
6. Exercise on QFT for many-body systems

Sommersemester 2020

TUTORIUM: Friday, 19.06.2020.

Consider the Hubbard-Hamiltonian given by

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

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 $\mu = \frac{U}{2}$.

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., $U=0$.

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

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

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

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 $\tau \rightarrow it$. 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

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

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

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

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 Exercise 3. From its Fourier transform $G_{i\sigma}(i\omega_n)$, extract the corresponding expression for the self-energy $\Sigma_{i\sigma}(i\omega_n)$. Is the atomic-limit expression derivable within conventional perturbation theory?

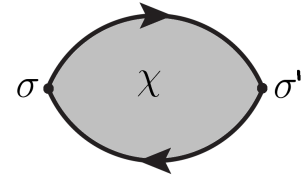
- e) Calcualte, analogously as in **d**), the local magnetic (spin) $\chi_i^s(\tau) = \langle T_\tau S_i^z(\tau) S_i^z \rangle$ and density (charge) $\chi_i^c(\tau) = \langle T_\tau n_i(\tau) n_i \rangle$ susceptibilities in the atomic limit of the Hubbard model (with $S_i^z = n_{i\uparrow} - n_{i\downarrow}$ 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: $\uparrow \text{---} U \text{---} \downarrow$



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

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

- Draw the (bubble) diagram of the free susceptibility $\chi_0^{\sigma\sigma'}(\mathbf{q}, \omega)$ and say which spin-combinations are possible.
- 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.
- 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 χ s was discussed in the lecture in the context of screening?

- (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 $T = 0$.