# Time-dependent electron driven tunneling phenomena for multipurpose terahertz applications:

## Self consistent computation of conduction and displacement current in mesoscopic systems


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# Outline

## 1. Theoretical development:

**1.1.- Introduction:**

1.1.1- From macroelectronic to nanoelectronic. THZ Gap

1.1.2- Total (conduction plus displacement) current conservation

**1.2- Time-dependent self-consistent solution of the Poisson and many-particle Schrödinger equations:**

1.2.1- Quantum trajectories with electron-electron interaction

1.2.2.- Current in terms of the Ramo-Shockley theorem.

## 2. THz applications:

**2.1.- Driven Tunneling Devices (DTD)**

**2.2.- Numerical DTD results:**

2.2.1.- Rectifier

2.2.2.- Harmonic Generator

## 3.- Conclusions

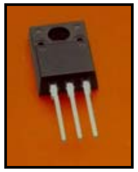
# 1.1.- From macroelectronic to nanoelectronic. THZ Gap

**Macroelectronic** — **Microelectronic** — **Nanoelectronic**

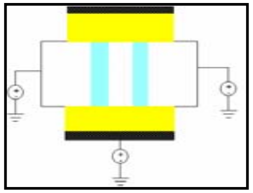
**Vacuum valve**

**Semiconductor Transistor**

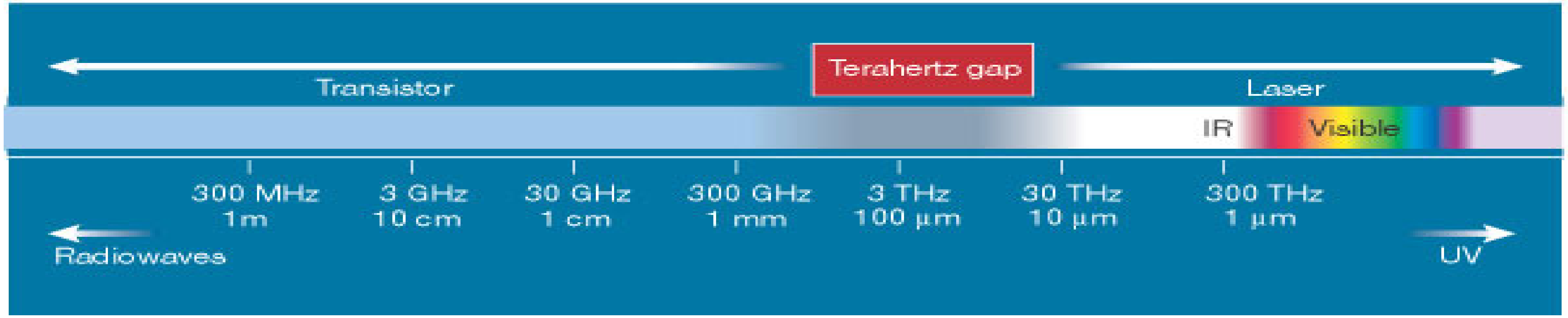
**MOS Transistor**



**DTD**



**Quantum Mechanics Description**




Goal ⇒ **Quantum electrons transport at THz frequencies** ⇒ **Time-dependent many-particle Schrödinger equation**

# 1.2.-Total (conduction + displacement) current conservation

Total current in high frequency electron devices:

$$J_T(r,t) = \underbrace{J_c(r,t)}_{\text{Conduction}} + \underbrace{\varepsilon(r)\frac{\partial E(r,t)}{\partial t}}_{\text{Displacement}}$$

**[Ya. M. Blanter and M. Büttiker, Phys. Rep. (2000)]**

1. $\nabla\left(\varepsilon(r)E(r,t)\right) = \rho(r,t)$ ⇐ 1st Maxwell (Poisson) equation (electron-electron interaction)

⇕

2. Many-particle Schrödinger equation

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# 2.1.- Quantum trajectories with electron-electron interaction

## The problem…

**Many-particle (Coulomb interaction) Schrödinger equation**

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

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

**Practical solution is inaccessible for more than very few electrons**

**Numerical viability 1 eq N-Dim:** N=100 electrons, L=100nm length (with Δx=0.1 nm)

nº of variables = $1000^{3N} = 1000^{300}$ variables !!!!!!!!!!!!

## The solution…

**Electron-electron approximations in the literature:**

**- Fermi liquid (no Coulomb interaction)**

**-Perturvative (Green-function) treatment**

**-Density Functional theory**

**. …….**

# 2.1.- Quantum trajectories with electron-electron interaction

## The solution…

**[D. Bohm, Phys. Rev, 1952 ]**

▶ New approximation to simplifying the evaluation of many-particle Schrödinger equation.

$$i\hbar\frac{\partial\Psi_a(\vec{r}_a,t)}{\partial t}=\left\{-\frac{\hbar^2}{2\cdot m}\nabla^2_{\vec{r}_a}+U_a(\vec{r}_a,\vec{R}_a[t],t)+G_a(\vec{r}_a,\vec{R}_a[t],t)+i\cdot J_a(\vec{r}_a,\vec{R}_a[t],t)\right\}\Psi_a(\vec{r}_a,t)$$

**[X.Oriols, Phs. Rev. Letters, 2007]**

**Numerical viability N-eqs 1-Dim:** N=100 electrons, L=100nm length (with $\Delta x$=0.1 nm)

nº of variables = 3·1000·N = 300 000 variables

The self-consistent coupling between the electron dynamics obtained from the last equation and the Coulomb potential (obtained from 3D Poisson solver) is achieved by using Bohm trajectories.

# 2.2.- Current in terms of the Ramo-Shockley theorem

Ramo-Shockley theorem with Bohm trajectories in volume Ω and total surface S

$$I_i(t) = \Gamma_i^q(t) + \Gamma_i^e(t) + \Gamma_i^m(t)$$

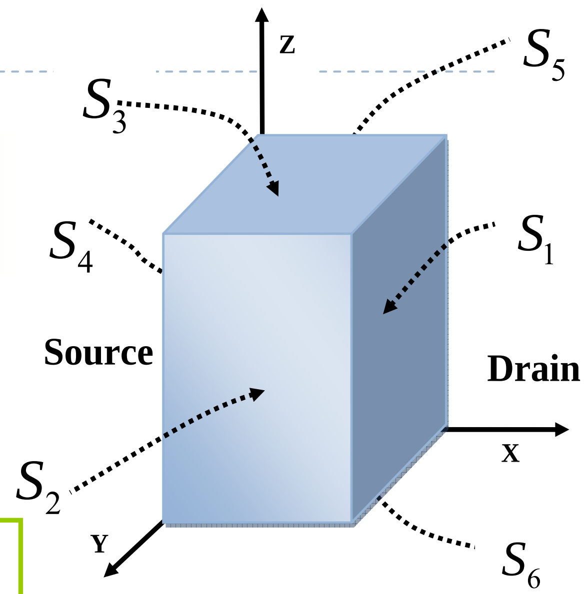
$$\Gamma_i^q(t) = -\int_\Omega F_i(r) \cdot J_c(r,t) \cdot d^3r$$

**Conduction current density**

$$\Gamma_i^e(t) = \int_S F_i(r) \cdot \varepsilon(r) \cdot \frac{\partial}{\partial t} V(r,t) \cdot ds$$

**Potential scalar**

$$\Gamma_i^m(t) = \int_\Omega F_i(r) \cdot \varepsilon(r) \cdot \frac{\partial^2 A(r,t)}{\partial t^2} \cdot d^3r$$




$$\vec{F}(\vec{r}) = -\nabla\Phi(\vec{r})$$

$$\nabla\left(\varepsilon(\vec{r}) \cdot \vec{F}(\vec{r})\right) = -\nabla\left(\varepsilon(\vec{r}) \cdot \nabla\Phi(\vec{r})\right) = 0$$

$$\Phi(\vec{r}) = 1 \ ; \ \vec{r} \in S_i$$

$$\Phi(\vec{r}) = 0 \ ; \ \vec{r} \in S_{h \neq i}$$

**[X.Oriols, A.Alarcon, et al. Phy. Rev. B, 2005]**

**[A.Alarcon, X.Oriols, et al. JSTAT, 2008 (Submitted)]**

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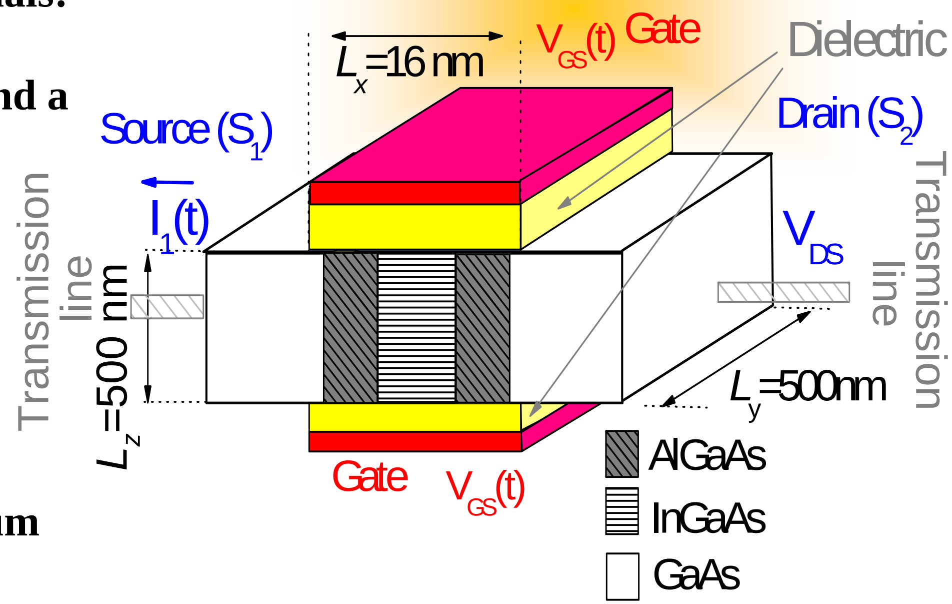
# 3.- Driven Tunneling Devices (DTD)

## DTD geometry

- **Field effect transistor with three terminals: double gate, drain and source. Inside active region, a double barrier and a quantum well**




## DTD operation

- **The output current (from a source to the drain) is controlled by the gate voltage.**
- **Coupling non-stationary (THz) quantum transport with electromagnetism.**
- **The density of states inside the active region is designed "by hand" (modifying the structure geometry).**

**[DTD was patented in the year 2005]**

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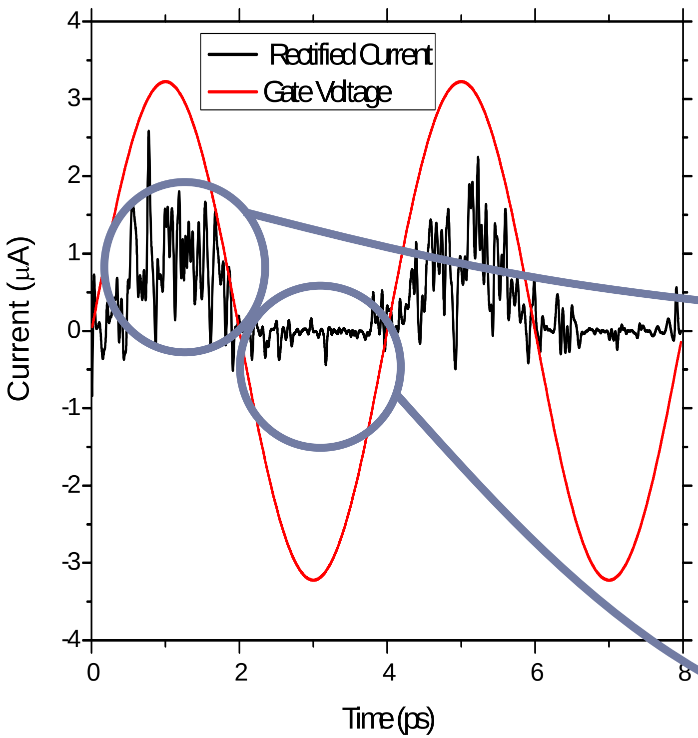
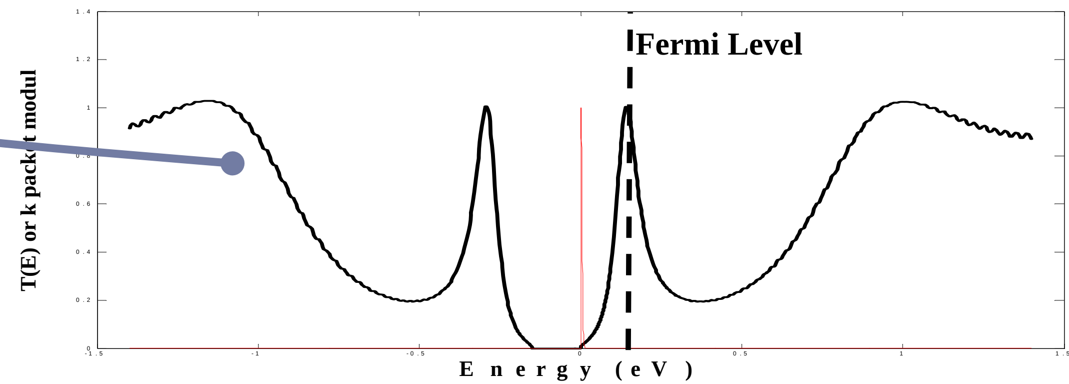
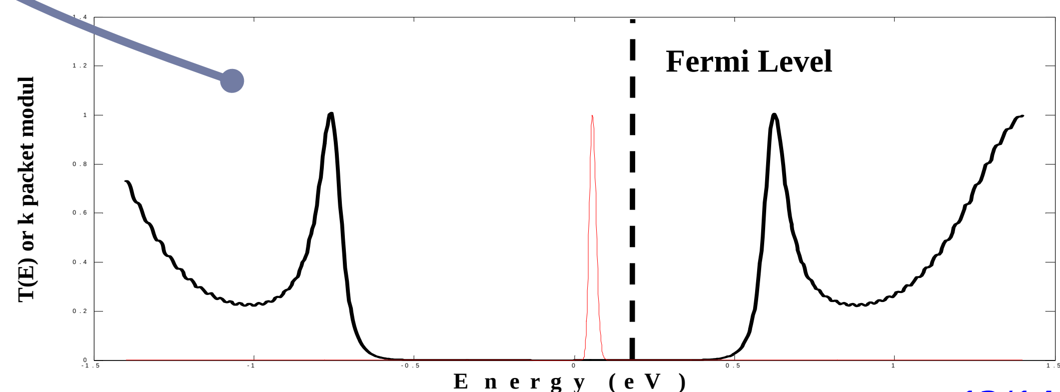
# 4.1.- DTD Applications: THz Rectifier




**"Qualitative" explanation "ON":**



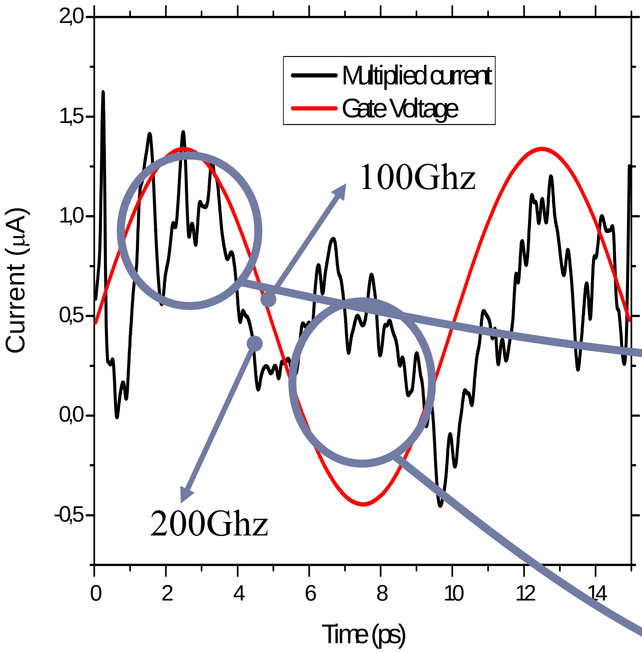

**"Qualitative" explanation "OFF":**



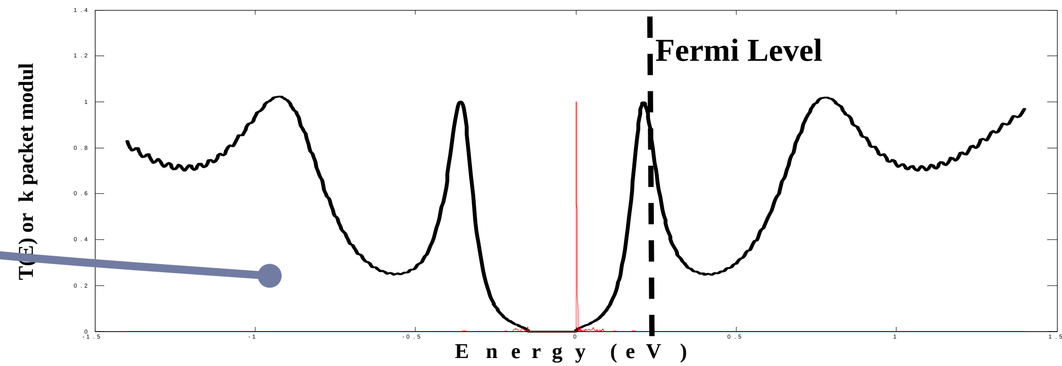

**DTD parameters:**

**Barriers: 1.5nm, 0.6eV**
**Quantum well: 2.4nm.**
**Gate frequency: 250 GHz**

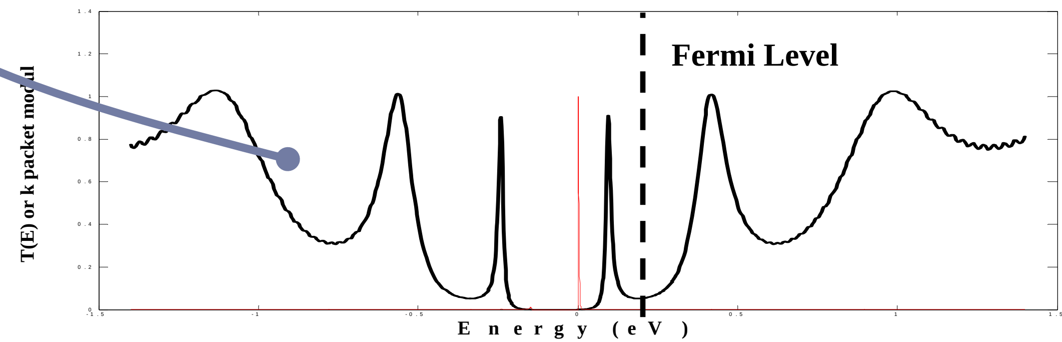
# 4.2.- DTD Applications: THz harmonic generator




**"Qualitative" explanation: Two resonances**




**"Qualitative" explanation: One resonance**




**DTD parameters:**

**Barriers: 1.5nm, 0.8eV**
**Quantum well: 5.1 nm.**
**Gate frequency: 100 GHz**

## 5. Conclusions

# Theoretical development:

- We have presented a novel approach for the self-consistent simulation of the time-dependent total current at the range of THz.
- The self-consistent solution of the 3D Poisson and Schrödinger equations are achieved using Bohm trajectories.
- Computation of the time-dependent total current using quantum version of the Ramo-Shockley theorem.

# THz applications:

- Driven Tunneling Devices: Geometry and Operation.
- This numerical approach is applied for the computing of tunneling currents in two different DTD configuration: Rectifier and a harmonic generator.