

COMPUTATIONAL STATISTICAL MECHANICS 2017 (BACHELET-MORONI)
SHORT TABLE OF CONTENTS

Self-consistent field (Giovanni Bachelet)

Schrödinger equation, variational principle
Interacting electrons
Hartree-Fock approximation
Density Functional Theory
Electrons in atoms: shell structure, Periodic Table
Electrons in crystals: Bloch, plane waves, pseudopotentials
Total energy and interatomic forces: Hellmann-Feynman

Quantum Monte Carlo (Saverio Moroni)

Variational Monte Carlo:

- Stochastic integration, Metropolis algorithm
- Correlated wavefunctions, local energy
- Expectation values
- Optimization by correlated sampling

Projection Monte Carlo:

- Imaginary time evolution
- Variational Path Integral, mixed and pure estimation
- Diffusion Monte Carlo, branching random walk
- Fermion sign problema and Fixed Node Approximation

NB

Theoretical, methodological and computational aspects of the above subject list are addressed by the course. More details, references, notes on <http://www.giovannibachelet.it/CSM-16-17/>.