Quantum many-particle computations with Bohmian trajectories

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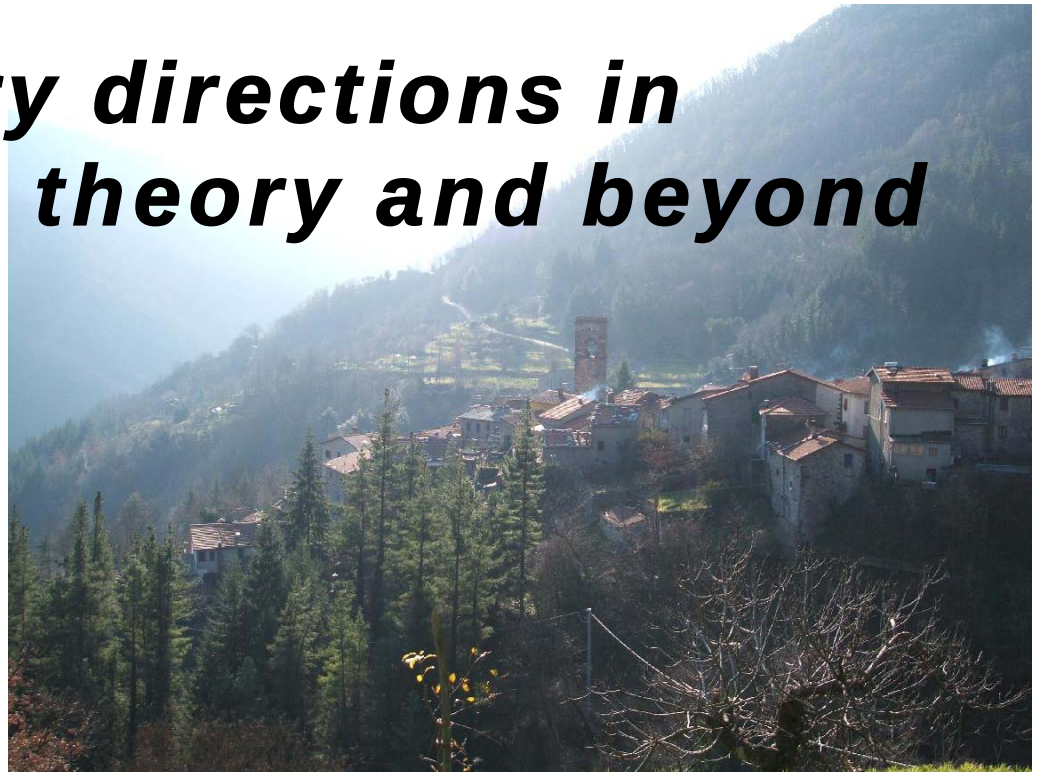
21st-century directions in de Broglie-Bohm theory and beyond



Saturday 28th August - Saturday 4th September 2010

Vallico Sotto, Tuscany, Italy

Quantum many-particle computations with Bohmian trajectories

1.- Quantum Many-Particle Computations with Bohmian Trajectories:

1.1.- Introduction

1.2.- Our Many-particle Bohmian trajectories (MPBT) theorem

2.- Application to Electron Transport in Nanoelectronic Devices:

2.1.- The electron transport problem at the nanoscale

2.2.- Our quantum Monte Carlo algorithm

3.- Conclusions and Future work

Quantum many-particle computations with Bohmian trajectories

1.- Quantum Many-Particle Computations with Bohmian Trajectories:

1.1.- Introduction

1.1.1.- Why to use Bohmian mechanics
1.1.2.- The “many-body” problem
1.1.3.- Does Bohmian mechanics provide any help?

1.2.- Our Many-particles Bohmian trajectories (MPBT) theorem

1.3.- Approximation

2.- Application to Electron Transport in Nanoelectronic Devices:

3.- Conclusions and Future work

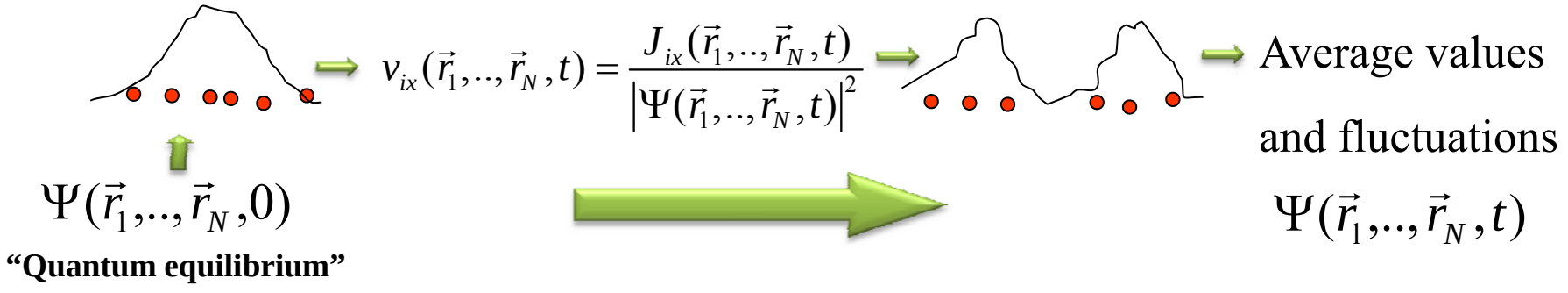
1.1.1.- Introduction: Why to use Bohmian mechanics?

Reason 1: Bohmian Thinking:

.-Looking for **extensions/limitations/contradictions** of 'Orthodox' QM.

Reason 2: Bohmian Explaining:

.- An **intuitive/simpler/causal** explanation of QM phenomena.



1.1.1.- Introduction: Why Bohmian mechanics?

Reason 3. Bohmian computing:

"Analytical" : Bohmian trajectories from the wavefunction

"Synthetical" : without explicitly computing the wavefunction

Quantum Hamilton-Jacobi equation

$$\frac{\partial S(\vec{r},t)}{\partial t}+\frac{(\nabla S)^2}{2m}+U(\vec{r},t)+Q(\vec{r},t)=0$$

Continuity equation

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

Quantum potential

$$Q(\vec{r},t)=-\frac{1}{R(\vec{r},t)}\frac{\hbar^2\nabla^2R(\vec{r},t)}{2m}$$

Unknowns: $R(\vec{r},t)$ $S(\vec{r},t)$

Synthetical examples from the Physical-Chemistry community:

Without trajectories: Hydrodynamic quantum equation: **B. Kendrix**

With trajectories: Lagrangian (moving with the flow): **Robert E.Wyatt**

Complex Action: **D.Tannor**

Valid for 1, 2, 3... degrees of freedom

1.1.2.- Introduction: The "**many-body**" problem

P.A.M. Dirac, 1929

"The general theory of quantum mechanics is now almost complete. The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble."

Max Born, 1960

"It would indeed be remarkable if Nature fortified herself against further advances in knowledge behind the analytical difficulties of the many-body problem."

1.2.- Introduction: The "**many-body**" problem

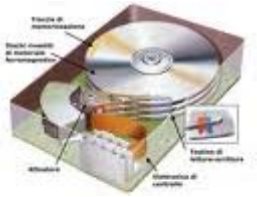
The many-particle (non-relativistic spinless) Schrödinger equation

$$i\hbar\frac{\partial\Phi(\vec{r}_1,..,\vec{r}_N,t)}{\partial t}=\left\{\sum_{k=1}^{N}-\frac{\hbar^2}{2m}\nabla^2_{\vec{r}_k}+U(\vec{r}_1,..,\vec{r}_N,t)\right\}\cdot\Phi(\vec{r}_1,..,\vec{r}_N,t)$$

$\Phi(\vec{r}_1,..,\vec{r}_N,t)$ Many particle wave function

The practical solution is **inaccesible for more than very few electrons**

Exercise: Number of hard disks to load the (finite-difference) wave-function in a PC memory for N=10 particles, L=50nm length (Δx=1 nm)



nº of variables (1 particle) = 50^3 = 125000 variables !!

nº of variables (Total degrees of freedom) = 50^{3N} = 50^{30} variables !!

nº of bits = 50^{30} variables *16 bits/variable ~ 1^{38} Terabytes !!

nº of PCs ~ 1000000000000000000000000000000 Hard disks

1.1.2.- Introduction: Some 'Orthodox' solutions available in the literature

Orthodox solutions:

Hartree-Fock

- Many-electron wave-functions having the form of antysimmetric product of single-particle wave-functions ("orbitals").
- Leads to an effective single-particle Schrodinger equation with a potential determined by all others "orbitals".

Density Functional Theory (W.Kohn)

- The "orbitals" are solutions of single-particle Schrodinger equation which depends on the charge density rather than the "orbitals" themselves.
- There are terms (the exchange potentials) that are **unknown and have to be approximated.**

Quantum Monte Carlo (ex: CASINO Mike Towler)

Pseudo-Bohmian solutions:

Quantum Fluid Density Functional framework: P.K. Chataraj

Hidrodynamic quantum Monte Carlo: Ivan. P. Christov

DFT Super symmetric quantum mechanics, E. Bittner

Quantum many-particle computations with Bohmian trajectories

1.- Quantum Many-Particle Computations with Bohmian Trajectories:

1.1.- Introduction

1.2.- Our Many-particles Bohmian trajectories (MPBT) theorem

- 1.2.1.- The basic idea
- 1.2.2.- The MPT theorem
- 1.2.3.- Good points
- 1.2.4.- Bad points

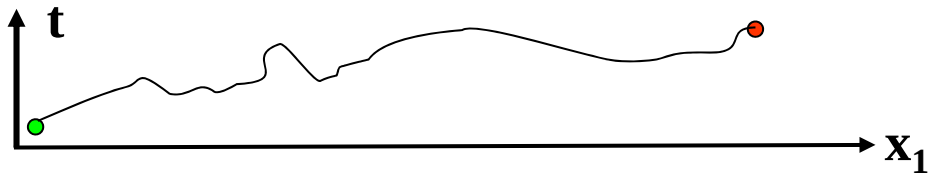
1.3.- Approximation

2.- Application to Electron Transport in Nanoelectronic Devices:

3.- Conclusions and Future work

1.2.1.- Our MPBT Theorem: the basic idea

Single-particle Bohmian trajectory $x_a[t]$,



$$\Psi(x_1,t)$$

$$v(x_1[t],t)=\left.\frac{\partial S(x_1,t)/\partial x_1}{m}\right|_{x1=x1[t]}$$

Many-particle Bohmian trajectory $x_a[t]$,

$$\Psi(x_1,...,x_N,t)$$

$$v_a(x_1[t],..,x_N[t],t)=\left.\frac{\partial S(x_1,....,x_N,t)/\partial x_a}{m}\right|_{x_1=x_1[t],....,x_N=x_N[t]}$$

$$v_a(x_1[t],..,x_N[t],t)=\left.\frac{\partial S(x_1[t],..,x_a,..,x_N[t],t)/\partial x_a}{m}\right|_{x_1=x_1[t]}$$

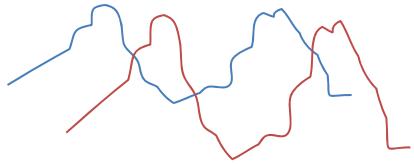
$$\Psi(x_1[t],....x_a,...,x_N[t],t)\equiv\Psi_a(x_a,t)$$

What is the equation satisfied by this single-particle wave-function ?

1.2.1.- Our MPBT Theorem: the basic idea

Any arbitrary complex "function":

$$\Psi_a(x_a,t)$$



can be written in Schrödinger-like equation:

$$i\hbar\frac{\partial\Psi_a(x_a,t)}{\partial t}=-\frac{\hbar^2}{2m^*}\frac{\partial^2\Psi_a(x_a,t)}{\partial x_a^2}+W(x_a,t)\cdot\Psi_a(x_a,t)$$

with a complex potential:

$$W_r(x_a,t)+iW_i(x_a,t)=\frac{i\hbar\frac{\partial\Psi_a(x_a,t)}{\partial t}+\frac{\hbar^2}{2m^*}\frac{\partial^2\Psi_a(x_a,t)}{\partial x_a^2}}{\Psi_a(x_a,t)}$$

What is the complex "potential" satisfied by this single-particle wave-function ?

1.2.1.- Our MPBT Theorem: the basic idea

What is the complex "potential" satisfied by this single-particle wave-function ?

$$W_r(x_a,t)+iW_i(x_a,t)=\frac{i\hbar\frac{\partial\Psi_a(x_a,t)}{\partial t}+\frac{\hbar^2}{2m^*}\frac{\partial^2\Psi_a(x_a,t)}{\partial x_a^2}}{\Psi_a(x_a,t)}$$

1st step

$$\frac{\partial\Psi_a(x_a,t)}{\partial t}=\frac{\partial\Psi(x_1[t],..,x_a,..,x_N[t],t)}{\partial t}$$

$$\frac{\partial^2\Psi_a(x_a,t)}{\partial x_a^{\,2}}=\frac{\partial^2\Psi(x_1[t],..,x_a,..,x_N[t],t)}{\partial x_a^{\,2}}$$

2nd step

$$\Psi(x_1[t],..x_a..,x_N[t],t)\equiv R(x_a,\vec{x}_b[t],t)\cdot e^{iS(x_a,\vec{x}_b[t],t)/\hbar}$$

3rd step

Use the quantum Hamiltonian-Jacobi equations

1.2.2.- Our MPBT Theorem: Good points

$$i\hbar\frac{\partial\Psi(x_a,t)}{\partial t}=\left\{-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial x_a^2}+U_a(x_a,\vec{x}_b[t],t)+G(x_a,\vec{x}_b[t],t)+i\cdot J(x_a,\vec{x}_b[t],t)\right\}\Psi(x_a,t)$$

Good points :

[X. Oriols, Phys. Rev. Lett. 98, 066803 (2007)]

1st An **exact** procedure for computing many-particle Bohmian trajectories

2nd The rest of trajectories in the potentials have to be Bohmian trajectories

3rd The correlations are introduced into the time-dependent potentials

4th The interacting potential for "classical" correlations

5th There is a real potential to account for "non-classical" correlations

6th There is a imaginary potential to account for non-conserving norms

7st **"Analytical" (for 1D,2D,..TDSE) + "Synthetical" (for the rest).**

1.2.2.- Our MPBT Theorem: Bad points

$$i\hbar\frac{\partial\Psi(x_a,t)}{\partial t}=\left\{-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial x_a^2}+U_a(x_a,\vec{x}_b[t],t)+G(x_a,\vec{x}_b[t],t)+i\cdot J(x_a,\vec{x}_b[t],t)\right\}\Psi(x_a,t)$$

Bad points :

1st The Bohm trajectories for the rest of particles have to be known

Ok! no problem, we will use a single-particle equation for each particles

2nd The terms G and J depends on the many-particle wave-function

$$G_a(x_a,\vec{x}_b,t)=U_b(\vec{x}_b,t)+\sum_{k=1,k\neq a}^{N}\left\{K_k(\vec{x},t)-Q_k(\vec{x},t)-\frac{\partial S(\vec{x},t)}{\partial x_k}\cdot v_k(x[t],t)\right\}$$

$$J_a(x_a,\vec{x}_b,t)=\frac{\hbar}{2\cdot R^2(\vec{x},t)}\left\{\sum_{k=1,k\neq a}^{N}\left\{\frac{\partial R^2(\vec{x},t)}{\partial x_k}\cdot v_k(\vec{x}[t],t)-\frac{\partial}{\partial x_k}\left(\frac{R^2(\vec{x},t)}{m}\cdot\frac{\partial S(\vec{x},t)}{\partial x_k}\right)\right\}\right\}$$

$$K_a(\vec{x},t)=\frac{1}{2\cdot m}\left(\frac{\partial S(\vec{x},t)}{\partial x_a}\right)^2 \quad ; \quad Q_a(\vec{x},t)=-\frac{\hbar^2}{2\cdot m}\frac{\partial^2 R(\vec{x},t)/\partial x_a^2}{R(\vec{x},t)}$$

¡ This is exactly the same difficulty found in the DFT (or TD-DFT) !

Quantum many-particle computations with Bohmian trajectories

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1.1.- Introduction

1.2.- Our Many-particles Bohmian trajectories (MPBT) theorem

1.3.- Approximation

1.3.1.- The simplest approximation
1.3.2.- Application to systems with non-identical particles
1.3.4.- Application to systems with ‘identical’ particles

2.- Application to Electron Transport in Nanoelectronic Devices:

3.- Conclusions and Future work

1.3.1.- Approximate methods for G and J terms: The simplest approximation

Exercise: What happens if the many-particle wave-function is separable ?

$$\Psi(x_1,...,x_N,t) = \bar{\Psi}_1(x_1,t)\cdot....\cdot\bar{\Psi}_N(x_N,t)$$

$$i\hbar\frac{\partial\Psi(x_a,t)}{\partial t} = \left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_a^2} + U(x_a,\vec{x}_b[t],t) + G(x_a,\vec{x}_b[t],t) + i\cdot J(x_a,\vec{x}_b[t],t)\right\}\Psi(x_a,t)$$

$$G(x_a,\vec{x}_b[t],t) = G(\vec{x}_b[t],t) = -\sum_{k=1,k\neq a}^{N}\frac{dS_k(x_k[t],t)}{dt}$$

$$J(x_a,\vec{x}_b[t],t) = J(\vec{x}_b[t],t) = -\sum_{k=1,k\neq a}^{N}\frac{\hbar}{2}\frac{d}{dt}\ln\left(R_k^2(x_k[t],t)\right)$$

$$\Psi_a(x_a,t) = \tilde{\Psi}_a(x_a,t)\cdot e^{\alpha_a(t)+i\cdot\beta_a(t)} = \bar{\Psi}_1(x_1[t],t)\cdot...\bar{\Psi}_a(x_a,t)..\cdot\bar{\Psi}_N(x_N[t],t)$$

1.3.1.- Approximate methods for G and J terms: The simplest approximation

$$i\hbar\frac{\partial\Psi(x_a,t)}{\partial t}=\left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_a^2}+U(x_a,\vec{x}_b[t],t)+G(x_a,\vec{x}_b[t],t)+i\cdot J(x_a,\vec{x}_b[t],t)\right\}\Psi(x_a,t)$$

Guess:

$$G(x_a,\vec{x}_b(t),t)=G(x_a(t),\vec{x}_b(t),t)+\ldots$$
$$J(x_a,\vec{x}_b(t),t)=J(x_a(t),\vec{x}_b(t),t)+\ldots$$

$$\Psi_a(x_a,t)=\tilde{\Psi}_a(x_a,t)\,e^{\alpha_a(t)+i\cdot\beta_a(t)}$$

The global time-dependent phase does not affect the velocity

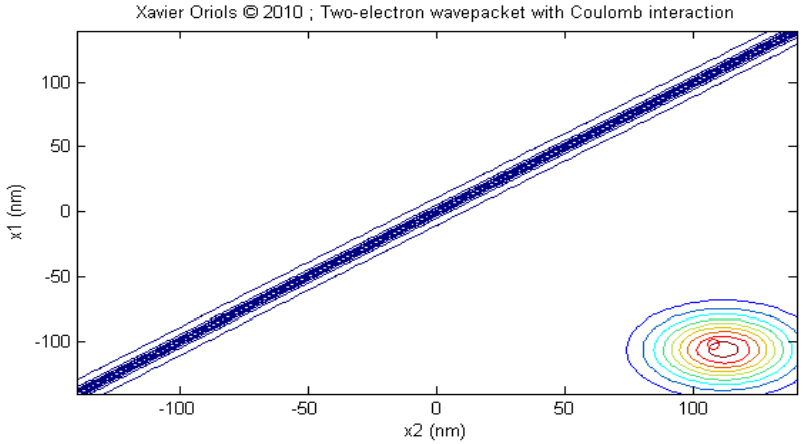
N=2 system

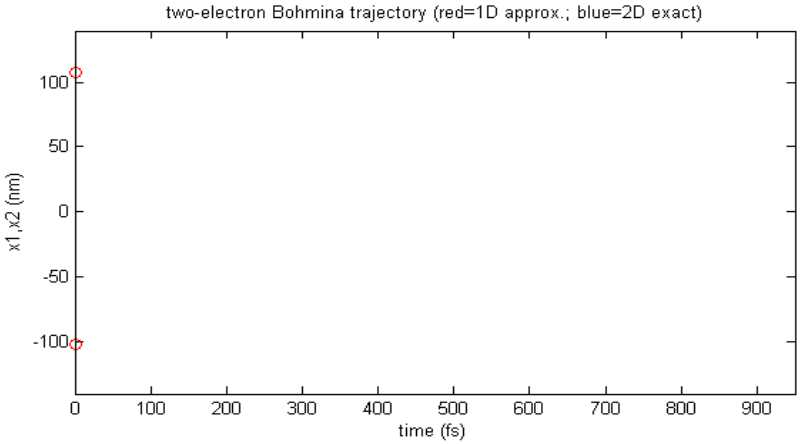
$$i\hbar\frac{\partial\tilde{\Psi}_1(x_1,t)}{\partial t}=\left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2}+U(x_1,x_2[t],t)\right\}\tilde{\Psi}_1(x_1,t)\quad;\quad x_1[t]=x_1[t_o]+\int_{t_o}^{t}dt\,\frac{\tilde{J}_1(x_1,t)}{|\tilde{\Psi}_1(x_1,t)|^2}\Bigg|_{x_1=x_1[t]}$$

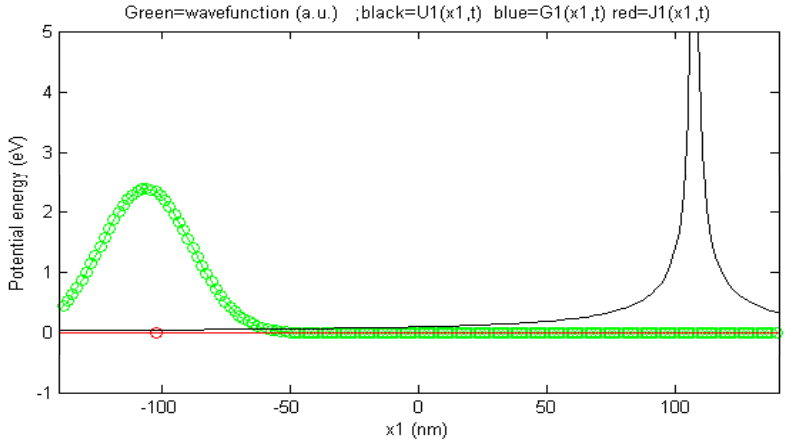
$$i\hbar\frac{\partial\tilde{\Psi}_2(x_2,t)}{\partial t}=\left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_2^2}+U(x_1[t],x_2,t)\right\}\tilde{\Psi}_2(x_2,t)\quad;\quad x_2[t]=x_2[t_o]+\int_{t_o}^{t}dt\,\frac{\tilde{J}_2(x_2,t)}{|\tilde{\Psi}_2(x_2,t)|^2}\Bigg|_{x_2=x_2[t]}$$

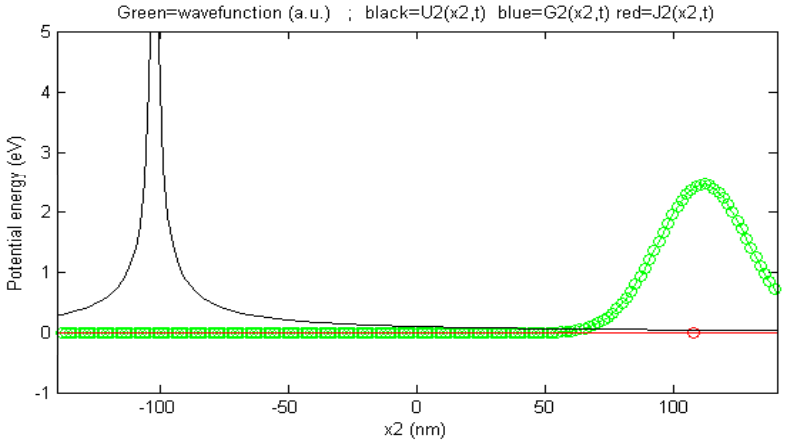
1.3.2.- Application to systems with non-identical particles

Example: two Coulomb interacting particles



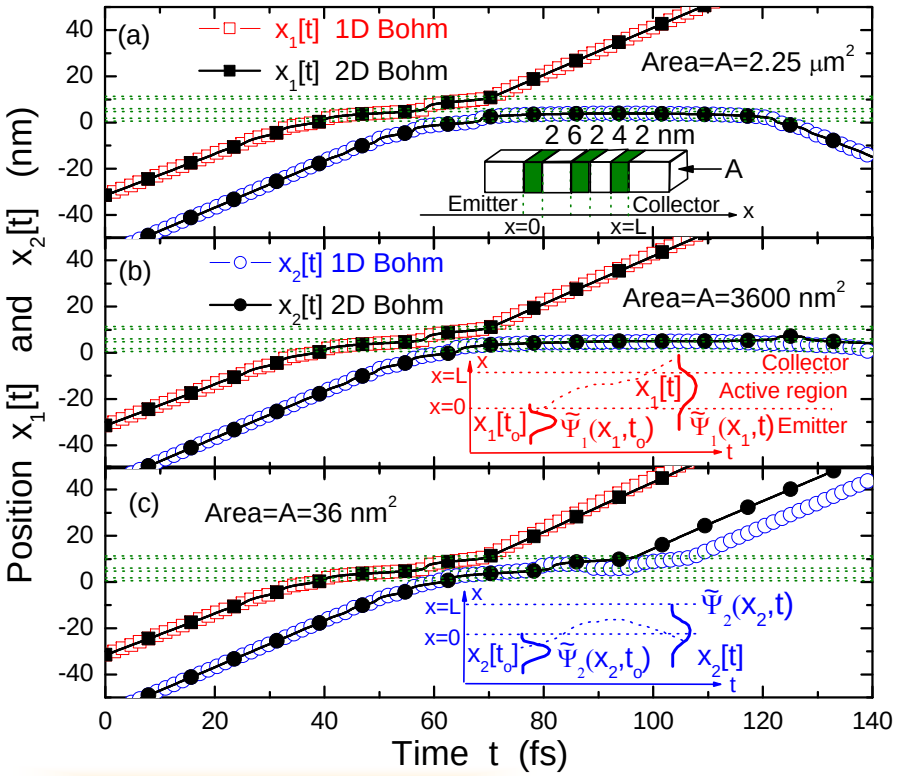


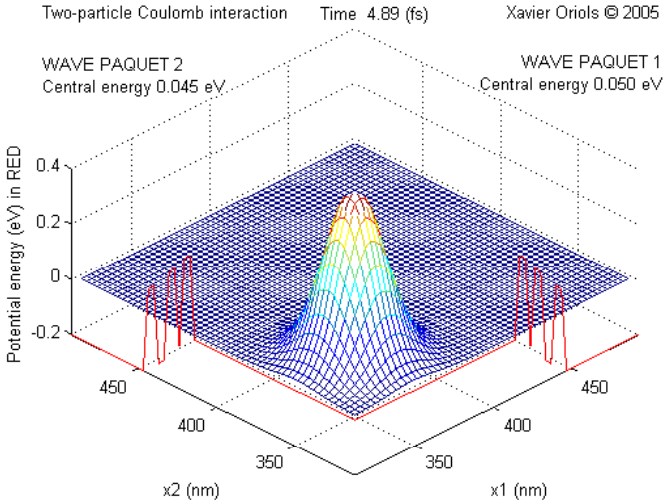


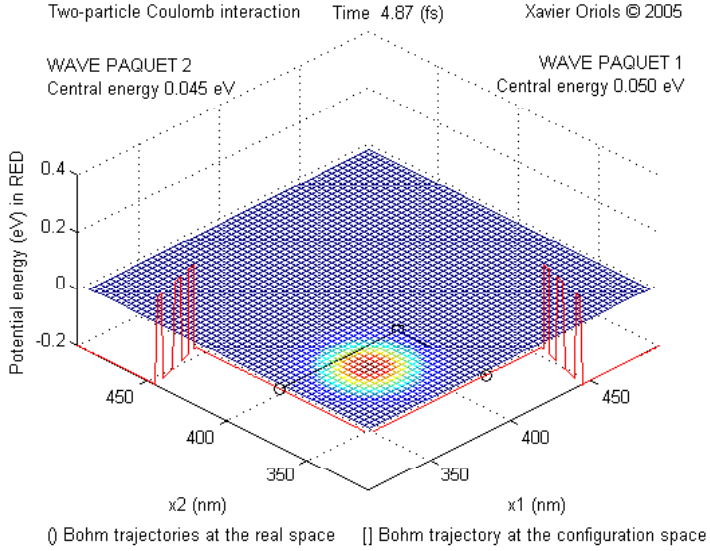


1.3.2.- Application to systems with non-identical particles

Example: two interacting tunneling particles







Electrostatic potential

$$V(x_1,x_2)=U_E(x_1)+U_E(x_2)+\frac{q^2}{4\pi\varepsilon\varepsilon_0\cdot|r_1-r_2|}$$

1.3.3.- Application to systems with “identical” particles

The exchange interaction appears in the symmetries of the many-particle wave-function (in the configuration space) when particles are exchanged

Where is the exchange interaction ?

$$i\hbar\frac{\partial\Psi(x_a,t)}{\partial t}=\left\{-\frac{\hbar^2}{2\,m^*}\frac{\partial^2}{\partial x_a^2}+U_a(x_a,\vec{x}_b(t),t)+G(x_a,\vec{x}_b(t),t)+i\cdot J(x_a,\vec{x}_b(t),t)\right\}\Psi(x_a,t)$$

$$G_a(x_a,\vec{x}_b,t)=U_b(\vec{x}_b,t)+\sum_{k=1,k\neq a}^{N}\left\{K_k(\vec{x},t)+Q_k(\vec{x},t)-\frac{\partial S(\vec{x},t)}{\partial x_k}\cdot v_k(x[t],t)\right\}$$

$$J_a(x_a,\vec{x}_b,t)=\frac{\hbar}{2\cdot R^2(\vec{x},t)}\left\{\sum_{k=1,k\neq a}^{N}\left\{\frac{\partial R^2(\vec{x},t)}{\partial x_k}\cdot v_k(\vec{x}[t],t)-\frac{\partial}{\partial x_k}\left(\frac{R^2(\vec{x},t)}{m}\cdot\frac{\partial S(\vec{x},t)}{\partial x_k}\right)\right\}\right\}$$

The exchange interaction appears (in the real space) as a potential energy !!

1.3.3.- Application to systems with "identical" particles

How we include the exchange interaction ?

Write, the fermionic/bosonic wave function as a sum of a wave-functions without exchange interaction.

One wave-function with exchange interaction:

$$\Phi(x_1, x_2, .., x_N, t) = C \cdot \sum \left(\Psi_P(x_{p(1)}, x_{p(2)}, .., x_{p(N)}, t) \right)$$

Many wave-functions without exchange interaction,

$$\Phi_a(x_a, t) = C \cdot \sum \tilde{\Psi}_{pa}(x_a, t) \cdot e^{\alpha_{pa}(t) + i \cdot \beta_{pa}(t)}$$

How can we know the phases without computing them ?

1.3.3.- Application to systems with "identical" particles

How can we know the phases without computing them ?

By imposing exchange conditions on the set of "no exchange" wave-functions

Example: N=2 fermions

$$\Phi(x_1,x_2,0)=\Psi_1(x_1,0)\cdot\Psi_2(x_2,0)-\Psi_1(x_2,0)\cdot\Psi_2(x_1,0)$$

$$\Psi_1(x_1,t)=\tilde{\Psi}_{11}(x_1,t)\cdot w_{11}(t)-\tilde{\Psi}_{21}(x_1,0)\cdot w_{21}(t)$$
$$\Psi_2(x_2,t)=\tilde{\Psi}_{12}(x_2,t)\cdot w_{12}(t)-\tilde{\Psi}_{22}(x_2,0)\cdot w_{22}(t)$$

2 Conditions:

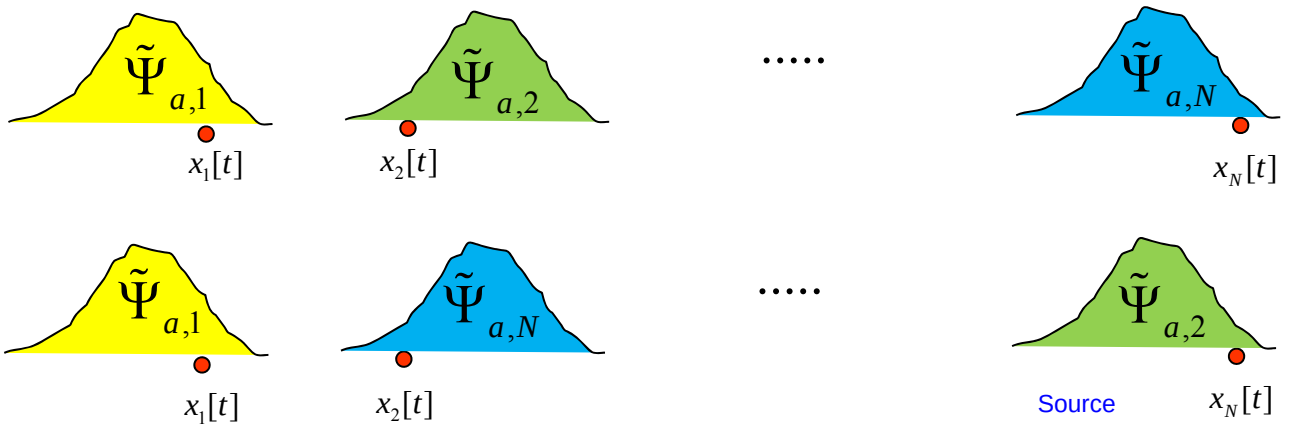
$$\Psi_1(x_2[t],t)=0$$

$$\Psi_2(x_1[t],t)=0$$

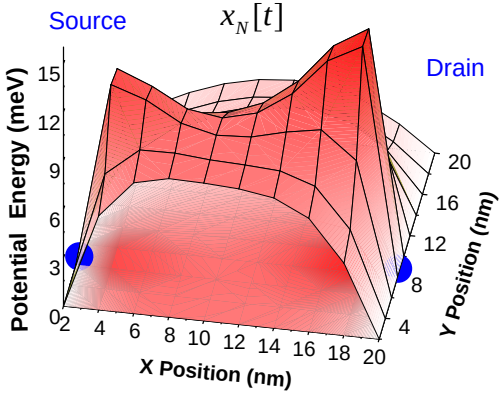
1.3.3.- Application to systems with "identical" particles

General expression:

$$\tilde{\Psi}_a(x_a,t)=\sum_{j=1}^{N!}\tilde{\Psi}_{a,p(j)_1}(x_1[t],t)\cdot\ldots\cdot\tilde{\Psi}_{a,p(j)_a}(x_a,t)\cdot\ldots\cdot\tilde{\Psi}_{a,p(j)_N}(x_N[t],t)\cdot s(\vec{p}(j))$$



$$i\hbar\frac{\partial\tilde{\Psi}_1(x_1,t)}{\partial t}=\left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2}+U(x_1,x_2[t],\ldots.,x_N[t],t)\right\}\tilde{\Psi}_1(x_1,t)$$



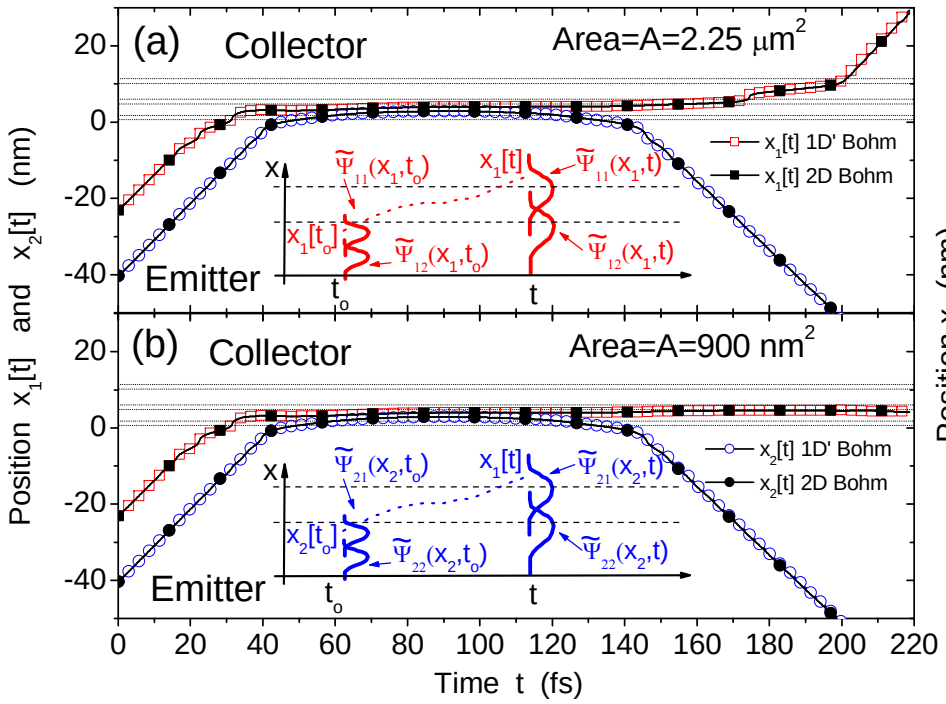
Only N·N wave-functions are needed!

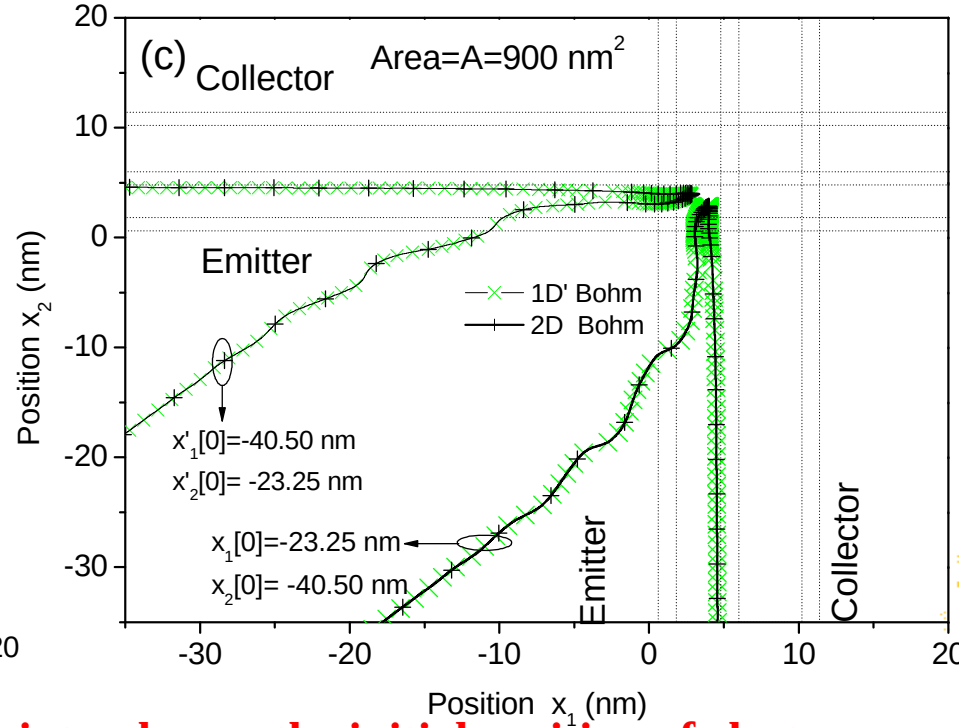
1.3.3.- Application to systems with "identical" particles

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

Quantum many-particle computations with Bohmian trajectories

1.- Quantum Many-Particle Computations with Bohmian Trajectories:

2.- Application to Electron Transport in Nanoelectronic Devices:

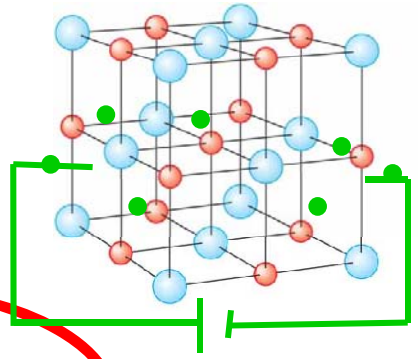
2.1.- Electron transport at the nanoscale

- 2.1.1.- The “many-body” problem
- 2.1.2.- Solid-state approximations
- 2.1.3.- The Bohmian prediction of the current

2.2.- BITLLES simulator: our quantum Monte Carlo algorithm

3.- Conclusions and Future work

Many-particle Schrödinger equation for electron devices:



$$\hat{H}_T = \left\{ \sum_k \left(-\frac{\hbar^2}{2m_0} \nabla_k^2 \right) + \sum_g \left(-\frac{\hbar^2}{2M_g} \nabla_g^2 \right) + \frac{1}{2} \sum_{k \neq j} \sum_j \frac{q^2}{4\pi\varepsilon\varepsilon_0 r_{kj}} \right.$$

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

kinetic energy of the electrons

kinetic energy of the atoms

electron-electron coulomb interaction

atom-atom coulomb interaction

electron-atom coulomb interaction

electron-potential due to external bias

atom potential due to external bias

2.1.1.- The electron transport at the nanoscale: the "many-body" problem

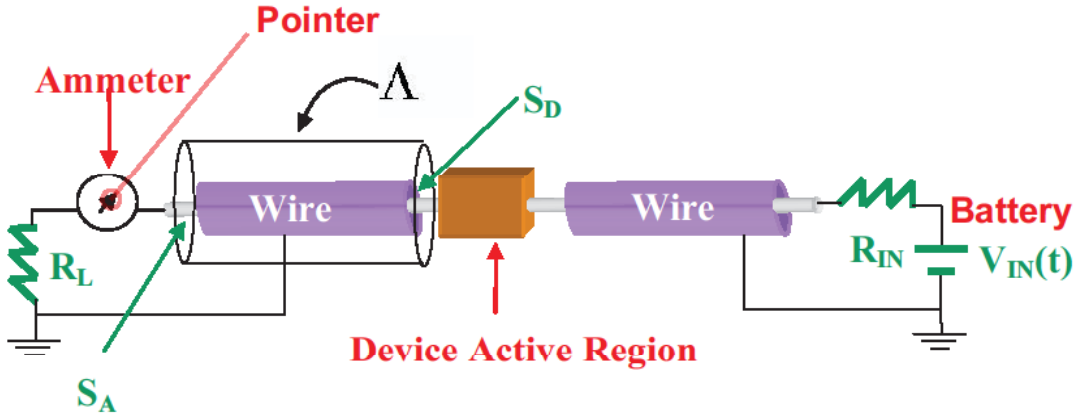
What is an electron device ?

1.- Open system

2.- Statistical system

3.- Far from equilibrium

4.- Strongly correlated system



What we measure ?

We measure the total (conduction + displacement) current in the ammeter, which is identical to that in a surface of the active region.

Continuity equation

$$\partial\rho/\partial t + \vec{\nabla}\cdot\vec{J}_c = 0 \Rightarrow \vec{\nabla}\cdot\left(\vec{J}_c + \partial\vec{D}/\partial t\right) = 0 \Rightarrow I_{S_A}(t) = I_{S_D}(t)$$

Quantum many-particle computations with Bohmian trajectories

1.- Quantum Many-Particle Computations with Bohmian Trajectories:

2.- Application to Electron Transport in Nanoelectronic Devices:

2.1.- Electron transport at the nanoscale

2.2.- Our quantum Monte Carlo algorithm

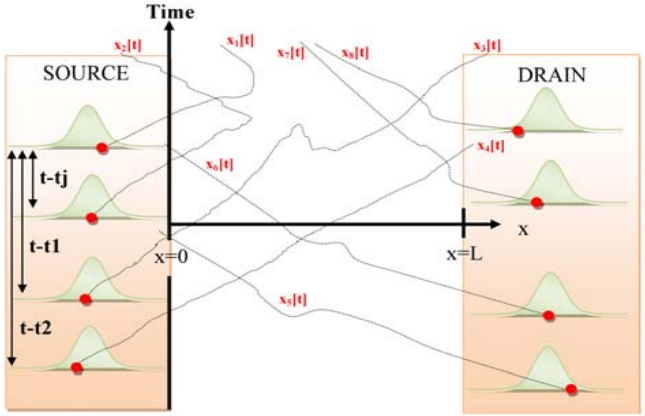
- 2.1.1.- The BITLLES simulator
- 2.1.2.- Numerical results for DC current
- 2.1.3.- Numerical results for current fluctautions
- 2.1.4.- Numerical results for transient and AC currents

3.- Conclusions and Future work

2.2.1.- Our quantum Monte Carlo algorithm: The Bittles simulator

Quantum Monte Carlo simulation for electron transport

Monte Carlo Casino (MONACO)



$$< I(t) >= \lim_{N_g, N_h \to \infty} \frac{1}{N_g \cdot N_h} \sum_{g=1}^{N_g} \sum_{h=1}^{N_h} I_{g,h}(t)$$

G-distribution:

initial position of Bohmian trajectory

H-distribution:

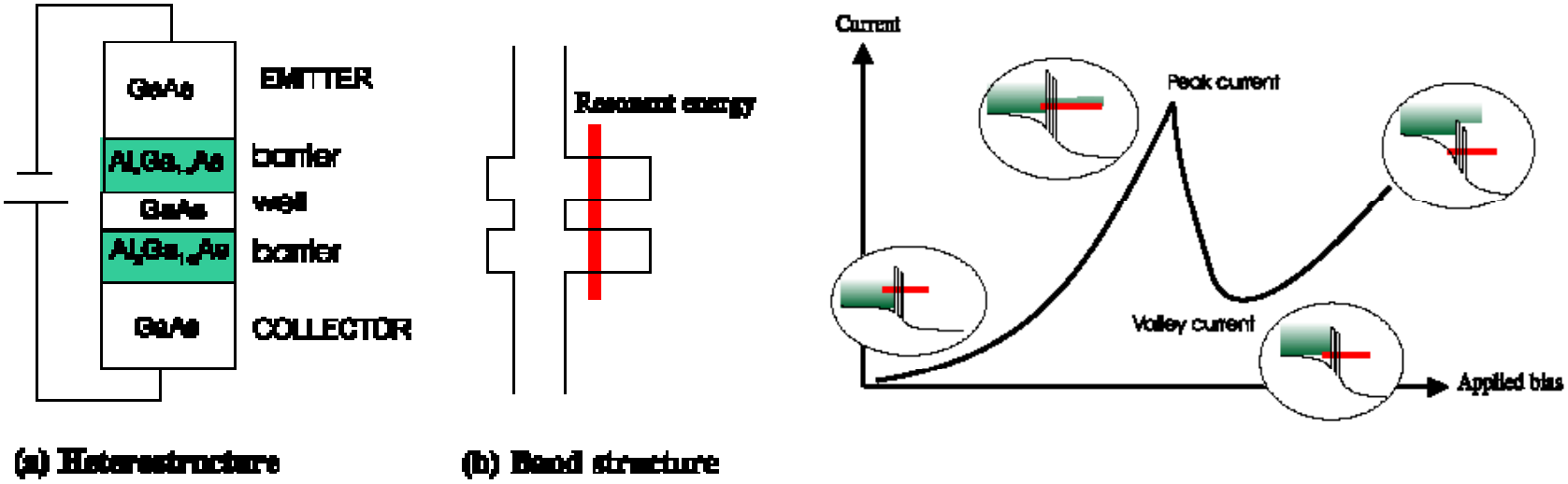
initial energy of the wave-packet

(Stationary and ergodic system)

$$\langle I \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T I_{g,h}(t') \cdot dt'$$

2.2.2.- Our quantum Monte Carlo algorithm: DC current

DC current for a Resonant Tunneling Device (RTD)



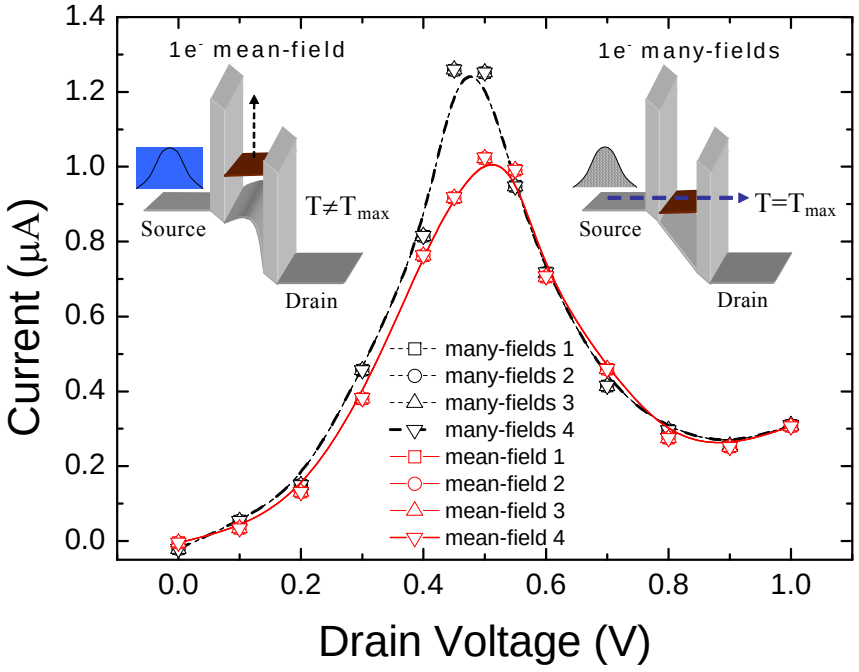
In the 80's, engineers expected that RTDs would substitute the FET transistor

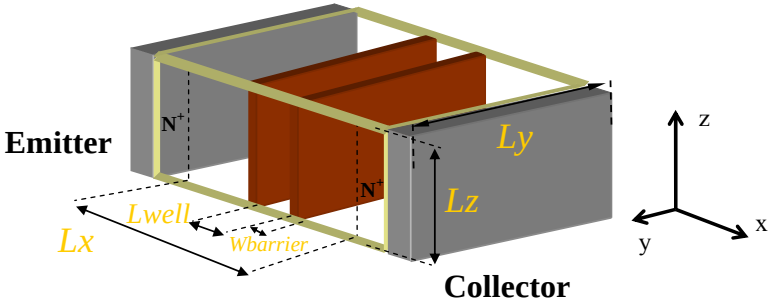
Now, it is a very useful scenario to understand QM phenomena at the nanoscale.

2.2.2.- Our quantum Monte Carlo algorithm: DC current

DC current for a Resonant Tunneling Device (RTD)

[G. Albareda et al. Phys. Rev. B 79, 075315 (2009)]

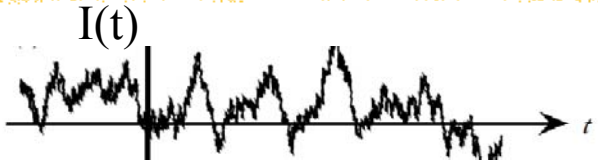




Electron transport **beyond the standard mean-field approximation**.
We include many-particle interaction effects on the current.

2.2.3.- Our quantum Monte Carlo algorithm: current fluctuations

Quantum Noise:



$$I(t) \qquad \Delta I(t) = I(t) - \bar{I} \qquad C_I(\tau) \qquad S_I(w)$$

Fluctuations — Autocorrelation — Fourier transform

Engineers do not like noise, it makes errors in the device.

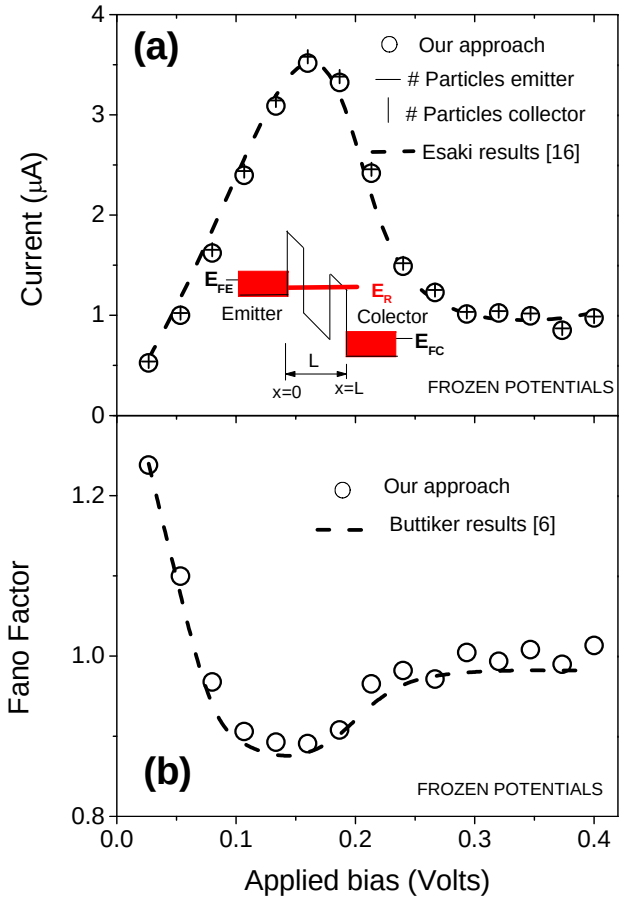
Physicist enjoy noise, because it shows phenomena that are not shown in DC

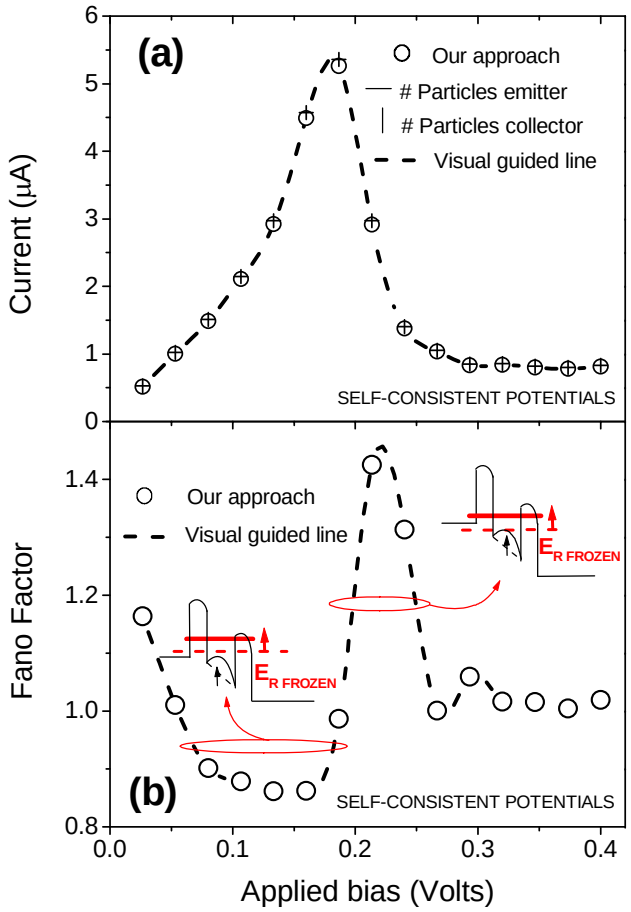
$$Fano\ Factor = F = \frac{S_I(w=0)}{< I >}$$

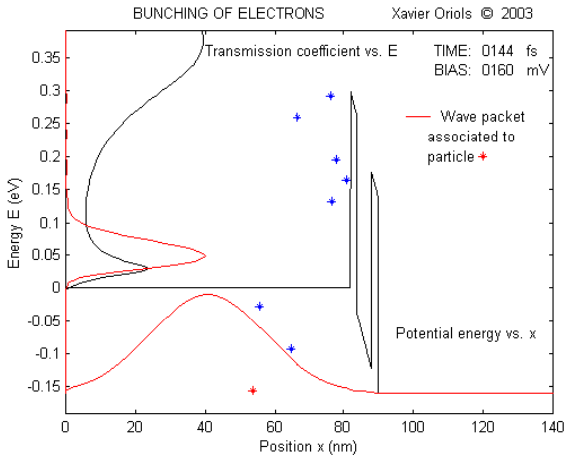
2.2.3.- Our quantum Monte Carlo algorithm: current fluctuations

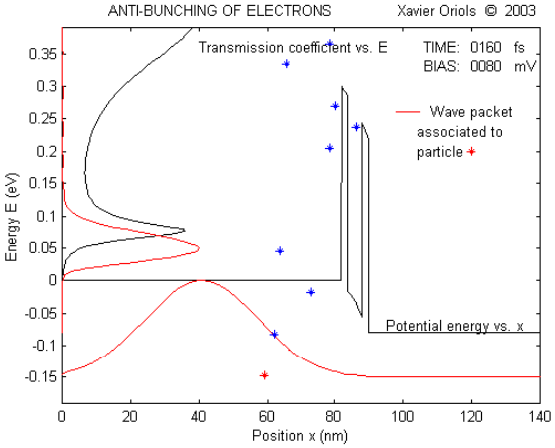
Effect of Coulomb correlation on current and noise

[X.Oriols, APL,85, 3596 (2004)]









2.2.4.- Our quantum Monte Carlo algorithm: transient and AC current

Time dependent (particle + displacement) current

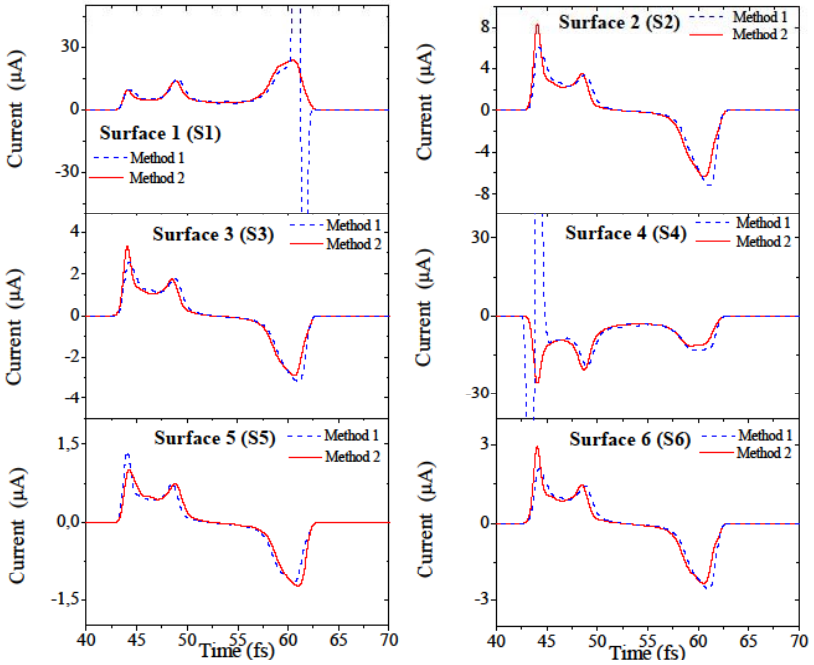
[A. Alarcon, JSTM, 2009(P01051) (2009)]

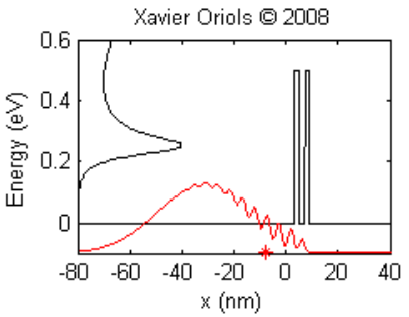
$$\vec{\nabla}\times\vec{H}=\vec{J}_c+\partial\vec{D}/\partial t \Rightarrow \vec{\nabla}\cdot\left(\vec{J}_c+\partial\vec{D}/\partial t\right)=0$$

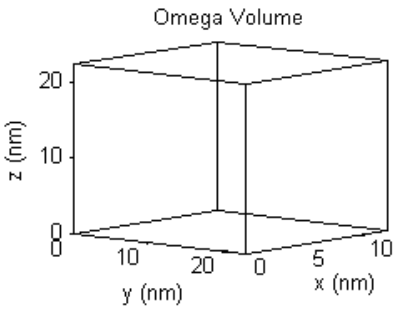
$$\vec{\nabla}\cdot\vec{D}=\rho \Rightarrow \text{Poisson equation}$$

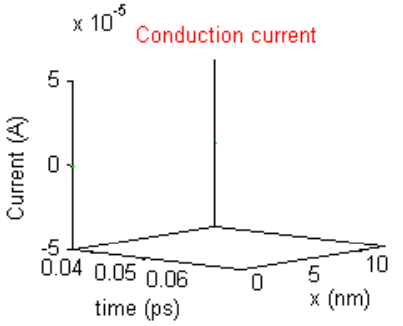
Continuity equation

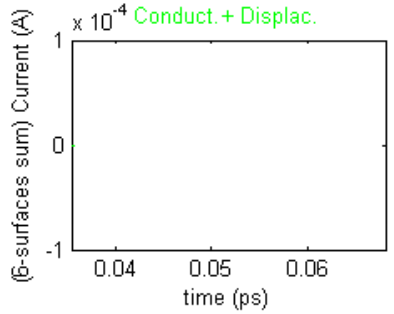
$$\partial\rho/\partial t+\vec{\nabla}\cdot\vec{J}_c=0$$







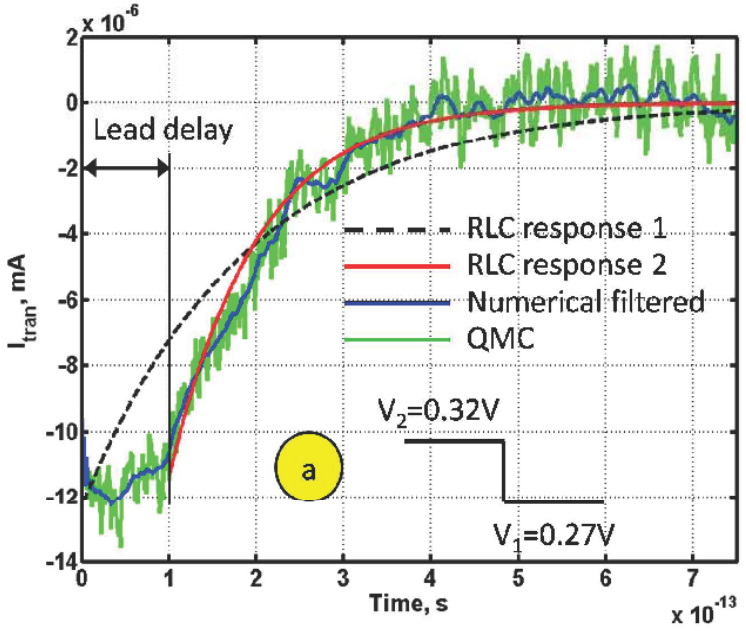


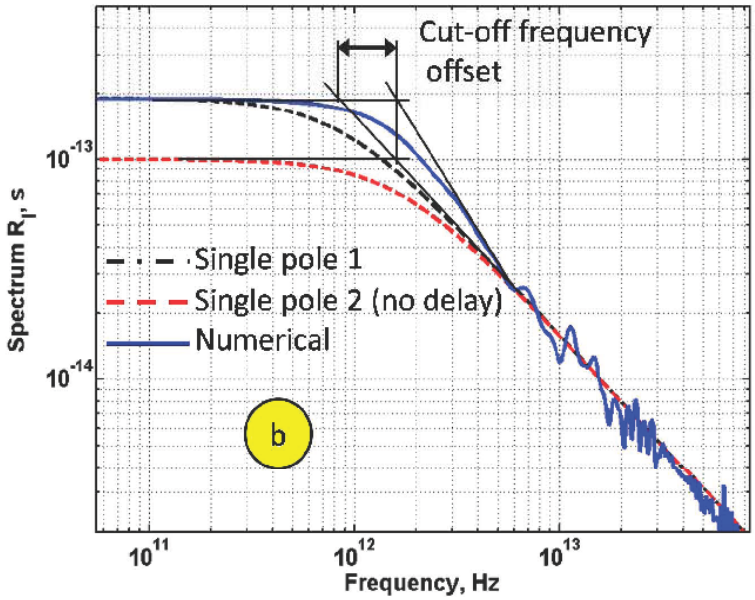


2.2.4.- Our quantum Monte Carlo algorithm: transient and AC current

Transit simulation:

[G. Albareda et al. Phys. Rev. B, 82, 085301 (2010)]





Non-ergodic system (ensemble average): $< I(t) >= \lim_{N_g, N_h \to \infty} \frac{1}{N_g \cdot N_h} \sum_{g=1}^{N_g} \sum_{h=1}^{N_h} I_{g,h}(t)$

Quantum many-particle computations with Bohmian trajectories

1.- Quantum Many-Particle Computations with Bohmian Trajectories:

2.- Application to Electron Transport in Nanoelectronic Devices:

3.- Conclusions and Future work

3.- Conclusions and future work

We have presented a algorithm to compute many-particle Bohmian trajectories.

1.-We have shown the existence of a single-particle Schrodinger equation that computes a many-particle Bohmian trajectory.

2.- Its practical application needs an educated guess on the potentials.

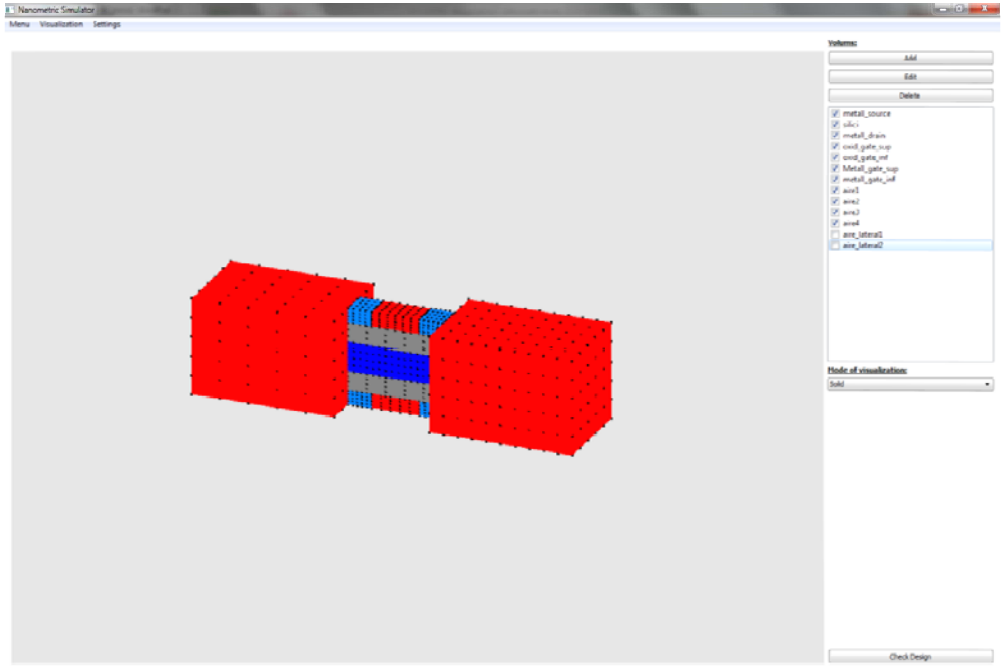
We apply the previous algorithm to a many-particle quantum MC simulator for computing electron quantum transport

We are able to compute DC, AC, transients and (current and voltage) noise with electron-electron correlations.

Simulation time 1-2 days for a complete I-V curve (N=100 electrons)

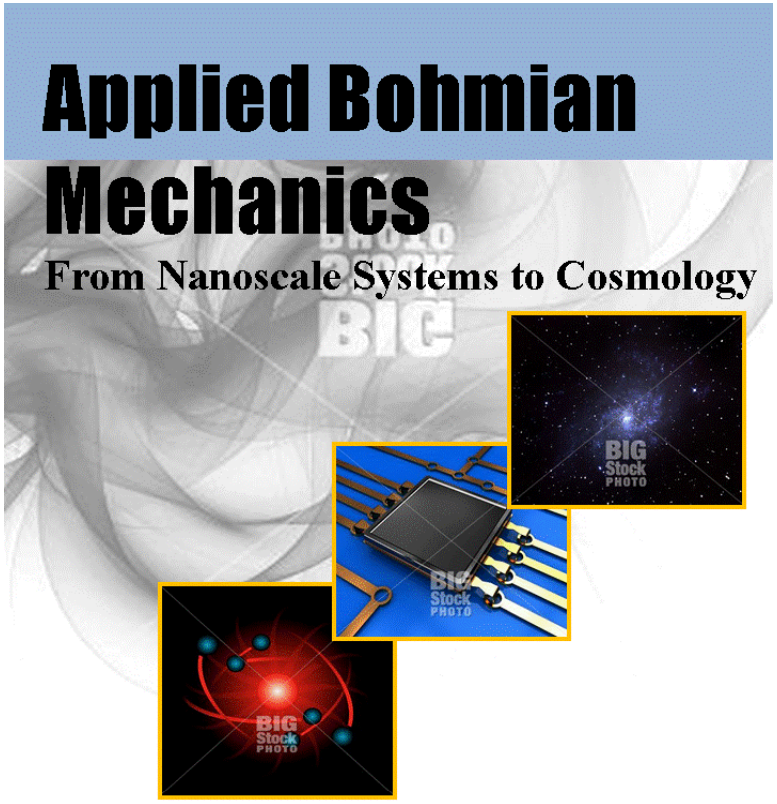
The BITLLES Simulator

Bohmian Interacting Transport in Electronic Structures



We have a three years project by the *Ministerio de Ciencia e Innovación* to develop the BITLLES simulator through project TEC2009-06986.

3.- Future work



• This book provides the first comprehensive discussion on the practical application of Bohmian ideas in several forefront research fields written by leading experts, with an extensive updated bibliography.

• This book provides a didactic introduction to Bohmian mechanics easily accessible for graduate and undergraduate students including a thorough list of exercises and easily programmable codes.

Readership

The book is addressed to students in physics, chemistry, electrical engineering, applied mathematics, nanotechnology, as well as both theoretical and experimental researchers who seek an intuitive understanding of the quantum world and new computational tools for their everyday research activity.

978-981-4316-39-2
Cloth, 400 pages (approx.)
Fall 2011, US$149

How to order

You can place an order from any good bookstores or email us at **sales@panstanford.com** for more information.

3.- Conclusions and future work

Acknowledgment

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- X.Cartoixà,
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Research Group of Computational Nanoelectronics
NANOCOMP

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Thank you very much for your attention