11 Statistical Physics

11.3 Classical gases with a microscopic thermometer (8 units)

This project can be done with knowledge of the course Statistical Physics.

1 Introduction

Consider a gas of N non-interacting classical particles. The momentum of the ith particle is $\mathbf{p}_i$ and its kinetic energy is E_i. The energy E_g of the gas is

$$E_g \;=\; \sum_{i=1}^{N} E_i \,.$$

To this system we add one additional degree of freedom, which acts as a thermometer. The thermometer stores energy, and can exchange it with the gas. The energy of the thermometer is E_d and the total energy $E = E_g + E_d$ is conserved (we consider the microcanonical ensemble). We will show that measuring the average value of E_d can be used to infer the temperature of different kinds of classical gas.

2 Algorithm

We use a stochastic (random) algorithm to calculate the statistical behaviour of this system. This is an example of a Monte Carlo algorithm. It operates as follows:

1. As an initial configuration, set $\mathbf{p}_i = \mathbf{e}_1$ for all i, where $\mathbf{e}_1$ is a unit vector in the x-direction. Initialise also $E_d = 0$.

2. Choose one of the N particles at random and compute its *current* energy E_{curr}. Generate a random vector $\Delta\mathbf{p}$ and propose a change of the particle's momentum, from $\mathbf{p}_i$ to $\mathbf{p}_i + \Delta\mathbf{p}$. A good choice is to take each component of the vector $\Delta\mathbf{p}$ to be a random number from $(-\varepsilon, \varepsilon)$ with $\varepsilon = 0.1$. Compute the energy that the particle would have if its momentum was $\mathbf{p}_i + \Delta\mathbf{p}$: this is the *proposed* energy E_{prop}.

3. Define $\Delta E \equiv E_{\text{prop}} - E_{\text{curr}}$. If $\Delta E \leqslant E_d$ then accept the change. That is, update the momentum of particle i to a new value $\mathbf{p}_i + \Delta\mathbf{p}$, and update E_d to a new value $E_d - \Delta E$. If $\Delta E > E_d$ then the change is rejected and no variables are updated.

4. Whether or not the change was accepted, record the value of E_d as a new value in an array (or list) which will later be used to plot a histogram. Also record the energy of the particle. (This is called the *single-particle energy.*) If the change was accepted, you should record these values *after* the update was performed.

5. Repeat steps 2-4 until the total number of attempted updates is N_{updates}. Since each update only affects one particle, it is useful to define $N_{\text{sweeps}} = N_{\text{updates}}/N$ so that N_{sweeps} is the typical number of times that each particle has been chosen for an update.

Question 1 In the microcanonical ensemble each microstate (of the whole system) is equally likely. For the thermometer, suppose that every possible value of E_d corresponds to a single microstate. Hence explain why the probability distribution for E_d behaves as

$$P(E_d) \propto \Omega_g(E_g) .$$

where $\Omega_g(E_g)$ gives the number of microstates of the gas.

Question 2 The temperature of the gas is related to its entropy as

$$\frac{1}{T} = \frac{\partial S_g}{\partial E_g} .$$

Assuming that $E_d \ll E_g$, use this fact to show that

$$P(E_d) \propto \exp\left(-\frac{E_d}{k_{\mathrm{B}}T}\right) . \tag{1}$$

where k_{B} is Boltzmann's constant. [It is also acceptable to take $k_{\mathrm{B}} = 1$.]

3 Ideal gas

Programming Task: Write a program to simulate a gas of N particles using the Monte Carlo algorithm outlined above. Consider a 3-dimensional gas of nonrelativistic particles, so $\mathbf{p} = (p_1, p_2, p_3)$ and

$$E(\mathbf{p}) = \frac{|\mathbf{p}|^2}{2} .$$

You will need to keep track of the momentum vectors for the N particles in the gas. It will be useful in later questions if your program includes a function which returns the particle energy, given $\mathbf{p}$ as input.

You will also need to plot histograms of the quantities that were recorded in step 4 of the algorithm: the value of E_d and the single-particle energy. Remember, a histogram is a graph of the relative frequency that a quantity such as E_d lies within a particular bin. This relative frequency is $f(E_d)$.

Your program should also calculate the average of E_d.

Throughout this project, should compare your results with the behaviour that you would expect from the theory of statistical physics. The results should be presented in such a way that this comparison is clear.

Question 3 For $N = 100$, plot a histogram of E_d for $N_{\mathrm{sweeps}} = 10, 100, 1000$. [You may wish to plot $\log f(E_d)$ instead of $f(E_d)$.] Your program should not take more than a few minutes to run. Discuss (and explain) the results, including the dependence on N_{sweeps}. Do the results depend on the parameter ε that appears in step 2 of the algorithm?

Question 4 If N_{sweeps} is large enough, the system should be in an equilibrium state. For this case, compare the histogram of E_d with Equation (1), and estimate the temperature of the gas. If the distribution of E_d is consistent with (1), you can also estimate the temperature from the average of E_d. Quantify the numerical uncertainties on these two estimates of the temperature.

Question 5 For the equilibrium state, plot a histogram of the single-particle energy. Show that the result is consistent with the theory of ideal gases from statistical physics.

Programming Task: Modify your program so that each particle is initialised with a randomly assigned momentum (instead of all starting with $\mathbf{p}_i = \mathbf{e}_1$). For example, assign each component of $\mathbf{p}_i$ independently at random from $(-a, a)$, with $a = 1$.
(Note: depending on a, you may want to change the parameter ε that appears in step 2 of the algorithm.)

Question 6 How does this change in initial conditions affect the histograms of E_d and the single-particle energy? What happens for different values of a? How does the temperature depend on a? Explain your observations, including their consistency with the theory of ideal gases from statistical physics.
(Note: depending on a, you may want to change the parameter ε that appears in step 2 of the algorithm.)

4 Relativistic gases

Programming Task: Continue with random initial conditions [each component of $\mathbf{p}_i$ chosen independently at random from $(-a, a)$]. Modify your program to consider ultra-relativistic particles that move in two dimensions: this means that $\mathbf{p}$ is a vector with two components and that

$$E = |\mathbf{p}| \ .$$

(For the purposes of statistical physics, we still refer to this system as a classical gas, because quantum mechanical effects have been neglected.)

Question 7 For $a = 1$, compute and plot histograms of E_d and of the single particle energy. Estimate the temperature of the gas. Vary a and compute the temperature. Plot this temperature as a function of the total energy of the system. Compare the result with the case considered in question 5 (non-relativistic particles in three dimensions), and discuss their consistency with the theory of ideal gases from statistical physics.

Programming Task: Consider relativistic particles in three dimensions so that $\mathbf{p}$ is a vector with three components, and

$$E(\mathbf{p}) = \sqrt{1 + |\mathbf{p}|^2} - 1 \ .$$

Question 8 Consider different values of the total energy by varying a in the range 0.1 to 2.0. How does the temperature depend on the total energy? By considering the behaviour of $E(\mathbf{p})$ for large and small values of $|\mathbf{p}|$, comment on the relation of this result to the cases from previous questions. Compare the histograms of single-particle energies for a few representative cases.

