Radial distribution function of hard-sphere fluid

Christian Vogt

Master thesis in Physics

Liquid molecules are constantly interacting with their neighbours, because of their dense nature. This implies that we need a technique which tells us the physical properties of a liquid, this tool will be the radial distribution function. In this work we will first discuss what the radial distribution function is and some of its important properties. Next, the Ornstein-Zernike equation will be introduced, which will be used mainly in the Percus-Yevick approximation for hard spheres, but also investigated briefly in the hypernetted-chain approximation. The derivation of the Ornstein-Zernike equation with help of the density functional theory will also be discussed. Furthermore, the Monte-Carlo simulation method will be treated, which provides a good estimation for the radial distribution function g(r). Finally, based on the known continued fraction method, we will try to generalise the approach to get an expression for infinite integral series. In the second part of the work, some results about the radial density function for hard spheres will be shown. These solutions were obtained by numerical simulations using different methods, but basically by solving the Ornstein-Zernike equation.

Professor Joseph Brader