Dissipative quantum transport using one-particle time-dependent (conditional) wave functions

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Dissipative quantum transport using one-particle time-dependent (conditional) wave functions

1.- Introduction:

1.1.- Potentialities of the BITLLES simulator

1.2.- Dissipation? Reversible laws for an irreversible world

2.- Dissipative quantum transport in the BITLLES simulator

3.- Conclusions
1. Microscopic electron’s path

2. Electron’s acceleration related to electric field

3. Powerful: DC, AC, transient, noise....

Quantum Monte Carlo (Bohmian) solution of the many-particle Schrödinger equation

1. Microscopic (Bohmian) electron’s path

2. Electron’s velocity related to (conditional) wave function

3. Powerful: DC, AC, transient, noise....

Bohmian Interacting Transport for non-equilibrium electronic structures

Freely available at http://euroep.uab.es/bitlles

IWCE, September 2015

X. Oriols, UAB Spain
1.1.- Potentialities of the BITLLES simulator

The BITLLES simulator:

General discussion:
[X. Oriols and D.K. Ferry, JCE, 12(3), 317-330 (2013)]

Beyond mean field:

Boundary conditions:
[X. Oriols, SEE 51, 306 (2007)]

DC and AC noise:
[G. Albareda et al. JCE 12(3), 405-419 (2013)]
[G. Albareda et al. Noise and fluct. 11(3) 1242008 (2012)]

Exchange interaction:
[A. Alarcón et al. J. Phys.: CM 25, 325601 (2013)]

Weak measurement:
[D. Marian et al. arxiv1508.00248]
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The problem of describing irreversible processes starting from reversible laws is indeed one of the deeper recurring problems of physics which has been widely discussed in the literature.

W. Frensley 1990

“The study of the fundamental origins of irreversibility in physical theory remains an area of active discussion and debate, more than a century after the question was first raised. ……it is clearly more profitable to adopt the view that irreversibility is a fundamental law of nature.
1.2. - Dissipation? Reversible laws for an irreversible world

**Reversible electron transport laws for 1,2,3 degrees of freedom**

- Schrödinger equation (wave function)
- Quantum Liouville equation (density matrix)

**Net effect**

The electron *evolves* from the state \( \{E, k\} \) to \( \{E', k'\} \)

**Irreversible electron transport laws for 1,2,3 degrees of freedom**

- Scattering rates (Fermi Golden rule)
- Relaxation time approximation

**Net effect**

The electron *changes* from the state \( \{E, k\} \) to \( \{E', k'\} \)
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2.- Dissipative quantum transport in the BITLLES simulator
   2.1.- Conditional (Bohmian) wave function
   2.2.- Single-particle (conditional) dissipative wave functions
   2.3.- Numerical results

3.- Conclusions
2.1.- Conditional (Bohmian) wave function

The many-particle wave function

\[ i\hbar \frac{\partial \Phi(x_1, x_2, \ldots, x_N, t)}{\partial t} = \left\{ \sum_{a=1}^{N} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_a^2} + U(x_1, x_2, \ldots, x_N, t) \right\} \Phi(x_1, x_2, \ldots, x_N, t) \]

The many-body problem

Linear
Unitary
"lives" in \( \mathbb{R}^{3N} \)
Non-Linear
Non-Unitary
"lives" in \( \mathbb{R} \)

The conditional wave function

Bohmian mechanics

\[ i\hbar \frac{\partial \Psi(x_a, t)}{\partial t} = \left\{ - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_a^2} + U(x_a, \bar{x}_b[t], t) + G(x_a, \bar{x}_b[t], t) + iJ(x_a, \bar{x}_b[t], t) \right\} \Psi(x_a, t) \]
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2.2.- Single-particle (conditional) dissipative wave functions

Usual single-particle Schrodinger equation:

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

“Conditional” single-particle Schrodinger equation:

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


Our goal effect:

Use \( G(x,t) \) and \( i\cdot J(x,t) \) to produce an electron changes from the state \( \{E,k\} \) to \( \{E',k'\} \)

\[ i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \left\{ \frac{1}{2m^*} \left( -i\hbar \frac{\partial}{\partial x} + \lambda\Phi(t_1) \right)^2 + U(x,t) \right\} \Psi(x,t) \]

\[ i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \left\{ -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x^2} + U(x,t) + i\frac{\hbar\Phi(t_1)}{m^*} \frac{\partial}{\partial x} + \frac{\lambda^2\Phi^2(t_1)}{2m^*} \right\} \Psi(x,t) \]
2.2.- Single-particle (conditional) dissipative wave functions

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

\[
i \hbar \frac{\partial \Psi(x,t)}{\partial t} = \left\{ \frac{1}{2m^*} \left( -i \hbar \frac{\partial}{\partial x} + \lambda \Phi(t) \right)^2 + U(x,t) \right\} \Psi(x,t)
\]
2.2.- Single-particle (conditional) dissipative wave functions

1st property:

Electron changes from the state \( \{E,k\} \) to \( \{E',k'\} \) according to the parabolic dispersion.

\[
\langle p(t^-_1) \rangle = p(t^-_1) \\
\langle E(t^-_1) \rangle = \left(\frac{p(t^-_1)}{2m^*}\right)^2 + \frac{\sigma^2}{2m^*} \\
\langle p(t^+_1) \rangle = p(t^-_1) + \lambda \\
\langle E(t^+_1) \rangle = \left(\frac{p(t^-_1) + \lambda}{2m^*}\right)^2 + \frac{\sigma^2}{2m^*}
\]

2nd property:

After \( t_1 \), when the \( \lambda \) becomes time-independent the wave functions evolves as a “normal” wave function with the new energy and momentum.

\[
\Psi = e^{-i\frac{\lambda \cdot x}{\hbar}} \Psi_{No\lambda}
\]

\[
i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \left\{ \frac{1}{2m^*} \left( -i\hbar \frac{\partial}{\partial x} + \lambda \right)^2 + U(x,t) \right\} \Psi(x,t) \\
i\hbar \frac{\partial \Psi_{No\lambda}(x,t)}{\partial t} = \left\{ -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x^2} + U(x,t) \right\} \Psi_{No\lambda}(x,t)
\]
2.2.- Single-particle (conditional) dissipative wave functions

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

\[ i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \left\{ \frac{1}{2m^*} \left( -i\hbar \frac{\partial}{\partial x} + \lambda \Phi(t_i) \right)^2 + U(x,t) \right\} \Psi(x,t) \]
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2.3.- Numerical results

Simulated time $T = 5 \text{ ps}$ (each bias point)

Computational time $4 \text{ (5 hours)}$

GaAs

AlGaAs

GaAs

AlGaAs

GaAs

1(6nm(2(4nm(1(6nm

Barrier height $0(5 \text{ eV}$

Scattering mechanisms

(Fermi Golden Rule

Acustic Phonons

Optial Phonons

Optial Phonons

Impurities

$N_D = 10^{17} \text{ cm}^3$

BITLLES:

0,0 0,2 0,4 0,6 0,8 1,0

0 5 10 15 20 25 30

DC Current (µA)

SCATTERING

With

# particles

Ramo-Shockley-Pellegrini

Without

# particles

Ramo-Shockley-Pellegrini

Without

# particles

DC Current (µA)

Applied bias (V)
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Thank you very much for your attention

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