BITLLES: a quantum-trajectory simulation tool for electron transport in large electronic structures

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Electron transport modeling for guiding electronic industry

Classical approaches (microelectronics)

Monte Carlo technique for the Boltzmann transport equation

Accurate and intuitive picture of the dynamics of electrons using trajectories

Difficulty for quantum effects

The quantum effects

Quantum approaches (nanoelectronics)

Single-particle approaches

Landauer formalism
Wigner function model

Difficulty to treat electron correlations

The many body problem

Many-particle approaches

DFT
Green's functions

Difficulty for AC and noise

Time-dependent correlations

Bohmian Interacting Transport for non-equiLibrium eLEctronic Structures

BITLLES: a quantum-trajectory simulation tool for electron transport in large electronic structures

1.- Introduction:

2.- Theoretical framework of BITLLES

2.1.- Bohmian Mechanics

2.2.- The many-body problem

2.3.- The time-dependent correlations

3.- Numerical application to electron devices:

4.- Conclusions and Future work

1.1.- Introduction: Bohmian mechanics

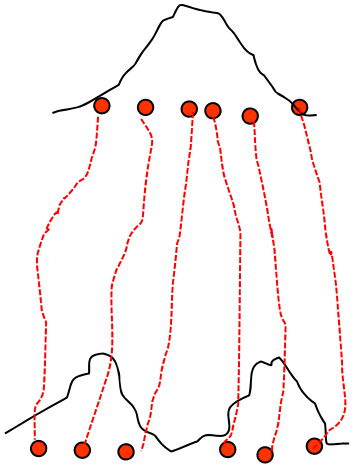
Playing with the many-particle Schrodinger equation,

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

L. De Broglie

D. Bohm

J.S. Bell



- Look for a continuity equation: $$\frac{\partial \left|\Psi(\vec{r}_1,..,\vec{r}_N,t)\right|^2}{\partial t} + \sum_{k=1}^{N} J_k(\vec{r}_1,..,\vec{r}_N,t) = 0$$

- Define a velocity: $$v_k(\vec{r}_1,..,\vec{r}_N,t) = \frac{J_k(\vec{r}_1,..,\vec{r}_N,t)}{\left|\Psi(\vec{r}_1,..,\vec{r}_N,t)\right|^2}$$

- Define a Bohmian trajectory: $$x_k[t] = x_k[t_o] + \int_{t_o}^{t} dt' \cdot v_k(\vec{r}_1[t'],..,\vec{r}_N[t'],t')$$

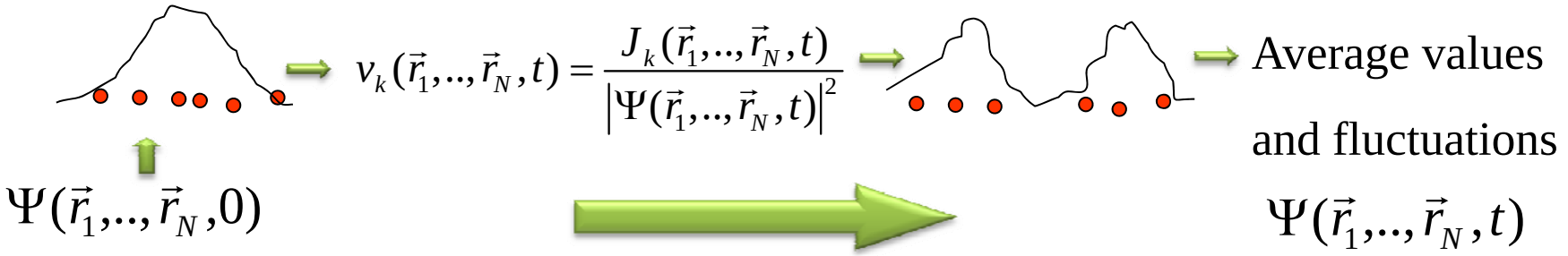
1.1- Introduction: Bohmian mechanics

…By construction, Bohmian mechanics reproduce all ensemble results.

Main criticism against Bohmian mechanics

"…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 comunication with Shelly Goldstein)



The many body problem

$$\Psi(x_1,\ldots,x_N,t) = R(x_1,\ldots,x_N,t)\cdot e^{iS(x_1,\ldots,x_N,t)/\hbar}$$

M grid points

M^N configuration point

$$v_a(x_1[t],..,x_N[t],t) = \left.\frac{\partial S(x_1,....,x_N,t)/\partial x_a}{m}\right|_{x_1=x_1[t],....,x_N=x_N[t]} = \left.\frac{J_a(x_1,\ldots,x_N,t)}{\left|\Psi(x_1,\ldots,x_N,t)\right|^2}\right|_{x_1=x_1[t],....,x_N=x_N[t]}$$

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

M grid points

$M\cdot N$ configuration point

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

1.2.- Introduction: the many body problem

The many body problem

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

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

Good points :

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

2rd The correlations are introduced into the time-dependent potentials

3th The interacting potential from (a classical-like) Bohmian trajectories

4th There is a real potential to account for “non-classical” correlations

5th There is a imaginary potential to account for non-conserving norms

6st The “N”D TDSE can be decomposed into 1D, 2D, 3D TDSE equations

1.2.- Introduction: the many body problem

The many body problem

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

Bad points :

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

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

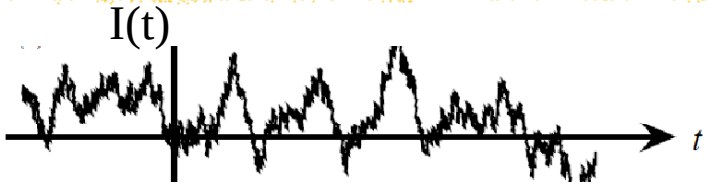
$$J_a(x_a,\vec{x}_b,t)=\frac{\hbar}{2\cdot R^2(\vec{x},t)}\left\{\sum_{k=1,k\neq a}^{N}\left\{\frac{\partial R^2(\vec{x},t)}{\partial x_k}\cdot v_k(\vec{x}[t],t)-\frac{\partial}{\partial x_k}\left(\frac{R^2(\vec{x},t)}{m}\cdot\frac{\partial S(\vec{x},t)}{\partial x_k}\right)\right\}\right\}$$

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

A similar difficulty found in the DFT (or TD-DFT) .....

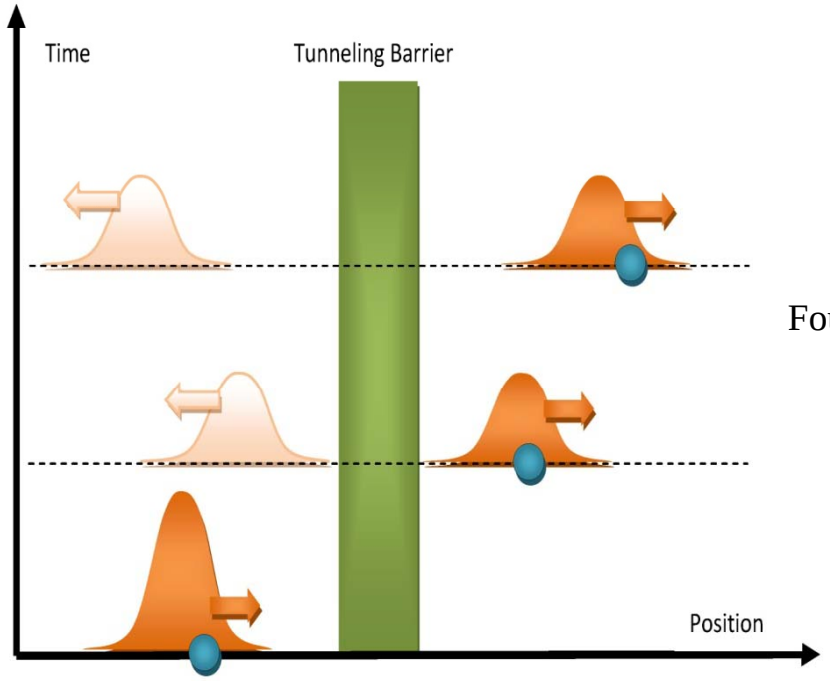
Time-dependent correlations

Quantum Noise:



$$\Delta I(t) = I(t) - \bar{I}$$

Fluctuations



$$\tau = t_2 - t_1$$

Autocorrelation $$R(\tau)=\overline{\Delta I(t)\Delta I(t+\tau)}$$

Fourier transform $$S(f)=\int_{-\infty}^{\infty} R(\tau)\, e^{-j2\pi f\tau}\, d\tau$$

$$Fano\ Factor = F = \frac{S_I(w=0)}{2 \cdot q \cdot < I >}$$

…By construction, Bohmian mechanics can also reproduce correlation results.

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1.- Introduction:

2.- Theoretical framework of BITLLES

3.- Numerical application to electron devices:

- 3.1.- Quantum Monte Carlo scheme
- 3.2.- DC current
- 3.3.- Transient current
- 3.4.- Noise in the current

4.- Conclusions and Future work

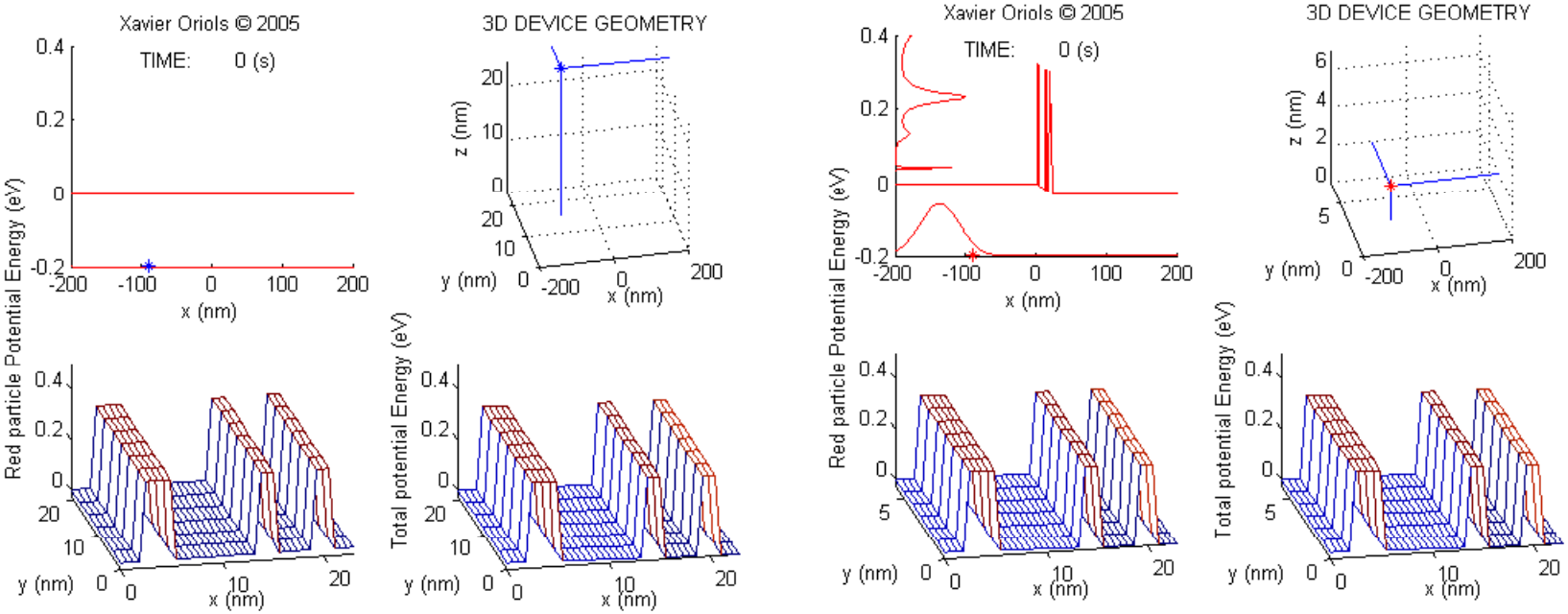
3.2.- Qauntum Monte Carlos Scheme

Quantum Monte Carlo scheme for current computation:

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

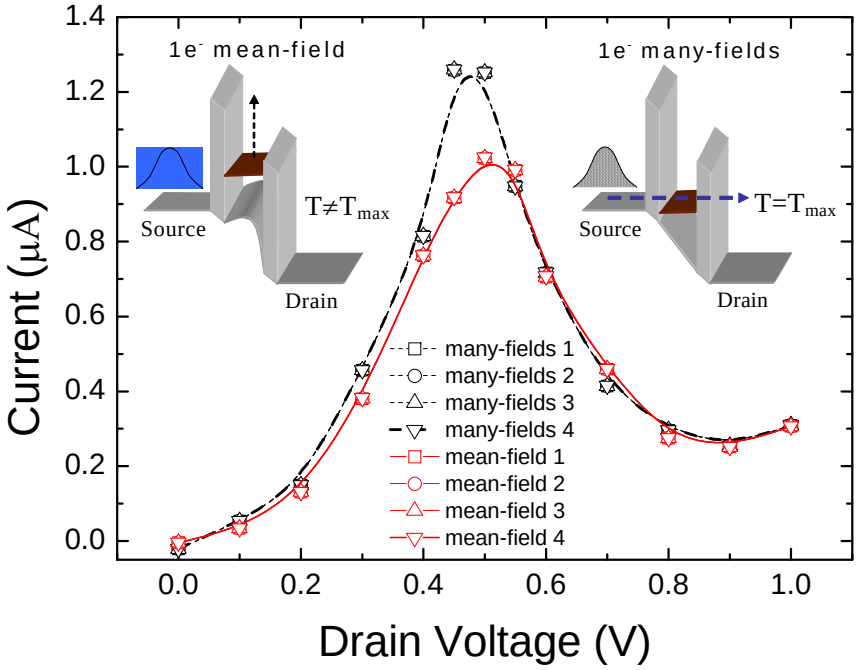
G-distribution: initial position of Bohmian trajectory

H-distribution: initial energy of the wave-packet

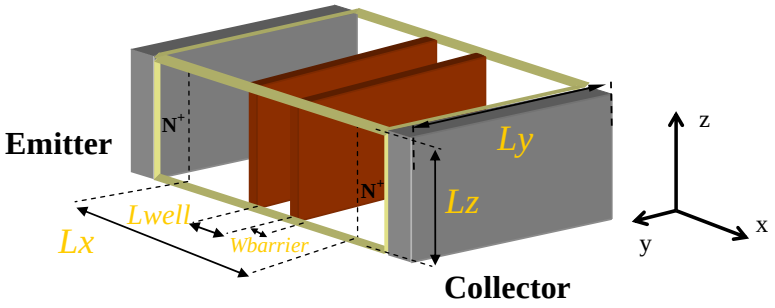


3.2.- DC current

DC current for a Resonant Tunneling Device (RTD)



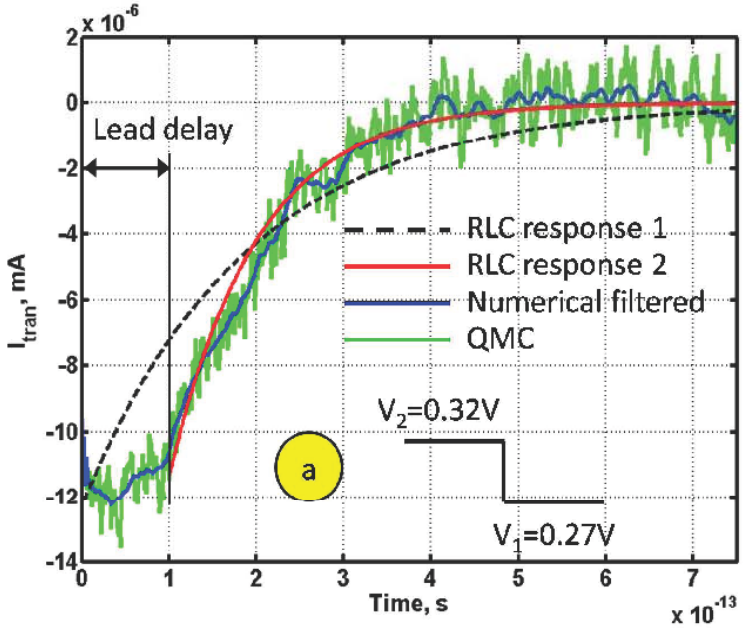
[G. Albareda et al. Phys. Rev. B 79, 075315 (2009)]

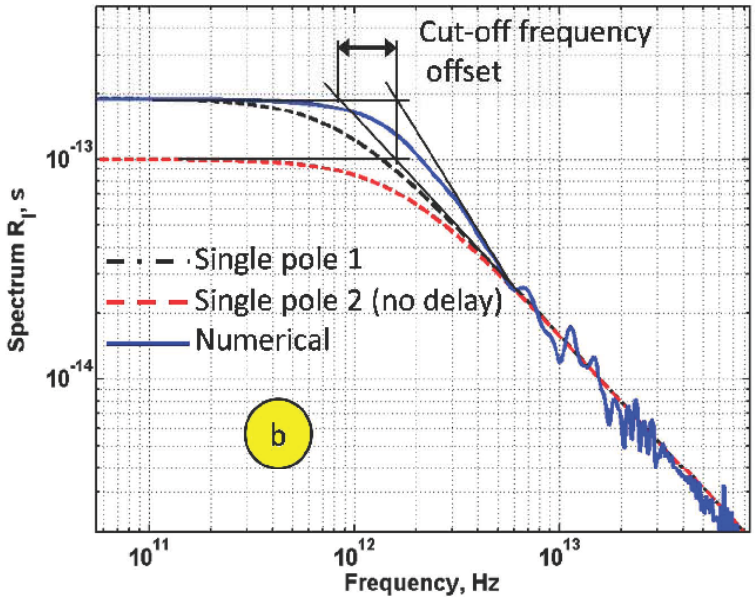


Electron transport **beyond the standard mean-field approximation**. We include many-particle (Coulomb and exchange) interaction effects on the current.

3.3.- Transient current

Transient simulation for a RTD in the NDC region for a step voltatge:



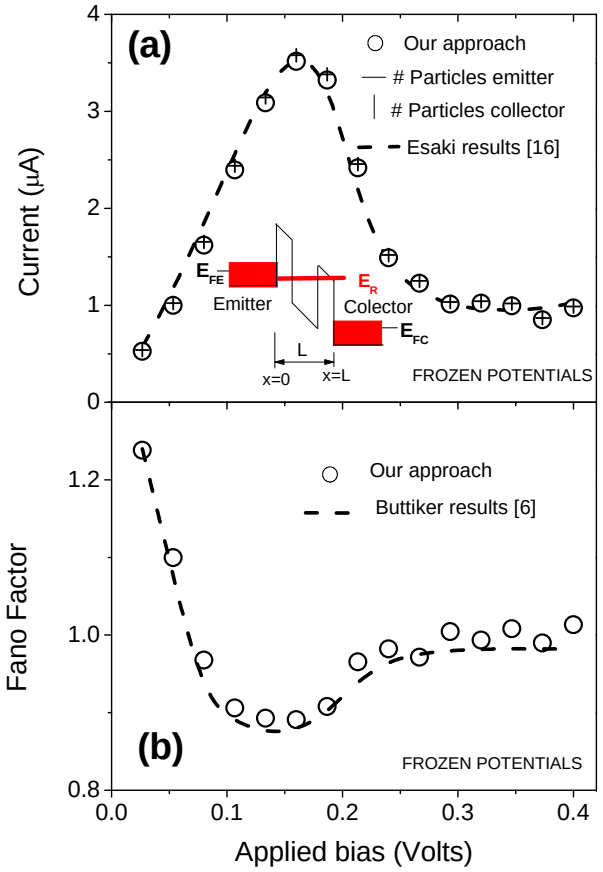


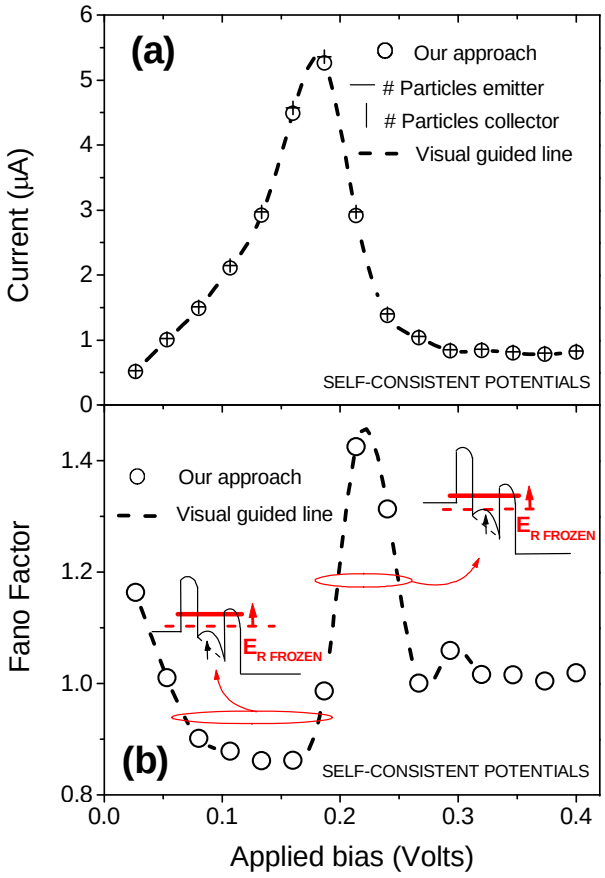
Non-ergodic system (ensemble average): $< I(t) >= \lim_{N_g, N_h \to \infty} \frac{1}{N_g \cdot N_h} \sum_{g=1}^{N_g} \sum_{h=1}^{N_h} I_{g,h}(t)$

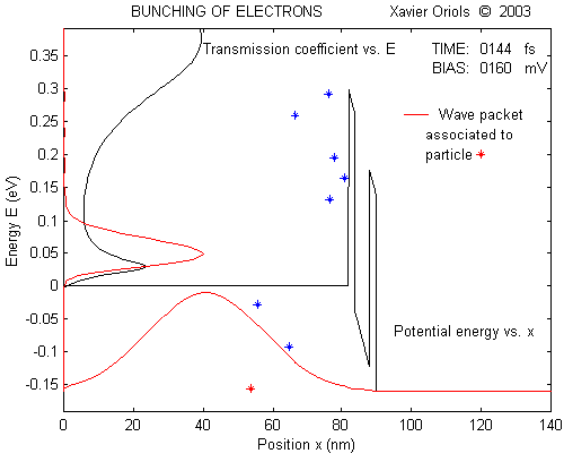
[F.Traversa, IEEE TED (2011)]

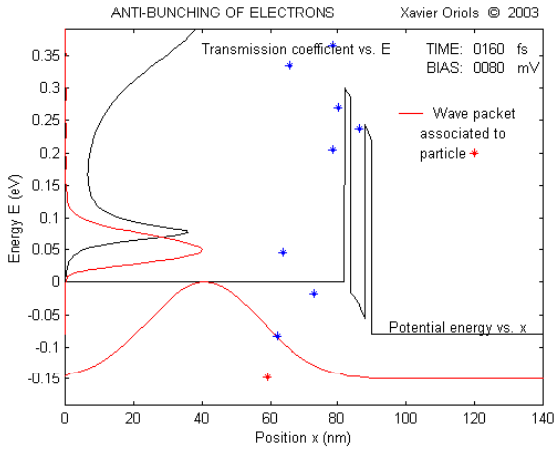
2.2.3.- Our quantum Monte Carlo algorithm: current fluctuations

current noise simulation: superpoissonian and subpoissonian Fano factor









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3.- Conclusions and future work

Bohmian Interacting Transport for non-equiLibrium eLEctronic Structures

Its ability to deal with many-particle Coulomb and exchan

The many body problem

Its ability to provide all moments of the current distribution (D

Time-dependent correlations

Computational burden:

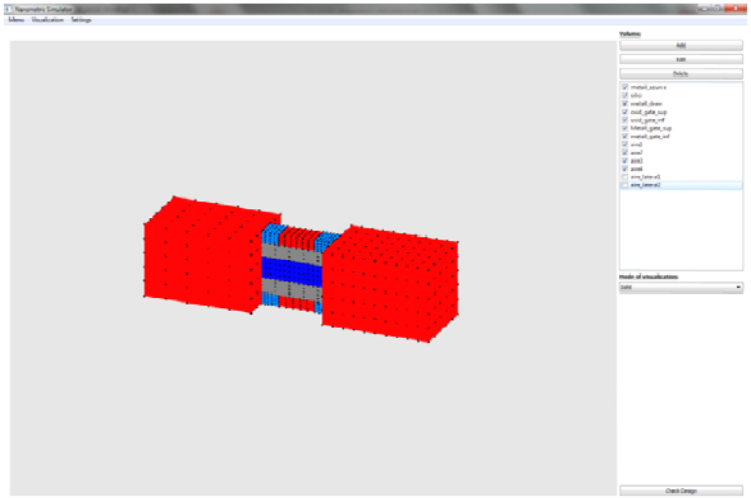
For each electron (maximum 100-200 electrons),
a 3D Poisson equation and a 1D time-dependent Schrodinger equation

3.- Conclusions and future work

The BITLLES code:

More than 15000 FORTRAN lines.

It has also a 3000 C++ lines for a (Windows, MAC and Linux compatible) user friendly environment to design an verify the simulated electronic structures.



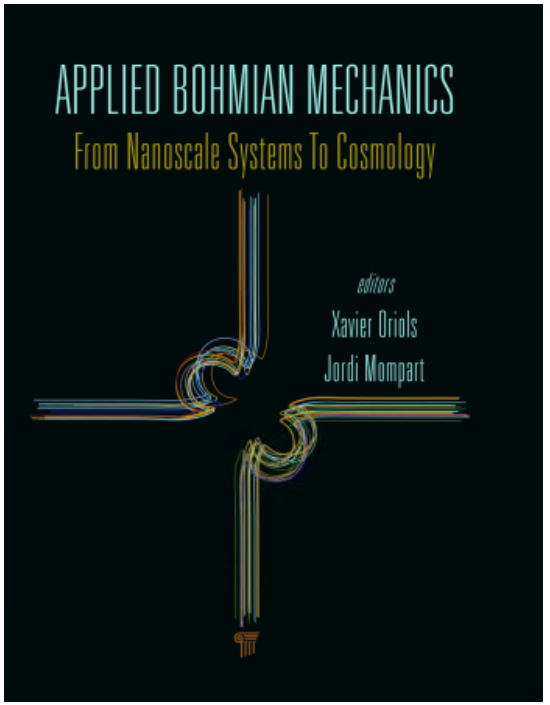
Simulation time:

One-two days for the complete I-V curve (DC, AC and noise) of a simulation box of hundred of electrons with a cluster of 40 Intel Xeon CPUs at 2.7GHz

3.- Conclusions and future work

Other works

➡ Photoionization with strong lasers



X.Oriols and J.Mompart, Applied Bohmian Mechanics: From Nanoscale Systems to Cosmology, (2011). ISBN: 978-981-4316-39-2]

Acknowledgment

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Thank you very much for your attention