Ex5980: BEC regarded as a phase transition

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The problem:

Consider N bosons that each have mass M in a box of volume V. The overall density of the particles is $\rho = N/V$. The temperature is T. Denote by m the number of particles that occupy the ground state orbital of the box. The canonical partition function of the system can be written as

$$Z = \sum_{m=0}^{N} Z_{N-m} = \sum_{m=0}^{N} e^{-\tilde{A}(m)} = \int d\varphi \ e^{-NA(\varphi) + \text{const}}$$

In this question you are requested to regard the the Bose-Einstein condensation as phase transition that can be handled within the framework of the canonical formalism where m is the order parameter. Whenever approximations are required assume that $1 \ll m \ll N$ such that $\varphi = (m/N)$ can be treated as a continuous variable. In the first part of the question assume that the gas is ideal, and that Z_{N-m} can be calculated using the Gibbs prescription. In item 5 you are requested to take into account the interactions between the particles. Due to the interactions the dispersion relation in the presence of m condensed bosons is modified as follows:

$$E_k = \sqrt{\left(\epsilon_k + 2g\frac{m}{V}\right)\epsilon_k}$$

where ϵ_k are the one-particle energies in the absence of interaction, and g is the interaction strength. For the purpose of evaluating Z_{N-m} for large m assume that the above dispersion relation can be approximated by a linear function $E_k \propto k$

- (1) Write an explicit expression for the probability p_m of finding m particles in the ground state orbital. Calculation of the overall normalization factor is not required.
- (2) Find the most probable value \bar{m} . Determine what is the condensation temperature T_c below which the result is non-zero.
- (3) Assuming $T < T_c$ write a Gaussian approximation for p_m
- (4) Using the Gaussian approximation determine the dispersion δm
- (5) Correct your answer for p_m in the large m range where the interactions dominate.
- (6) On the basis of your answer to item3, write an expression for $A(\varphi; f)$ that involves a single parameter f whose definition should be provided using ρ, M, T .
- (7) On the basis of your answer to item5, write an expression for $A(\varphi; a)$ that involves a single parameter a whose definition should be provided using ρ, M, T and g.

The solution:

(1) By Gibbs prescription the probability p_m of finding m atoms in the ground state is given by

$$p_m \propto \frac{1}{(N-m)!} z^{N-m} = \frac{1}{(N-m)!} \left(V \left(\frac{MT}{2\pi}\right)^{\frac{3}{2}} \right)^{N-m}$$

(2) To find the most probable \bar{m} we donote $\tilde{A}(m)$ and find its externum

$$\tilde{A}(m) = \ln\left((N-m)!\right) - (N-m)\ln z$$

$$\tilde{A}'(m) = -\ln(N-m) + \ln z = 0$$

$$\bar{m} = N - V \left(\frac{MT}{2\pi}\right)^{\frac{3}{2}}$$

We find the condensation temperature by demanding $\bar{m} > 0$

$$N - V\left(\frac{MT}{2\pi}\right)^{\frac{3}{2}} > 0$$
$$T_c = \frac{2\pi}{M} \left(\frac{N}{V}\right)^{\frac{2}{3}}$$

and so if $T < T_c$ there will be \bar{m} condensed atoms.

(3) Assuming $T < T_c$ we can rewrite the action $\tilde{A}(m)$ in the Gaussian approximation, to do that we'll make some approximations on $\tilde{A}(m)$:

$$\tilde{A}(m) = \ln\left((N-m)!\right) - (N-m)\ln z$$

Using Stirling:

$$\tilde{A}(m) \approx (N-m)\ln(N-m) - (N-m)\ln z = (N-m)[\ln N + \ln(1-\frac{m}{N})] - (N-m)(N-m)\ln z$$

Remembering that $N \gg m$ we can make the following approximation:

$$\ln\left(1-x\right) \approx -x - \frac{1}{2}x^2$$

Now we see that

$$\tilde{A}(m) \approx \frac{1}{2} \frac{m^2}{N} + (N-m) \ln\left(\frac{N}{z}\right) + O(m^3)$$

and see that the probability p_m is:

$$p_m \propto \exp\left[-\frac{1}{2N}m^2 - \ln\left(\frac{N}{z}\right)(N-m)\right]$$

(4) From the result in item 3 we see immediately that the dispersion is

$$\delta m = \sqrt{N}$$

(5) Due to the add interaction that dominates now, we can approximate the energy as follows:

$$E_k = \sqrt{(\epsilon_k + 2g\frac{m}{V})\epsilon_k} \approx \sqrt{2g\frac{m}{V}\epsilon_k} = \sqrt{2g\frac{m}{V}\frac{k^2}{2M}} = \sqrt{\frac{gm}{VM}}k$$

Let us find the new one particle partition function:

$$z' = \int \exp(-\beta E_k) \frac{d^3 x d^3 p}{(2\pi)^3} = \frac{4\pi V}{(2\pi)^3} \int_0^\infty \exp(-\beta \sqrt{\frac{gm}{VM}}k)$$
$$z' = \frac{VT^3}{\pi^2} \left(\frac{VM}{gm}\right)^{\frac{3}{2}}$$

Since the only thing in the probability that changes is z' we can follow the previous procedure for the probability p_m :

$$p_m \propto \exp\left[-\frac{1}{2N}m^2 + \frac{3}{2}(N-m)\ln\frac{z'}{N}\right]$$

(6) If we set $\ln \frac{V}{N} \left(\frac{MT}{2\pi}\right)^{\frac{3}{2}} = f(T)$ and recall $\varphi = \frac{m}{N}$ we can easly rewrite the answer in item 3 as

$$A(\varphi; f) = -\frac{1}{2}\varphi^2 - f(T)(1-\varphi)$$

(7) Again from the answer in item 5 we set $\frac{VT^3}{\pi^2} \left(\frac{VM}{gm}\right)^{\frac{3}{2}} = \left(\frac{a(T)}{\varphi}\right)^{\frac{3}{2}}$ we can rewrite to get:

$$A(\varphi; a) = \frac{1}{2}\varphi^2 + \frac{3}{2}(1-\varphi)\ln\left(\frac{\varphi}{a(T)}\right)$$