Università degli Studi di Trento – Dipartimento di Fisica

Computational Physics 1

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Self-consistent methods for liquid structure

Contents

1 The radial (Hankel) transform

Implement the direct and inverse radial (Hankel) transform and test them by calculating the structure factor $S(q)$ corresponding to the low-density pair distribution function of the Lennard-Jones potential $v(r)$, that is

$$g(r) = \exp\left[-\beta v(r)\right].$$

What would you put as the value of the density ρ?

2 Percus-Yevick and Hypernetted Chain approximations

Calculate the pair distribution function of the Lennard-Jones liquid and the repulsive-Lennard-Jones liquid, by solving the Percus–Yevick and Hypernetted Chain closure of the Ornstein–Zernicke equation. Use your results to estimate the average energy per particle and the pressure of the system for selected values of the (reduced) density and temperature.

Compare your result with the outcome of molecular dynamics simulation.