Exam solutions
Statistical Mechanics
15 December 2015, 14:00-16:00

The total score is 20 points!

Problem 1 (2.5 points)

Consider three identical non-interacting fermions in three different energy levels described by the wave functions $\phi_k(\vec{q})$, $\phi_m(\vec{q})$ and $\phi_l(\vec{q})$. Use this to determine the three particle wave function $\Psi(\vec{q}_1, \vec{q}_2, \vec{q}_3)$.

Solution: The wave function of a many body system of non-interacting fermions should be antisymmetric under interchange of the positions of the particles. This leads to the many-body wave function

$$\begin{aligned}\Psi(\vec{q}_1, \vec{q}_2, \vec{q}_3) = c[&\phi_k(\vec{q}_1)\phi_l(\vec{q}_2)\phi_m(\vec{q}_3) + \phi_k(\vec{q}_3)\phi_l(\vec{q}_1)\phi_m(\vec{q}_2) + \phi_k(\vec{q}_2)\phi_l(\vec{q}_3)\phi_m(\vec{q}_1) \\ &- \phi_k(\vec{q}_1)\phi_l(\vec{q}_3)\phi_m(\vec{q}_2) - \phi_k(\vec{q}_3)\phi_l(\vec{q}_2)\phi_m(\vec{q}_1) - \phi_k(\vec{q}_2)\phi_l(\vec{q}_1)\phi_m(\vec{q}_3)]\,,\end{aligned} \tag{1}$$

whee c is a normalization constant. This can be expressed compactly as the following determinant

$$\Psi(\vec{q}_1, \vec{q}_2, \vec{q}_3) = c\begin{vmatrix} \phi_k(\vec{q}_1) & \phi_k(\vec{q}_2) & \phi_k(\vec{q}_3) \\ \phi_l(\vec{q}_1) & \phi_l(\vec{q}_2) & \phi_l(\vec{q}_3) \\ \phi_m(\vec{q}_1) & \phi_m(\vec{q}_2) & \phi_m(\vec{q}_3) \end{vmatrix}\,. \tag{2}$$

If we assume that the single-particle wave functions are properly normalized, i.e.

$$\int |\phi_k(\vec{q})|^2 d\vec{q} = 1\,. \tag{3}$$

and imposing

$$\int |\Psi(\vec{q}_1, \vec{q}_2, \vec{q}_3)|^2 d\vec{q}_1 d\vec{q}_2 d\vec{q}_3 = 1\,, \tag{4}$$

fixes

$$c = \frac{1}{\sqrt{6}}\,. \tag{5}$$

Problem 2 (2.5 points)

Consider a three-dimensional quantum harmonic oscillator with energy levels given by

$$\epsilon = \hbar\omega\left(n_1 + n_2 + n_3 + \frac{3}{2}\right)\,,$$

where $n_{1,2,3} = 0, 1, 2, 3, \ldots$. With this at hand:

1. Calculate the average energy of the system E as a function of the temperature T.
2. Analyze the low and high temperature behavior of E. Show that at high temperatures the system behaves according to the equipartition theorem.

Solution: The three-dimensional quantum harmonic oscillator has energy levels given by

$$\epsilon = \hbar\omega\left(n_1 + n_2 + n_3 + \frac{3}{2}\right), \tag{6}$$

where $n_{1,2,3} = 0, 1, 2, 3, \ldots$.

The partition function is

$$Z = \sum_{n_{1,2,3}=0}^{\infty} e^{-\beta\epsilon} = \left[\sum_{n=0}^{\infty} e^{-\beta\hbar\omega(n+\frac{1}{2})}\right]^3 = \left[e^{-\frac{\beta\hbar\omega}{2}} \sum_{n=0}^{\infty} \left(e^{-\beta\hbar\omega}\right)^n\right]^3$$
$$= \left[\frac{e^{-\frac{\beta\hbar\omega}{2}}}{1 - e^{-\beta\hbar\omega}}\right]^3 = \frac{1}{8\sinh^3(\frac{\beta\hbar\omega}{2})}. \tag{7}$$

where we have used the explicit summation of the geometric series

$$\sum_{n=0}^{\infty} q^n = \frac{1}{1-q}, \qquad 0 < q < 1. \tag{8}$$

The average energy of the system is then

$$E = -\frac{\partial}{\partial\beta}\log(Z) = \frac{3}{2}\hbar\omega\coth\left(\frac{\beta\hbar\omega}{2}\right). \tag{9}$$

At low temperatures we have $\beta \gg 1$ and we can use $\coth(x) \approx 1$ for $x \gg 1$ to find

$$E \approx \frac{3}{2}\hbar\omega(1 + 2e^{-\beta\hbar\omega}). \tag{10}$$

Thus at low temperature the average energy, to leading order, is equal to the energy of the ground state, i.e. $E \approx \epsilon|_{n_1=n_2=n_3=0}$.

At high temperatures we have $\beta \ll 1$ and we can use $\coth(x) \approx \frac{1}{x} + \frac{x}{3}$ for $x \ll 1$ to find

$$E \approx 3k_BT + \frac{\hbar^2\omega^2}{4}\frac{1}{k_BT} + \mathcal{O}(\beta^3)\hbar\omega. \tag{11}$$

Thus at high temperature, and to leading order, we recover the expected result from the equipartition theorem $E = \frac{n}{2}k_BT$ where $n = 6$ is the number of "quadratic" degrees of freedom of the oscillator.

Problem 3 (3 points)

Consider a quantum system with two non-interacting particles which can be each in 4 different quantum states. A ground state with energy 0 and 3 degenerate states with energy ϵ. Calculate the canonical partition functions $Z(T)$ for the case that the two particles are two identical bosons or two identical fermions.

Solution: Let us call the available energy states $(0, 1, 2, 3)$. With the notation (p, q) we will mean that one particle occupies state p and the other state q.

Consider the case of two indistinguishable bosons first. There is one possible configuration, namely $(0, 0)$, for which both particles are in the ground state with energy 0. There are 3 possible configurations, $(0, 1)$, $(0, 2)$ and $(0, 3)$ for which one particle is in the ground state and one in one of the 3 degenerate excited states of energy ϵ. Finally there are 6 possible configurations, $(1, 1)$, $(2, 2)$, $(3, 3)$, $(1, 2)$, $(1, 3)$, and $(2, 3)$, for which both particles are in an excited state. Thus the total partition functions is

$$Z_B = 1 + 3e^{-\beta\epsilon} + 6e^{-2\beta\epsilon} , \tag{12}$$

where $\beta \equiv k_B T$.

Now let us study the fermionic system. The particles are again indistinguishable. Due to the Pauli exclusion principle there cannot be two fermions occupying the same quantum state. Thus there are 3 configurations with one particle in the ground state and one in an excited state: $(0, 1)$, $(0, 2)$ and $(0, 3)$. There are also 3 configurations with two particles in excited states: $(1, 2)$, $(1, 3)$, and $(2, 3)$. Therefore the partition function is

$$Z_F = 3e^{-\beta\epsilon} + 3e^{-2\beta\epsilon} . \tag{13}$$

Problem 4 (4 points)

Atoms in a solid vibrate about their respective equilibrium positions with small amplitudes. Debye approximated the normal vibrations with the elastic vibrations of an isotropic continuous body and assumed that the number of vibrational modes $g(\omega)d\omega$, having angular frequencies between ω and $\omega + d\omega$, is given by

$$\begin{aligned} g(\omega) &= \frac{V}{2\pi^2}\left(\frac{1}{c_L^3} + \frac{2}{c_T^3}\right)\omega^2 \equiv \frac{9N}{\omega_D^3}\omega^2 , \qquad && \omega \leq \omega_D , \\ g(\omega) &= 0 , \qquad \omega > \omega_D , \end{aligned}$$

where c_L and c_T denote the velocities of longitudinal and transversal waves, respectively. The Debye frequency ω_D is determined by

$$\int_0^{\omega_D} g(\omega)d\omega = 3N .$$

where N is the number of atoms and hence $3N$ is the number of degrees of freedom. Use this to

1. Calculate the specific heat at constant volume for this model.
2. Examine its temperature dependence at high as well as low temperatures.

Solution: Using the Bose distribution and the density of states proposed by Debye we find that the average energy is

$$E = \int_0^\infty \frac{\hbar\omega g(\omega)}{e^{\beta\hbar\omega} - 1} d\omega = \frac{9N}{\omega_D^3} \int_0^{\omega_D} \frac{\hbar\omega^3}{e^{\beta\hbar\omega} - 1} d\omega . \tag{14}$$

Now we use that the specific heat at constant volume is $c_V = \frac{\partial E}{\partial T}$ to find

$$c_V = 9k_B N \left(\frac{T}{T_D}\right)^3 \int_0^{T_D/T} \frac{x^4 e^x}{(e^x - 1)^2} dx . \tag{15}$$

Here we have defined the Debye temperature $T_D \equiv \frac{\hbar\omega_D}{k_B}$.

At temperatures much higher than T_D we have that $T_D/T \ll 1$ and thus we can approximate the integral as (we have used $e^x \approx 1 + x$ for $|x| \ll 1$)

$$c_V \approx 9k_B N \left(\frac{T}{T_D}\right)^3 \int_0^{T_D/T} x^2 dx = 3k_B N\,. \tag{16}$$

At temperatures much lower than T_D we have that $T_D/T \gg 1$ and we find

$$c_V \approx 9k_B N \left(\frac{T}{T_D}\right)^3 \int_0^{\infty} \frac{x^4 e^x}{(e^x-1)^2} dx = \frac{12\pi^4}{5} k_B N \left(\frac{T}{T_D}\right)^3 . \tag{17}$$

Here we have used the relation

$$\int_0^{\infty} \frac{x^4 e^x}{(e^x-1)^2} dx = \frac{4\pi^4}{15} . \tag{18}$$

Problem 5 (8 points)

What is the pressure of a gas of free bosons in the limit of vanishing temperature, $T \to 0$? Argue that for $T \to 0$ an ideal Fermi gas will have non-vanishing pressure $p_0 > 0$. We will now use this fact to study a system of two ideal Fermi gases in three dimensions.

A free sliding piston separates two compartments labeled 1 and 2 with volumes V_1 and V_2 respectively. An ideal Fermi gas with N_1 particles with spin 1/2 is placed in compartment 1 and an ideal Fermi gas with N_2 particles with spin 3/2 is placed in compartment 2.

1. Find the density of states $g_{1/2}(\epsilon)$ and $g_{3/2}(\epsilon)$ of the two gases.[1]

2. Find the pressure of the two gases as a function of their densities N_1/V_1 and N_2/V_2 in the limit $T \to 0$.

3. Find the relative densities of the two gases at mechanical equilibrium in the limit $T \to 0$.

4. What are the equilibrium densities in the classical limit $T \to \infty$?

Solution: We use that the pressure for a gas of non-interacting bosons/fermions is given by

$$\frac{pV}{k_B T} = \log \Xi = \mp \sum_\gamma \log\left(1 \mp e^{\beta(\mu-\epsilon_\gamma)}\right) , \tag{19}$$

where the upper sign is for bosons and the lower sign is for fermions. For bosons we have that the chemical potential is bounded above $\mu \le \min_\gamma \epsilon_\gamma$ and thus at low temperatures, $\beta \to \infty$, we have $\log\left(1 \mp e^{\beta(\mu-\epsilon_\gamma)}\right) \to 0$ and thus the pressure of the free boson gas vanishes. In the case of fermions we can use a continuous approximation to write

$$\lim_{\beta\to\infty} p = \frac{1}{V}\int_0^{\epsilon_F} d\epsilon g(\epsilon)(\epsilon_F - \epsilon) = p_0 > 0\,, \tag{20}$$

where ϵ_F is the Fermi energy.

[1]Hint: A particle of spin s has $2s+1$ possible spin orientations.

We can use that for free particles we have $\epsilon = \frac{|p|^2}{2m}$ and that for free particles in a box we have $\vec{p} = \frac{h}{L}\vec{n}$ where $\vec{n} = \{n_1, n_2, n_3\}$ is a vector of integers to find that that the density of states for a spin s particle is

$$(2s+1)\frac{V}{h^3}4\pi p^2 dp = (2s+1)\frac{4\pi V}{h^3}m^{3/2}\sqrt{2\epsilon}d\epsilon \equiv g_s(\epsilon)d\epsilon\,. \tag{21}$$

the particle density for $\beta \gg 1$ is given approximately by

$$\frac{N}{V} = \frac{1}{V}\int_0^\infty d\epsilon \frac{g(\epsilon)}{e^{\beta(\epsilon-\mu)}+1} \approx \int_0^{\epsilon_F} d\epsilon g(\epsilon)\,. \tag{22}$$

Thus for a particle of spin s one finds

$$\frac{N}{V} = (2s+1)\frac{8\sqrt{2}\pi m^{3/2}}{3h^3}\epsilon_F^{3/2}\,. \tag{23}$$

We can now use (20), (21) and (23) to find the pressure at zero temperature

$$p_0 = \frac{2}{5}\left((2s+1)\frac{8\sqrt{2}\pi m^{3/2}}{3h^3}\right)^{2/3}\left(\frac{N}{V}\right)^{5/3}\,. \tag{24}$$

For the problem at hand we find

$$\begin{aligned} p_0 &= \frac{2}{5}\left(\frac{16\sqrt{2}\pi m_1^{3/2}}{3h^3}\right)^{2/3}\left(\frac{N_1}{V_1}\right)^{5/3}\,, \qquad & s = \frac{1}{2}\,, \\ p_0 &= \frac{2}{5}\left(\frac{32\sqrt{2}\pi m_2^{3/2}}{3h^3}\right)^{2/3}\left(\frac{N_2}{V_2}\right)^{5/3}\,, \qquad & s = \frac{3}{2}\,. \end{aligned} \tag{25}$$

At mechanical equilibrium we have that the pressure of the two gases is the same and thus for the relative density we find

$$\frac{N_1/V_1}{N_2/V_2} \approx 2^{2/5}\left(\frac{m_2}{m_1}\right)^{3/5}\,. \tag{26}$$

At high temperatures we have $\beta \ll 1$ and we can use the classical ideal gas approximation to find

$$p_1 \approx k_B T\frac{N_1}{V_1}\,, \qquad p_2 \approx k_B T\frac{N_2}{V_2}\,, \tag{27}$$

and thus at mechanical equilibrium, i.e. $p_1 = p_2$, we have

$$\frac{N_1/V_1}{N_2/V_2} \approx 1\,. \tag{28}$$