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5. Exercise on QFT for many-body systems

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Consider the Hubbard-Hamiltonian given by

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

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

12. The Green function in limiting cases *1.5+1+0.5+1+1+1+2*=6+2* 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 function $G_\sigma(\tau, \mathbf{k})$ by directly calculating the trace in the definition

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

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

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

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

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

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 $A(k, \omega)$.

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

d) Compute the (local) Green function for site i, $G_{i\sigma}(\tau)$, defined as

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

by directly evaluating the trace using the Lehmann representation.

Hint: Consider that the different atoms are completely independent and, hence, one can evaluate the trace by using the occupation-basis for one site, which consists of four states. Which are these?

e) Calculate the Green function $G_{i\sigma}(i\omega_n)$ in frequency-space by performing the Fourier transform for the result obtained in **d)**.

f) From the exact expression of $G_{i\sigma}(i\omega_n)$ in the atomic limit, extract the corresponding expression for the self-energy $\Sigma_{i\sigma}(i\omega_n)$. Is the atomic-limit expression derivable within conventional perturbation theory?

g) Perform the analytic continuation of $G_{i\sigma}(i\omega_n)$ on the real axis, and calculate the corresponding spectral function $A_{i\sigma}(\omega)$. How can we interpret the spectral function result?

13. Charge susceptibility in RPA

2+2=4 points

As it will be discussed in the next Lecture (11/06/2015 on linear response theory), the reaction of an electronic system to a (weak) external perturbation potential $V_{\rm ext}(\mathbf{q},\omega)$ can be obtained via the polarization function $\Pi(\mathbf{q},\omega)$, which is the proportionality factor between the induced charge density $n_{\rm ind}(\mathbf{q},\omega)$ and the external potential. Assuming the perturbation is weak (so that the induced density is directly proportional to it), we have

$$n_{\rm ind}(\mathbf{q},\omega) = \Pi(\mathbf{q},\omega) V_{\rm ext}(\mathbf{q},\omega),$$

where the polarization function can be calculated in imaginary time $\tau > 0$ as

$$\Pi(\mathbf{q},\tau) = -\langle T_\tau n_{\rm ind}(\mathbf{q},\tau) n_{\rm ind}(-\mathbf{q},0)\rangle \tag{5}$$

where

$$n_{\rm ind}(\mathbf{q},\tau) = n(\mathbf{q},\tau) - n_0\,\delta(\mathbf{q}), \quad n(\mathbf{q},\tau) = \sum_{\mathbf{k}} c^\dagger_{\mathbf{k}}(\tau) c_{\mathbf{k}+\mathbf{q}}(\tau)$$

and n_0 is the average filling of the non-interacting system.

a) Evaluate the polarization for the non-interacting case $U = 0$, i.e. $\Pi_0(\mathbf{q}, i\omega_n)$, by first using Wick's theorem and second performing a Fourier transform to Matsubara frequencies.

b) Let us consider now the case of an Hubbard model at finite $U > 0$. Use the random phase approximation (RPA) to calculate the polarization at $U \neq 0$, i.e. $\Pi_{\rm RPA}(\mathbf{q}, i\omega_n)$. What is the physical meaning of the result? How would the physics change, if we considered an *attractive* Hubbard model ($U < 0$)? Why?

Hint: For the final physical questions it is sufficient to consider the static limit of the polarization, i.e. $\omega_n = 0,\ \mathbf{q} \to 0$.

* Bonus points

Viel Spaß!