Bohmian solution to the measurement of many-body systems: Sequential current in mesoscopic electron devices

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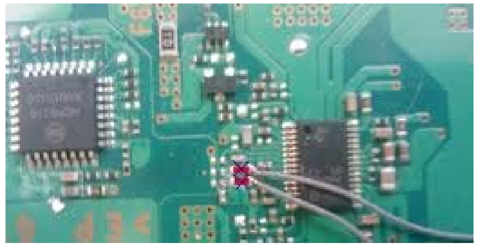
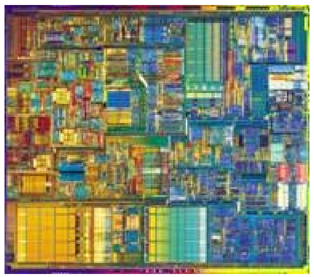
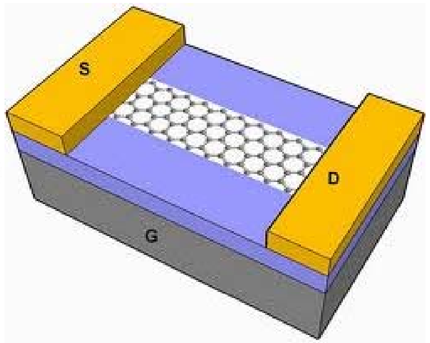
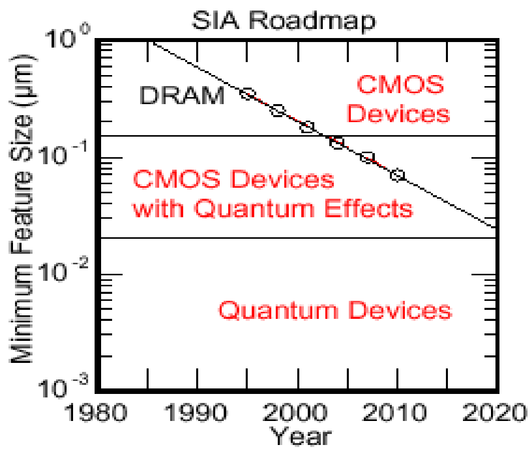
What is the relation between **electronics** and **Bohmian solution to the measurement of many-body systems**

Electron devices









1.000.000.000 transistors per CPU !!!

Bohmian mechanics

Bohmian solution to the measurement of many-body systems: Sequential current in mesoscopic electron devices

1.- Introduction:

2.- The use of quantum (Bohmian) trajectories

3.- Numerical results with the BITLLES simulator

4.- Conclusions and Future work

Bohmian solution to the measurement of many-body systems: Sequential current in mesoscopic electron devices

1.- Introduction:

1.1.- Why we have to worry about **many-body systems** ?

1.2.- Why we have to worry about **sequential measurement** ?

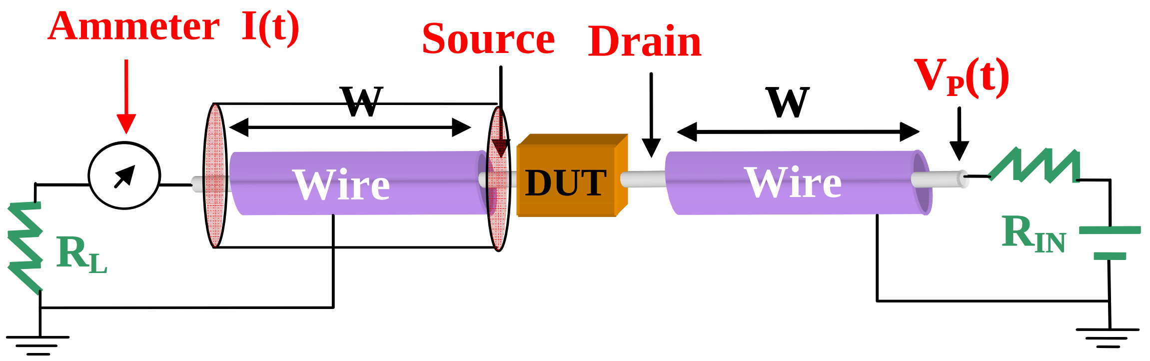
2.- The use of quantum (Bohmian) trajectories

3.- Numerical results with the BITLLES simulator

4.- Conclusions and Future work

1.1.- Why we have to worry about **many-body systems** ?

What we measure when we measure the current ?



→ **I(t) measured** in the ammeter

→ **I(t) computed** in the DUT

Integral (surface) conservation

$$\int_s J_T(\vec{r},t)\,d\vec{s} = 0$$

→

Differential (local) conservation

$$\nabla J_T(\vec{r},t) = 0$$

Which magnitude accomplish the differential (local) conservation ?

The many body problem

Continuity equation $\frac{d\rho}{dt} + \vec{\nabla}\cdot\vec{J}_c = 0$ →

$$\nabla\cdot\left(\vec{J}_c(\vec{r},t) + \varepsilon\frac{d\vec{E}(\vec{r},t)}{dt}\right) = 0$$

Poisson (Coulomb) equation $\vec{\nabla}\cdot\vec{E}(\vec{r},t) = \rho(\vec{r},t)/\varepsilon$

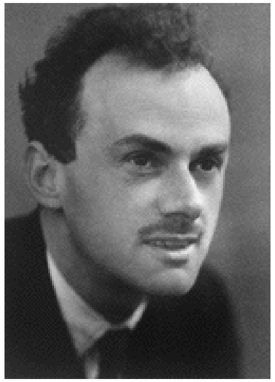
The **total current** measured at the ammeter is equal to that computed at the DUT

1.1.- Why we have to worry about **many-body systems** ?

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."

Multi-time measurement and displacement current in time-dependent quantum transport

1.2.- Why we have to worry about **sequential measurement** ?

Two "orthodox" dynamical law for describing the evolution of a quantum system:

1-law: Unitary-evolution (when no measure): Schrodinger equation

$$i\hbar\frac{d}{dt}\langle x|\psi(t)\rangle = H\langle x|\psi(t)\rangle \Rightarrow |\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle = U|\psi(0)\rangle$$

2-law: Non-unitary-evolution (when measure): "Collapse"

$$\langle x|\psi(0)\rangle \to \langle x|u_i(t)\rangle \Rightarrow |\psi(t)\rangle = |u_i\rangle\langle u_i||\psi(0)\rangle$$

Example: a single-time (ensemble) measurement

$$<I>=\sum_i I_i P(I_i)=\sum_i I_i\langle\psi|u_i\rangle\langle u_i|\psi\rangle = \sum_i \langle\psi|\hat{I}u_i\rangle\langle u_i|\psi\rangle = \langle\psi|\hat{I}\psi\rangle$$

$$P(I_i)=\langle\psi|u_i\rangle\langle u_i|\psi\rangle = |\langle u_i|\psi\rangle|^2 \quad \hat{I}|u_i\rangle = I_i|u_i\rangle \quad 1=\sum_i |u_i\rangle\langle u_i|$$

For ergodic system ⇒ Time-average is equal to ensemble average

The prediction of DC current can be computed without worrying about "collapse"

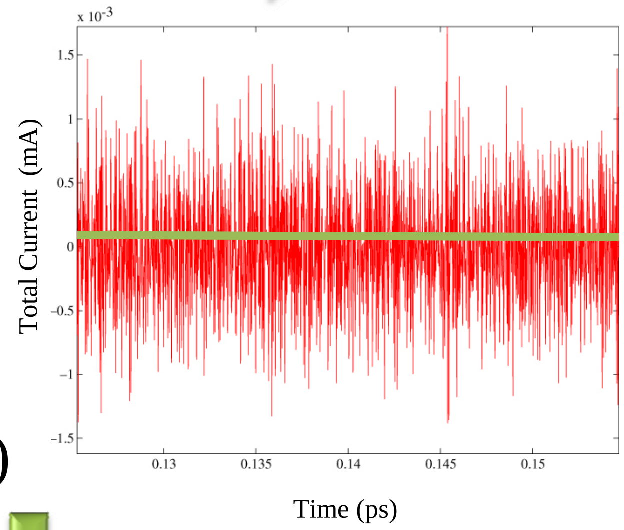
1.2.- Why we have to worry about **sequential measurement** ?

Sequential measurement

Example: noise (current fluctuations) measurement

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

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



$I(t)$ → fluctuations → $\Delta I(t) = I(t) - \bar{I}$ → Autocorrelation → $R(\tau)$ → Fourier transform → $S(f)$

$$\tau = t_2 - t_1 \quad R(\tau) = \langle \Delta I(t) \Delta I(t+\tau) \rangle$$

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

$$R(\tau) = \langle I(t_2) I(t_1) \rangle - (I_{DC})^2$$

We need the measurement of **I(t2)** after the measurement **I(t1)**.

1.2.- Why we have to worry about multi-time measurement ?

Sequential measurement

How we can compute the quantum two-times correlations ?

$$\langle I(t_2)I(t_1)\rangle = \sum_j \sum_i I_j(t_2)\cdot I_i(t_1)\cdot P\left(I_j(t_2),I_i(t_1)\right)$$

$$P\left(I_j(t_2),I_i(t_1)\right) = \langle\psi(0)|u_i\rangle\langle u_i|\hat{U}^\dagger(\tau)|u_j\rangle\langle u_j|\hat{U}(\tau)|u_i\rangle\langle u_i||\psi(0)\rangle$$

How we can compute the probability ?

With the modulus of the wavefunction

Time			
t1	Measuring at t1	2-law:	$|\psi(t_1)\rangle = |u_i\rangle\langle u_i||\psi(0)\rangle$
	Time-evolution	1-law:	$|\psi(t_2^-)\rangle = \hat{U}(\tau)|\psi(t_1)\rangle$
t2	Measuring at t2	2-law:	$|\psi(t_2)\rangle = |u_j\rangle\langle u_j||\psi(t_2^-)\rangle$

Final state

$$|\psi(t_2)\rangle = |u_j\rangle\langle u_j|\hat{U}(\tau)|u_i\rangle\langle u_i||\psi(0)\rangle$$

Bohmian solution to the measurement of many-body systems: Sequential current in mesoscopic electron devices

2.1.- Bohmian mechanics (quantum hydrodynamics)

L. De Broglie

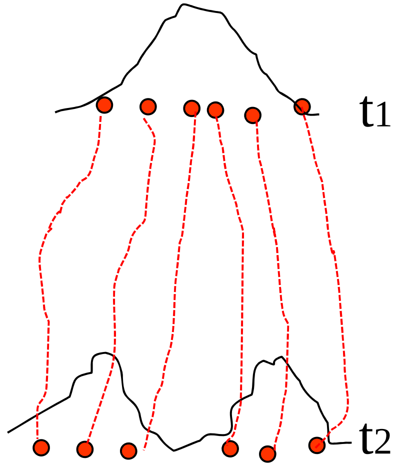
1924

D. Bohm

1952

J.S. Bell

1960



“Playing” with the many-particle Schrodinger equation....

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

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

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

- Define a Bohmian trajectory: $$\vec{r}_1[t] = \vec{r}_1[t_0] + \int_{t_0}^{t} dt' v_k(\vec{r}_1[t'],..,\vec{r}_N[t'],t')$$

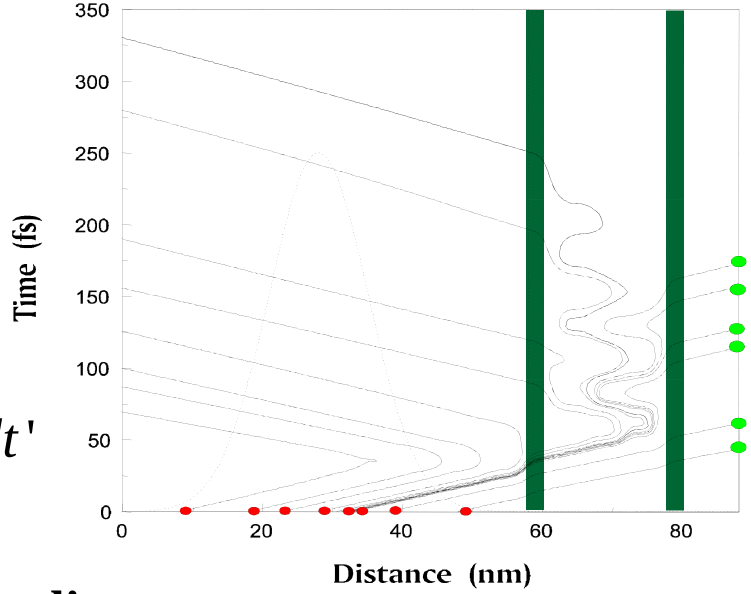
The computation of many-particle trajectories exactly reproduce the evolution of the modulus of the wavefunction.

Example: A wave packet impinging upon a double barrier structure

1.- First, $\psi(x,t)$

2.- Second, $v(x,t)=\dfrac{J(x,t)}{|\psi(x,t)|^2}$

3.- Third: $x^i[t]=x_o^i+\int_0^t v(x^i[t'],t')\cdot dt'$



Main criticism against Bohmian formalism:

"…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)

Bohmian solution to the measurement of many-body systems: Sequential current in mesoscopic electron devices

2.2.- The conditional wave function: a successful tool

The many body problem

The "BIG" many-particle wave-function for N particles:

$$\Rightarrow \quad \Psi(x_1,\dots,x_N,t)$$

M^N **configuration point**

$$\Downarrow$$

$$v_1(x_1[t],..,x_N[t],t) = \left. \frac{J_1(x_1,\dots,x_N,t)}{|\Psi(x_1,\dots,x_N,t)|^2} \right|_{x_1=x_1[t],\dots,x_N=x_N[t]}$$

$$\Downarrow$$

$$v_1(x_1[t],..,x_N[t],t) = \left. \frac{J_1((x_1,x_2[t],..,x_N[t],t)}{|\Psi(\vec{r}_1,x_2[t],..,x_N[t],t)|^2} \right|_{x_1=x_1[t]}$$

$$\Downarrow$$

The "LITTLE" **conditional** wave-functions for N particles:

$$\Rightarrow \quad \Psi(x_1,x_2[t],..,x_N[t],t) \equiv \Psi_1(x_1,t)$$

$M \cdot N$ **configuration point**

The computation of many-particle trajectories from one BIG or from N LITTLE conditional wave functions are exactly identical.

What is the equation satisfied by the conditional wave-function ?

2.2.- The conditional wave function: a successful tool

$$i\hbar\frac{\partial\Psi_1(x_1,t)}{\partial t}=\left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2}+U_1(x_1,\vec{x}_b[t],t)+G_1(x_1,\vec{x}_b[t],t)+i\cdot J_1(x_1,\vec{x}_b[t],t)\right\}\Psi_1(x_1,t)$$

Good points :

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

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

The correlations are introduced into the time-dependent potentials

4^{th} The interacting potential from (a classical-like) Bohmian trajectories

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

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

Bad points :

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

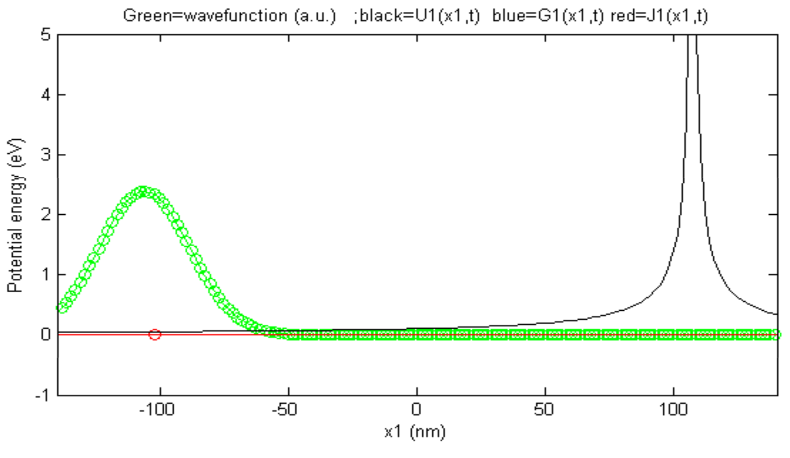
This is exactly the same difficulty found in the DFT (or TD-DFT)

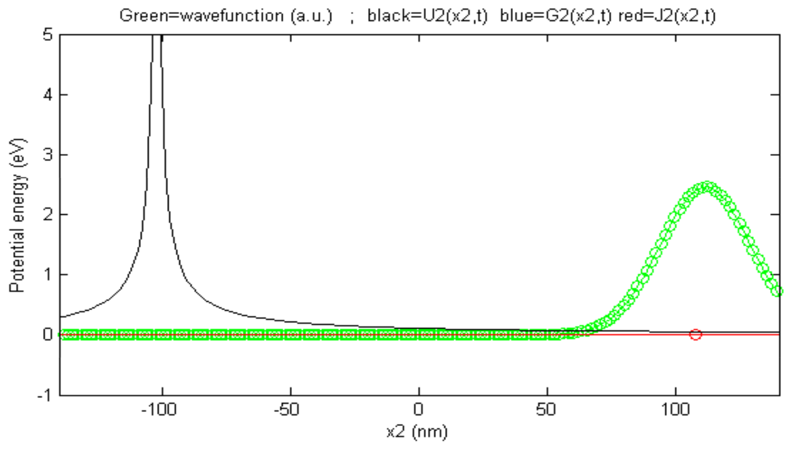
2.2.- The conditional wave function: a successful tool

Example: two Coulomb interacting particles

$$i\hbar\frac{\partial\Psi_1(\vec{r}_1,t)}{\partial t}=\left\{-\frac{\hbar^2}{2m^*}\nabla_1^2+\frac{q^2}{4\pi\varepsilon\varepsilon_0\left|\vec{r}_1-\vec{r}_2[t]\right|}\right\}\Psi_1(\vec{r}_1,t)\quad;\quad\vec{r}_1[t]=\vec{r}_1[t_o]+\int_{t_o}^{t}dt\left.\frac{J_1(\vec{r}_1,t)}{|\Psi_1(\vec{r}_1,t)|^2}\right|_{\vec{r}_1=\vec{r}_1[t]}$$

$$i\hbar\frac{\partial\Psi_2(\vec{r}_2,t)}{\partial t}=\left\{-\frac{\hbar^2}{2m^*}\nabla_2^2+\frac{q^2}{4\pi\varepsilon\varepsilon_0\left|\vec{r}_1[t]-\vec{r}_2\right|}\right\}\Psi_2(\vec{r}_2,t)\quad;\quad\vec{r}_2[t]=\vec{r}_2[t_o]+\int_{t_o}^{t}dt\left.\frac{J_2(\vec{r}_2,t)}{|\Psi_2(\vec{r}_2,t)|^2}\right|_{\vec{r}_2=\vec{r}_2[t]}$$

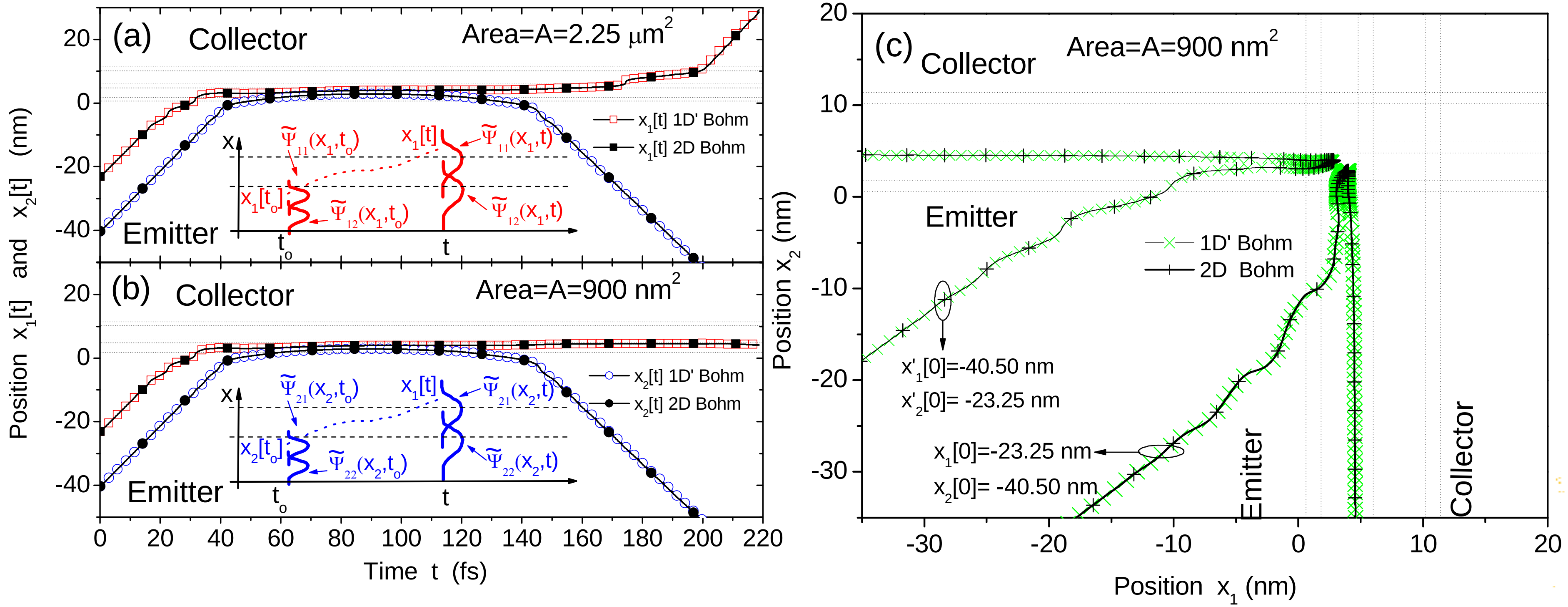




Example: two (Coulomb and Exchange) interacting particles

Ensemble results associated to x1 are indistinguishable from those associated to x2.

But, Bohmian trajectories associated to particle x1 or to x2 are distinguishable.



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

2.2.- The conditional wave function: a successful tool

Is it possible to improve the estimations of G and J functions ?

$$i\hbar\frac{\partial\Psi_1(x_1,t)}{\partial t}=\left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2}+U_1(x_1,\vec{x}_b[t],t)+G_1(x_1,\vec{x}_b[t],t)+i\cdot J_1(x_1,\vec{x}_b[t],t)\right\}\Psi_1(x_1,t)$$

Taylor expansion of the many-particle wave function:

$$\Psi(x_1,x_2,t)=\Psi(x_1,x_2,t)\Big|_{x_2=x_2[t]}+\frac{\partial\Psi(x_1,x_2,t)}{\partial x_2}\Bigg|_{x_2=x_2[t]}(x_2-x_2[t])+\frac{1}{2!}\frac{\partial^2\Psi(x_1,x_2,t)}{\partial x_2^2}\Bigg|_{x_2=x_2[t]}(x_2-x_2[t])^2+....$$

The "LITTLE" **conditional** wave-functions for the derivatives:

$$\Psi(x_1,x_2,t)\Big|_{x_2=x_2[t]}\equiv\Psi_1(x_1,t)\qquad\qquad \frac{\partial^n\Psi(x_1,x_2,t)}{\partial x_2^n}\Bigg|_{x_2=x_2[t]}\equiv\Psi_1^n(x_1,t)$$

A coupled system of equations for the derivatives **conditional** wave-functions

$$i\hbar\frac{\partial\Psi_1^n(x_1,t)}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi_1^n(x_1,t)}{\partial x_1^2}-\frac{\hbar^2}{2m}\Psi_1^{n+2}(x_1,t)+i\hbar\Psi_1^{n+1}(x_1,t)\frac{d\,x_2[t]}{dt}+\sum_{i=0}^{n}\binom{n}{i}\frac{\partial^{n-i}U(x_1,x_2,t)}{\partial x_2^{n-i}}\Bigg|_{x_2=x_2[t]}\Psi_1^i(x_1,t)$$

For n=0,1,2,3,4,5....... **[T.Norsen, Found. Phys 40, 1858 (2010)]**

Bohmian solution to the measurement of many-body systems: Sequential current in mesoscopic electron devices

2.3.- The computation of the displacement current

The TOTAL time-dependent current:

$$\langle I(t)\rangle = \int_{S_D} \langle \vec{J}_c(t)\rangle d\vec{s} + \int_{S_D} \varepsilon \frac{\partial \langle \vec{E}(r,t)\rangle}{\partial t} \cdot d\vec{s}$$

Quantum ensemble average value

Ensemble over all position distributions weighted by the probability

$$\langle \vec{E}(\vec{r},t)\rangle = \int d\vec{r}_1 \ldots \int d\vec{r}_N \left|\Psi(\vec{r}_1,\ldots,\vec{r}_N,t)\right|^2 \vec{E}(\vec{r},\vec{r}_1,\ldots,\vec{r}_N,t)$$

Solving the N-particle Poisson equation

$$\nabla \vec{E}(\vec{r},\vec{r}_1,\ldots,\vec{r}_N,t) = \sum_{i=1}^{N} q\delta(\vec{r}-\vec{r}_i)$$

Solving the N-particle Schrodinger equation ¿?

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

The many body problem

2.3.- The computation of the displacement current

The TOTAL time-dependent "Bohmian"current:

$$\langle I(t)\rangle = \int_{S_D} \langle \vec{J}_c(t)\rangle \cdot d\vec{s} + \int_{S_D} \varepsilon \frac{\partial \langle \vec{E}(r,t)\rangle}{\partial t} \cdot d\vec{s}$$

$$\langle \vec{E}(\vec{r},t)\rangle = \int d\vec{r}_1 .....\int d\vec{r}_N \left|\Psi(\vec{r}_1,...,\vec{r}_N,t)\right|^2 \vec{E}(\vec{r},\vec{r}_1,...,\vec{r}_N,t)$$

An ensemble of Bohmian trajectories reproduces the wavefunction modulus

$$\left|\Psi(\vec{r}_1,...,\vec{r}_N,t)\right|^2 = \lim_{M\to\infty} \frac{1}{M} \sum_{j=1}^{M} \delta(\vec{r}_1 - \vec{r}_1^{\,j}[t]) \cdot \cdots \cdot \delta(\vec{r}_N - \vec{r}_N^{\,j}[t])$$

The prediction of AC current can be computed from an ensemble over trajectories.

$$\left.\begin{array}{l} \vec{r}_1^{\,j}[t] \quad ; \quad \psi_1^j(\vec{r}_1,t) \\ \quad .... \\ \vec{r}_N^{\,j}[t] \quad ; \quad \psi_N^j(\vec{r}_N,t) \end{array}\right\} \nabla \vec{E}^j(\vec{r},\vec{r}_1^{\,j}[t],...,\vec{r}_N^{\,j}[t],t) = \sum_{i=1}^{N} q\delta(\vec{r} - \vec{r}_i^{\,j}[t])$$

$$\langle \vec{E}(\vec{r},t)\rangle = \lim_{M\to\infty} \frac{1}{M} \sum_{j=1}^{M} \vec{E}^j(\vec{r},\vec{r}_1^{\,j}[t],...,\vec{r}_N^{\,j}[t],t)$$

2.3.- The computation of the displacement current

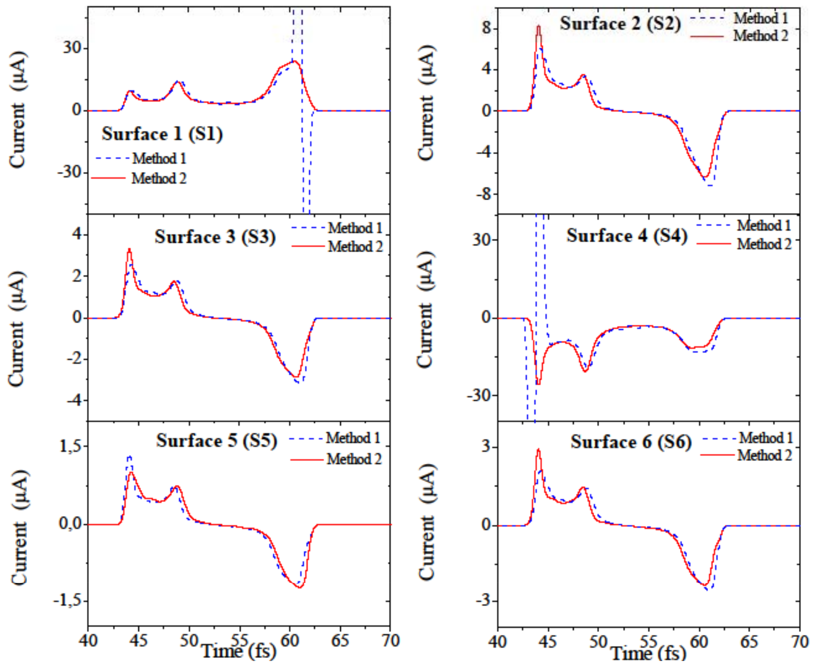
The TOTAL time-dependent "Bohmian" current:

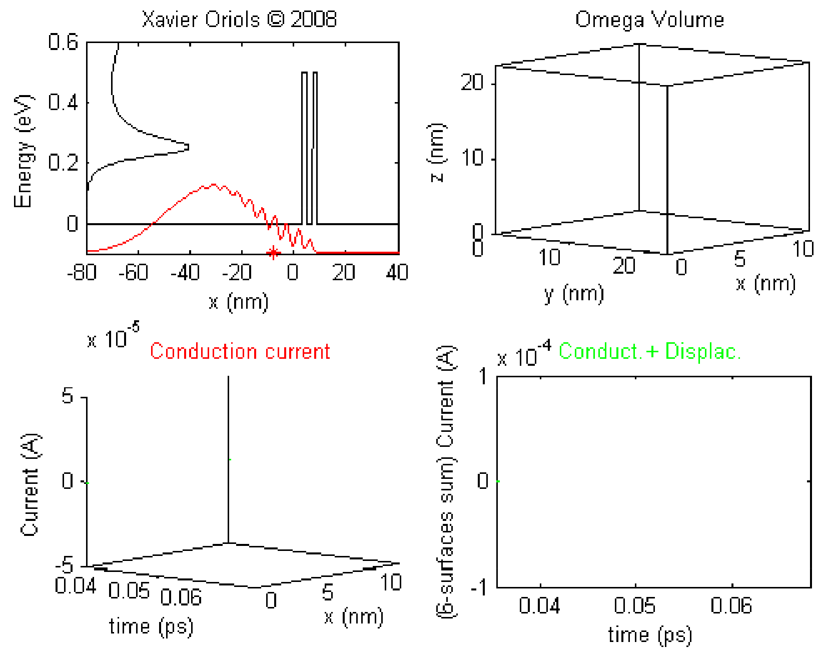
[A. Alarcon, JSTM (2009)]

$$\langle I(t)\rangle = \int_{S_D} \langle \vec{J}_c(t)\rangle \cdot d\vec{s} + \int_{S_D} \varepsilon \frac{\partial \langle \vec{E}(r,t)\rangle}{\partial t} \cdot d\vec{s}$$

$$\nabla \cdot \left(\vec{J}_c(\vec{r},t) + \varepsilon \frac{d\vec{E}(\vec{r},t)}{dt} \right) = 0$$

Each trajectory of the ensemble fulfils the TOTAL current conservation law.

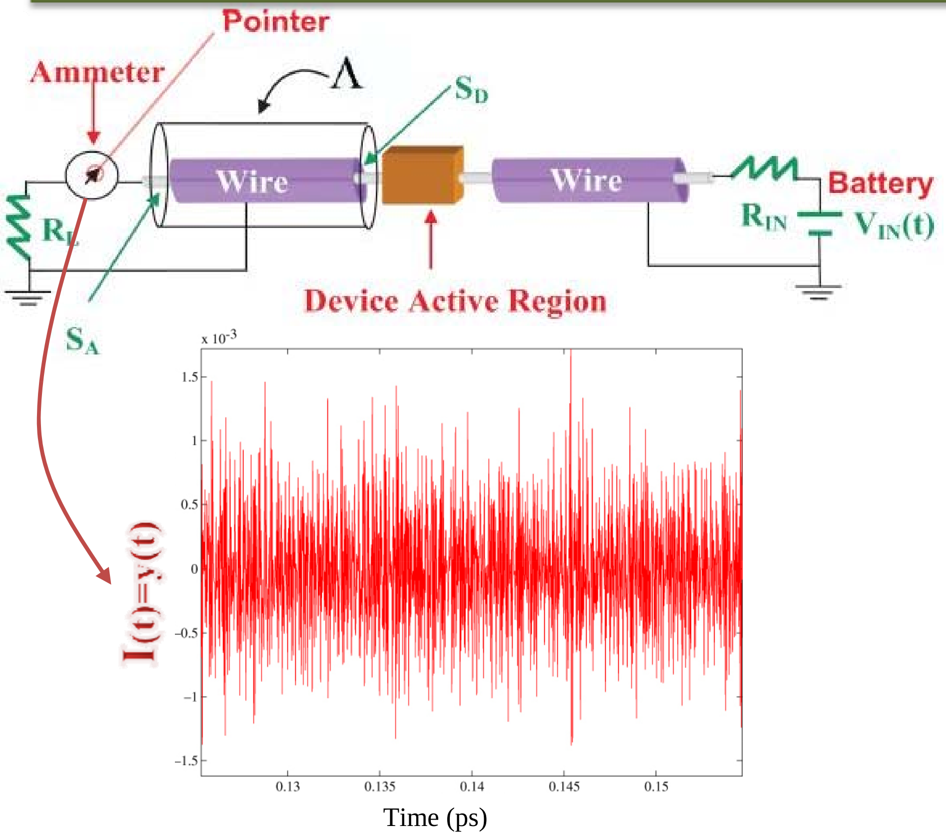




Bohmian solution to the measurement of many-body systems: Sequential current in mesoscopic electron devices

2.4- The computation of multi-time measurement

A “simple” explanation on Bohmian measurement……



The wavefunction:

$$\Psi\left(\vec{r}_1,...,\vec{r}_N,y,t\right)$$

The trajectories:

$$\vec{r}_1^{\,j}[t],\vec{r}_2^{\,j}[t],\vec{r}_3^{\,j}[t],...,\vec{r}_N^{\,j}[t],$$ yj[t]= I(t)

The conditional wavefunction:

$$\Psi\left(\vec{r}_1,...,\vec{r}_N,y^j[t],t\right)$$

The many body problem

[A.Alarcón *et. al.* Chapter 6, Applied Bohmian Mechanics (2012)]

2.1.3.- Multi-time Bohmian measuremen of the current

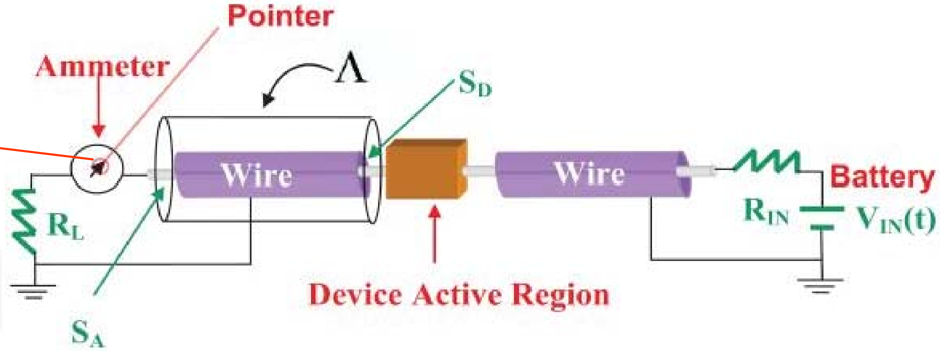
Is the Bohmian solution of the measurement equal to the Orthodox solution ?

Bohmian trajectory

I(t)=y[t]

Copenhagen operators

I(t)= eigenvalue of an Operator



What would happen if **I(t)** were not equal to **I(t)** ?

Copenhagen supporters: The measuring apparatus is wrong, because Bohmian mechanics has to reproduce orthodox quantum mechanics.

Bohmian supporters: The operator is wrong, because orthodox quantum mechanics has to reproduce Bohmian mechanics.

"Naïve realism about operators"

[D. Durr, S. Goldstein, N. Zanghi, J. Stat. Phys., 116, 959-1055, (2004)]

2.4- The computation of multi-time measurement

Is the Bohmian solution of the measurement equal to the Orthodox solution ?

$$\hat{I}_1 = \frac{1}{L_x m}\left(\sum_{k=1}^{k=N} q_k \hat{p}_{k_x}\right)$$

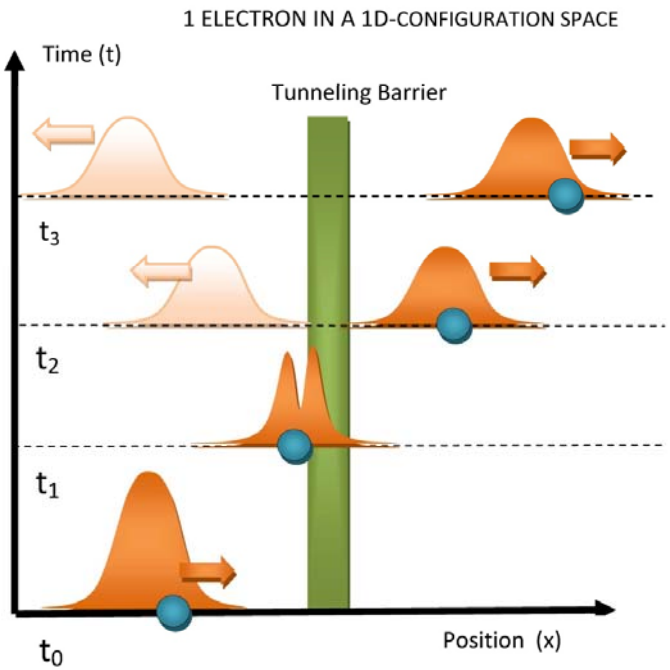
Total current operator

$$\hat{M}_{I_1(t)} = \sum_{\vec{p}_x} |\vec{p}_x\rangle\langle\vec{p}_x| \cdot \delta_{I_1(t),I(p_x)}$$

Its associated (degenerate) projector=POVM

$$|\Psi^f(t)\rangle = \hat{M}_{I_1(t)} |\Psi^0(t)\rangle$$

Final (unnormalized) state after measurement is a **total momentum** eigenstate.



A.- Following a collapsed wave function

The probability of being transmitted at t_2 and reflected at t_3 is zero.

B.- Following a trajectory

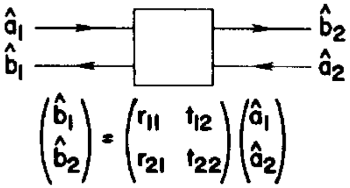
The probability of being transmitted at t_2 and reflected at t_3 is zero.

2.4- The computation of multi-time measurement

Partition “Noise” comparison for electron devices without (many-body) Coulomb ?

[M.Buttiker PRL1990]

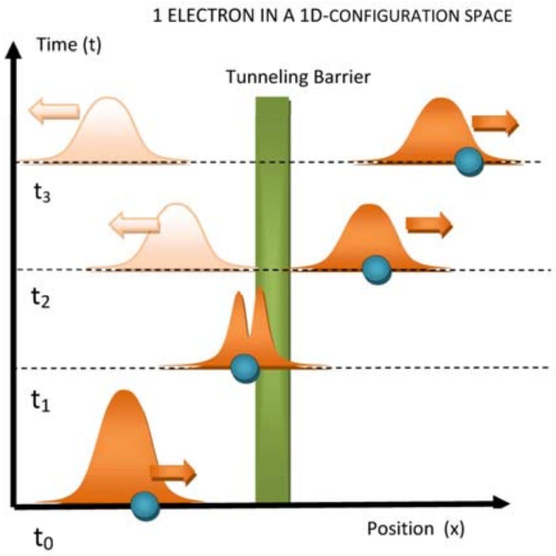
2nd quantization approach

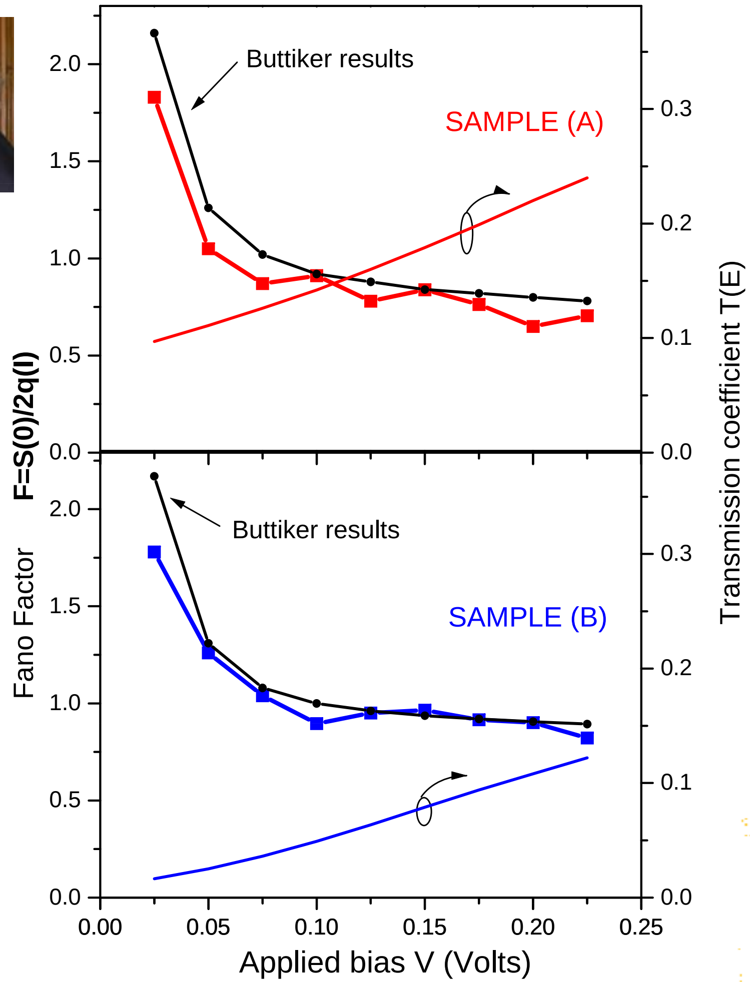


An electron “created” at one contact $|1> = \hat{a}_1^+ |0>$

can not “emerge” at two different contacts

$$< n_T n_R > = < 1 | \hat{b}_1^+ \cdot \hat{b}_1 \cdot \hat{b}_2^+ \cdot \hat{b}_2 | 1 > = 0$$





Bohmian solution to the measurement of many-body systems: Sequential current in mesoscopic electron devices

1.- Introduction:

2.- Theoretical discussion

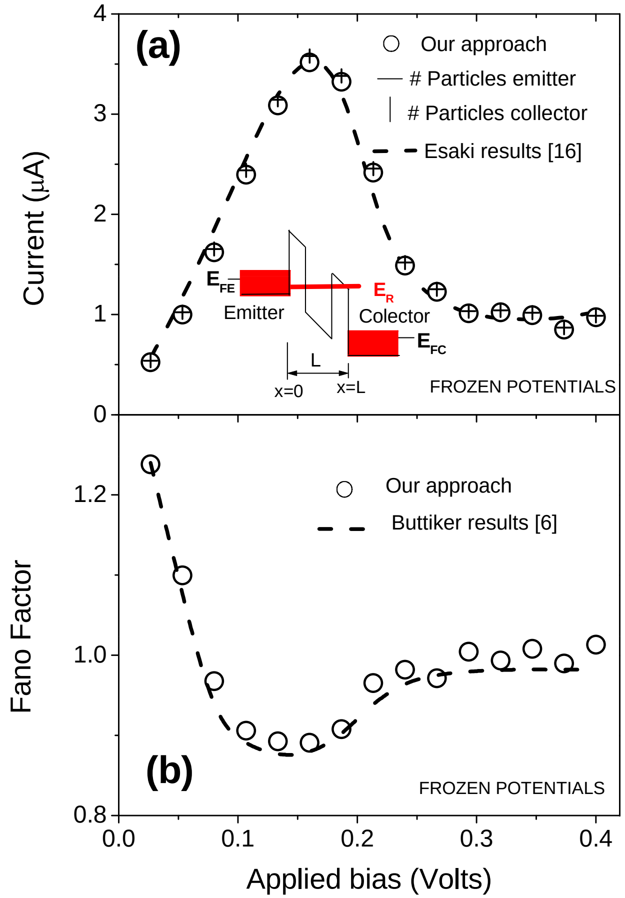
3.- Numerical results with the BITLLES simulator

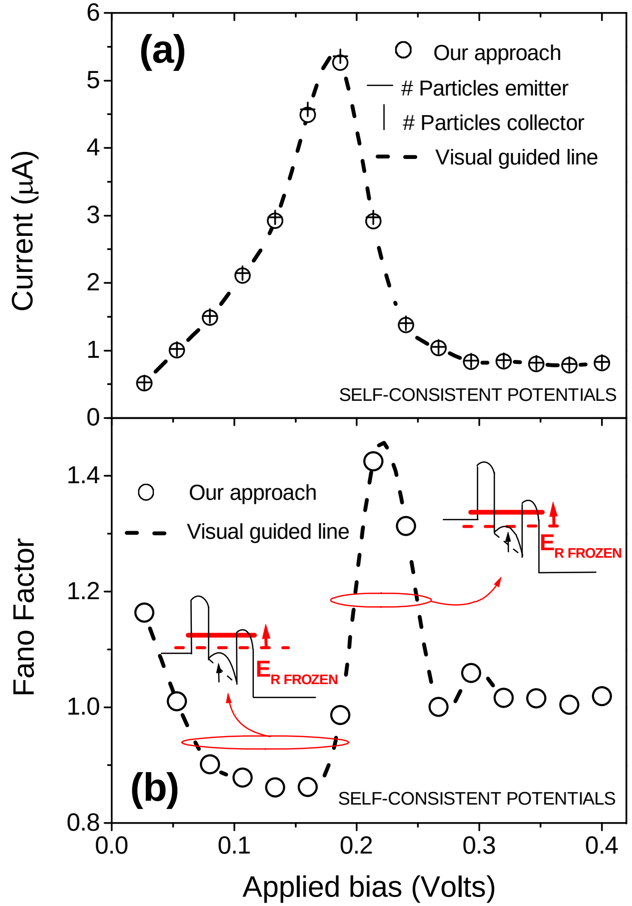
4.- Conclusions and Future work

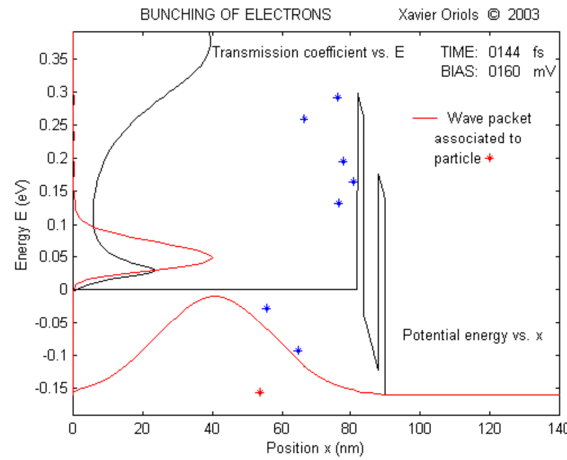
3.2.- DC current beyond mean field

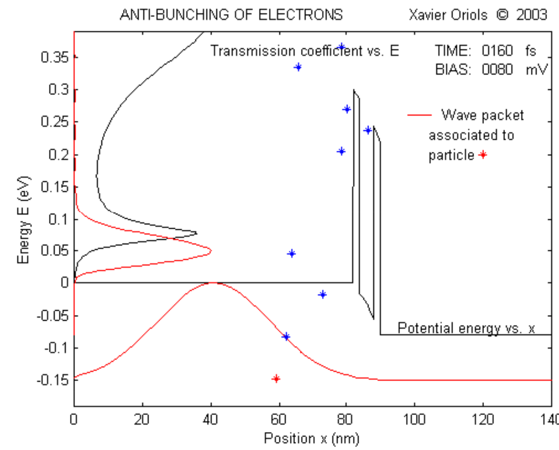
Effect of Coulomb correlation on current and noise

[X.Oriols, APL(2005)]









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There is a need for predictions of the dynamics properties of quantum devices…..

1.- FORMALISM: We have shown the ability of many-particle Bohmian trajectories (extracted from conditional wave functions) to accurately and efficiently compute time dependent transport (AC, noise, transients,…).

2.- SIMULATOR: Using these ideas, we have developed a user-friendly, hand-made simulator for time-dependent electron transport, named:

Bohmian Interacting Transport for non-equiLibrium eLEctronic Structures

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

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

[F. L. Traversa, et al. IEEE Trans. on Electron devices, 58(7) 2104 (2011)]

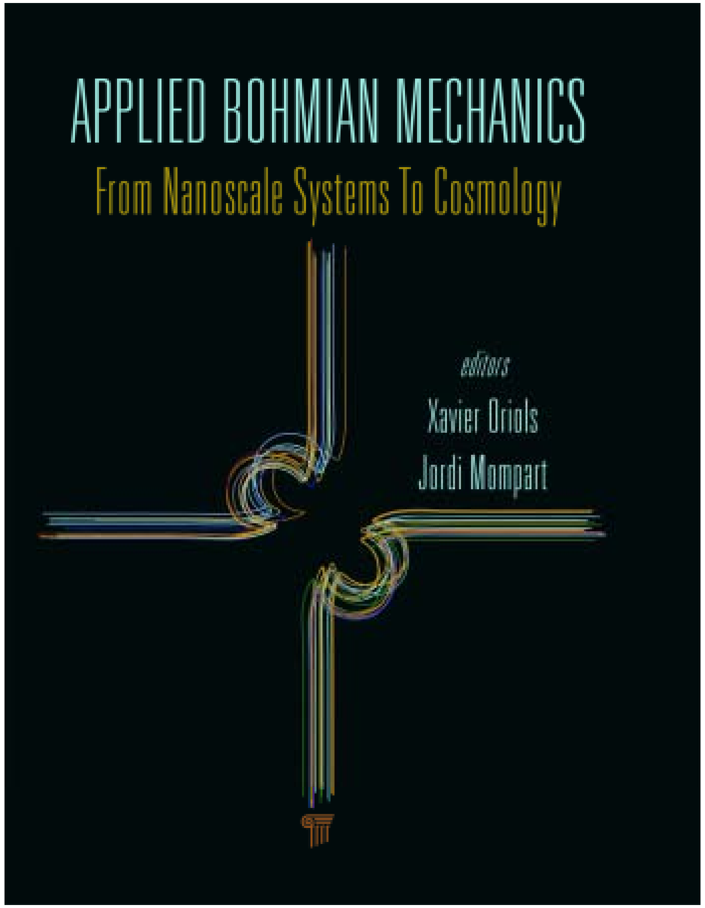
Freely available at **http:\europe.uab.es\bitlles**

4.- Conclusions and future work

Acknowledgment

This work has been partially supported by the Ministerio de Ciencia e Innovación under Project No. TEC2009-06986 and by the DURSI of the Generalitat de Catalunya under Contract No. 2009SGR783.

Research Group of Computational Nanoelectronics
NANOCOMP



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

Thank you very much for your attention

BITLLES freely available
at **http:\europe.uab.es\bitlles**