6. Exercise on QFT for many-body systems

Sommersemester 2023

TUTORIUM: Friday, 30.06.2023.

Consider the Hubbard-Hamiltonian given by

$$\hat{H} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma} \hat{c}^{\dagger}_{\mathbf{k}\sigma} + U \sum_i \underbrace{\hat{c}^{\dagger}_{i\uparrow}\hat{c}_{i\uparrow}}_{\hat{n}_{i\uparrow}} \underbrace{\hat{c}^{\dagger}_{i\downarrow}\hat{c}_{i\downarrow}}_{\hat{n}_{i\downarrow}} - \mu \sum_i \underbrace{(n_{i\uparrow} + n_{i\downarrow})}_{\hat{n}_i}. \tag{1}$$

The term containing μ fixes the number of particles. Specifically, we consider the case of half-filling where we have $\langle \hat{n}_i \rangle = 1$ particle per site. This corresponds to $\boldsymbol{\mu = \frac{U}{2}}$.

12. The Green's function in limiting cases

1+1+0.5+0.5+2=5 points

First, assume that the electrons governed by the Hamiltonian in Eq. (1) are non-interacting, i.e., $\boldsymbol{U=0}$.

a) Compute the one-particle Green's function $G_\sigma(\mathbf{k}, \tau)$ by directly calculating the trace in the definition

$$G_\sigma(\mathbf{k}, \tau) = -\frac{1}{\mathcal{Z}} \mathrm{Tr}\left[e^{-\beta \hat{H}} \hat{c}_{\mathbf{k}\sigma}(\tau) \hat{c}^{\dagger}_{\mathbf{k}\sigma} \right], \quad \beta \geq \tau \geq 0 \tag{2}$$

of the Green's function. (The partition function is defined as $\mathcal{Z} = \mathrm{Tr}[e^{-\beta \hat{H}}]$.)

Hint: Use the Lehmann representation, i.e. perform the trace over the basis of the eigenvalues and insert the completeness relation, where needed.

b) Continue the result obtained in **a)** for $G_\sigma(\mathbf{k}, \tau)$ to real times by the inverse Wick-rotation $\tau \to it$. Give a physical interpretation for the result.

c) Calculate the Green's function $G_\sigma(\mathbf{k}, i\omega_n)$ in Matsubara frequency space by performing the Fourier-transform

$$G_\sigma(\mathbf{k}, i\omega_n) = \int_0^\beta d\tau \; e^{i\omega_n \tau} G_\sigma(\mathbf{k}, \tau), \tag{3}$$

where $\omega_n = \frac{\pi}{\beta}(2n+1),\ n \in \mathbb{Z}$ is a fermionic Matsubara frequency. Then continue the results on the real frequency axis and calculate the corresponding spectral function $A(\mathbf{k}, \omega)$.

Now, consider the *opposite* limit where the kinetic energy appearing in the Hamiltonian in Eq. (1) is negligible compared to the interaction, i.e., $\varepsilon_{\mathbf{k}} = 0$ (atomic limit).

d) The (local) Green's function for site i, $G_{i\sigma}(\tau)$ is defined as

$$G_{i\sigma}(\tau) = -\langle T_\tau \hat{c}_{i\sigma}(\tau) \hat{c}^{\dagger}_{i\sigma} \rangle = -\frac{1}{\mathcal{Z}} \mathrm{Tr}\left[e^{-\beta \hat{H}} \hat{c}_{i\sigma}(\tau) \hat{c}^{\dagger}_{i\sigma} \right], \quad \beta \geq \tau \geq 0. \tag{4}$$

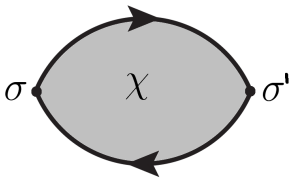
Note that the different atoms are completely independent in this case and the local Green's function is thus the same as already calculated in Problem 6 of Excercise 3. From its Fourier transfrom $G_{i\sigma}(i\omega_n)$, extract the corresponding expression for the self-energy $\Sigma_{i\sigma}(i\omega_n)$. Is the atomic-limit expression derivable within conventional perturbation theory?

e) Calcualte, analogously as in **d)**, the local magnetic (spin) $\chi_i^s(\tau) = \langle T_\tau S_i^z(\tau) S_i^z \rangle$ and density (charge) $\chi_i^c(\tau) = \langle T_\tau n_i(\tau) n_i \rangle$ susceptibilities in the atomic limit of the Hubbard model (with $S_i^z = n_{i\uparrow} - n_{i\downarrow}$ and $n_i = n_{i\uparrow} + n_{i\downarrow}$), as well as their Fourier transform to Matsubara frequencies. Then, analytically continue the expressions to real frequencies. What can you say about the temperature dependence?

13. RPA for the Hubbard model

1+2.5+1.5+2=5+2* points*

In the Hubbard model (Hamiltonian in Eq. (1)), the interaction is purely local and penalizes double occupations: $U \sum_i n_{i\uparrow} n_{i\downarrow}$. Therefore, the interaction only couples electrons with opposite spin: 

Then also susceptibilities can acquire a spin-dependence: $\chi_{\sigma\sigma'}$: 

Remembering that momentum, energy and spin need to be conserved at each vertex:

a) Draw the (bubble) diagram of the free susceptibility $\chi_0^{\sigma\sigma'}(\mathbf{q}, \omega)$ and say which spin-combinations are possible.

b) Draw the random phase approximation (RPA) series for $\chi_{RPA}^{\uparrow\uparrow}$ and $\chi_{RPA}^{\uparrow\downarrow}$. What can you say about the allowed powers of U in both series? Translate the diagrams into formulas and rewrite them using the geometric series. In all of this you can omit the labels for momentum and frequency.

c) The charge and spin susceptibilities (the local versions of which were already introduced in Problem 12 **e)**) are given by:

$$\chi^c = \chi^{\uparrow\uparrow} + \chi^{\uparrow\downarrow}, \quad \chi^s = \chi^{\uparrow\uparrow} - \chi^{\uparrow\downarrow}.$$

Using the result from (b) give expressions for these susceptibilities in the RPA. Which of the two χs was discussed in the lecture in the context of screening?

d) (Bonus points) Using the results of Problem 11 of Exercise 5, consider the electronic system for $d = 2$ in presence of the Hubbard interaction $U > 0$, and calculate within the RPA the two (ferromagnetic and antiferromagnetic) spin susceptibilities. On the basis of your RPA calculations, make your final considerations about the tendency of the system towards a given magnetic order at $T = 0$.