

Statistical Physics (MSc)

Homework 2.

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PROBLEM 1.

QUESTION

Using the second quantized formalism show that for non-interacting fermions

$$\Omega_0^F = -k_B T \sum_i \ln \left(1 + e^{-\beta(\epsilon_i - \mu)} \right)$$

where ϵ_i denotes the i -th one-particle level.

SOLUTION

On the lecture using the second quantization we derived, that for non-interacting bosons the grand-canonical potential is

$$\Omega_0^B = k_B T \sum_i \ln \left(1 - e^{-\beta(\epsilon_i - \mu)} \right) \quad (1)$$

We know, that the grand-canonical partition function at fixed T and μ is

$$Z_0 = e^{-\beta \Omega_0^{F,B}} = \text{Tr} \left(e^{-\beta \hat{K}_0} \right) \quad (2)$$

where

$$\hat{K}_0 = \hat{H} - \mu \hat{N} \equiv \sum_{k,s} (\epsilon_k - \mu) a_{k,s}^\dagger a_{k,s} \quad (3)$$

Here, ϵ_k is the 1 particle kinetic energy of the k -th particle and the Hamiltonian $\hat{H} = \sum_{k,s} \epsilon_k a_{k,s}^\dagger a_{k,s}$. We can expand equation (2) in the second quantization in the following way:

$$Z_0 = \sum_{n_1} \sum_{n_2} \dots \left\langle n_1, n_2 \dots \left| e^{-\beta \sum_{k,s} (\epsilon_k - \mu) a_{k,s}^\dagger a_{k,s}} \right| n_1, n_2 \dots \right\rangle \quad (4)$$

The operator inside the sandwich could be expanded into the product

$$e^{-\beta \sum_{k,s} (\epsilon_k - \mu) a_{k,s}^\dagger a_{k,s}} = e^{-\beta(\epsilon_1 - \mu) a_1^\dagger a_1} \cdot e^{-\beta(\epsilon_2 - \mu) a_2^\dagger a_2} \cdot \dots \quad (5)$$

Using this, the equation (4) could be further expanded into another product:

$$Z_0 = \left(\sum_{n_1=0}^{\infty} \left\langle n_1 \left| e^{-\beta(\epsilon_1 - \mu) a_1^\dagger a_1} \right| n_1 \right\rangle \right) \cdot \left(\sum_{n_2=0}^{\infty} \left\langle n_2 \left| e^{-\beta(\epsilon_2 - \mu) a_2^\dagger a_2} \right| n_2 \right\rangle \right) \cdot \dots \quad (6)$$

Since $a_k^\dagger a_k = n_k$, therefore the exponents could be rewritten in the following form:

$$Z_0 = \left(\sum_{n_1=0}^{\infty} \langle n_1 | e^{-\beta(\epsilon_1 - \mu)n_1} | n_1 \rangle \right) \cdot \left(\sum_{n_2=0}^{\infty} \langle n_2 | e^{-\beta(\epsilon_2 - \mu)n_2} | n_2 \rangle \right) \cdot \dots \quad (7)$$

The operators could be multiply out from the sandwiches:

$$\langle n_k | e^{-\beta(\epsilon_k - \mu)n_k} | n_k \rangle = e^{-\beta(\epsilon_k - \mu)n_k} \underbrace{\langle n_k | n_k \rangle}_{=1} \quad (8)$$

Thus equation (7) could be rewritten into the form of a product of sum of exponentials

$$Z_0 = \prod_{k=1}^{\infty} \left(\sum_{n_k=0}^{\infty} e^{-\beta(\epsilon_k - \mu)n_k} \right) . \quad (9)$$

The n_k occupation number can take the following values:

$$n_k = \begin{cases} 0, 1 & \text{for fermions} \\ 0, 1, 2, \dots & \text{for bosons} \end{cases}$$

Since our task is to derive the Ω_0 for fermions, we use the first fermionic case here, $n_k \in \{0, 1\}$. With this, the equation (9) could be rephrased in the following way:

$$Z_0 = \prod_{k=1}^{\infty} \left(\sum_{n_k=0}^1 e^{-\beta(\epsilon_k - \mu)n_k} \right) = \prod_{k=1}^{\infty} \left(e^{-\beta(\epsilon_k - \mu) \cdot 0} + e^{-\beta(\epsilon_k - \mu) \cdot 1} \right) = \prod_{k=1}^{\infty} \left(1 + e^{-\beta(\epsilon_k - \mu)} \right) \quad (10)$$

Substituting back to equation (2), $\Omega_0^{F,B}$ could be expressed with

$$\Omega_0^{F,B} = -\frac{1}{\beta} \ln(Z_0) \quad (11)$$

$$\Omega_0^F = -k_B T \ln \left(\prod_{k=1}^{\infty} \left(1 + e^{-\beta(\epsilon_k - \mu)} \right) \right) = -k_B T \sum_{k=0}^{\infty} \ln \left(1 + e^{-\beta(\epsilon_k - \mu)} \right) \quad (12)$$

Thus we've reached to our goal.

PROBLEM 2.**QUESTION**

Using the result for Ω_0 calculate Ω_0 and N as a function of $(T; V; \mu)$ for a fermionic homogeneous system (non-interacting fermions in a box with periodic boundary conditions). Express your results with Fermi-Dirac integrals. Give the first three terms of the high temperature expansion for Ω_0 and N .

SOLUTION

PROBLEM 3.**QUESTION**

For non-interacting fermions one can define a characteristic temperature T_{deg} by that temperature where the chemical potential is equal to zero:

$$\mu(T = T_{\text{deg}}) = 0. \quad (13)$$

By dimensional analysis

$$k_B T_{\text{deg}} = z \frac{\hbar^2}{2m} \left(\frac{N}{V} \right)^{2/3} \quad (14)$$

where z is a dimensionless number. Calculate this number z exactly and numerically.

SOLUTION

PROBLEM 4.**QUESTION**

Let us suppose that we have N non-interacting, spinless bosons confined in a 3 dimensional harmonic oscillator potential

$$V(\mathbf{r}) = \frac{1}{2}m\omega_1^2x^2 + \frac{1}{2}m\omega_2^2y^2 + \frac{1}{2}m\omega_3^2z^2. \quad (15)$$

Calculate T_c , where the Bose-Einstein condensation occurs.

SOLUTION