Studies of Quantum Dots using Machine Learning

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December 9, 2019

Outline

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

Motivation

Why quantum dots?

- Technology[1,2]
- Experimentally[3]
- Physically

Why is it challenging?

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

How to overcome the challenges?

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

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

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

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).

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,

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

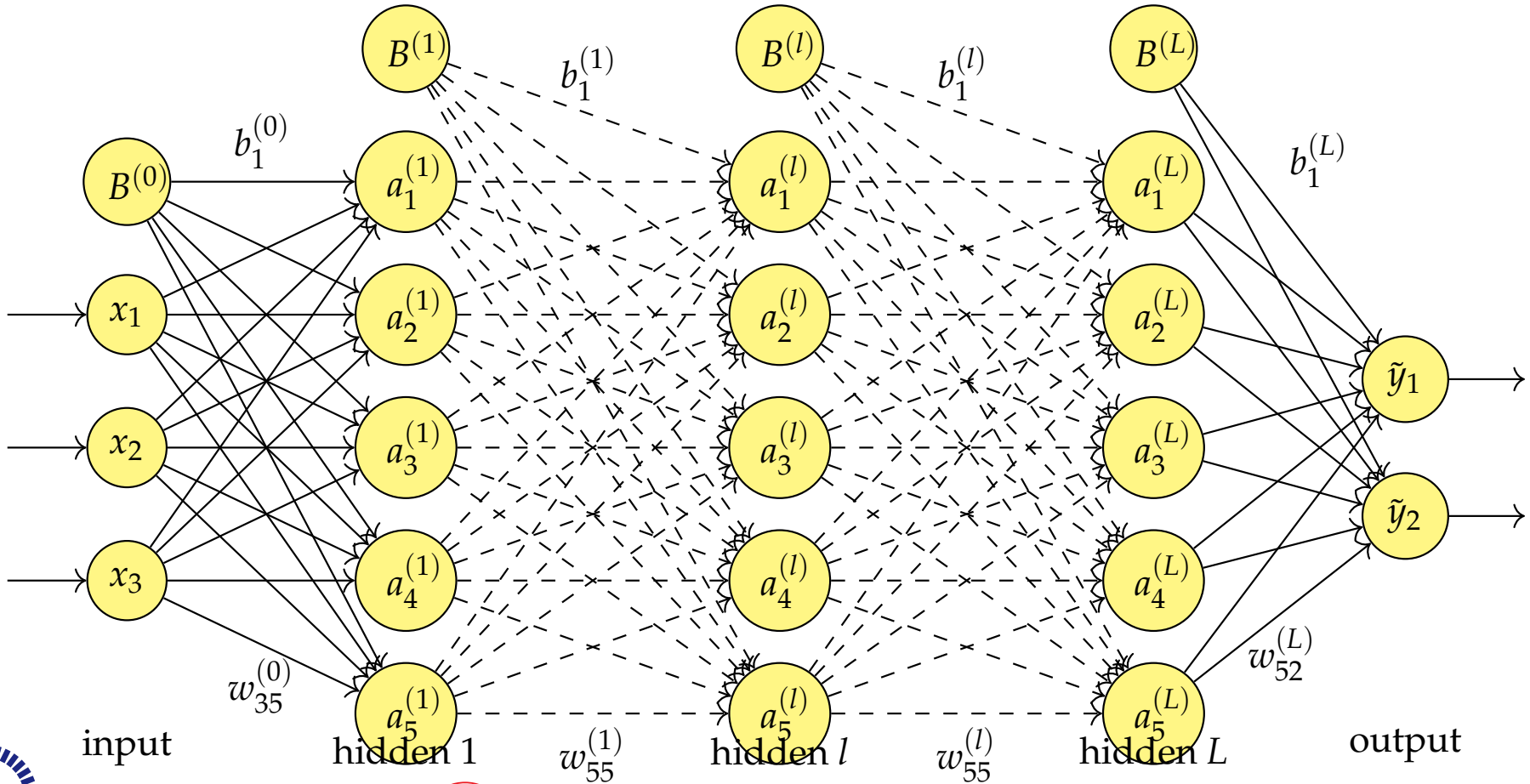
Thus, by minimizing the obtained energy, E, we can estimate the ground state energy.

Machine Learning Theory

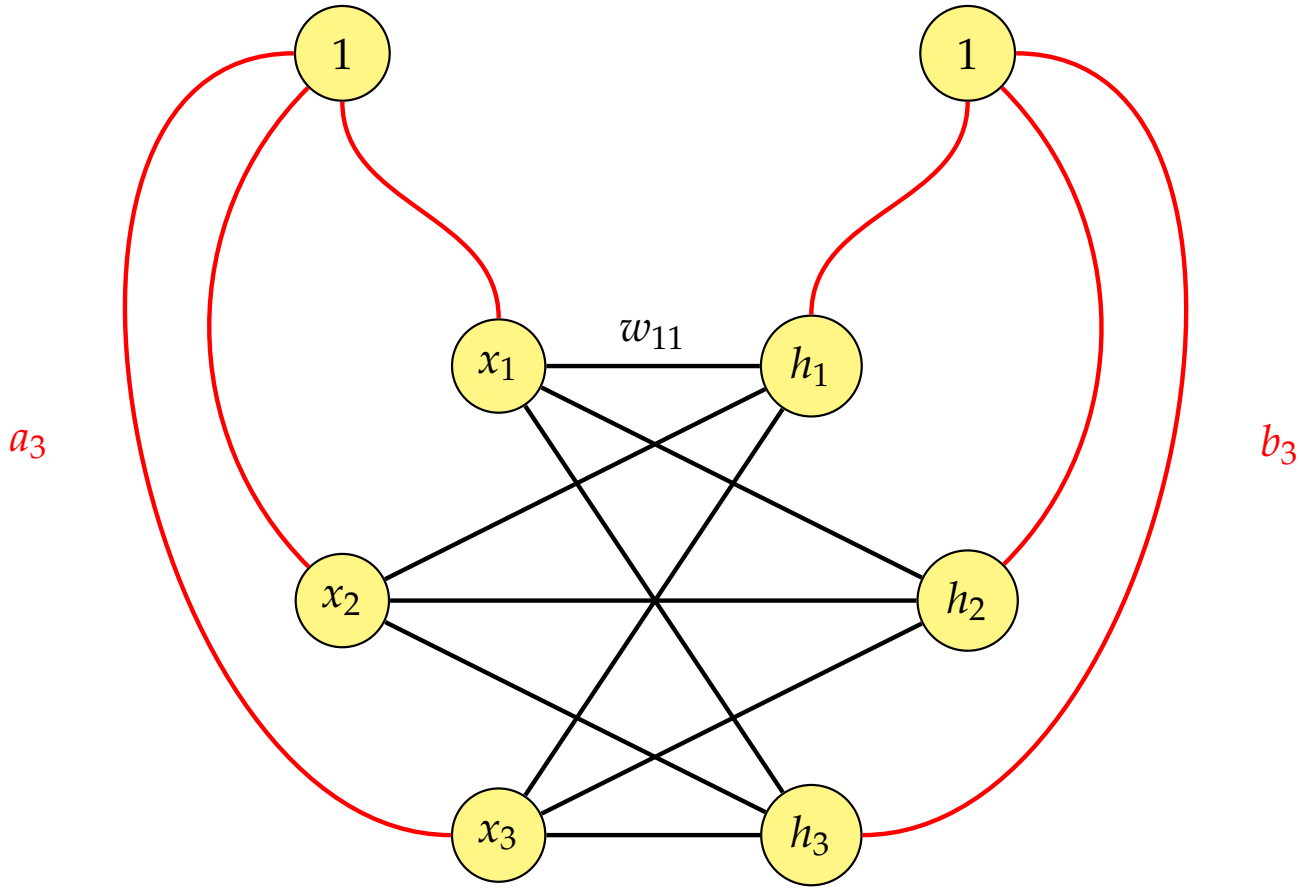
Machine Learning

> *Machine learning is the science of getting computers to act without being explicitly programmed.*
> *Stanford University*[6]

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 [7].

†Semi-analytical ground state energy calculated by Taut, 1993 [8].

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)

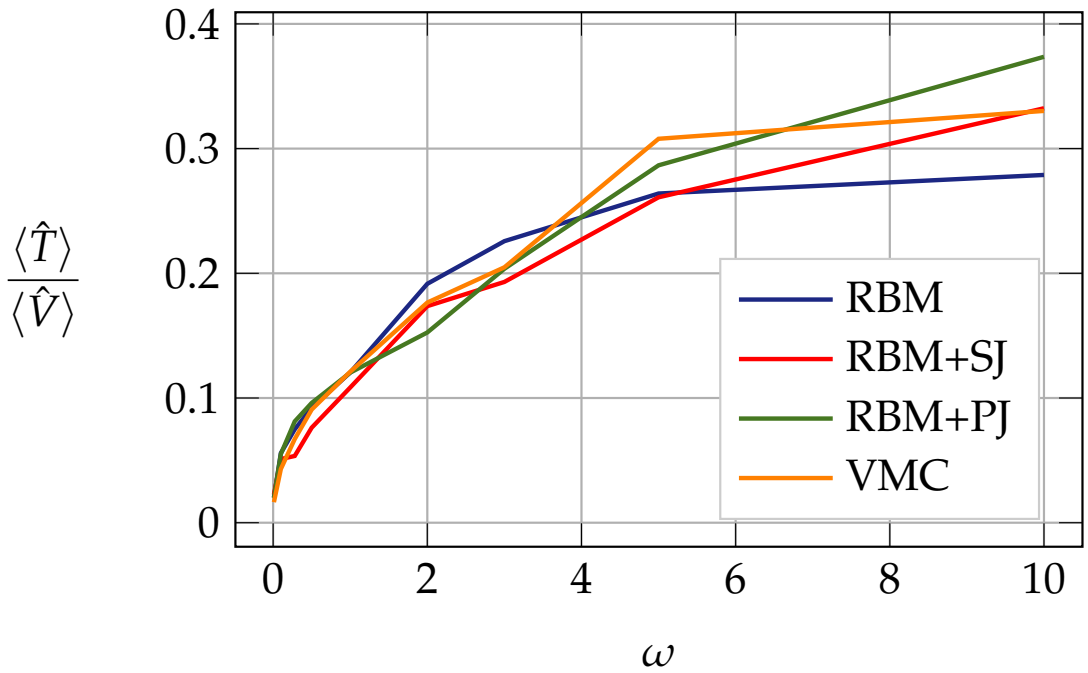
[‡]Computation of the Hartree-Fock limit by Mariadason, 2018 [7].

[§]Ground state energy estimate using the diffusion Monte Carlo method. By Høgberget, 2013 [9].

Energy distribution

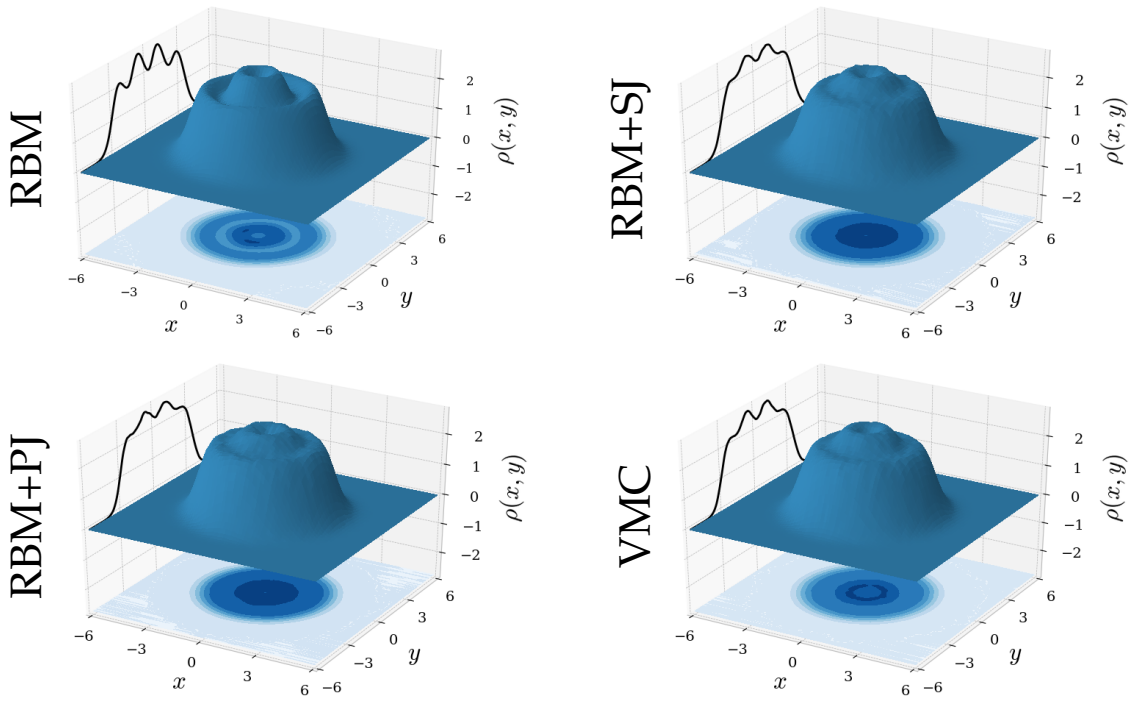
Number of electrons: $N = 20$. Frequency: ω.

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: $\omega = 1.0$.



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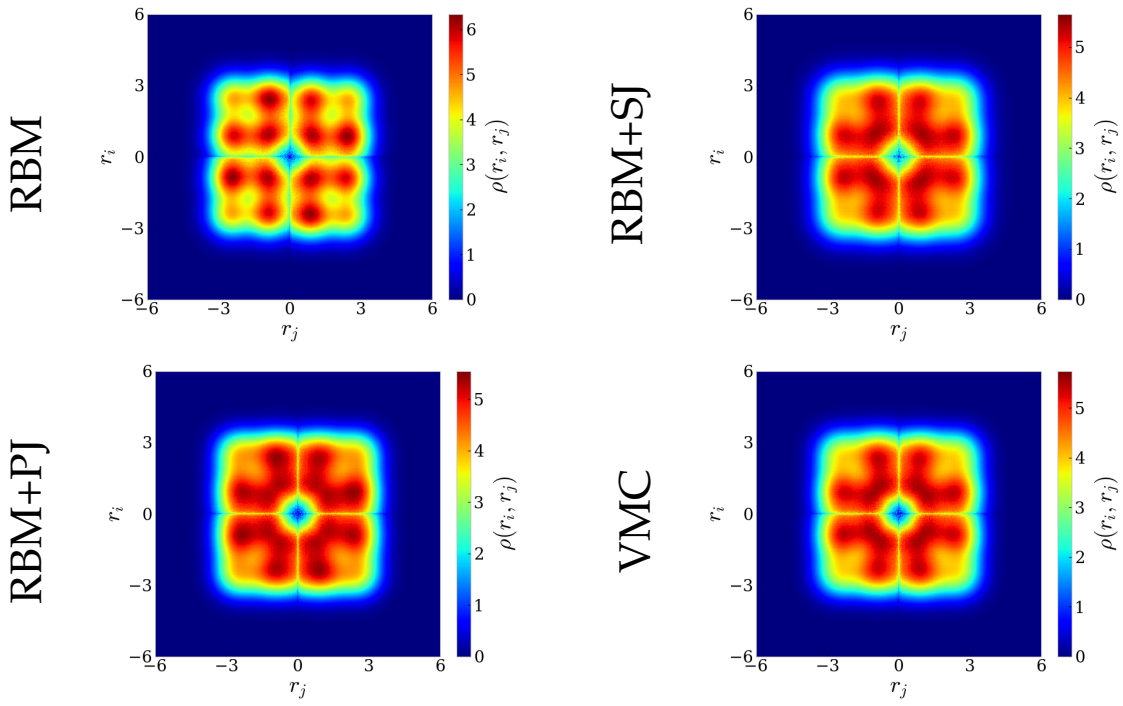
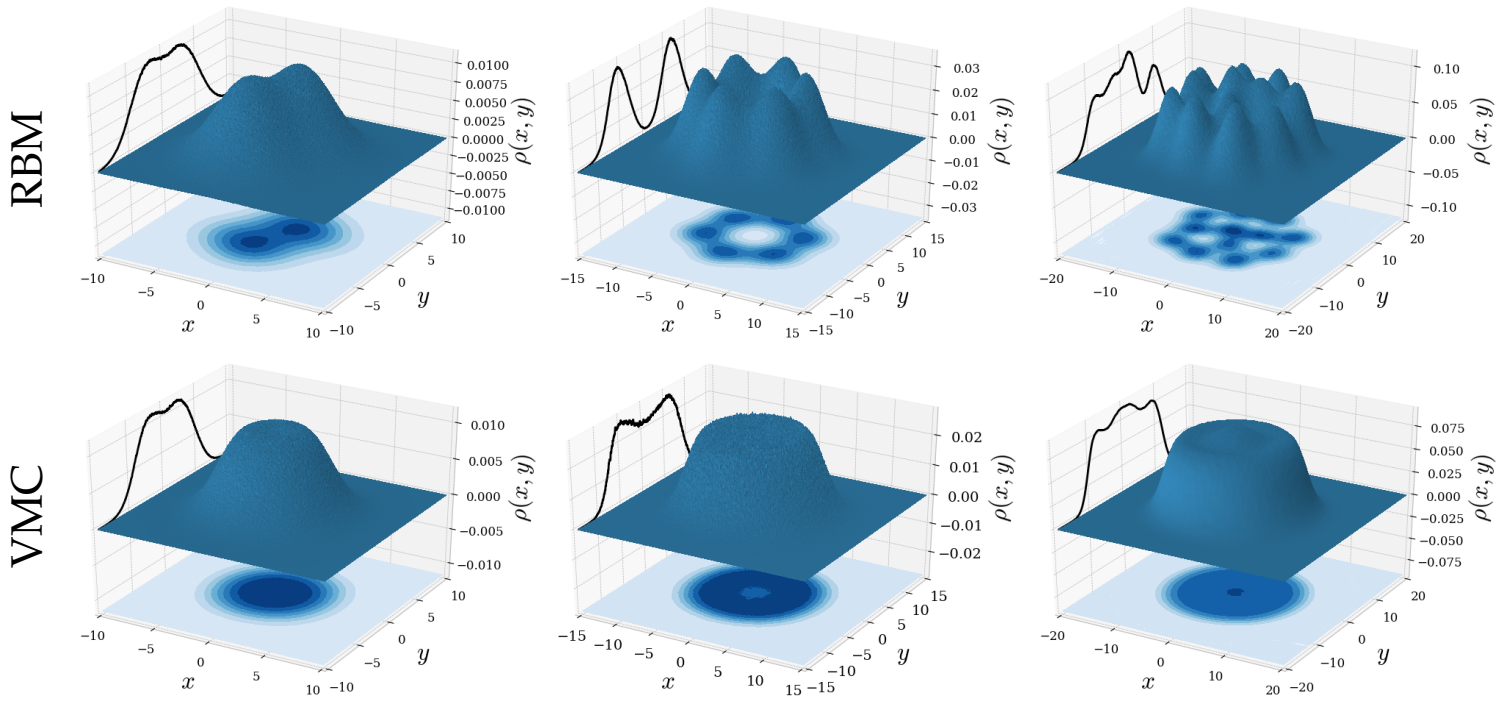
Two-body density

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



Low-frequency dots

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



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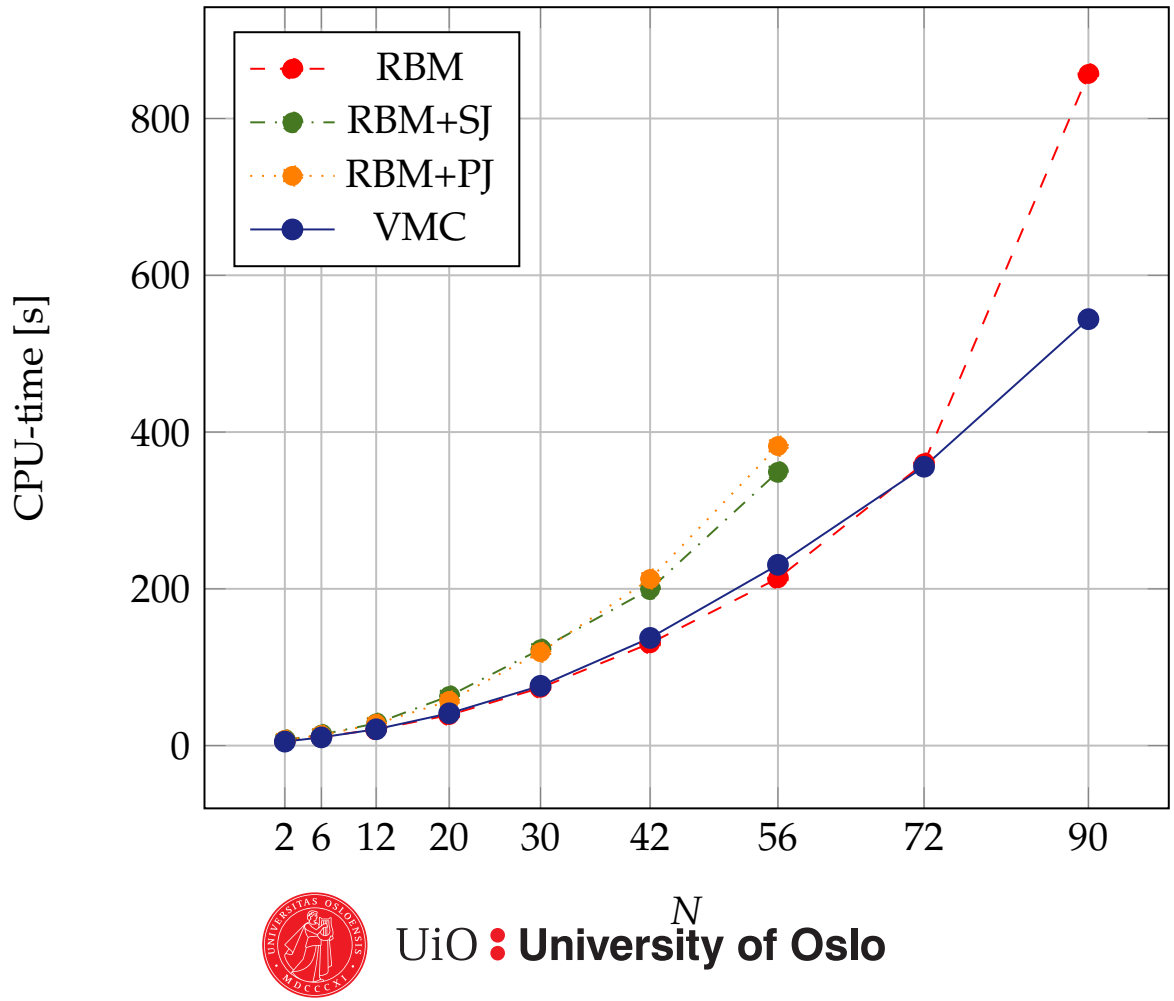
Computational Cost

Number of electrons: N.



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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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