Condensed-Matter Theory - Special Topics

Problem 16 — DMFT for the Hubbard model on the Bethe lattice
Consider the Bethe lattice with coordination number q in the $q \to \infty$ limit and argue that we have

$$\frac{1}{G_{\rm loc}(\omega)} = \omega + \mu - t_{ii} - \Sigma(\omega) - qt^2 G_{\rm loc}(\omega)$$

for the interacting ($U \neq 0$) local Green's function. (Hint: see problem 6, where the noninteracting Green's function on the Bethe lattice was discussed).

Solving this equation for $G_{\rm loc}(\omega)$ for given self-energy is obviously much simpler than solving Dyson's equation. Formulate a simplified self-consistency cycle as an algorithm for DMFT of the Hubbard model on the Bethe lattice with $q \to \infty$!

Problem 17 — DMFT for a two-sublattice model
The Bethe lattice is a bipartite lattice, i.e., it is composed of two "sublattices" (two sets of sites) such that the nearest neighbors of any site in sublattice 1 belong to sublattice 2. Sketch a Bethe lattice consisting of two sublattices with different coordination numbers q_1 and q_2, e.g., $q_1 = 3$, $q_2 = 2$!

We will study the Hubbard model on such a Bethe lattice in the limit $q_1 \to \infty$, $q_2 \to \infty$ with $0 < q_1/q_2 < \infty$. To this end, we assume a scaling of the hopping like $t = t^*/\sqrt{q_1 + q_2}$, such that the model is well-defined and nontrivial in the limit. The self-energy $\Sigma_\alpha(\omega)$ is local but dependent on the sublattice index $\alpha = 1, 2$. The problem on the Bethe lattice is mapped onto two impurity models specified by the hybridization functions

$$\Delta_\alpha = q_\alpha t^2 G_{\overline{\alpha}}(\omega)$$

where $G_\alpha(\omega)$ is the local Green's function for a site on sublattice α of the Hubbard model, and where $\overline{\alpha} = 2$ if $\alpha = 1$ (and $\overline{\alpha} = 1$ if $\alpha = 2$).

Justify this self-consistency condition!

Write down the full DMFT self-consistency cycle!

In the spirit of the linearized DMFT, we start the cycle (at half-filling and for $U \to U_{\rm c}$) with a one-pole hybridization function:

$$\Delta_\alpha = \frac{V_\alpha^2}{\omega} \; .$$

This gives two different two-site SIAMs with hybridization V_α, respectively. The approximate solution for $V_\alpha \to 0$ and at low frequencies (the "coherent" part of the Green's function) is (see lecture):

$$G_{{\rm imp},\alpha}(\omega) = \frac{z_\alpha}{\omega} \; ,$$

where

$$z_\alpha = \frac{36V_\alpha^2}{U^2} \, .$$

Show that the linearized-DMFT self-consistency cycle can be formulated solely for V_α^2!

Write this self-consistency cycle as a 2×2 matrix equation!

Iterate the matrix self-consistency cycle and find the fixed point at $U = U_\mathrm{c}$!

Show that the critical interaction for the Mott transition is

$$U_\mathrm{c} = 6t(q_1 q_2)^{1/4} \, !$$

What is the meaning of the eigenvector of the matrix eigenvalue problem at $U = U_\mathrm{c}$?

Discuss the limits $q_1 = 0$ and $q_1 = q_2$!

The problem can be generalized to $s > 2$ sublattices. Compute U_c!

Discuss the $s \to \infty$ limit!