Computer Simulations
1st exam

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Theory exam
July 1, 2025
Available time: 1 hour

Write your name and student number on every sheet you submit.

1. Sampling methods

We want to draw random numbers distributed according to the distribution

$$g(x) = x \exp(-x) \quad \text{for } x \geq 0,$$

which has the cumulative distribution function $G(x) = 1 - (1 + x)\exp(-x)$.

(a) Can the inverse transformation method be used to sample from the distribution $g(x)$? Explain.

(b) We construct an envelope function based on

$$h(x) = \frac{\exp(-\sqrt{x})}{2\sqrt{x}}.$$

Show that the cumulative distribution function of $h(x)$ is given by

$$H(x) = 1 - \exp(-\sqrt{x}).$$

(c) Calculate the inverse cumulative distribution function $H^{-1}(u)$ and explain why $h(x)$ can be used as the basis of an envelope function for $g(x)$.

(d) Explain the steps necessary to use $H^{-1}(u)$, where u is a uniformly distributed random number, to draw samples from the distribution $g(x)$.

2. Monte Carlo simulations

We perform a Monte Carlo simulation of N magnetic particles that can translate and rotate in three dimensions. When an external magnetic field with intensity B_x is applied in x direction, the Hamiltonian is given by

$$\mathcal{H} = \mathcal{H}_0 - M_x B_x,$$

with M_x being the total magnetization in x direction.

(a) Write down an expression for the ensemble average $\langle M_x \rangle$. The phase space consists of the positions $\boldsymbol{r}^N$ and orientations $\boldsymbol{\omega}^N$ of the particles, but may also be approximated as a discrete set of microstates.

(b) To simulate the translations, the following Monte Carlo moves are proposed

$$\boldsymbol{r}' = \boldsymbol{r} + \alpha \boldsymbol{u},$$

where α is the step size and $\boldsymbol{u}$ is a vector with three numbers, each drawn from the uniform distribution between 0 and 1. Explain whether this Monte Carlo algorithm will converge to a stationary distribution.

(c) We are interested in the magnetic susceptibility

$$\chi = \mu_0 \left(\frac{\partial \langle M_x \rangle}{\partial B_x} \right)_{T,V},$$

with μ_0 being the constant magnetic vacuum permeability. Write down an expression that can be used to estimate χ from simulations at two different values of B_x, $B_x^{(1)}$ and $B_x^{(2)}$.*

(d) As an alternative to performing simulations at different values of B_x, the susceptibility can be calculated using the expression

$$\chi = \frac{\mu_0}{k_B T} \left(\langle M^2 \rangle - \langle M \rangle^2 \right).$$

Explain the conditions under which this expression provides an accurate estimate of χ and discuss the simulation parameters that have to be used for this alternative expression to be valid.

3. **Molecular dynamics simulations**

(a) In the long-time limit, the time average of an observable A is defined as

$$\bar{A} = \frac{1}{\mathcal{N}_{init}} \sum_{j=1}^{\mathcal{N}_{init}} \left(\lim_{t \to \infty} \int_0^t dt' \, A(\boldsymbol{r}_j^N(0), \boldsymbol{p}_j^N(0), t') \right),$$

where we have additionally averaged over $\mathcal{N}_{init}$ initial conditions characterized by positions and momenta $\boldsymbol{r}_j^N(0)$ and $\boldsymbol{p}_j^N(0)$. In the limit where $\mathcal{N}_{init}$ equals the total number of configurations compatible with a given ensemble, the ensemble average is defined as

$$\langle A(t) \rangle = \frac{1}{\mathcal{N}_{init}} \sum_{j=1}^{\mathcal{N}_{init}} A(\boldsymbol{r}_j^N(0), \boldsymbol{p}_j^N(0), t)$$

Under which circumstances are the expressions for $\bar{A}$ and $\langle A(t) \rangle$ the same?

(b) In the case of a pairwise additive interaction potential, how does the computational cost of the force calculation scale with the number of particles N in the system? You may discard the effects of boundary conditions and cutoff distances.

*If you did not succeed in answering part (a), the ensemble averages at these values may be denoted as $\langle M_x \rangle_1$ and $\langle M_x \rangle_2$, respectively.