Heinrich-Heine-Universität Düsseldorf Institut für Theoretische Physik II Computational Physics Wintersemester 2018/2019 Prof. Dr. J. Horbach M. Eshraghi (mojtaba.eshraghi@hhu.de) M. Golkia (mehrdad.golkia@hhu.de) Blatt 10 vom 18.12.2018 Abgabe bis 16:00 Uhr am 08.01.2019

Problem 10.1: Metropolis Method in the Canonical Ensemble

In the Metropolis Monte-Carlo method random configurations are generated and accepted or rejected according to a given probability criterion. Let $\Delta U_{kk'}$ the difference between the potential energy of a system at the transition from the configuration k to the configuration k'. The new configuration k' is accepted with a probability $w_{kk'}$ given by

$$w_{kk'} = \begin{cases} 1 & \text{if } \Delta U_{kk'} \le 0, \\ \exp\left(\frac{-\Delta U_{kk'}}{k_B T}\right) & \text{if } \Delta U_{kk'} > 0. \end{cases}$$
 (1)

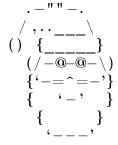
When $\Delta U_{kk'} > 0$ a new uniform random number ζ between 0 and 1 is generated, and the new configuration is accepted only if $\zeta < w_{kk'}$. If the new configuration is rejected the system stays in the old configuration k. New configurations are generated by random displacements of particles selected randomly

$$(x_i, y_i) \leftarrow (x_i, y_i) + \delta(u_x, u_y) , \qquad (2)$$

where δ is the maximal displacement and u_x and u_y are two uniform random numbers in the interval [-0.5, 0.5].

- a) Implement the Metropolis algorithm for the simulation of the two-dimensional WCA potential in the canonical ensemble. Use as initial configuration particles arranged in a regular square lattice.
- b) Determine the acceptance rate for different values of the maximum displacement $\delta \in [0.1, 1]$.
- c) Calculate the mean-squared displacement for the 2d-WCA system. Plot the mean-squared displacement as function of the Monte-Carlo sweeps. Hint: Use $\delta=0.1$.
- d) How do the results in c) change for $\delta = 0.2$? Describe the difference to the choice $\delta = 0.1$.
- e) Determine the pair correlation function g(r) and compare the result with the one obtained from molecular dynamics simulation in the previous exercise sheet (Problem 8.1).

Note: Perform the simulations at the same reduced density and temperature as in Problem 8.2, i.e. at $\rho = 0.74$ and T = 1.0.



***** Merry Christmas and Happy New Year *****