

VARIATIONAL MONTE CARLO METHODS FOR QUANTUM DOTS

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What are quantum dots?
The algorithm
The 2-electrons system
The 6-electrons system
Analytical derivatives
Conclusion

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The algorithm

The 2-electrons system

The 6-electrons system

Analytical derivatives

Conclusion

2015-07-16

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└ What are quantum dots?

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WHAT ARE QUANTUM DOTS?

Quantum dots can be thought as [artificial atoms](#).

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└ What are quantum dots?

└ Quantum dots as artificial atoms

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Like natural atoms, they are... While in natural atoms the attractive potential is generated by a charged nucleus, in quantum dots there is no such a thing.

To understand how the confinement is generated in this case, we have to take a look at the internal structure of such devices.

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Similarities with natural atoms:

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- They have a shell-structure with its relative **magic numbers**

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- *Shape of the potential* (2D isotropic harmonic potential)
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Building technique: stack up different layers of **semiconductor** materials.

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└ What are quantum dots?

└ Structure

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In the etched quantum dots figure, the white bars have a length of $0.5 \mu\text{m}$.

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Then, an electron gas forms at the interface between two layers.

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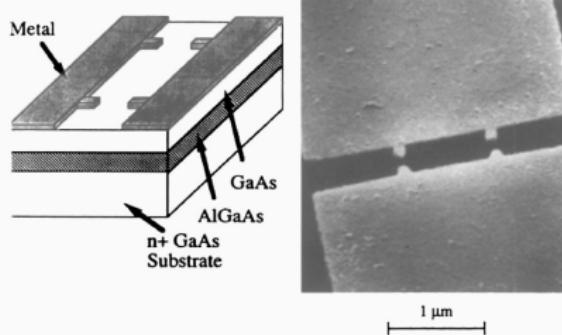
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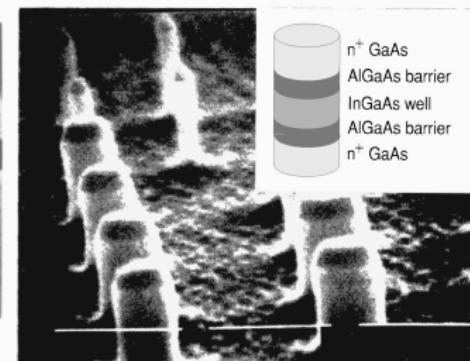
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(a) Lateral quantum dot.



(b) Etched quantum dots.

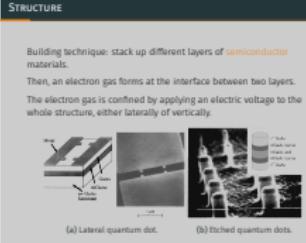
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A quantum dot can be schematized as a *single-electron transistor*.

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└ What are quantum dots?

└ The single-electron transistor

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In figure, scheme of a single electron transistor. The island has index 0, the source has index 1, the drain index 2 and the gate index 3. The capacitances are meant to be intrinsic capacitances of the respective electrode (source, drain or gate)

THE SINGLE-ELECTRON TRANSISTOR

A quantum dot can be schematized as a *single-electron transistor*.

Its charge is a multiple of the elementary charge and transport proceeds one electron at the time.

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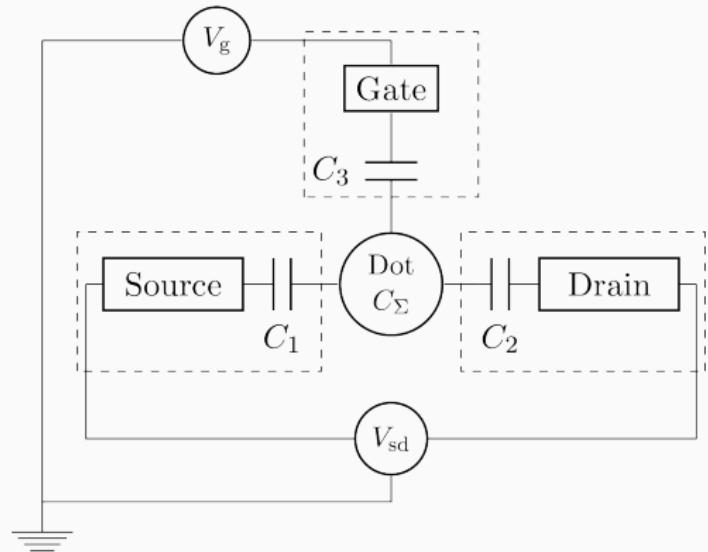
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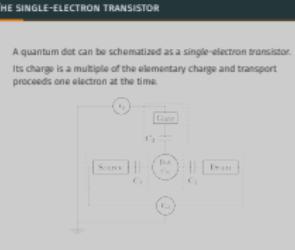


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└ What are quantum dots?

└ The Coulomb blockade effect

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In figure, Coulomb oscillations in a lateral quantum dot.

- The electron island is weakly coupled with source and drain via tunnel barriers.
- When the thermal energy is not enough to make an electron tunnel the barriers, the conduction is blocked.

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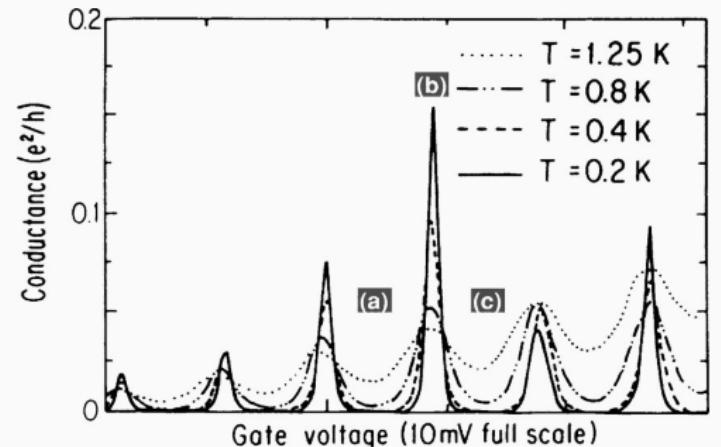
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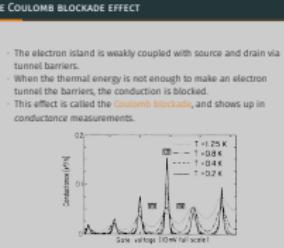
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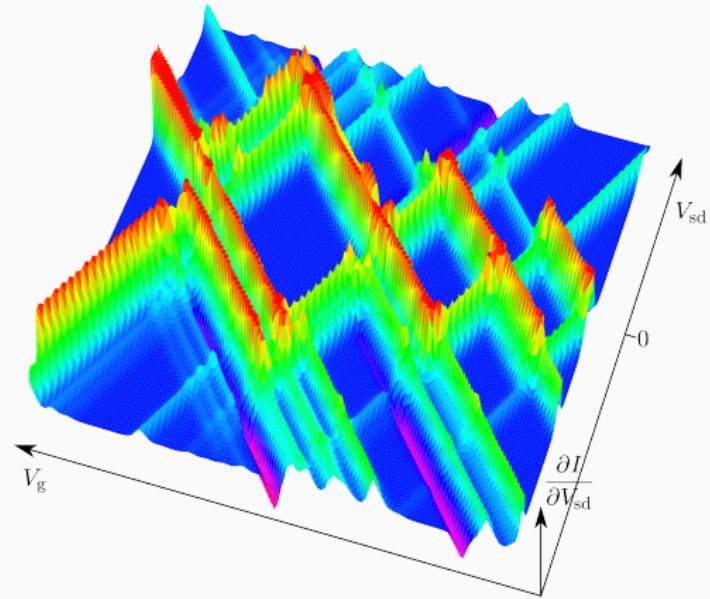


Figure 2: Differential conductance measurements in a nanowire.

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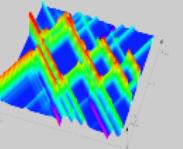
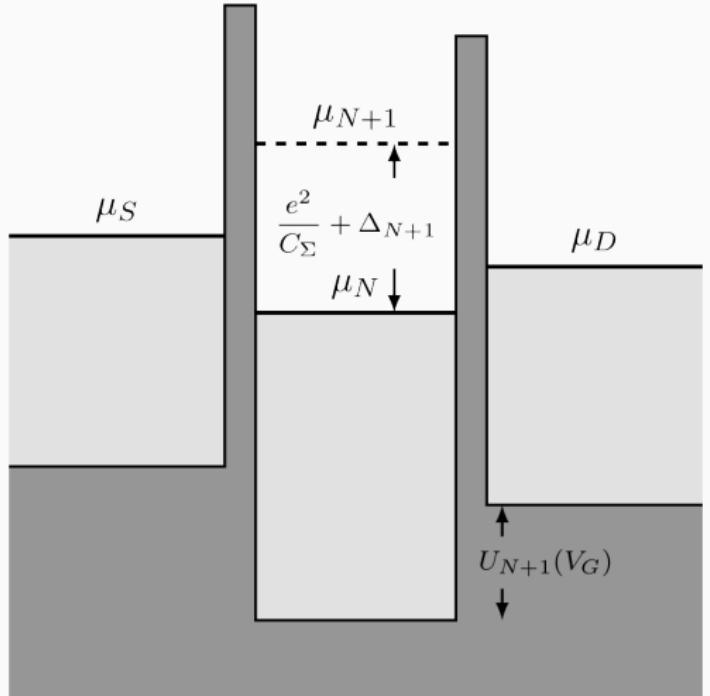


Figure 2: Differential conductance measurements in a nanowire.

BAND DIAGRAM



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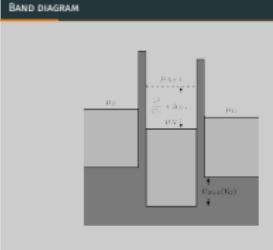
└ What are quantum dots?

└ Band diagram

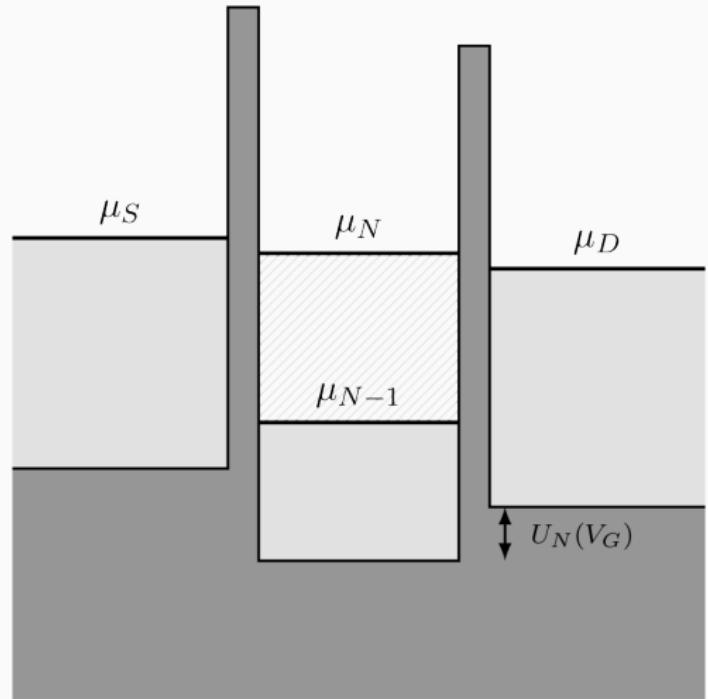
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Let's see what happens in terms of the electrochemical potential.

$\mu_N < \mu_D$: the transport is blocked due to the Coulomb blockade. The number of electrons inside the dot is N .



BAND DIAGRAM



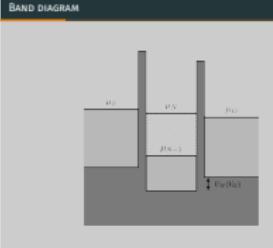
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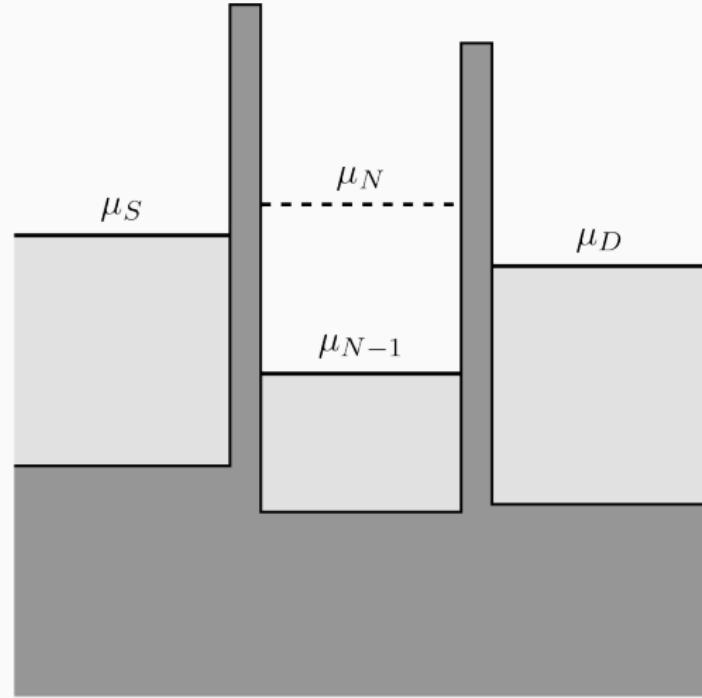
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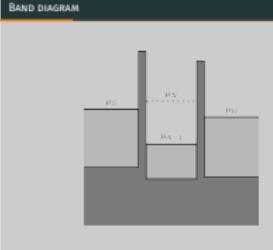
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$\mu_N > \mu_S$: the transport is blocked again due to the Coulomb blockade. The number of electrons inside the dot is $N - 1$. This situation is obtained by further lowering V_G .



THE ALGORITHM

The **variational principle** is a powerful tool that allows, for *any* system, to calculate an *upper bound* estimate for the *ground state energy*.

Being E_{gs} the ground-state energy, $|\psi\rangle$ a state whatsoever and \hat{H} the Hamiltonian of the system, the principle states that

$$E_{\text{gs}} \leq \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle}. \quad (1)$$

We are going to use this principle by calculating the quantity on the right hand side, for a chosen *trial wave-function* ψ_T . We will come back later on how to guess a realistic ψ_T .

Variational Monte Carlo methods for quantum dots

- └ The algorithm

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In the function-representation of the states, we can recast the above relation as

$$E_{\text{gs}} \leq \int d\vec{r} \mathcal{P}(\vec{r}) E_L(\vec{r}) \simeq \frac{1}{n} \sum_{i=1}^n E_L(\vec{r}), \quad (2)$$

where

$$\mathcal{P}(\vec{r}) = \frac{|\psi_T|^2}{\int d\vec{r} |\psi_T|^2} \quad \text{and} \quad E_L(\vec{r}) = \frac{1}{\psi_T} \hat{H} \psi_T. \quad (3)$$

The quantity E_L is called the **local energy**.

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Let's do a brief recap.

Variational Monte Carlo methods for quantum dots

└ The algorithm

└ The local energy

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- Since the E_L 's have a certain distribution, we should sample more points where the probability is higher and less points where the probability is lower, in order to be sure to have a consistent set of samples.

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The solution is to use the [Metropolis algorithm](#).

Let's suppose that we have just sampled E_L at a certain point in space, let's call it \bar{r}^{old} . Then, we make a [random move](#) to another point in space, \bar{r}^{new} .

To check whether we moved to a higher probability region, we calculate the ratio of the respective probabilities, that is

$$R \doteq \frac{\mathcal{P}(\bar{r}^{\text{new}})}{\mathcal{P}(\bar{r}^{\text{old}})} = \frac{|\psi(\bar{r}^{\text{new}})|^2}{|\psi(\bar{r}^{\text{old}})|^2}. \quad (4)$$

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- If $R \geq 1$, we accept this move because we are moving to a higher probability region and we sample E_L in the new position.

Variational Monte Carlo methods for quantum dots

└ The algorithm

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Solution: generate a random number $r \in (0, 1)$, and accept the move (i.e., sample E_L) if $r \leq R$. Otherwise, the sample is rejected.

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Variational Monte Carlo methods for quantum dots

└ The algorithm

└ The Metropolis algorithm

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2015-07-16

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CHOOSE THE PROPER STEP-LENGTH

Problem:

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Here, the random variable ε is no more uniform! For importance sampling, it's a *Gaussian* random variable.

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$$r^{\text{new}} = r^{\text{old}} + D\vec{F}(r^{\text{old}})\Delta t + \varepsilon, \quad (6)$$

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THE 2-ELECTRONS SYSTEM

Variational Monte Carlo methods for quantum dots

└ The 2-electrons system

└ The unperturbed system

Hamiltonian of the system:

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We begin with the unperturbed Hamiltonian, without the electron-electron repulsion.

Unlike the one-dimensional case, for two dimensions we need two quantum numbers: n_x and n_y for the x and y directions, respectively. This causes a degeneracy in the energy levels. The principal quantum number is

$$n = n_x + n_y.$$

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└ The 2-electrons system

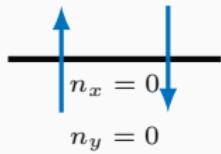
└ The unperturbed system

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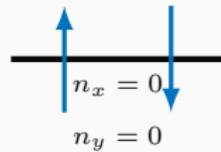
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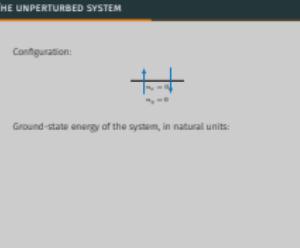
Ground-state energy of the system, in natural units:

Variational Monte Carlo methods for quantum dots

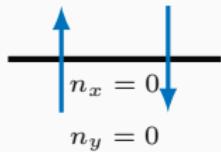
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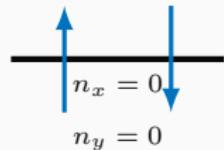


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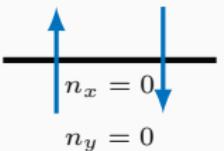
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$$\psi_T(\vec{r}_1, \vec{r}_2) = \exp(-\alpha\omega(r_1^2 + r_2^2)/2). \quad (13)$$

where α is a **variational parameter**.

For $\alpha = 1$ we expect to obtain a variational energy **exactly** equal to the ground state energy $E_{\text{gs}} = 2\omega$.

Variational Monte Carlo methods for quantum dots

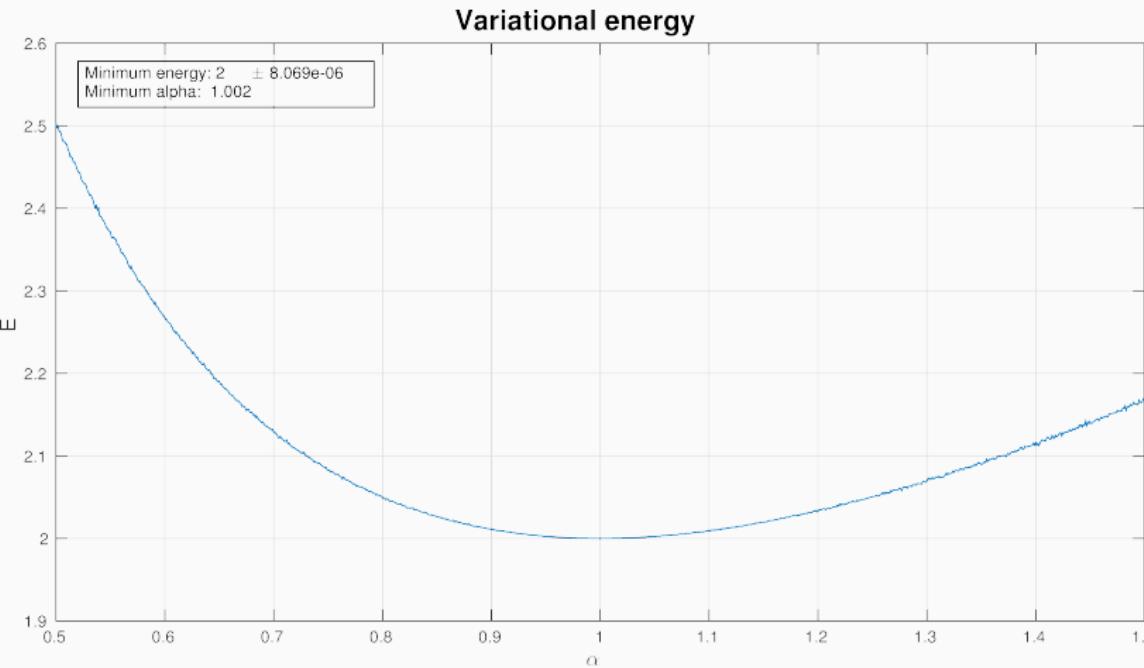
└ The 2-electrons system

└ The unperturbed system

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$\omega = 1$ 

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Variational Monte Carlo methods for quantum dots

└ The 2-electrons system

└ $\omega = 1$

The variational energy versus the variational parameter α . The settings used are: brute force sampling with step length 2, no Jastrow factor, no parallelization, 1000 variations of α around 1 with step 0.001, 1×10^7 Monte Carlo steps. Acceptance ratio varies from 40 to 60 %.



The full Hamiltonian is

Variational Monte Carlo methods for quantum dots

└ The 2-electrons system

└ The complete system

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$$\hat{H} = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 + \frac{1}{2}\omega r_1^2 + \frac{1}{2}\omega r_2^2 + \frac{1}{|\vec{r}_1 - \vec{r}_2|}. \quad (14)$$

Variational Monte Carlo methods for quantum dots

└ The 2-electrons system

└ The complete system

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Variational Monte Carlo methods for quantum dots

└ The 2-electrons system

└ The complete system

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Variational Monte Carlo methods for quantum dots

└ The 2-electrons system

└ The complete system

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Variational Monte Carlo methods for quantum dots

└ The 2-electrons system

└ The complete system

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Variational Monte Carlo methods for quantum dots

└ The 2-electrons system

└ The complete system

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Variational Monte Carlo methods for quantum dots

└ The 2-electrons system

└ The complete system

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In two dimensions

$$a = \begin{cases} 1 & \text{anti-parallel spin} \\ 1/3 & \text{parallel spin} \end{cases} \quad (16)$$

The calculated upper bound coincides with the ground state energy calculated by Taut theoretically.

Variational Monte Carlo methods for quantum dots

└ The 2-electrons system

└ The complete system

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a is a parameter that depends on the spin, while β is a *variational parameter*.

Variational Monte Carlo methods for quantum dots

└ The 2-electrons system

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Variational Monte Carlo methods for quantum dots

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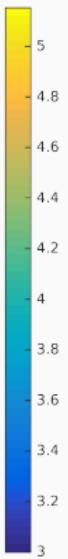
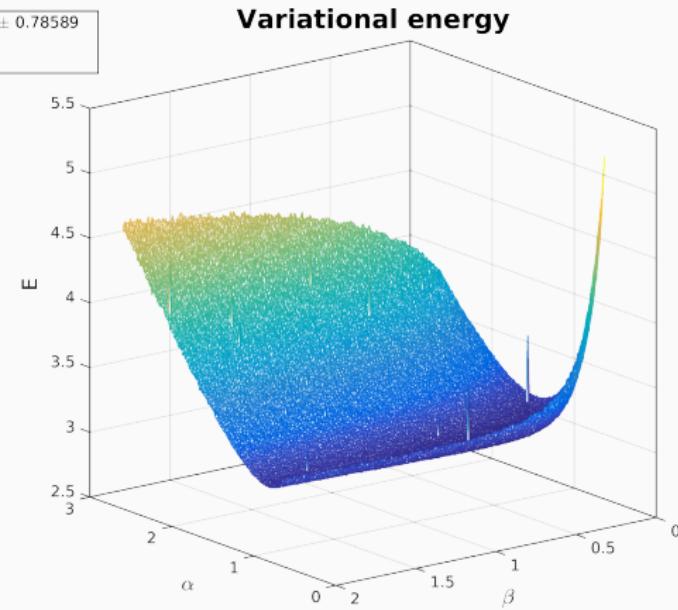
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The calculated upper bound coincides with the ground state energy calculated by Taut theoretically.

THE COMPLETE SYSTEM

Minimum energy: 2.9985 ± 0.78589
Minimum alpha: 1.02
Minimum beta: 0.36

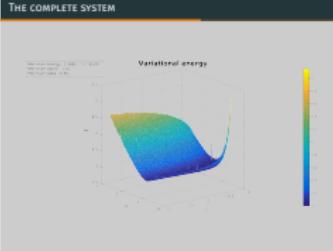


Variational Monte Carlo methods for quantum dots

└ The 2-electrons system

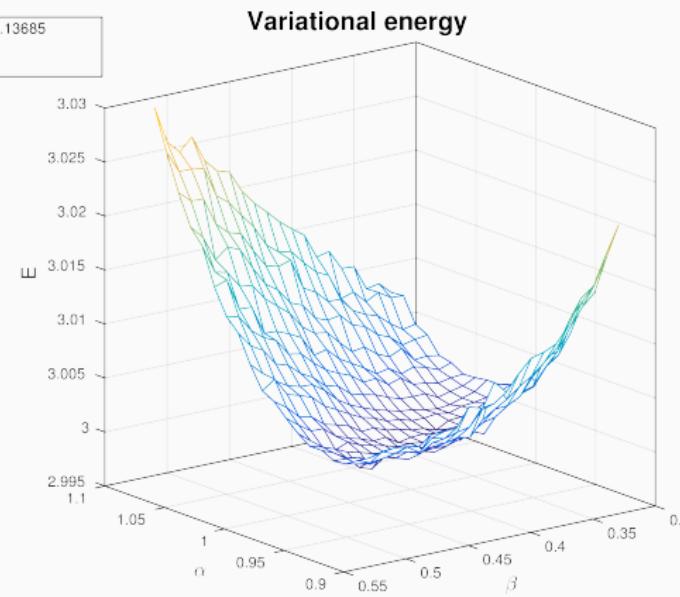
└ The complete system

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The variational energy versus the variational parameters α and β . The settings used are: brute force sampling with step length 2, Jastrow factor, no parallelization, 200 variations of α and β with step 0.01, 1×10^5 Monte Carlo steps. Acceptance ratio varies from 45 to 55 %.

Minimum energy: 2.9998 +/- 0.13685
Minimum alpha: 0.98
Minimum beta: 0.38

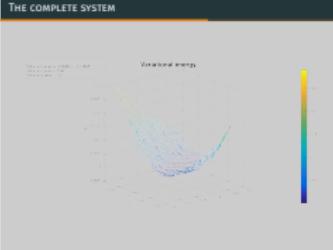


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Variational Monte Carlo methods for quantum dots

└ The 2-electrons system

└ The complete system



The variational energy versus the variational parameters α and β . The settings used are: brute force sampling with step length 2, Jastrow factor, no parallelization, 20 variations of α and β with step 0.01, 1×10^6 Monte Carlo steps. Acceptance ratio varies from 45 to 55 %. The relative distance is about 1.64 in natural units.

Idea: take multiple measurements for each point in order to lower the error.

Variational Monte Carlo methods for quantum dots

└ The 2-electrons system

└ Parallelization

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If we take n measurements of the same quantity, its error falls like

Variational Monte Carlo methods for quantum dots

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Variational Monte Carlo methods for quantum dots

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We obtain more precise energy values even with less Monte Carlo steps.

Variational Monte Carlo methods for quantum dots

└ The 2-electrons system

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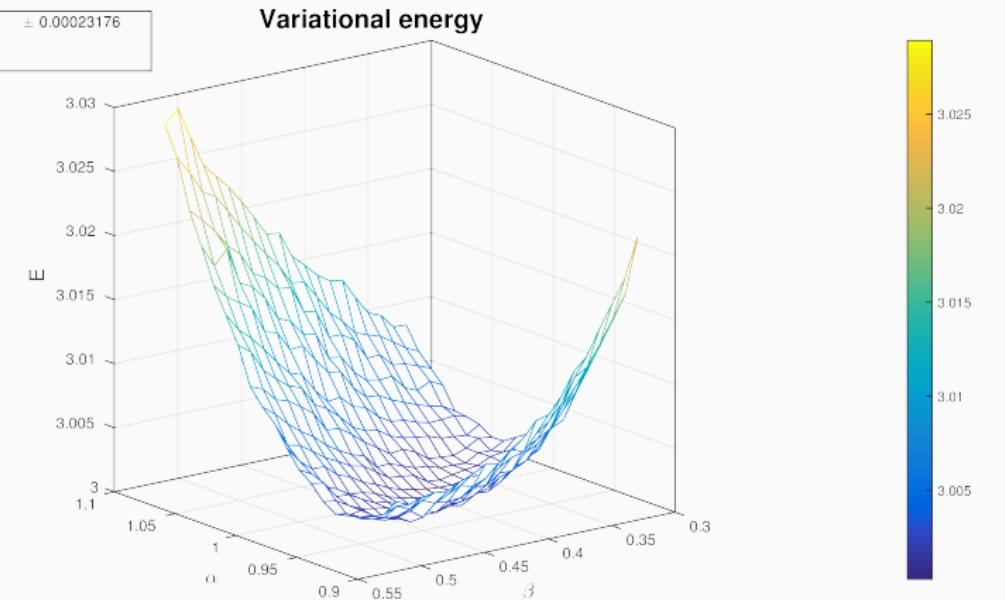
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$\omega = 1$

Minimum energy: 3.0003 ± 0.00023176
Minimum alpha: 0.99
Minimum beta: 0.4



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Variational Monte Carlo methods for quantum dots

└ The 2-electrons system

└ $\omega = 1$

The variational energy versus the variational parameters α and β . The settings used are: brute force sampling with step length 2, Jastrow factor, parallelization (8 threads), 20 variations of α and β with step 0.01, 2×10^5 Monte Carlo steps. Acceptance ratio varies from 45 to 55 %.

Idea: implement importance sampling in order to waste less points.

Variational Monte Carlo methods for quantum dots

└ The 2-electrons system

└ Importance sampling

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Variational Monte Carlo methods for quantum dots

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Variational Monte Carlo methods for quantum dots

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Variational Monte Carlo methods for quantum dots

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- For a given time-step, increase the number of Monte Carlo cycles until the acceptance ratio is slightly below 100 %.

The 2-electrons system

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Variational Monte Carlo methods for quantum dots

└ The 2-electrons system

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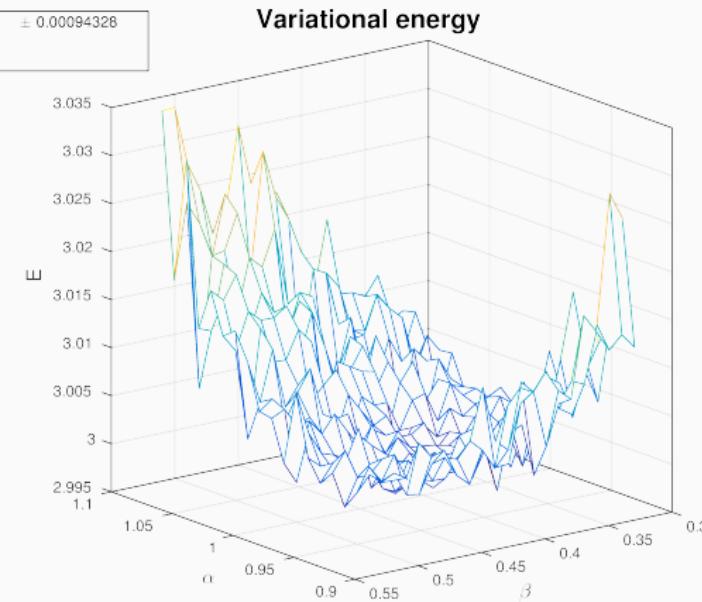
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$\omega = 1$

Minimum energy: 2.9975 ± 0.00094328
Minimum alpha: 0.95
Minimum beta: 0.39



Variational Monte Carlo methods for quantum dots

└ The 2-electrons system

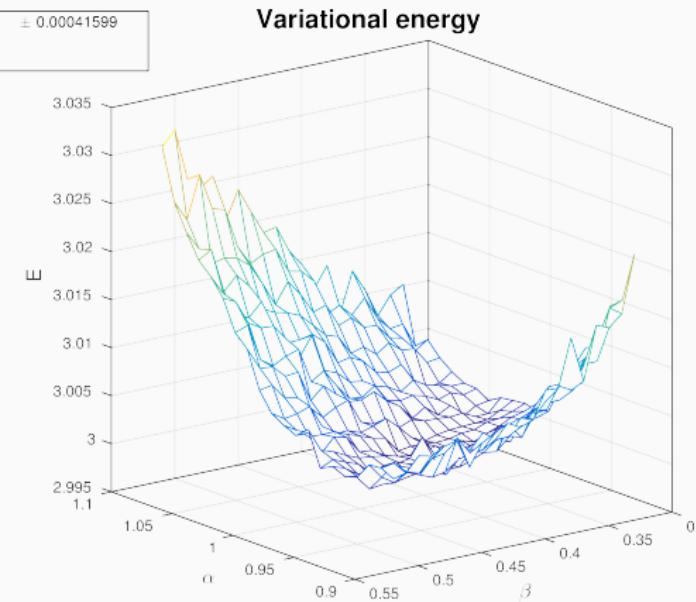
└ $\omega = 1$

The variational energy versus the variational parameters α and β . The settings used are: importance sampling with $\Delta t = 0.001$, Jastrow factor, parallelization (8 threads), 20 variations of α and β with step 0.01, 2×10^5 Monte Carlo steps. Acceptance ratio is about 99.999 %.

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$\omega = 1$

Minimum energy: 2.9999 ± 0.00041599
Minimum alpha: 1.01
Minimum beta: 0.39



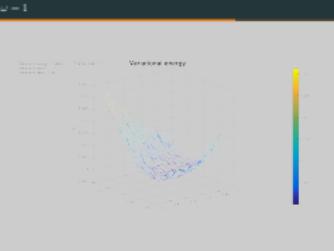
34

Variational Monte Carlo methods for quantum dots

└ The 2-electrons system

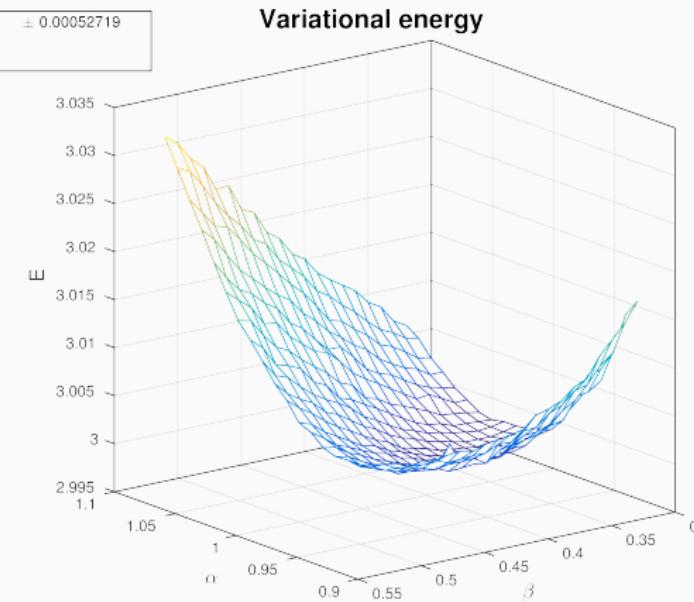
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$\omega = 1$

Minimum energy: 2.9989 ± 0.00052719
Minimum alpha: 1
Minimum beta: 0.36



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Variational Monte Carlo methods for quantum dots

└ The 2-electrons system

└ $\omega = 1$

The variational energy versus the variational parameters α and β . The settings used are: importance sampling with $\Delta t = 0.1$, Jastrow factor, parallelization (8 threads), 20 variations of α and β with step 0.01, 2×10^5 Monte Carlo steps. Acceptance ratio is about 99.793 %.

THE 6-ELECTRONS SYSTEM

The trial wave-function is like the one we used for 2 electrons, but this time is more general.

Variational Monte Carlo methods for quantum dots

└ The 6-electrons system

└ The trial wave-function

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Variational Monte Carlo methods for quantum dots

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$$\psi_T(\vec{r}_1, \vec{r}_2) = \phi(\vec{r}_1)\phi(\vec{r}_2) \exp\left(\frac{ar_{12}}{1 + \beta r_{12}}\right) \quad (19)$$

Variational Monte Carlo methods for quantum dots

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where ϕ is the single-particle spatial wave-function for $(n_x, n_y) = (0, 0)$, that is equal for both electron 1 and electron 2, and r_{12} is the inter-particle distance.

Variational Monte Carlo methods for quantum dots

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For N electrons, the generalization is straightforward:

Variational Monte Carlo methods for quantum dots

└ The 6-electrons system

└ The trial wave-function

2015-07-16

For N electrons, the generalization is straightforward:

$$\psi_T(\vec{r}_1, \dots, \vec{r}_N) = |S| \prod_{i < j}^N \exp\left(\frac{ar_{ij}}{1 + \beta r_{ij}}\right) \quad (20)$$

Variational Monte Carlo methods for quantum dots

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Variational Monte Carlo methods for quantum dots

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where $|S|$ is the **Slater determinant**.

$$|S| = \begin{vmatrix} \phi_1(\vec{r}_1) & \phi_2(\vec{r}_1) & \dots & \phi_N(\vec{r}_1) \\ \phi_1(\vec{r}_2) & \phi_2(\vec{r}_2) & \dots & \phi_N(\vec{r}_2) \\ \vdots & & & \vdots \\ \phi_1(\vec{r}_N) & \phi_2(\vec{r}_N) & \dots & \phi_N(\vec{r}_N) \end{vmatrix} \quad (21)$$

Variational Monte Carlo methods for quantum dots

└ The 6-electrons system

└ The trial wave-function

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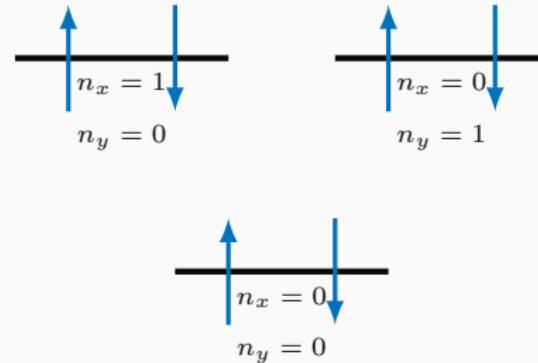
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THE TRIAL WAVE-FUNCTION

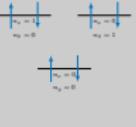


Smart thing:

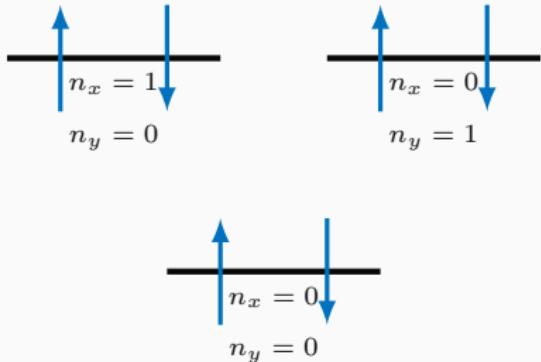
Variational Monte Carlo methods for quantum dots
└ The 6-electrons system
└ The trial wave-function

2015-07-16

THE TRIAL WAVE-FUNCTION



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Smart thing: for spin-independent Hamiltonians, the Slater determinant can be split in a product of **two** Slater determinants, one for the single-particle orbitals with spin up and the other for single-particle orbitals with spin down.

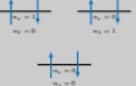
Variational Monte Carlo methods for quantum dots

└ The 6-electrons system

└ The trial wave-function

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THE TRIAL WAVE-FUNCTION



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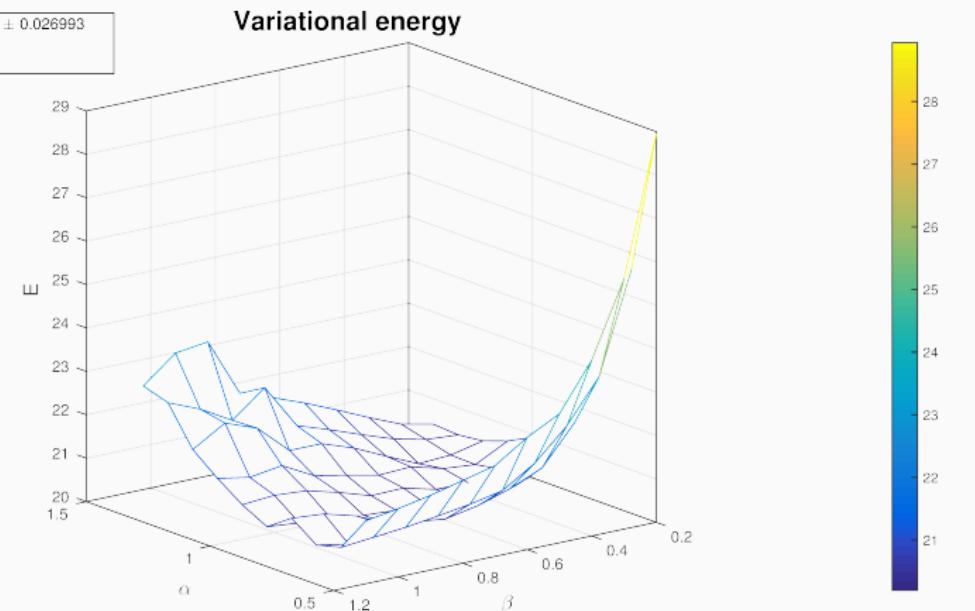
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$\omega = 1$

Minimum energy: 20.1947 ± 0.026993
Minimum alpha: 0.9
Minimum beta: 0.6



Variational Monte Carlo methods for quantum dots

└ The 6-electrons system

└ $\omega = 1$

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The variational energy versus the variational parameters α and β . The settings used are: importance sampling with $\Delta t = 0.1$, Jastrow factor, parallelization (8 threads), 10 variations of α and β with step 0.1, 2×10^5 Monte Carlo steps. $\omega = 1.00$.

Our result is in very good accordance with the one calculated by DMC, that is $20.1597(2)$ a.u..

ANALYTICAL DERIVATIVES

Idea: speed up the calculation of the acceptance ratio by performing analytical derivatives.

and

Variational Monte Carlo methods for quantum dots

└ Analytical derivatives

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Doing the calculations

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$$\frac{1}{\psi_T} \nabla_i \psi_T = \frac{\nabla_i |S^\alpha|}{|S^\alpha|} + \frac{\nabla_i J}{J} \quad (26)$$

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Further simplifications give

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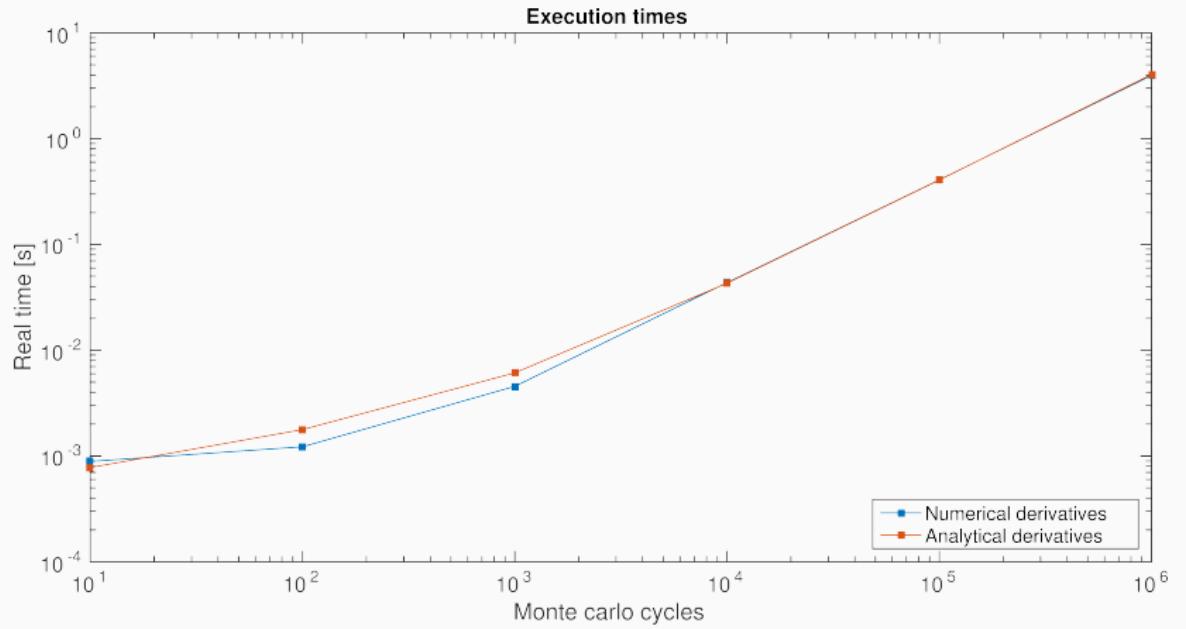
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EXECUTION TIMES – 2 ELECTRONS



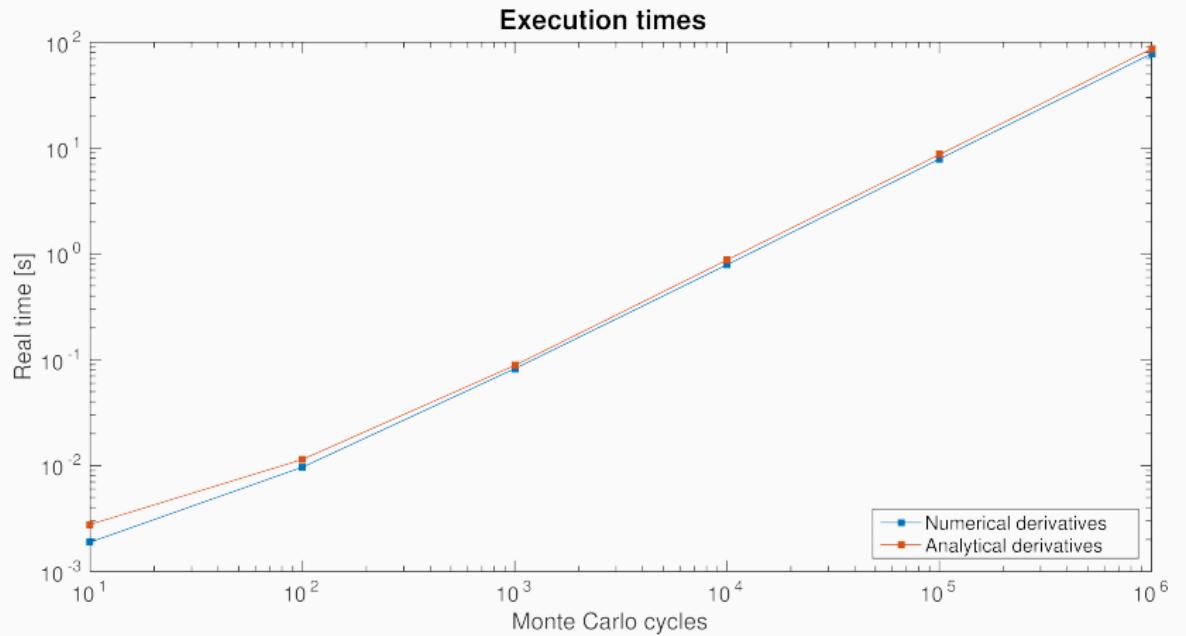
Variational Monte Carlo methods for quantum dots

└ Analytical derivatives

└ Execution times – 2 electrons

Execution times for 2-electrons and a single pair of variational parameters (α, β) . The GNU/Linux system tool `time` was used to take the measurements.

EXECUTION TIMES – 6 ELECTRONS



Variational Monte Carlo methods for quantum dots

└ Analytical derivatives

└ Execution times – 6 electrons

Execution times for 6-electrons and a single pair of variational parameters (α, β). The GNU/Linux system tool `time` was used to take the measurements.

CONCLUSION

Variational Monte Carlo methods for quantum dots
└ Conclusion

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Something to summarize here.

Variational Monte Carlo methods for quantum dots

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└ Summary

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QUESTIONS?