Computational Physics Sommersemester 2025

Exercise Sheet 03

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Contents

1 Part a

After we implemented the 3rd Dimension we obtain following Energy Plot:

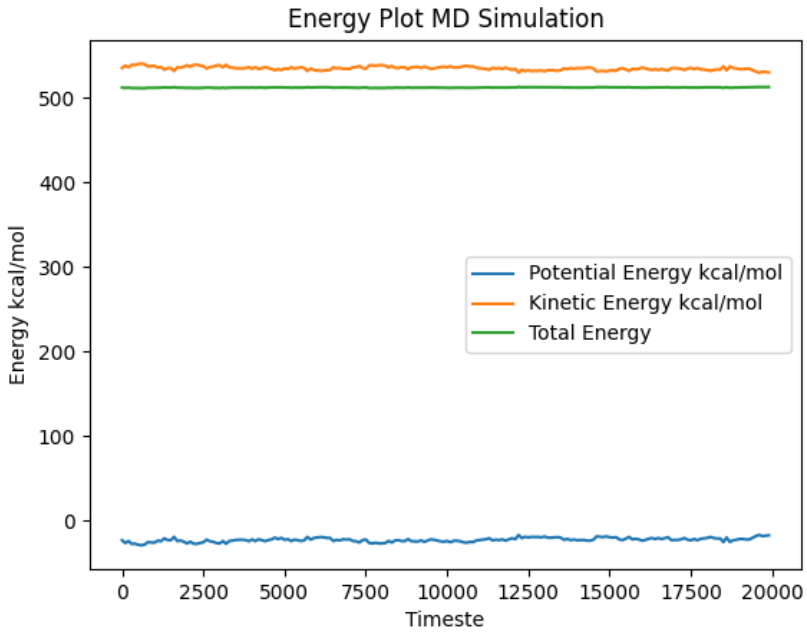

Figure 1: Energy Plot of our Simulation in 3D. $\rho = 0.01$ and $n^3 = 512$

The mean of the potential energy is $\bar{U} = -22.7\,\text{kcal/mole}$.

2 Part b

The radial distribution function $g(r)$ in the low-density limit for particles interacting via the Lennard-Jones potential is given by:

$$g(r) \approx \exp\left(-\frac{U(r)}{k_B T}\right)$$

with the Lennard-Jones potential:

$$U(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

Combining both:

$$g(r) \approx \exp\left(-\frac{4\varepsilon}{k_B T}\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]\right) \tag{1}$$

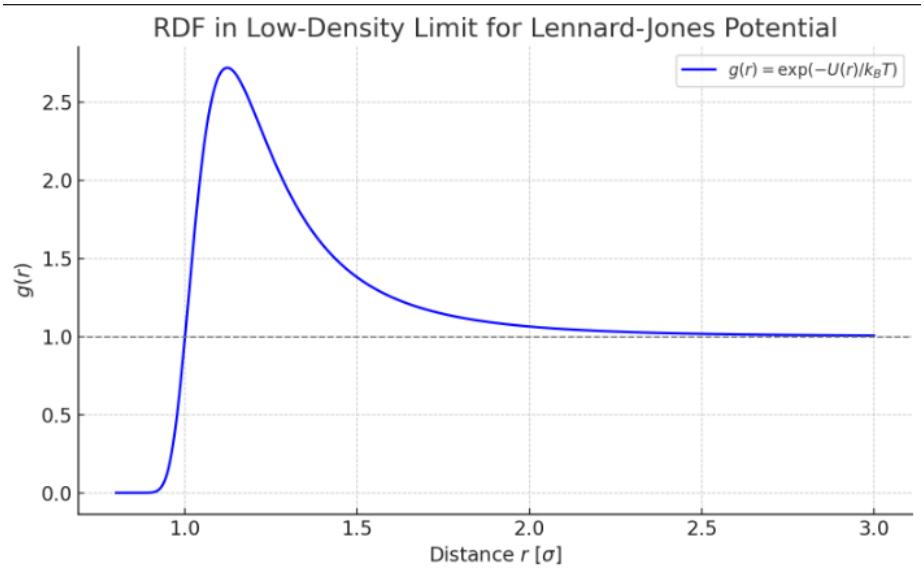

Figure 2: Theoretical low density limit

Our result of the MD Simulation can be seen in fig. 3.

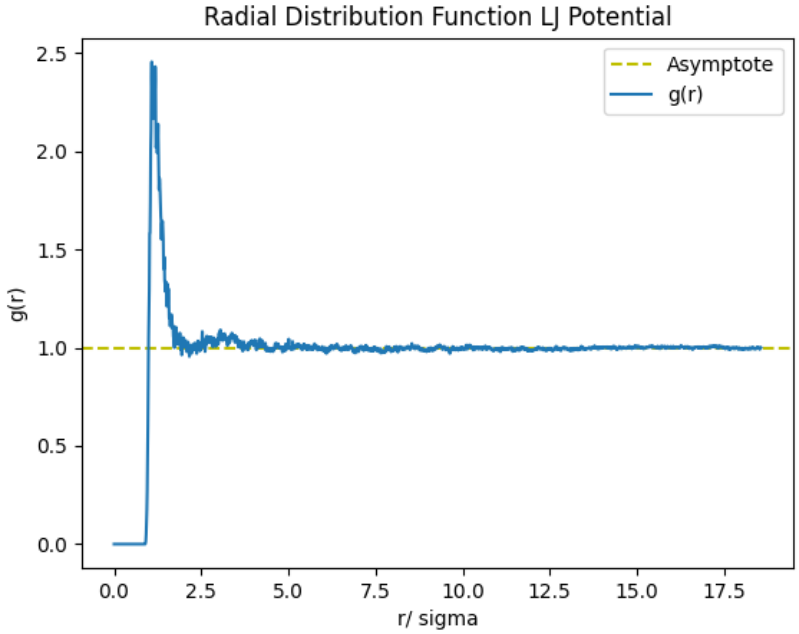

Figure 3: Result of our Simulation with $n^3 = 512$ and $\rho = 0.01$

For both, one can see that the graph is zero for values below 1, because particles dont overlap. Further, it can be seen that our $g(r)$ looks very similar to the

low density limit as shown in fig. 2. The only notable difference is that in our plot, an oscillation with another small peak after the first peak already starts to form, whereas in the low density limit, $g(r)$ decays monotonically as can be seen in eq. (1).

3 Part c

For a density of $\rho = 0.5$, we get the following $g(r)$:

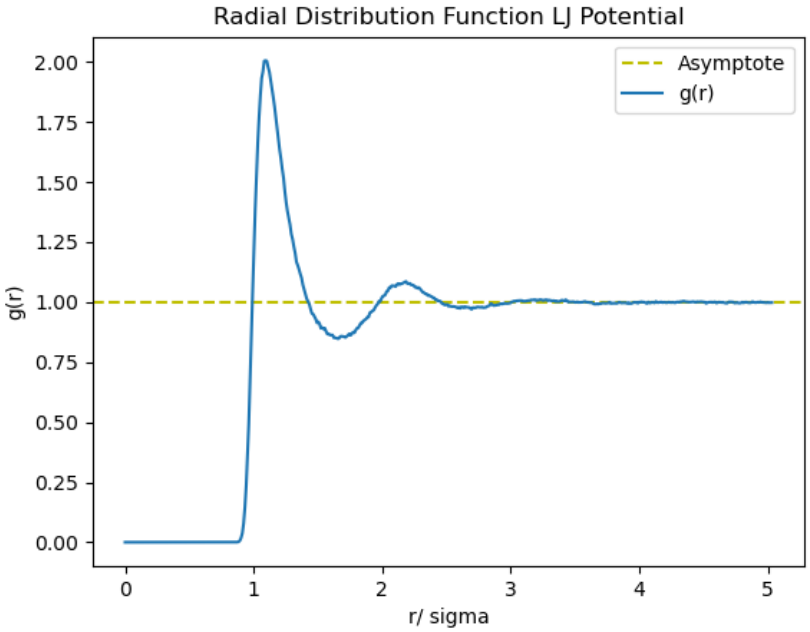

Figure 4: Result with $\rho = 0.5$ and $n^3 = 512$

The characteristic properties of this $g(r)$ are:

$g(r_{max})$	2.01
r_{max}	1.09 r/σ
$g(r_{minlokal})$	0.85
$r_{minlokal}$	1.65 r/σ

Table 1: Results of RDF with $\rho = 0.5$ and $n^3 = 512$

Here, the first peak means that particles have a tendency to be in a distance of $r_{\max} = 1.09\,\sigma$ and thus very close to each other since σ can be interpreted as the diameter. When comparing to the low density limit one can see that this does not result from a higher density but rather from the intrinsic particle distribution. The higher density only causes the oscillations.

4 Part d

We implemented the given integral for the mean potential energy per particle U/N as given on the exercise sheet. For this implementation, we integrated over the whole space, leaving us with a factor $4\pi \cdot r^2$.
The term "integrating" is a bit misleading here since our values were discrete; thus, we summed over our values and weighted them with the corresponding value of r in the volume factor.
The implementation can be found in *part_ de.py*. Note that for a better comparison, we directly multiplied with N.

By this, we were able to calculate the mean of U for both $\rho = 0.01$ and $\rho = 0.5$. We ended up with the values

$$U_{g(r),\,\rho=0.01} = -22.5\,\text{kcal/mole}, \qquad U_{g(r),\,\rho=0.5} = -861.5\,\text{kcal/mole}.$$

If we compare this to the values we obtained by taking the mean of the energies from separate snapshots, we can see that for both, the absolute values obtained via $g(r)$ are smaller:

$$\bar{U}_{\rho=0.01} = -22.7\,\text{kcal/mole}, \qquad \bar{U}_{\rho=0.5} = -874.5\,\text{kcal/mole}.$$

($\bar{U}_{\rho=0.5}$ was obtained in the same way we used in part a).

If we remember that we didn't really integrate, but rather summed over discrete value, it becomes clear why the absolute values $U_{g(r)}$ are slightly smaller than the mean values $\bar{U}$: while the value for $g(r)$ features particles in the interval $[r, r+\delta r)$, we only weight with a factor $4\pi \cdot r^2$ instead of $4\pi \cdot (r+\delta r)^2$ in the integral. In the limit of $\delta r \to 0$, both converge to the same, but at out system size there wasn't enough statistics to decrease the size of δr further.

5 Part e

With the formula given in the exercise sheet we obtain a $\kappa_T = 0.7563\,\text{mole} \cdot \text{nm}^3/\text{kcal}$ for $\rho = 0.01$. If we change the density to $\rho = 0.5$ the isothermal compressibility changes to $\kappa_T = 0.0059\,\text{mole} \cdot \text{nm}^3/\text{kcal}$.
It makes perfectly sense that for higher densities, it becomes much harder to compress the gas, which is clearly shown by our calculated values.