PHYS-463

Computational quantum physics

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Cursus	Sem.	Type
Ing.-phys	MA2, MA4	Opt.
Minor in Quantum Science and Engineering	E	Opt.
Physicien	MA2, MA4	Opt.
Quantum Science and Engineering	MA2, MA4	Opt.

Language of teaching	English
Credits	4
Session	Summer
Semester	Spring
Exam	Oral
Workload	120h
Weeks	14
Hours	**4 weekly**
Lecture	2 weekly
Exercises	2 weekly
Number of positions	

Summary

The numerical simulation of quantum systems plays a central role in modern physics. This course gives an introduction to key simulation approaches, through lectures and practical programming exercises. Simulation methods based both on classical and quantum computers will be presented.

Content

1. **Single-particle Problems:** Numerical solutions of the Schroedinger equation, Numerov's integration, the split operator method

2. **Quantum Spin Models**: Choice and representations of basis sets for the many-body problem, the Trotter decomposesition for real and imaginary-time evolution

3. **Electronic Structure**: Second Quantization, Full Configuration Interaction, Hartree-Fock, Density Functional Theory

4. **Variational Methods**: Variational Monte Carlo. Machine Learning Based Techniques, Time-dependent Variational Approaches

5. **Quantum Monte Carlo Methods**: Path Integral Monte Carlo at finite and zero temperature

6. **Quantum Computing**: Quantum simulation on a quantum computer, Adiabatic State preparation, Variational Quantum Eigensolver

Keywords

Quantum simulation, Variational Monte Carlo, Machine Learning in Physics, Density Functional Theory, Lanczos, Path Integral Monte Carlo, Quantum Computing, Second Quantization, Time-Dependent Variational Principle

Learning Prerequisites

Required courses

A solid understanding of quantum mechanics (I and II) is required.
Students should have a good working knowledge of at least one common programming language (Python, C, C++, Fortran, Julia...). Knowledge of Matlab is typically sufficient, but it is strongly advised to be familiar with Python, since the exercises will be typically presented and discussed in Python.

Recommended courses

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Learning Outcomes

By the end of the course, the student must be able to:

- Model a quantum problem through numerical tools
- Identify suitable algorithms to solve or approximately solve a certain quantum problem
- Discuss the limitations of a given algorithm
- Carry out computer simulations

Teaching methods

Ex cathedra with exercises

Expected student activities

Practical assignments will be given every week.
Solutions to the assignements will be handed out and the homework will not be graded.
It is strongly advised however to make the effort to do the homework weekly, since the final exam will also evaluate the understanding of the practical implementation aspects of the computational methods.

Assessment methods

The course is graded through an oral exam.
The oral exam will assess both the general theory as well as the understanding of the practical implementation of the algorithms, as presented during the practical weekly exercises.

Resources

Bibliography

Suggested books to acquire a broader view on the topics discussed in the lecture notes
"Quantum Monte Carlo Approaches for Correlated Systems", F. Becca & S. Sorella, (Cambridge University Press, 2017)
"Computational Physics", J. M. Thijssen, (Cambridge University Press)
"Statistical Mechanics: Algorithms and Computations", W. Krauth, (Oxford Master Series in Physics)

Ressources en bibliothèque

- Computational Physics / Thijssen
- Statistical Mechanics: Algorithms and Computations / Krauth
- Quantum Monte Carlo Approaches for Correlated Systems / Becca

Moodle Link

- https://go.epfl.ch/PHYS-463