1 Maxwell-Boltzmann distribution

In statistical mechanics, the velocity distribution of each particle in a gas is given by the Probability Distribution Function:

$$f(v_i)dv_i = \frac{1}{\sqrt{2\pi}} \cdot \sqrt{\frac{m}{k_B T}} e^{-\frac{mv_x^2}{2 \cdot k_B T}} dv_i, \tag{1}$$

for $v_i \in \{v_x, v_y, v_z\}$. Using the normalised velocity found in the lectures, given by $v_i = \sqrt{\frac{\epsilon}{m}}\tilde{v}_i$ we then obtain:

$$\sqrt{\frac{\epsilon}{m}} f(\tilde{v}_i)d\tilde{v}_i = \frac{1}{\sqrt{2\pi}} \cdot \sqrt{\frac{\epsilon}{k_B T}} e^{-\frac{\epsilon \tilde{v}_x^2}{2 \cdot k_B T}} d\tilde{v}_i. \tag{2}$$

Defining the normalised temperature $\tilde{T}$ according to the relation $\frac{1}{\tilde{T}} = \frac{\epsilon}{k_B T}$, we obtain:

$$\sqrt{\frac{\epsilon}{m}} f(\tilde{v}_i)d\tilde{v}_i = \tilde{f}(\tilde{v}_i)d\tilde{v}_i = \frac{1}{\sqrt{2\pi}} \cdot \frac{1}{\sqrt{\tilde{T}}} e^{-\frac{\tilde{v}_x^2}{2 \cdot \tilde{T}}} d\tilde{v}_i. \tag{3}$$

Note that the RHS is indeed a Probability Distribution as it integrates to 1. Actually, it is a Gaussian centred at 0 and with variance $\tilde{T}^2$.

Recall that, in the case of Argon, we have $\frac{\epsilon}{k_b} = 119.8\text{K}$. So, if we take $T \sim 119.8\text{K}$ $\Rightarrow \tilde{T} \sim 1 = 10^0$.

2 Handling of the velocities and temperatures (rescaling)

The kinetic energy is given by the expression:

$$K = \frac{3}{2}(N-1)k_B T, \tag{4}$$

with N the number of particles and T the temperature. Now, taking the normalised temperature $\tilde{T}$ defined before, we get:

$$K = \frac{3}{2}(N-1)\epsilon\tilde{T} \quad \overset{K=\epsilon\tilde{K}}{\longrightarrow} \quad \tilde{K} = \frac{3}{2}(N-1)\tilde{T} \Leftrightarrow \tilde{T} = \frac{2}{3}\cdot\frac{\tilde{K}}{N-1}. \tag{5}$$

From this later formula we can obtain the normalised temperature at every time-step in the simulation as we know the kinetic energy.

Let us now get the rescaling factor

$$\lambda = \sqrt{\frac{3(N-1)k_BT}{\sum_i mv_i^2}}$$

with the normalised parameters. First of all, the normalised velocity verifies $v_i = \sqrt{\frac{\epsilon}{m}}\tilde{v}_i \implies \sum_i mv_i^2 = \epsilon\sum_i v_i^2 =: \epsilon V$. Hence, we deduce:

$$\lambda = \sqrt{\frac{3(N-1)k_BT}{\epsilon V}} = \sqrt{\frac{3(N-1)\tilde{T}}{\sum_i \tilde{v}_i^2}}, \tag{6}$$

which gives the rescaling factor λ in terms of the normalised parameters. Note that the sum i is done over all the particles in the system.

3 FCC initialization

The FCC, or face-centered cubic, is one of the most important Bravais lattices in Solid State Physics. In this lattice, the atoms arrange in the vertices of cubes but also in the centre of the faces. This geometrical arrangement can be visualized in Figure 1.

The positions of the atoms in this lattice can be parametrized using the following primitive basis vectors:

$$\{a_1 = \begin{pmatrix} a/2 \\ a/2 \\ 0 \end{pmatrix}, a_2 = \begin{pmatrix} 0 \\ a/2 \\ a/2 \end{pmatrix}, a_3 = \begin{pmatrix} a/2 \\ 0 \\ a/2 \end{pmatrix}\}, \tag{7}$$

where a is the length of the unit cube and what we refer in the code as lattice constant. Thus, any position in the lattice can be expresses as an integer linear combination of these

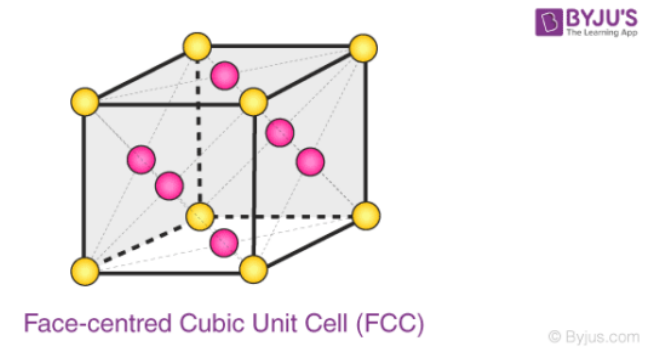

Figura 1: Geometrical arrangement of FCC Bravais lattice.

vectors:

$$r(n_1, n_2, n_3) = n_1 a_1 + n_2 a_2 + n_3 a_3; \quad n_1, n_2, n_3 \in \mathbb{Z} \tag{8}$$

However, our Argon simulation takes place in a limited space, a box of length L. Thus, we need to figure out what is the range of n_1, n_2 and n_3. For the sake of simplicity, let us assume that the coordinate origin is in one of the vertices of the box and the centre of the box is therefore in $(a/2, a/2, a/2)$.

First, we notice that the vertices that are in the Cartesian axes can be reached setting two integers the same, and the other to the negative of that number. We find by trial and error that the range of n_1 has to be between $-L/a = r$ and $2L/a = 2r$. To find out the range of n_2 and n_3, we first expand Equation 8 and impose the box constraints:

$$0 \leq r(n_1, n_2, n_3) = \frac{a}{2} \begin{pmatrix} n_1 + n_3 \\ n_1 + n_2 \\ n_2 + n_3 \end{pmatrix} \leq L \tag{9}$$

From this we obtain the range of n_2 and n_3:

$$-n_1 \leq n_2 \leq 2r - n_1 \tag{10}$$

$$-n_1 \leq n_3 \leq 2r - n_1 \quad and \quad -n_2 \leq n_3 \leq 2r - n_2 \tag{11}$$

This last condition is equivalent to:

$$-min(n1, n2) \leq n_3 \leq 2r - max(n_1, n_2) \tag{12}$$

To sum up, we have obtained the range of the three integers that parametrize the positions of a FCC lattice constrained to a box of length L. This can be implemented by three for loops. Finally, in our code the origin is in the centre of the box, so we have to shift all the positions by the vector $-(L/2, L/2, L/2)$.

One last modification was done to take into account that atoms in opposite faces of the box are at distance 0 due to periodic boundary conditions. It consists of multiplying the positions by 0.9 so that no atom lies on the surface of the box.