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Statistical Methods in Physics (14P058)

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Exercise IV – Monte Carlo integration II

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In this exercise, we will firstly revisit the Maxwell-Boltzmann distribution for the kinetic energy E_k of atoms in a three-dimensional (3D) classical system at room temperature. We will start directly from the energy distribution and compute the physical properties with Monte Carlo techniques. Then, we will turn to the case of 3D quantum Fermi gases at low temperature, where a Fermi-Dirac distribution should be applied to describe the system.

Task 1: *Revisit of the Maxwell-Boltzmann Distribution*

Consider a box system containing a large number of ^{40}K with mass $m = 40m_0$ at room temperature T, where m_0 is the atomic mass unit. The kinetic energy of the system E_k follows the probability density function

$$f(E_k) = 2\left(\frac{1}{k_B T}\right)^{3/2}\sqrt{\frac{E_k}{\pi}}e^{-\frac{E_k}{k_B T}} \tag{1}$$

In Exericse II, we computed the expectation value and the variance of E_k based on the facts that $f(v_i)$ follows a Gaussian (which can be directly generated with the *numpy.random* function) and that $f(E_k)$ can be obtained from $f(v_i)$ with a change of variables. In this exercise, we assume that we do not have any knowledge of $f(v_i)$ and we try to compute the statistical properties of E_k directly from Eq. (1) with Monte Carlo methods.

1. Prove analytically that the function $f(E_k)$ has its maximum at

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

2. Use the accept-reject method to generate E_k for $N = 10\,000$ particles in the range $[0, 10k_B T]$. Fill the values into a histogram, plot it and fit it with Eq. (1).

   Hint: We suggest to define python functions to generate the Maxwell-Boltzmann distribution. This will simplify the process of solving the following questions.

3. Based on the results of question 2, compute the expectation value for E_k

$$\langle E_k \rangle = \int E_k f(E_k) dE_k \tag{3}$$

   and show that it satisfies $\langle E_k \rangle = 1.5\, k_B T$.

4. Compute the variance of E_k and compare it with $(k_B T)^2$.

5. Compute $\langle E_k \rangle$ defined in Eq. (3) with the inverse transform method.

   Hint: One should take advantage of the term $\exp\left(-\frac{E_k}{k_B T}\right)$ in $f(E_k)$.

6. Assume the generated values of E_k are measurement from an actual experiment. From this data, we can obtain the corresponded velocity $v = \sqrt{2mE_k}$. What's the standard deviation for the velocity σ_v? Compute it both numerically and analytically.

Task 2: *Fermi-Dirac distribution*

Now, we move to the Monte Carlo generator of three-dimensional Fermi gas at low temperature. Consider a 3D box system which contains a large number of ^{40}K atoms with mass $m = 40\, m_0$, where m_0 is the atomic mass unit. At low enough temperatures and a particle density of $n = 1$, the energy ϵ of the atoms follows the Fermi-Dirac distribution

$$f(\epsilon) = A \frac{\sqrt{\epsilon}}{\exp\left(\beta(\epsilon - \mu)\right) + 1} \tag{4}$$

where $\beta = 1/(k_B T)$ denotes the inverse energy scale related to the temperature T, μ is the chemical potential of the system, and A is a pre-factor related to the properties of the system. Let's consider $T = 3\,\mathrm{K}$ and $\mu = 30\, k_B T$. Under these conditions, we have $A \simeq 3.5 \times 10^{31}$.

1. Build a MC process to generate this probability density function for a large number of data points $N = 10\,000$. Fill your results in a histogram, plot them and verify their correctness by comparing them with the curve of the analytical form in Eq. (4).

2. At low temperatures, the fermions show quantum behavior, which means that the mean energy per particle follows

$$\mathbb{E}\left[\epsilon\right] \simeq \frac{3}{5} n\mu. \tag{5}$$

   Compute the sample mean $\langle \epsilon \rangle$ and compare with the expectation value. Also, compute $\langle \epsilon \rangle / k_B T$ and comment.