Exercise sheet 3
Theoretical Physics 5 : WS 2019/2020
Lecturer : Prof. M. Vanderhaeghen

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Exercise 0.

How much time did it take to complete the task?

Exercise 1. (30 points) : Fermionic operators

Let c and $c^\dagger$ be two operators satisfying the anticommutation relations

$$\{c, c^\dagger\} = 1, \qquad \{c, c\} = \{c^\dagger, c^\dagger\} = 0.$$

a) (*5 p.*) Prove the relations $[N, c] = -c$ and $[N, c^\dagger] = c^\dagger$, where $N = c^\dagger c$.

b) (*5 p.*) Applying these relations on the eigenstates of N ($|0\rangle$ and $|1\rangle$), show that with suitable choice of phases

$$c|0\rangle = 0, \qquad c|1\rangle = |0\rangle, \qquad c^\dagger|0\rangle = |1\rangle, \qquad c^\dagger|1\rangle = 0; \tag{1}$$

c) (*5 p.*) Show that c and $c^\dagger$ are the hermitian conjugate operators (*i.e.* $\langle m|c^\dagger|n\rangle = \langle n|c|m\rangle^*, \quad \forall m, n$).

d) (*15 p.*) Show that for a system of fermions, the particle number operator $N = \sum_i a_i^\dagger a_i$ commutes with the Hamiltonian

$$H = \sum_{i,j} \langle i|H_0|j\rangle\, a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l} \langle i, j|V|k, l\rangle\, a_i^\dagger a_j^\dagger a_l a_k.$$

Hint: You could prove first that $[AB, C] = A[B, C] + [A, C]B = A\{B, C\} - \{A, C\}B$.

Exercise 2. (35 + [30 bonus] points) : Ground state energy of high-density e^- gas in 1^{st} order perturbation theory

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

$$\hat{H}_0 = \sum_{\vec{k},s} \frac{\hbar^2 k^2}{2m}\, a^\dagger_{\vec{k},s} a_{\vec{k},s} \quad \text{and} \quad \hat{H}_1 = \frac{e^2}{2V} \sum_{\vec{k},\vec{p}} \sum_{\vec{q}\neq\vec{0}} \sum_{s,s'} \frac{4\pi}{q^2}\, a^\dagger_{\vec{k}+\vec{q},s} a^\dagger_{\vec{p}-\vec{q},s'} a_{\vec{p},s'} a_{\vec{k},s}.$$

In the high-density limit, $\hat{H}_1$ is a perturbation to $\hat{H}_0$. Using techniques of perturbation theory, it is possible to estimate in this regime the ground state energy of the interacting electron gas.

a) (*5 p.*) Express the Fermi momentum k_F in terms of the interparticle spacing r_0.
Hint: $\frac{4}{3}\pi r_0^3 = V/N$.

b) (*15 p.*) Determine $\frac{E^{(0)}}{N}$ in terms of k_F.
Hints:

- $E^{(0)} = \langle \Psi_0 | \hat{H}_0 | \Psi_0 \rangle$
- In the limit that the volume of the system becomes infinite, the sums over states can be replaced by integrals:

$$\sum_{\vec{k},s} f_s(\vec{k}) \longrightarrow \frac{V}{(2\pi)^3} \sum_s \int \mathrm{d}\vec{k}\; f_s(\vec{k})$$

c) (*15 p.*) To 1^{st} order of perturbation theory, the energy shift due to the interaction is given by $E^{(1)} = \langle \Psi_0 | \hat{H}_1 | \Psi_0 \rangle$. Show that

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

Hint: The creation and annihilation operators need to be paired in a way that the matrix element is non-vanishing

d) (*20 p.*)[*Bonus*] Determine $E^{(1)}/N$ in terms of k_F.
Hint: Changing integration variables $\vec{k} \to \vec{P}$ you could show that the region of integration corresponds to the intersection of two spheres with radii $\vec{P} \pm \vec{q}/2$.

e) (*10 p.*)[*Bonus*] Express $(E^{(0)} + E^{(1)})/N$ in terms of $r_s \equiv r_0/a_0$ and $a_0 \equiv \hbar^2/me^2$. Evaluate numerically the coefficients and check the validity of the perturbative approach in the high-density limit.

Exercise 3. (35 points) : Helium atom

Helium is composed of two electrons bound by the electromagnetic force to a nucleus containing two protons along with either one or two neutrons, depending on the isotope

a) (*5 p.*) Write down the Hamiltonian of the two-electron system in the Helium atom in the approximation of an infinitely heavy nucleus.

b) (*10 p.*) Under the assumption that the interaction between electrons is a small perturbation, we can factorize the wave function into a product of wave functions for separate electrons. The total wave function of the fermion system should be antisymmetric and is given by product of coordinate and spin wave functions. If both electrons are in the 1s state, then the coordinate wave function must be symmetric, and the spin wave function is antisymmetric. Write down the spin wave function for this state. What is the total spin (S) and the spin projection (S_z) for this state ?
Hint: The spin operator is given by $\vec{S} = \hbar\frac{\vec{\sigma}}{2}$ with $\vec{\sigma}$ the Pauli matrices

c) (*10 p.*) For electrons in different states we can construct symmetric and antisymmetric combinations of coordinate wave functions. Write down the wave functions of all possible states with electrons in 1s and 2s states assuming that the 1s and 2s state wave functions are known, ϕ_{1s} and ϕ_{2s}. Find S and S_z for these states.

d) (*10 p.*) Find the energy levels for the states considered in (c) in first order of perturbation theory. The difference between energies is given by two exchange integrals. Express it in terms of the wave functions for 1s and 2s states, ϕ_{1s} and ϕ_{2s}. Discuss the result.