PHYS3020 Module 3 Problem Set

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Q1

Allowed occupancies are 0, 1, and 2, with energies 0, E, and 2E

Hence,

$$\mathcal{Z} = \sum_s e^{-(E(s)-\mu N(s))/kT}$$

$$= e^{(-0-\mu\cdot 0)/kT} + e^{-(E-\mu\cdot 1)/kT} + e^{-(2E-\mu\cdot 2)/kT}$$

$$= 1 + e^{-(E-\mu)/kT} + e^{-2(E-\mu)/kT}$$

$$= 1 + e^{-(E-\mu)/kT} + \left(e^{-(E-\mu)/kT}\right)^2$$

The average occupancy is given by

$$\langle N \rangle = \sum_n n\,P(n)$$

where $P(n) = \frac{1}{\mathcal{Z}} e^{-(E(n)-\mu N(n))/kT}$

So,

$$\langle N \rangle = 0\cdot P(0) + 1\cdot P(1) + 2\cdot P(2)$$

$$= \frac{1}{\mathcal{Z}}\left(e^{-(E-\mu)/kT} + 2e^{-(2E-2\mu)/kT}\right)$$

$$= \frac{e^{-(E-\mu)/kT} + 2e^{-2(E-\mu)/kT}}{1 + e^{-(E-\mu)/kT} + e^{-2(E-\mu)/kT}}$$

$$= \frac{1 + 2e^{-(E-\mu)/kT}}{e^{(E-\mu)/kT} + 1 + e^{-(E-\mu)/kT}}$$

This is considering a "system" consisting of two single-particle states in contact with a reservoir with temperature T and chemical potential μ.

Q2

- May be unoccupied, or occupied by one particle in one of two states of energy 0 or E.

a. The Gibbs sum is given by

$$\mathcal{Z} = \sum_s e^{-(E(s)-\mu N(s))/k_BT}$$

$$= e^{-(0-0)/k_BT} + e^{-(0-\mu\cdot 1)/k_BT} + e^{-(E-\mu\cdot 1)/k_BT}$$

$$= 1 + e^{\mu/k_BT} + e^{(\mu-E)/k_BT}$$

This assumes just one particle which can only occupy one state.

b. The thermal average occupancy of the system is given by

$$\langle N \rangle = \sum_n n\,P(n)$$

$$\frac{1}{\ \ }\left(\ldots e^{-(E(n)-\mu\cdot n)/k_BT}\right)$$

by
$$\langle N\rangle = \sum_n n P(n)$$
$$= \frac{1}{\mathcal{Z}}\left(\sum_n n e^{-(E(n)-\mu\cdot n)/k_BT}\right)$$
$$= \frac{1}{\mathcal{Z}}\left(0 + 1\cdot e^{-(0-\mu\cdot 1)/k_BT} + 1\cdot e^{-(E-\mu\cdot 1)/k_BT}\right)$$
$$= \frac{e^{\mu/k_BT} + e^{(\mu-E)/k_BT}}{\mathcal{Z}}$$
as required.

c. The thermal average occupancy of the state of energy E is given by
$$\langle N(E)\rangle = n P(n)$$
$$= 1\cdot \frac{1}{\mathcal{Z}} e^{-(E-\mu\cdot 1)/k_BT}$$
$$= \frac{e^{(\mu-E)/k_BT}}{\mathcal{Z}}$$
as required.

d. We'd expect that the thermal average energy of the system is the sum of the thermal average occupancy multiplied by the energy of each state:
$$\langle U\rangle = \sum_s E(s)\langle N(s)\rangle$$
Since only the occupied second state has energy, the the thermal average energy of this system will be
$$\langle U\rangle = E\cdot\langle N(E)\rangle$$
$$= \frac{E e^{(\mu-E)/k_BT}}{\mathcal{Z}}$$

e. For the state where the first and second orbitals are occupied simultaneously, we'll have energy
$$E_{tot} = E_1 + E_2 = 0 + E = E$$
and $N=2$ due to a total of two particles.
So,
$$\mathcal{Z} = \sum_s e^{-(E(s)-\mu N(s))/k_BT}$$
$$= e^{-(0-0)/k_BT} + e^{-(0-\mu\cdot 1)/k_BT} + e^{-(E-\mu\cdot 1)/k_BT} + e^{-(E-\mu\cdot 2)/k_BT}$$
$$= 1 + e^{\mu/k_BT} + e^{(\mu-E)/k_BT} + e^{(2\mu-E)/k_BT}$$
let $a = e^{\mu/k_BT}$ and $b = e^{(\mu-E)/k_BT}$
$$\Rightarrow \mathcal{Z} = 1 + a + b + ab$$
$$= (1+a)(1+b)$$
$$\Rightarrow \mathcal{Z} = (1+e^{\mu/k_BT})(1+e^{(\mu-E)/k_BT})$$
as required.