University of Oslo
FYS4411
Computational physics II: Quantum mechanical systems

Project 2: The Restricted Boltzmannn Machine Applied to the Quantum Many Body Problem

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Abstract

Abstract here, please. All material referenced in this report is available at `https://github.com/bsamseth/FYS4411`.

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1 Introduction

A physicist faced with a quantum many body system is quickly forced to abandon any hope of solving the Schrödinger equation (or one of its even worse relativistic siblings) exactly. Instead he must resort to one of two general workarounds: 1) make simplifying assumptions until the equation is solvable, or 2) make an educated guess for the solution. In either case, the desired quantity which solving the Schrödinger equation would yield is the quantum mechanical wavefunction. If we want to stay away from potentially faulty, or limiting assumptions, we must therefore somehow produce a guess for this wavefunction, without actually solving the equation.

The last project utilized the Variational Monte Carlo (VMC) approach, in which a specific, parametrized form is assumed for the wavefunction, with the subsequent optimization of the parameters.

The main limitation of VMC is that a specific form for the wavefunction is assumed. If this form contains the true optimum that works fine, but if not we are inherently limited in how accurate the final results can be.

Aiming to be overcome this issue, we may observe that the task at hand falls into the general field of function approximation. We wish to approximate the function that takes as input the configuration of the system, and outputs a probability amplitude for the given state. Function approximation is a task which lends itself to techniques from machine learning (ML).

In this project we will attempt to represent the wavefunction with a specific type of ML-model, the Restricted Boltzmann Machine (RBM). The use of RBMs for such applications was presented recently by Carleo & Troyer [1], with encouraging results. We shall therefore attempt to apply the same techniques to a different type of system, namely that of two interacting quantum particles confined in a harmonic oscillator trap.

2 Theory

We consider a system of electrons confined in a pure two-dimensional isotropic harmonic oscillator potential, with an idealized total Hamiltonian given by:

$$\begin{aligned}\hat{H} &= \sum_{i=1}^{N}\left(-\frac{1}{2}\nabla_i^2 + V_{ext}(\boldsymbol{r}_i)\right) + \sum_{i<j} V_{int}(\boldsymbol{r}_i, \boldsymbol{r}_j) \\ &= \sum_{i=1}^{N}\left(-\frac{1}{2}\nabla_i^2 + \frac{1}{2}\omega^2 r_i^2\right) + \sum_{i<j}\frac{1}{r_{ij}},\end{aligned} \tag{1}$$

where natural units ($\hbar = c = m_e = 1$) are used with energies in atomic units (a.u.), N denotes the number of particles in the system, and ω is the oscillator frequency of the trap. Further, $\boldsymbol{r}_i$ denotes the position vector of particle i, with $r_i \equiv \|\boldsymbol{r}\|$ and $r_{ij} \equiv \|\boldsymbol{r}_i - \boldsymbol{r}_j\|$ defined for notational brevity.

In this project we limit ourselves to the case of $N = 2$ interacting electrons in a trap with a frequency such that $\hbar\omega = 1$. We do this because for this case we have exact, analytical solutions for the ground state energy. With the interaction term included, the ground state energy is $E_0 = 3$ a.u. [2]. This limitation is purely one of convenience, as having exact benchmarks makes for better verification of results. The methods discussed in the project should extend to other systems.

2.1 Simple Non-Interacting Case

If we omit the interacting terms in Equation 1 we have the standard harmonic oscillator Hamiltonian:

$$\hat{H}_0 = \sum_{i=1}^{N}\left(-\frac{1}{2}\nabla_i^2 + \frac{1}{2}\omega^2 r_i^2\right). \tag{2}$$

This Hamiltonian lends it self to analytical solutions, and the stationary states are:

$$\phi_{n_x,n_y}(x,y) = AH_{n_x}(\sqrt{\omega}x)H_{n_y}(\sqrt{\omega}y)e^{-\frac{\omega}{2}\left(x^2+y^2\right)}, \tag{3}$$

for quantum numbers $n_x, n_y = 0, 1, \ldots$, and the Hermite polynomials H_n. The ground state, $n_x = n_y = 0$ is simply

$$\phi_{00}(x, y) = \sqrt{\frac{\omega}{\pi}} e^{-\frac{\omega}{2}(x^2+y^2)}. \tag{4}$$

Using this wavefunction we can calculate the ground state energy[1],

$$\epsilon_{00} = \frac{\langle\phi_{00}|\hat{H}_0|\phi_{00}\rangle}{\langle\phi_{00}|\phi_{00}\rangle} = \omega = 1\,\text{a.u.} \tag{5}$$

The ground state wavefunction for the (unperturbed) two-electron case is simply the product of the one-electron wavefunctions,

$$\begin{aligned}\Phi(\boldsymbol{r}_1, \boldsymbol{r}_2) &= \phi_{00}(\boldsymbol{r}_1)\phi_{00}(\boldsymbol{r}_2) \\ &= \frac{\omega}{\pi} e^{-\frac{\omega}{2}(r_1^2+r_2^2)}.\end{aligned} \tag{6}$$

The ground state energy can once again be evaluated analytically[1] and yields

$$E_0 = \frac{\langle\Phi|\hat{H}_0|\Phi\rangle}{\langle\Phi|\Phi\rangle} = 2\omega = 2\,\text{a.u.} \tag{7}$$

This result is not surprising, as adding one more particle, without any interactions, should simply double the energy. Another way to look at it is that the simple harmonic oscillator solution gives $\omega/2$ per degree of freedom, so adding another two yields and extra ω.

When the two particles are electrons, we may say something about their total spin. As electrons are fermions, their total wavefunction must be anti-symmetric upon interchanging the labels 1 and 2. Equation 6 is obviously symmetric, and so the spin-wavefunction must necessarily be anti-symmetric. For the combination of two spin-1/2 particles, there is only one candidate, namely the spin-0 singlet:

$$\chi_0 = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle). \tag{8}$$

References

1. Carleo, G. & Troyer, M. Solving the quantum many-body problem with artificial neural networks. *Science* **355,** 602–606. ISSN: 0036-8075 (2017).
2. Taut, M. Two electrons in an external oscillator potential: Particular analytic solutions of a Coulomb correlation problem. *Phys. Rev. A* **48,** 3561–3566 (5 Nov. 1993).

[1] See `projects/python/Sympy.ipynb` in the Github reposirepository for an explicit calculation of the ground state energy