QUALIFYING EXAMINATION, Part 4

Solutions

Problem 1: Statistical Mechanics I

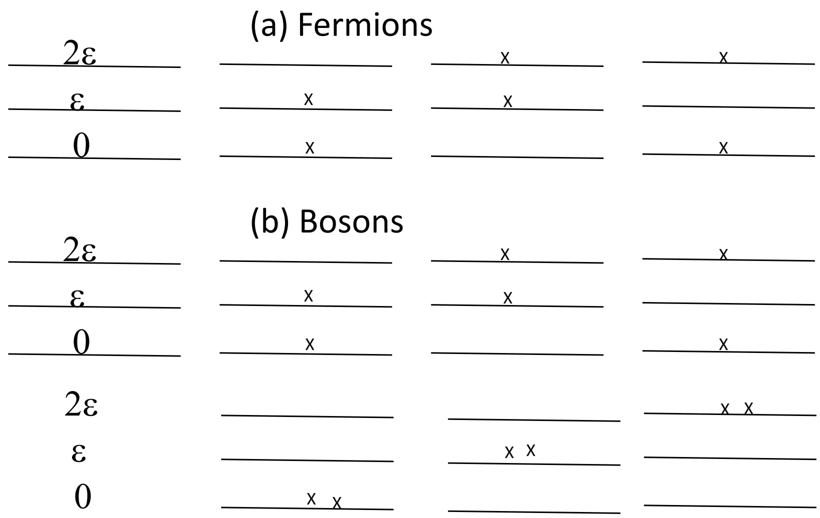


Figure 1: (a) 3 configurations for 2 fermions, (b) 6 configurations for 2 bosons.

(a) See Fig. 1(a).

(b) See Fig. 1(b).

(c) The canonical partition function for 2 fermions in 3 single-particle levels $0, \varepsilon, 2\varepsilon$ is given by

$$Z = e^{-\beta\varepsilon} + e^{-3\beta\varepsilon} + e^{-2\beta\varepsilon} ,$$

and the average energy is

$$\langle E \rangle = -\frac{d \ln Z}{d\beta} = \frac{\varepsilon e^{-\beta\varepsilon} + 3\varepsilon e^{-3\beta\varepsilon} + 2\varepsilon e^{-2\beta\varepsilon}}{Z} .$$

(d) The canonical partition function for 2 bosons in 3 single-particle levels $0, \varepsilon, 2\varepsilon$ is

$$Z = e^{-\beta\varepsilon} + e^{-3\beta\varepsilon} + e^{-2\beta\varepsilon} + 1 + e^{-2\beta\varepsilon} + e^{-4\beta\varepsilon} ,$$

and the average energy is

$$\langle E \rangle = -\frac{d \ln Z}{d\beta} = \frac{\varepsilon e^{-\beta\varepsilon} + 3\varepsilon e^{-3\beta\varepsilon} + 2\varepsilon e^{-2\beta\varepsilon} + 0 + 2\varepsilon e^{-2\beta\varepsilon} + 4\varepsilon e^{-4\beta\varepsilon}}{Z} .$$

(e) For non-interacting fermions, the explicit form of the grand-canonical partition function in Eq. (1) is

$$Z(\mu,\beta) = 1(N=0)+e^{\beta\mu}(1+e^{-\beta\varepsilon}+e^{-2\beta\varepsilon})(N=1)+e^{2\beta\mu}(e^{-\beta\varepsilon}+e^{-2\beta\varepsilon}+e^{-3\beta\varepsilon})(N=2)+e^{3\beta\mu}e^{-3\beta\varepsilon}(N=3)\ .$$

Treating each of the 3 levels as an independent system of fermions, the partition function is a product of the partition functions of each of the 3 levels. A single level can have an occupation of $n=0$ or $n=1$. We find

$$Z(\mu,\beta) = (1+e^{\beta\mu}) \times (1+e^{\beta(\mu-\varepsilon)}) \times (1+e^{\beta(\mu-2\varepsilon)})\ .$$

Opening the parentheses in this equation, we recover the explicit form of Eq. (1) above.

(f) For bosons each level can have occupations of $n = 0,1,2,\ldots$. For the level with energy ε, we find a partition function of

$$\sum_{n=0}^{\infty} e^{n\beta(\mu-\varepsilon)} = (1-e^{\beta(\mu-\varepsilon)})^{-1}\ ,$$

where the geometric series $\sum_{n=0}^{\infty}[e^{\beta(\mu-\varepsilon)}]^n$ has been summed.

For the 3 level system we find

$$Z(\mu,\beta) = (1-e^{\beta\mu})^{-1} \times (1-e^{\beta(\mu-\varepsilon)})^{-1} \times (1-e^{\beta(\mu-2\varepsilon)})^{-1}\ .$$

Problem 2: Statistical Mechanics II

(a) Using the boundary conditions that the single-particle wave function vanishes on the sides of the cubic box, each state has a volume $(\pi/L)^3$ in momentum space. The states with energy below $\epsilon = \hbar^2k^2/2m$ occupy a sphere of radius k in momentum space whose volume is $\frac{1}{8}\frac{4}{3}\pi k^3$ (the factor of 1/8 is to count only states with positive k_i). We thus find that the number of states with energy less than ϵ is $N_\epsilon = \frac{L^3}{6\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\epsilon^{3/2}$. Then $\mathcal{D} = \mathrm{d}N_\epsilon/\mathrm{d}\epsilon$ and we find the given result.

The density of states $\mathcal{D}(\epsilon)$ can also be calculated directly from the density of states in momentum space $\mathcal{D}(\vec{k}) = (L/\pi)^3$

$$\frac{1}{8}\left(\frac{L}{\pi}\right)^3 d^3\vec{k} = \frac{1}{8}\left(\frac{L}{\pi}\right)^3 4\pi k^2 dk = \frac{L^3}{2\pi^2}k^2\frac{dk}{d\epsilon}d\epsilon = C\sqrt{\epsilon}\,d\epsilon\ ,$$

where we have used $\epsilon = \hbar^2k^2/(2m)$ and $d\epsilon = (\hbar^2/m)k\,dk$.

(b) In the grand-canonical ensemble, the independent variables are $(\mu_{\mathrm{B}}, \mu_{\mathrm{F}}, T)$. In principle, the volume V is also one of the independent variables but here we consider it to be constant $V = L^3$.

The proper potential is the grand (or Landau) potential given by

$$\Omega = U - TS - \mu_{\mathrm{B}} N_{\mathrm{B}} - \mu_{\mathrm{F}} N_{\mathrm{F}} \; .$$

(c) The average number of bosons N_B is given by

$$N_{\mathrm{B}} = -\left(\frac{\partial \Omega}{\partial \mu_{\mathrm{B}}}\right)_{T,\mu_{\mathrm{F}},V} \; .$$

The equation for N_{F} is obtained by swapping the subscripts F and B in the above equation.

(d) Since the bosonic and fermionic subparts are noninteracting, they can be treated independently (at the same temperature T) and the total partition function is

$$Z = Z_{\mathrm{F}}(\mu_{\mathrm{F}}, T) Z_{\mathrm{B}}(\mu_{\mathrm{B}}, T) \; .$$

The grand potential $\Omega = -kT \ln Z$ can thus be written as the sum of the grand potentials for the Bose and Fermi gases

$$\Omega = \Omega_{\mathrm{B}} + \Omega_{\mathrm{F}} \; .$$

Using the explicit expression for Z_{B} given in the useful formulas, and converting the sum over single-particle states to an integral, we have

$$\ln Z_{\mathrm{B}} = -\int_0^\infty \mathcal{D}(\epsilon) \ln[1 - e^{-\beta(\epsilon - \mu_{\mathrm{B}})}] \, d\epsilon \; .$$

Using the formula for N_{B} in part (c) with $\Omega \to \Omega_{\mathrm{B}}$ and $\Omega_{\mathrm{B}} = -kT \ln Z_{\mathrm{B}}$, we find

$$N_{\mathrm{B}} = \int_0^\infty \frac{\mathcal{D}(\epsilon)}{e^{\beta(\epsilon - \mu_{\mathrm{B}})} - 1} \mathrm{d}\epsilon \; .$$

Carrying out a similar calculation for the fermions, we find

$$N_{\mathrm{F}} = \int_0^\infty \frac{\mathcal{D}(\epsilon)}{e^{\beta(\epsilon - \mu_{\mathrm{F}})} + 1} \mathrm{d}\epsilon \; .$$

(e) The energy U is given by $U = -\partial \ln Z / \partial \beta$. Following a similar method to the calculation in (d), we find

$$U = U_{\mathrm{B}} + U_{\mathrm{F}} = \int_0^\infty \mathcal{D}(\epsilon) \epsilon \left(\frac{1}{e^{\beta(\epsilon - \mu_{\mathrm{F}})} - 1} + \frac{1}{e^{\beta(\epsilon - \mu_{\mathrm{B}})} + 1} \right) \mathrm{d}\epsilon \; .$$

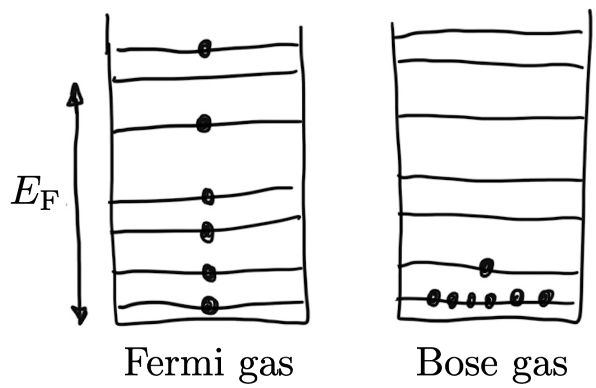
(f) At $T = 0$, the Fermi-Dirac distribution is a step function at $\mu(T = 0) = \epsilon_F$. At $T = 0$, all bosons occupy the ground state of a single particle in the box of zero energy. Thus

$$U = \frac{3}{5} N_F \epsilon_F \ ,$$

where $\epsilon_F = C^{-2/3}(3/2)^{2/3}(N_F/L^3)^{2/3} = \frac{\hbar^2}{2m}(6\pi^2 n_F)^{2/3}$ and $n_F = N_F/L^3$.

The state of the system is a mixture of a Fermi sea (filled up to energy $\mu_F = \epsilon_F$) and a pure Bose-Einstein condensate (with $\mu_B = 0$).

(g) At a very low temperature, only the lowest excited many-particle states contribute (in addition to the ground state). Such excited states are sketched in the figure for both the Bose and Fermi gases.



(energy levels not to scale)