Heinrich–Heine–Universität Düsseldorf
Institut für Theoretische Physik II
Computational Physics
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Problem 11.1: **Grand-Canonical Monte Carlo**

Consider a set of hard segments of length σ disposed on a straight line of length L and confined between hard boundaries at $x = 0$ and $x = L$. The interaction between segments is given by

$$U(r) = \begin{cases} \infty & \text{if } r \leq \sigma, \\ 0 & \text{if } r > \sigma, \end{cases} \tag{1}$$

with r the distance between the segment centers. The possible configurations of this system can be sampled by grand-canonical Monte Carlo simulation. The method consists of the following steps

a) generate random number $u \in [0, 1]$, if $u < 0.5$ perform a trial removal and continue with step b) otherwise perform a trial insertion; step c).

b) randomly choose a segment and accept its removal with probability $P_{\text{acc}}(N \to N - 1)$ and return to step a).

c) generate a random coordinate $x \in [\sigma/2, L - \sigma/2]$ for the new segment and accept the insertion with probability $P_{\text{acc}}(N \to N + 1)$ and return to step a).

The acceptance probability of the particle insertion is given by

$$P_{\text{acc}}(N \to N+1) = \min\left[1, \frac{L}{\lambda\,(N+1)} e^{\beta\mu} e^{-\beta[U(N+1)-U(N)]}\right] \tag{2}$$

and the acceptance probability of particle removal is given by

$$P_{\text{acc}}(N \to N-1) = \min\left[1, \frac{\lambda N}{L} e^{-\beta\mu} e^{-\beta[U(N)-U(N-1)]}\right] \tag{3}$$

where N is the number of segments, L the distance between walls, $\beta = 1/(k_B T)$ and λ the thermal de Broglie wavelength. Consider here $k_B = 1$, $\sigma = 1$ and $\lambda = 1$.

a) Use the grand canonical Monte Carlo (MC) to compute density profiles of hard segments (1d) in confinement for $L = 100$, $T = 1$ and three different values of the chemical potential $\mu = 1$, $\mu = 5$ and $\mu = 20$.
Hints: Consider at least 10^6 particle insertion/removal trials and averages over 10^3 configurations. Use a resolution of $\Delta x = 0.1\sigma$ for the calculation of the density profile.

b) Plot the number of particles versus number of MC sweeps (write N only each 10^3 steps).

c) Find for $T = 1$ and each value of μ the global density.

d) Interpret your results in a).