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

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Problem 12.1: **Widom insertion method**

In this exercise you calculate the chemical potential μ of a system using the Widom insertion method.

a) Derive Widom's formula:

$$\mu - \mu_{\text{ideal}} = \mu_{\text{ex.}} = -k_{\text{B}}T \ln\Big(\int d\mathbf{s}_{N+1} \Big\langle \exp(-\frac{\Delta U}{k_{\text{B}}T}) \Big\rangle_N \Big) \,, \tag{1}$$

with μ_{ideal} and $\mu_{\text{ex.}}$ the ideal gas and excess chemical potential, respectively, $\langle \cdots \rangle_N$ the canonical average of a system with N particles, T the temperature, k_{B} Boltzmann's constant, $\mathbf{s}_{N+1}$ the position of the trial particle, and ΔU the energy change due to the insertion of the trial particle.

b) Write a code to calculate the chemical potential of the system that you have worked with in Ex. 10 (two-dimensional WCA potential in the canonical ensemble at $T = 1.0$), but use a smaller density $\rho = 0.3$.

c) Now change the temperature to $T = 2.0$ and $T = 3.0$. Plot the chemical potential as a function of T. By increasing the temperature, do you expect an increase or a decrease in $\mu_{\text{ex.}}$?