Statistical Physics

The solution of this computer exercise can be done individually or by groups of maximum 3 persons. The solution should contain the working computer program, the outputs and clear description of what you did and why. You can use a separate PDF file to write your discussions. The preferred program is Mathematica, Python or C/C++. You can use other tools and languages but support is not guaranteed. You can upload your solution to the StudIP before 12:00 on the submission day.

If you have questions or comments about this exercise, please, contact me via

anas.abdelwahab@itp.uni-hannover.de .

[H19] Deviation from ideal gas   (12 points)

Consider a system of atoms in a box of volume $V = L^3$ and temperature τ. The number of particles is N. The position of particle i is given by $r_i = (x_i, y_i, z_i)$, and they fulfill periodic boundary conditions, i.e. $x_i \simeq x_i + L$, $y_i \simeq y_i + L$, and $z_i \simeq z_i + L$. The interaction between these particles can be described using the Lennard-Jones potential

$$\Phi_{LJ}(|r_i - r_j|) = 4\epsilon \left[\left(\frac{\sigma}{|r_i - r_j|} \right)^{12} - \left(\frac{\sigma}{|r_i - r_j|} \right)^6 \right], \tag{1}$$

where σ and ϵ are Lennard-Jones parameters (we choose $\sigma = 1$ and $\epsilon = 1$). However, we restrict the range of interaction to be zero after a certain length r_{cut}, i.e.

$$\Phi(|r_i - r_j|) = \begin{cases} \Phi_{LJ}(|r_i - r_j|) - \Phi_{cut} & \text{if } |r_i - r_j| \leq r_{cut} \\ 0 & \text{if } |r_i - r_j| > r_{cut} \end{cases} \tag{2}$$

where $\Phi_{cut} = \Phi_{LJ}(r_{cut})$. The average pressure is given by

$$\langle p \rangle = n\tau - \frac{1}{3V} \left\langle \sum_{i=1}^{N-1} \sum_{j=1+1}^{N} 48\epsilon \left[\left(\frac{\sigma}{|r_i - r_j|} \right)^{12} - \left(\frac{\sigma}{|r_i - r_j|} \right)^6 \right] \right\rangle, \tag{3}$$

where $\langle ... \rangle$ denotes the average over the configuration $\{r_1, ..., r_N\}$ generated below, and $n = N/V$.

One can use the Metropolis algorithm to calculate the average pressure similar to what has been done in the previous computer exercise, but instead of flipping a randomly selected spin a randomly selected particle is given a random displacement. Therefore, the calculations contain the following steps:

1. Set the initial configuration by locating the particles orderly in a cube with the volume V (e.g. construct a simple cubic crystal structure).

2. Calculate the energy of the configuration,

$$E_c = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \Phi(|r_i - r_j|). \tag{4}$$

3. Give a random displacement for the selected particle such that $x_i \rightarrow x_i + l\delta_1$, $y_i \rightarrow y_i + l\delta_2$ and $z_i \rightarrow z_i + l\delta_3$, where δ_i are random numbers in the range $[-1, 1]$ and l is the amplitude of the displacement.

4. Calculate the energy difference between the new and the previous configuration, and accept or reject the new configuration applying the same condition as used for the Ising model.

5. Continue the iteration and calculate the average quantities.

For $N = 265$, $\Phi_{cut} = 2.5 \ \epsilon$, $l = \frac{L}{2}$ and $\tau = 2$ calculate the pressure for several values of n up to $n = 1$, and fit the pressure to the virial expansion

$$p(n) = n\tau + B_2 n^2 + B_3 n^3 + \dots \ . \tag{5}$$

How many terms are needed for each value of n? Repeat your calculations for $\tau = 0.4, 0.6, 0.8, 1.1$ and discuss your results. Produce dynamical visualizations of your results.