E2050: Pressure by particle in a spring-box system

Submitted by: Shay Izbitski and Hamody Agbaria

The problem:

A spring that has an elastic constant K and natural length L is connected between a wall at $x = 0$ and a piston at $x = X$. A classical particle of mass m is attached to the middle point of the spring. The system is at equilibrium, the temperature is T.

(a) Write the Hamiltonian (careful!!!).
(b) Write the integral that defines the partition function $Z(\beta, X)$.
(c) Write a formal expression for the force F on the piston.
(d) Find elementary expressions (that do not involve exotic functions) in the limits of high and low temperatures. Explain the results that you get.

The solution:

(a) We define the coordinate x which is the position of the particle. We take notice to the fact that the particle is placed in the middle of the spring and therefore turning the spring into two springs with elastic constant $2K$. The Hamiltonian is:

$$\mathcal{H} = \frac{p^2}{2m} + \frac{1}{2}2K(\frac{L}{2} - x)^2 + \frac{1}{2}2K(X - x - \frac{L}{2})^2$$

After a little algebra we get the "effective" Hamiltonian

$$\mathcal{H} = \frac{p^2}{2m} + \frac{1}{2}K(X - L)^2 + 2 \cdot \frac{1}{2}2K(x - \frac{X}{2})^2$$

In this Hamiltonian the second term is contributed by the force applied by the spring on the piston and the third term by the force applied by the particle.

(b) The partition function is:

$$Z = \int \frac{dp}{2\pi} e^{-\beta T} \int dx e^{-\beta V(x)} = \frac{1}{\lambda_T} e^{-\beta \frac{1}{2} K(X-L)^2} \int_0^X dx e^{-\beta 2K(x-\frac{X}{2})^2} =$$

$$= \frac{1}{\lambda_T} e^{-\beta \frac{1}{2} K(X-L)^2} \sqrt{\frac{\pi}{2\beta K}} \text{erf}(\sqrt{2\beta K}\frac{X}{2})$$

(c) The force on the piston is given by:

$$\langle F \rangle_X = \frac{1}{\beta}\frac{\partial lnZ}{\partial X} = -K(X - L) + \frac{1}{\text{erf}(\sqrt{2\beta K}\frac{X}{2})} \cdot \sqrt{\frac{2K}{\pi\beta}} e^{-2\beta K(\frac{X}{2})^2}$$

We can see that the first term is the force applied by the spring and the second term is the force applied by the particle.

(d) In the case of high temperature $T \gg KX^2$ we expect the particle to fluctuate violently and hence eliminate the effect of the spring and essentially exert the force of a free particle gas in $1D$ box in length L on the piston. Let's take a look on the ideal gas law:

$$PV = NT$$

Convert it into the quantities in our problem gives us the force:

$$FX = 1 \cdot T \longrightarrow F = \frac{1}{\beta X}$$

The expansion for erf(x) is:

$$\text{erf(x)} = \frac{2}{\sqrt{\pi}}(x - \frac{x^3}{3} + \frac{x^5}{10} + \cdots)$$

Taking the first order expansion gives us:

$$\langle F \rangle_X \mid_{T \gg KX^2} \approx -K(X-L) + \frac{1}{\frac{2}{\sqrt{\pi}}\sqrt{2\beta K}\frac{X}{2}} \cdot \sqrt{\frac{2K}{\pi\beta}} \cdot 1 = -K(X-L) + \frac{1}{\beta X}$$

In the case of low temperature $T \ll KX^2$ we expect the particle to "freeze" in its position and hence not exerting force on the piston.

$$\langle F \rangle_X \mid_{T \ll KX^2} \approx -K(X-L) + \frac{1}{1} \cdot 0 \cdot 0 = -K(X-L)$$