VARIATIONAL MONTE CARLO METHODS FOR QUANTUM DOTS

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July 2015

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Variational Monte Carlo methods for quantum dots

015-07-15

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WHAT ARE QUANTUM DOTS?

Variational Monte Carlo methods for quantum dots

What are quantum dots?

WHAT ARE QUANTUM DOTS?

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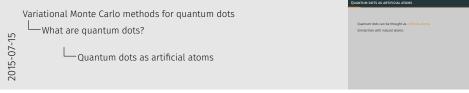
Quantum dots can be thought as artificial atoms.

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Variational Monte Carlo methods for quantum dots What are quantum dots?	Quantum dots can be thought as artificial atoms.
Quantum dots as artificial atoms	

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.

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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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Differences:

- · Shape of the potential (2D isotropic harmonic potential)
- · Dimensions (quantum dots are a few hundred angstroms big)

Variational Monte Carlo methods for quantum dots

What are quantum dots?

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Observations

Definences

- Stage of the potential (26 instruction, patients)

- Binerical (quantum dots as a New houself along proteins (pig).

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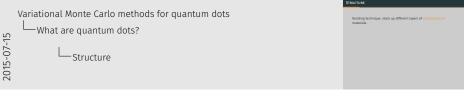
Differences:

- · Shape of the potential (2D isotropic harmonic potential)
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- · Structure and source of the potential



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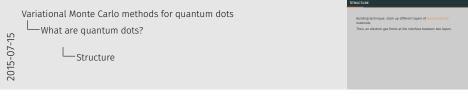
Building technique: stack up different layers of semiconductor materials.



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.

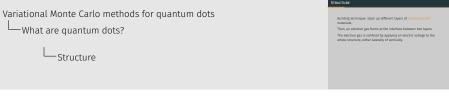


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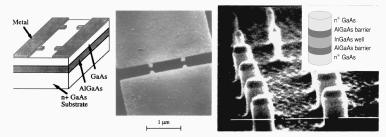


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(a) Lateral quantum dot.

(b) Etched quantum dots.

Variational Monte Carlo methods for quantum dots

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THE SINGLE-ELECTRON TRANSISTOR

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

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—What are quantum dots?	
The single-electron transistor	

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

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

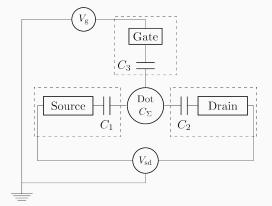
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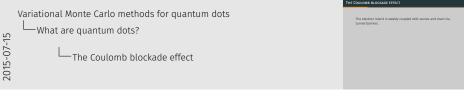
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In figure, Coulomb oscillations in a lateral quantum dot.

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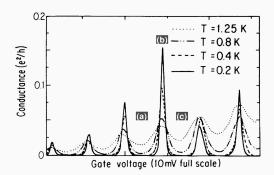
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- This effect is called the Coulomb blockade, and shows up in conductance measurements.



THE COULOMB BLOCKADE EFFECT

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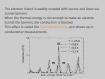
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Variational Monte Carlo methods for quantum dots

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The Coulomb blockade effect

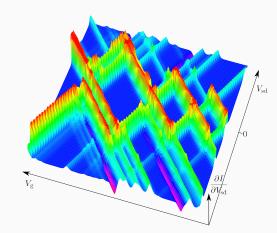


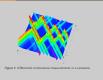
Figure 2: Differential conductance measurements in a nanowire.

Variational Monte Carlo methods for quantum dots

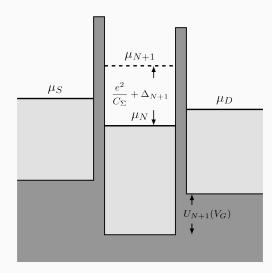
What are quantum dots?

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____The Coulomb blockade effect



BAND DIAGRAM



Variational Monte Carlo methods for quantum dots
—What are quantum dots?

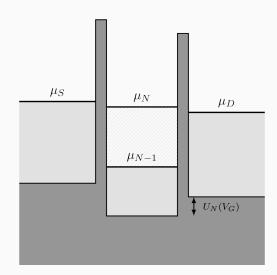
Band diagram



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



Variational Monte Carlo methods for quantum dots

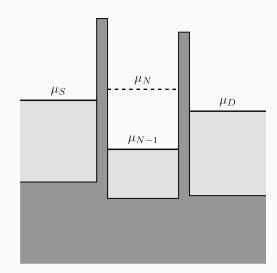
What are quantum dots?

Band diagram



 $\mu_S \gtrsim \mu_N \gtrsim \mu_D$: one electron can tunnel the barrier. The number of electrons inside the dot varies from N-1 to N. This configuration is obtain by lowering V_G , in order to increase μ_N .

BAND DIAGRAM



Variational Monte Carlo methods for quantum dots

What are quantum dots?

Band diagram



 $\mu_N>\mu_S$: 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

Variational Monte Carlo methods for quantum dots

The algorithm

THE ALGORITHM

THE VARIATIONAL PRINCIPLE

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

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

$$E_{\rm gs} \le \frac{\left\langle \psi \, \middle| \, \hat{H} \, \middle| \, \psi \right\rangle}{\left\langle \psi \, \middle| \, \psi \right\rangle}.\tag{1}$$

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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THE VARIATIONAL PRINCIPLE

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 $E_{\mathbb{R}^{4}} \le \frac{\langle \psi \mid \hat{H} \mid \psi \rangle}{\langle \psi \mid \psi \rangle}$.

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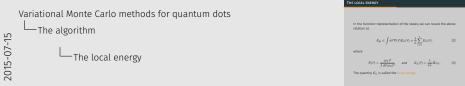
In the function-representation of the states, we can recast the above relation as

$$E_{\rm gs} \le \int d\vec{\tau} \, \mathcal{P}(\vec{\tau}) E_L(\vec{\tau}) \simeq \frac{1}{n} \sum_{i=1}^n E_L(\vec{\tau}),$$
 (2)

where

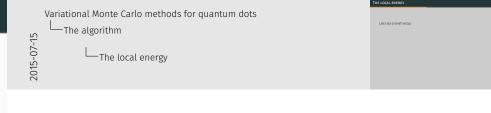
$$\mathcal{P}(\vec{\tau}) = \frac{|\psi_T|^2}{\int d\vec{\tau} \, |\psi_T|^2} \quad \text{and} \quad E_L(\vec{\tau}) = \frac{1}{\psi_T} \hat{H} \psi_T. \tag{3}$$

The quantity E_L is called the local energy.



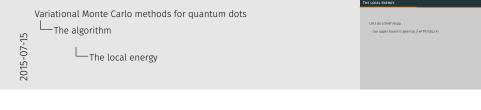
I dunno anything, fuck yeah!

Let's do a brief recap.



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· Our upper bound is given by $\int d\vec{\tau} \, \mathcal{P}(\vec{\tau}) E_L(\vec{\tau})$



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Variational Monte Carlo methods for quantum dots

The algorithm

The local energy

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- \cdot 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.

Variational Monte Carlo methods for quantum dots The algorithm

—The local energy

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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.
- But how can we achieve such a distribution of samples?

Variational Monte Carlo methods for quantum dots
—The algorithm

—The local energy

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THE LOCAL ENERGY

THE METROPOLIS ALGORITHM

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 \vec{r}^{old} . Then, we make a random move to another point in space, \vec{r}^{new} .

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

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

Variational Monte Carlo methods for quantum dots

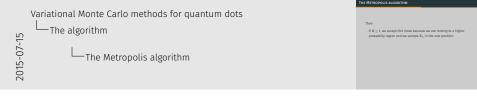
The algorithm

The algorithm

The Metropolis ALGORITHM

Then

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



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- · If $R \ge 1$, we accept this move because we are moving to a higher probability region and we sample E_L in the new position.
- · If R < 1, we can't blindly reject this move just because we are moving to a lower probability region; after all, we also have to populate the tails of the distribution! However, we can't accept all of this kind of moves.

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 < R. Otherwise, the sample is rejected.

Variational Monte Carlo methods for quantum dots

—The algorithm

The Metropolis algorithm

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Solidon generates a random number $r \in (0, 1)$, and accept the R < (0, 1), and R > 0. The remaining the sample is rejected.

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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.

This procedure is known as the brute force Metropolis algorithm.

Variational Monte Carlo methods for quantum dots

_____The algorithm

___The Metropolis algorithm

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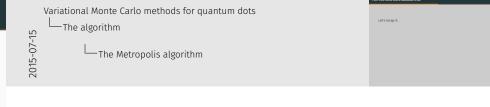
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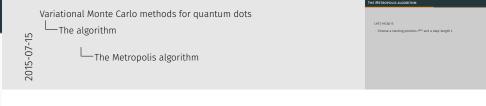
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Variational Monte Carlo methods for quantum dots

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- · Generate a new random number r in the interval (0,1).
- · If $R \geq r$, accept the step and store the position by letting $\bar{r}^{\rm old} = \bar{r}^{\rm new}$.

Variational Monte Carlo methods for quantum dots

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- · Generate a new random number r in the interval (0,1).
- · If $R \geq r$, accept the step and store the position by letting $\vec{r}^{\rm old} = \vec{r}^{\rm new}$.
- · If R < r, reject the step and discard the position by letting $ec{r}^{
 m new} = ec{r}^{
 m old}$

Variational Monte Carlo methods for quantum dots

Letting algorithm

Letting algorithm

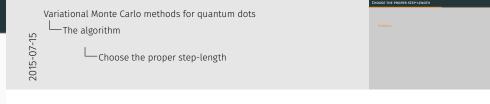
The Algorithm

The Metropolis algorithm

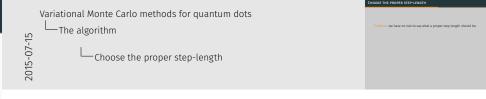
In the Algorithm

Letting and the Algorithm a

Problem:



Problem: we have no rule to say what a proper step length should be.



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Variational Monte Carlo methods for quantum dots

The algorithm

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- · If it's too much, our walker will make huge jumps all around and will sample very few points inside our distribution; the measurement will not be good.
- · If it's *too less*, our walker will wander around the starting point and will not cover all the distribution space; the measurement will not be good as well.

Variational Monte Carlo methods for quantum dots

_____The algorithm

Choose the proper step-length

CHOOSE THE PROPER STEP-LENGTH

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Solution:

CHOOSE THE PROPER STEP-LENGTH Variational Monte Carlo methods for quantum dots The algorithm 2015-07-15 If it's too less, our walker will wander around the starting point -Choose the proper step-length not be good as well.

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Solution: as a rule of thumb, one can test different step lengths and then choose the one that gives an acceptance of around 50%.

Variational Monte Carlo methods for quantum dots The algorithm

-Choose the proper step-length

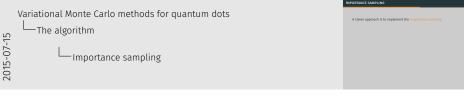
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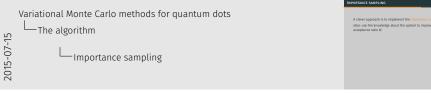
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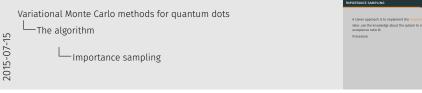
Idea: use the knowledge about the system to improve the acceptance ratio $\it R$.



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Procedure:

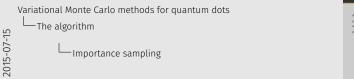


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Procedure:

· Recast the Schrödinger equation a *diffusion problem*, in which the walker is pushed in those regions where the trial wave-function is larger.



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Procedure

IMPORTANCE SAMPLING

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Procedure:

- · Recast the Schrödinger equation a *diffusion problem*, in which the walker is pushed in those regions where the trial wave-function is larger.
- · The force \vec{F} responsible for pushing the walker is called the quantum force, and can be expressed as

Variational Monte Carlo methods for quantum dots

The algorithm

Importance sampling

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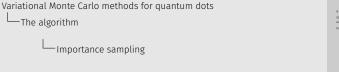
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$$\vec{F} = 2\frac{1}{\psi_T} \nabla \psi_T \tag{5}$$



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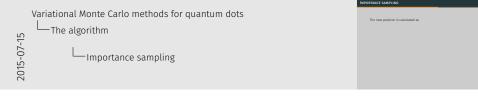
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MPORTANCE SAMPLING

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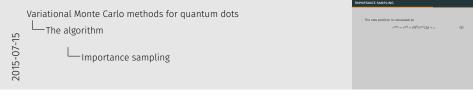
An improved acceptance ratio wastes less points.

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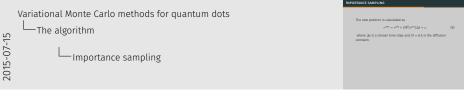
$$r^{\text{new}} = r^{\text{old}} + D\vec{F}(r^{\text{old}})\Delta t + \varepsilon,$$
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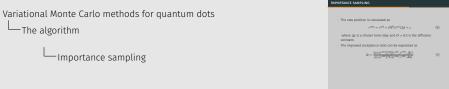
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$$R = \frac{|\psi_T(r^{\text{new}})|^2 G(r^{\text{old}}, r^{\text{new}}, \Delta t)}{|\psi_T(r^{\text{old}})|^2 G(r^{\text{new}}, r^{\text{old}}, \Delta t)}.$$
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Here, the random variable ε is no more uniform! For importance sampling, it's a *Gaussian* random variable.

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where $G(x, y, \Delta t)$ is the Green's function

$$G(y, x, \Delta t) = \frac{1}{(4\pi D\Delta t)^{3N/2}} \exp(-(y - x - D\Delta t F(x))^2 / 4D\Delta t).$$
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THE 2-ELECTRONS SYSTEM

Variational Monte Carlo methods for quantum dots

_____The 2-electrons system

THE 2-ELECTRONS SYSTEM

THE UNPERTURBED SYSTEM

Hamiltonian of the system:

Variational Monte Carlo methods for quantum dots

The 2-electrons system

The unperturbed system

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

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 $n = n_x + n_y$.

$$\hat{H}_0 = \sum_{i=1}^2 \left(-\frac{1}{2} \nabla_i^2 + \frac{1}{2} \omega^2 r_i^2 \right),\tag{9}$$

Variational Monte Carlo methods for quantum dots

The 2-electrons system

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$$E_s = \hbar\omega(n_x + n_y + 1). \tag{10}$$

Variational Monte Carlo methods for quantum dots

The 2-electrons system

The unperturbed system



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THE UNPERTURBED SYSTEM

Configuration:

Variational Monte Carlo methods for quantum dots

The 2-electrons system

The unperturbed system

The factor 2 in the ground-state energy stems from the fact that we have two particles in the ground state (spin degeneracy).

C is a normalization constant.

Configuration:





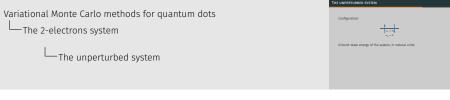
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Ground-state energy of the system, in natural units:



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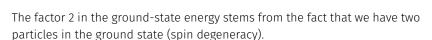
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$$E_{\rm gs} = 2\omega. \tag{11}$$

Variational Monte Carlo methods for quantum dots

The 2-electrons system

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Exact wave-function:

Variational Monte Carlo methods for quantum dots

The 2-electrons system

The unperturbed system

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$$n_x = 0$$

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

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Exact wave-function:

$$\phi(\vec{r}_1, \vec{r}_2) = C \exp\left(-\omega \left(r_1^2 + r_2^2\right)/2\right). \tag{12}$$

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Variational Monte Carlo methods for quantum dots

The 2-electrons system

The unperturbed system

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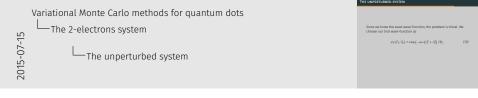
 ${\cal C}$ is a normalization constant.

Since we know the exact wave-function, the problem is trivial. We choose our trial wave-function as



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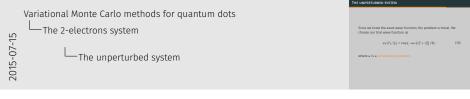
$$\psi_T(\vec{r}_1, \vec{r}_2) = \exp(-\alpha\omega(r_1^2 + r_2^2)/2).$$
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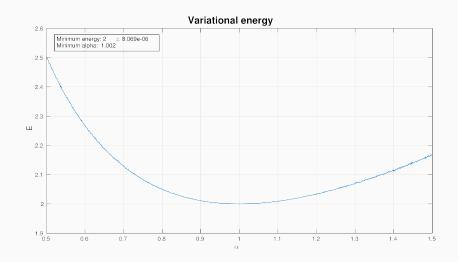
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For $\alpha=1$ we expect to obtain a variational energy exactly equal to the ground state energy $E_{\rm gs}=2\omega$.





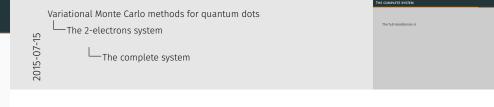


Variational Monte Carlo methods for quantum dots The 2-electrons system

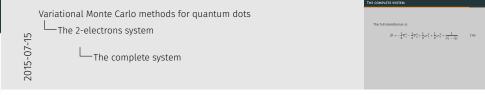
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The variational energy versus the variational parameter α . The settings used are: brute force sampling with step length 2, no Jastrow factor, no parallelization, 1000 variations of α around 1 with step 0.001, 1×10^7 Monte Carlo steps. Acceptance ratio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

The full Hamiltonian is



$$\hat{H} = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 + \frac{1}{2}\omega r_1^2 + \frac{1}{2}\omega r_2^2 + \frac{1}{|\vec{r_1} - \vec{r_2}|}.$$
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Problem:

Variational Monte Carlo methods for quantum dots

The 2-electrons system

The complete system

The complete system

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Problem: the term

$$\frac{1}{|\vec{x}-\vec{x}|} \tag{15}$$

could be a division by zero.

Variational Monte Carlo methods for quantum dots

The 2-electrons system $\begin{aligned}
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could be a division by zero.

Solution: add, in the wave-function, a factor that cancels the divergence in the Hamiltonian.

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The complete system

The extra factor is usually modeled as

In two dimensions

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

$$\exp\left(\frac{ar}{(1+\beta r)}\right) \tag{17}$$

Variational Monte Carlo methods for quantum dots

The 2-electrons system

The complete system

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that is called the Padé-Jastrow factor.

Variational Monte Carlo methods for quantum dots

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a is a parameter that depends on the spin, while β is a $\emph{variational parameter}.$

Variational Monte Carlo methods for quantum dots

The 2-electrons system

The complete system

The complete system

The complete system

In two dimensions

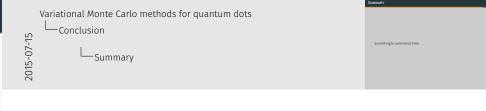
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CONCLUSION

Variational Monte Carlo methods for quantum dots —Conclusion

CONCLUSION

Something to summarize here.



QUESTIONS?

Variational Monte Carlo methods for quantum dots —Conclusion