

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.giovanibachelet.it/CSM-17-18/>.