Molecular Dynamics and Monte Carlo Simulations

Written Exam Spring Semester 2023

Name: _____ **SCIPER:** _____

1. What are some of the approximations made when moving from the time evolution of a quantum mechanical system to the one of a classical system? What do you gain and what do you lose?

2. Explain the following terms (provide examples or mathematical definitions and formulas where possible):
    a. Ergodicity and ergodic theorem
    b. Partition function
    c. Phase space versus configuration space
    d. Stochastic matrix
    e. Microstate
    f. Thermal equilibrium

3. Describe differences between Monte Carlo and Molecular Dynamics sampling of an ensemble. Which advantages/disadvantages do you see for the two methods?

4. Consider a Metropolis Monte Carlo sampling procedure for a box of liquid water at room temperature. Which probability distribution would you use for accepting a trial move for this specific system? Suggest one trial move for this specific water system that obeys detailed balance and one that violates it. Are living systems obeying detailed balance? Why?

5. Which ones of the following equations and time integration algorithms are time-reversible, i.e. describe the same trajectory when reversing time from t to $-t$? Why?
    a. Newton's equation of motion
    b. Position Verlet
    c. Leap frog
    d. Gear predictor-corrector

6. Give at least one physical and one practical reason for the fact that in most water models van der Waals interactions of the hydrogen atoms are neglected.

Bonus: a) What is the principal idea of the Car-Parrinello Method (in words)? b) Write down the extended Lagrangian.