Exercises

3.4 **Pressure computation.**[1] [2] (Computation) ②

Microscopically, pressure comes from atomic collisions onto a surface. Let us calculate this microscopic pressure for an ideal gas, both analytically and using a molecular dynamics simulation. You may download our molecular dynamics software [10] from the text web site [129].

Run a simulation of the ideal gas in a system with reflective walls. Each time an atom collides with a wall, it undergoes *specular reflection*, with the parallel momentum components unchanged and the perpendicular momentum component reversed.

(a) *Remembering that pressure $P = F/A$ is the force per unit area, and that force $F = \mathrm{d}p/\mathrm{d}t = (\sum \Delta P)/\Delta t$ is the net rate of momentum per unit time. Suppose a wall of area A at $x = L$ is holding atoms to values $x < L$ inside a box. Write a formula for the pressure in terms of $\rho_c(p_x)$, the expected number of collisions at that wall per unit time with incoming momentum p_x.* (Hint: Check the factors of two, and limits of your integral. Do negative momenta contribute?)

The simulation provides an 'observer', which records the magnitudes of all impacts on a wall during a given time interval.

(b) *Make a histogram of the number of impacts on the wall during an interval Δt with momentum transfer Δp. By what factor must you multiply $\rho_c(p_x)$ from part (a) to get this histogram?*

Unlike the distribution of momenta in the gas, the probability $\rho_c(p_x)$ of a wall collision with momentum p_x goes to zero as p_x goes to zero; the ideal gas atoms which are not moving do not collide with walls. The density of particles of momentum p_x per unit volume per unit momentum is the total density of particles N/V times the probability that a particle will have momentum p_x (eqn 3.19):

$$\frac{N}{V}\frac{1}{\sqrt{2\pi m k_B T}} \exp\left(-\frac{{p_x}^2}{2mk_BT}\right). \tag{3.60}$$

(c) *In a time Δt, from how far away will will atoms of incoming momentum p_x collide with the wall? What should the resulting formula be for $\rho_c(p_x)$? Does it agree with your histogram of part (b)? What is your resulting equation for the pressure P? Does it agree with the ideal gas law?*

[1] From *Statistical Mechanics: Entropy, Order Parameters, and Complexity* by James P. Sethna, copyright Oxford University Press, 2007, page 54. A pdf of the text is available at pages.physics.cornell.edu/sethna/StatMech/ (select the picture of the text). Hyperlinks from this exercise into the text will work if the latter PDF is downloaded into the same directory/folder as this PDF.

[2] This exercise and the associated software were developed in collaboration with Christopher Myers.