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Exercises for Computational Methods in Solid State Theory
SS 2013

Exercise Set 4

(Due date: Monday, June 4, 2013)

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

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

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

a) Use the decoupling

(2)
$$\begin{aligned} \langle\langle d^\dagger_{\sigma'} c_{k\sigma'} d_\sigma ; d^\dagger_\sigma \rangle\rangle &\approx \langle d^\dagger_{\sigma'} c_{k\sigma'} \rangle \langle\langle d_\sigma ; d^\dagger_\sigma \rangle\rangle \\ \langle\langle c^\dagger_{k\sigma'} d_{\sigma'} d_\sigma ; d^\dagger_\sigma \rangle\rangle &\approx \langle c^\dagger_{k\sigma'} d_{\sigma'} \rangle \langle\langle d_\sigma ; d^\dagger_\sigma \rangle\rangle \\ \langle\langle d^\dagger_{\sigma'} c_{k'\sigma'} c_{k\sigma} ; d^\dagger_\sigma \rangle\rangle &\approx \langle d^\dagger_{\sigma'} c_{k'\sigma'} \rangle \langle\langle c_{k\sigma} ; d^\dagger_\sigma \rangle\rangle \\ \langle\langle c^\dagger_{k'\sigma'} d_{\sigma'} c_{k\sigma} ; d^\dagger_\sigma \rangle\rangle &\approx \langle c^\dagger_{k'\sigma'} d_{\sigma'} \rangle \langle\langle c_{k\sigma} ; d^\dagger_\sigma \rangle\rangle \end{aligned}$$

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

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

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

(4)
$$\Delta(i\omega_n) = \sum_k \frac{V^2}{i\omega_n - \varepsilon_k}$$

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.

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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.