MONASH UNIVERSITY
School of Physics & Astronomy

ASSESSMENT COVER SHEET

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Unit Name	**Statistical Mechanics**	**Unit Code**	**PHS4200/PHS4021**

Title of Assignment & Assignment Number	Statistical Mechanics: Assignment 2
Name of Lecturer	**Michael J. Morgan**

Due Date: 09/06/2023	**Date Submitted: 09/06/2023**

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(1) Deduce density operator for canonical ensemble starting from entropy definition:

$$S = -k_B \mathrm{Tr}(\hat{\rho}\ln(\hat{\rho}))$$

Solution.

Constraints: $\mathrm{Tr}(\hat{\rho}) = 1$ and $\mathrm{Tr}(\hat{H}\hat{\rho}) = \langle E \rangle$

Introduce Lagrange multipliers α, β. We can form an analogue of the auxilliary function by incorporating these constraints:

$$\Rightarrow \mathrm{Tr}(\alpha\hat{\rho} + \beta\hat{H}\hat{\rho} - k_B\hat{\rho}\ln(\hat{\rho}))$$

The extremisation condition is:

$$= \delta(\mathrm{Tr}(\alpha\hat{\rho} + \beta\hat{H}\hat{\rho} - k_B\hat{\rho}\ln(\hat{\rho}))\delta\rho = 0$$

$$\therefore \mathrm{Tr}(\alpha + \beta\hat{H} - k_B\ln(\hat{\rho}) - k_B) = 0 \quad (\text{since } \delta\rho = \text{arbitr}$$

$$\Rightarrow ((\alpha - k_B)\underset{\text{identity}}{\hat{\mathbb{I}}} + \beta\hat{H} - k_B\ln(\hat{\rho})) = 0$$

$$\therefore k_B\ln(\hat{\rho}) = (\alpha - k_B)\mathbb{I} + \beta\hat{H}$$

$$\therefore \ln(\hat{\rho}) = \frac{\alpha}{k_B} - 1 + \frac{\beta\hat{H}}{k_B}$$

$$\therefore \hat{\rho} = \exp\left[\frac{\alpha}{k_B} - 1 + \frac{\beta\hat{H}}{k_B}\right]$$

Using the constraints, we can determine α and β. Using ~~(7.27)~~ $Tr(\hat{\rho}) = 1$, we have:

$$\cancel{\hat{\rho}} = Tr\left[\exp\left(\left(\frac{\alpha}{k_B} - 1\right)\hat{\mathbb{I}} + \frac{\beta \hat{H}}{k_B}\right)\right] = 1$$

$$\Rightarrow \cancel{\sum_i \exp\left(\frac{\alpha}{k_B} - 1\right)\mathbb{I}} = \cancel{e}$$

$$\therefore \cancel{Tr\left(e^{-\beta \hat{H}/k_B}\right)} = \cancel{\exp}$$

$$\therefore \exp\left(1 - \frac{\alpha}{k_B}\right) = Tr\left(e^{\beta \hat{H}/k_B}\right)$$

We can now determine β. Multiply constraint eqn ("auxilliary function") by $\hat{\rho}$ and take trace:

$$\therefore Tr\left[(\alpha - k_B)\hat{\rho} + \beta \hat{H}\hat{\rho} - k_B \hat{\rho}\ln(\hat{\rho})\right] = 0$$

$$= \cancel{\text{Since } \hat{\rho} = \exp\left[\left(\frac{\alpha}{k_B} - 1\right)\hat{\mathbb{I}} + \frac{\beta}{k_B}\hat{H}\right]}$$

~~we have~~

$$= -k_B \ln\left(\cancel{\tfrac{?}{?}}\, Z(\beta)\right) + \beta \underbrace{\langle E \rangle}_{U} + S = 0 \quad (\star)$$

$$\text{where } \exp\left(1 - \frac{\alpha}{k_B}\right) = \underbrace{Z(\beta)}_{\text{partition function}} = Tr\left(e^{\beta \hat{H}/k_B}\right)$$

$(\star)$ looks like $\underbrace{F - U}_{\text{expression for Helmholtz free energy}} + ST = 0$. Hence, we have

~~$\beta = -\frac{1}{T}$ (by~~ $\beta = -\frac{1}{T}$ by comparing the expressions

- We can also identify that:

$$F = -k_B T \ln(Z(\beta T)) \quad (**)$$

Since $Z(T) = \mathrm{Tr}\left(e^{-\beta \hat{H}_N / k_B}\right)$

$$\Rightarrow \mathrm{Tr}\left(e^{-\beta' \hat{H}}\right) \quad \left(\text{where } \beta' = \frac{1}{k_B T}\right)$$

It is also evident that: (from (**))

$$\frac{-F}{k_B T} = \ln(Z(T))$$

$$e^{-\beta' F} = Z(T)$$

Hence, we can write

$$\hat{\rho} = e^{-\beta'(\hat{H} - F)} = \frac{e^{-\beta' \hat{H}}}{\mathrm{Tr}\left(e^{-\beta \hat{H}_N}\right)} \Rightarrow \text{as required}$$

(2) Dynamical state of system represented by ~~dia~~ density operator:

$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{Tr(e^{-\beta \hat{H}})}$$

a. Want to show that:

$$Z(\beta) = \frac{e^{-\beta \hbar \omega/2}}{1 - e^{-\beta \hbar \omega}}$$

Solution:

$$Z(\beta) = Tr(\exp(-\beta \hat{H}))$$

$$\hat{H} = \left(n + \frac{1}{2}\right)\hbar\omega, \quad n = 0, 1, 2, \ldots$$

$$\therefore Z(\beta) = Tr\left(\exp\left(-\beta\left(n + \frac{1}{2}\right)\hbar\omega\right)\right)$$

$$\sum_n \langle \varphi_n | e^{-\beta(n+1/2)\hbar\omega} | \varphi_n \rangle$$

$$= \sum_n e^{-\beta(n+1/2)\hbar\omega} \langle \varphi_n | \varphi_n \rangle$$

orthonormal basis vect φ_n

$$= \sum_{n=0}^{\infty} e^{-\beta(n+1/2)\hbar\omega}$$

$$= e^{-\beta\hbar\omega/2} + e^{3\beta\hbar\omega/2} + \ldots = Z(\beta)$$

= Geometric series with first term $e^{-\beta\hbar\omega/2}$ and common ratio $e^{-\beta\hbar\omega}$ $\Rightarrow$ The above simplifies to

$$\therefore Z(\beta) = \frac{e^{-\beta \hbar \omega/2}}{1 - e^{-\beta \hbar \omega}} = \frac{\cancel{e^{\beta \hbar \omega/2}}}{\ }$$

$\Rightarrow$ QED

b. Ensemble average is defined by:

$$\langle E \rangle = T_r(\hat{\rho}\hat{H}) = \frac{T_r(\hat{H} e^{-\beta \hat{H}})}{T_r(e^{-\beta \hat{H}})}$$

$\therefore$ From (7.24), we have that:

$$\langle \hat{H} \rangle = \frac{T_r(\hat{H} e^{-\beta \hat{H}})}{T_r(e^{-\beta \hat{H}})} = -\frac{\partial}{\partial \beta} \ln\left(T_r(e^{-\beta \hat{H}})\right)$$

$$= -\frac{\partial}{\partial \beta}\left(\frac{\cancel{e^{-\beta \hbar \omega/2}}}{\ } \ln\left(\frac{e^{-\beta \hbar \omega/2}}{1 - e^{-\beta \hbar \omega}}\right)\right)$$

$$= \frac{-\partial}{\partial \beta}\left(\ln\left(e^{-\beta \hbar \omega/2}\right) - \ln\left(1 - e^{-\beta \hbar \omega}\right)\right)$$

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

$$= \frac{\hbar \omega}{2} + \frac{\partial}{\partial \beta}\left(\ln\left(1 - e^{-\beta \hbar \omega/\cancel{2}}\right)\right)$$

$$= \frac{\hbar \omega}{2} + \frac{\hbar \omega e^{-\beta \hbar \omega}}{1 - e^{-\beta \hbar \omega}}$$

$$= \frac{\hbar \omega}{2} + \frac{\hbar \omega}{e^{\beta \hbar \omega} - 1}$$ (Multiply numerator and denom by $e^{\beta \hbar \omega}$)

$$\therefore \langle E \rangle = \frac{\hbar\omega}{2} + \frac{\hbar\omega}{e^{\beta\hbar\omega}-1} \Rightarrow \underline{\underline{QED}}$$

In the low temp' limit, $\beta \to \infty \Rightarrow$

$$\therefore \lim_{\beta\to\infty} (\langle E \rangle) = \lim_{\beta\to\infty} \left(\frac{\hbar\omega}{2} + \frac{\hbar\omega}{e^{\beta\hbar\omega}-1} \right) = \frac{\hbar\omega}{2}$$

In the high temp. limit $\Rightarrow \beta \to 0$

$$\therefore \lim_{\beta\to 0} \left(\frac{\hbar\omega}{2} + \frac{\hbar\omega}{e^{\beta\hbar\omega}-1} \right) \sim \cancel{\frac{\hbar\omega}{2}}$$

$$= \lim_{\beta\to 0} \left(\frac{\hbar\omega}{2} + \frac{\hbar\omega}{\underbrace{(1+\beta\hbar\omega+O(\beta^2))}-1} \right)$$

Taylor expand $\cancel{\beta\hbar\omega}$ $e^{\beta\hbar\omega}$

To leading order, this is:

$$\lim_{\beta\to 0} \left(\frac{\hbar\omega}{2} + \frac{\hbar\omega}{\beta\hbar\omega} \right) = \frac{\hbar\omega}{2} + \frac{1}{\beta}$$

As $\beta \to 0$, $\frac{1}{\beta} \to \infty \Rightarrow \frac{\hbar\omega}{2}$ is negligible in this limit.

$\Rightarrow$ High temp limit $\Rightarrow \lim_{\beta\to 0} \langle E \rangle = \frac{1}{\beta} = \underline{\underline{k_B T}}$

with consistent equipartition theorem

c. $\langle n_\omega \rangle = \frac{1}{e^{\beta\hbar\omega} - 1}$

$\therefore$ For sodiumlight, $\beta = \frac{1}{(1.38\times10^{-23})(300)}$

$= 2.42\times10^{20}$

$\omega = 5.09\times10^{14}$ Hz $\hbar = 1.05\times10^{-34}$

$\therefore e^{\beta\hbar\omega} = e^{(2.42\times10^{20})(1.05\times10^{-34})(5.09\times10^{14})}$

$= \cancel{4.1\times10^{5}}$ $\frac{1}{e^{\beta\hbar\omega}-1} = 2.42\times10^{-6}$

For radio interferometer:

$\beta = 2.42\times10^{20}$, $\omega = \cancel{9\times10}$ 9.19×10^{9} Hz,

$\hbar = 1.05\times10^{-34}$

$\therefore e^{\beta\hbar\omega} - 1 = e^{(2.42\times10^{20})(1.05\times10^{-34})(9.19\times10^{9})} - 1$

$= 2.33\times10^{-4}$

$\langle n_\omega \rangle = \frac{1}{2.33\times10^{-4}} = 4.3\times10^{3}$

(3) Riemann zeta function:

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} \quad (s \in \mathbb{C})$$

Want to show that canonical partition function of system of primons = zeta functi

Energy of each pole: $\ln(p_n)$ $(n \geq 1)$ ($n = n^{th}$ prin number)

Since n is a prime number, it has a unique factorisation.

$$n = p_1^{m_1} p_2^{m_2} \cdots p_k^{m_k} \quad (m = \text{no. of poles in the sta } |p\rangle)$$

Total energy of system in state $|n\rangle$ is:

$$E_n = m_1 \ln(p_1) + m_2 \ln(p_2) + \dots + m_k \ln(p_k)$$

$$= \ln\left(p_1^{m_1} p_2^{m_2} \cdots p_k^{m_k}\right) = \ln(n)$$

$\therefore$ Partition function $= \sum_{n=1}^{\infty} \exp(-\beta E_n) = Z(\beta)$

$$\therefore Z(\beta) = \sum_{n=1}^{\infty} \exp(-\beta(\ln(n))) = \sum_{n=1}^{\infty} \exp\left(\ln\left(\frac{1}{n^{\beta}}\right)\right)$$

$$= \sum_{n=1}^{\infty} \frac{1}{n^{\beta}} = \zeta(\beta)$$

The partition function is well behaved for $\beta > 1$ (as the sum to infinity of $\frac{1}{n}$ diverges). It is not well behaved for $\beta \leq 1$

$n \cdot x$

Average internal energy $\langle E \rangle$ is given by:

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

$$= -\frac{1}{\zeta(\beta)} \frac{\partial \zeta(\beta)}{\partial \beta} \approx \frac{1}{\beta - 1}$$

The internal energy of the gas diverges when $\beta = 1$
This corresponds to a temperature of $T = \frac{1}{k_B}$

Hagedron temperature.

Helmholtz free energy:

$$F = -k_B T \ln(Z) = -k_B T (\ln(\zeta(\beta)))$$

$$C_v = \left(\frac{\partial U}{\partial T}\right)_V = \frac{\partial}{\partial T}\left(\frac{1}{\left(\frac{1}{k_B T}\right) - 1}\right)$$

$$= \frac{\partial}{\partial T}\left(\frac{1}{\left(\frac{1 - k_B T}{k_B T}\right)}\right) = \frac{\partial}{\partial T}\left(\frac{k_B T}{1 - k_B T}\right)$$

$$= \frac{k_B (1 - k_B T) + k_B (k_B T)}{(1 - k_B T)^2}$$

$$= \frac{k_B - k_B^2 T + k_B^2 T}{(1 - k_B T)^2} = \frac{k_B}{(1 - k_B T)^2} \sim \frac{1}{T^2}$$

$p = -\left(\frac{\partial F}{\partial V}\right)_{T,N} = 0$ (as expected, as this is a gas of "numbers"). Similar for μ $= -\left(\frac{\partial F}{\partial N}\right)_{T,V} = 0$

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

$$= k_B\left(\ln(\zeta(\beta)) + \frac{\partial}{\partial T}\left(\ln(\zeta(\beta))\right)\right)$$

$$= k_B \ln(\zeta(\beta)) + \left(\frac{1}{\zeta(\beta)}\frac{\partial \zeta}{\partial \beta}\frac{\partial \beta}{\partial T}\right) k_B$$

$$= k_B \ln(\zeta(\beta)) - \frac{1}{\zeta(\beta)}\frac{\partial \zeta}{\partial \beta}\frac{1}{T^2}$$

Expand $\zeta(\beta) \approx -\frac{1}{2} - \frac{\beta}{2}\ln(2\pi) + \dots$

$$\therefore \frac{\partial \zeta}{\partial \beta} = -\frac{1}{2}\ln(2\pi)$$

$$= -k_B \ln\left(-\frac{1}{2} - \frac{\beta}{2}\ln(2\pi)\right) \cdot \frac{1}{2T^2}\ln(2\pi)$$

$$= -k_B \ln\left(-\frac{1}{2} - \frac{1}{2k_BT}\ln(2\pi)\right) \cdot \frac{1}{2T^2}\ln(2\pi)$$

~~As T→0~~ Entropy appears to be inversely proportional to temperature.

(4) Want to show that the quantal distribution of an ideal gas is:

$$\langle n \rangle = \frac{1}{e^{\beta(\hbar\omega - \mu)} - \underbrace{\eta}}$$

-1 for bosons
+1 for fermions

$$\langle n \rangle = \frac{\mathrm{Tr}\left(\hat{a}^{\dagger}\hat{a}\, e^{-\beta\hat{H}}\right) \text{ I}}{\mathrm{Tr}\left(e^{-\beta\hat{H}}\right) \text{ II}}, \quad \text{where } \hat{H} = \hat{N}\hbar\omega - \mu\hat{N}$$

(1) Bosons:

(I) $$\mathrm{Tr}\left(\hat{a}^{\dagger}\hat{a}\, e^{-\beta\hat{H}}\right) = \sum_{n=0}^{\infty} \langle n | \hat{a}^{\dagger}\hat{a}\, e^{-\beta\hat{N}(\hbar\omega-\mu)} | n \rangle$$

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

By Mathematica, this ~~expression~~ sum ~~has~~ evaluates to:

$$\frac{e^{\beta(\hbar\omega-\mu)}}{\left(e^{\beta(\hbar\omega-\mu)} - 1\right)^2}$$

(II) $$\mathrm{Tr}\left(e^{-\beta\hat{H}}\right) = \sum_{n=0}^{\infty} \langle n | e^{-\beta\hat{N}(\hbar\omega-\mu)} | n \rangle$$

$$= \sum_{n=0}^{\infty} e^{-\beta n(\hbar\omega-\mu)}$$

This is an infinite geometric series with first term ~~(I)~~ 1 and common ratio $= e^{-\beta(\hbar\omega-\mu)}$

$$\therefore \sum_{n=0}^{\infty} e^{-\beta n(\hbar\omega-\mu)} = \frac{1}{1-e^{-\beta(\hbar\omega-\mu)}}$$

$$\therefore \cancel{(I) \div (II)} = \quad = \frac{e^{\beta(\hbar\omega-\mu)}}{e^{\beta(\hbar\omega-\mu)}-1}$$

$\therefore$ (I) $\div$ (II) $: = \langle n_b \rangle$

$$\frac{e^{\beta(\hbar\omega-\mu)}}{\left(e^{\beta(\hbar\omega-\mu)}-1\right)^2} \times \frac{e^{\beta(\hbar\omega-\mu)}-1}{e^{\beta(\hbar\omega-\mu)}}$$

$$= \frac{1}{e^{\beta(\hbar\omega-\mu)}-1} \Rightarrow \text{QED}$$

(2) Fermions:

(I) $Tr\left(\hat{a}^{+}\hat{a}\, e^{-\beta\hat{H}}\right)$

$$= \sum_{n=0}^{1} \langle n|\hat{a}^{+}\hat{a}\, e^{-\beta\hat{N}(\hbar\omega-\mu)}|n\rangle$$

$$= \sum_{n=0}^{1} n\, e^{-\beta n(\hbar\omega-\mu)} \langle n|n\rangle$$

$$= e^{-\beta(\hbar\omega-\mu)}$$

(II) $Tr\left(e^{-\beta \hat{H}}\right)$

$$= \sum_{n=0}^{1} e^{-\beta n(\hbar\omega-\mu)}$$

$$= 1 + e^{-\beta(\hbar\omega-\mu)}$$

$\therefore$ (I) $\div$ (II) :

$$\frac{e^{-\beta(\hbar\omega-\mu)}}{1+e^{-\beta(\hbar\omega-\mu)}} \times \frac{e^{\beta(\hbar\omega-\mu)}}{e^{\beta(\hbar\omega-\mu)}}$$

$$= \frac{1}{e^{\beta\hbar\omega}+1} = \langle n_f \rangle$$

$\therefore$ Combining (1) and (2):

$$\langle n \rangle = \frac{1}{e^{\beta(\hbar\omega-\mu)}-\eta} \qquad \eta = \begin{cases} +1 & \text{for Bose gas} \\ -1 & \text{for Fermi gas} \end{cases}$$

$\Rightarrow$ QED

(5) Calculate the Slater sum for the quantum harmonic oscillator:

Solution:

$$P(q) = \rho(q, q'=q) = \frac{\sum_n e^{-\beta E_n} |\psi_n(q)|^2}{\sum_n e^{-\beta E_n}}$$

$$\rho(q, q') = \frac{1}{Z(\beta)} \langle q | e^{-\beta \hat{H}} | q' \rangle$$

$$= \frac{1}{Z(\beta)} \sum_{n=0}^{\infty} e^{-\beta E_n} \psi_n^*(q') \psi_n(q)$$

From lectures:

$$\langle q | e^{-\beta \hat{H}} | q' = \cancel{q} \rangle = \left(\frac{m\omega}{\pi\hbar} \right)^{1/2} e^{-\xi^2} \sum_{n=0}^{\infty} \frac{1}{2^n n!} e^{-\beta(n+1/2)\hbar\omega} H_n(\xi)^2$$

From Kubo, this is equal to:

$$\cancel{\left(\frac{m\omega}{\pi\hbar} \right)^{1/2}}$$

$$\left(\frac{m\omega}{2\pi\hbar \sinh(\beta\hbar\omega)} \right)^{1/2} \exp\left(-\frac{m\omega}{4\hbar} (2q)^2 \tanh\left(\frac{\beta\hbar\omega}{2} \right) \right)$$

$$= \left(\frac{m\omega}{2\pi\hbar \sinh(\beta\hbar\omega)} \right)^{1/2} \exp\left(-\frac{m\omega q^2}{\hbar} \tanh\left(\frac{\beta\hbar\omega}{2} \right) \right)$$

and $Z(\beta) = \dfrac{1}{2\sinh\left(\frac{\beta\hbar\omega}{2}\right)}$

$$\therefore P(q) = \left(\frac{m\omega}{2\pi\hbar\sinh(\beta\hbar\omega)}\right)^{1/2} \exp\left(-\frac{m\omega q^2}{\hbar}\tanh\left(\frac{\beta\hbar\omega}{2}\right)\right) \times 2\sinh\left(\frac{\beta\hbar\omega}{2}\right)$$

$$= \boxed{2\left(\frac{m\omega}{2\pi\hbar\sinh(\beta\hbar\omega)}\right)^{1/2} \exp\left(-\frac{m\omega q^2}{\hbar}\tanh\left(\frac{\beta\hbar\omega}{2}\right)\right)\sinh\left(\frac{\beta\hbar\omega}{2}\right)}$$

(6) Long range order parameter: $L(T) := \frac{M(T)}{M(0)}$

$$L(T) = \tanh\left(\frac{T_c L(T)}{T}\right)$$

a. Want to show that:

$$L(T) = \sqrt{3\left(1 - \frac{T}{T_c}\right)} \quad 0 < 1 - \frac{T}{T_c} \ll 1$$

In the abovementioned limit, $\frac{T_c}{T} L(T)$ is small

$\Rightarrow$ we can Taylor expand RHS in $\frac{T_c}{T} L(T)$

$$\therefore L(T) = \left(\frac{T_c}{T} L(T)\right) = \frac{T_c}{T} L(T) - \left(\frac{T_c}{T} L(T)\right)^3 \cdot \frac{1}{3} + O\left(\frac{T_c}{T} L(T)^5\right)$$

$$\Rightarrow L(T) = \frac{T_c}{T} L(T) - \left(\frac{T_c}{T}\right)^3 \frac{L(T)^3}{3} + O\left(\frac{T_c}{T} L(T)^5\right)$$

To order $L(T)^3$:

$$L(T) = \frac{T_c}{T} L(T) - \frac{T_c^3}{T^3} \frac{L(T)^3}{3}$$

$$\therefore \frac{T_c}{T} - \frac{T_c^3}{T^3} \frac{L(T)^2}{3} = 1$$

$$\therefore -\cancel{\frac{T_c^3}{T^3} \frac{L(T)^2}{3}} = 1 - \cancel{\frac{T_c}{T}} \qquad \frac{T^3}{T_c^3} - T_c$$

$$\therefore 1 - \frac{T_c}{T} = \frac{-T_c^3}{T^3} \frac{L(T)^2}{3}$$

$$\therefore \frac{T^3}{T_c^3} - \frac{T^3 T_c}{T T_c^3} = \frac{T^2}{T_c^2} \quad \frac{T^3}{T_c^3} - \frac{T^2}{T_c^2} = -\frac{L(T)^2}{3}$$

$$\therefore \frac{T^2}{T_c^2} - \frac{T^3}{T_c^3} = \frac{L(T)^2}{3}$$

$$\therefore \frac{3T^2}{T_c^2}\left(1 - \frac{T}{T_c}\right) = L(T)^2$$

$$\therefore L(T) = \sqrt{3\left(1 - \frac{T}{T_c}\right) \times \left(\frac{T}{T_c}\right)}$$

Since $\left(\frac{T}{T_c}\right)$ is small in this limit, we can set the prefactor $\left(\frac{T}{T_c}\right)$ to 1:

$$\therefore L(T) = \sqrt{3\left(1 - \frac{T}{T_c}\right)} \Rightarrow \underline{\underline{QED}}$$

b. Want to show that: for $\frac{T}{T_c} \ll 1$, we obtain:

$$L(T) = 1 - 2e^{-2T_c/T}$$

For this, we can write RHS of the expression for $L(T)$ ~~in~~ as:

$$\tanh\left(\frac{T_c}{T} L(T)\right) = \frac{e^{T_c/T} - e^{-T_c/T}}{e^{T_c/T} + e^{-T_c/T}}$$

(since ~~assuming~~ $L(T)$ is ≈ 1 ~~small~~).

~~For $\frac{T}{T_c} << 1$~~

Multiply previous expression by $\frac{e^{-T_c/T}}{e^{-T_c/T}}$

$$\Rightarrow L(T) = \frac{1 - e^{-2T_c/T}}{1 + e^{-2T_c/T}}$$

~~In the given limit,~~

$$\therefore L(T) = \left(1 - e^{-2T_c/T}\right)\left(1 + e^{-2T_c/T}\right)^{-1}$$

- Since $\cancel{\frac{T_c}{T}}$ $e^{-2T_c/T}$ is small, we can write this as: (by binomial expansion):

$$L(T) \approx \left(1 - e^{-2T_c/T}\right)\left(1 - e^{-2T_c/T}\right)$$

$$\therefore L(T) \approx 1 - 2e^{-2T_c/T} + O\left(\left(e^{-T_c/T}\right)^4\right)$$

$$\therefore L(T) \; 1 - 2e^{-2T_c/T} \quad \text{(neglecting higher order terms)}$$

c) Given that:

$$C(B=0, T) = \begin{cases} -\frac{1}{2} pNJ \left(\frac{\partial L^2(T)}{\partial T}\right) & T < T_c \\ 0 & T > T_c \end{cases}$$

It is evident that:

$$C(B=0,T) = -\frac{1}{2} pNJ \frac{\partial}{\partial T}\left(3\left(1-\frac{T}{T_c}\right)\right)$$

$$= -\frac{1}{2} pNJ \left(\frac{-3}{T_c}\right)$$

$$= \frac{3}{2} \frac{pNJ}{T_c} = \frac{3}{2} N k_B \quad (\text{since } pJ = k_B T_c)$$

(7) 1D Ising model with 3-valued spin: $\sigma_i = 0, \pm 1$

Determine if transition temperature exists.

Solution:

Partition function:

$$Z(\beta, B, N) = \sum_{\{\sigma = 0, \pm 1\}} e^{-\beta E(\{\sigma\})}$$

$$= \sum_{\sigma_1 = 0, \pm 1} \sum_{\sigma_2 = 0, \pm 1} \cdots \sum_{\sigma_N = 0, \pm 1} \exp\left(\beta \sum_{i=1}^{N} \left[J \sigma_i \sigma_{i+1} + \frac{1}{2} B (\sigma_i + \sigma_{i+1})\right]\right)$$

To compute this, introduce 3×3 transfer matrix.

$$\hat{T} = \begin{pmatrix} \langle \sigma_i = 0 | T | \sigma_i = 0 \rangle & \langle \sigma_i = 0 | T | \sigma_i = +1 \rangle & \langle \sigma_i = 0 | T | \sigma_i = -1 \rangle \\ \langle \sigma_i = +1 | T | \sigma_i = 0 \rangle & \langle \sigma_i = +1 | T | \sigma_i = +1 \rangle & \langle \sigma_i = +1 | T | \sigma_i = -1 \rangle \\ \langle \sigma_i = -1 | T | \sigma_i = 0 \rangle & \langle \sigma_i = -1 | T | \sigma_i = 1 \rangle & \langle \sigma_i = -1 | T | \sigma_i = -1 \rangle \end{pmatrix}$$

where $\langle \sigma_i | T | \sigma_{i+1} \rangle = \exp\left(\beta \left(J \sigma_i \sigma_{i+1} + \frac{B}{2} (\sigma_i + \sigma_{i+1})\right)\right)$

$$\hat{T} = \begin{pmatrix} 1 & e^{\beta B/2} & e^{-\beta B/2} \\ e^{\beta B/2} & e^{\beta (J+B)} & e^{-\beta J} \\ e^{-\beta B/2} & e^{-\beta J} & e^{\beta (J-B)} \end{pmatrix}$$

In order to compute $Tr(T^N)$ which gives the partition function, which ~~is~~ can be written as:

$$Z(\beta, B; N) = \mathrm{Tr}(T^N) = \lambda_+^N + \lambda_-^N + \lambda_0^N$$

Compute characteristic polynomial:

$$\begin{vmatrix} 1-\lambda & e^{\beta B/2} & e^{-\beta B/2} \\ e^{\beta B/2} & e^{\beta(J+B)} - \lambda & e^{-\beta J} \\ e^{-\beta B/2} & e^{-\beta J} & e^{\beta(J-B)} - \lambda \end{vmatrix}$$

$$\Rightarrow (e^{\beta J} - \lambda)^2 (1-\lambda) - 2(e^{\beta J} - \lambda) + 2e^{-\beta J} - e^{-2\beta J}(1-\lambda) = 0$$

Solving the above equation by Mathematica yields:

$$\lambda_0 = \frac{e^{2\beta J} - 1}{e^{\beta J}}, \quad \lambda_\pm = \frac{1 + e^{\beta J} + e^{2\beta J} \pm \sqrt{1 - 2e^{\beta J} + 11e^{2\beta J} - 2e^{3\beta J} + e^{4\beta J}}}{2e^{\beta J}}$$

The largest of the above roots is:

$$\lambda_+ = \frac{1 + e^{\beta J} + e^{2\beta J} + \sqrt{1 - 2e^{\beta J} + 11e^{2\beta J} - 2e^{3\beta J} + e^{4\beta J}}}{2e^{\beta J}}$$

This will contribute to the partition function

$$\therefore \cancel{Z(\beta)} \cancel{B} = \cancel{Z(\beta, B, N)}$$

$$\therefore Z(\beta) = \cancel{1+e}^{\cancel{2}} \lambda_+$$

$\therefore$ Compute thermodynamic parameters:

∴ Helmholtz free energy:

$$F = -k_B T \ln(Z):$$

$$= -k_B T \ln\left(\frac{1+e^{\beta J}+e^{2\beta J}+\sqrt{1-2e^{\beta J}+11e^{2\beta J}-2e^{3\beta J}+e^{4\beta J}}}{2e^{\beta J}}\right)$$

$$= -k_B T \ln\left(\frac{1}{2}e^{-\beta J}\left(1+e^{\beta J}+e^{2\beta J}-\sqrt{e^{2\beta J}\left(11-\cancel{\cos}\,4\cosh(\beta J)\right.}\right.\right.$$
$$\left.\left.\cancel{\sqrt{2\cosh(2J\beta)}}\right)\right)$$

$$\ldots + \underbrace{\sqrt{2\cosh(2J\beta)}}$$

this term is included under square root on previous line.

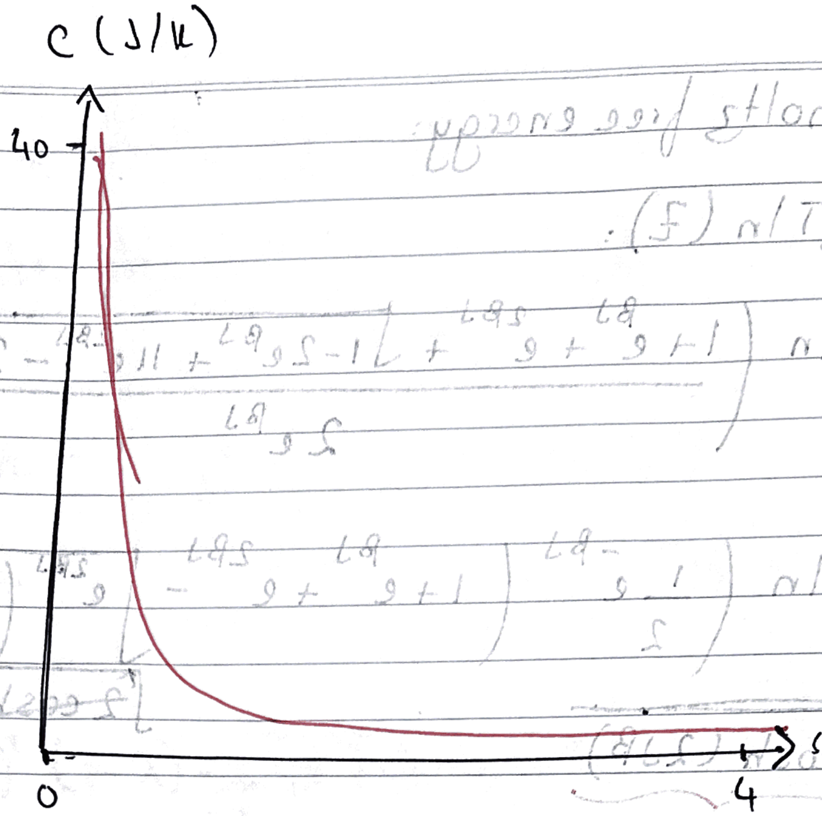
The heat capacity, C is defined as:

$$C = -T\left(\frac{\partial^2 F}{\partial T^2}\right)$$

$$\Rightarrow C = -T\frac{\partial^2}{\partial T^2}\left(-k_B T \ln(\lambda_+)\right)$$

Plotting this as a function of temperature using Mathematica yields the following:

(8)



From this, it is evident that there is no transition temperature. Furthermore, there is no magnetisation since the partition function is independent of B. (as the external field is vanishing).