Sheet 2:

Hand-out: Monday, Oct. 30, 2023; Solutions: Tuesday, Nov. 7, 2023

Problem 1 RPA of Hubbard model

In this exercise, we want to calculate the charge response functions χ_c and spin response function χ_s of electrons with Hubbard interactions in D dimensions. Assume $\mu_{\mathrm{B}} = 1$. *Note: Do not evaluate any integrals.*

(1.a) Draw the Feynman diagram of $\chi_0(q, i\omega_n)$, and express the analytical form as an integral over momentum.

(1.b) Write down the expression for $\chi^T_{ab}(q)$. Find the RPA expression for χ_c. Argue that the RPA of χ_s vanishes.
Hint: use the form II.1.12 in lecture notes.

(1.c) To evaluate the spin response, find an expression for the ladder approximation to χ_s.
Hint: The diagrammatic representation of the ladder approximation is depicted in II.1.14 in lecture notes.

Problem 2 Two-particle self-consistent theory

In this exercise, we will derive a sum rule that allows us to show the violation of Pauli's principle by the RPA spin and charge response functions. The sum rules are the starting point to derive the two-particle self-consistent theory (TPSC): the Hubbard interactions U are renormalized such that the sum rule, and hence the Pauli principle, is fulfilled.

In Problem 1, we have derived the RPA charge $(+)$ and spin $(-)$ response of the Hubbard model at momentum q and Matsubara frequency ω_n, which are given by (for spin-$1/2$)

$$\chi_\pm(q, i\omega_n) = \frac{\chi_0(q, \omega_n)}{1 \pm \frac{1}{2} U \chi_0(q, i\omega_n)} \tag{1}$$

with the retarded susceptibility $\chi_0(q, i\omega_n)$. The charge and spin structure factor in momentum space is defined as

$$S^\pm(q) = \frac{1}{V^2} \sum_j \sum_d e^{iqd} \left[\langle \hat{n}^\pm_j \hat{n}^\pm_{j+d} \rangle - \langle \hat{n}^\pm_j \rangle \langle \hat{n}^\pm_{j+d} \rangle \right], \tag{2}$$

where V is the volume of the system, j and d are lattice sites, and $\hat{n}^\pm_j = \hat{n}_{j\uparrow} \pm \hat{n}_{j\downarrow}$. Further, we use the following expression for the fluctuation-dissipation theorem at temperature T,

$$S^\pm(q) = -\frac{T}{n} \sum_{i\omega_n} \chi^\pm(q, i\omega_n), \tag{3}$$

at particle density $n = N/V$ and total number of fermions N.

(2.a) Derive the sum rule for the spin and charge structure factor $\sum_q S^{\pm}(q)$. Use the Pauli exclusion principle, $\hat{n}_{j\sigma}^2 = \hat{n}_{j\sigma}$, to find expressions that only depend on particle densities and the density-density correlation function.

(2.b) The density-density correlation function is typically hard to determine in an interacting system. Show that the combined sum rule is given by $\frac{1}{V}\sum_q [S^+(q) + S^-(q)] = 2n - n^2$. This is a very generic expression that only depends on the particle density.

(2.c) Show that the RPA charge and spin response violate the above combined sum rule and therefore the Pauli exclusion principle.
Hint: Expand the denominator of Eq. (1) *in* U. *You can assume that non-interacting fermions are consistent with the sum rule.*

The trick of TPSC is to renormalize the interaction strength for charge $U \to U_+$ and spin $U \to U_-$ separately such that the sum rule is fulfilled.

(2.d) Write down the sum rules as in (2.a) with the expressions for the renormalized interactions up to $\mathcal{O}(U_+^2, U_-^2)$.

(2.e) We make the ansatz $U_- \langle \hat{n}_{j\uparrow} \rangle \langle \hat{n}_{j\downarrow} \rangle = U \langle \hat{n}_{j\uparrow} \hat{n}_{j\downarrow} \rangle$. Find an expression for U_-.
Hint: Do not solve the sum/integral.

(2.f) Solve the combined sum rule self-consistently to find U_+.