Karlsruhe Institute of Technology

Institute for Theoretical Condensed Matter physics

Condensed Matter Theory I WS 2022/2023

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Sheet 9

Tutorial: 12.01.2022

The last task is a bonus exercise. It will be corrected during the tutorial only if we have enough time. In any case, its correction will be uploaded on Ilias with the other exercises.

Category A

1. Correlation functions of an ideal Fermi gas $(5 + 10 + 5 + 10 + 5 = 35$ Points)

Consider a 3D system with a finite volume V of N non-interacting fermions in the ground state $|\Psi_0\rangle$. One can express the density operator for particles in the spin state σ using the creation and annihilation operators:

$$\hat{n}(\boldsymbol{r}, \sigma) = \frac{1}{V} \sum_{\boldsymbol{k},\boldsymbol{k}'} e^{-i(\boldsymbol{k}-\boldsymbol{k}')\boldsymbol{r}} a^\dagger_{\boldsymbol{k},\sigma} a_{\boldsymbol{k}',\sigma}.$$

where $\sigma = \downarrow, \uparrow$ is one of the eigenstate of the σ_z operator. The operator $a^\dagger_{\boldsymbol{k},\sigma}$ increases the number of particles in the state $\boldsymbol{k}$ and σ to 1. The operator $a_{\boldsymbol{k},\sigma}$ reduces the number of particles in this state to 0. The creation and annihilation operators satisfy the anti-commutation relations:

$$\{\hat{a}_{\boldsymbol{k},\sigma}, \hat{a}_{\boldsymbol{k}',\sigma'}\} = \{\hat{a}^\dagger_{\boldsymbol{k},\sigma}, \hat{a}^\dagger_{\boldsymbol{k}',\sigma'}\} = 0, \qquad \{\hat{a}^\dagger_{\boldsymbol{k},\sigma}, \hat{a}_{\boldsymbol{k}',\sigma'}\} = \delta_{\sigma,\sigma'}\delta_{\boldsymbol{k},\boldsymbol{k}'}.$$

The ground state of the free Fermi gas can be expressed as follows:

$$|\Psi_0\rangle = \prod_{|\boldsymbol{k}|<k_F,\sigma} \hat{a}^\dagger_{\boldsymbol{k},\sigma}|0\rangle,$$

where all momenta from $|k| = 0$ up to k_F are filled.

(a) Show that, the Fermi momentum in 3D is given by:

$$k_F = (3\pi^2 n)^{1/3},$$

where

$$n = \frac{N}{V} = \sum_\sigma \langle\Psi_0|\hat{n}(\boldsymbol{r}, \sigma)|\Psi_0\rangle,$$

is the particle density.

We now introduce the fermionic field operators:

$$\hat{\psi}_\sigma(\boldsymbol{r}) = \frac{1}{\sqrt{V}} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\boldsymbol{r}} \hat{a}_{\boldsymbol{k},\sigma}, \qquad \hat{\psi}^\dagger_\sigma(\boldsymbol{r}) = \frac{1}{\sqrt{V}} \sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\boldsymbol{r}} \hat{a}^\dagger_{\boldsymbol{k},\sigma},$$

whose effect are: $\hat{\psi}_\sigma(\boldsymbol{r})$ destroys a particle with spin σ at $\boldsymbol{r}$, while $\hat{\psi}^\dagger_\sigma(\boldsymbol{r})$ creates a particle with spin σ at $\boldsymbol{r}$. Show that these field operators satisfy the canonical anti-commutation relations:

$$\{\hat{\psi}_\sigma(\boldsymbol{r}), \hat{\psi}^\dagger_{\sigma'}(\boldsymbol{r}')\} = \delta(\boldsymbol{r} - \boldsymbol{r}')\delta_{\sigma,\sigma'}.$$

(b) The one-particle correlation function is defined as follows:

$$G_\sigma(\boldsymbol{r}-\boldsymbol{r}') = \langle \Psi_0 | \hat{\psi}^\dagger_\sigma(\boldsymbol{r}) \hat{\psi}_\sigma(\boldsymbol{r}') | \Psi_0 \rangle.$$

This correlation function can be interpreted as the probability amplitude of an electron with spin σ being destroyed at $\boldsymbol{r}'$ and recreated at $\boldsymbol{r}$. Demonstrate that it gives:

$$G_\sigma(\boldsymbol{r}-\boldsymbol{r}') = \frac{3n}{2} \frac{\sin x - x\cos x}{x^3}, \qquad x = k_F|\boldsymbol{r}-\boldsymbol{r}'|.$$

Hint: Use the Fourier transform

(c) The two-particle correlation function gives the probability amplitude to find a particle with spin σ' at $\boldsymbol{r}'$ when a particle with spin σ is already at $\boldsymbol{r}$. It is defined as follows:

$$g_{\sigma,\sigma}(\boldsymbol{r}-\boldsymbol{r}') = \frac{4}{n^2} \langle \Psi_0 | \hat{n}(\boldsymbol{r},\sigma) \hat{n}(\boldsymbol{r}',\sigma') | \Psi_0 \rangle = \frac{4}{n^2} \langle \Psi_0 | \hat{\psi}^\dagger_\sigma(\boldsymbol{r}) \hat{\psi}^\dagger_{\sigma'}(\boldsymbol{r}') \hat{\psi}_{\sigma'}(\boldsymbol{r}') \hat{\psi}_\sigma(\boldsymbol{r}) \Psi_0 \rangle.$$

Show that in the case where $\sigma \neq \sigma'$ (for any $\boldsymbol{r}$ and $\boldsymbol{r}'$)

$$g_{\sigma,\sigma'}(\boldsymbol{r}-\boldsymbol{r}') = 1.$$

(d) Show that only when we are in the case $\sigma = \sigma'$ the two -particle correlation function can be expressed using the one-particle correlation function such that:

$$g_{\sigma,\sigma}(\boldsymbol{r}-\boldsymbol{r}') = 1 - \frac{4}{n^2} \left[G_\sigma(\boldsymbol{r}-\boldsymbol{r}') \right]^2.$$

Compare this result with the one of question (d) and and think about what all this has to do with the Pauli principle.

(e) To understand the Pauli principle, calculate the following Integral:

$$\frac{n}{2} \int d^3r \left[g_{\sigma,\sigma'}(\boldsymbol{r}-\boldsymbol{r}') - 1 \right].$$

How could you interpret the result?

Category B

2. Thermodynamic perturbation theory (5 + 10 = Points)

We consider a gas of spinless bosons of mass m in a volume $V = L^3$, with periodic boundary conditions for the wave functions. The particles interact via a potential $U(\vec{r}_1 - \vec{r}_2) = U_0\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)$ with $U_0 > 0$. The interaction part of the Hamiltonian ($\widehat{H} = \widehat{H}_0 + \widehat{U}$) has the following form in secondary quantization representation:

$$\widehat{U} = \frac{U_0}{2V} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4} \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3-\boldsymbol{k}_4}\, \hat{a}^\dagger_{\boldsymbol{k}_3} \hat{a}^\dagger_{\boldsymbol{k}_4} \hat{a}_{\boldsymbol{k}_2} \hat{a}_{\boldsymbol{k}_1}$$

The chemical potential μ and the temperature T are given.

(a) Consider $\widehat{U}$ as a small perturbation and show that the first-order correction in U_0 to the grand canonical potential is given by

$$\delta\Omega = \langle \widehat{U} \rangle_{H_0} = \frac{\operatorname{tr}\left\{ \widehat{U} e^{-\beta\left(\widehat{H}_0 - \mu\widehat{N}\right)} \right\}}{\operatorname{tr}\left\{ e^{-\beta\left(\widehat{H}_0 - \mu\widehat{N}\right)} \right\}} .$$

(b) Calculate $\delta\Omega$. The relevant matrix element can be generated either by different states $\vec{k}_1 \neq \vec{k}_2$ or by the same state $\vec{k}_1 = \vec{k}_2$. Consider these two cases separately.

3. Operators in the secondary quantized representation (bonus exercise) (25 Points)

In the lecture, the second quantization for bosonic operators $\hat{F}^{(1)} = \sum_a \hat{f}^{(1)}_{x_a}$ has been derived: $\hat{F}^{(1)} = \sum_{ij} \langle i|\hat{f}^{(1)}|j\rangle\, \hat{b}^\dagger_i \hat{b}_j$. Here, $|i\rangle$ are the single particle states and the operator $\hat{f}^{(1)}_{x_a}$ acts on coordinates x_a. The diagonal elements ($i = j$) of the bosonic operators are given by

$$\langle N_1, N_2, \ldots |\hat{F}^{(1)}| N_1, N_2, \ldots \rangle = \sum_i N_i \langle i|\hat{f}^{(1)}|i\rangle, \tag{1}$$

where $|N_1, N_2, ...\rangle = \left(\frac{N_1! N_2! \ldots}{N!} \right)^{1/2} \sum_P \phi_{P_1}(x_1)\phi_{P_2}(x_2) \ldots \phi_{P_N}(x_N)$ is the symmetrized bosonic wavefunction. $\phi_i(x_i)$ are the single particle wave functions (i is a quantum number). The non-diagonal elements ($i \neq j$) are

$$\langle \ldots, N_i, \ldots, N_j - 1, \ldots |\hat{F}^{(1)}| \ldots, N_i - 1, \ldots, N_j, \ldots \rangle = \sqrt{N_i N_j}\, \langle i|\hat{f}^{(1)}|j\rangle \tag{2}$$

where $N = \sum_i N_i$. Analogously to the single-particle operators, the two-particle bosonic operators $\hat{F}^{(2)}$ are introduced

$$\hat{F}^{(2)} = \frac{1}{2} \sum_{iklm} \langle ik|\hat{f}^{(2)}|lm\rangle\, \hat{a}^\dagger_i \hat{a}^\dagger_k \hat{a}_m \hat{a}_l \tag{3}$$

with the matrix elements $\langle ik|\hat{f}^{(2)}|lm\rangle = \iint dx_1\, dx_2\, \phi^\star_i(x_1)\, \phi^\star_k(x_2)\, \hat{f}^{(2)}\, \phi_l(x_1)\, \phi_m(x_2)$.

Derive the expression for $\hat{F}^{(2)} = \sum_{a<b} f_{ab}^{(2)}$ of the form (3) where the operator acts on coordinates x_a and x_b. To do that, find the expressions for two-particle operators that are analogous to (1) and (2). Distinguish whether $f^{(2)}$ acts twice on the same single-particle state or on two different ones.