Graduate stat. Mech

HW # 5 - solution

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① 1D H.O with $H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2$

a) $Q_{classical} = \frac{1}{\tau} \int dq\, dp\, e^{-\beta H}$

$$= \frac{1}{\tau} \int_{-\infty}^{\infty} dq\, e^{-\frac{\beta m\omega^2 q^2}{2}} \int_{-\infty}^{\infty} dp\, e^{-\frac{\beta p^2}{2m}}$$

$$= \frac{1}{\tau} \left(\frac{\pi}{\beta m\omega^2/2} \right)^{1/2} \left(\frac{\pi}{\beta/2m} \right)^{1/2} = \frac{1}{\tau} \frac{2\pi}{\beta\omega} = \frac{2\pi}{\beta \tau \omega}$$

b) $Q_{quantum} = \sum_{n=0}^{\infty} e^{-\beta E_n}$; $E_n = (n + 1/2)\hbar\omega$; $n = 0, 1, 2 \dots$

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

$$= e^{-\beta \frac{\hbar\omega}{2}} \frac{1}{1 - e^{-\beta\hbar\omega}}$$; using $\sum_{n=0}^{\infty} x^n = \frac{1}{1-x}$

c) when $\beta \Rightarrow 0$, $e^{-\beta\hbar\omega} \approx 1 - \beta\hbar\omega$

$$\Rightarrow Q_{quantum} \approx \frac{1}{1 - 1 + \beta\hbar\omega} = \frac{1}{\beta \frac{h}{2\pi}\omega} = \frac{2\pi}{\beta h \omega}$$

compare with $Q_{classical}$, we get $\tau = h$

Planck's constant

② a) for a single spin $Q_1 = \sum_s e^{-\beta E_s} = e^{\beta \mu_0 B} + e^{-\beta \mu_0 B}$

for N spins $Q_N = Q_1^N = (e^{\beta \mu_0 B} + e^{-\beta \mu_0 B})^N$

b) $\langle M \rangle = -\frac{1}{\beta} \frac{\partial}{\partial B} \ln Q_N$; $\ln Q_N = N \ln (e^{\beta \mu_0 B} + e^{-\beta \mu_0 B})$

$= N \ln 2 \cosh (\beta \mu_0 B)$

$$= -\frac{N}{\beta} \left[\frac{2 \beta \mu_0 \sinh (\beta \mu_0 B)}{2 \cosh (\beta \mu_0 B)} \right]$$

$$= -\frac{N}{\beta} \beta \mu_0 \tanh (\beta \mu_0 B) = - N \mu_0 \tanh (\beta \mu_0 B)$$

c) $\langle M^2 \rangle - \langle M \rangle^2 = \frac{1}{\beta^2} \frac{\partial^2}{\partial B^2} \ln Q_N$

Now $\frac{\partial}{\partial B} \ln Q_N = N \frac{2 \beta \mu_0 \sinh (\beta \mu_0 B)}{2 \cosh (\beta \mu_0 B)} = N \beta \mu_0 \tanh (\beta \mu_0 B)$

$$\frac{\partial^2}{\partial B^2} \ln Q_N = N \beta \mu_0 \quad \operatorname{sech}^2 (\beta \mu_0 B) \times \beta \mu_0$$

$$= N \beta^2 \mu_0^2 \operatorname{sech}^2 (\beta \mu_0 B)$$

$$= \frac{N \beta^2 \mu_0^2}{\cosh^2 (\beta \mu_0 B)}$$

$$\Rightarrow \langle M^2 \rangle - \langle M \rangle^2 = \frac{N \mu_0^2}{\cosh^2 (\beta \mu_0 B)} = \frac{4 N \mu_0^2}{(e^{\beta \mu_0 B} + e^{-\beta \mu_0 B})^2}$$

③ Pathria 5.1

In the normal representation where the field is applied in the z-direction, the Pauli matrices are

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Note that $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1$, meaning the eigenvalues of σ_x is ± 1, , for σ_y ± 1, and for σ_z ± 1. we note also that in this representation only σ_z is diagonal, i.e the diagonal elements represent the eigenvalues and the off diagonal elements are all zeros.

in this representation, $\rho = \dfrac{e^{-\beta H}}{\mathrm{Tr}\, e^{-\beta H}}$; $H = -\mu_B \vec{\sigma}\cdot\vec{B}$

$$= -\mu_B \sigma_z B$$

$$= \begin{pmatrix} -\mu_B B & 0 \\ 0 & \mu_B B \end{pmatrix}$$

$$\Rightarrow \rho = \frac{1}{e^{\beta\mu_B B} + e^{-\beta\mu_B B}} \begin{pmatrix} e^{\beta\mu_B B} & 0 \\ 0 & e^{-\beta\mu_B B} \end{pmatrix}$$

and $\langle \sigma_z \rangle = \mathrm{Tr}(\rho\sigma_z)$

$$= \mathrm{Tr}\, \frac{1}{e^{\beta\mu_B B} + e^{-\beta\mu_B B}} \begin{pmatrix} e^{\beta\mu_B B} & 0 \\ 0 & e^{-\beta\mu_B B} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$= \frac{e^{\beta\mu_B B} - e^{-\beta\mu_B B}}{e^{\beta\mu_B B} + e^{-\beta\mu_B B}} = \tanh(\beta\mu_B B) \quad \text{--- (1)}$$

Now to transfer to a new representation when σ_x is diagonal, we apply the unitary transformation U

where $u = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & +1 \\ -1 & 1 \end{pmatrix}$; $u^{+} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$; $uu^{+} = I$

in the new representation $\sigma_x \to \sigma_x'$, $\sigma_y \to \sigma_y'$, $\sigma_z \to \sigma_z'$

$$\sigma_x' = u\sigma_x u^{+} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2 & 0 \\ 0 & -2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Note that in the new representation, σ_x' is diagonal

similarly $\sigma_y' = u\sigma_y u^{+} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ and $\sigma_z' = u\sigma_z u^{+} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

Note that in this rep, σ_z is no longer diagonal and σ_y is still not diagonal.

Now $\rho \to \rho' = u\rho u^{+} = \dfrac{1}{e^{\beta\mu_B B} + e^{-\beta\mu_B B}}\begin{pmatrix} \cosh(\beta\mu_B B) & -\sinh(\beta\mu_B B) \\ -\sinh(\beta\mu_B B) & \cosh(\beta\mu_B B) \end{pmatrix}$

$$= \frac{1}{2}\begin{pmatrix} 1 & -\tanh(\beta\mu_B B) \\ -\tanh(\beta\mu_B B) & 1 \end{pmatrix}$$

in this new rep, we have

$$\langle \sigma_z' \rangle = Tr(\rho'\sigma_z') = \frac{2\sinh(\beta\mu_B B)}{e^{\beta\mu_B B} + e^{-\beta\mu_B B}} = \tanh(\beta\mu_B B) \quad \text{--(2)}$$

same result in the old representation i.e $\langle \sigma_z \rangle = \langle \sigma_z' \rangle$

<u>Remark!</u> to go to a new representation where σ_y is diagonal, we use the unitary transformation

$u = \frac{1}{2}\begin{pmatrix} 1-i & 1+i \\ -1+i & 1+i \end{pmatrix}$; $u^{+} = \frac{1}{2}\begin{pmatrix} 1+i & -1-i \\ 1-i & 1-i \end{pmatrix}$

check that $uu^{+} = I$, find ρ' and $\langle \sigma_z' \rangle$ in this representation

④ a) $\rho = 1/2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

$S_x = \frac{\hbar}{2}\sigma_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$; $S_y = \frac{\hbar}{2}\sigma_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$,

and $S_z = \frac{\hbar}{2}\sigma_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$\langle S_z \rangle = Tr\, \rho S_z = Tr\, \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar}{4}\, Tr \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
$= 0$

similarly $\langle S_y \rangle = \langle S_x \rangle = 0$

meaning, the electrons beam is not polarized in any direction. Note that the density matrix has equal probabilities for spin up and spin down stated.

b) $\rho = 1/2 \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}$

$\langle S_x \rangle = \langle S_z \rangle = 0$;

$\langle S_y \rangle = \frac{\hbar}{2}$

the electrons beam is 100 % polarized in the y direction; more precisly in the + y direction.

(5) $\chi_{n+} = \begin{pmatrix} e^{-i\phi/2} \cos\frac{\theta}{2} \\ e^{i\phi/2} \sin\frac{\theta}{2} \end{pmatrix}$; $\rho = |\chi_{n+}\rangle\langle\chi_{n+}|$

a)

$$\rho = \underbrace{\begin{pmatrix} e^{-i\phi/2} \cos\frac{\theta}{2} \\ e^{i\phi/2} \sin\theta/2 \end{pmatrix}}_{2\times 1} \underbrace{\begin{pmatrix} e^{i\phi/2} \cos\frac{\theta}{2} & e^{-i\phi/2} \sin\frac{\theta}{2} \end{pmatrix}}_{1\times 2} \rightarrow 2\times 2$$

$$= \begin{pmatrix} \cos^2\frac{\theta}{2} & e^{-i\phi} \sin\frac{\theta}{2}\cos\frac{\theta}{2} \\ e^{i\phi} \sin\frac{\theta}{2}\cos\frac{\theta}{2} & \sin^2\frac{\theta}{2} \end{pmatrix},$$ see that $\mathrm{Tr}\,\rho = 1$

b)

$\rho_z(\theta = 0, \phi = 0) \Rightarrow \rho_z = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$

$\rho_x(\theta = \frac{\pi}{2}, \phi = 0) \Rightarrow \rho_x = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$

$\rho_y(\theta = \frac{\pi}{2}, \phi = \frac{\pi}{2}) \Rightarrow \rho_y = \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}$

c) $\rho_y = \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}$

$$\langle S_y \rangle = \mathrm{Tr}\,\rho_y S_y = \mathrm{Tr}\,\frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{\hbar}{4}\mathrm{Tr}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}$$

$$= \frac{\hbar}{4} \cdot \times 2 = \frac{\hbar}{2}$$

$$\langle S_x \rangle = \mathrm{Tr}\,\rho_y S_x = \mathrm{Tr}\,\frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \cdot \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$= \frac{\hbar}{4}\mathrm{Tr}\begin{pmatrix} -i & 1 \\ 1 & i \end{pmatrix} = 0$$

$$\langle S_z \rangle = \mathrm{Tr}\,\rho_y S_z = \mathrm{Tr}\,\frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \cdot \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$= 0$ as expected for a beam polarized in the y direction

⑥ $\rho = A e^{-H/k_B T}$; $H|n\rangle = E_n|n\rangle$; $E_n = (n+1/2)\hbar\omega$

$n = 0, 1, 2, \ldots$

a) $\sum \rho_{nn} = 1 \Rightarrow$ where $\rho_{nn} = \langle n|\rho|n\rangle$

$= A e^{-(n+1/2)\hbar\omega/k_B T}$

Normalization

$$A \sum_n e^{-(n+1/2)\hbar\omega/k_B T} = 1 \Rightarrow A e^{-\frac{\hbar\omega}{2k_B T}} \underbrace{\sum_n \left(e^{-\frac{\hbar\omega}{k_B T}}\right)^n}_{\frac{1}{1-x}} = 1$$

$$\Rightarrow A e^{-\frac{\hbar\omega}{2k_B T}} \frac{1}{1 - e^{-\hbar\omega/k_B T}} = 1$$

Geometric Series

$$\sum_n x^n = \frac{1}{1-x}$$

$$\Rightarrow A = \frac{1 - e^{-\hbar\omega/k_B T}}{e^{-\hbar\omega/2k_B T}}$$

b) $$\rho_{nn} = \frac{1 - e^{-\hbar\omega/k_B T}}{e^{-\hbar\omega/2k_B T}} \cdot e^{-(n+1/2)\hbar\omega/k_B T}$$

$$= \frac{1 - e^{-\hbar\omega/k_B T}}{\cancel{e^{-\hbar\omega/2k_B T}}} \cancel{e^{-\frac{\hbar\omega}{2k_B T}}} \cdot e^{-n\frac{\hbar\omega}{k_B T}}$$

$$= \left(1 - e^{-\frac{\hbar\omega}{k_B T}}\right) e^{-n\hbar\omega/k_B T}$$

c) $\langle E \rangle = \mathrm{Tr}(\rho E_n) = \mathrm{Tr}\ (1-e^{-\frac{\hbar\omega}{k_BT}})e^{-n\frac{\hbar\omega}{k_BT}}(n+1/2)\hbar\omega$

$$= \mathrm{Tr}\,(1-e^{-\frac{\hbar\omega}{k_BT}})e^{-n\frac{\hbar\omega}{k_BT}} \cdot \frac{1}{2}\hbar\omega$$

$$+ \mathrm{Tr}\,(1-e^{-\frac{\hbar\omega}{k_BT}})e^{-n\frac{\hbar\omega}{k_BT}}\, n\hbar\omega$$

$$= \frac{1}{2}\hbar\omega(1-e^{-\frac{\hbar\omega}{k_BT}}) \underbrace{\sum_{n=0}^{\infty}\left(e^{-\frac{\hbar\omega}{k_BT}}\right)^n}_{\to \frac{1}{1-x}}$$

$$+ (1-e^{-\frac{\hbar\omega}{k_BT}})\hbar\omega \underbrace{\sum_{n=0}^{\infty} n\left(e^{-\frac{\hbar\omega}{k_BT}}\right)^n}_{\to \frac{x}{(1-x)^2}}$$

$$= \frac{1}{2}\hbar\omega\,\cancel{(1-e^{-\frac{\hbar\omega}{k_BT}})} \cdot \frac{1}{\cancel{(1-e^{-\frac{\hbar\omega}{k_BT}})}}$$

$$+ \cancel{(1-e^{-\frac{\hbar\omega}{k_BT}})}\,\frac{\hbar\omega\, e^{-\frac{\hbar\omega}{k_BT}}}{(1-e^{-\frac{\hbar\omega}{k_BT}})^{\cancel{2}}}$$

$$= \frac{1}{2}\hbar\omega + \frac{\hbar\omega\, e^{-\hbar\omega/k_BT}}{1-e^{-\hbar\omega/k_BT}}$$

$$= 1/2\,\hbar\omega + \hbar\omega/(e^{\hbar\omega/k_BT}-1)$$

$$= \hbar\omega\left[1/2 + \frac{1}{e^{\hbar\omega/k_BT}-1}\right]$$