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Statistical Methods in Physics (14P058)

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Exercise II – Maxwell-Boltzmann distribution

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Consider a box system containing a large number of ^{85}Rb atoms with mass $m = 85\, m_0$ 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

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

where v_i is the velocity along each direction and k_B is the Boltzmann constant. Here, we assume the $f(v_i)$ of each direction to be independent of each other. *N.B.* The values of the universal constants are $m_0 = 1.66 \times 10^{-27}$ kg as well as $k_B = 1.38 \times 10^{-23}\,\mathrm{J\,K^{-1}}$.

1. What is the average and variance of the distribution $f(v_i)$? Generate an array which contains the velocity information on the x-axis, v_x, for $N_{par} = 5000$ particles, and plot a histogram of this array.

   Hint: One can draw random numbers from a Gaussian distribution in python with the function *np.random.normal(μ, σ)*. Some other, possibly useful functions in this exercise are:

   matplotlib.pyplot.hist(), *np.var()*, *scipy.stats.skew()*, *scipy.stats.kurtosis()*.

2. Based on the array you created, 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 $E_k = \frac{1}{2} m v^2$. Then show that your numerical data follows that function. Compute its skewness and kurtosis numerically, and comment.

4. Generate the kinetic energy for $N_{par} = 900$ particles. Compute the expectation value and variance of your data, and check if you recover the results from statistical physics: $E(E_k) = 1.5\, k_B T$, $V(E_k) = 1.5\, (k_B T)^2$.

5. Application of the central limit theorem: we define an experiment as the following: generate the kinetic energy, E_k, for $N_{par} = 900$ particles and compute the expectation value $E(E_k)$. Repeat the experiment $N_{exp} = 400$ times and plot the obtained $E(E_k)$ in a histogram.

6. What should be the standard deviation of the $E(E_k)$ distribution? Fit your results from question 5 with a Gaussian, compute $\sigma_{E(E_k)}/\sigma_{E_k}$ and comment on what you get.

   Hint: The python function *spo.curve_fit* cannot work efficiently if the fitting parameters are too far from the scale of 1.