

*La simulation du courant et du bruit dans  
les composants quantiques:  
Méthode des trajectoires de Bohm pour  
l'étude des interactions entre les électrons*

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**I.- Introduction:** *“La simulation du courant et du bruit  
dans les composants quantiques”*

**II.- Our approach:** *“Méthode des trajectoires de Bohm pour  
l'étude des interactions entre les électrons”*

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**JOURNÉES "SIMULATION ET CARACTÉRISATION  
DES NANOCOMPOSANTS"**



Universitat  
Autònoma  
de Barcelona

## Outline of the talk:

### I.- Introduction: *“La simulation du courant et du bruit dans les composants quantiques”*

I.1.- From the “many-particle” to the “single-particle” Schrödinger equation.

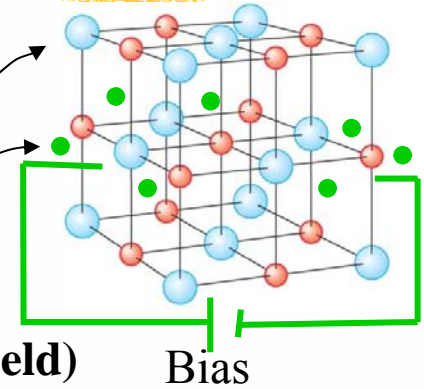
I.2.- The computation of DC/AC and noise current in quantum devices.

### II.- Our approach: *“Méthode des trajectoires de Bohm pour l'étude des interactions entre les électrons”*

# I.1.- From the “many-particle” to the “single-particle” Schrödinger equation

## ▶ Many-particle Schrödinger equation:

$$i\hbar \frac{\partial \Psi_T(\bar{r}_1, \bar{r}_2, \dots, \bar{R}_1, \bar{R}_2, \dots, t)}{\partial t} = \hat{H}_T \cdot \Psi_T(\bar{r}_1, \bar{r}_2, \dots, \bar{R}_1, \bar{R}_2, \dots, t)$$



## ▶ Full Hamiltonian (spinless electrons, no magnetic field)

kinetic energy of the electrons    kinetic energy of the atoms    electron-electron coulomb interaction

$$\hat{H}_T = \left\{ \sum_k \left( -\frac{\hbar^2}{2m_0} \nabla_k^2 \right) + \sum_g \left( -\frac{\hbar^2}{2M_g} \nabla_g^2 \right) + \frac{1}{2} \sum_k \sum_{j \neq k} \frac{q^2}{4\pi \epsilon \epsilon_0 r_{kj}} \right.$$

$$\left. + U_0(\bar{R}_1, \bar{R}_2, \bar{R}_3, \dots) + \sum_k U_C(\bar{r}_k, \bar{R}_1, \bar{R}_2, \bar{R}_3, \dots) + \sum_k U_E(\bar{r}_k) + \sum_g U'_E(\bar{R}_g) \right\}$$

atom-atom coulomb interaction

electron-atom coulomb interaction

electron-potential due to external bias

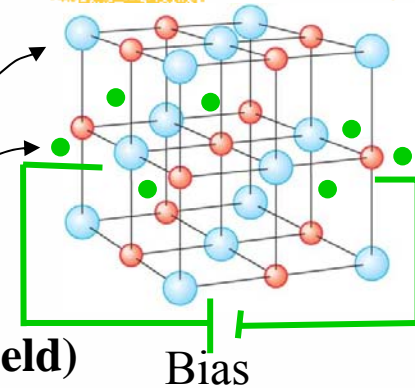
atom potential due to external bias

# I.1.- From the “many-particle” to the “single-particle” Schrödinger equation

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## ▶ Many-particle Schrödinger equation:

$$i\hbar \frac{\partial \Psi_T(\bar{r}_1, \bar{r}_2, \dots, \bar{R}_1, \bar{R}_2, \dots, t)}{\partial t} = \hat{H}_T \cdot \Psi_T(\bar{r}_1, \bar{r}_2, \dots, \bar{R}_1, \bar{R}_2, \dots, t)$$



## ▶ Full Hamiltonian (spinless electrons, no magnetic field)

$$\hat{H}_T = \left\{ \sum_k \left( -\frac{\hbar^2}{2m_0} \nabla_k^2 \right) + \sum_g \left( -\frac{\hbar^2}{2M_g} \nabla_g^2 \right) + \frac{1}{2} \sum_{k \neq j} \sum_j \frac{q^2}{4\pi \epsilon \epsilon_0 r_{kj}} \right. \\ \left. + U_0(\bar{R}_1, \bar{R}_2, \bar{R}_3, \dots) + \sum_k U_C(\bar{r}_k, \bar{R}_1, \bar{R}_2, \bar{R}_3, \dots) + \sum_k U_E(\bar{r}_k) + \sum_g U'_E(\bar{R}_g) \right\}$$

## ▶ Numerical viability of solving the many-particle Schrödinger equation ?

For a 3D system with N=100 electrons, L=100nm length (with Δx=0.1 nm)

n° of variables in 3D = 1000<sup>3N</sup> ~ 10<sup>1000</sup> variables !!!!!!!

# I.1.- From the “many-particle” to the “single-particle” Schrödinger equation

▶ **1<sup>st</sup> approximation:**

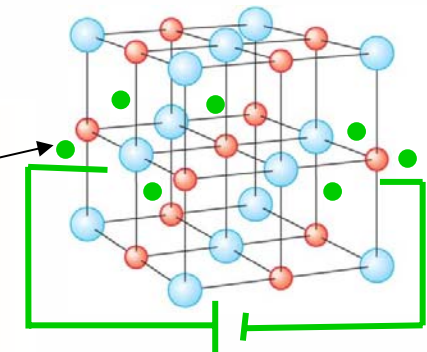
**Born-Oppenheimer approximation** (being the mass of the atoms much larger than the mass of electrons, we can assume they are always at rest at the electronic time scale).

$$\hat{H}_T = \left\{ \sum_k \left( -\frac{\hbar^2}{2m_0} \nabla_k^2 \right) + \sum_g \left( -\frac{\hbar^2}{2M_g} \nabla_g^2 \right) + \frac{1}{2} \sum_{k \neq j} \sum_j \frac{q^2}{4\pi \epsilon \epsilon_0 r_{kj}} \right. \\ \left. + U_0(\bar{R}_1, \bar{R}_2, \bar{R}_3, \dots) + \sum_k U_C(\bar{r}_k, \bar{R}_1, \bar{R}_2, \bar{R}_3, \dots) + \sum_k U_E(\bar{r}_k) + \sum_g U_F(\bar{R}_g) \right\}$$

**The suppressed terms can be included later, perturbatively, as a phonon scattering.**

**Many-particle Schrodinger equation:**

$$i\hbar \frac{\partial \Psi_T(\bar{r}_1, \bar{r}_2, \dots, t)}{\partial t} = \hat{H}_T \cdot \Psi_T(\bar{r}_1, \bar{r}_2, \dots, t)$$



X.Oriols, UAB Spain

# I.1.- From the “many-particle” to the “single-particle” Schrödinger equation

▶ **2<sup>nd</sup> approximation:**

**Effective-mass approximation** (for infinite structures, only one band involved, and a parabolic dispersion, then, the atom-electron interaction is included into an “effective” value of the electron mass).

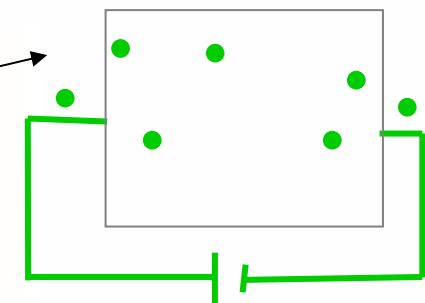
$$\hat{H} = \left\{ \sum_k \left( -\frac{\hbar^2}{2m_0^*} \nabla_k^2 \right) + \frac{1}{2} \sum_{k \neq j} \sum_j \frac{q^2}{4\pi\epsilon\epsilon_0 r_{kj}} + \sum_k U_C(\bar{r}_k, \bar{R}_1, \bar{R}_2, \bar{R}_3, \dots) + \sum_k U_E(\bar{r}_k) \right\}$$

**This was an important simplification and it used to divide the study of a system of electrons between those involved in:**

- (i) Electron band-structure** + **(ii) Electron transport**

**Many-particle Schrödinger equation:**

$$i\hbar \frac{\partial \Psi(\bar{r}_1, \bar{r}_2, \dots, \bar{r}_N, t)}{\partial t} = \hat{H} \cdot \Psi(\bar{r}_1, \bar{r}_2, \dots, \bar{r}_N, t)$$



X.Oriols, UAB Spain

# I.1.- From the “many-particle” to the “single-particle” Schrödinger equation

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## ▶ 3<sup>rd</sup> approximation:

**Mean-field approximation** (the term of the Coulomb interaction among electrons is changed by an average potential)

$$\hat{H} = \left\{ \sum_k \left( -\frac{\hbar^2}{2m^*} \nabla_k^2 \right) + \cancel{\frac{1}{2} \sum_{k \neq j} \sum_j \frac{q^2}{4\pi\epsilon\epsilon_0 r_{kj}}} + \sum_k U_E(\bar{r}_k) \right\} = \sum_i H_i$$

$\sum_k U_{coul}(\bar{r}_k)$

↑

**The total Hamiltonian is just a sum of single-particle Hamiltonian.  
But there is still another source of correlation between electrons.**



# I.1.- From the “many-particle” to the “single-particle” Schrödinger equation

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▶ 4<sup>th</sup> approximation:

**For electrons, only antisymmetrical wave-functions are valid**

$$i\hbar \frac{\partial \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N, t)}{\partial t} = \hat{H} \cdot \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N, t) \quad \Rightarrow \quad \Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \dots, t) = -\Psi(\vec{r}_2, \vec{r}_1, \vec{r}_3, \dots, t)$$

$$\text{if } \vec{r}_1 = \vec{r}_2 = \vec{r}_o \Rightarrow \Psi(\vec{r}_o, \vec{r}_o, t) = -\Psi(\vec{r}_o, \vec{r}_o, t)$$

$$\Psi(\vec{r}_o, \vec{r}_o, t) = 0$$



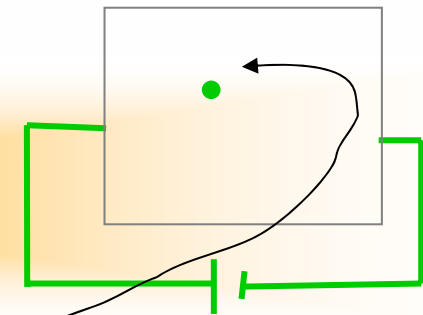
**Pauli exclusion principle**

**No exchange-interaction** (a multiplicative wave-function is assumed)

$$\Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \dots, \vec{r}_N, t) = \Psi_1(\vec{r}_1, t) \cdot \Psi_2(\vec{r}_2, t) \cdot \Psi_3(\vec{r}_3, t) \dots \Psi_N(\vec{r}_N, t)$$

**Single-particle Schrödinger equation (no correlations):**

$$i\hbar \frac{\partial \Psi_i(x, t)}{\partial t} = \hat{H}_i \cdot \Psi_i(x, t) = \left\{ -\frac{\hbar^2}{2 \cdot m_x^*} \frac{\partial^2}{\partial x^2} + U_E(x) \right\} \Psi_i(x, t)$$





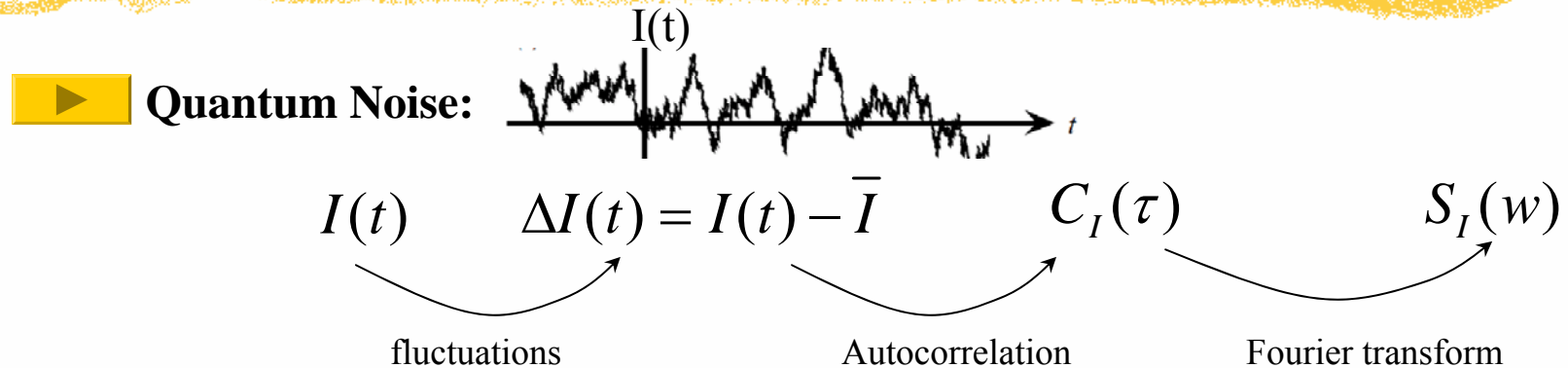
# I.2.- The computation of DC/AC and noise in quantum devices

► Computation of DC current in quantum systems

		Quantum function			Approximations				Name
		Schrö	Wigner	Green	Born- Oppen.	Effective- mass	Mean field	No exchange	
Transport		●			●	●	●	●	Landauer method
			●		Perturbative	●	●	●	Wigner distribution
				●	Perturbative	●	●	●	Non-Equil. Green Funct.
		●			Buttiker probes	●	●	Second quantization	Buttiker method
Band structure		●		●	Perturbative	Pseudo	●	●	k.p method
		●		●	Perturbative	Pseudo	●	●	Tight-binding method
		●		●	●	Ab initio	Ab initio	Ab initio	Dens Func Theory
				●	Perturbative	Ab initio	Ab initio	Ab initio	Time Dependent DFT

## I.2.- The computation of DC/AC and noise in quantum devices

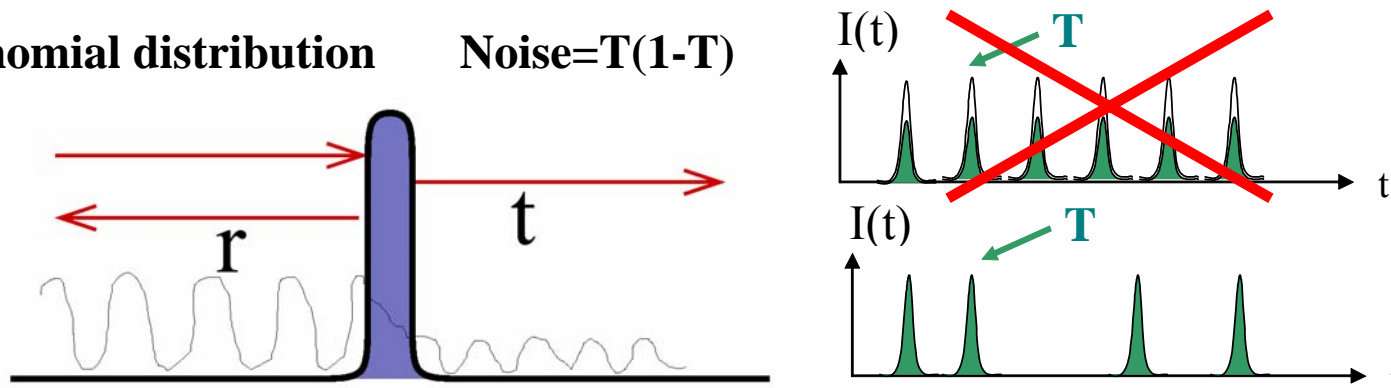
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► **Example: Partition noise due to the tunneling probability**

Binomial distribution

Noise =  $T(1-T)$



**Electrons are transmitted or reflected, but not both !**

**The noise measured by the amperimeter takes into account the wave and the particle nature of electrons.**

## I.2.- The computation of DC/AC and noise in quantum devices

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### ► Computation of noise in quantum systems

	Quantum function			Approximations			Name	
	Schrö	Wigner	Green	Born- Oppen.	Effective- mass	Mean field		No exchange
Transport	●		●	Perturbative	●	●	Second quantization	Full counting statistics
			●	Perturbative	●	●	Second quantization	Non-equil. Green funct.
	●			Buttiker probes	●	●	Second quantization	Buttiker method

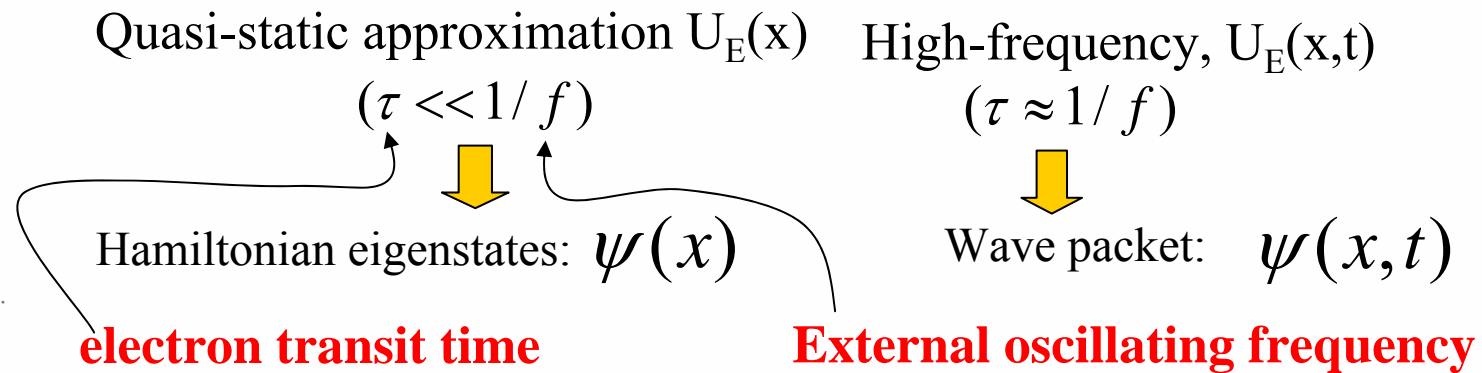
### ► Mixed techniques

Example, Once you know the Noise expression, for example,  $T(1-T)$ , you compute  $T$  with approaches for DC current

## I.2.- The computation of DC/AC and noise in quantum devices

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### ▶ Quantum high-frequency effects (“Driven Tunneling”):



### ▶ Displacement current (Maxwell equations):

**The amperimeter measures the particle (conduction) current plus the displacement current !!**

$$\vec{\nabla} \times \vec{H} = \vec{J}_c + \partial \vec{D} / \partial t \quad \Rightarrow \quad \vec{\nabla} \cdot (\vec{J}_c + \partial \vec{D} / \partial t) = 0$$

Continuity equation

$$\vec{\nabla} \cdot \vec{D} = \rho \quad \Rightarrow \quad \text{Poisson equation}$$

$$\partial \rho / \partial t + \vec{\nabla} \cdot \vec{J}_c = 0$$

**A time-dependent self-consistent Schrödinger and Poisson solver !!**

# I.2.- The computation of DC/AC and noise in quantum devices

▶ **Computation of time-dependent current in quantum systems**

Assume a quasi-static approximation

Computation of current with DC models and some capacitive coupling

	Quantum function			Approximations				Name
	Schrö	Wigner	Green	Born- Oppen.	Effective- mass	Mean field	No exchange	
Transport	●			●	●	●	●	Non-periodic potentials
		●	●	Perturbative	●	●	●	Wigner / Green funct.
	●		●	Perturbative	●	●	Second quantization	Floquet theory

## Outline of the talk:

I.- Introduction: *“La simulation du courant et du bruit dans les composants quantiques”*

II.- Our approach: *“Méthode des trajectoires de Bohm pour l'étude des interactions entre les électrons”*

II.1.- Single-particle Bohm trajectories.

II.2.- Many-particle Bohm trajectories

II.3.- Our quantum Monte Carlo approach

II.4.- Numerical results

## II.- Our approach: “*Méthode des trajectoires de Bohm pour l’étude des interactions entre les électrons*”

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Most of the quantum electron transport in nanoelectronic devices is understood under a non-interacting (Fermi liquid) picture.

**Our goal: Go beyond the non-interacting (Fermi liquid) pattern, to develop a formalism that introduces Coulomb and exchange interactions (correlations) among electrons.**

Quantum function			Approximations				Name
Schor	Wigner	Green	Born-Oppen.	Effective-mass	Mean field	No exchange	
●			●	●	Exact.	Exact.	Many-particle Bohm traj.

**We extract quantum trajectories from the Schrödinger equation**



# II.1.- Single-particle Bohm trajectories

**▶ A simple mathematical development**

[D. Bohm, Phys. Rev, 1952 ]

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \left\{ -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x^2} + U(x,t) \right\} \Psi(x,t)$$

**Polar form**



$$\Psi(x,t) = R(x,t) \cdot \exp(iS(x,t)/\hbar)$$

$$\frac{\partial S}{\partial t} + \frac{(\partial S / \partial x)^2}{2m^*} + U(x,t) + Q(x,t) = 0$$

**Quantum potential**

$$Q(x,t) = -\frac{1}{R(x,t)} \left( \frac{\hbar^2 \partial^2 R(x,t) / \partial x^2}{2m^*} \right)$$

**Hamilton-Jacobi equation**

$$\frac{\partial S}{\partial t} + H(\partial S / \partial x, x, t) = 0$$

**Newton-like equation**

$$\frac{d^2 x(t)}{dt^2} = -\frac{\partial}{\partial x} (U(x,t) + Q(x,t)) \Big|_{x=x(t)}$$

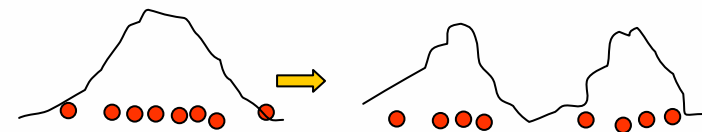
$$\frac{\partial R^2(x,t)}{\partial t} + \frac{\partial}{\partial x} \left( R^2(x,t) \cdot \frac{\partial S(x,t) / \partial x}{m^*} \right) = 0$$

**Current density**

$$J(x,t) = R^2(x,t) \cdot \frac{\partial S(x,t) / \partial x}{m^*}$$

**Continuity equation**

$$\frac{\partial R^2(x,t)}{\partial t} + \frac{\partial}{\partial x} (J(x,t)) = 0$$



# II.1.- Single-particle Bohm trajectories



Example: Plane wave  $\Psi(x,t) \propto \exp(ik \cdot x)$



$$v(x,t) = \frac{\hbar}{m} \cdot \frac{\partial(k \cdot x)}{\partial x} = \frac{\hbar k}{m}$$



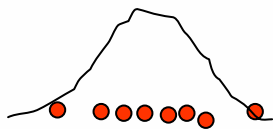
Example: double barrier

Equation of Motion:

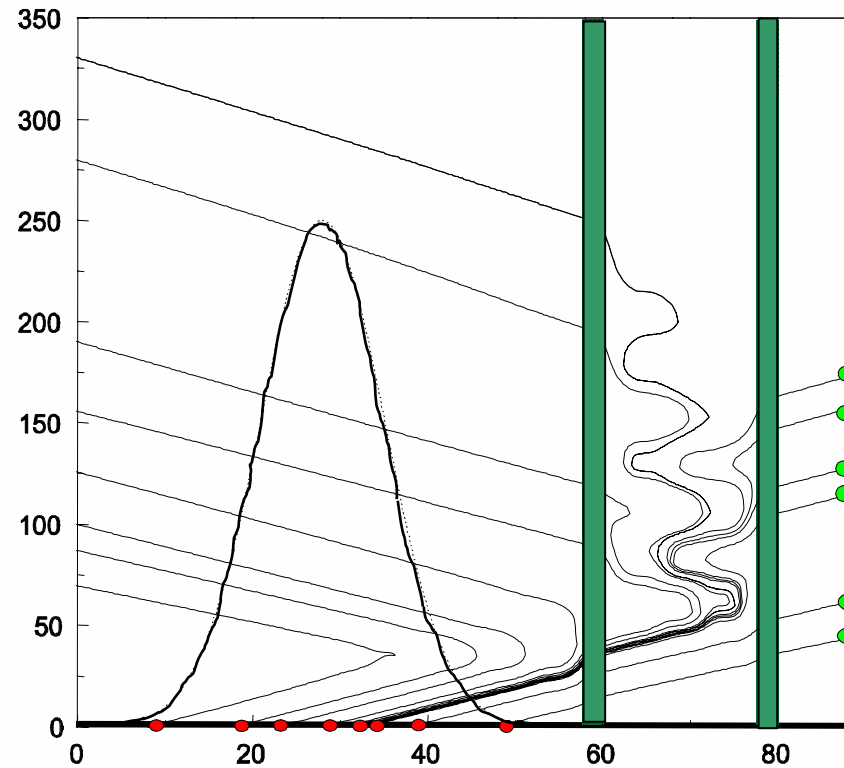
$$\psi(x,t) \downarrow v(x,t) = \frac{1}{m} \frac{\partial S(x,t)}{\partial x}$$

$$x(t) = x(t_0) + \int_{t_0}^t v(x(t),t) \cdot dt \quad \rightarrow$$

Quantum uncertainty



Time (fs)



Continuity equation:

$$\frac{\partial R^2(x,t)}{\partial t} + \frac{\partial}{\partial x} (J(x,t)) = 0$$

Distance (nm)

[X.Oriols *et al.* S.S.C. 1996 ]

## II.2.- Many-particle Bohm trajectories

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### ▶ N particles in 3D space

$$i\hbar \frac{\partial \Psi(\vec{r}_1, \dots, \vec{r}_N, t)}{\partial t} = \left\{ \sum_{k=1}^N \left( -\frac{\hbar^2}{2m^*} \nabla_k^2 \right) + U(\vec{r}_1, \dots, \vec{r}_N, t) \right\} \Psi(\vec{r}_1, \dots, \vec{r}_N, t)$$

**Polar form**

$$\Psi(\vec{r}_1, \dots, \vec{r}_N, t) = R(\vec{r}_1, \dots, \vec{r}_N, t) \cdot \exp(iS(\vec{r}_1, \dots, \vec{r}_N, t)/\hbar)$$

**Hamilton-Jacobi equation**

$$\frac{\partial S(\vec{r}_1, \dots, \vec{r}_N, t)}{\partial t} + \sum_{k=1}^N \frac{(\nabla_k S)^2}{2m^*} + U(\vec{r}_1, \dots, \vec{r}_N, t) + Q(\vec{r}_1, \dots, \vec{r}_N, t) = 0$$

**Continuity equation**

$$\frac{\partial R^2(\vec{r}_1, \dots, \vec{r}_N, t)}{\partial t} + \sum_{k=1}^N \nabla_k \left( R^2(\vec{r}_1, \dots, \vec{r}_N, t) \cdot \nabla_k \frac{S(\vec{r}_1, \dots, \vec{r}_N, t)}{m^*} \right) = 0$$

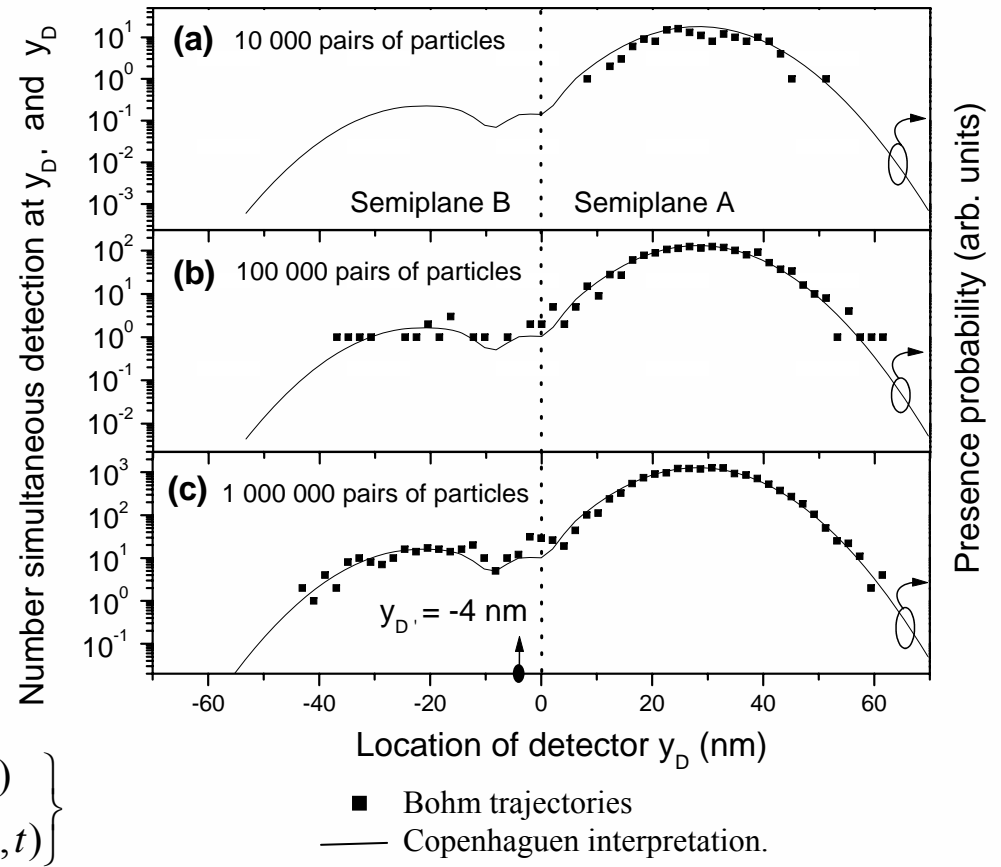
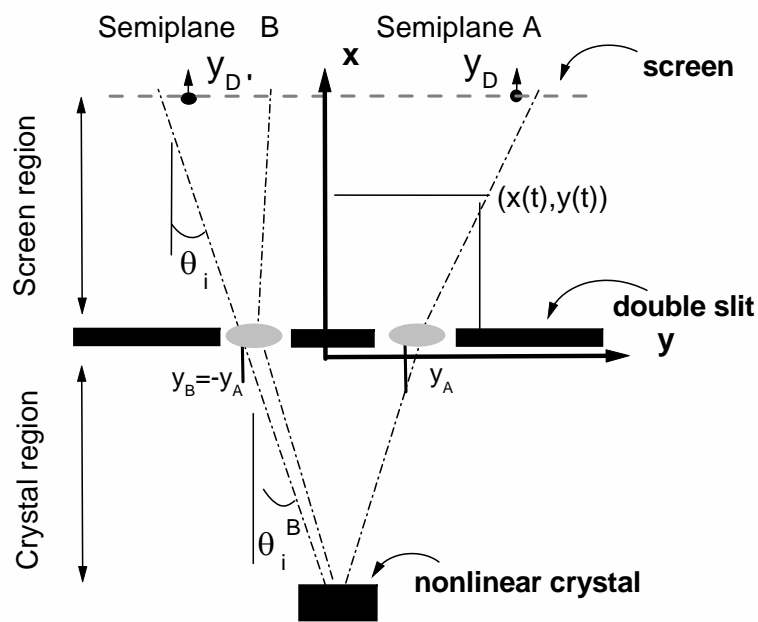
$$\left. \begin{array}{c} \dots\dots \\ \frac{d^2 \vec{r}_i}{dt^2} = -\nabla_i (U(\vec{r}_1, \dots, \vec{r}_N, t) + Q(\vec{r}_1, \dots, \vec{r}_N, t)) \Big|_{\vec{r}_1 = \vec{r}_1(t), \dots, \vec{r}_N = \vec{r}_N(t)} \\ \dots\dots \end{array} \right\}$$

A system of N coupled equations

The wave function evolution (i.e the correlations among electrons) can be calculated using many-particle Bohm trajectories.

## II.2.- Many-particle Bohm trajectories

▶ **Example: Two symmetric boson system**



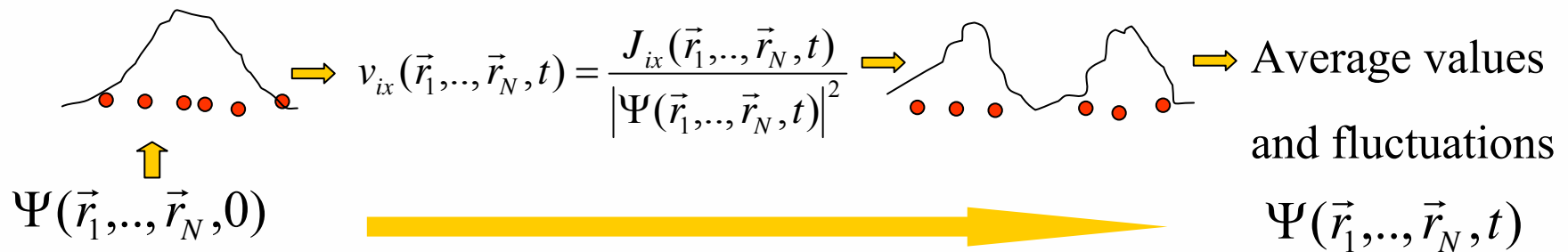
$$\Psi(x_1, x_2, y_1, y_2, t) = \frac{1}{\sqrt{2}} \left\{ \begin{aligned} &\Psi_A(x_1, y_1, t) \cdot \Psi_B(x_2, y_2, t) \\ &+ \Psi_A(x_2, y_2, t) \cdot \Psi_B(x_1, y_1, t) \end{aligned} \right\}$$

[X.Oriols, Phys. Rev A, 2005]

## II.2.- Many-particle Bohm trajectories

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### ▶ Summary of Bohm trajectories



### ▶ Main criticism against Bohm trajectories approach:

“...In any case, the basic reason for not paying attention to the Bohm approach is not some sort of ideological rigidity, but much simpler...It is just that we are all too busy with our own work to spend time on something that doesn't seem likely to help us make progress with our real problems”.

Steven Weinberg (private communication with Shelly Goldstein)

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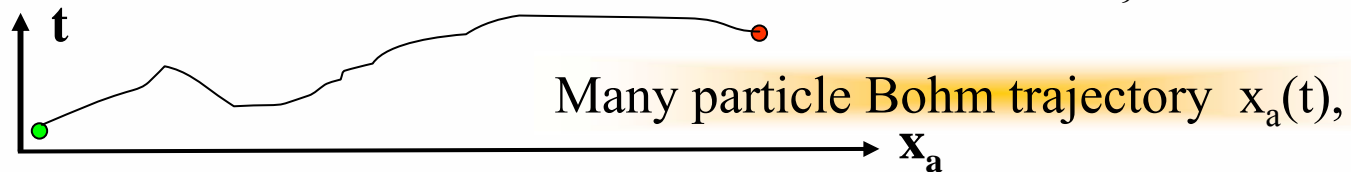
**II.3.- Our quantum Monte Carlo approach**

II.4.- Numerical results

## II.3.- Our Quantum Monte Carlo approach

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▶ 
$$i\hbar \frac{\partial \Psi(\vec{r}_1, \dots, \vec{r}_N, t)}{\partial t} = \left\{ \sum_{k=1}^N \left( -\frac{\hbar^2}{2m^*} \nabla_k^2 \right) + \sum_{k=1}^N U_E(\vec{r}_k, t) + \frac{1}{2} \sum_{k=1}^N \sum_{\substack{j=1 \\ k \neq j}}^N \frac{q^2}{4\pi \epsilon \epsilon_0 |\vec{r}_k - \vec{r}_j|} \right\} \Psi(\vec{r}_1, \dots, \vec{r}_N, t)$$



▶ Theorem: Many-particle Bohm trajectory from single-particle pseudo-Schrodinger equation

$$i\hbar \frac{\partial \Psi(\vec{r}_a, t)}{\partial t} = \left\{ -\frac{\hbar^2}{2m^*} \nabla_a^2 + U_E(\vec{r}_a, t) + \frac{1}{2} \sum_{\substack{k=1 \\ k \neq a}}^N \frac{q^2}{4\pi \epsilon \epsilon_0 |\vec{r}_k(t) - \vec{r}_a|} + G(\vec{r}_a, \vec{r}_b(t), t) + iJ(\vec{r}_a, \vec{r}_b(t), t) \right\} \Psi(\vec{r}_a, t)$$

DEMO: See X.Oriols, Phys. Rev Lett, 2007 (in press)



## II.3.- Our Quantum Monte Carlo approach

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$$G(\vec{r}_a, \vec{r}_b(t), t) \approx G(\vec{r}_a(t), \vec{r}_b(t), t)$$

► **Approximation:**

$$J(\vec{r}_a, \vec{r}_b(t), t) \approx J(\vec{r}_a(t), \vec{r}_b(t), t)$$

► Thus, we can obtain many-particle Bohm trajectories by solving a system of N single-particle Schrödinger equations with time dependent potentials

$$\left\{ \begin{array}{l} i\hbar \frac{\partial \Psi_1(\vec{r}_1, t)}{\partial t} = \left\{ -\frac{\hbar^2}{2m^*} \nabla_1^2 + U_E(\vec{r}_1) + \sum_{k=2}^N \frac{q^2}{4\pi \varepsilon \varepsilon_0 |\vec{r}_k(t) - \vec{r}_1|} \right\} \Psi_1(\vec{r}_1, t) \quad ; \quad \vec{r}_1(t) = \vec{r}_1(t_o) + \int_{t_o}^t dt \frac{J_1(\vec{r}_1, t)}{|\Psi_1(\vec{r}_1, t)|^2} \Big|_{\vec{r}_1 = \vec{r}_1(t)} \\ \dots \\ i\hbar \frac{\partial \Psi_N(\vec{r}_N, t)}{\partial t} = \left\{ -\frac{\hbar^2}{2m^*} \nabla_N^2 + U_E(\vec{r}_N) + \sum_{k=1}^{N-1} \frac{q^2}{4\pi \varepsilon \varepsilon_0 |\vec{r}_k(t) - \vec{r}_N|} \right\} \Psi_N(\vec{r}_N, t) \quad ; \quad \vec{r}_N(t) = \vec{r}_N(t_o) + \int_{t_o}^t dt \frac{J_N(\vec{r}_N, t)}{|\Psi_N(\vec{r}_N, t)|^2} \Big|_{\vec{r}_N = \vec{r}_N(t)} \end{array} \right.$$

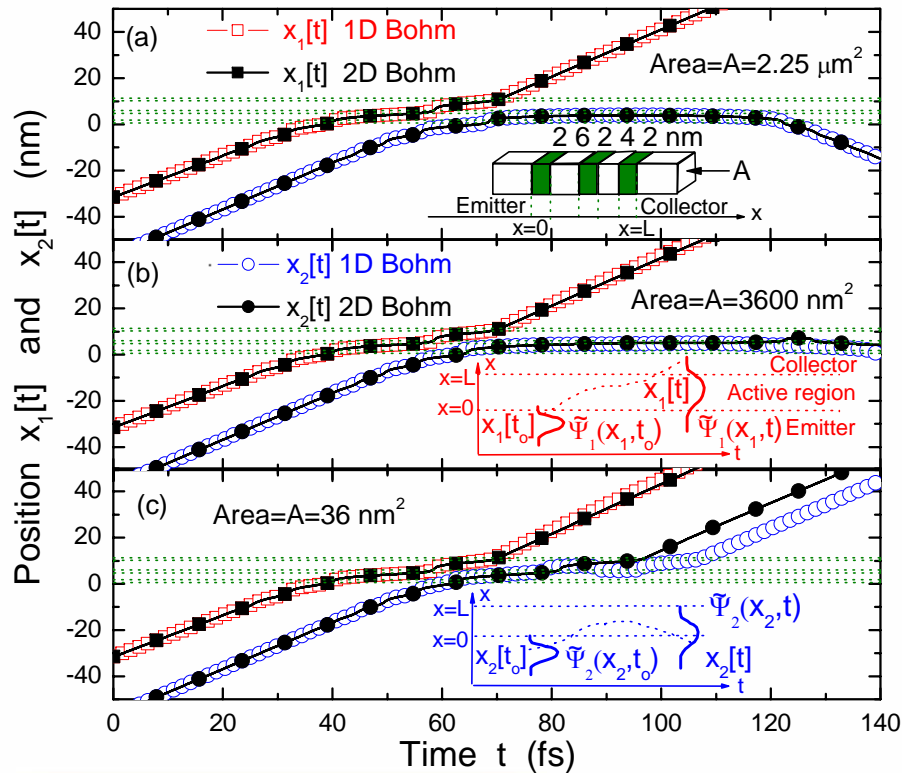
► **Numerical viability:** N=100 electrons, L=100nm length (with  $\Delta x=0.1$  nm) in 1D

n° of variables =  $1000 \cdot N = 100\,000$  variables

X.Oriols, Phys. Rev Lett, 2007 (in press)

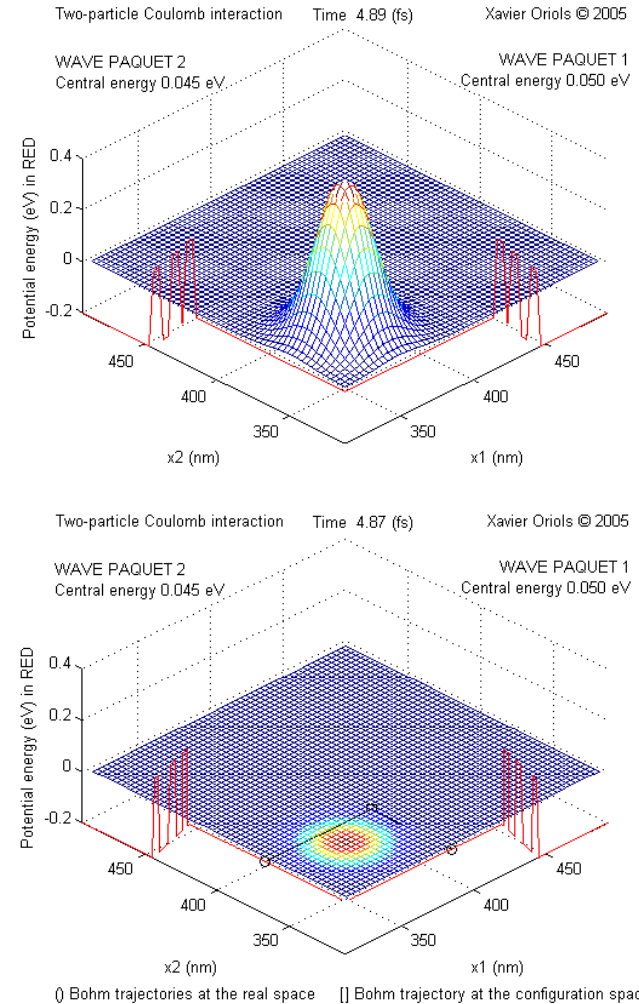
# II.3.- Our Quantum Monte Carlo approach

## ▶ Example: two interacting particles



Electrostatic potential

$$V(x_1, x_2) = U_E(x_1) + U_E(x_2) + \frac{q^2}{4\pi\epsilon\epsilon_0 \cdot |r_1 - r_2|}$$



## II.3.- Our Quantum Monte Carlo approach

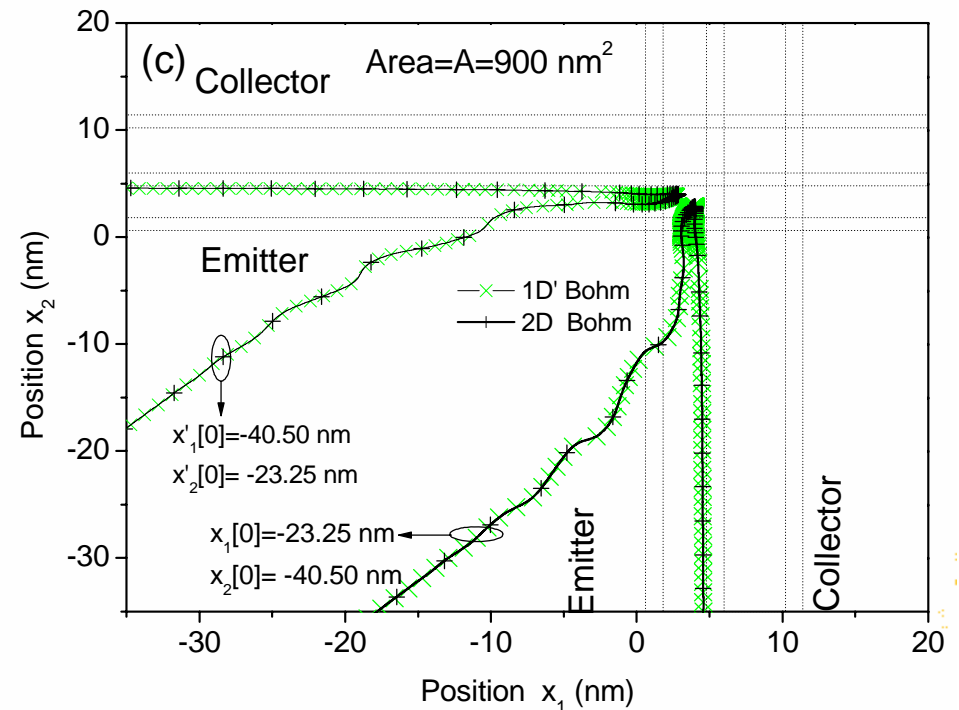
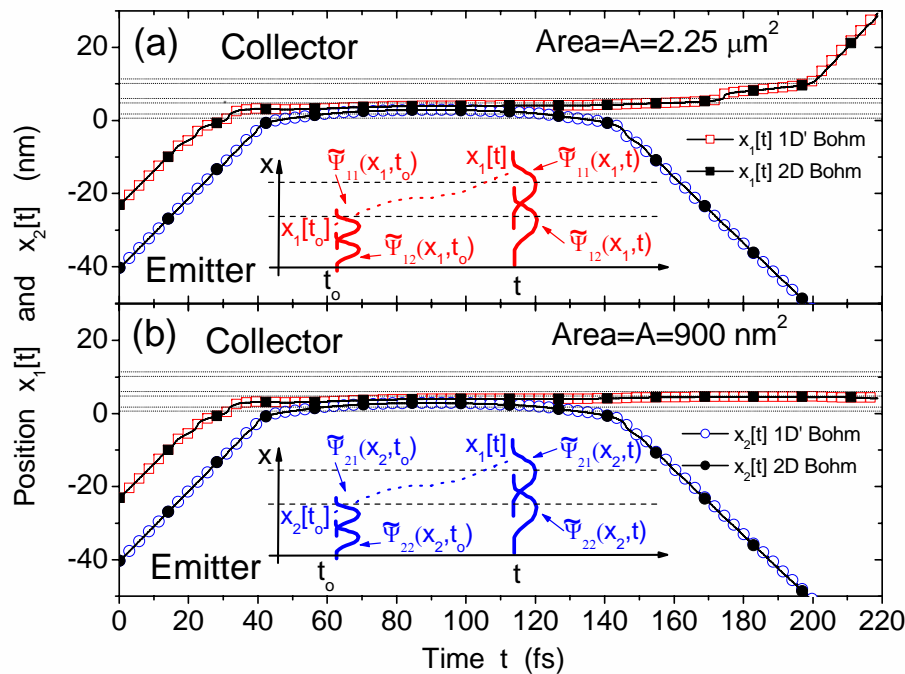
▶ Example: two (Coulomb and Exchange) interacting particles



Only antisymmetrical wave-functions are valid



What is the difference due to the Exchange interaction?



Observable results are identical when we interchange the initial position of electrons

# Outline of the talk:

I.- Introduction: *“La simulation du courant et du bruit dans les composants quantiques”*

II.- Our approach: *“Méthode des trajectoires de Bohm pour l'étude des interactions entre les électrons”*

II.1.- Single-particle Bohm trajectories.

II.2.- Many-particle Bohm trajectories

II.3.- Our quantum Monte Carlo approach

**II.4.- Numerical results**

**II.3.1.- Coulomb Blockade and resonant tunneling**

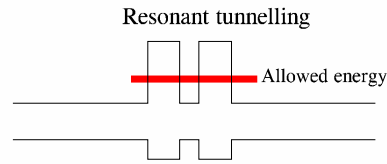
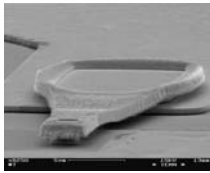
**II.3.2.- Current noise with Coulomb correlations**

**II.3.3.- AC conductance**

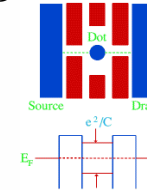
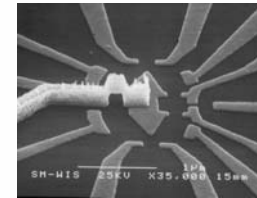
# II.3.1.- Numerical results: Coulomb Blockade and Resonant tunneling

▶ **Double/triple barrier structure**

**Resonant tunneling diode**



**Coulomb blockade (Single electrons)**

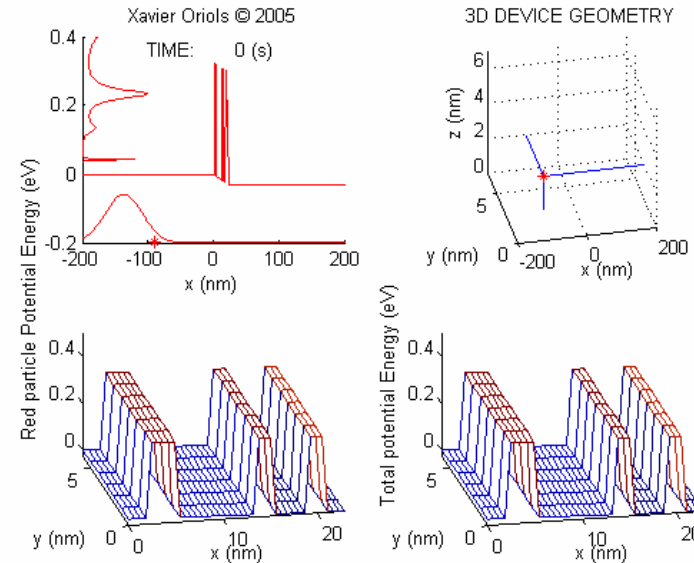
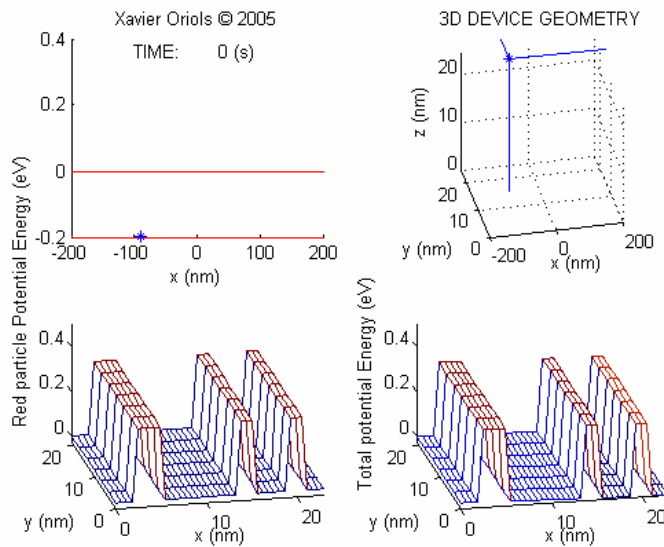


▶ **Example: Coulomb correlation as a function of the lateral area**

Area=20 nm x 20 nm

**Dimensions**

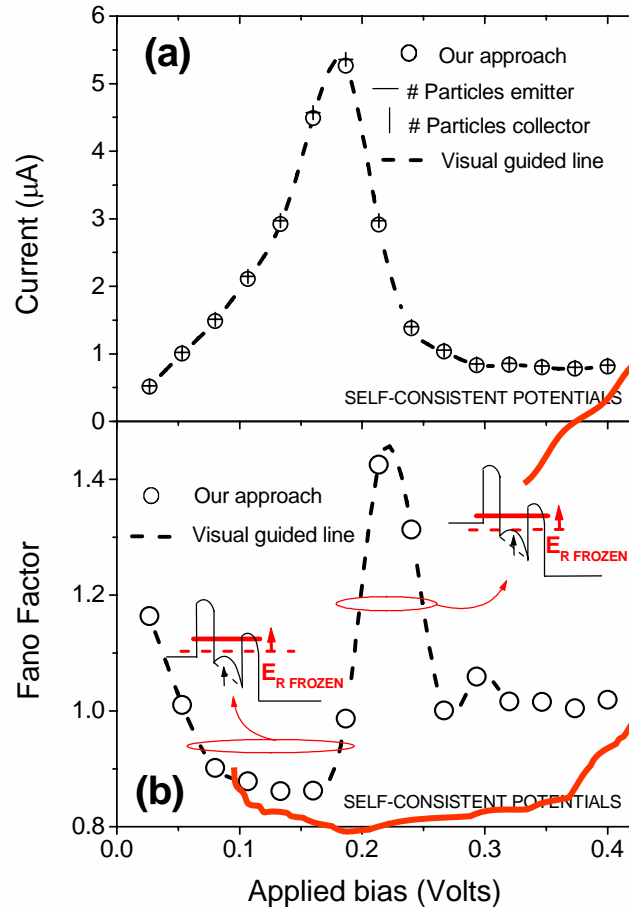
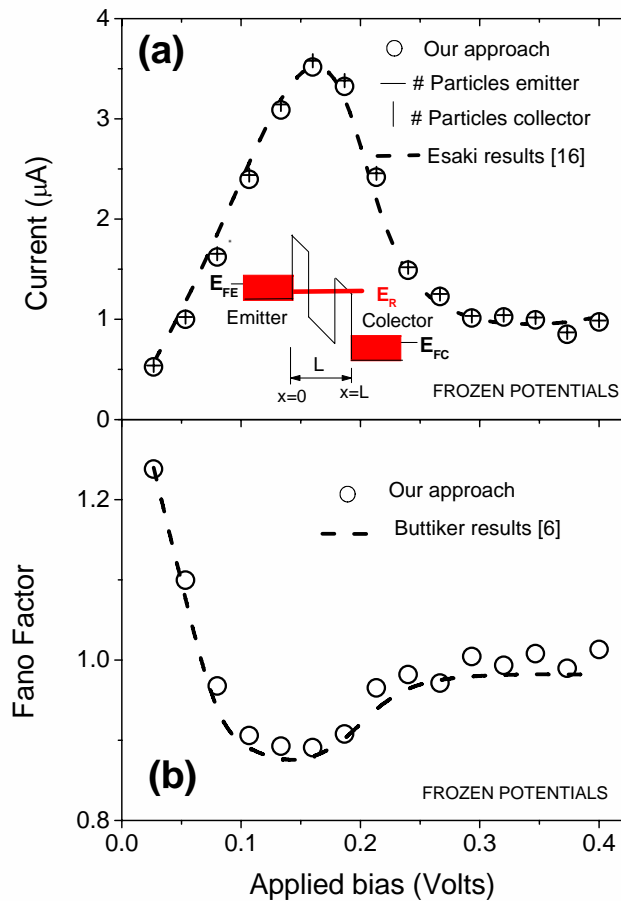
Area=6 nm x 6 nm



## II.3.2.- Numerical results: Current noise with Coulomb correlations

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### ▶ Example: Effect of Coulomb correlation on current and noise for RTD



Bunching of electrons

Anti-bunching of electrons

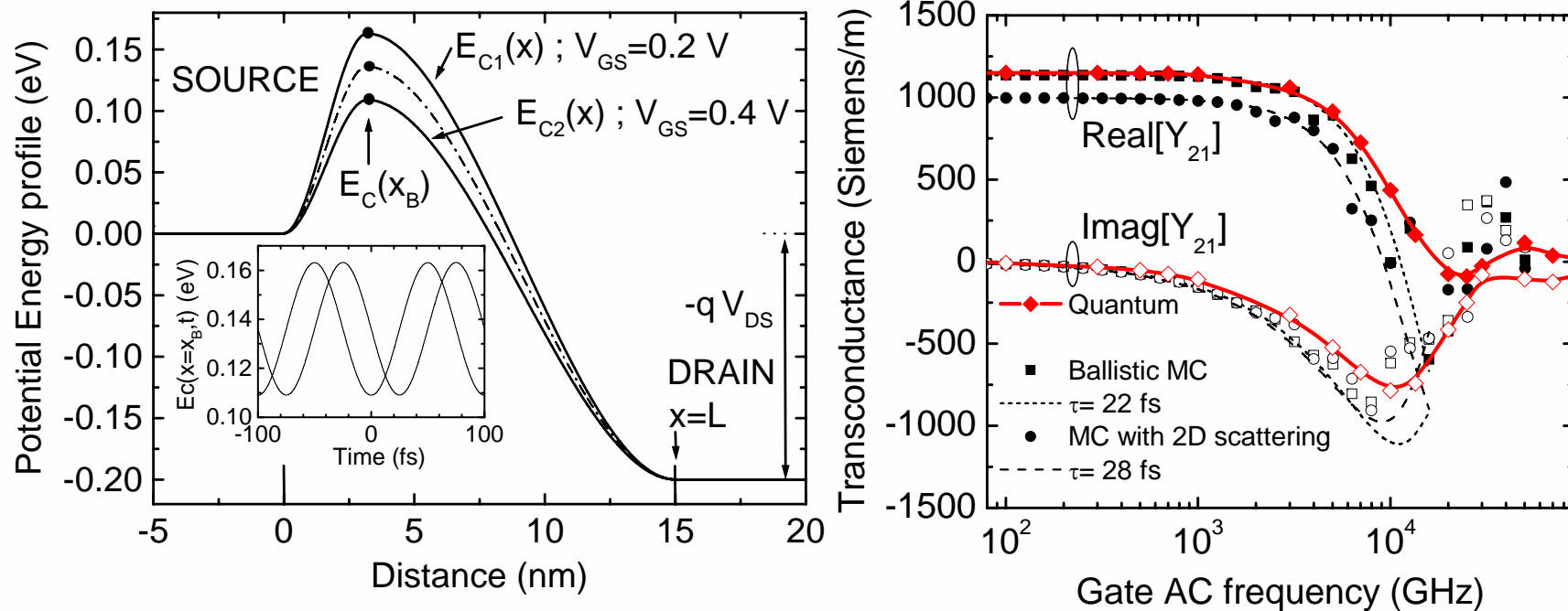
[X.Oriols *et al.*, APL, 2004]



## II.3.4.- Numerical results: AC conductance

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### ▶ Quantum-frequency limits for nanoscale Si MOSFET



[X.Oriols *et al.*, Phys. Rev B, (2005)]

[E. Fernandez-Diaz, A.Alarcon and X.Oriols *et al.*, IEEE TON, (2005)]



## Summary:

- ▶ We have developed a quantum Monte Carlo formalism, based on Bohm trajectories, to study Coulomb and Exchange correlations in nanoscale devices.
- ▶ Our approach is accurate, **intuitive** and provides an **unified formalism** to study average current, instantaneous current and noise in different transport regimes, from resonant tunneling to Coulomb Blockade in nanoelectronic devices.

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