ICTS Summer Course

Computational Methods for Quantum Many-Body Physics

Summer Semester: May – July 2023

Instructors:

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Course description: The course is aimed at introducing some of the most ubiqutiously used computational methods in quantum many-body physics to PhD students and interested postdocs. There will be a certain focus on kinds of settings commonly encountered in condensed matter and statistical physics, such as interacting fermionic, bosonic or spin systems on lattices. Some of the topics that will be covered are extracting eigenvalues and eigenstates using (sparse) exact diagonalisation, time-evolution methods for non-equilibrium quantum dynamics, classical and quantum Monte-Carlo methods and using them to understand critical behaviour, a basic introduction to simulating dynamics of open quantum systems, and finally, time permitting, some tensor network methods. The emphasis will be on both, the algorithms and the physics behind them, as well as their implementations. Hence, it is required that the students have completed courses on quantum mechanics and statistical mechanics at the Master's level. Some basic experience with programming (in any language) is also desirable.

Course contents:

- **Exact diagonalisation:** (2 lectures)
  - representing Hamiltonians as sparse matrices
  - Lanczos algorithms for diagonalisation
  - Shift-invert and Polynomially filtered exact diagonalisation
- **Time-evolution of quantum systems:** (2 lectures)
  - time-evolution using exact diagonalisation
  - (truncated) Krylov space methods
  - Kernel polynomial methods
  - time-evolving block decimation
- **Classical and Quantum Monte Carlo:** (4 lectures)
  - Basic principles of Monte Carlo algorithms: importance sampling, detailed balance, autocorrelation timescales, error analysis

- Illustrating classical Monte Carlo using the 2D Ising model: local, worm and cluster type algorithms
- Some other useful tricks: parallel tempering, overrelaxation etc
- Illustrating quantum Monte Carlo (QMC) using the 2D $S = 1/2$ Heisenberg antiferromagnet and the 2D J-Q model: Stochastic series expansion (SSE) QMC and its implementation
- Introduction to sign problem (time permitting)

- **Tensor Network Methods** (2 lectures)
  - matrix product states
  - matrix product operators
  - introduction to DMRG and tDMRG algorithms (time permitting)

Logistical details

- **Venue**: Emmy Noether Seminar Room and online
- **Zoom link**: https://icts-res-in.zoom.us/j/87633971378?pwd=eE4yQU44S0RFYjdRM3VnN2pzcV
  Meeting ID: 876 3397 1378
  Passcode: 171723
- **Class timings**: Wednesdays 15:00-17:00 hrs
- **First class**: 17th May 2023
