

Solving Many-body Quantum Problem using Machine Learning

by

Even M. Nordhagen

THESIS

for the degree of

MASTER OF SCIENCE



Faculty of Mathematics and Natural Sciences
University of Oslo

September 18, 2018

Abstract

Abstract should be written here

Acknowledgements

Acknowledgements should be written here

-One of my mottos used to be that everything has a reason, which I used to point out whenever people were talking about things that apparently could not be described immediately. It was first when I learned about quantum mechanics that I understood I was wrong, and that is one of the reasons why quantum mechanics caught me so hardly.

Contents

1	Introduction	7
2	Background theory	7
2.1	Hamiltonian and wavefunction	7
2.2	Born-Oppenheimer approximation	7
2.3	Wave function properties	7
2.4	Slater determinant	8
2.4.1	More specifcly	9
2.4.2	6 fermion example	9

List of abbreviations

Letters	Meaning
RBM	- Restricted Boltzmann Machine
MC	- Monte Carlo
VMC	- Variational Monte Carlo
DMC	- Diffusion Monte Carlo
ML	- Machine Learning
WF	- Wave Function
SPF	- Single Particle Function

Table 1: List of symbols used with explanation.

Source Code

The source code is given in [`https://github.com/evenmn`](https://github.com/evenmn)

1 Introduction

Write introduction here

- Introduce the wavefunction - Mention the uncertainty principle and also quantum entanglement to catch the readers interest

2 Background theory

Here I might present basic quantum mechanics briefly.

2.1 Hamiltonian and wavefunction

Quantum quantities can be found by solving eigenvalue equations with the wavefunction as eigenfunction.

$$\hat{H}\Psi_n(\mathbf{x}) = \epsilon_n \Psi_n(\mathbf{x}) \quad (1)$$

2.2 Born-Oppenheimer approximation

The Born-Oppenheimer approximation is the assumption that we can split the Hamiltonian in a one-body part and a two-body part, and calculate the energies separately.

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

In atomic units.

2.3 Wave function properties

Assume we have a permutation operator \hat{P} which switches two coordinates in the wave function,

$$\hat{P}\Psi_n(\mathbf{x}_1, \dots, \mathbf{x}_i, \dots, \mathbf{x}_j, \dots, \mathbf{x}_M) = p\Psi_n(\mathbf{x}_1, \dots, \mathbf{x}_j, \dots, \mathbf{x}_i, \dots, \mathbf{x}_M), \quad (3)$$

where p is just a factor which comes from the transformation. If we again apply the \hat{P} operator, we should switch the same coordinates back, and we expect to end up with the initial wave function. For that reason, $p = \pm 1$.¹

¹This was true until 1976, when J.M. Leinaas and J. Myrheim discovered the anyon, <https://www.uio.no/studier/emner/matnat/fys/FYS4130/v14/documents/kompendium.pdf>.

The particles that have an antisymmetric wave function under exchange of two coordinates are called fermions, while the particles that have a symmetric wave function under exchange of two coordinates are named bosons.

Mention fermions and bosons and why they are the only particles (or maybe mention anions as well?).

Read <https://manybodyphysics.github.io/FYS4480/doc/pub/secondquant/html/secondquant.html> Read <https://www.uio.no/studier/emner/matnat/fys/FYS4130/v14/documents/kompen>

2.4 Slater determinant

For a system of more particles we can define a total wavefunction, which is a composition of all the single particle wavefunctions (SPF) and contains all the information about the system. The way we compile the SPFs needs to be based on Pauli's exclusion, which states that two identical fermions cannot possibly be in the same state at the same time. If this happens, we set the total wavefunction to zero, which is done by defining the wavefunction as a determinant.

Consider a system of two identical fermions with SPFs ϕ_1 and ϕ_2 at positions \mathbf{r}_1 and \mathbf{r}_2 respectively. The way we define the wavefunction of the system is then

$$\Psi_T = \begin{vmatrix} \phi_1(\mathbf{r}_1) & \phi_2(\mathbf{r}_1) \\ \phi_1(\mathbf{r}_2) & \phi_2(\mathbf{r}_2) \end{vmatrix} = \phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2) - \phi_2(\mathbf{r}_1)\phi_1(\mathbf{r}_2), \quad (4)$$

which is set to zero if the particles are at the same position. This is called a Slater determinant, and yields the same no matter how big the system is.

Notice that we denote the wavefunction with the ' T ', which indicates that it is a trial wavefunction. We do this because the spin part is avoided with ψ as the radial parts only, thus this wavefunction is not the true wavefunction. We will look closer at how we can factorize out the spin part later. The spin part is assumed to not affect the energies. For bosons the total wavefunction is defined similarly, but with no negative signs since the Pauli principle does not apply for fermions.

A general Slater determinant for a system of N particles takes the form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \begin{vmatrix} \psi_1(\mathbf{r}_1) & \psi_2(\mathbf{r}_1) & \dots & \psi_N(\mathbf{r}_1) \\ \psi_1(\mathbf{r}_2) & \psi_2(\mathbf{r}_2) & \dots & \psi_N(\mathbf{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_1(\mathbf{r}_N) & \psi_2(\mathbf{r}_N) & \dots & \psi_N(\mathbf{r}_N) \end{vmatrix} \quad (5)$$

where the ψ 's are the true single particle wavefunctions, which are the tensor products

$$\psi = \phi \otimes \xi \quad (6)$$

with ξ as the spin part.

2.4.1 More specifcly

NOT SURE WHERE TO PUT THIS

For our purpose we will study fermions with spin $\sigma = \pm 1/2$ only, so the Slater determinant can be simplified to

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \begin{vmatrix} \phi_1(\mathbf{r}_1)\xi_{\uparrow} & \phi_1(\mathbf{r}_1)\xi_{\downarrow} & \dots & \phi_{N/2}(\mathbf{r}_1)\xi_{\downarrow} \\ \phi_1(\mathbf{r}_2)\xi_{\uparrow} & \phi_1(\mathbf{r}_2)\xi_{\downarrow} & \dots & \phi_{N/2}(\mathbf{r}_2)\xi_{\downarrow} \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\mathbf{r}_N)\xi_{\uparrow} & \phi_1(\mathbf{r}_N)\xi_{\downarrow} & \dots & \phi_{N/2}(\mathbf{r}_N)\xi_{\downarrow} \end{vmatrix}. \quad (7)$$

This is called the wavefunction ansatz, because assumptions are raised, like two particles with opposite spins are found to be at the same position all the time, i.e, an equal number of fermions have spin up as spin down, are applied. Further the...

SHOULD END UP WITH SPLITTED DETERMINANTS HERE

For a detailed walkthrough, see appendix I in REF(The Stochastic Gradient Approximation: an application to Li nanoclusters, Daniel Nissenbaum).

2.4.2 6 fermion example

Wave function:

$$\Psi_T(\vec{x}, \vec{a}, \vec{b}, \hat{W}, \sigma) = \frac{1}{Z} \det(\hat{D}^{\uparrow}) \det(\hat{D}^{\downarrow}) e^{\sum_i^M \frac{(X_i - a_i)^2}{2\sigma^2}} \prod_j^N (1 + e^{b_j + \sum_i^M \frac{X_i W_{ij}}{\sigma^2}}) \quad (8)$$

Inspired by statistical mechanics = partition function