Problem 1:

(a) $E_n = (n + \frac{1}{2})\hbar\omega$

We are considering a single quantum oscillator: $N=1$.

we have discrete energies: quantum

$\hookrightarrow$ 1D HO : $n = 0, 1, \ldots, \infty$

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

$\leftarrow$ using the canonical ensemble

this is the partition function

"normalization factor"

probability to find system in state n

Look at denominator:

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

$$= e^{-\beta\hbar\omega/2} \sum_{n=0}^{\infty} \underbrace{\left(e^{-\beta\hbar\omega}\right)}_{x}{}^{n}$$

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x}$$

using info from exam

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

$$\Rightarrow \boxed{P_n = e^{-n\beta\hbar\omega}\left(1 - e^{-\beta\hbar\omega}\right)}$$

(b) Since the temperature and the number of particles are fixed, I worked in the canonical ensemble.

In principle, we should be able to work in any ensemble. However, the ensembles can give differing results in the small particle limit, where particle number fluctuations are large compared to the number of particles. Here, we do not have a particle reservoir. Thus, we do not know how to "set" the chemical potential. Working in the micro-canonical ensemble is not trivial for answering this problem. In the microcanonical ensemble, all states are equally likely. To connect with the temperature, we would need to establish the connection between E and T.

Problem 2:

(a) $P = k_B T n - \frac{b}{2} n^2 + \frac{c}{6} n^3$ (*) $\quad b, c > 0$

$n = \frac{N}{V}$

Demand: $\frac{\partial P}{\partial V} = 0$ (**)

$\frac{\partial^2 P}{\partial V^2} = 0$ (***)

these two conditions ensure that the P-V curve for fixed T does not have a turning point.

We have three equations and three quantities to determine, namely $k_B T_c$, n_c, and P_c.

(b) Start with (*) and divide both sides by $\frac{1}{6}\frac{b^3}{c^2}$:

$$\frac{P}{P_c} = \frac{k_B T n}{\frac{1}{6}\frac{b^3}{c^2}} - \frac{b n^2}{2 \frac{1}{6}\frac{b^3}{c^2}} + \frac{c n^3}{6 \frac{1}{6}\frac{b^3}{c^2}}$$

$$\frac{c n^3}{6 \frac{1}{6}\frac{b^3}{c^2}} = \left(\frac{n}{n_c}\right)^3$$

$$\frac{b n^2}{2 \frac{1}{6}\frac{b^3}{c^2}} = \frac{n^2}{\frac{1}{3}\frac{b^2}{c^2}} = 3\left(\frac{n}{n_c}\right)^2$$

$$\frac{k_B T n}{\frac{1}{6}\frac{b^3}{c^2}} = \frac{k_B T}{\frac{1}{6}\frac{b^2}{c}} \cdot \frac{n}{\frac{b}{c}}, \qquad \frac{k_B T}{\frac{1}{6}\frac{b^2}{c}} = 3\frac{k_B T}{k_B T_c}, \qquad \frac{n}{\frac{b}{c}} = \frac{n}{n_c}$$

$$\Rightarrow \boxed{\frac{P}{P_c}} = 3\boxed{\frac{k_B T}{k_B T_c}\left(\frac{n}{n_c}\right)} - 3\boxed{\left(\frac{n}{n_c}\right)^2} + \boxed{\left(\frac{n}{n_c}\right)^3}$$

dimensionless ⇒ units are ok!

Add-on for (a):

$$P = k_B T \frac{N}{V} - \frac{b}{2}\left(\frac{N}{V}\right)^2 + \frac{c}{6}\left(\frac{N}{V}\right)^3$$

$$= k_B T N V^{-1} - \frac{b}{2} N^2 V^{-2} + \frac{c}{6} N^3 V^{-3}$$

$$\Rightarrow \frac{\partial P}{\partial V} = - k_B T N V^{-2} + b N^2 V^{-3} - \frac{c}{2} N^3 V^{-4} \quad (**')$$

$$\Rightarrow \frac{\partial^2 P}{\partial V^2} = 2 k_B T N V^{-3} - 3 b N^2 V^{-4} + 2 c N^3 V^{-5} \quad (***')$$

Set $(**')$ and $(***')$ to zero:

$$- k_B T N V^2 + b N^2 V - \frac{c}{2} N^3 = 0 \quad (**'')$$

$$2 k_B T N V^2 - 3 b N^2 V + 2 c N^3 = 0 \quad (***'')$$

Add: $2 \cdot (**'') + (***'')$: $- b N^2 V + c N^3 = 0$

$$\Rightarrow \frac{b}{c} = \frac{N}{V} = n \Rightarrow \boxed{n_c = \frac{b}{c}}$$

Rewrite $(**')$: $k_B T = b \underbrace{\left(\frac{N}{V}\right)}_{=\frac{b}{c}} - \frac{c}{2} \underbrace{\left(\frac{N^2}{V^2}\right)}_{=\frac{b^2}{c^2}} = \frac{b^2}{c} - \frac{1}{2}\frac{b^2}{c}$

$$\Rightarrow \boxed{k_B T_c = \frac{1}{2}\frac{b^2}{c}}$$

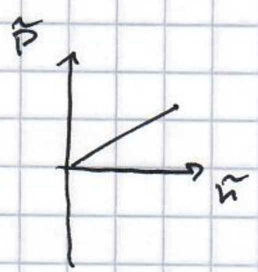
Plug into $(*)$: $P_c = \frac{1}{2}\frac{b^2}{c}\frac{b}{c} - \frac{b}{2}\left(\frac{b}{c}\right)^2 + \frac{c}{6}\left(\frac{b}{c}\right)^3 \Rightarrow \boxed{\frac{1}{6}\frac{b^3}{c^2} = P_c}$

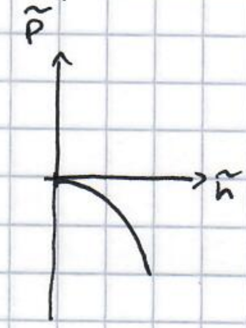
(c)

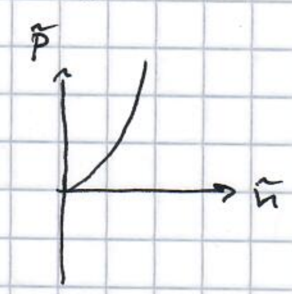
$$\frac{P}{P_c} = 3 \, \frac{k_B T}{k_B T_c} \, \frac{n}{n_c} - 3 \left(\frac{n}{n_c}\right)^2 + \left(\frac{n}{n_c}\right)^3$$

$$\tilde{P} = 3 \, \tilde{T} \, \tilde{n} - 3 \, \tilde{n}^2 + \tilde{n}^3$$

linear | quadratic | cubic



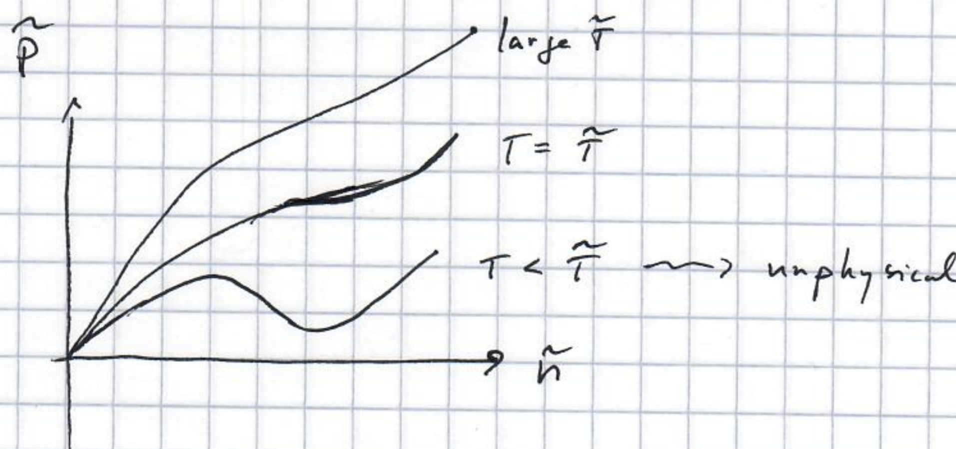




small $\tilde{n}$: linear term dominates

large $\tilde{n}$: cubic term dominates

intermediate $\tilde{n}$: the quadratic term can lead to a "turn-around"



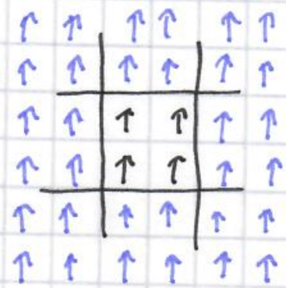
Problem 3:

Ising model Hamiltonian $\mathcal{H} = -J \sum_{(i,j)} s_i s_j \underbrace{- B \sum_i s_i}_{\text{this problem: } B=0}$

only nearest neighbor interactions

We are considering a 2×2 lattice with periodic boundary conditions.

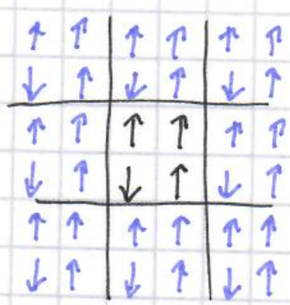
(a) Let's consider a configuration with four up spins:



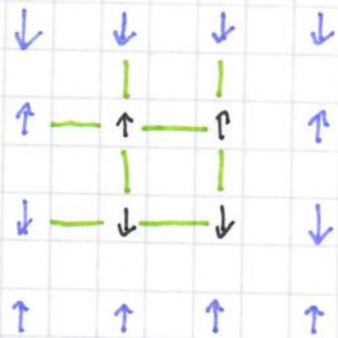
The black spins show the actual system (2×2 lattice)

The purple spins show replica (or "image" boxes) that shift the black box down, up, to the left/right, ...

Different example:



How many nearest neighbor interactions does the 2×2 square lattice have?

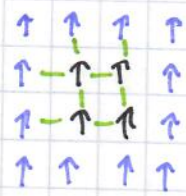


Each of the green lines corresponds to a NN (nearest neighbor) interaction.

Note: I used the "images" to the left and the top to "connect" the actual 2×2 box with the images. If I had used the right and top images instead, I would have obtained the same result.

(b) Let's write down (using pictures) the allowed microstates and then make a table.

4 spins up:



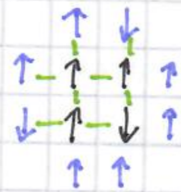
$E = -8J$

deg. = 1

$\langle M \rangle = 4$

$\langle M^2 \rangle = 16$

3 spins up:

 or $\begin{matrix}\uparrow & \uparrow \\ \downarrow & \uparrow\end{matrix}$ or $\begin{matrix}\uparrow & \downarrow \\ \uparrow & \uparrow\end{matrix}$ or $\begin{matrix}\downarrow & \uparrow \\ \uparrow & \uparrow\end{matrix}$

4 $\uparrow - \downarrow$ interactions and 4 $\uparrow - \uparrow$ interactions

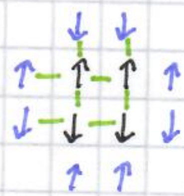
$\Rightarrow E = -4J + 4J = 0$

$\langle M \rangle = 2$

$\langle M^2 \rangle = 4$

degeneracy = 4

2 spins up:

a  or $\begin{matrix}\downarrow & \downarrow \\ \uparrow & \uparrow\end{matrix}$ or $\begin{matrix}\uparrow & \downarrow \\ \uparrow & \downarrow\end{matrix}$ or $\begin{matrix}\downarrow & \uparrow \\ \downarrow & \uparrow\end{matrix}$

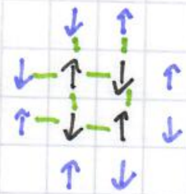
4 $\uparrow - \downarrow$ and 4 $\uparrow - \uparrow / \downarrow - \downarrow$ interactions

$\Rightarrow E = 0$

$\langle M \rangle = 0$

$\langle M^2 \rangle = 0$

degeneracy 4

(b)  or $\begin{matrix}\downarrow & \uparrow \\ \uparrow & \downarrow\end{matrix}$

8 ↑-↓ interactions

$\Rightarrow E = 8J$

$\langle M \rangle = 0$

$\langle M^2 \rangle = 0$

degeneracy $= 2$

1 spin up: same as 3 spins up

$E = 0$

$\langle M \rangle = -2$ (this differs from 3 spin-up case)

$\langle M^2 \rangle = 4$

degeneracy $= 4$

0 spin up: similar to 4 spins up

$E = -8J$

deg. $= 1$

$\langle M \rangle = -4$

$\langle M^2 \rangle = 16$

Let's collect the information in a table:

# of ↑ spins	E/J	deg.	$\langle M \rangle$	$\langle M^2 \rangle$
4	−8	1	4	16
3	0	4	2	4
2	0	4	0	0
	8	2	0	0
1	0	4	−2	4
0	−8	1	−4	16

16 microstates

So, the number of allowed microstates is 16.

(c) Let's calculate Q_N:

$$Q_N = \sum_j e^{-\beta E_j}$$

(j goes from 1 to 16; sum over all microstates)

$$Q_N = 2e^{8\beta J} + 2e^{-8\beta J} + 12$$

How do we obtain $\langle \mathcal{H} \rangle$?

$$U = \left(-\frac{\partial}{\partial \beta} Q_N\right) \Big/ Q_N = \frac{16J\left(e^{8\beta J} - e^{-8\beta J}\right)}{2e^{8\beta J} + 2e^{-8\beta J} + 12}$$

How do we obtain U^2 ?

$$U^2 = \left(\frac{\partial^2}{\partial \beta^2} Q_N\right) \Big/ Q_N$$

$$= \frac{8 \cdot 16\, J^2 \left(e^{8\beta J} + e^{-8\beta J}\right)}{2e^{8\beta J} + 2e^{-8\beta J} + 12}$$

$$= \frac{64\, J^2 \left(e^{8\beta J} + e^{-8\beta J}\right)}{e^{8\beta J} + e^{-8\beta J} + 6}$$

What about $\langle M \rangle$?

M_j is the magnetization of microstate j w/ energy E_j

$$\langle M \rangle = \frac{\sum_j M_j\, e^{-\beta E_j}}{\sum_j e^{-\beta E_j}}$$

$$= \frac{4e^{8\beta J} + 4 \cdot 2 - 4 \cdot 2 - 4e^{8\beta J}}{2e^{8\beta J} + 2e^{-8\beta J} + 12} = 0$$

What about $\langle M^2 \rangle$?

$$\langle M^2 \rangle = \frac{\sum_j M_j^2\, e^{-\beta E_j}}{\sum_j e^{-\beta E_j}}$$

$$= \frac{2 \cdot 16\, e^{8\beta J} + 8 \cdot 4}{2e^{8\beta J} + 2e^{-8\beta J} + 12} = \frac{16\left(e^{8\beta J} + 1\right)}{e^{8\beta J} + e^{-8\beta J} + 6}$$

Problem 4:

$$\hat{\mathcal{H}} = -\mu_B \, \vec{\hat{\sigma}} \cdot \vec{B} \qquad \text{for (a) } \vec{B} = \begin{pmatrix} 0 \\ 0 \\ B \end{pmatrix} \Rightarrow \hat{\mathcal{H}} = -\mu_B B \hat{\sigma}_z$$

$$\text{for (b) } \vec{B} = \begin{pmatrix} B \\ 0 \\ 0 \end{pmatrix} \Rightarrow \hat{\mathcal{H}} = -\mu_B B \hat{\sigma}_x$$

We want $\hat{\rho}_{can}$ and $\langle \hat{\mathcal{H}} \rangle = Tr\left(\hat{\rho}_{can} \hat{\mathcal{H}}\right)$.

$$\hat{\rho}_{can} = \frac{1}{Q} \underbrace{\sum_k}_{\text{sum over all eigenstates}} e^{-\beta E_k} |k\rangle\langle k|$$

(a) $\hat{\mathcal{H}} = -\mu_B B \hat{\sigma}_z$ $\qquad$ Need: $e^{-\beta \hat{\mathcal{H}}} = e^{-\beta \hat{\mathcal{H}}} \overset{\text{identity}}{\hat{\mathbb{1}}} = e^{-\beta \hat{\mathcal{H}}} \Big(\underbrace{|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|}_{\text{complete set of basis states}} \Big)$

→ eigenenergies are: $-\mu_B B$ for state $|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$\mu_B B$ $\qquad$ $|\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$$\Rightarrow \hat{\rho}_{can} = \frac{1}{Q}\left(e^{\beta \mu_B B} |\uparrow\rangle\langle\uparrow| + e^{-\beta\mu_B B} |\downarrow\rangle\langle\downarrow| \right)$$

$$\text{with } Q = e^{\beta\mu_B B} + e^{-\beta\mu_B B}$$

(b) $\hat{\mathcal{H}} = -\mu_B B \hat{\sigma}_x$

eigenvalues of $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$$\det\begin{pmatrix} -\lambda & 1 \\ 1 & -\lambda \end{pmatrix} = 0 \Rightarrow \lambda^2 - 1 = 0$$

$$\Rightarrow \lambda = \pm 1$$

$\lambda = 1$: $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} u \\ v \end{pmatrix} \Rightarrow u = v \Rightarrow |+\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right)$

$\lambda = -1$: $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = -\begin{pmatrix} u \\ v \end{pmatrix} \Rightarrow u = -v \Rightarrow |-\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle - |\downarrow\rangle\right)$

$\Rightarrow$ eigenenergies are: $-\mu_B B$ for state $|+\rangle$

$\mu_B B$ for state $|-\rangle$

$$\Rightarrow \hat{\rho}_{can} = \frac{1}{Q}\left(e^{\beta \mu_B B} |+\rangle\langle+| + e^{-\beta\mu_B B} |-\rangle\langle-| \right)$$

these are the eigen-states of $\hat{\sigma}_x$!

Q is the same as above

(c) let $\vec{B} = \begin{pmatrix} 0 \\ 0 \\ B \end{pmatrix}$

$$\Rightarrow \langle \hat{\mathcal{H}} \rangle = \frac{1}{Q}\left(-\mu_B B e^{\beta\mu_B B} + \mu_B B e^{-\beta\mu_B B} \right)$$

for $\vec{B} = \begin{pmatrix} B \\ 0 \\ 0 \end{pmatrix}$, the answer is the same (we can argue by rotating the system – alternatively, we can do the calculation).

$$\langle \hat{\mathcal{H}} \rangle = \frac{1}{Q}\left(-\mu_B B \underbrace{|\langle+|+\rangle|^2}_{=1} e^{+\beta\mu_B B} + \mu_B B \underbrace{|\langle-|-\rangle|^2}_{=1} e^{-\beta\mu_B B} \right)$$

I'm using the $|+\rangle, |-\rangle$ basis:

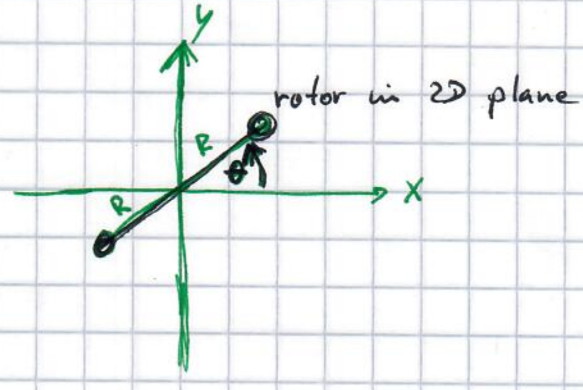
$$\sum_{|a\rangle = |+\rangle, |-\rangle} |a\rangle\langle a| \, e^{-\beta E_a}$$

So: $\langle \hat{\mathcal{H}} \rangle = \frac{1}{Q}\left(-\mu_B B e^{\beta\mu_B B} + \mu_B B e^{-\beta\mu_B B} \right)$

Problem 5:

(a)

$$\hat{\mathcal{H}} = -\frac{\hbar^2}{2J}\frac{d^2}{d\theta^2}$$



$\psi_l \propto e^{il\theta}$ → we require: $e^{il\theta} = e^{il(\theta+2\pi)}$

not normalized

$\Rightarrow e^{il2\pi} = 0$

$\Rightarrow l = 0, \pm 1, \pm 2, \ldots$

$$E_l = \frac{\hbar^2 l^2}{2J}$$

(b)

$$\hat{\rho}_{can} = \frac{1}{Q}\sum_{l=-\infty}^{\infty} |\psi_l\rangle\langle\psi_l| \, e^{-\beta E_l}$$

E_l is given above

ψ_l is given above but we need to normalize:

$$\psi_l(\theta) = \frac{1}{\sqrt{2\pi R}} e^{il\theta}$$

$$Q = \sum_{l=-\infty}^{\infty} e^{-\beta\frac{\hbar^2 l^2}{2J}}$$

(c)

valid for large T → $\approx \int_{-\infty}^{\infty} e^{-\beta\frac{\hbar^2 l^2}{2J}} \, dl$

$$= \sqrt{\pi}\sqrt{\frac{2J}{\beta\hbar^2}} = \sqrt{\frac{2\pi J}{\hbar^2}}\sqrt{k_B T}$$

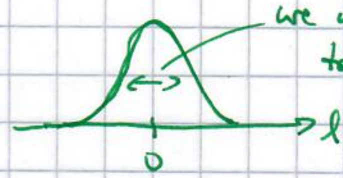
Let's look at the approximate sign:

write $e^{-\beta\frac{\hbar^2 l^2}{2J}}$ in terms of width:

$$\exp\left(-\beta\frac{\hbar^2 l^2}{2J}\right) = \exp\left(-\frac{\beta\hbar^2}{2J}l^2\right)$$

$$= \exp\left(-\frac{l^2}{\frac{2J}{\beta\hbar^2}}\right)$$

Gaussian in l:



we want this width to be much larger than 1 (to convert sum into integral)

$$\Rightarrow \frac{2J}{\beta\hbar^2} \gg 1 \quad \text{or} \quad \underbrace{k_B T \gg \frac{\hbar^2}{2J}}_{\text{temperature much larger than the typical energy level spacing}}$$

(d) The $T \to 0$ limit is governed by $l = 0$ energy state:

$$\hat{\rho}_{can} = |0\rangle\langle 0| \quad \text{and } Q = 1$$