Lectures:

Monday, 10.6.: Spectral function, ARPES, mean field approach
Thursday, 12.6.: Hartree Fock method, Bose Hubbard model

Exercises:
All solutions must be handed in by **Tue. 18.6.** noon in box on 5th floor of Building 46 or electronically to laschwar@rptu.de

Consider the Hubbard Model for spin-1/2 Fermions in one-dimension:

$$H = \sum_j \left[-t \sum_{\sigma=\uparrow,\downarrow} \left(\psi^\dagger_{j,\sigma} \psi_{j+1,\sigma} + \psi^\dagger_{j+1,\sigma} \psi_{j,\sigma} \right) + U n_{j,\uparrow} n_{j,\downarrow} \right].$$

At each site we define operators for the local particle number $n_j = n_{j,\uparrow} + n_{j,\downarrow}$, the local magnetization $m_j = n_{j,\uparrow} - n_{j,\downarrow}$

14a) Show that the interaction can be re-written by the following expressions

$$U n_{j,\uparrow} n_{j,\downarrow} = \frac{U}{2} n_j (n_j - 1) = \frac{U}{2} (n_j - m_j^2)$$

b) Show that $N_\sigma = \sum_j n_{j,\sigma} = \sum_{k \in 1BZ} n_{k,\sigma}$, for each value of $\sigma = \uparrow, \downarrow$, i.e. the total number of spin-up and spin-down particles can be determined in k-space or real space. Argue that $[N_\sigma, H] = 0$, so that the number of spin up and down particles are conserved separately. (hint: for the commutator with the interaction this is easier to show using the real space expression of N_σ, while the k-space expression can be used for the commutator with the kinetic energy).[1]

15.) In the following we want to determine if mean field theory predicts an overall magnetization in the ground state.
Use a mean field decoupling for the interaction $U n_{j,\uparrow} n_{j,\downarrow}$ (using $A = n_{j,\downarrow}$ and $B = n_{j,\uparrow}$). If the average occupation is uniform, show that the problem becomes diagonal in k-space (using $N_\sigma = \sum_j n_{j,\sigma} = \sum_{k \in 1BZ} n_{k,\sigma}$ from above). Assume an average total density of $\langle n \rangle = \langle n_\uparrow \rangle + \langle n_\downarrow \rangle = 1/2$ (i.e. "quarter filling"). What are the lowest energy eigenstates in terms of occupied k-states in the cosine dispersion, in case $\langle n_\uparrow \rangle = \langle n_\downarrow \rangle = 1/4$ or in case $\langle n_\uparrow \rangle = 1/2$ and $\langle n_\downarrow \rangle = 0$, respectively? Note that both states remain eigenstates of the mean field model for any U. Calculate the mean field energies as a function of U for both cases. Determine the value of U beyond which the spin-polarized $\langle m_j \rangle = 1/2$ mean field state has lower energy and becomes the ground state.[2]

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[1] Therefore, for each given magnetization and given total density there is a lowest energy eigenstate. Note, that above relations are valid for any dimension, but we use the one-dimensional model here..

[2] Note, that it is known that there is no such phase transition to a ferromagnetic state in the 1D Hubbard model. This is an example where mean field theory fails due to strong quantum correlations.