
5. Exercise on QFT for many-body systems

Sommersemester 2018

TUTORIUM: Friday, 8.06.2018.

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

10. The Green's function in limiting cases

1.5+1+0.5+1.5=4.5 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

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

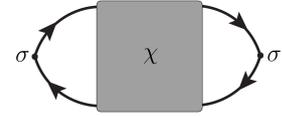
Note that the different atoms are completely independent in this case and the local Green's function is thus the same as already calculated in Problem 6 of Exercise 3. From its Fourier transform $G_{i\sigma}(i\omega_n)$, extract the corresponding expression for the self-energy $\Sigma_{i\sigma}(i\omega_n)$.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

11. RPA for the Hubbard model

1+2.5+2+2* = 5.5+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: $\uparrow \overset{U}{\text{---}} \downarrow$



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 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.
- It is customary to define charge and spin susceptibilities:

$$\chi_c = \chi^{\uparrow\uparrow} + \chi^{\uparrow\downarrow}, \quad \chi_s = \chi^{\uparrow\uparrow} - \chi^{\uparrow\downarrow}.$$

Using the result from (b) give expressions for these susceptibilities in the random phase approximation. Which of the two χ s was discussed in the lecture in the context of screening?

- (Bonus points) Consider now non-interacting electrons on a one-dimensional lattice with dispersion $\epsilon_k = -2t \cos(ka)$ at half-filling ($U = 0, \mu = 0$). Is there a Q -point in the Brillouin zone, $Q \in [0, 2\pi]$, for which $\epsilon_{k+Q} = -\epsilon_k = 0$? What is the signature of this “nesting” property in the free (bubble) susceptibility $\chi_0(Q, \omega = 0)$ at $T = 0$? Remember that the sum over k, \sum_k , can be replaced by $\int d\epsilon \mathcal{N}(\epsilon)$ with the density of states $\mathcal{N}(\epsilon)$ from Exercise 1.