EX. 1 (27/10/2011) (T.CM)

- DETERMINE THE PARTITION FUNCTION $Z = Z(\beta)$ IN THE CANONICAL ENSEMBLE FOR A ONE-DIMENSIONAL HARMONIC OSCILLATOR WITH FREQUENCY ω.

  DETERMINE ALSO $\langle E \rangle$, $\Delta E = \sqrt{\langle E^2 \rangle - \langle E \rangle^2}$, AND THE ENTROPY S.

- CONSIDER THE CASE IN WHICH A PARTICLE CAN BE DESCRIBED BY THE HILBERT-SPACE $\{|E_1\rangle, |E_2\rangle, |E_3\rangle\}$

  DETERMINE $Z(\beta)$ (CANONICAL), THE ENERGY AND THE ENTROPY.

- CONSIDER THE POTENTIAL

  $$V(x) = \frac{1}{2} m \omega_1^2 x^2 + \frac{1}{2} m \omega_2^2 y^2 + \frac{1}{2} m \omega_3^2 z^2$$

  DETERMINE $Z(\beta)$ FOR A SINGLE PARTICLE (CANONICAL).

- CONSIDER THE HILBERT-SPACE $\{|+\rangle, |-\rangle\}$ (SPIN OF A SINGLE ELECTRON). CONSIDER:

  $$Z = \langle + | e^{-\gamma S_z} | + \rangle + \langle - | e^{-\gamma S_z} | - \rangle \qquad S_z |+\rangle = \frac{1}{2} |+\rangle$$
  $$S_z |-\rangle = -\frac{1}{2} |-\rangle$$

  DETERMINE THE PROBABILITY THAT THE SYSTEM IS DESCRIBED BY $|+\rangle$ ($P_{|+\rangle}$) OR BY $|-\rangle$ ($P_{|-\rangle}$).

  IN WHICH LIMIT DOES $P_{|+\rangle} = 1$ HOLD?

  IN WHICH CASE $P_{|+\rangle} = P_{|-\rangle}$?

SOL. 1

$$E_n = \omega (n + 1/2)$$

$$Z(\beta) = \sum_{n=0}^{\infty} e^{-\beta E_n} = \sum_{n=0}^{\infty} e^{-\beta\omega \cdot n} e^{-\beta\omega/2}$$

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

Note, for very small β one has $Z \sim \frac{1}{\beta\omega} = \frac{T}{\omega}$

For very large β (small T) $\to Z \simeq e^{-\beta\omega/2} = e^{-\omega/2T}$

$$P_n = \frac{e^{-\beta(n+1/2)\omega}}{Z} = \frac{e^{-\beta\omega n} \cancel{e^{-\beta 1/2 \omega}}}{\cancel{e^{-\beta\omega/2}}} \left(1 - e^{-\beta\omega}\right) = e^{-\beta\omega n}\left(1 - e^{-\beta\omega}\right).$$

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

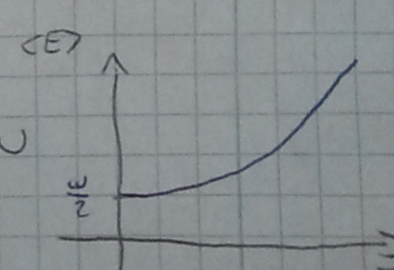
$$\ln Z = \ln\left(\frac{e^{-\beta\omega/2}}{1 - e^{-\beta\omega}}\right) = -\beta\omega/2 - \ln\left(1 - e^{-\beta\omega}\right)$$

$$\partial_\beta \ln Z = -\omega/2 - \frac{\left[-(-\omega) e^{-\beta\omega}\right]}{1 - e^{-\beta\omega}}$$

$$\boxed{\langle E \rangle = \frac{\omega}{2} + \omega \frac{e^{-\beta\omega}}{1 - e^{-\beta\omega}}}$$

$\beta = \infty \quad \langle E \rangle = \omega$

$\beta = 0 \quad \langle E \rangle = \infty$



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

$$= -\omega\,\frac{-\omega e^{-\beta\omega}(1-e^{-\beta\omega}) - (-(-\omega)e^{-\beta\omega})e^{-\beta\omega}}{(1-e^{-\beta\omega})^2}$$

$$= \omega\,\frac{\omega e^{-\beta\omega}(1-e^{-\beta\omega}) + \omega e^{-\beta\omega}\, e^{-\beta\omega}}{(1-e^{-\beta\omega})^2}$$

$$= \omega^2\,\frac{e^{-\beta\omega}}{(1-e^{-\beta\omega})^2}$$

$$\boxed{\Delta E = \omega\,\frac{e^{-\beta\omega/2}}{(1-e^{-\beta\omega})}}$$

$$S = \ln Z + \beta\langle E\rangle$$

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

$$\boxed{S = \beta\omega\frac{e^{-\beta\omega}}{1-e^{-\beta\omega}} - \ln(1-e^{-\beta\omega})}$$

2) 3 states only: $\{|E_1\rangle, |E_2\rangle, |E_3\rangle\}$

$$Z = e^{-\beta E_1} + e^{-\beta E_2} + e^{-\beta E_3}.$$

$$P_1 = \frac{e^{-\beta E_1}}{Z}, \quad P_2 = \frac{e^{-\beta E_2}}{Z}, \quad P_3 = \frac{e^{-\beta E_3}}{Z}.$$

$$\langle E \rangle = E_1 P_1 + E_2 P_2 + E_3 P_3 =$$

$$= \frac{E_1 e^{-\beta E_1} + E_2 e^{-\beta E_2} + E_3 e^{-\beta E_3}}{Z}$$

or alternatively,

$$-\partial_\beta \ln Z = -\frac{\partial Z}{\partial \beta} \cdot \frac{1}{Z} = \frac{1}{Z}\left(E_1 e^{-\beta E_1} + E_2 e^{-\beta E_2} + E_3 e^{-\beta E_3}\right) \checkmark.$$

$$S = \ln Z + \beta \langle E \rangle =$$

$$= \ln\left(e^{-\beta E_1} + e^{-\beta E_2} + e^{-\beta E_3}\right) + \frac{\beta}{Z}\left(E_1 e^{-\beta E_1} + E_2 e^{-\beta E_2} + E_3 e^{-\beta E_3}\right).$$

3)

$$Z = \frac{e^{-\beta\omega_1/2}}{(1-e^{-\beta\omega_1})} \cdot \frac{e^{-\beta\omega_2/2}}{(1-e^{-\beta\omega_2})} \frac{e^{-\beta\omega_3/2}}{(1-e^{-\beta\omega_3})}$$

$$= \frac{e^{-\beta(\omega_1+\omega_2+\omega_3)/2}}{(1-e^{-\beta\omega_1})(1-e^{-\beta\omega_2})(1-e^{-\beta\omega_3})} .$$

4)

$$Z = e^{-\gamma/2} + e^{\gamma/2} .$$

$$P_{|+\rangle} = \frac{e^{\gamma/2}}{Z}$$

$$P_{|-\rangle} = \frac{e^{-\gamma/2}}{Z}$$

$P_{|+\rangle} = 1$ holds for $\gamma = -\infty$. $P_{|-\rangle} = 1$ for $\gamma = +\infty$.

$P_{|+\rangle} = P_{|-\rangle}$ for $\gamma = 0$ (equiprobables).