VARIATIONAL MONTE CARLO METHODS FOR QUANTUM DOTS

Matteo Seclì

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University of Trento – Department of Physics

Contents

WHAT ARE QUANTUM DOTS?

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The term "quantum dots" refers to finite fermion systems consisting of an artificial 3D confinement of a few electrons, that have a size of only a few hundred angstroms.

Although this definition is quite precise, I prefer a more immediate one: "quantum dots are *artificial atoms*". Despite its simplicity, this definition contains a good amount of relevant information. Like natural atoms, in fact, quantum dots are made up of electrons confined in an attractive potential; and as one may guess, they show a similar shell-like structure with its relative *magic numbers*.

Such confinement is usually achieved by restricting the two-dimensional electron gas that forms at the interface between two different semiconductor materials (or heterostructure), either laterally or vertically.

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Building technique: stack up different layers of semiconductor materials.

Quantum dots are built by stacking up different layers of semiconductors. The electron gas forms at the interface of different layers, and the confinement is obtained by applying a voltage to the top metal electrodes – called *gates*. In the Figure, the white bars have a length of 0.5 μm.; so, the gates are created by lithographic patterning.

Another common method to fabricate quantum dots is to build heterostructure pillars by etching techniques. Here, the electrodes are at the top and at the bottom of the pillars.

Other fabricating processes include self-growth mechanisms, in which the growth conditions determine the form of the structure (that can be pyramidal, disk shaped or lens shaped), and cleaved-edge overgrowth, that consists in two separate Molecular Beam Epitaxy growths on a specific substrate.

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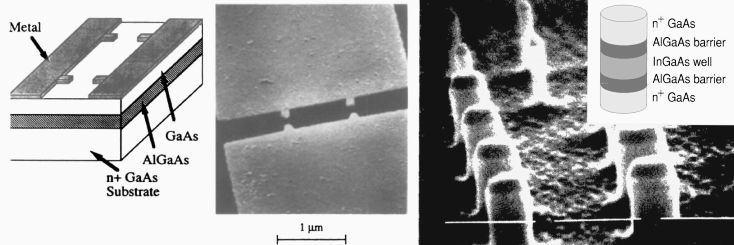Building technique: stack up different layers of semiconductor materials.

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(a) Lateral quantum dot.   (b) Etched quantum dots.

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The Variational Principle is a method of general validity that can be used to gather information about a system with a Hamiltonian that we are unable to diagonalize. Specifically, this principle gives us an *upper bound* for the energy of the ground state. The formulation is really simple: if you pick *any state $|\psi\rangle$ whatsoever*, then SHOW FORMULA ON SLIDE.

In practice, one chooses a class of states for $|\psi\rangle$ parametrized by one or more parameters – the so-called *variational parameters*, and then calculates the quantity E_T for multiple sets of values of the variational parameters $\alpha_1 \ldots, \alpha_n$. The lower value of E_T obtained in this way is the required upper bound. If one manages to find an even lower value for E_T with a more clever wave-function, then he has found a better upper bound for the ground state energy.

The only trouble with this method is that we never know for sure how close we are to the *actual* ground state energy; all we get for sure is just an upper bound. However, if one manages to guess a *realistic $|\psi\rangle$*, he often gets values for the ground state energy that miraculously match the actual ones.

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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.

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The quantity E_L is called the local energy.

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· But how can we achieve such a distribution of samples?

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

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This procedure is known as the brute force Metropolis algorithm.

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- If $R < r$, reject the step and discard the position by letting $\vec{r}^{\text{new}} = \vec{r}^{\text{old}}$.

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An improved acceptance ratio wastes less points. A better approach is to implement the *Importance sampling*, that consists in doing more clever assumptions on the shape of the transition probability.

Since we know the system we are working on, we know that if we recast the Schrödinger equation as a diffusion problem, the transition probability is going to be a Gaussian distribution (or a modified Gaussian).

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READ THE NEW POSITION.

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IMPORTANCE SAMPLING

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$$G(y, x, \Delta t) = \frac{1}{(4\pi D\Delta t)^{3N/2}} \exp(-(y - x - D\Delta t F(x))^2/4D\Delta t). \tag{8}$$

THE 2-ELECTRONS SYSTEM

Hamiltonian of the system:

Let's apply this algorithm to two electrons in an harmonic oscillator, without the electron-electron repulsion.

The unperturbed Hamiltonian is SHOW THE HAMILTONIAN.

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, and this causes a degeneracy in the energy levels. The principal quantum number is $n = n_x + n_y$.

For a single electron in a 2D harmonic potential, the energy can be expressed as SHOW THE ENERGY.

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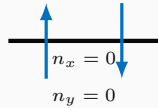For a single electron in a 2D harmonic potential, the energy can be expressed as SHOW THE ENERGY.

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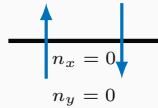
Configuration:

This is the configuration of the system.

You see that the spatial parts of the wave-functions are equal because of the spin degeneracy, so the ground state energy of the complete system has a factor of 2 to take this thing into account.

For the same reason, the exact wave-function (or at least, its spatial part) can be expressed as the product of the single-particle wave-functions.

C is a normalization constant.

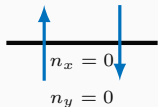Configuration:

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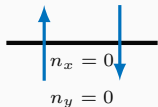Ground-state energy of the system, in natural units:

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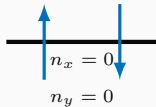
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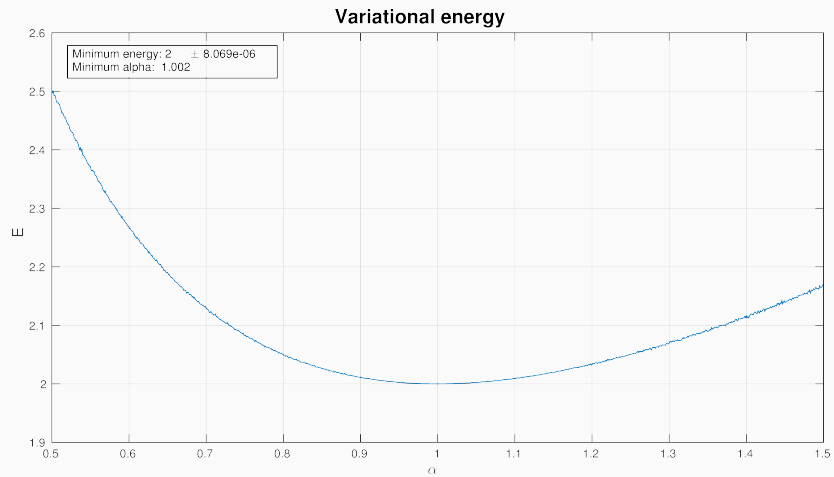
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The variational energy versus the variational parameter α. The settings used are: brute force sampling with step length 2, no Jastrow factor, no parallelization, 1000 variations of α around 1 with step 0.001, 1×10^7 Monte Carlo steps. Acceptance ratio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

Variational energy

Minimum energy: 2 $\pm$ 8.069e-06
Minimum alpha: 1.002

The full Hamiltonian is

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

The extra factor is usually modeled as

An extra factor to the non-interacting wave-function is added, that has the form READ THE SLIDE.

In two dimensions

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

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

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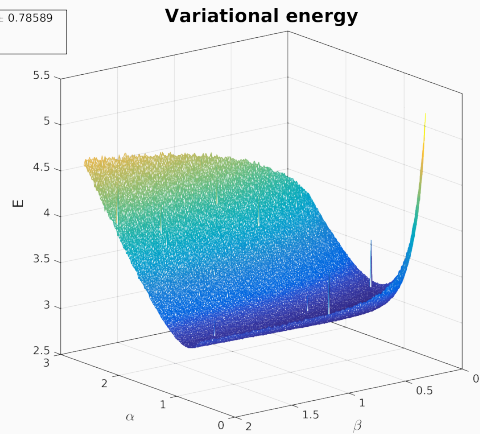
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The variational energy versus the variational parameters α and β. The settings used are: brute force sampling with step length 2, Jastrow factor, no parallelization, 200 variations of α and β with step 0.01, 1×10^5 Monte Carlo steps. Acceptance ratio varies from 45 to 55 %.
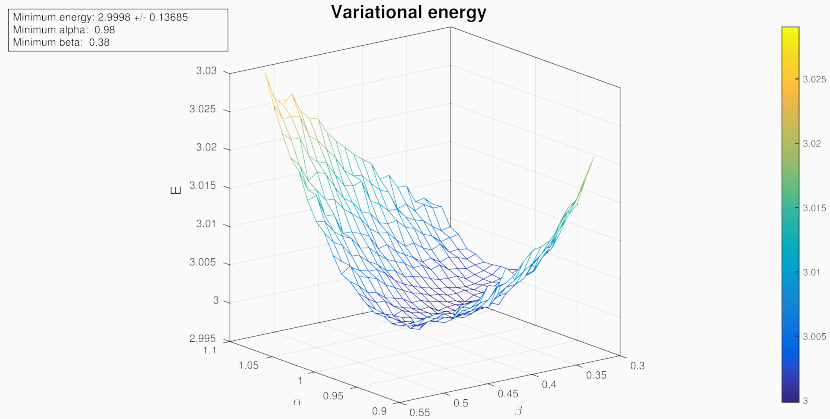
Minimum energy: 2.9985 ± 0.78589
Minimum alpha: 1.02
Minimum beta: 0.36

Variational energy

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.

Variational energy

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

Parallelization

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

Despite the fact that we have very good values, you see that the error is still quite large.

We can improve it by taking multiple measurements at each point of the grid, and then take the mean. If we do that, the error falls like the $1/\sqrt{n}$ and we can obtain more precise energy values even with less Monte Carlo steps.

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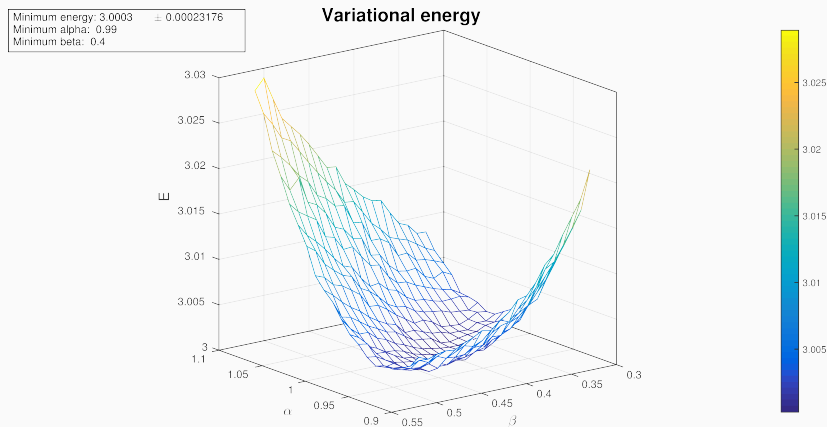
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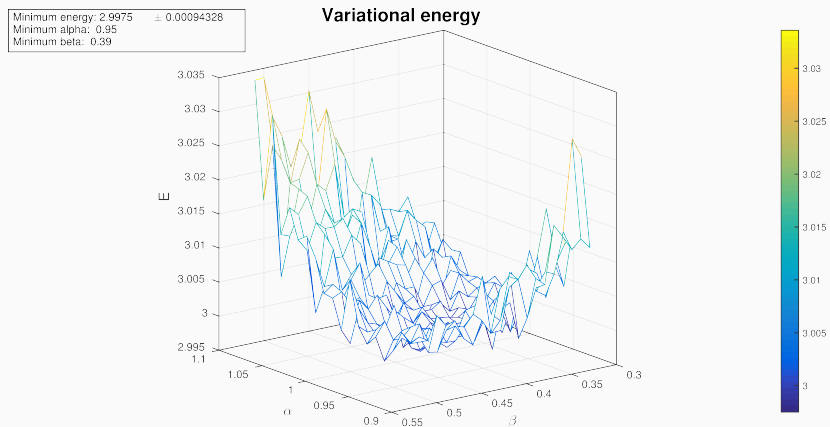
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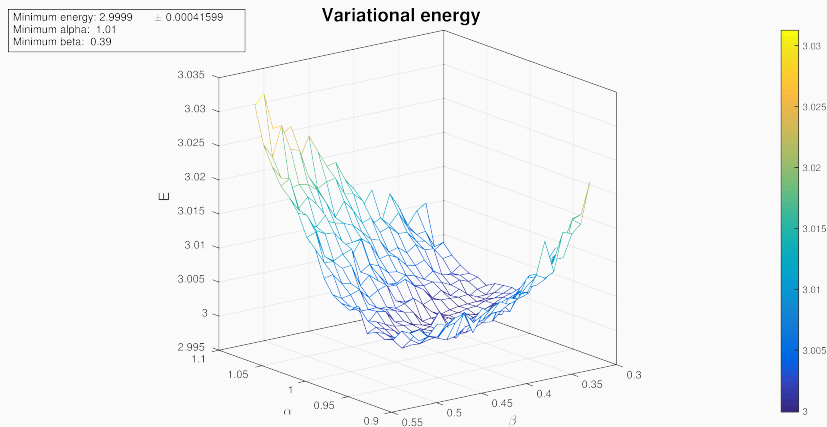
The variational energy versus the variational parameters α and β. The settings used are: importance sampling with $\Delta t = 0.001$, Jastrow factor, parallelization (8 threads), 20 variations of α and β with step 0.01, 2×10^5 Monte Carlo steps. Acceptance ratio is about 99.999 %.

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

Variational energy

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Minimum energy: 2.9999   ± 0.00041599
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Variational energy

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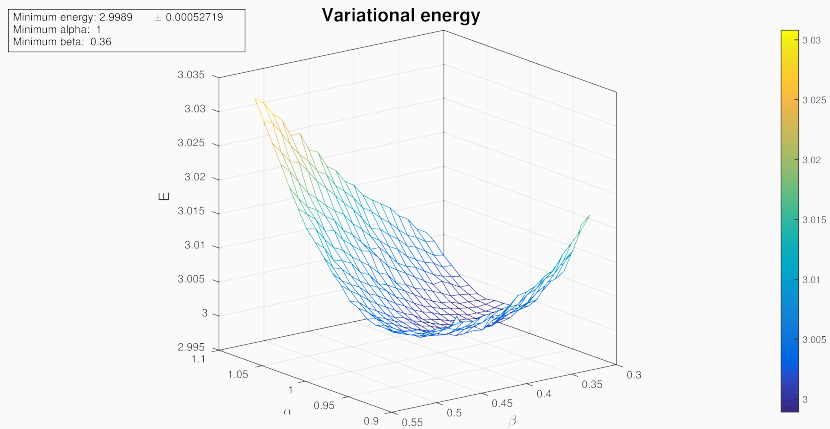
THE 6-ELECTRONS SYSTEM

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Recall that, for 2-electrons, the wave-function had this form. That is, it was the product among the single-particle wave-functions and a repulsion factor called the Jastrow factor.

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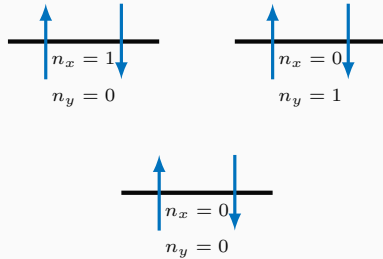
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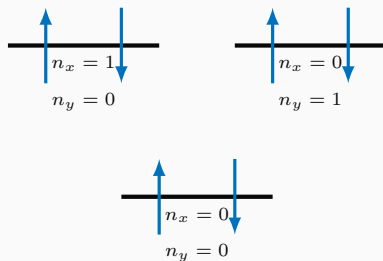
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Now, let's take a look at the configuration of the system. You see that we are free to label the particles in whatever way we want; for example, we can say that (INDICATE ALL SPIN UP) this is particle 1, this is particle 2 and this is particle 3, and the others are numbered accordingly. If we do that, we can split the Slater determinant into two smaller determinants; one for spin-up particles, and one for spin-down particles.

SHOW NEXT SLIDE WITHOUT COMMENTS.

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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.

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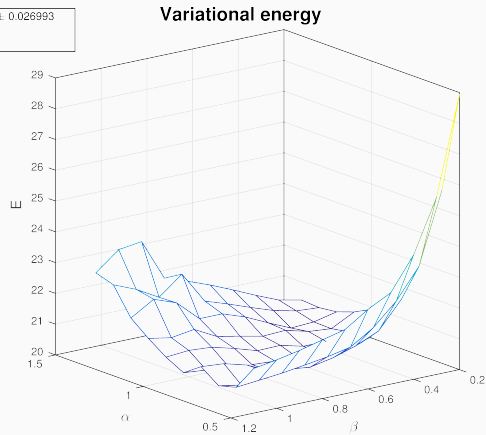
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and J is the Jastrow factor.

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..

CONCLUSION

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· Thanks for your attention!

Questions?