Studies of Quantum Dots using Machine Learning

Even Marius Nordhagen

University of Oslo

evenmn@fys.uio.no

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- Glad so many of you could attend this presentation
- Present myself
- Present topic/master thesis
- Practical information (Present a years work in 30 min - leave details in the thesis)
- Feel free to ask questions if anything is unclear

Outline

- Motivation
- Quantum Theory
- Machine Learning Theory
- Methods
- Results
- Conclusion
- (Code)

Outline

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We will start with some motivation. Thereafter, we present the essential theory, the methods and the results. I will try to spend most of the time on the results. In the end, I will address a brief conclusion, and show how to use the developed software if we have time.

Motivation

Why quantum dots?

- **Technologically:**
  Quantum dots are expected to be the next big thing in display technology[1,2].
- **Experimentally:**
  Researchers have managed to study two-dimensional quantum dots in the laboratory[3].
- **Physically:**
  An array of interesting physical phenomena can be observed in quantum dots.

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As mentioned initially, we have focused on quantum dots throughout this thesis.

But what are quantum dots?

Quantum dots are small artificial particles, often called artificial atoms because of their many common features with atoms. For instance, both quantum dots and atoms have discrete energy spectra.

Why quantum dots?

Technologically: Quantum dots are expected to be the next big thing in display technology. They have, for instance, the ability to emit light of specific wave lengths, meaning that the color can be controlled with high precision. Samsung already claim that they use quantum dots in their high-end TVs.

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- **Physically:**
  An array of interesting physical phenomena can be observed in quantum dots.

Experimentally: Quantum dots can be investigated in laboratory experiments. This encourages computational experiments as well, since we can use the results from the laboratory experiments as references. Researchers have managed to study quantum dots squeezes between two plates, making the confinement in z-direction absent. This makes them essentially two-dimensional, which is the reason why we have decided to also focus on two-dimensional systems.

Physically: From a physical point of view, the quantum dots are interesting as they are simple systems that can model a long range of phenomena. An example is the Wigner localization.

We will look at circular quantum dots with electron.

Why is it challenging?

- Many-body problem
- Fermi-Dirac statistics
- Hard to compute the wave function

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- Hard to compute the wave function

The many-body problem is encountered when simulating a quantum many-body system. The problem is caused by the correlations between the particles. A many-body system means more than two particles.

Fermionic systems need to obey Fermi-Dirac statistics. This results in the requirement of an anti-symmetric wave function under exchange of two particle coordinates.

The wave function is categorized as nondeterministic polynomial hard to compute, which means that...

How to overcome the challenges?

- Hartree-Fock (HF) theory
- Variational Monte Carlo (VMC) method
- Our approach: VMC with Machine Learning[4,5]

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There are several different ways to overcome the many-body problem. The Hartree-Fock method is a popular approach, which, loosely speaking, attempts to replace the electron-electron interactions with a mean field.

Then we have the variational Monte Carlo method, which attempts to solve the Schrödinger equation accurately using Monte Carlo integration. It is called variational because we need to introduce a trial wave function ansatz, which we vary. Our approach is to let machine learning define this ansatz, inspired by Carleo & Troyer[4] and Flugsrud[6]. Also Pfau *et al.*[5] has done something similar.

Quantum Theory

The Time-independent Schrödinger Equation

A stationary quantum mechanical system is described by the time-independent Schrödinger equation,

$$\hat{\mathcal{H}}\Psi_n = E_n\Psi_n,$$

where Ψ_n is the wave function of state n and E_n is the corresponding energy. $\hat{\mathcal{H}}$ is the Hamiltonian, which for a quantum dot is given by

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

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The Schrödinger equation describes the motion of any quantum mechanical system. Since we will limit us to stationary systems only, the time-independent Schrödinger equation will be our focus. It is shown here. In linear algebra terms, it is an eigenvalue equation with the Hamilton operator, $\hat{\mathcal{H}}$, as a matrix and the wave function, Ψ_n, as the eigen function. E_n is the energy of state n, and is the eigenvalue.

For quantum dots, the Hamiltonian is given by

The Time-independent Schrödinger Equation

By solving the Schrödinger equation with respect to the energy, we obtain

$$E_n = \frac{\int d\boldsymbol{X}\Psi_n^*(\boldsymbol{X})\hat{\mathcal{H}}\Psi_n(\boldsymbol{X})}{\int d\boldsymbol{X}\Psi_n^*(\boldsymbol{X})\Psi_n^*(\boldsymbol{X})},$$

where $\boldsymbol{X}$ are the collective coordinates (spin and position).

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where $\boldsymbol{X}$ are the collective coordinates (spin and position).

There are several ways to solve the equation, where an approach is to solve it as an eigenvalue problem. However, this quickly gets infeasible as the Hamilatonian matrix gets large. Instead, we can express the energy on an integral form, as shown here. This integral is hard to solve because of the interaction term in the Hamiltonian.

The Variational Principle

The variational principle serves as a way of finding the ground state energy. For an arbitrary trial wave function $\Psi_T(\boldsymbol{X})$, it states that the obtained energy is larger or equal to the ground state,

$$E_0 \leq E = \frac{\int d\boldsymbol{X}\Psi_T^*(\boldsymbol{X})\hat{\mathcal{H}}\Psi_T(\boldsymbol{X})}{\int d\boldsymbol{X}\Psi_T^*(\boldsymbol{X})\Psi_T^*(\boldsymbol{X})}.$$

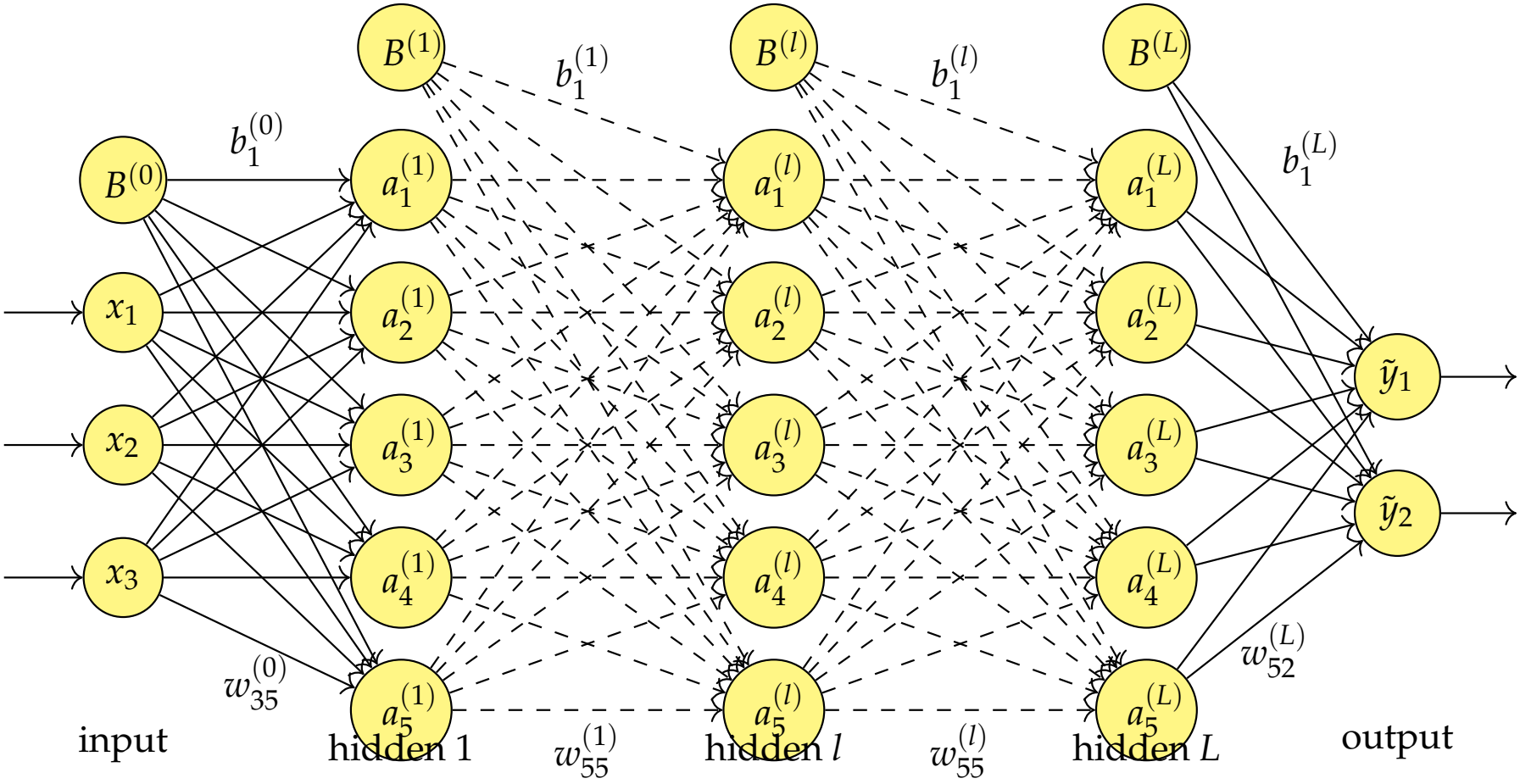
Thus, by minimizing the obtained energy, E, we can estimate the ground state energy.

Machine Learning Theory

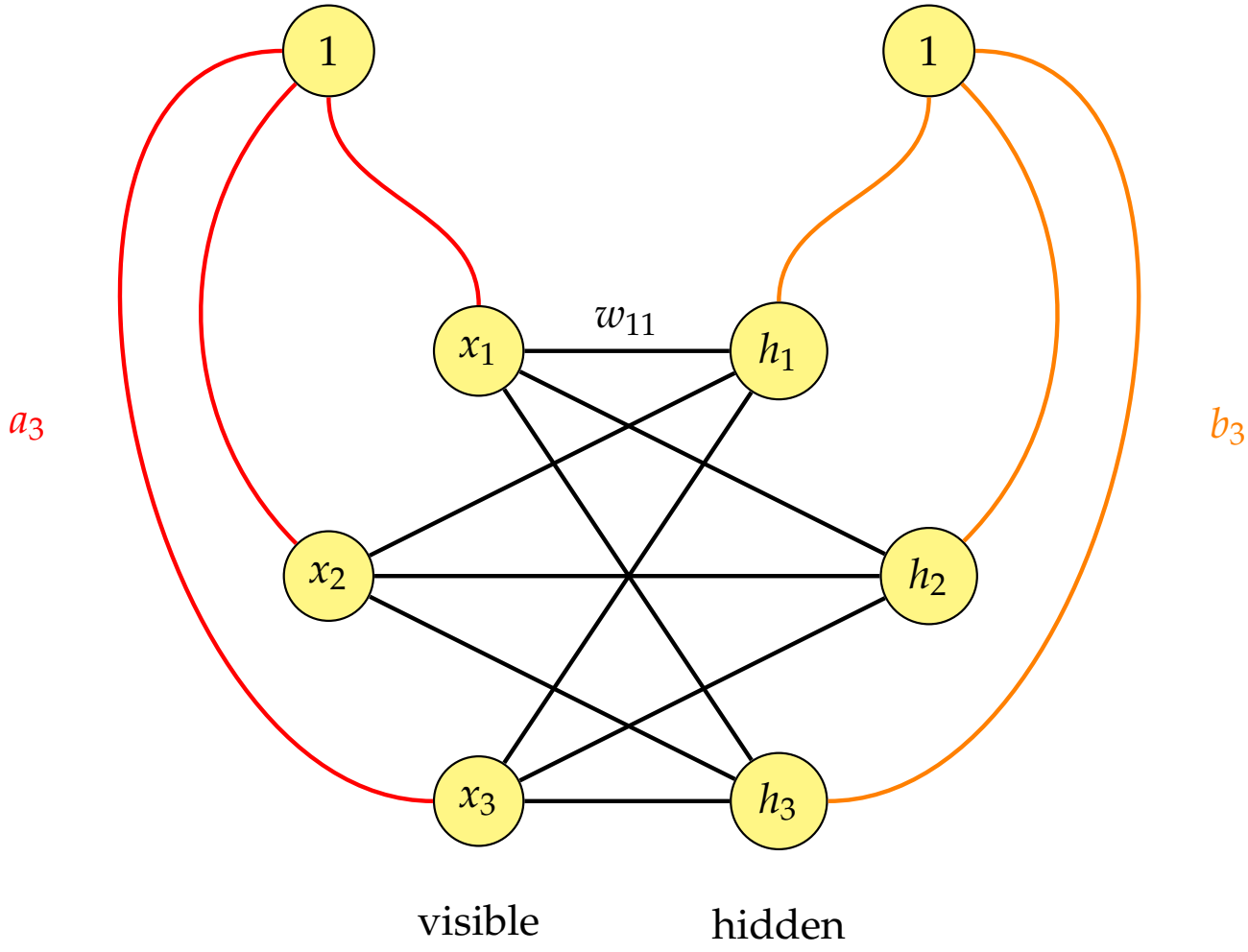
Machine Learning

> *Machine learning is the science of getting computers to act without being explicitly programmed.*
> *Stanford University*[7]

Feed-forward Neural Network



Restricted Boltzmann machines



Methods

Variational Monte Carlo (VMC)

Exploit the variational principle in order to obtain the ground state energy

$$
\begin{aligned}
E_0 < E_{\mathrm{VMC}} &= \frac{\int d\boldsymbol{R}\Psi_T(\boldsymbol{R})^*\hat{\mathcal{H}}\Psi_T(\boldsymbol{R})}{\int d\boldsymbol{R}\Psi_T(\boldsymbol{R})^*\Psi_T(\boldsymbol{R})} \\
&= \int d\boldsymbol{R}\, \underbrace{\frac{\Psi_T(\boldsymbol{R})^*\Psi_T(\boldsymbol{R})}{\int d\boldsymbol{R}\Psi_T(\boldsymbol{R})^*\Psi_T(\boldsymbol{R})}}_{P(\boldsymbol{R})} \cdot \underbrace{\frac{1}{\Psi_T(\boldsymbol{R})}\hat{\mathcal{H}}\Psi_T(\boldsymbol{R})}_{E_L(\boldsymbol{R})}
\end{aligned}
$$

Monte Carlo Integration

We attempt to solve the integral by sampling from the probability density function $P(\boldsymbol{R})$

$$E_{\mathrm{VMC}} = \int d\boldsymbol{R} E_L(\boldsymbol{R}) P(\boldsymbol{R})$$

$$\approx \frac{1}{M} \sum_{i=1}^{M} E_L(\boldsymbol{R}_i)$$

Trial Wave Function

$$P(\boldsymbol{R}) \propto \Psi_T(\boldsymbol{R})^* \Psi_T(\boldsymbol{R})$$

Use the Slater-Jastrow function as our trial wave function

$$\Psi_T(\boldsymbol{R}) = |\hat{D}(\boldsymbol{R})| J(\boldsymbol{R})$$

where the Slater matrix, $\hat{D}(\boldsymbol{R})$, contains all the single-particle functions

$$\hat{D}(\boldsymbol{R}) = \begin{pmatrix} \phi_1(\boldsymbol{r}_1) & \phi_2(\boldsymbol{r}_1) & \dots & \phi_N(\boldsymbol{r}_1) \\ \phi_1(\boldsymbol{r}_2) & \phi_2(\boldsymbol{r}_2) & \dots & \phi_N(\boldsymbol{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\boldsymbol{r}_N) & \phi_2(\boldsymbol{r}_N) & \dots & \phi_N(\boldsymbol{r}_N) \end{pmatrix}$$

Single-particle Functions

The Hermite functions,

$$\phi_n(\boldsymbol{r}) \propto H_n(\boldsymbol{r}) \exp\left(-\frac{1}{2}\alpha\omega|\boldsymbol{r}|^2\right),$$

are used as the single-particle functions for quantum dots in standard VMC. The Gaussian can be factorized out from the Slater determinant.

$$|\hat{D}(\boldsymbol{R};\alpha)| \propto \exp\left(-\frac{1}{2}\alpha\omega|\boldsymbol{R}|^2\right) \begin{vmatrix} H_1(\boldsymbol{r}_1) & H_2(\boldsymbol{r}_1) & \dots & H_N(\boldsymbol{r}_1) \\ H_1(\boldsymbol{r}_2) & H_2(\boldsymbol{r}_2) & \dots & H_N(\boldsymbol{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ H_1(\boldsymbol{r}_N) & H_2(\boldsymbol{r}_N) & \dots & H_N(\boldsymbol{r}_N) \end{vmatrix}$$

Restricted Boltzmann Machine

We use the marginal distribution of the visible units as the single-particle functions in the Slater determinant, and see if them can model the correlations

$$\phi_n(\boldsymbol{r}) \propto H_n(\boldsymbol{r})P(\boldsymbol{r};\boldsymbol{a},\boldsymbol{b},\boldsymbol{W})$$

where $P(\boldsymbol{r})$ is the marginal distribution of the visible units.

$$|\hat{D}(\boldsymbol{r};\boldsymbol{a},\boldsymbol{b},\boldsymbol{W})| \propto P(\boldsymbol{r};\boldsymbol{a},\boldsymbol{b},\boldsymbol{W}) \begin{vmatrix} H_1(\boldsymbol{r}_1) & H_2(\boldsymbol{r}_1) & \dots & H_N(\boldsymbol{r}_1) \\ H_1(\boldsymbol{r}_2) & H_2(\boldsymbol{r}_2) & \dots & H_N(\boldsymbol{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ H_1(\boldsymbol{r}_N) & H_2(\boldsymbol{r}_N) & \dots & H_N(\boldsymbol{r}_N) \end{vmatrix}$$

Jastrow Factor

The Jastrow factor is added to account for the correlations
Simple Jastrow factor

$$J(\boldsymbol{r};\boldsymbol{\beta}) = \exp\left(\sum_{i=1}^{N}\sum_{j>i}^{N}\beta_{ij}r_{ij}\right).$$

Padé-Jastrow factor

$$J(\boldsymbol{r};\beta) = \exp\left(\sum_{i=1}^{N}\sum_{j>i}^{N}\frac{a_{ij}r_{ij}}{1+\beta r_{ij}}\right).$$

Results

Ground State Energy

Number of electrons: $N = 2$. Frequency: ω.

ω	RBM	RBM+SJ	RBM+PJ	VMC	HF *	Exact †
1/6	0.7036(1)	0.67684(7)	0.66715(6)	0.66710(1)	0.768675	2/3
1	3.0803(2)	3.02108(5)	2.999587(5)	2.99936(1)	3.16190	3

*Computation of the Hartree-Fock limit by Mariadason, 2018 [8].

†Semi-analytical ground state energy calculated by Taut, 1993 [9].

Ground State Energy

Number of electrons: $N = 20$. Frequency: ω.

ω	RBM	RBM+SJ	RBM+PJ	VMC	HF [‡]	DMC [§]
0.1	30.824(2)	30.567(3)	30.1553(9)	30.0403(2)	31.1902	29.9779(1)
1.0	159.428(3)	156.816(4)	156.104(1)	155.8900(4)	158.004	155.8822(1)

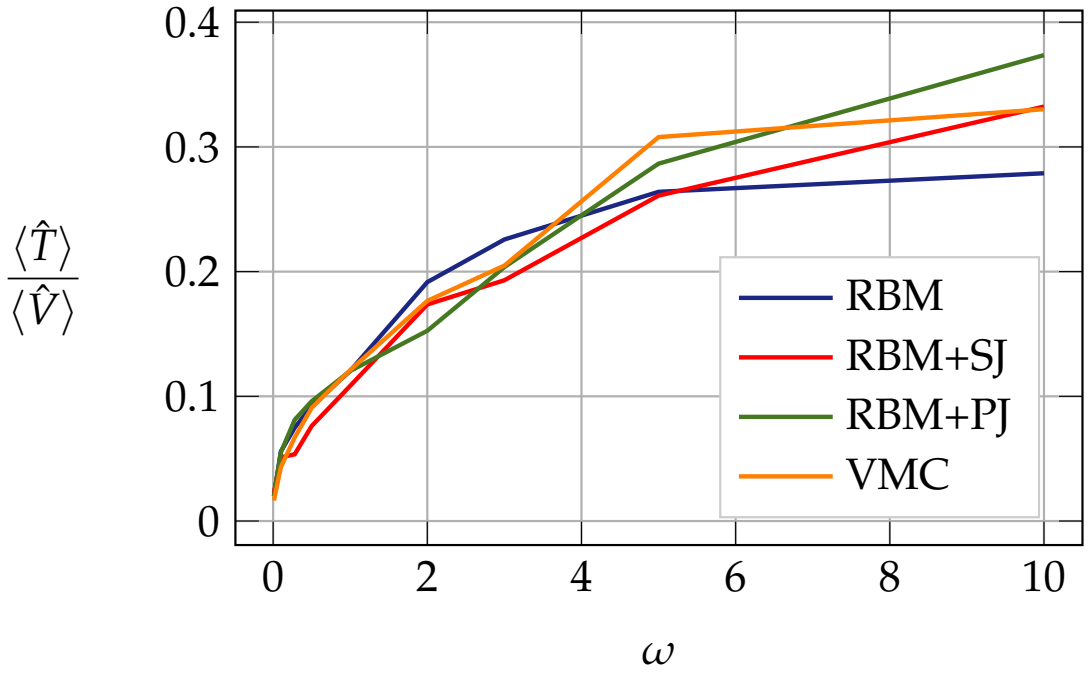
[‡]Computation of the Hartree-Fock limit by Mariadason, 2018 [8].

[§]Ground state energy estimate using the diffusion Monte Carlo method. By Høgberget, 2013 [10].

Energy distribution

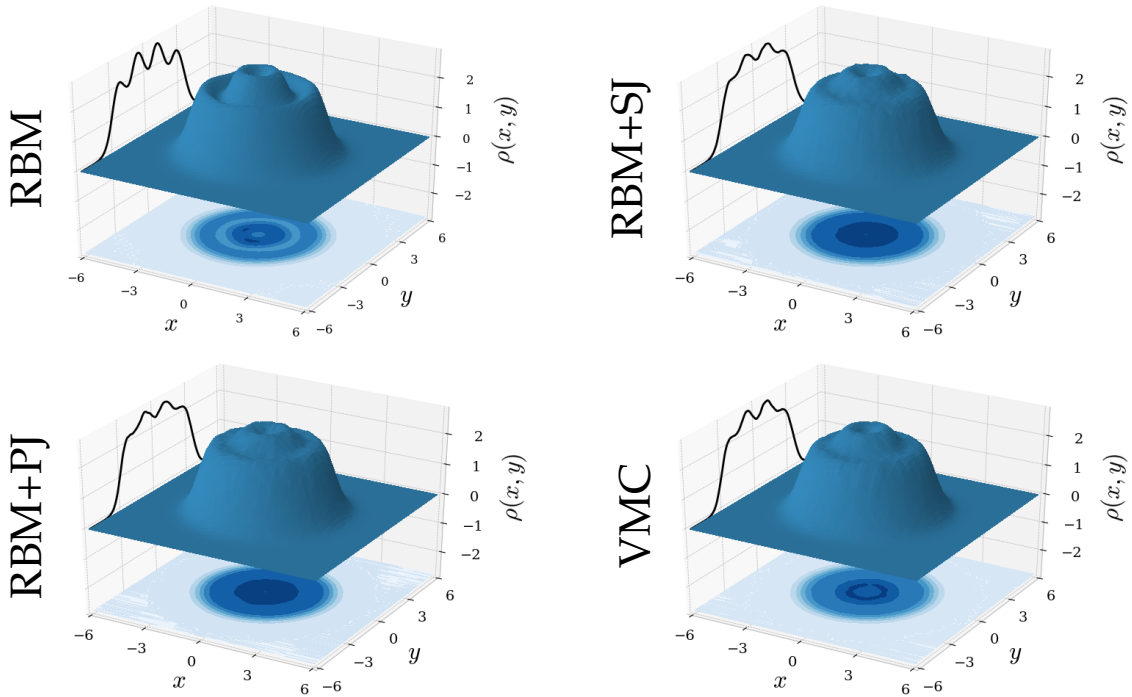
Number of electrons: $N = 20$. Frequency: ω.

Ratio between the kinetic energy, $\langle \hat{T} \rangle$, and the total potential energy, $\langle \hat{V} \rangle$.



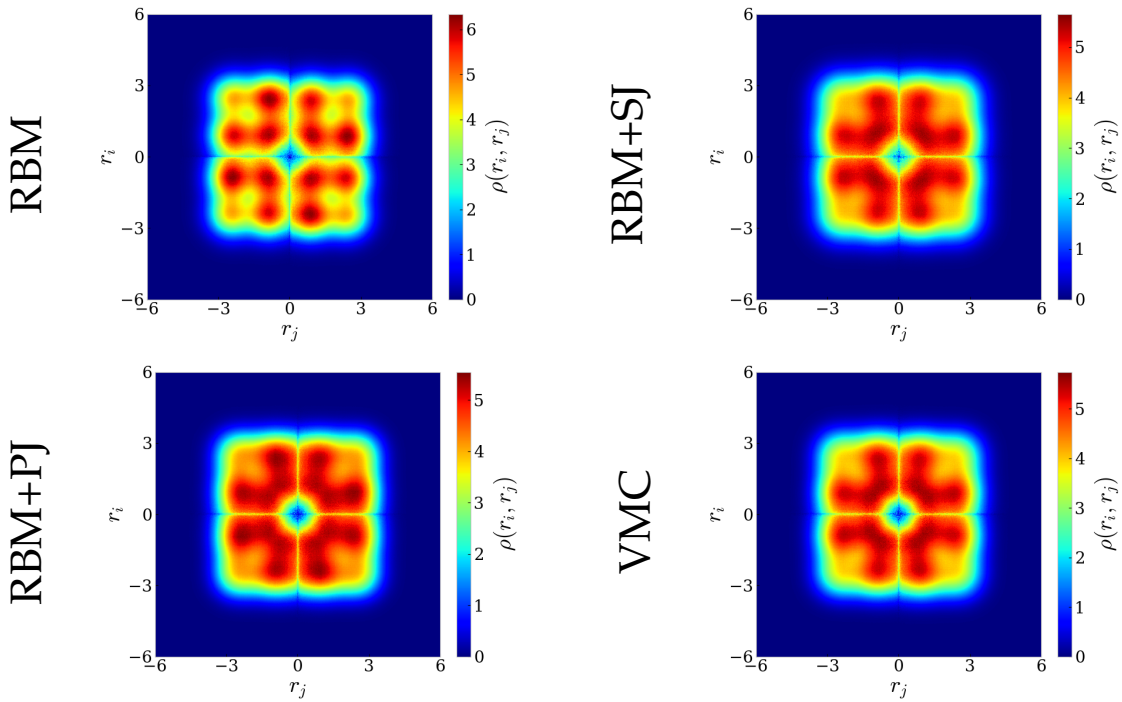
One-body density

Number of electrons: $N = 20$. Frequency: $\omega = 1.0$.



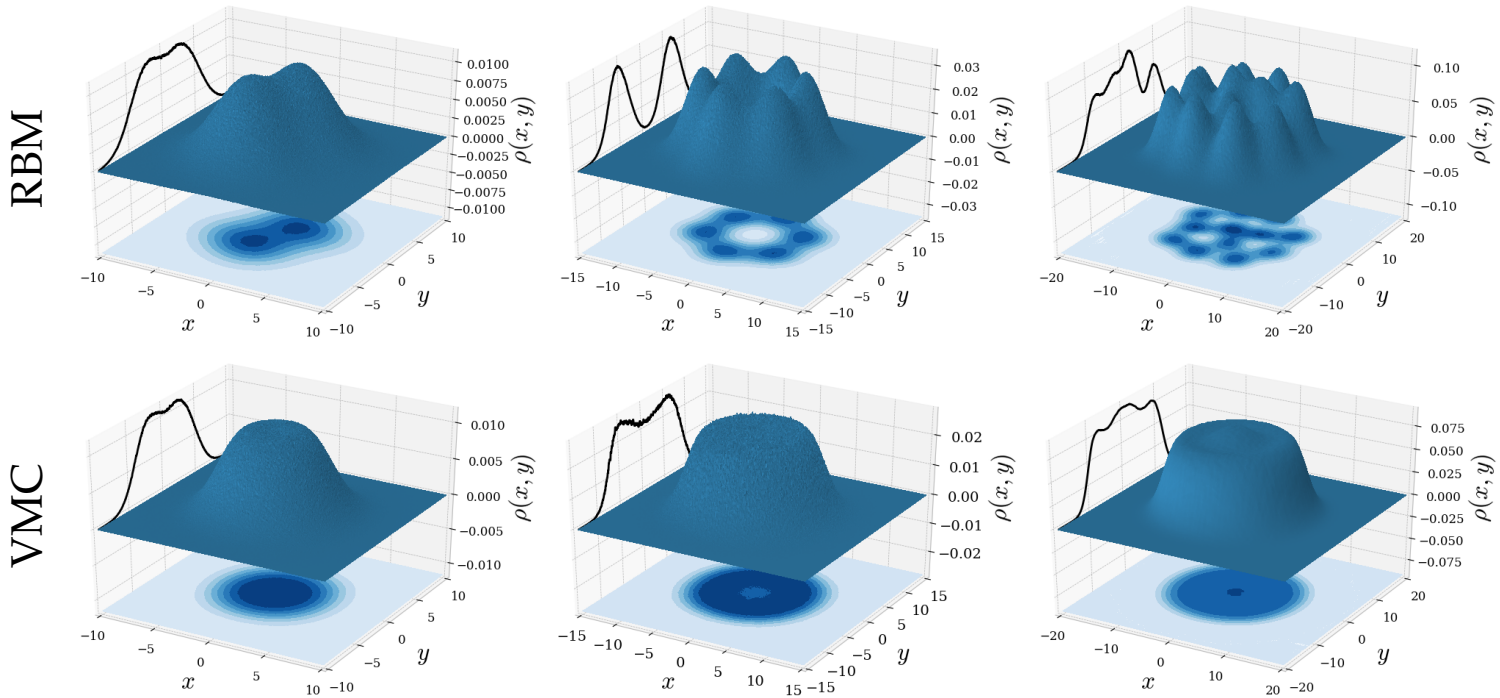
Two-body density

Number of electrons: $N = 20$. Frequency: $\omega = 1.0$.



Low-frequency dots

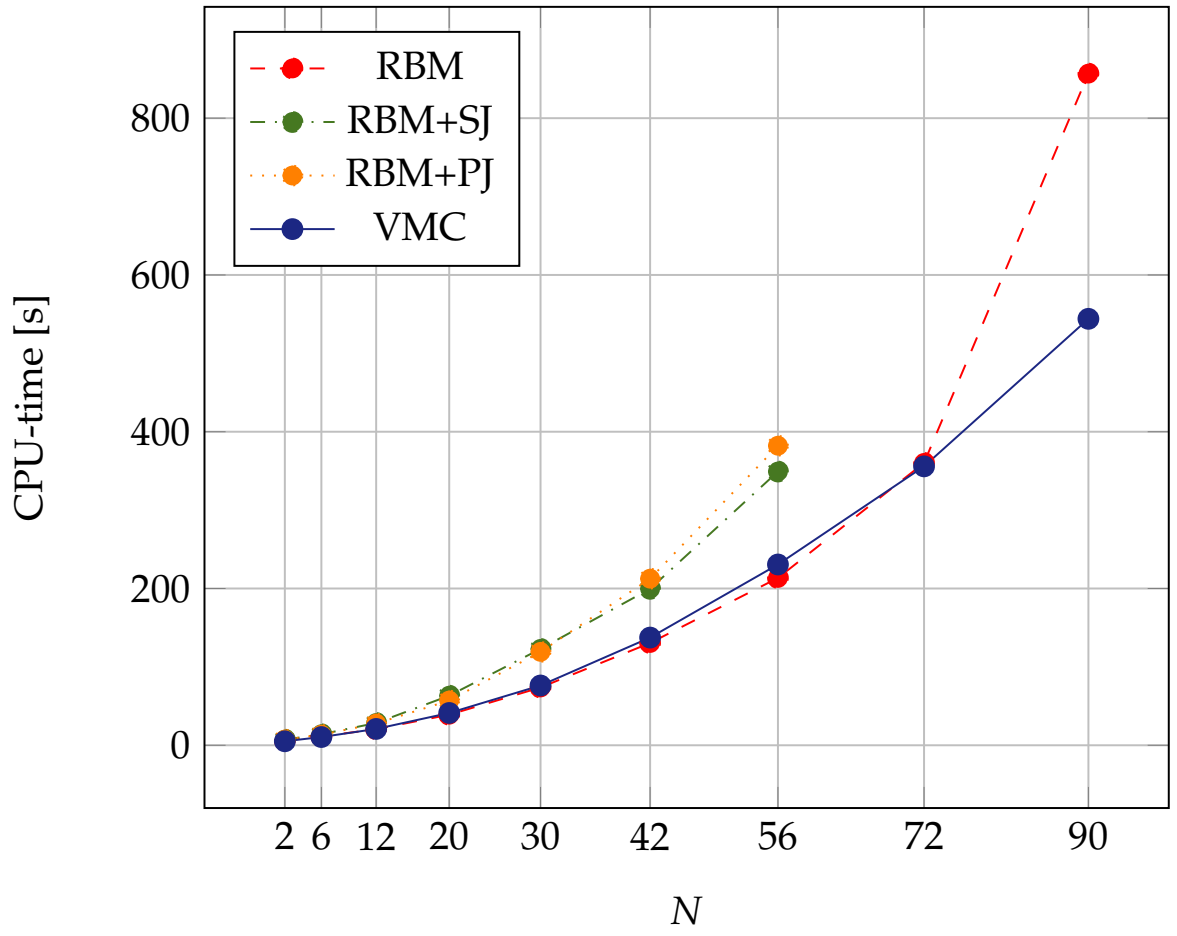
Number of electrons: N. Frequency: $\omega = 0.1$.



UiO : University of Oslo

Computational Cost

Number of electrons: N.



Conclusion

Conclusions

- RBM is able to account for most of the correlations
- RBM+PJ implies to give a lower ground state energy and model the correlations better than a traditional VMC
- RBM+SJ is both more expensive and less accurate than its fellow methods, and we see no reason to choose it

Future Work

- Repeat the exercise using spherical coordinates - interactions are easier to model in spherical coordinates
- Check the ability of modeling the three-body correlations, considering nuclear systems
- Reduce the computational cost

Thank you!

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