Heinrich–Heine–Universität Düsseldorf
Institut für Theoretische Physik II
Computational Physics
Wintersemester 2018/2019

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Problem 13.1: **Grand-Canonical Monte Carlo of a 2D WCA fluid**

Consider a set of particles of diameter σ disposed in a 2D square box of length L. The interactions between the particles are modeled via the pairwise-additive Weeks-Chandler-Andersen (WCA) potential. Here, the interaction between two particles, separated by a distance r, is given by

$$u(r) = \begin{cases} 4\varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] + \varepsilon, & \text{if } r \leq 2^{1/6}\sigma \\ 0, & \text{if } r > 2^{1/6}\sigma \end{cases} \tag{1}$$

where the two parameters σ and ε have units of length and energy, respectively. The number of particles is $N = 144$ and the number density of the system is $\rho = 0.3$. Consider three temperatures $T = 1.0, 2.0, 3.0$ (same set up as Ex. 12).

Use the values which you obtained in Ex. 12 for $\mu_{\text{ex.}}$ at $T = 1.0, 2.0, 3.0$ and perform grand canonical Monte Carlo (MC) simulations to compute the probability distribution of the number of particles $P(N)$. Compare the results which you obtain for different values of $\mu_{\text{ex.}}$.