Advanced numerical methods in many-body physics

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General information

This course is recommended for students who

- would like to dive into the fascinating field of computational physics
- would like to learn about state-of-the-art methods relevant in many areas in Science (also in non-academic areas)
- intend to do a computationally oriented project in future (e.g. Master- or PhD-thesis)
- would like to strengthen their understanding in many-body physics
- enjoy programming and would like to get more practice in programming

Content

In this course you will learn about modern computational methods for the simulation of many-body systems in condensed matter physics, including systems from classical statistical physics and quantum many-body problems. Covered topics include:

- Monte Carlo methods for classical spin systems (Metropolis algorithm, cluster algorithms and flat-histogram methods)
- Numerical study of first and second order phase transitions in magnetic systems (the Ising model and generalizations)
- Solution of quantum one-body problems
- Quantum many-body problems and effective lattice models (e.g. spin chains and Hubbard model)
- Hartree Fock
- Exact diagonalization of quantum lattice models
- Quantum Monte Carlo methods and the negative sign problem
- The density matrix renormalization group and tensor network methods

Objectives

The learning objectives of this course is that you are able to

- explain, implement, and apply computational methods to study many-body systems, ranging from Monte Carlo simulations in classical statistical physics to tensor network algorithms for quantum many-body systems (see course content). This includes also being able to select the right algorithm for a given problem
- describe and understand the challenges and the physics of many-body systems
- evaluate, analyze, and interpret numerical simulation results

Course format and exercises

- In each 4 hour session (on Tuesdays 9-13 and on Fridays 9-13) there will be 2 hours of lectures followed by 2 hours of exercise classes
- Location of the lectures: SP G2.13 (Tuesdays 9-11), SP B0.203 (Fridays 9-11)
- For the exercise classes we will be in the computer rooms SP F2.04 (Tuesdays 11-13 and Fridays 11-13), but you are encouraged to bring your own laptop if you have one!
- The exercises consist mostly of programming tasks in Python. We will do an introduction / warm-up in the first week, assuming that you already have previous programming experience (see prerequisites below)
- The exercises (homework) do not have to be handed in, but everyone is supposed to work on the exercises, since they are important for the understanding of the course and also relevant for the exam. There will be 3 specially marked and particularly important exercises which everyone needs to complete in a satisfactorily way in order to get admitted to the exam (see assessment below).
- Solutions to the exercises will be provided
- Schelto Crone (S.P.G.Crone@uva.nl) will be teaching assistant of the course

Prerequisites

- Previous programming experience (preferably Python)
- Knowledge in statistical physics and quantum mechanics (including second quantization). The course *Statistical Physics and Condensed Matter Theory I* from the first semester is recommended

Assessment

- Final written exam at the end of the course (one part of the exam will include programming tasks). Details about the exam will be given during the course.
  Important note: In order to be admitted to the exam 3 specific exercises have to be completed in a satisfactorily way (to get a ”pass”). These special exercises will be announced during the course.

Course material

- Lecture notes will be provided

Additional references

- D. Landau and K. Binder, *A Guide to Monte Carlo Simulations in Statistical Physics*, Cambridge University Press (2000), ISBN 0521653665
- J.M. Thijssen, *Computational Physics*, Cambridge University Press (1999), ISBN 0521575885
- U. Schollwöck, *The density-matrix renormalization group in the age of matrix product states*, Annals of Physics 326, 96192 (2011).
  Open-access version: `http://arxiv.org/abs/1008.3477`

Useful Python resources and links

We will use Python version v2.7.x, and make use of the additional packages Numpy, Scipy, Matplotlib, and IPython. I recommend installing the nice cross-plattform IDE called Spyder (available for free e.g. at `https://pythonhosted.org/spyder/`) which comes with all the required packages. There are many good tutorials and books to get started with Python, see examples below. I will do the introduction in the first week mostly based on the first reference.

- Python Scientific Lecture Notes: `http://scipy-lectures.github.io/`
- Quick tutorial: `http://www.tutorialspoint.com/python/python_quick_guide.htm`
- Python main page: `http://www.python.org`
- Book: "Learning Python" by Mark Lutz (O'Reilly).
- Online Python course: http://www.python-course.eu