Theoretical Physics 5 : WS 2024/2025
Exercise sheet 3

04.11.2024

Exercise 0.

How much time did it take to complete this exercise sheet?

Exercise 1. (20 points): Fermion wave functions & operators

a) (*5 p.*) Explicity write the following N-fermion wave functions in terms of single-fermion wave functions $\psi_i(x_j)$:

- $\Phi_{0011\cdots 0}(x_1, x_2)$
- $\Phi_{1101\cdots 0}(x_1, x_2, x_3)$
- $\Phi_{1210\cdots 0}(x_1, x_2, x_3, x_4)$

b) (*15 p.*) The creation and annihilation operators for fermions satisfy

$$\{c_i, c_j^\dagger\} = \delta_{ij}, \qquad \{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0.$$

Show that for a system of fermions the particle number operator $n = \sum_i c_i^\dagger c_i$ commutes with the Hamiltonian

$$\mathcal{H} = \sum_{i,j} \langle i|H_0|j\rangle \, c_i^\dagger c_j + \frac{1}{2} \sum_{i,j,k,l} \langle i,j|V|k,l\rangle \, c_i^\dagger c_j^\dagger c_l c_k.$$

Hint: To save some effort, after you show that $\left[n, c_i^\dagger c_j\right] = 0$ you can try to manipulate $\left[n, c_i^\dagger c_j^\dagger c_l c_k\right]$ into a form whose terms are all similar to $\left[n, c_i^\dagger c_j\right]$.

Exercise 2. (80 points): High-density electron gas and perturbation theory

The Hamiltonian of a homogeneous electron gas is given by $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$, with

$$\mathcal{H}_0 = \sum_{\boldsymbol{k}} \sum_{s} \frac{\hbar^2 k^2}{2m} c^\dagger_{\boldsymbol{k},s} c_{\boldsymbol{k},s} \quad \text{and} \quad \mathcal{H}_1 = \frac{e^2}{2V} \sum_{\boldsymbol{k},\boldsymbol{p}} \sum_{\boldsymbol{q}\neq\boldsymbol{0}} \sum_{s,s'} \frac{4\pi}{q^2} c^\dagger_{\boldsymbol{k}+\boldsymbol{q},s} c^\dagger_{\boldsymbol{p}-\boldsymbol{q},s'} c_{\boldsymbol{p},s'} c_{\boldsymbol{k},s},$$

where m is the electron mass, $k \equiv |\boldsymbol{k}|$, and $q \equiv |\boldsymbol{q}|$.

In the lecture notes you have seen that it is possible to rewrite this Hamiltonian using dimensionless variables, including $r_s \equiv r_0/a_0$, where r_0 is the interparticle spacing. We claimed that in the high-density limit, where $r_s \to 0$, $\mathcal{H}_1$ is a perturbation to $\mathcal{H}_0$.

In this exercise you are going to put this claim to the test by calculating the correction from $\mathcal{H}_1$ to the ground state energy, and checking whether this correction is indeed small as compared to the ground state energy.

a) (*10 p.*) Derive the magnitude of the Fermi momentum and show that it is given by

$$k_F = \left(\frac{9\pi}{4}\right)^{1/3} \frac{1}{r_0}.$$

Here, the interparticle spacing r_0 is defined via $V/N = (4\pi/3)r_0^3$, where N is the number of electrons.

b) (*20 p.*) Let us denote the (unperturbed) ground state and the corresponding ground state energy by $|\Psi_0\rangle$ and $E^{(0)} = \langle\Psi_0|\mathcal{H}_0|\Psi_0\rangle$, respectively. Show that

$$\frac{E^{(0)}}{N} = \frac{3}{5}\frac{\hbar^2 k_F^2}{2m}$$

Hints:

- You do not need an explicit form for $|\Psi_0\rangle$. Think about what the Fermi momentum means, physically, and how this relates to the sum over $\boldsymbol{k}$ of the creation and annihilation operators.
- You might find it useful to use the Heaviside step function,

$$\Theta(x) = \begin{cases} 1 & \text{if } x > 0, \\ 0 & \text{if } x < 0. \end{cases}$$

- In the limit of $V \to \infty$ you can replace

$$\sum_{\boldsymbol{k},s} f_s(\boldsymbol{k}) \to \frac{V}{(2\pi)^3} \sum_s \int \mathrm{d}^3k \, f_s(\boldsymbol{k}).$$

c) (*20 p.*) Recall that the first-order correction to the energy is given by

$$E^{(1)} = \langle \Psi_0 | \mathcal{H}_1 | \Psi_0 \rangle \,. \tag{1}$$

In order to calculate this correction, it is helpful to consider which combinations of states the operator $\mathcal{H}_1$ can act on.

Show that

$$\sum_{\boldsymbol{k},\boldsymbol{p}} \sum_{\boldsymbol{q}\neq\boldsymbol{0}} \sum_{s,s'} \langle \Psi_0 | c^\dagger_{\boldsymbol{k}+\boldsymbol{q},s} c^\dagger_{\boldsymbol{p}-\boldsymbol{q},s'} c_{\boldsymbol{p},s'} c_{\boldsymbol{k},s} | \Psi_0 \rangle$$
$$= -2 \left(\frac{V}{(2\pi)^3} \right)^2 \int \mathrm{d}^3 k \; \Theta(k_F - k) \int \mathrm{d}^3 q \; \Theta(k_F - |\boldsymbol{k} + \boldsymbol{q}|),$$

and then fill in the constants and the $1/q^2$ factor from $\mathcal{H}_1$ to get an integral expression for $E^{(1)}$.

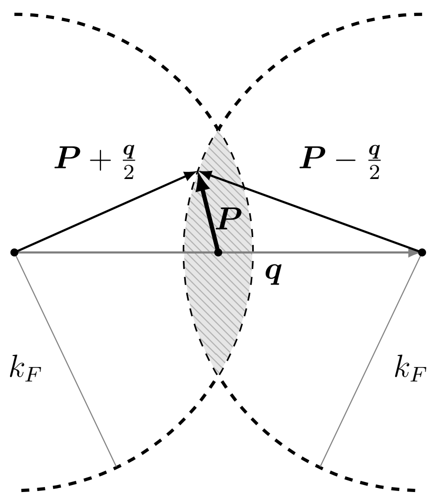
Hints:

- Consider the order of the annihilation and creation operators acting on $|\Psi_0\rangle$. Since the initial and final state are both the ground state, can you draw any conclusions about the relationship between $\boldsymbol{k}$, $\boldsymbol{q}$ and $\boldsymbol{p}$? What about the relationship between s and s'? Can you express these restrictions with delta functions?
- The annihilation and creation operators must all act on occupied states, otherwise the matrix element of the transition would be zero. What does it mean for a state with momentum $\boldsymbol{k}$ to be occupied? Can you express these restrictions with Heaviside functions?
- Remember the $V \to \infty$ limit from the previous question!

d) (*20 p.*) Perform the integrations to show that

$$\frac{E^{(1)}}{N} = -\frac{e^2}{4\pi} 3k_F.$$

Hint: If you change integration variables from $\boldsymbol{k} \to \boldsymbol{P}$, using $\boldsymbol{k} = \boldsymbol{P} - \boldsymbol{q}/2$, you can visualize the $\boldsymbol{P}$ integral over the two step functions as the volume of the overlap region of two spheres with radius k_F, whose centers are at a distance q from each other:



Remember that these are **spheres** and not circles. **Explain why the $\boldsymbol{P}$ integral over the Θ functions is equivalent to this volume**, and then try to calculate such a volume by integrating in spherical coordinates!

After you get the $\boldsymbol{P}$ integration out of the way, the $\boldsymbol{q}$ integration should be more straightforward.

e) (*10 p.*) Express $(E^{(0)} + E^{(1)})/N$ in terms of $r_s = r_0/a_0$, where $a_0 = \hbar^2/(me^2)$. Fill in physical values for the constants. Is $E^{(1)}$ indeed small as compared to $E^{(0)}$ in the high-density limit, i.e. is it valid to use perturbation theory here?