

Frankfurt, May 15, 2012

Exercises for Computational Methods in Solid State Theory
 SS 2012

Exercise Set 4

(Due date: Monday, May 28, 2012)

Exercise 4 (Dynamical mean field theory and Hubbard I approximation)
 (20 points)

We use equations of motion together with the decoupling scheme given in J. Hubbard, Proc. Roy. Soc. A **281**, 401 (1964) and L. M. Roth, Phys. Rev. **184**, 451 (1969) to solve the Anderson impurity model

$$(1) \quad \mathcal{H} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \sum_{\sigma} \varepsilon_d d_{\sigma}^{\dagger} d_{\sigma} + \frac{U}{2} \sum_{\sigma\sigma'} \hat{n}_{\sigma} \hat{n}_{\sigma'} + \sum_{\mathbf{k}\sigma} (V_{\mathbf{k}\sigma}^* c_{\mathbf{k}\sigma}^{\dagger} d_{\sigma} + V_{\mathbf{k}\sigma} d_{\sigma}^{\dagger} c_{\mathbf{k}\sigma})$$

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

a) Use the decoupling

$$(2) \quad \begin{aligned} \langle\langle d_{\sigma}^{\dagger} c_{\mathbf{k}\sigma'} d_{\sigma}; d_{\sigma}^{\dagger} \rangle\rangle &\approx \langle d_{\sigma'}^{\dagger} c_{\mathbf{k}\sigma'} \rangle \langle\langle d_{\sigma}; d_{\sigma}^{\dagger} \rangle\rangle \\ \langle\langle c_{\mathbf{k}\sigma'}^{\dagger} d_{\sigma'} d_{\sigma}; d_{\sigma}^{\dagger} \rangle\rangle &\approx \langle c_{\mathbf{k}\sigma'}^{\dagger} d_{\sigma'} \rangle \langle\langle d_{\sigma}; d_{\sigma}^{\dagger} \rangle\rangle \\ \langle\langle d_{\sigma'}^{\dagger} c_{\mathbf{k}'\sigma'} c_{\mathbf{k}\sigma}; d_{\sigma}^{\dagger} \rangle\rangle &\approx \langle d_{\sigma'}^{\dagger} c_{\mathbf{k}'\sigma'} \rangle \langle\langle c_{\mathbf{k}\sigma}; d_{\sigma}^{\dagger} \rangle\rangle \\ \langle\langle c_{\mathbf{k}'\sigma'}^{\dagger} d_{\sigma'} c_{\mathbf{k}\sigma}; d_{\sigma}^{\dagger} \rangle\rangle &\approx \langle c_{\mathbf{k}'\sigma'}^{\dagger} d_{\sigma'} \rangle \langle\langle c_{\mathbf{k}\sigma}; d_{\sigma}^{\dagger} \rangle\rangle \end{aligned}$$

to show that the d electron Greens function can be written as

$$(3) \quad \langle\langle d_{\sigma}; d_{\sigma}^{\dagger} \rangle\rangle = \frac{1 - \frac{\langle n_{\sigma'} \rangle}{i\omega_n - \varepsilon_d - U - \Delta(i\omega_n)}}{i\omega_n - \varepsilon_d - \Delta(i\omega_n)}$$

where the hybridization function $\Delta(i\omega_n)$ is given as

$$(4) \quad \Delta(i\omega_n) = \sum_{\mathbf{k}} \frac{V^2}{i\omega_n - \varepsilon_{\mathbf{k}}}$$

b) Use this expression for the 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.

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