\sigma} \rangle = \langle \mathbf{n}_{\bar{\sigma}} \rangle$.

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.