

## Quantum Mechanics II

### Exercise 6: 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

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

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

Consider  $N$  bosons of spin zero in an isotropic harmonic trap of angular frequency  $\omega$ . 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  $\mu$  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

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

Reminder: 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 ( $k_b T \gg \hbar \omega$ ) 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

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

where the Riemann  $\zeta(n)$  function.

Reminder:

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

(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  $\rho$  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.

Reminder: Fermi momentum  $p_F$  is the maximal absolute value of the momentum of a particle in the Fermi gas.

(b) Express the average energy of the fermions in terms of the *Fermi energy*  $\varepsilon_F$  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.

Reminder: 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 ( $k_B T \approx 0,025$  eV). That is why the “zero temperature” approximation is applicable for the conduction electrons in metals even at room temperature.

Note. 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