Condensed-Matter Theory - Special Topics

Problem 14 — Charge compressibility
The charge compressibility is defined as

$$\kappa = \frac{1}{L}\frac{\partial\langle N\rangle}{\partial\mu} \, .$$

What can be said about κ for a Mott insulator?

Show that for the metallic phase of the Hubbard model at temperature $T = 0$ one has

$$\kappa = \frac{1}{L}\sum_{\boldsymbol{k}\sigma}\delta(\mu - \varepsilon(\boldsymbol{k}) - \Sigma_{\boldsymbol{k}}(0))\left(1 - \frac{\partial\Sigma_{\boldsymbol{k}}(0)}{\partial\mu}\right) \, !$$

(Hint: Luttinger's theorem holds). Use

$$\frac{\partial}{\partial\mu}\Sigma_{\boldsymbol{k}}(0) = \frac{\partial}{\partial\omega}\Sigma_{\boldsymbol{k}}(0) + \frac{\partial\Sigma_{\boldsymbol{k}}(0)}{\partial n}\frac{\partial n}{\partial\mu}$$

to derive the Fermi-liquid relation

$$\kappa = \frac{1}{1+F_0^s}\frac{1}{L}\sum_{\boldsymbol{k}\sigma}A_{\boldsymbol{k}\sigma}(0)z_{\boldsymbol{k}\sigma}^{-1} \, !$$

Here, $A_{\boldsymbol{k}\sigma}(\omega)$ is the spectral function, $z_{\boldsymbol{k}\sigma}$ is the quasi-particle weight, $n = \langle N\rangle/L$, and

$$F_0^s = \frac{1}{L}\sum_{\boldsymbol{k}\sigma}\delta(\mu - \varepsilon(\boldsymbol{k}) - \Sigma_{\boldsymbol{k}}(0))\frac{\partial\Sigma_{\boldsymbol{k}}(0)}{\partial n}$$

is a Fermi-liquid parameter.

Problem 15 — Real-space DMFT
Consider the Hubbard model on a lattice of sites $i = 1, ..., L$ with a hopping matrix t_{ij}, which is not assumed as invariant under translations, i.e., all sites i are generically inequivalent. Assume that the coordination number of each site $q_i = \infty$.

Give at least 6 examples of possible geometries!

One example is a $D = \infty$ hypercubic lattice where one site is missing. How must the nearest-neighbor hopping scale with D?

Argue that the self-energy is local but site-dependent:

$$\Sigma_{ij}(\omega) = \delta_{ij}\Sigma_i(\omega) \, !$$

Argue that the skeleton-diagram expansion reads

$$\Sigma_i(\omega) = \Sigma[G_{ii}(\omega)]$$

i.e., the self-energy at i is a functional of the local Green's function $G_{ii}(\omega)$ at the same site only!

Define the hybridization function of a single-impurity Anderson model at site i as

$$\Delta_i(\omega) = \omega + \mu - t_{ii} - \Sigma_i(\omega) - \frac{1}{G_{ii}(\omega)} \; !$$

How would you set up the real-space DMFT self-consistency cycle?