Exercise sheet 4 Theoretical Physics 5 : SS 2023

08.05.2023

Write your name and your tutor's name on every page you hand in. Please staple said pages together.

Exercise 0.

How much time did you take to complete this homework sheet?

Exercise 1. (15 points): Fermion varia

- a) (4 p.) How many terms does the fermion wave function $\Psi_{11110...0}(x_1, x_2, x_3, x_4, x_5)$ have? Explain your reasoning.
- b) (1 p.) What is unphysical about the fermion wave function $\Psi_{11212...1}(x_1, x_2, x_3, x_4, x_5, \ldots, x_{\infty})$?
- b) (10 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

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

Exercise 2. (85 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 and $|\mathbf{k}| = k$, $|\mathbf{q}| = q$.

In the lecture notes you have seen that it is possible to rewrite this Hamiltonian using dimensionless variables. One of these variables was r_s . We defined a so-called high-density limit, where $r_s \to 0$, and claimed that \mathcal{H}_1 was 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) (5 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 may replace

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

c) (15 p.) Recall from your introductory quantum mechanics classes 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 quite helpful to build some intuition as to what the operator \mathcal{H}_1 does. To that end, we've started drawing a diagram below

that represents the action of \mathcal{H}_1 in between $\langle \Psi_0 |$ and $|\Psi_0 \rangle$. Each line represents a different momentum, and it is up to you to finish the diagram.

Label the four solid lines and single dashed line with the relevant momenta. Use a circle, \bigcirc , to mark the two annihilated particles and a dot, \bigcirc , to mark the two created particles. Connect the relevant annihilated particles with the relevant created particles.

Using your diagram and the fact that you are looking at the ground state, derive a relation between the spins, constraints for the magnitudes of \boldsymbol{k} , \boldsymbol{p} , $\boldsymbol{p} - \boldsymbol{q}$ and $\boldsymbol{k} + \boldsymbol{q}$, and a relation between two of these four momenta. You can express the constraints in terms of step functions and the relations in terms of a delta function. These constraints kill the sums in $\langle \Psi_0 | \mathcal{H}_1 | \Psi_0 \rangle$. Do not simply state the constraints and relations. Explain, in words, why they are true.

Hint: Remember that $q \neq 0$.



d) (15 p.) Show that

$$E^{(1)} = -\frac{4\pi e^2 V}{(2\pi)^6} \int d^3k \,\theta(k_F - k) \int d^3q \,\frac{1}{q^2} \theta(k_F - |\mathbf{k} + \mathbf{q}|).$$

Mind the sign!

e) (20 p.) Do the integrals to show that

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

Hint: If you change integration variables from $\mathbf{k} \to \mathbf{P}$, using $\mathbf{k} = \mathbf{P} - \mathbf{q}/2$, you will see that the \mathbf{P} integral over the two step functions reduces to an integral over the overlap region of two spheres with radii $\mathbf{P} \pm \mathbf{q}/2$. By drawing a picture you should be able to figure out how the step functions constrain the integration limits of \mathbf{P} . The remaining integral over \mathbf{q} should then be rather easy.

f) (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. In the high-density limit is $E^{(1)}$ indeed small as compared to $E^{(0)}$, i.e. is it valid to use perturbation theory here?