Universität Freiburg – Institut für Physik
Applied Theoretical Physics
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Exercise 7 for '*Computational Physics - Material Science*', SoSe 2021

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Please provide a well documented submission of your solution. Your submission should include

- A pdf file containing the solution to the questions with the corresponding equations that are implemented in your codes. Figures must contain axis titles with corresponding units and a caption.
- The source code should be commented, and the equations given in the pdf file have to be referenced in the source code.
- There is no need to provide the trajectory files.
- In case your code is not working properly, please provide a description of the debugging attempts you did.

Exercise 7.1: From the radial distribution function to the structure factor

The objective of this exercise is to recover the relationships between the radial distribution function, the structure factor, and the isothermal compressibility.

a) Using the canonical ensemble engine implemented in Sheet #6 with $T_d = 300$ K, simulate the trajectory of N atoms interacting through a LJ potential distributed in a simulation box of volume V such that the number density is $\rho = 0.5\sigma^{-3}$. 2000 steps are used for the equilibration run, and 20000 steps are used for the production run. Save the trajectory obtained during the production run every 10 steps. Calculate and plot $g(r)$ versus r.

b) Noting the wave vectors, $\mathbf{k_i}$ with $\mathbf{i} = (i_1, i_2, i_3) \in \mathbb{N}^3$, as $\mathbf{k_i} = (i_1 k_x, i_2 k_y, i_3 k_z)$ with $k_x = 2\pi/L_x$, $k_y = 2\pi/L_y$, $k_z = 2\pi/L_z$ (L_x, L_y, and L_z being the box size along x, y, and z), and $k = |\mathbf{k_i}| = ((i_1 k_x)^2 + (i_2 k_y)^2 + (i_3 k_z)^2)^{1/2}$, the structure factor, $S(k)$ of a monodisperse system (a system containing only atoms of identical size) of N atoms with position $\mathbf{r_i}$ is defined as:

$$S(\mathbf{k}) = \frac{1}{N} < |\sum_{i=1}^{N} \cos(\mathbf{k}.\mathbf{r_i})|^2 + |\sum_{i=1}^{N} \sin(\mathbf{k}.\mathbf{r_i})|^2 >$$

Using the trajectory file obtained in (a), implement an analysis routine that calculates the structure factor, $S(k)$, averaged over the whole production run. The number ($\mathbf{i} = (i_1, i_2, i_3)$) of wave vectors used for the calculation of $S(k)$ needs to be an input. A pseudo code for building the wave vectors saved in the list of class *Wavevector*, is:

nk = 0
for nx = 0 to nx $< i_1$
for ny = 0 to ny $< i_2$

for nz = 0 to nz $< i_3$
Wavevector[nk].x $=$ *nx***k_x*; *Wavevector[nk].y* $=$ *ny***k_y*; *Wavevector[nk].z* $=$ *nz***k_z*
nk += 1

Calculate and plot $S(k)$ vs k for $\mathbf{i} = (50, 50, 50)$. The limit value of $S(0)$ is related to the isothermal compressibility as $\lim_{k\to 0} S(k) = \rho k_B T_d \kappa_T$. What is the magnitude of the isothermal compressibility obtained from $S(0)$?

c) The structure factor, $S(k)$, can also be derived directly from the radial distribution function, $g(r)$, as

$$S(k) = 1 + 4\pi\rho_0 \int_{0^+}^{\infty} dr (g(r) - 1) r^2 \frac{sin(kr)}{kr}.$$

Using $g(r)$ calculated in (a), implement an analysis code that calculates and plots $S(k)$ versus k, for k in the same range as in (b) (the integration can be performed using trapezoidal integration e.g. $\int_a^b f(x)dx \approx \Delta x(\frac{f(x_N)+f(x_0)}{2} + \sum_{l=1}^{N-1} f(x_l))$ with $\Delta x = \frac{b-a}{N}$, and $x_0 = a$ and $x_N = b$). How does the variation of the structure factor compare with the ones obtained in (b)? What is the magnitude of $S(k)$ in the limit $k \to 0$, and how does it compare with the limit obtained in (b)? Interpret the structure factor, in particular, the position of the first peak.

d) Calculate the isothermal compressibility, κ_T, directly from the radial distribution function (see exercise sheet #3). How does it compare with the magnitude of κ_T obtained in (b) and (c)?

Numerical values of quantities to be used:

quantity	value (units)
k_B	1.38×10^{-23} (m^2 kg s^{-2} K^{-1})
ϵ	0.5 k_BT
σ	2.55×10^{-10} (m)
T_d	300 (K) or see text
mass	105.52×10^{-27} (kg)
Δt	10^{-15} (s)