Exercise 5. Classical Monte Carlo simulation of a liquid–solid phase transition in a two-dimensional Lennard-Jones system

Objective: To simulate a liquid–solid transition in a two-dimensional system with a Lennard-Jones interaction potential.

Outline

1. Develop a classical Monte Carlo code for a (N, V, T) ensemble for a Lennard-Jones (LJ) system in two dimensions. Use $N = 242$ atoms. Remember that the LJ potential has the following form:
$$U_{LJ}(r) = 4\varepsilon[(\sigma/r)^{12} - (\sigma/r)^6]$$

2. Run a annealing simulation for argon at density $\rho^* = 0.96$ in a square box of size $L \times L$. Use an annealing method to obtain the particle configuration having minimal energy. Physically, this configuration corresponds to a perfect crystal lattice.

3. Run a MC simulation for argon at $T^* = 0.5$ and $\rho^* = 0.96$. Remember the criterium to choose the displacement amplitude Δ is to obtain an acceptance of $\approx 50\%$.

4. Compute the energy E^*, its standard deviation σ_E, and the radial distribution function $g(r)$. Note that for a two dimensional system of area S and density $\rho = N/S$ it is
$$\frac{E}{N} = \frac{2}{2}k_BT + \frac{1}{N}\left\langle \sum_{i=1}^{N}\sum_{j>i}^{N} U(r_{ij}) \right\rangle \quad (1)$$
$$g(r) = \frac{1}{\rho}\frac{n(r)}{2\pi r dr} = \frac{n(r)}{n_{id}(r)} \quad (2)$$

5. Repeat the simulation for the following temperatures: T^*= 1.0, T^* =1.5, T^*=2.0, T^* =2.5 and T^*=3.0.

6. List the technical parameters (the number of iterations, the displacement amplitude Δ and the acceptance rate) of all the simulations.

7. Plot the radial distribution functions $g(r)$ obtained for the different temperatures.

Report

1. snapshots of the particle coordinates in the crystal and gas phases

2. Radial distribution function in the crystal and gas phases

3. Energy per particle E/N and its statistical error for temperatures $T^\star = 0.5; 1; 1.5; 2; 2.5; 3$

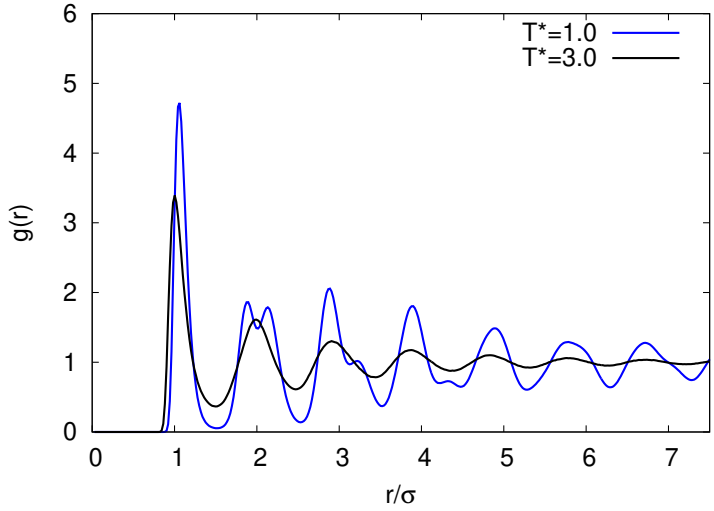
4. List the technical parameters (the number of iterations, the displacement amplitude Δ and the acceptance rate) for temperatures $T^\star = 0.5; 1; 1.5; 2; 2.5; 3$.

Lennard-Jones parameters

While the specific parameters of the LJ potential are needed for making comparisons with experiments, it is convenient to perform simulations using dimensionless units chosen in a such way that typical distances and energies are of the order of unit. In the case of the LJ potentials, it is common to use σ as a unit of length and ϵ as a unit of energy.

atom	mass(uma)	ϵ/k_B (K)	σ ($\mathring{A}$)
Ar	39.948	119.8	3.405

Some results to compare with:



Radial distribution functions for the Lennard-Jones system at different temperatures.

Some observations

- pair distribution function $g(r)$ quantifies the probability of finding two particles separated by distance r. Essentially, it corresponds to the histogram of relative distances $r = |\mathbf{r}_i - \mathbf{r}_j|$ found in the Monte Carlo simulation. It is common to divide the histogram by $(4\pi r^2 \Delta r)$ in three dimensions, and $2\pi r \Delta$

- periodic boundary conditions have to be implemented in a box of size $L_x \times L_y$. This means that points $(x + n_x L_x, y + n_y L_y)$ with arbitrary integer n_x and n_y are actually equivalent to point (x, y).

- if a particle is moved in the Metropolis move, check if the final position is inside the box. In case the particle is outside, put it back to the box
  $x := x - (floor)(x/L_x) * L_x$
  $y := y - (floor)(y/L_y) * L_y$;

- now, any distance between two particles should be seen as the minimal distance between their images. A simple way to implement this is, to calculate $\Delta x = x_i - x_j$ and minimize its difference with respect to 0, i.e.
  $\Delta x := \Delta x - (floor)(\Delta x/L_x + 0.5) * L_x$
  $\Delta y := \Delta y - (floor)(\Delta y/L_y + 0.5) * L_y$