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

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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

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

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

$$(x_i, y_i) \leftarrow (x_i, y_i) + \delta(u_x, u_y) \ , \tag{2}$$

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 $T = 1.0$.

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