REVIEW OF STATISTICAL MECHANICS


2) Consistency of thermodynamics and classical mechanics: reversibility and Poincare' return time. Huang, sec. 4.5 (a better discussion appears in Falcioni, Vulpiani, Meccanica Statistica Elementare, in Italian). Tuckerman, sec. 3.2, 3.5.

3) Microcanonical ensemble, canonical ensemble, isobaric-isothermal ensemble, grandcanonical ensemble. The ideal gas. Tuckerman, sec. 4.3, 4.5.1, 5.4, 5.5, 6.4, 6.5. [note: derivations of the different partition functions are not required].

4) Virial pressure. Pair distribution function. Average kinetic energy and equipartition theorem. Tuckerman, sec. 16.6, 4.6.

THE MONTE CARLO METHOD


3) Simple algorithms for spin models and molecular systems of monoatomic molecules in the canonical ensemble. Determination of the average energy and pressure. Frenkel, Smit, sec. 3.2, 5.2

4) Computation of the chemical potential with Widom method. Simulations in the isobaric/isothermal ensemble. Frenkel, Smit, sec. 7.2.1, 5.4, 7.2.2 (p. 161 only)


6) Reweighting data. Notes on biased methods: Sec. 2.
7) Combining reweighting data.  
Notes on biased methods: Sec. 3.

8) Umbrella sampling, simulated tempering, parallel tempering  
Notes on biased methods: Sec. 4.1, 4.2, 6.1

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MOLECULAR DYNAMICS (09/05 - 06/06)

Frenkel, Smit, Sec. 4.1 and 4.2  
Tuckerman, sec. 3.8, sec. 3.13 (p.120, 121 only).

Tuckerman, sec. 3.10, Frenkel, Smit, Sec. 4.3.3

3) Properties of Liouvillian and existence of a conserved Hamiltonian.  
Tuckerman, sec. 3.13.

4) Multiple-time step algorithms.  
Tuckerman, sec. 3.11

5) Constraints.  
Tuckerman, sec. 3.9.1. Frenkel, Smit, sec. 10.1

6) Nose–Hoover.  
Tuckerman, sec. 4.8.1, 4.9.4. Frenkel, Smit, sec. 6.1.2.  

7) Langevin equation.