ETH Zurich
Department of Mechanical and Process Engineering
Statistical Mechanics of Elasticity
Exercise 6 - Summer 2007

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Useful Definitions

General definition of fluctuations

Given a phase function F, its mean square fluctuation is defined by

$$\overline{\Delta F^2} = \overline{(F - \overline{F})^2} = \overline{F^2} - \overline{F}^2. \tag{1}$$

The relative fluctuation is given by

$$\frac{\sqrt{\overline{\Delta F^2}}}{\overline{F}} = \frac{\sqrt{\overline{F^2} - \overline{F}^2}}{\overline{F}}. \tag{2}$$

Fluctuations of conjugate forces

The mean value of a conjugate (microscopic) force

$$F^m = \frac{\partial H}{\partial A}, \tag{3}$$

where H is the Hamiltonian and A the kinematic control variable, is given by

$$\overline{F^m} = \frac{\partial \Psi}{\partial A}, \tag{4}$$

where Ψ is the Helmholtz free energy of the system. The relative fluctuation of F^m is calculated from

$$\frac{\sqrt{\overline{(\Delta F^m)^2}}}{\overline{F^m}} = \frac{\sqrt{kT}\left(\overline{\frac{\partial^2 H}{\partial A^2}} - \frac{\partial^2 \Psi}{\partial A^2}\right)^{1/2}}{\partial \Psi / \partial A} \tag{5}$$

Useful integrals

The following integrals are useful for problem 1:

$$\int_0^\infty \exp(-ax)\mathrm{d}x = \frac{1}{a} \text{ and } \int_0^\infty x^2 \exp(-ax)\mathrm{d}x = \frac{2}{a^3}. \tag{6}$$

Problem 1 - The thermally vibrating pencil

Consider a cylindrical pencil standing up on a flat surface under the influence of gravity (see Figure 1). At nonzero temperature, the position of its center of gravity will fluctuate due to thermal excitation. We want to determine the temperature at which the expected fluctuations are so large that the pencil will tip over. Do do so, we take advantage of the axissymmetry of the problem and consider the plane problem. We then go through the following steps:

a) Compute the Hamiltonian $H(\theta, \dot{\theta})$ if the moment of inertia for rotations about the edges is I. Assume that the vertical position of the center of gravity varies linearly with θ (and chose a monotonically increasing θ). Since higher energies will make less and less contributions in the negative exponent, all integrations can be carried out for $0 < \theta < \infty$.

b) Compute the partition function Z of the system.

c) Compute the mean position $\overline{\theta}$.

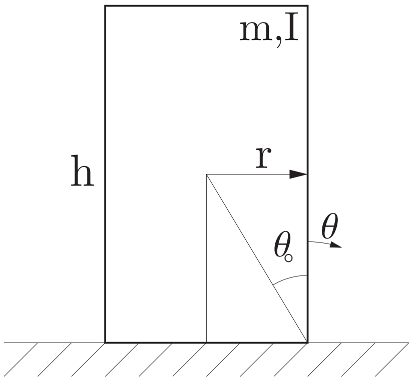

Figure 1: The idealized pencil on a flat surface.

d) Compute the mean square position $\overline{\theta^2}$.

e) If the pencil has the following properties: $m = 0.005kg$, $r = 0.003m$ and $h = 0.15m$, what is the temperature T_o for which $\sqrt{\overline{\Delta\theta^2}} > \theta_o$, where θ_o is the tipping angle $\theta_o = \arctan(2r/h)$.

Homework 1 - Fluctuation of energy in the canonical ensemble

Show that the mean cubic fluctuation of the energy in the canonical ensemble is

$$\overline{\Delta E^3} = k^2 \left(T^4 \frac{\partial^2 U}{\partial T^2} + 2T^3 \frac{\partial U}{\partial T} \right). \tag{7}$$

To do so, go through the following steps

a) First show that

$$\overline{\Delta E^3} = \overline{E^3} - 3U\overline{E^2} + 2U^3, \tag{8}$$

where $U = \overline{E}$.

b) Using the definition

$$U = \frac{\int_\Gamma H \exp(-\beta H) \mathrm{d}y}{\int_\Gamma \exp(-\beta H) \mathrm{d}y} \tag{9}$$

show that very conveniently

$$\frac{\partial^2 U}{\partial \beta^2} = \overline{E^3} - 3U\overline{E^2} + 2U^3. \tag{10}$$

c) By rewriting derivatives $\frac{\partial}{\partial\beta}$ in terms of $\frac{\partial}{\partial T}$, show that (7) follows directly from (10).

d) Now evaluate calculate the relative mean cubic fluctuation $\overline{(\Delta E/U)^3}$ for the ideal gas by inserting $U = \frac{3}{2}NkT$ in (7) and compare the result to the relative mean square fluctuation in an ideal gas, $\overline{(\Delta E/U)^2} = 2/(3N)$.

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