Sample problems and solutions

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Problem 1

One kilogram of Argon gas is in equilibrium at temperature T in a container of volume V. At time $t = 0$ a very small hole is drilled in one of the walls of the container. Find:

1. The number of particles escaping the container per unit area of the hole per unit time *immediately* after the hole is drilled.

2. Find the average kinetic energy of the particles leaving the container. Show that this is 4/3 times the average energy of the particles inside the container and explain your answer.

Solution

Let us assume, without loss of generality, that the normal to the hole surface coincides with the x-direction. The number of particles of velocity U_x that will collide with this surface in time Δt is equal to the number of particles in a volume $AU_x\Delta t$, where A is the area of the hole. Since the particles are uniformly distributed, the latter is given by $nfAU_x\Delta t$. To find the total number of particles escaping we need to integrate over all velocity classes i.e.,

$$\frac{N}{A\Delta t} = \frac{1}{A\Delta t}\int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty nfA\Delta t dU_x\, dU_y\, dU_z$$

where $n = 1/40 \times 6.023 \times 10^{26}/V$. Because we are interested in the moment immediately after the hole is opened, we can assume that the gas is still in equilibrium, i.e.

$$f\left(\vec{U}\right) = \left(\frac{m}{2\pi kT}\right)^{3/2} \exp\left(-\frac{mU^2}{2kT}\right)$$

Plugging in we get

$$\frac{N}{A\Delta t} = \frac{1}{A\Delta t}\int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty nfA\Delta t dU_x\, dU_y\, dU_z = n\sqrt{\frac{kT}{2\pi m}}$$

To find the average energy of the escaping particles we integrate to find the energy flux of the escaping particles and divide that by the flux of particles. The energy flux is given by

$$\frac{E}{A\Delta t} = \frac{1}{A\Delta t}\int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty nfA\Delta t \left(\frac{1}{2}m(U_x^2+U_y^2+U_z^2)\right) dU_x\, dU_y\, dU_z = 2kTn\sqrt{\frac{kT}{2\pi m}}$$

The average particle energy is

$$\frac{\frac{E}{A\Delta t}}{\frac{N}{A\Delta t}} = 2kT$$

The average energy of particles inside the container is

$$\bar{E} = \frac{1}{n}\int_{-\infty}^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty nf\left(\frac{1}{2}m(U_x^2+U_y^2+U_z^2)\right) dU_x\, dU_y\, dU_z = \frac{3}{2}kT$$

The reason that particles leaving have on average a higher energy than the ones inside the container, is that particles with higher velocities (energy) have a higher probability of escaping.

Problem 2

Consider a perfect fcc crystal made from N atoms of a Lennard-Jones material at zero temperature. In terms of Lennard-Jones parameters, find

1. The total energy of the crystal
2. The equilibrium value for the nearest neighbor spacing

Hint: Express the distances of all atoms (j) from a given atom (i) as $r_{ij} = RP_{ij}$ where R is the nearest neighbor distance and

$$\sum_j \frac{1}{P_{ij}^{12}} = 12.13188$$

and

$$\sum_j \frac{1}{P_{ij}^{6}} = 14.45392$$

for an fcc crystal.

Solution

Let us denote the Lennard-Jones potential by

$$\Phi(r_{ij}) = 4\varepsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right]$$

At zero temperature there is no kinetic energy; we thus obtain for the total energy

$$U_{tot} = \frac{1}{2} N 4\varepsilon \left[\sum_j \left(\frac{\sigma}{P_{ij}R} \right)^{12} - \sum_j \left(\frac{\sigma}{P_{ij}R} \right)^{6} \right]$$

For an fcc structure

$$\sum_j \frac{1}{P_{ij}^{12}} = 12.13188$$

and

$$\sum_j \frac{1}{P_{ij}^{6}} = 14.45392$$

Note that there are 12 nearest neighbors in an fcc crystal so the series above converge fast, that is, most of the energy is contributed by the nearest neighbors.

The equilibrium value for R, R_o, is found by

$$\frac{dU_{tot}}{dR} = 0 = -2N\varepsilon \left[12(12.13188)\frac{\sigma^{12}}{R^{13}} - 6(14.45392)\frac{\sigma^{6}}{R^{7}} \right]$$

$$\Rightarrow R_o = 1.09\sigma$$

Problem 3

Using simple mean free path arguments, obtain a theoretical *estimate* for the thermal conductivity of a dilute gas.

On the course webpage you will find a DSMC code which performs simulations of a shear flow and estimates the viscosity of gas. Modify this code and perform simulations which allow you to calculate the thermal conductivity of a dilute gas. Compare your above estimate and simulation results with the theoretical value given by

$$\kappa = \frac{75k}{64\sigma^2}\sqrt{\frac{kT}{\pi m}}$$

Solution

Consider an imaginary surface in the gas and a temperature gradient normal to this surface. We will evaluate the thermal conductivity as the heat flux across this surface per degree of temperature difference. To get an *approximate estimate* for the thermal conductivity, we will consider particles crossing the surface from left to right: these particles, *on average*, start a distance $\lambda/2$ to the left of the surface and end up $\lambda/2$ to the right of the interface. The *average* energy flux associated with them is $n\bar{c}_1(0.5m\bar{c}_1^2)$, where 1 denotes the location from which these particles originated. Similarly for particles traveling from right to left, the *average* energy flux associated with them is $n\bar{c}_2(0.5m\bar{c}_2^2)$. The net heat flux is thus $q \approx 0.5nm(\bar{c}_1^3 - \bar{c}_2^3) = 0.5nm[8k/(\pi m)]^{3/2}(T_1^{3/2} - T_2^{3/2}) = 0.5nm[8k/(\pi m)]^{3/2}T_1^{3/2}(1 - T_2^{3/2}/T_1^{3/2})$.

Clearly if $T_1 = T_2$ there is no heat flux. Let us assume that a temperature gradient is present such that $T_2 = T_1 + \Delta T$. Then

$$\frac{T_2^{3/2}}{T_1^{3/2}} = \left(1 + \frac{\Delta T}{T_1}\right)^{3/2} \approx 1 + \frac{3}{2}\frac{\Delta T}{T_1} \approx 1 + \frac{3}{2T_1}\lambda\frac{dT}{dx}$$

Thus the thermal conductivity is

$$\kappa \approx \frac{-q}{dT/dx} = \frac{3}{4}nm\sqrt{\left(\frac{8k}{\pi m}\right)^3}\lambda T_1^{1/2} = \frac{12k}{\pi^2\sigma^2}\sqrt{\frac{kT_1}{\pi m}}$$

Problem 4

When characteristic flow lengthscales (H) approach the molecular mean free path (λ), the typical continuum approaches fail. A typical criterion used is that when the Knudsen number $Kn = \lambda/H$ exceeds 0.01 (approximately) continuum approaches are unreliable. You may assume that for air $\sigma \approx 3.5 \times 10^{-10}$m.

1. Explain (qualitatively) why this is so.
2. Find the approximate lengthscale for which continuum descriptions fail at atmospheric pressure at sea level where the atmospheric density is $\rho_o = 1.23\text{Kg/m}^3$.
3. By assuming that the air density drops with altitude from sea level (h) as $\rho/\rho_o = \exp(-\alpha h)$, where $\alpha = 1.3 \times 10^{-4}\text{m}^{-1}$, *estimate* the altitude above which calculating the aerodynamic forces on the re-entering space shuttle using a continuum description would be unreliable.

Solution

1. Continuum descriptions fail because when the characteristic flow lengthscale becomes of the order of the mean free path, particle motion and thus transport is no longer diffusive. In other words, Fick's diffusion law, Newton's shear stress law, and Fourier's heat flux law are no longer valid.

2. At atmospheric pressure $\lambda = \frac{m}{\sqrt{2}\pi\rho\sigma^2} \approx 70$nm. For $Kn \approx 0.01$ we need $H \approx 7\mu$m

3. Let us assume that the characteristic lengthscale for the space shuttle is 7 cm (wing leading edge). Then, for $Kn \approx 0.01$ we need $\lambda \approx 7 \times 10^{-4}$m. From our previous calculation and the fact that $\lambda \propto \rho^{-1}$, we conclude that $\rho \approx 0.0001\rho_o$ and $h = \ln(\rho_o/\rho)/\alpha \approx 70$Km.