Ex2050: Pressure by a particle in a spring-box system

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A spring that has an elastic constant K and natural length L is connected between a wall at $x = 0$ and a piston at $x = X$. Consequently the force that acts of the piston is $F_0 = -K(X - L)$. A classical particle of mass m is attached to the middle point of the spring. The system is at equilibrium, the temperature is T.

(1) Write the Hamiltonian (be careful).

(2) Write an expression for the partition function $Z(\beta, X)$. The answer is an expression that may contain a definite integral.

(3) Write an expression for the force F on the piston. The answer is an expression that may contain a definite integral.

(4) Find a leading order (non-zero) expression for $F - F_0$ in the limit of high temperature.

(5) Find a leading order (non-zero) expression for $F - F_0$ in the limit of low temperature.

Your answers should not involve exotic functions, and should be expressed using (X, L, K, m, T).

The Solution:

1. When cutting a spring in half its spring constant is doubled. This is understood by viewing the whole spring as 2 identical halves connected in series, so

$$K_{whole}^{-1} = K_{half}^{-1} + K_{half}^{-1} \Rightarrow K_{half} = 2K_{whole}\,.$$

The Hamiltonian is therefore,

$$\mathcal{H} = \frac{p^2}{2m} + \frac{2K\left(x - L/2\right)^2}{2} + \frac{2K\left[(X - x) - L/2\right]^2}{2}\,. \tag{1}$$

Here, x is the position of the particle, p is its momentum, the second term is due to the left spring and the third term is due to the right spring.

2. Writing the partition function we have,

$$Z = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}p \int_0^X \mathrm{d}x\, e^{-\beta\left[p^2/2m + 2K(x-L/2)^2/2 + 2K(X-x-L/2)^2/2\right]}\,. \tag{2}$$

Let us rewrite the argument of the spatial exponent,

$$\begin{aligned}(x - L/2)^2 - (X - x - L/2)^2 &= 2x^2 + L^2/2 + X^2 - 2Xx - LX = \\ &= 2\left(x^2 - xX + X^2/4\right) + \left(L^2 - 2LX + X^2\right)/2 = 2\left(x - X/2\right)^2 + \left(L - X\right)^2/2\,.\end{aligned}$$

Substituting the above and solving the kinetic part we get,

$$Z = \frac{1}{\lambda_T} e^{-\beta K(L-X)^2/2} \int_0^X \mathrm{d}x\, e^{-2\beta K(x - X/2)^2}\,. \tag{3}$$

3. The generalized force associated with the parameter X is the force F on the piston. By definition it is,

$$\langle F\rangle = \frac{1}{\beta}\frac{\partial \ln Z}{\partial X} = \frac{1}{\beta}\left[\beta K\left(L-X\right) + \frac{\partial}{\partial X}\ln\left(\int_0^X \mathrm{d}x\, e^{-2\beta K(x-X/2)^2}\right)\right] \tag{4}$$

$$= F_0 + \frac{1}{\beta}\frac{\partial}{\partial X}\ln\left(\int_0^X \mathrm{d}x\, e^{-2\beta K(x-X/2)^2}\right)\,. \tag{5}$$

4. In the limit of high temperatures, or $\beta \to 0$, we can expand the exponent in the intergal and have:

$$\langle F\rangle - F_0 \approx \frac{1}{\beta}\frac{\partial}{\partial X}\ln\left(\int_0^X \mathrm{d}x\, 1\right) = \frac{1}{\beta}\frac{\partial}{\partial X}\ln X = \frac{1}{\beta X}\,. \tag{6}$$

5. Let us denote

$$I\left(X,\beta\right) = \int_0^X \mathrm{d}x\, e^{-2\beta K(x-X/2)^2} = \frac{2}{\sqrt{2\beta K}}\int_0^{\sqrt{\frac{\beta K}{2}}X} \mathrm{d}y\, e^{-y^2}\,, \tag{7}$$

(in the last equality we just changed variables) giving us:

$$\langle F\rangle - F_0 = \frac{1}{\beta I\left(X,\beta\right)}\frac{\partial}{\partial X}I\left(X,\beta\right)\,. \tag{8}$$

Notice that in the limit $\beta \to \infty$ we have $I\left(X,\beta\right) \to \sqrt{\pi}/2$ becase of the upper bound of the integral. This gives as the approximated value:

$$\langle F\rangle - F_0 \approx \sqrt{\frac{2K}{\pi\beta}}e^{-\beta K\frac{X^2}{2}}\,, \tag{9}$$

where the last exponent came from the fundamental theorem of calculus.