10.4: A simple example - the quantum harmonic oscillator

As a simple example of the trace procedure, let us consider the quantum harmonic oscillator. The Hamiltonian is given by

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2$$

and the eigenvalues of H are

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \qquad n = 0, 1, 2, \dots$$

Thus, the canonical partition function is

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

This is a geometric series, which can be summed analytically, giving

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

The thermodynamics derived from it as as follows:

1. **Free energy**:

   The free energy is

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

2. **Average energy**:

   The average energy $E = \langle H \rangle$ is

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

3. **Entropy**

   The entropy is given by

   $$S = k\ln Q(\beta) + \frac{E}{T} = -k\ln\left(1 - e^{-\beta\hbar\omega}\right) + \frac{\hbar\omega}{T}\frac{e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}}$$

Now consider the classical expressions. Recall that the partition function is given by

$$Q(\beta) = \frac{1}{h}\int dpdx e^{-\beta\left(\frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2\right)} = \frac{1}{h}\left(\frac{2\pi m}{\beta}\right)^{1/2} = \frac{2\pi}{\beta\omega h} = \frac{1}{\beta\hbar\omega}$$

Thus, the classical free energy is

$$A_{\text{cl}} = \frac{1}{\beta}\ln(\beta\hbar\omega)$$

In the classical limit, we may take $\hbar$ to be small. Thus, the quantum expression for A becomes, approximately, in this limit:

$$A_{\text{Q}} \longrightarrow \frac{\hbar\omega}{2} + \frac{1}{\beta}\ln(\beta\hbar\omega)$$

and we see that

$$A_{\mathrm{Q}} - A_{\mathrm{cl}} \longrightarrow \frac{\hbar\omega}{2}$$

The residual $\frac{\hbar\omega}{2}$ (which truly vanishes when $\hbar \to 0$) is known as the quantum *zero point* energy. It is a pure quantum effect and is present because the lowest energy quantum mechanically is not $E = 0$ but the ground state energy $E = \frac{\hbar\omega}{2}$.