-Project 5 - FYS3150/FYS4150-

Quantum Monte Carlo of confined electrons
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1 Abstract

[3] [1]

2 Introduction

The purpose of this article is to apply the Variational Monte Carlo (VMC) method to two electrons in a quantum dot modelled by a 3- dimensional harmonic oscillator potential. This is in order to evaluate their ground state energy, relative distance, and the expectation values of their kinetic and potential energies.
In order to benchmark the results of this method, we are comparing the results of the ground state energy with analytical solutions for specific harmonic oscillator frequencies (henceforth ω) as found in M. Taut's [4] and our previous article [3] on the topic of electron confinement in 3- dimensional harmonic oscillator potentials.

The idealized Hamiltonian used in this article, models the Coulombic interaction between electrons and the 3- dimensional harmonic oscillator potential:

$$\hat{H} = \sum_{i=1}^{N} \left(-\frac{1}{2}\nabla_i^2 + \frac{1}{2}\omega^2 r_i^2 \right) + \sum_{i<j} \frac{1}{r_{ij}} \tag{1}$$

[2] with r_{ij} being the distance between electrons i and j with position moduli r_i and r_j respectively.

3 Methods

4 Results

5 Conclusion

6 Critique

7 Appendix

7.1 Figures

7.2 Tables

7.3 List of programs

All programs can be found on `https://github.com/adrian2208/FYS3150_collab` in the folder "Project5".

1. b.cpp - Program with several options of writing to file, different matrices etc., for a given temperature and lattice size

2. e_not_parallel.cpp - Like b, but can run over several lattices and temperatures, more efficient
3. e.cpp - Same as above, but parallelized with openMPI
4. vecop.hpp - Several functions
5. vecop.cpp - Functions, out of which some are used.
6. tests_main.cpp - Unit testing.
7. a.py - Analytical solution. Not properly up to date!
8. plot_cv.py - Creates 2×2 plot for the larger simulations, also calculates $T_C(L_{\to\infty})$
9. plot_distribution.py Plots the distribution histograms at different temperatures.
10. plot_energy_simulation_step.py Plots the avg. energy, the avg. magnetisation and the amount of accepted steps as a function of simulation step.
11. functions.hpp & functions.cpp - Contains functions for parallelization, and all the integrands, and some more.

8 References

[1] Brian L Hammond, William A Lester, and Peter James Reynolds. *Monte Carlo methods in ab initio quantum chemistry*, volume 1. World Scientific, 1994.

[2] Morten Hjort-Jensen. Problem set 5- quantum monte carlo of confined electrons fall 2019.

[3] Simon Schrader and Adrian Kleven. Project 2. 2019.

[4] M. Taut. Two electrons in an external oscillator potential: Particular analytic solutions of a coulomb correlation problem. *Phys. Rev. A*, 48:3561–3566, Nov 1993.