ETH Zurich
Department of Mechanical and Process Engineering
Statistical Mechanics of Elasticity
Exercise 4 - Summer 2007

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Useful Definitions

The canonical ensemble

The distribution function of a system interacting with a heat bath of temperature T is given by

$$\rho(\mathbf{q},\mathbf{p}) = C \cdot e^{-\frac{H(\mathbf{q},\mathbf{p})}{k_B T}} = e^{\frac{\Psi - H(\mathbf{q},\mathbf{p})}{k_B T}}, \tag{1}$$

where $H(\mathbf{q},\mathbf{p})$ is the Hamiltonian of the considered system, T the temperature of the surrounding heat bath (in degree Kelvin), $k_B = 1.38044 \cdot 10^{-23} J/K$ and $C = e^{\Psi}$ is determined from the normalization condition

$$\int_\Gamma \rho(\mathbf{q},\mathbf{p})\, \mathrm{d}\mathbf{q}\, \mathrm{d}\mathbf{p} = 1, \tag{2}$$

where Γ is the entire phase space spanned by the coordinates and momenta of the system.

Monoatomic ideal Gas

A collection of N distinguishable monoatomic particles is called a monoatomic ideal gas if the particles are weakly interacting and hence - for phase space calculations exclusively - its Hamiltonian can be approximated by

$$H(\mathbf{q},\mathbf{p}) = \sum_i^{3N} \frac{p_i^2}{2m_i}. \tag{3}$$

Heat capacity

The heat capacity C is defined in terms of microscopic properties as

$$C = \left(\frac{\partial \bar{E}}{\partial T}\right) = \left(\frac{\partial}{\partial T} \int_\Gamma \rho(\mathbf{q},\mathbf{p}) H(\mathbf{q},\mathbf{p})\, \mathrm{d}\mathbf{q}\, \mathrm{d}\mathbf{p}\right), \tag{4}$$

where $\rho(\mathbf{q},\mathbf{p})$ is the distribution function and $H(\mathbf{q},\mathbf{p})$ the Hamiltonian of the system.

Useful integrals

For $a > 0$, we have

$$\int_{-\infty}^{+\infty} e^{-ax^2} \mathrm{d}x = \sqrt{\frac{\pi}{a}} \tag{5}$$

and

$$\int_{-\infty}^{+\infty} x^2 e^{-ax^2} \mathrm{d}x = \frac{\sqrt{\pi}}{2a^{3/2}}. \tag{6}$$

More generally we have

$$\int_0^{+\infty} x^n e^{-ax^2} \mathrm{d}x = \frac{1}{2}\Gamma\left(\frac{n+1}{2}\right) a^{-\frac{n+1}{2}}, \tag{7}$$

where Γ is defined by

$$\int_0^{+\infty} x^n e^{-x} \mathrm{d}x \tag{8}$$

and

$$\Gamma(1/2) = \sqrt{\pi}, \qquad \Gamma(n) = (n-1)\Gamma(n-1). \tag{9}$$

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Problem 1 - Maxwell velocity distribution

Derive the canonical distribution of an ideal monoatomic gas with masses m at absolute temperature T. For the derivation, use the fact that the N particles are only weakly interacting and assume the gas is confined to a box of volume L^3. Use your result to compute the velocity distribution of an ideal gas in the canonical ensemble.

Problem 2 - Equation of state of ideal gas

Using the canonical distribution computed above, derive the equation of state of an ideal gas at absolute temperature T. To do so, compute the pressure p exerted on an area element of the wall pointing in the z-direction from the rate of momentum transfer through that area element.

Homework 1 - Heat capacity of surface particles

Monoatomic molecules adsorbed on a surface are free to move on this surface and can be treated as a classical ideal two-dimensional gas. The particles have absolute temperature T.

a) What is the Hamiltonian H of this system?

b) Derive the distribution function ρ of the system.

c) Calculate the mean energy $\bar{E}$.

d) Compute the heat capacity C using (4).

Questions/Comments/Suggestions? Felix Hildebrand - CLA H23.1 - 044/632-7755 - felixhi@ethz.ch