Course title:
Computational Statistical Mechanics

Instructors:
Giovanni Bachelet (giovanni.bachelet@roma1.infn.it), Saverio Moroni (saveriomoroni@gmail.com)
Fermi building, room 304, ext. 2-3474

Subject and scope:
Computational Statistical Mechanics aims at the evaluation of macroscopic collective and average properties of many-body systems (up to ~10^{22} particles) through the microscopic numerical evolution (e.g. by Molecular Dynamics or Monte Carlo methods) of very large (yet much smaller) samples of their constituent (classical or quantum) particles. In this context the course will focus on "realistic" many-body systems like electrons in atoms, molecules and solids, or atoms in classical and quantum solids and fluids. To attack them we will need tools common to other branches of Computational Physics (series expansions, matrix inversion and diagonalization, root-finding algorithms, numerical approaches to eigenvalue-eigenfunction systems), and specific tools (like Monte Carlo methods or molecular dynamics). This course will deal with some of these tools. On one hand, it will deal with the electronic structure theories which over the last 40 years, along with the ever-increasing computer power, have allowed a reliable description of many molecular and solid-state systems, and, in particular, a very accurate prediction of their interatomic forces, and thus their structural and dynamical properties "from first-principles". On the other hand, it will deal with quantum Monte Carlo methods, which over the last 40 years have proved a powerful, "numerically exact" simulation tool for realistic and model quantum many-body systems. In particular, the course will deal with:

1. the Density Functional theory, which reduces the many-electron problem to a self-consistent-field problem, and the pseudopotential theory, which further simplifies atoms by eliminating their inner-core electrons: two crucial ingredients for the first-principles prediction of the stability of a compund and of its lattice and molecular dynamics;
2. quantum (variational, diffusion, path-integral) Monte Carlo methods, their applicability and the motivations of their use in the numerical study of quantum many-body interacting systems (like the electron gas, electrons in atoms and molecules, solid or liquid helium).

At the end of the course the student should:

a. have clear ideas on the theories and algorithms which presently allow the calculation from first principles of many properties of atoms, molecules, and solids, and also on their limits and on the directions of development of this field of research;
b. be able to implement on a computer at least one of the methods learned from this course to a quantum many-body system (electrons in an isolated atom or in a periodic crystal; a quantum liquid or solid).

Teaching methods:
Along with the essential elements of the theory (frontal lectures), examples and applications will be both presented and tested in practice (computer lab). Hands-on sessions will represent a larger portion of the Monte Carlo part of the course. A numerical project within the methods spanned by the course, conceived, implemented on the computer, summarized and presented (with a short report or slide presentation) by a single individual or a small group is an integral part of the student's responsibilities.

Evaluation method:
The final examination consists of an individual discussion of (i) one or more subjects covered by the course, as listed in the short table of contents; and (ii) the numerical project which the student has performed.

Frontal lecture plan (very approximate):
Hartree and Hartree-Fock method for interacting electrons (7 hours) / Periodic Table (2 hours) / Density Functional Theory (6 hours) / Electrons in solids and pseudopotentials (7 hours)
Variational Monte Carlo (6 hours) / Diffusion Monte Carlo (6 hours) / Path-Integral Monte Carlo (6 ore)

References:

prerequisites for attending the course

N.W. Ashcroft and N.D. Mermin, Solid State Physics, Holt, Rinehart and Winston 1976*
L.D. Landau e E.M. Lifsic, Fisica teorica. Vol. 3: Meccanica quantistica. Teoria non relativistica. Editori Riuniti 1999*

self-consistent field, Density Functional theory (DFT)

DFT: an introduction, N. Argaman and G. Makov, Am. J. Phys. 68, 69-79 (2000)
DFT of Atoms and Molecules, R.G. Parr and W. Yang, Oxford University Press 1989*
Pseudopotentials that work: from hydrogen to plutonium, G.B. Bachelet, D.R. Hamann, and M. Schlüter, Phys. Rev. B. 26, 4199-4228 (1982)
Iterative minimization techniques for ab initio calculations: molecular dynamics and conjugate gradients, M.C. Payne et al, Rev. Mod. Phys. 64, 1046-1097 (1992)
Phonons and related crystal properties from density-functional perturbation theory, S. Baroni et al, Rev. Mod. Phys. 73, 515-562, (2001)

quantum Monte Carlo (QMC)

Microscopic Simulations in Physics, D.M. Ceperley, Rev. Mod. Phys. 71, S438-443 (1999)
Path integrals in the theory of condensed helium, D.M. Ceperley, Rev. Mod. Phys. 67, 279-355 (1995)
Worm algorithm and diagrammatic MC: A new approach to continuous-space PIMC simulations, M. Boninsegni, N. V. Prokof'ev, and B. V. Svistunov, Phys. Rev. E 74, 036701 (2006)
QMC simulations of solids, W.M.C. Foulkes et al, Rev. Mod. Phys. 73, 33-83 (2001)
Applications of QMC methods in condensed systems, Jindrich Kolorenc and Lubos Mitas, Rep. Prog. Phys. 74, 026502 (28pp) (2011)

Short table of contents: