Advanced Quantum Mechanics

Prof. Dr. J. Krug, Dr. J. Åberg

Exercise sheet 7 (Due: Monday December, 5th.)

7.1 Bose-Einstein and Fermi-Dirac statistics

The state of the grand canonical ensemble is characterized by the density operator (not to be confused with the particle density operator)

$$\rho = \frac{1}{Z} e^{-\beta(H-\mu N)}, \quad Z = \mathrm{Tr} e^{-\beta(H-\mu N)}, \quad \beta = \frac{1}{k_B T}, \tag{1}$$

where H is the Hamiltonian of the system, T the absolute temperature, k_B Boltzmann's constant, N the total particle number operator, and μ is the chemical potential (which is a real number). Hence, not only can heat flow between the system and the heat bath, but there can also be a flow to and from a reservoir of particles. Suppose that the particles are non-interacting, and that the single-particle eigenenergies are ε_j, and that a_j, $a_j^\dagger$, and $n_j = a_j^\dagger a_j$ are the corresponding bosonic or fermionic annihilation, creation, and number operators. The many-body Hamiltonian can thus be written $H = \sum_j \epsilon_j n_j$. We shall show that the average occupation of state j is given by

$$\langle n_j \rangle \equiv \mathrm{Tr}(\rho n_j) = \frac{1}{e^{\beta(\epsilon_j - \mu)} \pm 1}, \tag{2}$$

where the "+"-sign corresponds to fermions, and the "−"-sign to bosons.

(a) For both bosons and fermions, show the following relations

$$[n_j, a_k] = -\delta_{jk} a_j, \quad [n_j, a_k^\dagger] = \delta_{jk} a_j^\dagger. \tag{3}$$

(3 points)

(b) Let A and B be two operators such that $[A, B] = \gamma B$ for $\gamma \in \mathbb{C}$. Show that

$$e^A B = e^\gamma B e^A.$$

Hint: First show that $A^k B = B(A + \gamma \hat{1})^k$, and then use an expansion. **(3 points)**

(c) For ρ as in (1) show that

$$\mathrm{Tr}(\rho a_j^\dagger a_j) = e^{-\beta(\epsilon_j - \mu)} \mathrm{Tr}(\rho a_j a_j^\dagger). \tag{4}$$

Hint: There was a reason for why we bothered to do (a) and (b). **(3 points)**

(d) Use (4) to prove (2). **(2 points)**

7.2 Weakly interacting bosons: Getting a finite ground state energy

In the lecture you derived the following expression (in the Bogoliubov approximation) for the ground state energy E_0 of a collection of N weakly interacting bosons of mass m enclosed in a volume V

$$E_0 = \frac{N^2}{2V} \hat{\mathcal{V}}^{(2)}(\vec{0}) - \frac{1}{2} \sum_{\vec{k} \neq 0} \left(w_{\vec{k}} - \varepsilon_{\vec{k}} \right), \quad \hat{\mathcal{V}}^{(2)}(\vec{k}) = \int \mathcal{V}^{(2)}(\vec{r}) e^{-i\vec{k}\cdot\vec{r}} \, d^3 r,$$

where

$$w_{\vec{k}} = \frac{\hbar^2 k^2}{2m} + n\hat{\mathcal{V}}^{(2)}(\vec{k}), \quad \varepsilon_{\vec{k}} = \sqrt{\frac{\hbar^4 k^4}{4m^2} + \frac{\hbar^2 k^2 n}{m}\hat{\mathcal{V}}^{(2)}(\vec{k})}, \quad n = \frac{N}{V},$$

and where $\mathcal{V}^{(2)}$ is the interaction potential between the particles. You also found that if one chooses $\mathcal{V}^{(2)}(\vec{r}) = \lambda\delta(\vec{r})$ for $\lambda > 0$, then $\hat{\mathcal{V}}(\vec{k}) = \lambda$, and the ground state energy E_0 diverges. This seems a bit annoying from a physical point of view, so here we are going to mend this by assuming a slightly less idealized interaction potential, namely a Gaussian

$$\mathcal{V}^{(2)}(\vec{r}) = (2\pi)^{-3/2}\frac{\lambda}{a^3}e^{-\frac{1}{2a^2}\|\vec{r}\|^2}, \quad a > 0, \quad \lambda > 0, \tag{5}$$

which has the Fourier transform

$$\hat{\mathcal{V}}^{(2)}(\vec{k}) = \lambda e^{-\frac{(ak)^2}{2}}, \quad k = \|\vec{k}\|. \tag{6}$$

We wish to show that the ground state energy E_0 is finite. The tricky part is the sum $\sum_{\vec{k}\neq 0}\left(w_{\vec{k}} - \varepsilon_{\vec{k}}\right)$. Like in the lecture, we here approximate this sum with the volume integral $\frac{V}{(2\pi)^3}\int \left(w_{\vec{k}} - \varepsilon_{\vec{k}}\right) d^3k$, which we can rewrite as $\frac{V}{2\pi^2}\int_0^\infty f(k)k^2 dk$, where we for the sake of notational simplicity write $f(k) = w_{\vec{k}} - \epsilon_{\vec{k}}$.

Remark: The potential $\mathcal{V}^{(2)}$ is constructed such that $\int \mathcal{V}^{(2)}(\vec{r})\, d^3r = \lambda$ for all $a > 0$.

(a) As the first step towards showing that the ground state energy is finite, show that

$$\frac{\lambda n}{2}\frac{e^{-(ak)^2}}{(lk)^2} \geq f(k) \geq 0, \quad k \geq 0, \quad l^2 = \frac{\hbar^2}{2mn\lambda}. \tag{7}$$

Hint: First show that $f(k) = \lambda n(lk)^2 g\left(\frac{e^{-\frac{(ak)^2}{2}}}{(lk)^2}\right)$, where $g(x) = 1 + x - \sqrt{1+2x}$, and then show that $\frac{1}{2}x^2 \geq g(x) \geq 0$ for all $x \geq 0$. **(4 points)**

Remark: Note that we have two characteristic length-scales l and a, and that the groups lk and ak are dimensionless.

(b) Show that

$$\frac{\lambda n\sqrt{\pi}}{4l^2}\frac{1}{a} \geq \int_0^{+\infty} f(k)k^2 dk. \tag{8}$$

From this result it follows that the ground state energy E_0 is finite. **(3 points)**

(c) By letting $a \to 0$ in (5) one does in some sense regain the contact potential $\mathcal{V}^{(2)}(\vec{r}) = \lambda\delta(\vec{r})$. Show that

$$\frac{V}{2\pi^2}\int_0^{+\infty} f(k)k^2 dk \sim \frac{1}{8\pi^{3/2}}\lambda n\frac{V}{l^2 a} \quad \text{as} \quad a \to 0. \tag{9}$$

In order to not make this the exercise from hell, you are provided with the following lower bound

$$\int_0^{+\infty} f(k)k^2 dk \geq \frac{\lambda n\sqrt{\pi}}{4l^2}\frac{1}{a} - \frac{\lambda n k_0}{2l^2} - \frac{\lambda n}{2l^4 k_0}e^{-\frac{3a^2k_0^2}{2}} + \frac{\lambda n}{2l^4}\sqrt{\frac{3\pi}{2}}a - \frac{3\lambda n k_0}{2l^4}a^2,$$

where k_0 is some constant that does not depend on a. **(2 points)**

Remark: The "asymptotic equivalence" $F(x) \sim G(x)$ as $x \to 0$ means that $\lim_{x\to 0}\frac{F(x)}{G(x)} = 1$. Hence F increases (or decreases) at the same rate as G as x decreases.