Exercise sheet 2

Structure factors and the thermodynamic limit

PUE Advanced Computational Physics

University of Vienna - Faculty of Physics

6 The thermodynamic limit

In simulations related to statistical mechanics one is often interested in the so-called thermodynamic limit—i.e. the properties of an infinitely large system.

a. Perform a series of simulations of liquid argon at the triple point with varying system size (at least $N = 108$, 256, 500).

b. Investigate the N-dependence of potential energy U, pressure p, and pair correlation function $g(r)$.

7 The structure factor

The structure factor and the pair correlation function are related by the following one-to-one correspondence:

$$S(k) = 1 + \frac{4\pi\rho}{k} \int_0^\infty \mathrm{d}r\, r \sin kr \,[g(r) - 1]\,,$$
$$g(r) = 1 + \frac{1}{2\pi^2\rho r} \int_0^\infty \mathrm{d}k\, k \sin kr \,[S(k) - 1]\,.$$

For one of the simulations performed previously, calculate the structure factor $S(k)$ from the obtained $g(r)$ and then try to reconstruct $g(r)$ from $S(k)$. *Hint:* In practice the integrals have to be truncated. In simulations the cutoff is given by the size of the simulation box used. Experimental data is usually truncated at wave numbers on the order of $k\sigma \approx 20$.