Blatt 8 - Hausaufgabe   Übung am 21. December 2018

Aufgabe 1: Canonical and Grand canonical ensembles

a) Show that the probability of finding N particles in a grand canonical microstate, p_N, is maximum if $\bar{N}(\mu) = N$.

b) Represent and interpret the probabilities p_n as a function of μ for a one dimensional system of hard rods in a cavity of length $L/\sigma = 4.9$.

c) Show that $\sum_{N=0}^{\infty} \exp(\beta\mu N)(N - \bar{N})Z_N = 0$.

Aufgabe 2: Ornstein-Zernike

Consider a homogeneous one dimensional fluid. Demonstrate the Ornstein-Zernike equation

$$h(x) = c(x) + \rho \int_{-\infty}^{\infty} dx' c(x')h(|x - x'|), \tag{1}$$

implies the continuity of $h(x) - c(x)$ everywhere. (Note: h and c remain finite everywhere.)

Aufgabe 3: Virial equation

Consider a homogeneous fluid with pairwise interactions given by the interparticle potential $\phi(r)$. The virial equation for the pressure is

$$p = k_B T \left(\frac{\partial \ln Z}{\partial V}\right) = k_B T\rho + \frac{1}{3V}\left\langle \sum_{i=1}^{N} \boldsymbol{r}_i \cdot \boldsymbol{f}_i \right\rangle, \tag{2}$$

with $\boldsymbol{f}_i$ the internal forces acting on the i-th particle.

(a) Show that

$$\sum_{i=1}^{N} \boldsymbol{r}_i \cdot \boldsymbol{f}_i = \sum_{i=1}^{N} \sum_{j,j<i} \boldsymbol{r}_{ij} \cdot \boldsymbol{f}_{ij}, (3)$$

with $\boldsymbol{f}_{ij}$ the force acting on the i-th particle due to the presence of particle j.

(b) Use the above results to find the virial equation

$$p = k_B T\rho - \frac{\rho^2}{6}\int d\boldsymbol{r} r\phi'(r)g(r), \tag{4}$$

with $g(r)$ the radial distribution function.

(c) Show that for hard-spheres (HS) of diameter σ, the virial equation simplifies to

$$p_{\text{HS}} = k_B T\rho + k_B T\frac{2\pi}{3}\rho^2\sigma^3 g(\sigma). \tag{5}$$

Hint: $g(r)\exp(\beta\phi(r))$ is continuous everywhere.

Blatt 8 - Präsenzübung

Übung am 21. December 2019

Aufgabe 4: Equation of state of hard rods in one dimension

The direct correlation function of a one-dimensional fluid of hard rods of length σ is

$$c(x) = \begin{cases} -\frac{1}{1-\eta} - \frac{\eta}{(1-\eta)^2}\left(1 - \frac{|x|}{\sigma}\right), & \text{if } |x| < \sigma \\ 0, & \text{otherwise} \end{cases}$$

where $\eta = \rho\sigma$ is the packing fraction.

a) Using the result of Aufgabe 2 obtain the contact value of the radial distribution function, that is $\lim_{x\to\sigma^+} g(x)$.

b) Using the contact value of the radial distribution function obtain the equation of state $P(\rho)$.