Computational Quantum Physics (M2)

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Course description

The quantum many-body problem represents one of the biggest scientific challenges of modern science, due to the exponential growth of the complexity of quantum systems with their size. This course aims at introducing some of the most successful methods for the numerical simulation of quantum many-body systems -- from condensed matter and statistical physics to quantum chemistry.

Tentative course plan

1) Introduction to the quantum many-body problem (second quantization, equilibrium and non-equilibrium physics) and its complexity (2h);
2) Exact diagonalization, Krylov space and Lanczos method (2h);
3) Variational approaches; the Monte Carlo method, and variational Monte Carlo for physics and chemistry (4h);
4) Improving on the variational approach: diffusion Monte Carlo, fixed-node approximation for strongly interacting fermions (4h);
5) Density-matrix approaches and tensor-network Ansätze for lattice quantum systems and beyond (4h);
6) Path-integral Monte Carlo methods for systems in continuous space: applications to quantum fluids and solids (4h);
7) Quantum Monte Carlo methods for systems on lattice: applications to condensed matter, statistical physics, etc. (4h).

The exam will be based on a report (written or oral) of either a work in the recent literature, or of an original coding project chosen by the students (either as individuals, or in two-student teams).

TD sessions

The TD sessions will be hands-on sessions, in which you will be required to *write a little computer code* - either alone or in a duo (binôme) - to solve a problem in quantum mechanics. You should bring with you your laptop (or have one shared with your duo partner) and choose a programming platform of your choice (Python, Matlab, Mathematica, Fortran, C, etc.), which is *operational* on your laptop — namely, you should make sure that you have installed the software that you need, e.g. a C/Fortran compiler or a working Python distribution.

Requirements

Introductory quantum mechanics and statistical physics; an introductory class in informatics (ex. Outils numériques (L3)); a minimal familiarity with computer coding (either Python, Matlab, Mathematica, Fortran, C, etc.).

Exam mode

The exam will be based on a report (written or oral) of either a work in the recent literature, or of an original coding project chosen by the students (either as individuals, or in two-student teams).

Bibliography

Our class will cover a variety of topics, which are treated in several different books / review articles

General references
A. Sandvik, *Computational studies of quantum spin systems*, https://arxiv.org/abs/1101.3281
H. Fehske, R. Schneider, A Weisse (Eds.), *Computational Many-Particle Physics* (Springer)

Quantum Monte Carlo
F. Becca and S. Sorella, *Quantum Monte Carlo Approaches for Correlated Systems* (Cambridge, 2017);
J. Gubernatis, N. Kawashima and P. Werner, *Quantum Monte Carlo Methods: Algorithms for Lattice Models* (Cambridge, 2016);
M. E. Tuckerman, *Statistical Mechanics: Theory and Molecular Simulation* (Oxford, 2010);
B. L. Hammond, W. A. Lester Jr, P. J. Reynolds, *Monte Carlo Methods in Ab Initio Quantum Chemistry* (World Scientific, 1994);
W. M. C. Foulkes, L. Mitas, R. J. Needs, and G. Rajagopal, *Quantum Monte Carlo simulations of solids*, Rev. Mod. Phys. 73, 33 (2001);
D. M. Ceperley, *Path integrals in the theory of condensed helium*, Rev. Mod. Phys. 67, 279 (1995).

Density-Matrix Renormalization Group
S. Montangero, *Introduction to Tensor Network Methods* (Springer);
H. Ma, U. Schollwöck, and Z. Shuai, *Density Matrix Renormalization Group (DMRG)-based approaches in Computational Chemistry* (Elsevier);
T. Xiang, *Density Matrix and Tensor Network Renormalization* (Cambridge).