Université de Genève Autumn term 2021

Statistical Methods in Physics (14P058)

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Exercise II – Maxwell-Boltzmann distribution

7 October 2021, 9.15 CEST, room: SCI–202

Consider a box system containing a large number of ^{85}Rb atoms with mass $m = 85m_0$ at room temperature T, where m_0 is the atomic mass unit. Along each single direction $i = x, y, z$, we assume the particles follow a probability density distribution

$$f(v_i) = \left(\frac{m}{2\pi k_B T}\right)^{1/2} e^{\frac{mv_i^2}{2k_B T}} \tag{1}$$

where v_i is the velocity along each direction and k_B is the Boltzmann constant. Here, we assume the $f(v_i)$ on each direction is independent with each other.

1. What is the average and variance of the distribution $f(v_i)$? Generate on your computer an array which contains the velocity information on the x-axis v_x for $N = 20\,000$ particles and plot a histogram for it. Compute its skewness and kurtosis numerically, and comment.

2. Now, we fix $N = 20\,000$. Based on the array you generated, generate a histogram for the speed of the particle $v = |\vec{v}|$, and prove that it fits the shape

$$f(v) = \left(\frac{m}{2\pi k_B T}\right)^{3/2} 4\pi v^2 e^{-\frac{mv^2}{2k_B T}} \tag{2}$$

3. Derive analytically the probability density function for the kinetic energy $E_k = \frac{1}{2}mv^2$. And then prove it with your numerical data.

4. Write a function on your computer: it should generate an array which contains the information of E_k for a given particle number N and a given temperature T. Then, plot the histogram of $f(E_k)$ for three different temperatures, $T = 100\,\mathrm{K}, 300\,\mathrm{K}, 600\,\mathrm{K}$, on the same plot.

5. At five given temperatures, $T = 10\,\mathrm{K}, 50\,\mathrm{K}, 100\,\mathrm{K}, 300\,\mathrm{K}, 600\,\mathrm{K}$, and fixed $N = 20000$ compute with your code the expectation value $\langle E_k \rangle$. We suppose it should follow the shape $\langle E_k \rangle = \alpha k_B T$. Estimate the value of α.

6. Redo the procedure from question 5 with $N = 500$ particles. Comment.

7. Compute the variance σ^2 of the distribution $f(E_k)$ for the case $N = 20\,000$ and $T = 300\,\mathrm{K}$ and check how it compares with $(k_B T)^2$. Compute also the skewness and kurtosis, and comment on your results.

Hints:

a) One can draw random numbers from a Gaussian distribution in python with the function "np.random.normal(μ, σ)".

b) Other possibly useful functions: plt.hist(), np.var(), scipy.stats.skew(), scipy.stats.kurtosis()

c) Universal constants: $m_0 = 1.66 \times 10^{-27}\,\mathrm{kg}$, $k_B = 1.38 \times 10^{-23}\,\mathrm{J\,K^{-1}}$.