VARIATIONAL MONTE CARLO METHODS FOR QUANTUM DOTS
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July 2015
University of Trento – Department of Physics

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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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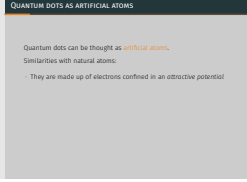

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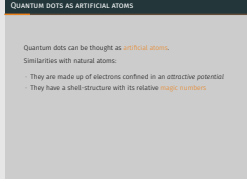

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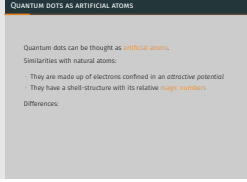

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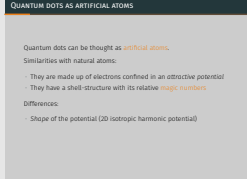

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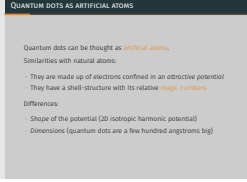

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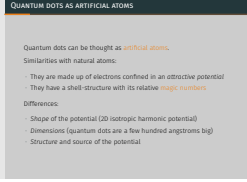

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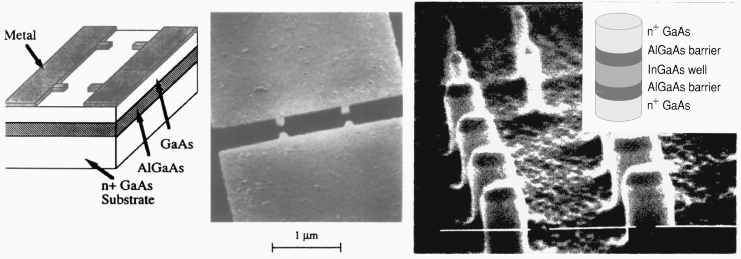

(a) Lateral quantum dot. (b) Etched quantum dots.

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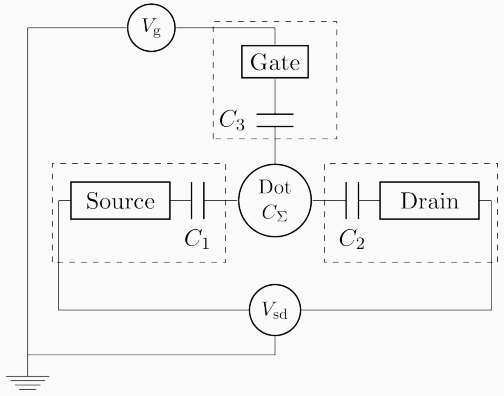

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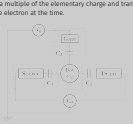

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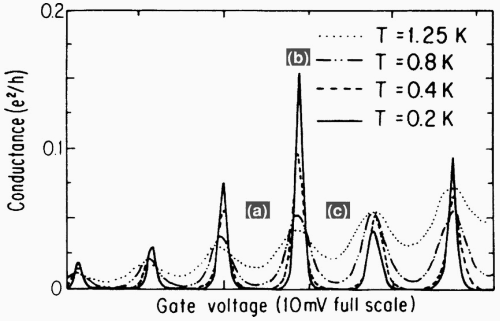

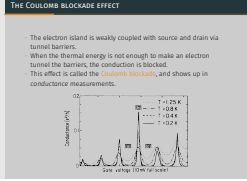

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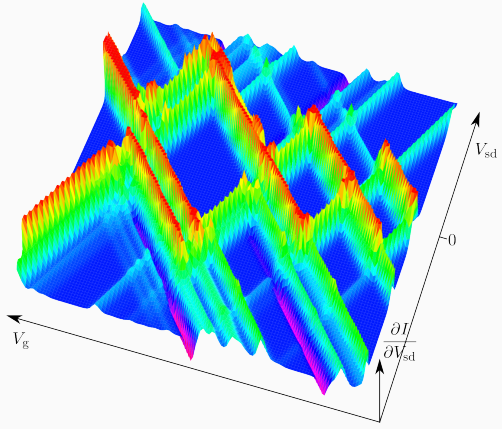
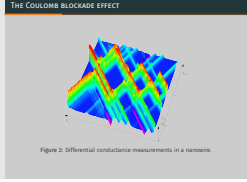
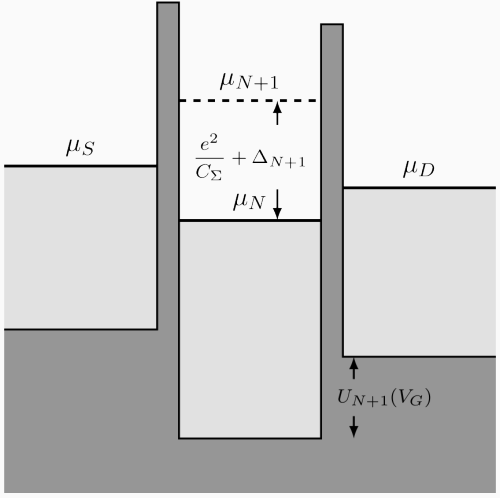
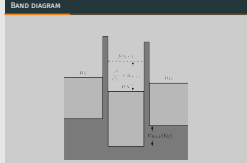


Figure 2: Differential conductance measurements in a nanowire.



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.

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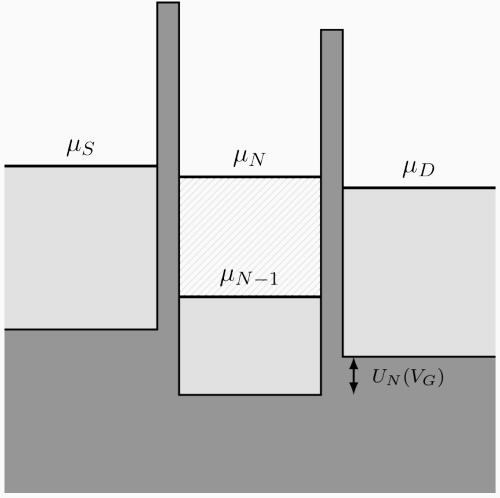

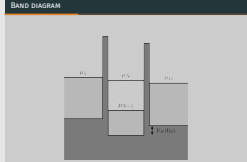

$\mu_S \gtrsim \mu_N \gtrsim \mu_D$: one electron can tunnel the barrier. The number of electrons inside the dot varies from $N-1$ to N. This configuration is obtain by lowering V_G, in order to increase μ_N.

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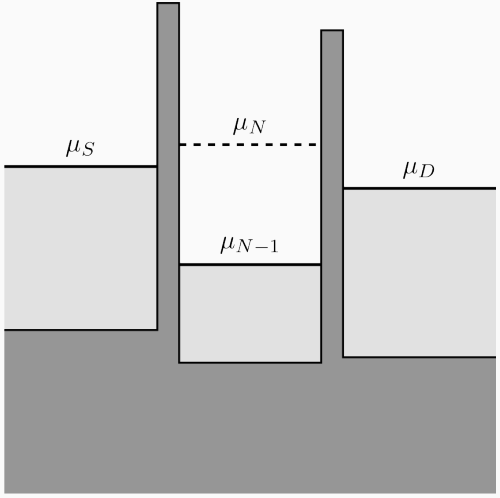

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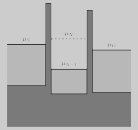

$\mu_N > \mu_S$: the transport is blocked again due to the Coulomb blockade. The number of electrons inside the dot is $N - 1$. This situation is obtained by further lowering V_G.

THE ALGORITHM

The variational principle

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

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

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.

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The local energy

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

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

where

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

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I dunno anything, fuck yeah!

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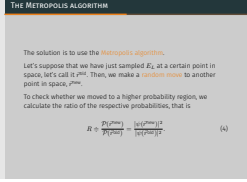
The Metropolis algorithm

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

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

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



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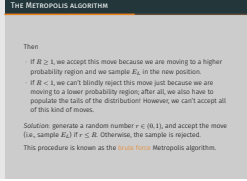
- If $R < 1$, we can't blindly reject this move just because we are moving to a lower probability region; after all, we also have to populate the tails of the distribution! However, we can't accept all of this kind of moves.

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.



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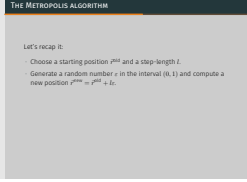

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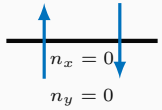

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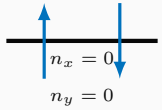

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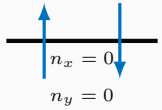

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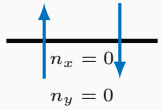

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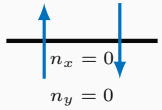

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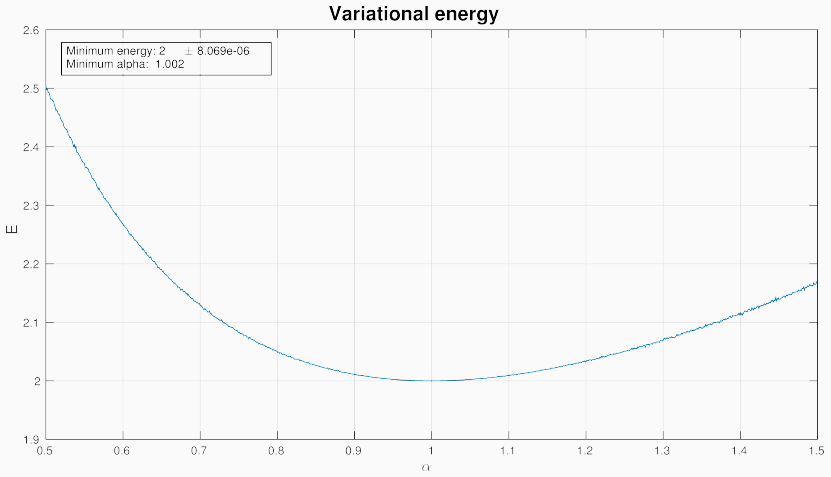

The variational energy versus the variational parameter α. The settings used are: brute force sampling with step length 2, no Jastrow factor, no parallelization, 1000 variations of α around 1 with step 0.001, 1×10^7 Monte Carlo steps. Acceptance ratio varies from 40 to 60 %.

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CONCLUSION

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Questions?