REVIEW OF STATISTICAL MECHANICS

1)
Introduction to thermodynamics. Thermodynamic potentials.
Extensive and intensive quantities. Chemical potential of the ideal gas. Relation between chemical potential
and the equation of state in the canonical ensemble.
Tuckerman, sec. 2.2, 3.2, 4.2, 5.2, 6.3.

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

1) Independent random data sets. Bias and errors. Jackknife method. Blocking.
Lecture I on MC methods.

2) Importance sampling. Dynamic Monte Carlo and Markov chains. Autocorrelation function and error estimates. Reversibility and detailed balance. Metropolis algorithm.
Lecture II on MC methods.

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)

5) Grand-canonical ensemble.
Frenkel, Smit, sec. 5.6.2, 5.6.3, 5.6.4.

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

MOLECULAR DYNAMICS (09/05 – 06/06)

1) Basics of MD simulations. Verlet updates. Verlet update for the harmonic oscillator. Some practical questions.
Frenkel, Smit, Sec. 4.1 and 4.2
Tuckerman, sec. 3.8, sec. 3.13 (p.120, 121 only).

2) Liouville operator in classical mechanics. Liouvillian formulation
of the dynamics. Verlet update in the Liouville approach.
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.
Frenkel, Smit, App. E.2.

7) Langevin equation.