Assignment 1: Question 1

Saturday, 13 May 2023 3:46 pm

(1) Consider a system of N free particles in which the energy of each particle can assume only two values, 0 and E. ($E>0$) The occupation numbers for the two states are denoted n_0 and n_1 respectively. The total energy of the system is U.

a. Find the entropy of the system.

Solution:

$n_0 =$ No. of particles with energy $E=0$
$n_1 =$ No. of pcles with energy E

Total energy of system $= n_1 E = U$

· Also have the constraint that $n_0 + n_1 = N$

∴ Number of ways of assigning N pcles into state n_0 or n_1:

$$\binom{N}{n_1} = \frac{N!}{n_0!\, n_1!} = \frac{N!}{n_1!\,(N-n_1)!} \quad (\text{where } n_1 E = U)$$

$$\therefore \frac{N!}{n_1!\,(N-n_1)!} = \frac{N!}{\left(\frac{U}{E}\right)!\left(N-\frac{U}{E}\right)!} \quad (\text{by the constraint } n_1 E = U)$$

$$\therefore \Omega(N) = \sum_{n_1=0}^{N} \frac{N!}{\left(\frac{U}{E}\right)!\left(N-\frac{U}{E}\right)!} = \sum_{n_1=0}^{N} t(n_1)$$

$$\therefore \ln(t_n) = \ln\left[\frac{N!}{(U/E)!\left(N-\frac{U}{E}\right)!}\right]$$

$$= \underset{①}{\ln(N!)} - \underset{②}{\ln\left(\left(\frac{U}{E}\right)!\right)} - \underset{③}{\ln\left(\left(N-\frac{U}{E}\right)!\right)}$$

Exploit Stirling's approximation for each of the above terms:

① $\ln(N!) \approx N\ln(N) - N + O(\ln(N))$

② $\ln\left(\left(\frac{U}{E}\right)!\right) = \frac{U}{E}\ln\left(\frac{U}{E}\right) - \frac{U}{E} + O\left(\ln\left(\frac{U}{E}\right)\right)$

③ $\ln\left(\left(N-\frac{U}{E}\right)!\right) = \left(N-\frac{U}{E}\right)\ln\left(N-\frac{U}{E}\right) - \left(N-\frac{U}{E}\right) + O\left(\ln\left(N-\frac{U}{E}\right)\right)$

① − ② − ③

$$= [N\ln(N) - N + O(\ln(N))] - \left[\frac{U}{E}\ln\left(\frac{U}{E}\right) - \frac{U}{E} + O\left(\ln\left(\frac{U}{E}\right)\right)\right] - \left[\left(N-\frac{U}{E}\right)\ln\left(\left(N-\frac{U}{E}\right)\right) - \left(N-\frac{U}{E}\right) + O\left(\ln\left(N-\frac{U}{E}\right)\right)\right]$$

$$= \left[N\ln(N) - N + O(\ln(N)) - \frac{U}{E}\ln\left(\frac{U}{E}\right) + \frac{U}{E} - O\left(\ln\left(\frac{U}{E}\right)\right) - \left(N-\frac{U}{E}\right)\ln\left(\left(N-\frac{U}{E}\right)\right) + N + \frac{U}{E} + O\left(\ln\left(N-\frac{U}{E}\right)\right)\right]$$

Neglect higher order terms:

$$= N\ln(N) - \cancel{N} - \frac{U}{E}\ln\left(\frac{U}{E}\right) + \cancel{\frac{U}{E}} - \left(N-\frac{U}{E}\right)\ln\left(\left(N-\frac{U}{E}\right)\right) + \cancel{N} - \cancel{\frac{U}{E}}$$

$$N\ln(N) - \frac{U}{E}\ln\left(\frac{U}{E}\right) - \left(N-\frac{U}{E}\right)\ln\left(\left(N-\frac{U}{E}\right)\right) = \ln(\Omega(N))$$

$$= N\ln(N) - \frac{U}{E}\ln\left(\frac{U}{E}\right) - N\ln\left(\left(N-\frac{U}{E}\right)\right) + \frac{U}{E}\ln\left(\left(N-\frac{U}{E}\right)\right)$$

$$= N\ln\left(\frac{N}{N-\frac{U}{E}}\right) + \frac{U}{E}\ln\left(\left[\frac{N-U/E}{U/E}\right]\right)$$

$$\therefore S = k_B\ln(\Omega) = k_B\left[N\ln\left(\frac{N}{N-\frac{U}{E}}\right) + \frac{U}{E}\ln\left(\frac{N-U/E}{U/E}\right)\right]$$

b Find the most probable values of n_0 and n_1. Calculate the mean square fluctuations in these quantities

Solution:

· Most probable value of n_1 can be determined by setting:

$$\frac{d(\ln(t(n_1)))}{dn_1} = 0$$

$$\therefore \ln(t(n_1)) = N\ln\left(\frac{N}{N-n_1}\right) + n_1\ln\left(\frac{N-n_1}{n_1}\right)$$

$$= N\ln\left(\frac{N}{N-n_1}\right) + n_1\ln\left(\frac{N}{n_1} - 1\right)$$

$$\therefore \frac{d(\ln(t(n_1)))}{dn_1} = \frac{N}{N-n_1} + \ln\left(\frac{N}{n_1} - 1\right) - \frac{N\,n_1}{n_1(N-n_1)}$$

$$= \frac{N}{N-n_1} + \ln\left(\frac{N-n_1}{n_1}\right) - \frac{N}{N-n_1} = 0$$

$$\Rightarrow \ln\left(\frac{N-n_1}{n_1}\right) = 0 \Rightarrow \frac{N-n_1}{n_1} = 1 \Rightarrow 2n_1 = N \Rightarrow \boxed{n_1^* = \frac{N}{2}}$$

· Similarly, one can rewrite $t(n_1)$ as $q(n_0)$ (which would have an identical form to $t(n_1)$). By symmetry, $n_0^* = \frac{N}{2}$.

· Since the two states have energy 0 and E, the partition function (using the canonical ensemble) is given by:

$$Z_1 = 1 + e^{-\beta E}$$

∴ For N particles this is given by:

$$Z_N = (1 + e^{-\beta E})^N$$

∴ Energy fluctuations in the CE are given by:

$$\sigma_U^2 = \langle U^2\rangle - \langle U\rangle^2 = \frac{\partial^2 \ln(Z(\beta))}{\partial\beta^2}$$

$$= \frac{\partial^2}{\partial\beta^2}\left(\ln\left(\left[1 + e^{-\beta E}\right]^N\right)\right)$$

$$= \frac{\partial^2}{\partial\beta^2}\left(N\ln(1 + e^{-\beta E})\right)$$

$$= N\frac{\partial^2}{\partial\beta^2}\left(\ln(1 + e^{-\beta E})\right) = \frac{E^2 e^{\beta E} N}{(e^{\beta E}+1)} = \frac{NE^2 e^{\beta E}}{(e^{\beta E}+1)} = \frac{NE^2}{(1+e^{-\beta E})}$$

· Given that $U = n_1 E \Rightarrow n_1 = \frac{U}{E} \Rightarrow \sigma_{n_1}^2 = \frac{N\cdot\frac{U^2}{n_1^2}}{(1+e^{-\beta U/n_1})} = \frac{NU^2}{n_1^2(1+e^{\beta U/n_1})}$ ⇒ this is equal to the mean square fluctuations for n_0 as well.

c. Solution:

$$S = k_B\left[N\ln\left(\frac{N}{N-\frac{U}{E}}\right) + \frac{U}{E}\ln\left(\frac{N-U/E}{U/E}\right)\right]$$

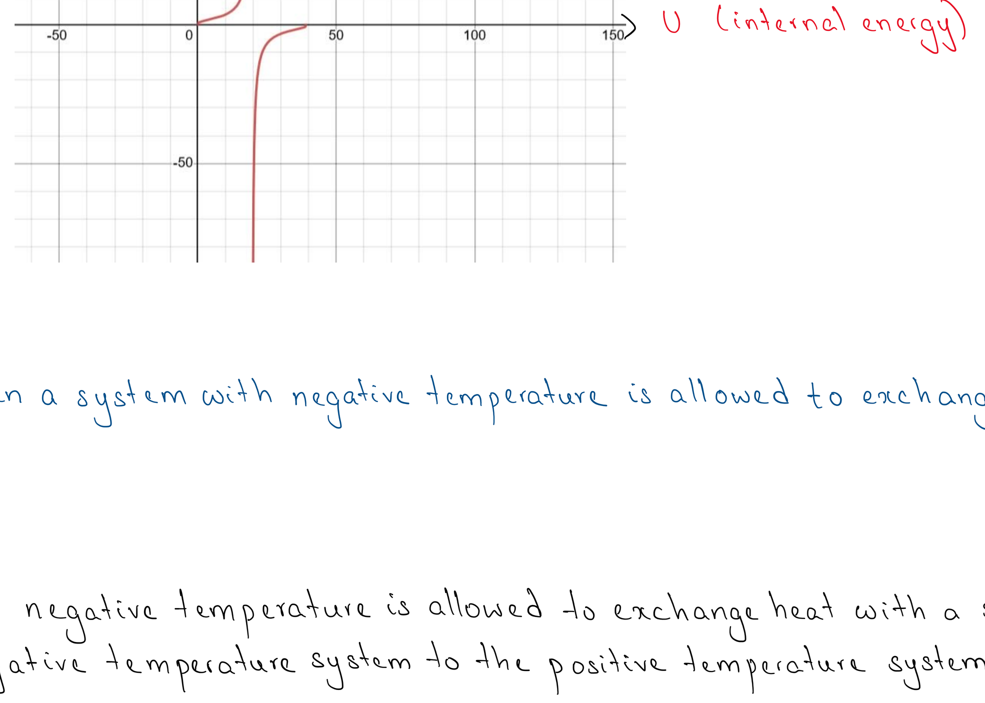
$$\therefore \frac{1}{T} = \left(\frac{\partial S}{\partial U}\right) = \frac{\partial}{\partial U}\left[N\ln\left(\frac{N}{N-\frac{U}{E}}\right) + \frac{U}{E}\ln\left(\frac{NE}{U} - 1\right)\right]$$

$$= \frac{-N}{U-EN} + \left[\frac{1}{E}\ln\left(\frac{NE}{U} - 1\right) - \frac{N}{EN-U}\right]$$

$$= \frac{N}{EN-U} + \frac{1}{E}\ln\left(\frac{NE}{U} - 1\right) - \frac{N}{EN-U}$$

$$= \frac{1}{E}\ln\left(\frac{NE}{U} - 1\right) = \frac{1}{T} \Rightarrow T = \frac{E}{\ln\left(\frac{NE}{U} - 1\right)} = \frac{E}{\ln\left(\frac{NE-U}{U}\right)} = \frac{E}{\ln(NE-U) - \ln(U)}$$

· One can examine how the temperature varies as a function of internal energy $T(U)$. This is plotted below for fixed N and E. By inspection, it is evident that the temperature can be negative



d. What happens when a system with negative temperature is allowed to exchange heat with a system having a positive temperature

Solution:

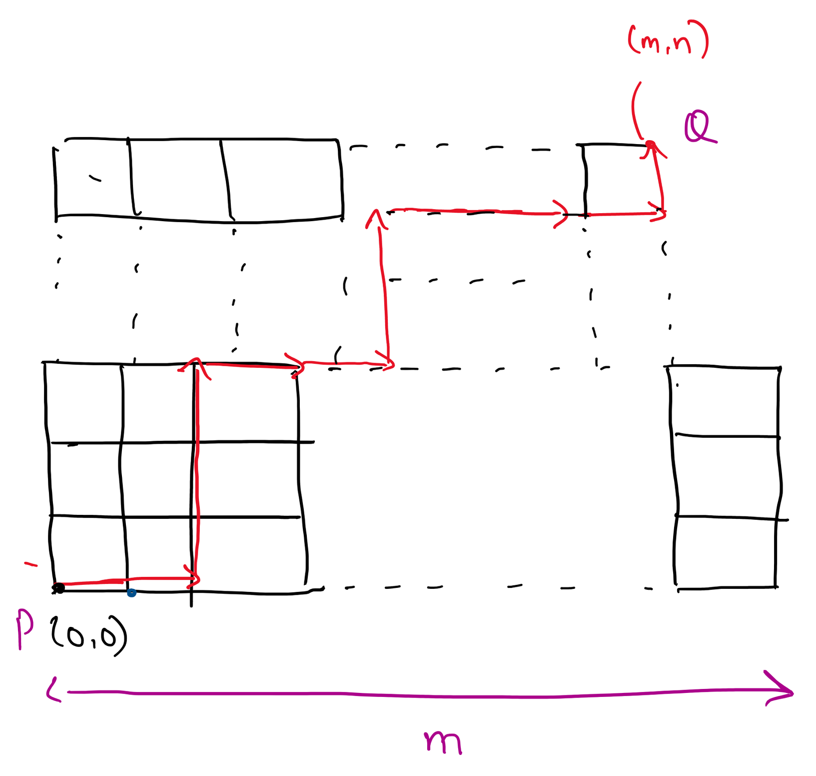
· If a system with negative temperature is allowed to exchange heat with a system having a positive temperature, heat would flow from the negative temperature system to the positive temperature system

Assignment 1: Question 2

Saturday, 13 May 2023 3:47 pm

(2) A physics student lives in a location P in a city. She walks to the lecture theatre at point Q. At each street, she has equal probability of going east or north. Because she wants to arrive on time for her lectures, she never doubles back.

a. If there are m streets east and n streets north of P, how many different ways can the student can go from P to Q?



Solution:

a. Total number of streets: mn

∴ Total number of ways in which the student can go from P to Q:

$$= \frac{(m+n)!}{n!\,m!}$$

b. We now relax the requirement that the student is not allowed to double back. She has equal probability of going east, west, north or south. Calculate the probability that after a large number of streets, the student has taken n_E streets eastward

Solution:

- This can be interpreted as two independent one-dimensional random walks, one in the east-west direction and the other in the north-south direction. Let there be k steps in the east-west direction and N-k steps in the north-south direction. Then:

① East-west direction:

$$m = \underbrace{a}_{\text{step size}}(\overset{\text{no. of east steps}}{n_E} - \underset{\text{no. of west steps}}{n_W}) = as \qquad (n_E + n_W = k) \qquad \overset{n_E - n_W = s}{\cancel{n_E}\ 2n_E - s = k} \Rightarrow \frac{k+s}{2}$$

$$\therefore\ N(n_E) = \frac{k!}{n_E!\,(k-n_E)!} \qquad \Rightarrow P(n_E) = \frac{k!}{n_E!\,(k-n_E)!}\left(\frac{1}{2}\right)^k$$

$$\therefore\ n_E + n_W = k \ \text{ and } \ n_E = \frac{1}{2}(k+s) \ \text{ and } \ n_W = \frac{1}{2}(k-s)$$

$$\therefore\ P(s) = \frac{k!}{\left[\frac{1}{2}(k+s)\right]!\left[\frac{1}{2}(k-s)\right]!}\left(\frac{1}{2}\right)^k$$

} Apply Stirling's approximation and simplify
Since k is presumably large, the continuum limit can be taken.

- From lectures ⇒ $P(x) = e^{-x^2/2ka^2}$ (where $m \to x = as$)

- Similarly, given that we must take N-k steps in the north-south direction, we have:

$$P(y) = e^{-y^2/2(N-k)a^2}$$

- Hence, the probability distribution can be written as:

$$P(n_E) = \exp\left(\frac{-x^2}{2(2n_E - s)a^2}\right) \cdot \exp\left(\frac{-y^2}{2(N-(2n_E-s))a^2}\right)$$

∴ Impose normalisation condition as follows:

$$\int_{-\infty}^{\infty} P(n_E)\,dx\,dy = 1$$

$$= \int_{-\infty}^{\infty} \exp\left(\frac{-x^2}{2(2n_E-s)a^2}\right)dx \int_{-\infty}^{\infty} \exp\left(\frac{-y^2}{2(N-(2n_E-S))a^2}\right)dy = 1$$

$$= \left(\sqrt{2}\sqrt{\pi}\,a\sqrt{2n_E - s}\right)\left(\sqrt{2}\sqrt{\pi}\,a\sqrt{(N-(2n_E-S))}\right) = 1$$

$$= \left(\sqrt{2\pi}\,a\sqrt{2n_E-s}\right)\left(\sqrt{2\pi}\,a\sqrt{N-(2n_E-S)}\right) = 1$$

$$= 2\pi a^2\sqrt{(2n_E-s)(N-2n_E+s)} = 1$$

$$\Rightarrow \text{Normalisation constant} = \frac{1}{2\pi a^2\sqrt{(2n_E-S)(N-2n_E+S)}}$$

$$\therefore\ P(x,y) = \frac{1}{2\pi a^2\sqrt{k(N-n_E-n_W)}} \exp\left(\frac{-x^2}{2(n_E+n_W)a^2} - \frac{y^2}{2(N-(n_E+n_W))a^2}\right)$$

c. Discuss the relationship between this random walk and diffusion in two dimensions

Solution:

- If a time dependence is introduced into the above probability distribution (i.e. $P(x,y) \to P(x,y,t)$), then this distribution must satisfy the two-dimensional diffusion equation of the form:

$$\frac{\partial P(x,y,t)}{\partial t} = D\left(\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2}\right)$$

where D is the diffusion coefficient.

Assignment 1: Question 3

Friday, 19 May 2023 10:34 am

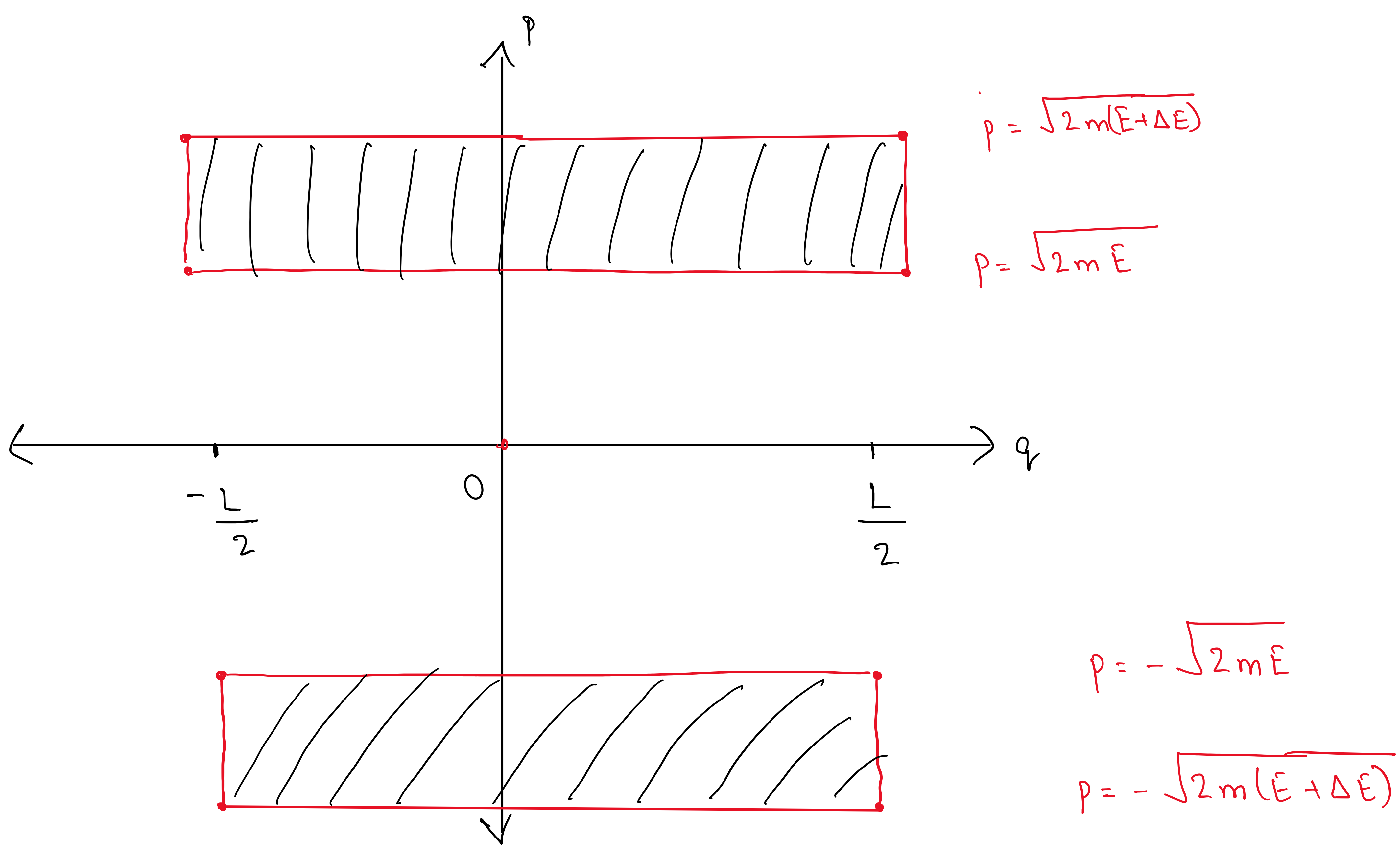
(3) Construct the classical phase space diagram for a particle of mass m confined to a one-dimensional box of size L. Assume that the energy of pcle lies between E and E+ΔE. Clearly label regions of phase space accessible to the pcle.

Solution:

. Hamiltonian for particle of mass m in a one-dimensional box of length L:

$$E = \frac{p^2}{2m} \qquad 0 < x \leq L$$

$$\Rightarrow p = \pm\sqrt{2mE} \quad , \quad 0 \leq x \leq L$$



Shaded region = region of phase space accessible to pcle

(4) Calculate the thermodynamic properties (F, p, S and μ) of an ultrarelativistic ideal gas whose Hamiltonian is given by:

$$H(q, p) = \sum_{i=1}^{N} E_i \quad \text{where} \quad E_i = \sqrt{|p_i|^2 c^2 + m_0 c^4} \longrightarrow |p_i| c \quad (|p_i| \gg m_0 c^2)$$

$= \omega(E)$

Solution:

$$H(q, p) = \sum_{i=1}^{N} |p_i| c$$

$$\therefore \quad Z(\beta, V, N) = \frac{1}{N!\, h^{3N}} \int_{\Gamma(E)} e^{-\beta H(q,p)}\, d^N q\, d^N p$$

$$= \frac{1}{N!\, h^{3N}} \int_{\Gamma(E)} e^{-\beta |p_i| c}\, d^N q\, d^N p$$

$$= \frac{V^N}{N!\, h^{3N}} \int_{\Gamma(E)} e^{-\beta |p_i| c}\, d^N p$$

$$\Rightarrow Z(\beta, V, N) = \frac{V^N}{N!\, h^{3N}} \prod_{i=1}^{N} \int_{-\infty}^{\infty} e^{-\beta |p_i| c}\, dp_i = \frac{V^N}{N!\, h^N} \cdot \prod_{i=1}^{N} \frac{2}{\beta c} = \frac{V^N}{N!\, h^N} \left[\frac{2 k_B T}{c}\right]^N = \frac{1}{N!} \left[\frac{2V}{\beta h c}\right]^N$$

$$F(T, V, N) = -k_B T \ln(Z(\beta, V, N))$$

$$= -k_B T \ln\left[\frac{1}{N!} \left[\frac{2 k_B T}{hc}\right]^N\right]$$

$$= -k_B T \left[\ln\left(\left(\frac{2 k_B T V}{hc}\right)^N\right) - \ln(N!)\right]$$

$$= -N k_B T \ln\left(\frac{2 k_B T V}{hc}\right) + k_B T \ln(N!)$$

$$= k_B T \left(\ln(N!) - N \ln\left(\frac{2 k_B T V}{hc}\right)\right)$$

$$= k_B T \left(\ln(N!) - N \ln(V) - N \ln\left(\frac{2 k_B T}{hc}\right)\right)$$

$$= k_B T \left(N \ln(N) - N - N \ln(V) - N \ln\left(\frac{2 k_B T}{hc}\right)\right)$$

$$= N k_B T \left(\ln(N) - \ln(V) - \ln\left(\frac{2 k_B T}{hc}\right) - 1\right)$$

$$= N k_B T \left[\ln\left(\frac{N}{V}\right) - \ln\left(\frac{2 k_B T}{hc}\right) - 1\right]$$

$$= N k_B T \left[\ln\left(\frac{N}{V} \times \frac{hc}{2 k_B T}\right) - 1\right]$$

$$= N k_B T \left[\ln\left(\frac{N h c}{2 k_B T V}\right) - 1\right]$$

$$= -N k_B T \left[1 - \ln\left(\frac{N h c}{2 k_B T V}\right)\right] = F(T, V, N)$$

$$\therefore \quad p = -\left(\frac{\partial F}{\partial V}\right)_{T,N} = -\frac{\partial}{\partial V}\left(-N k_B T \left[1 - \ln\left(\frac{N h c}{2 k_B T V}\right)\right]\right)$$

$$= \frac{\partial}{\partial V}\left(N k_B T \left[1 - \ln\left(\frac{N h c}{2 k_B T V}\right)\right]\right)$$

$$= \frac{\partial}{\partial V}\left[-\ln\left(\frac{N h c}{2 k_B T V}\right)\right] \times N k_B T$$

$$= \frac{\partial}{\partial V}\left[\ln\left(\frac{2 k_B T V}{N h c}\right)\right] \times N k_B T$$

$$\Rightarrow \frac{\partial}{\partial V}\left[\ln(\alpha V)\right] \times N k_B T$$

$$p = \frac{N k_B T}{V} \Rightarrow \boxed{pV = N k_B T}$$

$$S = -\left(\frac{\partial F}{\partial T}\right)_{V,N}$$

$$= -\frac{\partial}{\partial T}\left[-N k_B T \left[1 - \ln\left(\frac{N h c}{2 k_B T V}\right)\right]\right]$$

$$= \frac{\partial}{\partial T}\left(N k_B T \left(1 - \ln\left(\frac{N h c}{2 k_B T V}\right)\right)\right)$$

$$= N k_B \left(1 - \ln\left(\frac{N h c}{2 k_B T V}\right)\right) + N k_B T \frac{\partial}{\partial T}\left(1 + \ln\left(\frac{2 k_B T V}{N h c}\right)\right)$$

$$= N k_B \left(1 + \ln\left(\frac{2 k_B T V}{N h c}\right)\right) + N k_B T \times \frac{1}{T}$$

$$= N k_B \left(1 + \ln\left(\frac{2 k_B T V}{N h c}\right)\right) + N k_B$$

$$= \boxed{N k_B \left(2 + \ln\left(\frac{2 k_B T V}{N h c}\right)\right)} = \underline{\underline{S}}$$

$$\mu = \left(\frac{\partial F}{\partial N}\right)_{T,V} = \frac{\partial}{\partial N}\left\{-N k_B T \left[1 - \ln\left(\frac{N h c}{2 k_B T V}\right)\right]\right\}$$

$$= -k_B T \left[1 - \ln\left(\frac{N h c}{2 k_B T V}\right)\right] - N k_B T \left[\frac{\partial}{\partial N}\left\{1 - \ln\left(\frac{N h c}{2 k_B T V}\right)\right\}\right]$$

$$= -k_B T + k_B T \ln\left(\frac{N h c}{2 k_B T V}\right) - N k_B T \left(\frac{-1}{N}\right)$$

$$= -k_B T + k_B T \ln\left(\frac{N h c}{2 k_B T V}\right) + k_B T$$

$$= \boxed{k_B T \ln\left(\frac{N h c}{2 k_B T V}\right) = \mu}$$

Assignment 1: Question 5

Thursday, 11 May 2023 7:52 pm

(5) The grand canonical partition function is defined as:

$$\Xi(\beta, V, N) = \sum_N z^N Z(\beta, V, N)$$

where $z = e^{\beta\mu}$ = fugacity, μ = chemical potential and $Z(\beta, V, N)$ = canonical partition function for N particles

a. Defining $D = z\frac{\partial}{\partial z}$, prove that the grand canonical average is given by:

$$\langle (N - \langle N\rangle)^2 \rangle = D^2 \ln(\Xi(\beta, V, N))$$

Solution:

$$\langle (N - \langle N\rangle)^2 \rangle = \langle N^2\rangle - \langle N\rangle^2$$

$$\therefore \langle N\rangle = \frac{\sum_{N=0}^{\infty} N z^N Z(\beta, V, N)}{\sum_{N=0}^{\infty} z^N Z(\beta, V, N)} = \frac{1}{\Xi(\beta, V, N)} \sum_{N=0}^{\infty} \frac{\partial}{\partial z}(\Xi(\beta, V, N)).z = \frac{1}{\Xi(\beta, V, N)} z\frac{\partial}{\partial z}(\Xi(\beta, V, N))$$

$$= z\frac{\partial}{\partial z}(\ln(\Xi(\beta, V, N))) = D\ln(\Xi(\beta, V, N)) \quad ①$$

$$\therefore \langle N^2\rangle = \frac{\sum_{N=0}^{\infty} N^2 z^N Z(\beta, V, N)}{\sum_{N=0}^{\infty} z^N Z(\beta, V, N)} = \frac{1}{\Xi(\beta, V, N)}\left(z\frac{\partial}{\partial z}\right)\left(z\frac{\partial}{\partial z}\right)(\Xi(\beta, V, N)) \quad ②$$

$$\therefore \langle N^2\rangle - \langle N\rangle^2$$

$$= \frac{1}{\Xi(\beta, V, N)}\left(z\frac{\partial}{\partial z}\right)\left(z\frac{\partial}{\partial z}\right)(\Xi(\beta, V, N)) - \frac{1}{\Xi^2(\beta, V, N)} z^2\left(\frac{\partial \Xi}{\partial z}\right)^2$$

$$= \frac{1}{\Xi(\beta, V, N)}\left(z\frac{\partial}{\partial z} + z^2\frac{\partial^2}{\partial z^2}\right)(\Xi(\beta, V, N)) - \frac{1}{\Xi^2(\beta, V, N)} z^2\left(\frac{\partial \Xi}{\partial z}\right)^2$$

$$= \frac{1}{\Xi(\beta, V, N)}\left[\left(z\frac{\partial}{\partial z} + z^2\frac{\partial^2}{\partial z^2}\right)(\Xi(\beta, V, N))\right] - \left[\frac{1}{\Xi^2(\beta, V, N)} z^2\left(\frac{\partial \Xi}{\partial z}\right)^2\right]$$

$$= \frac{1}{\Xi(\beta, V, N)}\left[\left(z\frac{\partial}{\partial z} + z^2\frac{\partial^2}{\partial z^2}\right)(\Xi(\beta, V, N)) - \frac{1}{\Xi(\beta, V, N)} z^2\left(\frac{\partial \Xi}{\partial z}\right)^2\right]$$

$$= \left(z\frac{\partial}{\partial z}\right)^2 \ln(\Xi(\beta, V, N)) = D^2\ln(\Xi(\beta, V, N)) \rightarrow \text{QED}$$

b. Does the result in Part (a) generalise? Is the following result valid:

$$\langle (N - \langle N\rangle)^n \rangle = D^n \ln(\Xi(\beta, V, N))$$

Solution:

- The result does not generalise. A counterexample is the $n = 4$ case, where $\left(z\frac{\partial}{\partial z}\right)^4 \ln(\Xi(\beta, V, N)) = D^4\ln(\Xi(\beta, V, N)) \neq \langle (N - \langle N\rangle)^4\rangle$

c. Prove that the internal energy is given by:

$$U = -\frac{\partial}{\partial \beta}\ln(\Xi(\beta, V, N))$$

$\therefore$ Solution:

$$\Xi(\beta, V, N) = \sum_{N=0}^{\infty}\sum_i e^{-\beta(E_i - \mu N)}$$

$$-\frac{\partial}{\partial \beta}(\ln(\Xi(\beta, V, N))) = \frac{1}{\Xi(\beta, V, N)} \cdot -\frac{\partial}{\partial \beta}\left(\sum_{N=0}^{\infty}\sum_i e^{-\beta(E_i - \mu N)}\right)$$

$$= \frac{1}{\Xi(\beta, V, N)} \times \sum_{N=0}^{\infty}\sum_i -\frac{\partial}{\partial \beta}\left(e^{-\beta(E_i - \mu N)}\right)$$

$$= \frac{1}{\Xi(\beta, V, N)} \sum_{N=0}^{\infty}\sum_i (E_i - \mu N) e^{-\beta(E_i - \mu N)}$$

$$= \frac{1}{\Xi(\beta, V, N)}\left(\sum_{N=0}^{\infty}\sum_i E_i e^{-\beta(E_i - \mu N)} - \sum_{N=0}^{\infty}\sum_i \mu N e^{-\beta(E_i - \mu N)}\right)$$

$$= \langle E\rangle - \mu\langle N\rangle$$

$$= U - \mu\langle N\rangle$$

Assignment 1: Question 6

Thursday, 11 May 2023 7:54 pm

(6) Consider a one dimensional Einstein solid with anharmonicity defined by a cubic term in the potential of the oscillator:

$$V(x) = \frac{1}{2} m\omega_0^2 x^2 - \frac{1}{3}\lambda x^3$$

where $\omega_0 = \sqrt{\frac{\kappa}{m}}$ and λ is small. The thermal expansion coefficient of this one-dimensional system is given by:

$$\alpha_L = \frac{1}{L_0}\left(\frac{\partial \langle x \rangle}{\partial T}\right)_p$$

where L_0 = unperturbed length of one-dimensional solid. Calculate α_L and comment on the case where $\lambda = 0$

Solution:

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} x e^{-\beta V(x)}\, dx \quad (1)}{\int_{-\infty}^{\infty} e^{-\beta V(x)}\, dx \quad (2)}$$

(1) $$\int_{-\infty}^{\infty} x e^{-\beta V(x)}\, dx = \int_{-\infty}^{\infty} x e^{-\beta\left(\frac{1}{2}m\omega_0^2 x^2 - 1/3\lambda x^3\right)}\, dx$$

$$= \int_{-\infty}^{\infty} x\, e^{-\beta(1/2 m\omega_0^2 x^2)} \cdot e^{\beta\lambda x^3/3}\, dx$$

$\therefore$ Noting that λ is small, one can write:

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} \Rightarrow e^{\beta\lambda x^3/3} = \left(1 + \frac{\beta\lambda x^3}{3} + O(x^6)\right)$$

$\therefore$ The integral (1) becomes:

$$\int_{-\infty}^{\infty} x e^{-\beta(1/2 m\omega_0^2 x^2)}\left(1 + \frac{\beta\lambda}{3}x^3 + O(x^6)\right) dx$$

$$= \int_{-\infty}^{\infty} x e^{-\beta m\omega_0^2 x^2/2}\left(1 + \frac{\beta\lambda}{3}x^3\right) dx \quad \text{(neglecting higher order terms)}$$

$$= \frac{\sqrt{2\pi}\,\lambda\beta}{(m\beta\omega^2)^{5/2}} = \left(\frac{2\pi\lambda^2\beta^2}{(m\beta\omega^2)^5}\right)^{1/2}$$

(2) $$\int_{-\infty}^{\infty} e^{-\beta V(x)}\, dx = \int_{-\infty}^{\infty} e^{-\beta\left(\frac{1}{2}\omega_0^2 x^2 - \frac{\lambda x^3}{3}\right)}\, dx = \int_{-\infty}^{\infty} e^{\frac{-\beta\hbar\omega_0^2 x^2}{2}} \cdot e^{\beta\lambda x^3/3}\, dx = \int_{-\infty}^{\infty} e^{-\beta\hbar\omega_0^2 x^2/2}\left(1 + \frac{\beta\lambda x^3}{3} + O(x^6)\right) dx$$

$$= \int_{-\infty}^{\infty} e^{-\beta\hbar\omega_0 x^2/2}\left(1 + \frac{\beta\lambda x^3}{3}\right) dx \quad \text{(neglecting higher order terms)}$$

$$= \left(\frac{2\pi}{m\beta\omega_0^2}\right)^{1/2} = \frac{1}{\omega_0}\left(\frac{2\pi}{m\beta}\right)^{1/2} \quad \text{(by Mathematica)}$$

$$\therefore \langle x \rangle = \frac{(1)}{(2)} = \frac{\sqrt{2\pi}\,\lambda\beta}{(m\beta\omega^2)^{5/2}} \div \left(\frac{2\pi}{m\beta\omega_0^2}\right)^{1/2}$$

$$= \left(\frac{\cancel{2\pi}\lambda^2\beta^2}{(m\beta\omega_0^2)^5}\right)^{1/2} \times \left(\frac{m\beta\omega_0^2}{\cancel{2\pi}}\right)^{1/2}$$

$$= \left(\frac{\lambda^2}{m^5\beta^3\omega_0^{10}}\right)^{1/2}(m\beta\omega_0^2)^{1/2}$$

$$= \frac{\lambda}{m^{5/2}\beta^{3/2}\omega^5} \cdot m^{1/2}\beta^{1/2}\omega_0$$

$$= \frac{\lambda}{m^2\beta\omega^4} = \frac{\lambda k_B T}{m^2\omega^4} \quad (3)$$

$$\therefore \alpha_L = \frac{1}{L_0}\left(\frac{\partial\langle x\rangle}{\partial T}\right)_p = \frac{1}{L_0}\frac{\partial}{\partial T}\left(\frac{\lambda k_B T}{m^2\omega^4}\right) = \boxed{\frac{1}{L_0}\frac{\lambda k_B}{m^2\omega^4}}$$

- When $\lambda = 0$, $\alpha_L = 0 \Rightarrow$ no thermal expansion occurs when $\lambda = 0$.

Assignment 1: Question 7

Thursday, 11 May 2023 9:01 pm

(7) Evaluate the classical and quantum partition functions for a simple harmonic oscillator. Show that the quantum oscillator reproduces the classical result in the case $T \to \infty$

Solution:

- Quantum harmonic oscillator in one dimension has quantised energies given by:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad (n = 0, 1, 2, \ldots)$$

$$\therefore Z(\beta, V, 1) = \sum_{n=0}^{\infty} e^{-\beta E_n} = e^{-\beta\hbar\omega/2} \sum_{n=0}^{\infty} e^{-\beta\hbar\omega n}$$

$$\therefore Z(\beta, V, 1) = \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}} = \frac{1}{e^{\beta\hbar\omega/2} - e^{-\beta\hbar\omega/2}} = \frac{1}{2\sinh\left(\frac{\beta\hbar\omega}{2}\right)} = \boxed{\frac{1}{2\sinh\left(\frac{\hbar\omega}{2k_BT}\right)}} \quad (1)$$

- Classical harmonic oscillator has a continuum of possible energies, and is described by the Hamiltonian:

$$H(q, p) = \frac{p^2}{2m} + \frac{1}{2} m\omega_0^2 q^2$$

$\therefore$ Partition function is given by:

$$Z(\beta, V, 1) = \frac{1}{h^3} \int_{\Gamma(E)} e^{-\beta H(p,q)} \, d^3p \, d^3q = \frac{1}{h^3} \int_{-\infty}^{\infty} e^{-\beta p^2/2m} \, d^3p \int_{-\infty}^{\infty} e^{-\beta m\omega_0^2 q^2/2} \, d^3q$$

$$= \frac{1}{h^3} \left(\frac{2m\pi}{\beta}\right)^{1/2} \left(\frac{2\pi}{\beta m\omega_0^2}\right)^{1/2} = \frac{2\pi}{\beta\omega_0 h} = \frac{2\pi k_B T}{\omega_0 h} = \boxed{\frac{k_B T}{\hbar\omega_0}} \quad (2) \qquad \left(\text{where } \hbar = \frac{h}{2\pi}\right)$$

- Seek to show that in the limit $T \to \infty$, the quantum oscillator reproduces the classical result

- $$Z(\beta, V, 1) = \frac{1}{2\sinh\left(\frac{\hbar\omega}{2k_BT}\right)} = \frac{1}{2\sinh\left(\frac{\beta\hbar\omega}{2}\right)}$$

- $T \to \infty \Rightarrow \hbar\omega \ll k_BT \Rightarrow$ Taylor expand denominator in β:

$$\therefore Z(\beta, V, 1) = \frac{1}{2\left[\left(\frac{\beta\hbar\omega}{2}\right) + \frac{1}{6}\left(\frac{\beta\hbar\omega}{2}\right)^3 + \ldots\right]} \qquad \left(\sinh(x) = \sum_{n=0}^{\infty} \frac{x^{2n+1}}{(2n+1)!}\right)$$

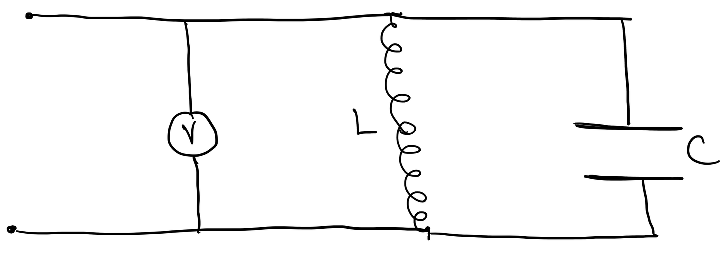
$$= \frac{1}{2\left[\left(\frac{\beta\hbar\omega}{2}\right) + O\left(\left(\frac{\beta\hbar\omega}{2}\right)^3\right)\right]} \approx \frac{1}{\beta\hbar\omega_0} = \boxed{\frac{k_B T}{\hbar\omega_0}} \text{ (to leading order)} = (2)$$

Hence, in the high temperature limit, the quantum oscillator reproduces the classical result $\Rightarrow$ QED

Assignment 1: Question 8

Saturday, 13 May 2023 1:33 pm

(8) An LC circuit can be used as a thermometer by measuring the noise voltage across the inductor and capacitor in parallel. Determine the relationship between the root mean square (RMS) noise voltage and the absolute temperature. You may assume the classical limit $k_B T \gg \hbar\omega$, where $\omega = (LC)^{-1/2}$ = frequency of the oscillator.



Solution:

- Hamiltonian describing oscillations in the LC circuit is:

$$H = \frac{1}{2} L \left(\frac{dQ(t)}{dt} \right)^2 + \frac{Q^2(t)}{2C}$$

Given that $V = \frac{Q}{C}$ (from circuit theory), one can deduce that $\frac{Q^2}{2C} = \frac{CV^2}{2}$

voltage

Additionally, letting $I = \frac{dQ}{dt}$ (from the definition of electric current), one can rewrite the Hamiltonian as:

$$H = \frac{1}{2} L I^2 + \frac{CV^2}{2}, \quad \text{where } I = I(t) \text{ and } V = V(t)$$

- Hence, one can compute the partition function for the circuit:

$$Z = \int_{-\infty}^{\infty} e^{-\beta\left(\frac{CV^2}{2} + \frac{LI^2}{2}\right)} \, dV \, dI$$

$$= \int_{-\infty}^{\infty} e^{-\beta C V^2/2} \, dV \int_{-\infty}^{\infty} e^{-\beta L I^2/2} \, dI$$

$$= \int_{-\infty}^{\infty} e^{-\frac{1}{2} a V^2} \, dV \int_{-\infty}^{\infty} e^{-\frac{1}{2} s I^2} \, dI$$

$a = \beta C$ $\quad$ $s = \beta L$

$$= \left(\frac{2\pi}{\beta C} \right)^{1/2} \left(\frac{2\pi}{\beta L} \right)^{1/2} = \frac{2\pi}{\beta (LC)^{1/2}} = \frac{2\pi}{\beta\omega}$$

- Noting that

$$U = \frac{-1}{Z} \frac{\partial Z}{\partial \beta}$$

$$= \frac{-1}{Z} \frac{\partial}{\partial \beta} \left(\frac{2\pi}{\beta\omega} \right)$$

$$= \frac{-1}{Z} \left(\frac{-2\pi}{\beta^2 \omega} \right)$$

$$= \left(\frac{\beta\omega}{2\pi} \right) \left(\frac{2\pi}{\beta^2 \omega} \right) = \frac{1}{\beta} = k_B T \qquad (1)$$

- Furthermore, one can note that:

$$U = \frac{1}{Z} \frac{\partial}{\partial \beta} \int e^{-\beta\left(\frac{CV^2}{2} + \frac{LI^2}{2}\right)} \, dV \, dI$$

$$= \frac{1}{Z} \int \left(\frac{CV^2}{2} + \frac{LI^2}{2} \right) e^{-\beta\left(CV^2/2 + \frac{LI^2}{2}\right)} \, dV \, dI$$

$$= \frac{C}{2} \langle V^2 \rangle + \frac{L}{2} \langle I^2 \rangle$$

- Since there exist two quadratic degrees of freedom in this system, one in V and the other in I,
- the equipartition theorem states that each of these must contribute equally to the internal energy U of the system:

$$\Rightarrow \quad \frac{C}{2} \langle V^2 \rangle = \frac{L}{2} \langle I^2 \rangle = \frac{U}{2}$$

$\therefore$ Since $\frac{C}{2} \langle V^2 \rangle = \frac{U}{2} \Rightarrow C \langle V^2 \rangle = U \qquad (2)$

- Hence $V_{RMS} = \sqrt{\langle V^2 \rangle} = \sqrt{\frac{U}{C}}$

$\therefore$ From (1), $U = k_B T \quad \Rightarrow \quad \boxed{V_{RMS} = \sqrt{\frac{k_B T}{C}}} \quad \Rightarrow \underline{V_{RMS} \propto T^{1/2}}$