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

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

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

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

where

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

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:

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

The operator inside the sandwich could be expanded into the product

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

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

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

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

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

The operators could be multiplied out from the sandwiches:

$$\left\langle n_k \middle| e^{-\beta(\epsilon_k - \mu) n_k} \middle| n_k \right\rangle = e^{-\beta(\epsilon_k - \mu) n_k} \underbrace{\langle n_k \,|\, n_k \rangle}_{=1} \tag{8}$$

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

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

The n_k occupation number can take the following values:

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

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:

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

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

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

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

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, μ) 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

In the previous task, we derived that for free, non-interacting fermions the grand canonical potential is

$$\Omega_0^F\left(T, V, \mu\right) = -k_B T \sum_k \ln\left(1 + e^{-\beta(\epsilon_k - \mu)}\right). \tag{13}$$

The particle number could be expressed using this potential as the following:

$$N = -\left.\frac{\partial \Omega_0^F}{\partial \mu}\right|_{T,V} = k_B T \frac{\partial}{\partial \mu}\left(\sum_k \ln\left(1 + e^{-\beta(\epsilon_k - \mu)}\right)\right) \tag{14}$$

Now we need to express the fermionic grand canonical potential Ω_0^F for enclosed fermions, using Fermi-Dirac integrals.

The Fermi-Dirac integrals could be derived from the distribution of the half-integer spin particles (Weisstein, 1999) and is defined as the following:

$$\mathcal{F}\left(s, \alpha\right) = \frac{1}{\Gamma\left(s\right)} \int_0^\infty \frac{x^{s-1}}{e^{x+\alpha} + 1}\, dx \tag{15}$$

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:

$$\mu\left(T = T_{\text{deg}}\right) = 0.$$

By dimensional analysis

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

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

SOLUTION

At hight temperature the chemical potential is negative, but for lower temperature its sign changes. There will be a certain T_{deg} temperature, where it is zero. It could be concluded (Lee, 1990), that for non-interacting fermions, this characteristic temperature could be expressed as follows:

$$\Gamma\left(1 + D/2\right) \cdot \left(\frac{\mu_0}{k_B T_{\text{deg}}}\right)^{D/2} = \left(1 - 2^{1-D/2}\right)\zeta\left(D/2\right) \tag{16}$$

Where Γ is the gamma function, ζ is the Riemann zeta function, D is the dimension number (here, $D := 3$) and μ_0 is the chemical potential at $T = 0$. For $D = 3$ the above equation could be rephrased in the following way:

$$\Gamma\left(5/2\right) \cdot \left(\frac{\mu_0}{k_B T_{\text{deg}}}\right)^{3/2} = \left(1 - 2^{-1/2}\right)\zeta\left(3/2\right) \tag{17}$$

$$\frac{3\sqrt{\pi}}{4} \cdot \left(\frac{\mu_0}{k_B T_{\text{deg}}}\right)^{3/2} = \left(1 - \frac{1}{\sqrt{2}}\right)\left(\frac{2}{\sqrt{\pi}}\int_0^\infty \frac{\sqrt{t}}{e^t - 1}\,dt\right) \tag{18}$$

$$\left(\frac{\mu_0}{k_B T_{\text{deg}}}\right)^{3/2} = \underbrace{\frac{8}{3\pi}\left(1 - \frac{1}{\sqrt{2}}\right)\left(\int_0^\infty \frac{\sqrt{t}}{e^t - 1}\,dt\right)}_{>0} \tag{19}$$

$$\frac{\mu_0}{k_B T_{\text{deg}}} = \frac{1}{\left(\frac{8}{3\pi}\left(1 - \frac{1}{\sqrt{2}}\right)\left(\int_0^\infty \frac{\sqrt{t}}{e^t-1}\,dt\right)\right)^{2/3}} \tag{20}$$

$$T_{\text{deg}} = \frac{\mu_0}{k_B}\left(\frac{8}{3\pi}\left(1 - \frac{1}{\sqrt{2}}\right)\left(\int_0^\infty \frac{\sqrt{t}}{e^t - 1}\,dt\right)\right)^{2/3} \tag{21}$$

The value of z could be expressed by simple reordering of the equation in the task description:

$$z = \frac{k_B T_{\text{deg}}}{\frac{\hbar^2}{2m}\left(\frac{N}{V}\right)^{2/3}} = \frac{k_B T_{\text{deg}} 2m}{\hbar^2}\left(\frac{N}{V}\right)^{-2/3} \tag{22}$$

Substituting the derived formula for T_{deg}, the k_B factor cancels out:

$$z = \frac{2m\mu_0}{\hbar^2}\left(\frac{8}{3\pi}\left(1 - \frac{1}{\sqrt{2}}\right)\left(\int_0^\infty \frac{\sqrt{t}}{e^t - 1}\,dt\right)\right)^{2/3}\left(\frac{N}{V}\right)^{-2/3} \tag{23}$$

At zero temperature the chemical potential is equals to the Fermi energy (E_F), which could be expressed for non-interacting half-integer spin particles as follows (Glyde, 2014):

$$\mu_0 = E_F = \frac{\hbar^2}{2m}\left(3\pi^2\right)^{2/3}\left(\frac{N}{V}\right)^{2/3} \tag{24}$$

Substituting back to the previous equation, we get the form

$$z = \frac{2m}{\hbar^2} \left(\frac{N}{V} \right)^{-2/3} \cdot \frac{\hbar^2}{2m} \left(3\pi^2\right)^{2/3} \left(\frac{N}{V} \right)^{2/3} \left(\frac{8}{3\pi} \left(1 - \frac{1}{\sqrt{2}} \right) \left(\int_0^\infty \frac{\sqrt{t}}{e^t - 1} \, dt \right) \right)^{2/3} \tag{25}$$

$$z = \left(3\pi^2\right)^{2/3} \left(\frac{8}{3\pi} \left(1 - \frac{1}{\sqrt{2}} \right) \left(\int_0^\infty \frac{\sqrt{t}}{e^t - 1} \, dt \right) \right)^{2/3} \tag{26}$$

Which is an exact value. It could be approximated numerically as

$$z \approx 6.62246... \tag{27}$$

PROBLEM 4.

QUESTION

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

$$V(\boldsymbol{r}) = \frac{1}{2}m\omega_1^2 x^2 + \frac{1}{2}m\omega_2^2 y^2 + \frac{1}{2}m\omega_3^2 z^2. \tag{28}$$

Calculate T_c, where the Bose-Einstein condensation occurs.

SOLUTION

Work in progress...

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