Computational Quantum Physics – Projects

1) *Ground-state calculation of the Helium atom with Hartree-Fock and Density Functional Theory*

Hartree-Fock is a method to compute the ground-state wave function of a quantum many body system. Density functional theory computes the electron density of a many-body system in the ground-state. Both methods are frequently used in computational chemistry.

2) *Calculation of the excitation spectrum of spin systems using the Lanczos algorithm*

The Lanczos method is an approximate method that iteratively obtains the lowest lying eigenvectors and eigenvalues of large matrices.

3) *Path Integral Ground State study of ground-state properties of* ^4He

The PIGS method is a projection technique that filters out the exact ground-state wave function out of an initial trial state and is used for the computation of the ground-state of many body quantum systems.

4) *Monte Carlo study of the critical coupling for the* ϕ^4 *theory*

ϕ^4 theory is one of the simplest lattice field theories. We look at one of the limiting cases of infinite coupling, where we can map this model onto the four-dimensional Ising model.

5) *Density Matrix Renormalization Group calculation of the one dimensional Heisenberg chain*

DMRG is the method of choice for obtaining the ground-state of large one-dimensional quantum systems.

6) *Quantum Monte Carlo study with operator loop updates of the Quantum Heisenberg model*

QMC with operator loop updates is an example of cluster QMC algorithms, for which the efficiency is improved due to non local update schemes.

We recommend that you work together in pairs on the projects. At the end of the semester you are requested to give a 15 min presentation of your project and to hand in a short report.