FYS4411 - Computational Physics II

Project 2

Dorthea Gjestvang
Even Marius Nordhagen

April 22, 2018

- Github repository containing programs and results:
  `https://github.com/evenmn/FYS4411/tree/master/Project%202`

Abstract

Abstract

Contents

1 Introduction

2 Theory

2.1 Presentation of potential

In this project, we simulate a system of P electrons trapped in a harmonic oscillator potential, with a Hamiltonian given by

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

where ω is the harmonic oscillaor potential and $r_i = \sqrt{x_i^2 + y_i^2}$ is the position of electron i. The term $\frac{1}{r_{ij}}$ is the interacting term, where $r_ij = |r_i - r_j|$ is the distance between a given pair of interacting electrons. Natural units have been used, such that $\hbar = c = m_e = e = 1$.

2.2 Solving with machine learning

Usually, when solving a system of particles as the one described in the previous system, we would need an anzats for the wave function, where we use our physical intuition to create the form of a wave function with different variational parameters, and then let it be up to the computer to find the optimal parameters through a minimization method. However, this method is only as good as the physical intuition; if the form of the wave function is unrealistic, the results will be the same, and there is no guarantee that we have actually found a ground state energy.

This challenge can be solved by using machine learning.

2.2.1 Restricted Boltzmann Machines

2.3 Energy calculation

2.4 Onebody density

2.5 Scaling

2.6 Error estimation

3 Method

3.1 Variational Monte Carlo

3.2 Metropolis Algorithm

3.2.1 Brute force

3.2.2 Importance sampling

3.2.3 Gibbs sampling

3.3 Minimalization method

3.3.1 Gradient decent

4 Code

4.1 Structure

4.2 Implementation

5 Results

6 Discussion

7 Conclusion

8 Appendix A

9 References

[1] Morten Hjorth-Jensen. Computational Physics 2: Variational Monte Carlo methods, Lecture Notes Spring 2018. Department of Physics, University of Oslo, (2018).

[2] J. L. DuBois and H. R. Glyde, H. R., *Bose-Einstein condensation in trapped bosons: A variational Monte Carlo analysis*, Phys. Rev. A **63**, 023602 (2001).

[3] J. K. Nilsen, J. Mur-Petit, M. Guilleumas, M. Hjorth-Jensen, and A. Polls, *Vortices in atomic Bose-Einstein condensates in the large-gas-parameter region*, Phys. Rev. A **71**, 053610, (2005).

[4] F. Dalfovo, S. Stringari, *Bosons in anisotropic traps: ground state and vortices* Phys. Rev. A **53**, 2477, (1996).

[5] J. Emspak, *States of Matter: Bose-Einstein Condensate*, LiveScience, (2016). `https://www.livescience.com/54667-bose-einstein-condensate.html` Downloaded March 15th 2018.

[6] S. Perkowitz *Bose-Einstein condensate* Encyclopaedia Britannica `https://www.britannica.com/science/Bose-Einstein-condensate` Downloaded March 15th 2018.

[7] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, E. A. Cornell, *Observation of Bose-Einstein Condensation in a Dilute Atomic Vapor*, Science **269**, (1995).

[8] J. K. Nilsen *Bose-Einstein condensation in trapped bosons: A quantum Monte Carlo analysis*, Master thesis 2004, Department of Physics, University of Oslo, (2004).

[9] E. P. Gross, *Structure of a quantized vortex in boson systems*, Il Nuovo Cimento, **20** (3): 454–457, (1961).

[10] L. P. Pitaevskii, *Vortex lines in an imperfect Bose gas*, Sov. Phys. JETP. **13** (2): 451–454, (1961).