Homework I

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1.6-1. Find a the most probable distribution P_n such that,

$$\begin{aligned}\sum_n P_n &= N\\ \sum_n nP_n &= Nn_a\\ \sum_n n^2 P_n &= Nn_d^2\end{aligned}$$

Here the most probable distribution is defined as the distribution P_n of which the following quantity

$$\begin{aligned}\ln\Omega\{P_n\} &= \text{In } N_p! - \sum_n \text{In } P_n!\\ &= \text{In } N_p! - \sum_n P_n \text{In } P_n + P_n\end{aligned}$$

is maximized.

Solve:

Using the Langrari Mulitlier

$$S(\alpha,\beta,\gamma,\{P_n\}) = \text{In }\Omega\{P_n\} - \alpha\left(\sum_n P_n - N\right) - \beta\left(\sum_n nP_n - Nn_a\right) - \gamma\left(\sum_n n^2 P_n - Nn_d^2\right)$$

$$\frac{\delta S}{\delta P_n} = -\text{In } P_n - \alpha - n\beta - n^2\gamma = 0$$

$$P_n = e^{-\alpha - n\beta - n^2\gamma}$$

Then apply P_n to the distribution properity,

$$P_n = \frac{1}{\sqrt{2\pi(n_d^2 - n_a^2)}} e^{-\frac{(n-n_a)^2}{2(n_d^2 - n_a^2)}}$$

$$P_n = \frac{N}{\sqrt{2\pi(n_d^2 - n_a^2)}} e^{-\frac{(n-n_a)^2}{2(n_d^2 - n_a^2)}}$$

1.6-2. For a ideal gas with distribution

$$P(v) = \prod_{i=1}^{3} \sqrt{\frac{m}{2\pi\kappa_B T}} e - \frac{m(v_i - \bar{v}_i)^2}{2k_B T}$$

Please find out the state equation

Solve:

energy may not equated in each direction

We known

$$\begin{aligned} P &= \frac{F}{A} = \\ P &= \frac{N}{V}\frac{1}{3}m\,\bar{v^2} \end{aligned}$$

Then, get the $\bar{v^2}$ from distribution.

$$\begin{aligned} <mv_i> &= m\bar{v_i} \\ <mv_i^2> &= \kappa_B T + <mv_i> \\ &= \kappa_B T + m\bar{v_i} \\ <mv^2> &= 3\kappa_B T + 3m\,\bar{v} \end{aligned}$$

Finally,

$$\begin{aligned} P &= \frac{N}{V}\frac{1}{3}m\,\bar{v^2} \\ &= \frac{N}{V}\frac{1}{3}(3\kappa_B T + 3m\,\bar{v}) \\ &= \frac{N}{V}\kappa_B T + \frac{N}{V}m\,\bar{v} \\ \Longrightarrow PV &= N\,(k_B T + m\,\bar{v}) \end{aligned}$$

2.6-2. Find a the most probable distribution $P(x)$ such that,

$$\begin{aligned} \int P(x) &= 1 \\ <x> &= \int P(x)x\,dx = \mu \\ <x^2> - <x>^2 &= \int P(x)x^2dx - \left(\int P(x)x\,dx\right)^2 = \sigma^2 \end{aligned}$$

Here the most distribution is defined as the distribution $P(x)$ of which the entropy

$$S = -\int P(x)\mathrm{InP}(x)dx$$

is maximized. Compared the result with the problem 1 of chapter 1. What do you find?

Solve:

Using the priciple of maximum entropy

$$\begin{aligned} \frac{\delta}{\delta P(x)}\left(S - \alpha\left(\int P(x) - 1\right) - \beta\left(\int P(x)x\,dx - \mu\right) - \gamma\left(\int P(x)x^2dx - \sigma^2 - \mu^2\right)\right) &= 0 \\ -\int(\mathrm{In}\,P(x) + 1)dx - \alpha\int 1dx - \beta\int x\,dx - \gamma\int x^2dx &= 0 \\ -\int 1dx - \alpha\int 1dx - \beta\int x\,dx - \gamma\int x^2dx &= \int \mathrm{In}\,P(x)\,dx \\ -\int(1 + \alpha + \beta x + \gamma x^2)dx &= \int \mathrm{In}\,P(x)dx \\ -1 - \alpha - \beta x - \gamma x^2 &= \mathrm{In}\,P(x) \\ e^{-1-\alpha-\beta x-\gamma x^2} &= P(x) \end{aligned}$$

using the constrain to determine α, β, γ

$$P(x)=\frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

This problem get more a normalize factor than problem 1 of chapter 1.

2.6-3. For different $N=1,10,100,1000$, numerically calculate the following fucntions,

$$\sum_{n=1}^{100}\exp[N/n^2]$$

Compared it with the function $\exp[N]$ (then $n=1$ term, the largest term, in the above function), what do you find?

Solve:

N	1	10	100	1000
$\sum_{n=1}^{100}\exp[N/n^2]$	102.397	22141.87	2.688exp(43)	1.97exp(434)
$\exp[N]$	2.718	22026.46	2.688exp(43)	1.97exp(434)

The larger N, the closer $\exp[N]$ and $\sum_{n=1}^{100}\exp[N/n^2]$. It is a example of rule of large number

2.6-4. The probability for observing a closed thermally equilibrate system with given energy E is in forms of

$$P(E)=C\Omega(E)\exp(-\beta E)$$

where C is the normalization constant and $\Omega(E)$ is the number of microsates with enery E. Both $\text{In}\Omega(E)$ and E are of the order of the particle number N.

1). Using the steepest descent method to verify that $P(E)$ is a very narrow distribution centered on the most probable value of E(denoted as E_0).

2). Use the expansion to estimated the probability for observing a spontaneous fluctuation in E of the order of $10^{-6}E_0$ for 1 *moles* of gas. (Hint: Expanding $\text{InP}(E)$ in powers of $\delta E=E-E_0$. Formular $S(E)=\kappa_B\text{In}\Omega(E)$, $\partial E/\partial S=T$, $\partial E/\partial T=C_v$, $E_0=3N\kappa_B T/2$ and $C_v=3N\kappa_B/2$ are needed in this calculation.

Solve:

1). Try to calculate the mean and variance to show $P(E)$ is narraow distribution.

$$\begin{aligned}\int EP(E)\,dE &= \int EC\Omega(E)\exp(-\beta E)dE\\ &= C\int \exp(\ln\Omega(E)+\text{In}\,E-\beta E)dE\\ &\cong\end{aligned}$$

$$\begin{aligned}\int E^2\,P(E)dE &= \int E^2C\Omega(E)\exp(-\beta E)dE\\ &= C\int \exp(\text{In}\,\Omega(E)+2\text{In}\,E-\beta E)dE\\ &=\end{aligned}$$

设 E_0 是极大值，将 $\text{In}(P)$ 在 E_0 处展开，

$$\text{In}\,P(E) = \text{In}\,P(E_0) - (E-E_0)\frac{\partial \text{In}\,P(E)}{\partial E}|_{E_0} + \frac{1}{2}(E-E_0)^2\frac{\partial^2 \text{In}\,P(E)}{\partial E^2}|_{E_0}$$
$$\text{In}\,P(E) = \text{In}\,P(E_0) + \frac{1}{2}\delta E^2\frac{\partial^2 \text{In}\,P(E)}{\partial E^2}|_{E_0}$$
$$\begin{aligned}
\frac{\partial \text{In}\,P(E)}{\partial E} &= \frac{\partial(C\Omega(E)\exp(-\beta E))}{\partial E} = C\frac{\partial(\exp(-\beta E + \text{In}\,\Omega(E)))}{\partial E} \\
&= C\left(-\beta + \frac{\partial \text{In}\,\Omega(E)}{\partial E}\right)\exp(-\beta E + \text{In}\,\Omega(E)) \\
\frac{\partial^2 \text{In}\,P(E)}{\partial E^2} &= C\left(\frac{\partial^2 \text{In}\,\Omega(E)}{\partial E^2}\right)\exp(-\beta E + \text{In}\,\Omega(E)) + C\left(-\beta + \frac{\partial \text{In}\,\Omega(E)}{\partial E}\right)^2\exp(-\beta E + \text{In}\,\Omega(E)) \\
&= C\left(\frac{\partial^2 \text{In}\,\Omega(E)}{\partial E^2} + \left(-\beta + \frac{\partial \text{In}\,\Omega(E)}{\partial E}\right)^2\right)\exp(-\beta E + \text{In}\,\Omega(E)) \\
&= ??? \\
&= \frac{1}{\kappa_B}\frac{\partial}{\partial E}\left(\frac{1}{T}\right) = \frac{-1}{\kappa_B T^2}\frac{\partial T}{\partial E} = \frac{-2}{\kappa_B T^2\,3N\kappa_B} = \frac{-2}{3\kappa_B^2 T^2} \\
\Rightarrow & \\
\text{In}\,P(E) &= \text{In}\,P(E_0) + \delta E^2\frac{1}{2}\frac{-2}{3\kappa_B^2T^2} = \text{In}\,P(E_0) - \delta E^2\frac{1}{3\kappa_B^2T^2} \\
P(E) &= P(E_0)e^{-\frac{\delta E^2}{3\kappa_B^2T^2}} = P(E_0)e^{-\frac{(E-E_0)^2}{3\kappa_B{}^2T^2}}
\end{aligned}$$

2).

$$\int_0^{10^{-6}E_0} P(E)dE =$$

$$\delta E = 10^{-6}E_0$$
$$\frac{P(E)}{P(E_0)} = e^{-\frac{10^{-6}E_0}{3\kappa_B^2T^2}} = ??? = \frac{1}{e^{10^9}}$$