Quantum Mechanics II

Exercise 4: Second quantization. *N*-body problems.

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- 1. Express two-particle operator $\hat{F} = \frac{1}{2} \sum_{\alpha \neq \beta} \hat{f}^{(2)}(x_{\alpha}; x_{\beta})$ in terms of creation and annihilation operators for the case of bosons as well as fermions.
- 2. Show that the number operator $\hat{N} = \sum_i \hat{a}_i^{\dagger} \hat{a}_i$ (for bosons and fermions) commutes with the Hamiltonian

$$\hat{H} = \sum_{ij} \hat{a}_i^{\dagger} \langle i|T|j \rangle \hat{a}_j + \frac{1}{2} \sum_{ijkm} \hat{a}_i^{\dagger} \hat{a}_j^{\dagger} \langle ij|V|km \rangle \hat{a}_m \hat{a}_k.$$

3. Bose-Einstein Condensate (BEC) in a harmonic trap.

Consider N bosons of spin zero in an isotropic harmonic trap of angular frequency ω . The interactions between particles are neglected and the mean number of particles at the energy level E is given by the Bose-Einstein law

$$n_E = \frac{1}{e^{(E-\mu)/k_b T} - 1},$$

where μ is chemical potential, T is temperature, and k_b is Boltzmann's constant. Show that:

- (a) The chemical potential satisfies $\mu < \frac{3}{2}\hbar\omega$.
- (b) The number of particles N outside the fundamental level of the trap satisfies

$$N \le F(\xi) = \sum_{n=1}^{\infty} \frac{(n+1)(n+2)}{2(e^{n\xi}-1)}, \qquad \xi = \frac{\hbar\omega}{k_b T}.$$

<u>Reminder</u>: The degeneracy of the energy level $E_n = (n + \frac{3}{2})\hbar\omega$ is $g_n = \frac{1}{2}(n+1)(n+2).$

(c) In the high temperature limit $(k_{\rm B}T \gg \hbar\omega)$ the discrete sum in the definition of $F(\xi)$ can be replaced by an integral. Show that the number of particles outside the fundamental level is majorized by

$$N_{\rm max}' = \zeta(3) \left(\frac{k_b T}{\hbar\omega}\right)^3,$$

where the Rieman $\zeta(n)$ fonction. Reminder:

$$\int_0^\infty \frac{x^{\alpha-1}}{e^x - 1} \mathrm{d}x = \Gamma(\alpha)\zeta(\alpha), \qquad \Gamma(3) = 2!, \qquad \zeta(3) \approx 1.202.$$

- (d) What happens if we place in the trap more than N'_{max} particles? At which temperature this phenomenon can be observed in a trap of frequency $\frac{\omega}{2\pi} = 100$ Hz containing 10^6 atoms?
- 4. Fermi gas : non-interacting fermions at low (zero) temperatures.
 - "non-interacting" particles the energy of the particles is only kinetic.
 - "low temperatures" the particles occupy the lowest possible energy levels.

Consider N non-interacting fermions of spin s at low temperature confined in a three-dimensional (cubic) box with the edge length L:

(a) Find a relation between the density of the Fermi gas ρ and the *Fermi momentum* p_F assuming that the number of fermions N is large. Use the momentum quantization of a free particle in a box with the momentum eigenvalues $\vec{p} = \frac{2\pi\hbar}{L}\vec{n}$, where $\vec{n} = (n_1, n_2, n_3)$ and all $n_i \neq 0$ integer. Take into account the maximal number of fermions of spin s which can occupy the same energy level.

<u>Reminder</u>: Fermi momentum p_F is the maximal absolute value of the momentum of a particle in the Femi gas.

- (b) Express the average energy of the fermions in terms of the *Fermi energy* ε_F corresponding to Fermi momentum p_F .
- (c) Express the Fermi energy as a function of the density of fermions and deduce an expression of the Fermi energy for electrons.

<u>Reminder</u>: The Fermi energy of electrons can attain large values ($\varepsilon_F = 3eV$ in sodium metal) which is much higher than the kinetic energy of the thermal motion at room temperature ($k_{\rm B}T \approx 0,025$ eV). That is why the "zero temperature" approximation is applicable for the conduction electrons in metals even at room temperature.

<u>Note.</u> Applications of the Fermi gas model:

- conduction electrons in a metal
- semi-conductors
- electronic degenerate gas in white dwarfs
- electronic degenerate gas in neutron stars