Homework problems #3

1. *Computer problem*: Verify the Maxwell-Boltzmann distibution of a velocity vector of magnitude v of ideal gas particles using a random number generator. Calculate the result for $N = 10^3$, 10^6 particles. Express the velocities relatively to $\sqrt{2kT/m}$. Hint: Let us assume that one has a function that generates random numbers in an interval $x \in [0,1]$ with uniform distribution. What transformation shall be performed to get a random variable from interval $y \in [-1,1]$? Using a computer experiment and histogram verify that a function $\mathrm{erf}^{-1}(y)$ gives a Gaussian distribution of random variable, where erf^{-1} is an inverse function to the error function $\mathrm{erf}(y) = 2/\sqrt{\pi}\int_0^y \exp(-t^2)\,\mathrm{d}t$. Maxwell-Boltzmann distibution of a magnitude of velocity vector can be derived by combining three random variables with Gaussian distribution

2. A system with two energy levels E_0 and E_1 is populated by N distinguishable particles at temperature T. Assuming canonical distribution determine

   (a) mean energy per particle,

   (b) limit of mean energy for temperatures $T \to 0$ and $T \to \infty$,

   (c) heat capacity of the system,

   (d) limit of the heat capacity of the system for $T \to 0$ and $T \to \infty$.

3. As a result of entanglement of rotational and vibrational movement of a diatomic molecule, angular momentum depends partially on the vibrational state. In such a case, the rotational-vibrational spectrum can be approximated by

$$E_{n,l} = \hbar\omega\left(n + \frac{1}{2}\right) + \frac{\hbar^2}{2I} l(l+1) + \alpha l(l+1)\left(n + \frac{1}{2}\right), \tag{1}$$

   where first two terms correspond to the vibrational and rotational movement and the last term is a small correction due to the entanglement of rotational and vibrational movement. The constant satisfy

$$\hbar\omega \gg \frac{\hbar^2}{2I} \gg \alpha. \tag{2}$$

   Determine energy of an ideal gas composed of diatomic molecules for temperature

$$\hbar\omega \gg kT \gg \frac{\hbar^2}{2I}.$$

The solution should be submitted not later than on April 13th.