Sheet 11:

Hand-out: Friday, July 08, 2022[1]

Problem 1 Small and large Fermi surfaces in the Hubbard model

In this problem we apply the Luttinger theorem for Fermi liquids, which states:
For a Fermi liquid, independent of the underlying interactions, the volume enclosed by the Fermi surface is given by the number of the underlying fermions $N_\uparrow = N_\downarrow = N/2$. In two dimenions:

$$\frac{V_{\text{FS}}}{2\pi^2} = \frac{N}{L_x L_y} \text{ mod} 2 \tag{1}$$

where L_x, L_y are the linear system sizes along x and y. Similar results hold in higher dimensions.

(2.a) When a translational symmetry is spontaneously broken, Luttinger's theorem can be applied for the resulting reduced Brillouin zone. Show for the case of a Néel state, i.e. for a square lattice with a broken sub-lattice symmetry, that Luttinger's theorem in the reduced magnetic Brillouin zone (MBZ) becomes:

$$\frac{V_{\text{FS}}^{\text{MBZ}}}{2\pi^2} = \mathbb{Z} - p \tag{2}$$

where p denotes the hole doping, i.e.

$$N = L_x L_y (1 - p). \tag{3}$$

Consider a spin-balanced system where $N_\uparrow = N_\downarrow = N/2$.

(2.b) Perform a particle-hole mapping, $\hat{c}_{\boldsymbol{j},\sigma} \to \hat{h}^\dagger_{\boldsymbol{j},\sigma}$, and show Luttinger's theorem formulated for the hole-fermi surface becomes:

$$\frac{V_{\text{FS}}^h}{2\pi^2} \equiv \frac{N_h}{L_x L_y} \mod 2. \tag{4}$$

Here N_h denotes the number of (spin-full) holes and $V_{\text{FS}}^h = (2\pi)^2 - V_{\text{FS}}$.

(2.c) Combine your results from (a) and (b) to show that:

$$\frac{V_{\text{FS}}^h}{2\pi^2} \equiv 1 + p \mod 2 \qquad \text{large FS} \tag{5}$$

for translationally invariant systems, and

$$\frac{V_{\text{FS}}^h}{2\pi^2} \equiv p \mod 1 \qquad \text{small FS} \tag{6}$$

for a broken translational symmetry in the case of a Néel state.

[1] If you would like to present your solution(s), feel free to send them to Henning Schlömer until Fri, July 15.

Problem 2 Generalized RPA calculation

Consider the Fermi-Hubbard model with nearest-neighbor tunneling t and on-site interactions U between the two spin states $\sigma =\uparrow,\downarrow$.

(2.a) Using the Hartree-Fock decoupling, derive the equations of motion for

$$\hat{\rho}_{p,q,\sigma} = \hat{c}^{\dagger}_{p+q,\sigma}\hat{c}_{p,\sigma} \tag{7}$$

in the generalized RPA approximation (as defined in the script) – i.e. include direct and exchange terms and approximate

$$\langle \hat{c}^{\dagger}_{p+q,\sigma}\hat{c}_{p,\sigma'}\rangle \approx \delta_{q,0}\delta_{\sigma,\sigma'} n^{\mathrm{F}}_{p}(T). \tag{8}$$

(2.b) From the equations of motion in (2.a) [the result can also be found in the script] derive the generalized RPA (gRPA) response functions for charge and spin:

$$\chi^{\mathrm{c}}_{\mathrm{gRPA}}(q,\omega) = \frac{\chi_0(q,\omega)}{1-\chi_0(q,\omega)U/L^d}, \qquad \chi^{\mathrm{s}}_{\mathrm{gRPA}}(q,\omega) = \frac{\chi_0(q,\omega)}{1+\chi_0(q,\omega)U/L^d}. \tag{9}$$

where L is the linear system size, d is the dimensionality and $\chi_0(q,\omega)$ denotes the free-fermion susceptibility.

Problem 3 Antiferromagnetism in the Fermi-Hubbard model

In this problem we consider the 2D Fermi-Hubbard model at half filling, $\langle \hat{n}_{\boldsymbol{j},\sigma}\rangle = 1/2$, and show that the model has an antiferromagnetic (AFM) instability.

(3.a) At weak coupling, $U \ll t$, show that the spin-susceptibility $\chi^{s}_{\mathsf{gRPA}}(q,\omega)$ has an instability (divergence) at $\omega = 0$ around $\boldsymbol{q} = (\pi,\pi) \equiv \boldsymbol{Q}$, indicating an AFM instability.

(3.b) At finite temperature T and weak coupling, $U \ll t$, it can be shown that (you don't have to show this):

$$\chi_0(\boldsymbol{Q},\omega=0,T)/L^d \approx \frac{1}{2\pi^2 t}\log^2\left(\frac{16e^{\gamma}}{\pi}\frac{t}{T}\right) + C_0\frac{1}{t}, \tag{10}$$

where $\boldsymbol{Q} = (\pi,\pi)$ and two constants $\gamma = 0.5772...$ (Euler's constant) and $C_0 = -0.0166...$ show up.

From Eq. (10), derive an estimate for the critical Néel temperature T_{N} where antiferromagnetism sets in and χ^{s}_{gRPA} diverges.

(3.c) At strong coupling, $U \gg t$, use second-order perturbation theory in t/U to show that the half-filled Fermi-Hubbard model can be mapped to a Heisenberg model:

$$\hat{\mathcal{H}} = J\sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle} \hat{\boldsymbol{S}}_{\boldsymbol{i}}\cdot\hat{\boldsymbol{S}}_{\boldsymbol{j}}, \qquad J = \frac{4t^2}{U} \tag{11}$$

up to an overall energy shift.