Quantum versus classical

Let the classical Hamiltonian be

$$\mathcal{H} = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2$$ $\rightsquigarrow$ 1D harmonic oscillator (single particle)

For the same system, let us assume that the quantum mechanical energy levels are given by

$$E_n = a + b\,n \quad , \text{ where } n = 0, 1, 2, \ldots$$

We do, of course, know what "a" and "b" are! However, for this problem, we will assume that we do not know what the values of these constants are.

(a) Compute the classical partition function Q_{cl} (canonical ensemble).

(b) Compute the quantum partition function Q_{qm} (also canonical ensemble) and determine b by matching Q_{qm} to Q_{cl} as high temperature.

(c) Compute the quantum mechanical energy in the canonical ensemble and expand the result for $\beta \to 0$; keep the leading two terms. Then match to the classical energy to find a.

(a)

We want to calculate

$$Q_{cl}(T) = \frac{1}{h} \iint e^{-\beta\left(\frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2\right)} \, dp\, dx$$

$$\xrightarrow{\text{Gaussian integrals}} = \ldots$$

$$= \frac{1}{h} \, 2\pi \, \frac{1}{\omega\beta} = \frac{1}{\hbar\omega\beta}$$

(b) Let's set up $Q_{qm}(T)$:

$$Q_{qm}(T) = \sum_{n=0}^{\infty} e^{-\beta E_n}$$

$$= \sum_{n=0}^{\infty} e^{-\beta(a+bn)}$$

$$= e^{-\beta a} \underbrace{\sum_{n=0}^{\infty} e^{-\beta b n}}_{\text{geometric series} \quad \frac{1}{1-e^{-\beta b}}}$$

$$= \frac{e^{-\beta a}}{1-e^{-\beta b}}$$

$$\xrightarrow[\text{for small } \beta]{\text{Taylor expanding}} \frac{1}{b\beta}$$

Enforce that the high-T limit of $Q_{qm}(T)$ agrees with $Q_{cl}(T)$:

$$\underbrace{\frac{1}{\beta b}}_{\substack{\text{from qm} \\ (Q_{qm})}} = \underbrace{\frac{1}{\hbar\omega\beta}}_{\substack{\text{from classical} \\ (Q_{cl})}} \implies b = \hbar\omega$$

(c) We want $\langle E \rangle_{qm}$:

$$\langle E \rangle_{qm} = -\frac{\partial}{\partial\beta} \log Q_{qm}(T)$$

$$= \underbrace{-\frac{\partial}{\partial\beta} \log\left(\frac{e^{-\beta a}}{1-e^{-\beta b}}\right)}_{\text{can be evaluated straightforwardly}}$$

$\rightsquigarrow$ I did this in Mathematica

Next, Taylor expand:

$$\langle E \rangle_{qm} \underset{\substack{\text{Taylor expansion} \\ \text{around } \beta = 0}}{\approx} \underset{\substack{\uparrow \\ \text{leading term}}}{\frac{1}{\beta}} + \underbrace{\frac{1}{2}(2a - b)}_{\text{sub-leading term}}$$

Also need $\langle E \rangle_{cl}$:

$$\langle E \rangle_{cl} = -\frac{\partial}{\partial\beta} \log(Q_{cl}(T))$$

$$= -\frac{\partial}{\partial\beta} \log\left(\frac{1}{\hbar\omega\beta}\right)$$

$$= -\frac{\partial}{\partial\beta}\left(\log\left(\frac{1}{\hbar\omega}\right) - \log(\beta)\right)$$

$$= +\frac{1}{\beta}$$

Match in high-T limit:

$$\underbrace{\frac{1}{\beta} + \frac{1}{2}(2a-b)}_{\text{from } \langle E \rangle_{qm}} = \underbrace{\frac{1}{\beta}}_{\text{from } \langle E \rangle_{cl}}$$

$$\Rightarrow 2a - b = 0 \Rightarrow a = \frac{b}{2} = \frac{1}{2}\hbar\omega$$

using earlier result

Thus, we determined $a = \frac{1}{2}\hbar\omega$ and $b = \hbar\omega$.

Hence: $\underbrace{E_n = (n + \frac{1}{2})\hbar\omega}$; $n = 0, 1, 2, \ldots$

not a surprising result!

But a neat illustration of how

qm and classical match