

COMPUTATIONAL STATISTICAL MECHANICS 2016 (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-15-16/>.