High frequency resonant tunneling behavior: Testing an analytical small signal equivalent circuit with time dependent many-particle quantum simulations

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Outline

- Introduction & Motivations

- I : QMC based on many-particle Bohm trajectories
  - ✓ Introduction to the model
  - ✓ current conservation
  - ✓ overall charge neutrality

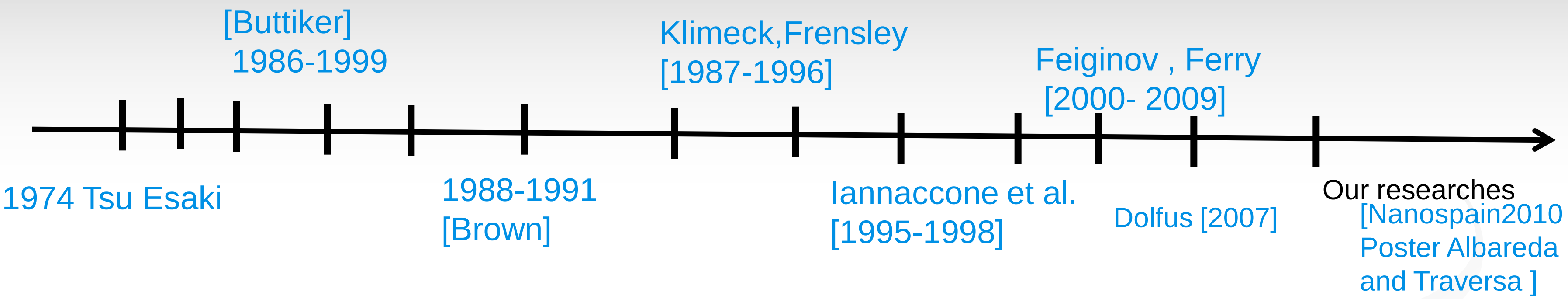
- II:Physics-Based Analytical Model
  - ✓ DC Analytical model
  - ✓ AC Analytical model

- Comparison :
  - ✓ current conservation
  - ✓ overall charge neutrality

- Conclusions

- Thanks to epitaxial technologies, Resonant Tunneling Diode (RTD) are commonly used realized using III-V semiconductor *[Yan-Kuin Su, IEEE EDL,2000]*
- RTD provides *a large amount of information* about electron transport in quantum devices.

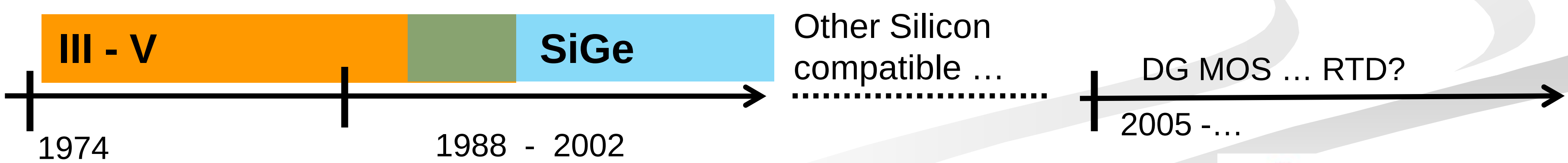
Physics understanding (DC,AC, noise...)



- These devices offer several advantages for analogical and digital applications (oscillator or logic circuits) *[De Los Santos, (2001)] ,[Lin Proceedings 1994]*

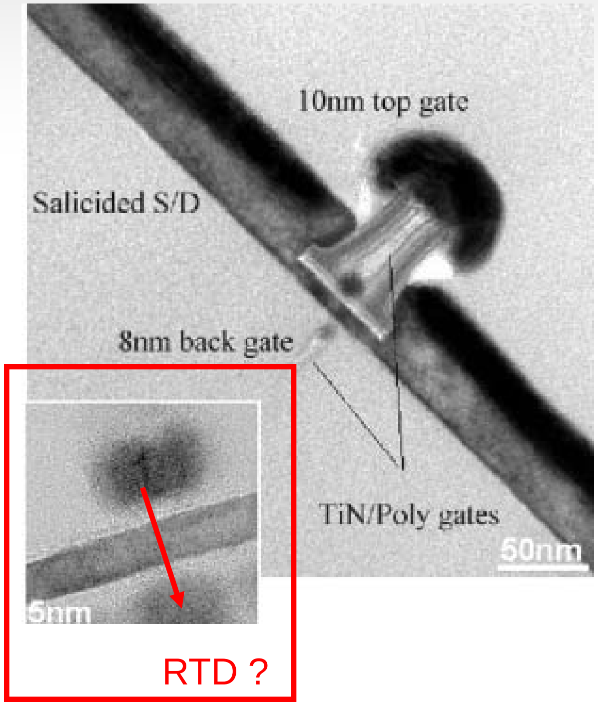
- However, III V materials can not be easily integrated in the mainstream Silicon technology.

Technological improvement on silicon compatible solutions:



- Progress in MOSFETs technology has made possible to realize Double Gate (DG) devices with very thin Body thicknesses (tsi < 10nm)

(Vinet, EDL 2005, Harrison IEDM 2003, Thean IEDM 2006, Collaert VLSI 2006 …)



Vinet et al. EDL 2005

- Recently, evidence of Resonant tunneling effects has been reported in Si/SiO_2 structures
  [Junichi Kubota,2005] [Rommel et Al.1998]

- Such RTD could be easy integrate in DG or ultra thin SOI technology

OBJECTIVE OF THIS WORK:

- The aim of this work is an accurate analysis of the frequency behavior of RTDs , comparing a numerical complete model and an analytical model

QMC based on many-particle Bohm trajectories

Quantum trajectories with electron-electron interactions

Standard Approaches :

- ✓ without solving Poisson equation [Frensley et al, 1987]
- ✓ small " simulation box" not ensure charge neutrality [Kluksdahl et al.1988]

The problem…

Many-particle (Coulomb interaction) Schrödinger equation

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

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

1 Equation **N variable**

Practical solution is inaccessible for more than very few electrons

The solution…

N equations **1 variable**

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

Using Bohm trajectories **[X.Oriols, Phs. Rev. Letters, 2007]**

(i) Solving Poisson equation: current conservation

The total current is :

$$\vec{J}_T(\vec{r},t) = \vec{J}_c(\vec{r},t) + \varepsilon(\vec{r})\frac{\partial \vec{E}(\vec{r},t)}{\partial t} = \vec{J}_c(\vec{r},t) + \vec{J}_d(\vec{r},t)$$

Conduction current

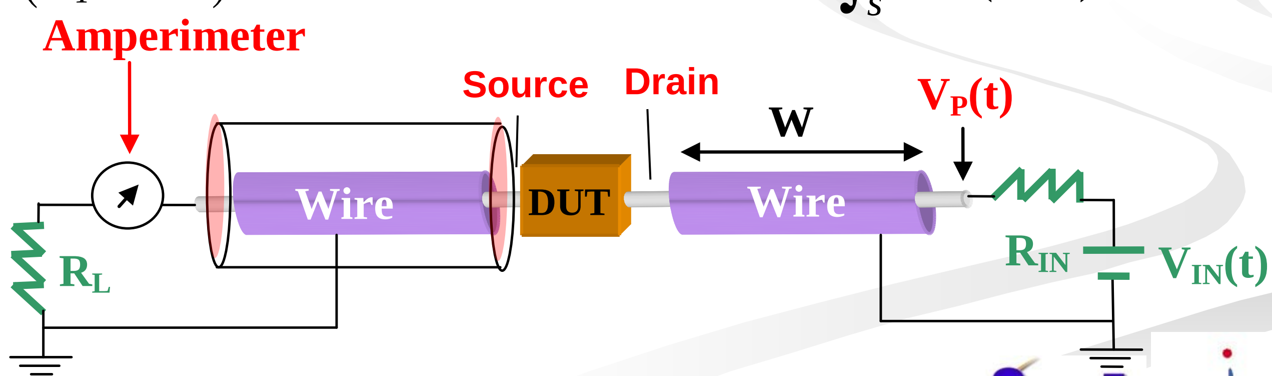
Displacement current:
related to temporal variations of the electric field

Differential (point) conservation

$$\nabla\left(J_T(r,t)\right) = 0$$

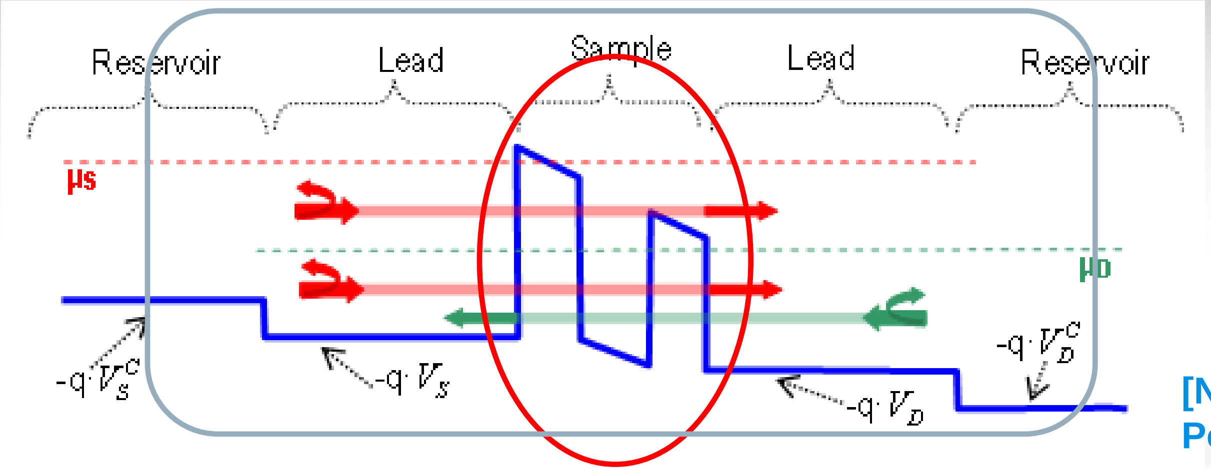
Integral (surface) conservation

$$\int_s J_T\left(r,t\right) ds = 0$$



(ii) Solving Poisson equation Overall charge neutrality

Screening deep inside the leads assures that the total charge tends to zero ⇒
Coulomb interaction is taking into account in a larger "simulation box "



[Nanospain2010 Poster Albareda et al.]

✓ The charge neutrality is a consequence of electrons to screen each other in order to minimize the electric field.

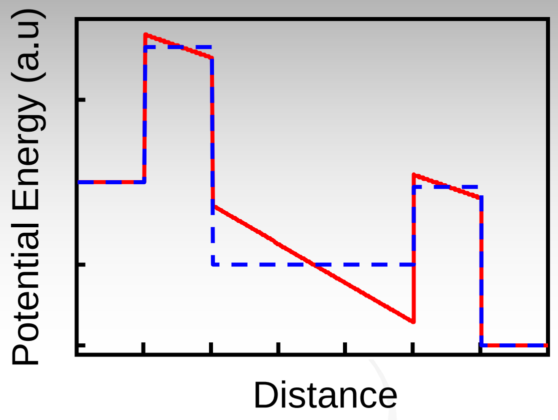
✓The charge neutrality is achieved in the dielectric relaxation time.

✓ Any increment/reduction of the charge in the leads implies a modification the bottom of the conduction band.

Physics-Based Analytical Model

DC I – V Analytical model

$$J(V) = q\frac{4\pi\, mkT}{h^3}\int_{E_c}^{\infty} T(E,V)\cdot \ln\left[\frac{1+e^{(E_f-E)/kT}}{1+e^{(E_f-E-eV)/kT}}\right]dE$$



Assuming for sake of simplicity :

- Effective Mass approximation
- Non self Consistent calculation (linear Energy Potential Profile)
- Ballistic model (coherent model →best case)

- Contrary to previous analytical model, the transparency has been analytically computed, approximating triangular barrier by squared barriers.

For each resonant peak E_n :

$$T(E,V) \approx \frac{T_{max}(E,V)}{1+\left(\frac{2\,(E-E_n)}{\Delta E(E,V)}\right)^2}$$

$$\Delta E = \frac{\Gamma_L+\Gamma_R}{2}$$

$$T_{max} = \frac{4\,\Gamma_L\Gamma_R}{(\Gamma_L+\Gamma_R)^2}$$

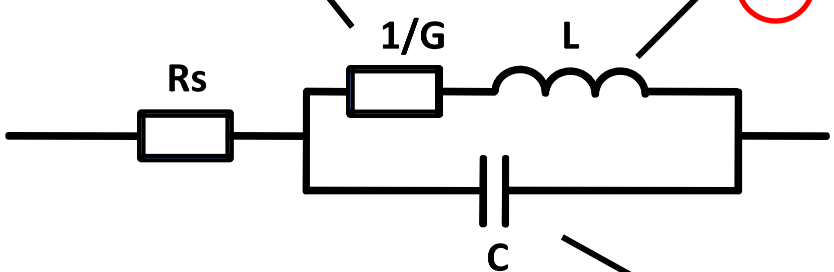
$$\Gamma_{L,R} = \left(\frac{2\hbar\cdot E_n\cdot T_{L,R}}{m\cdot t_{si}(1-T_{L,R})}\right)^{1/2}$$

AC Analytical model

- Following the approach of *Liu et al. TED 2004,* the previous DC model has been extended in the AC regime.
- It leads to an equivalent circuit model.
- Contrary to previous models, all elements are computed versus device and material parameters.

$$G = \frac{dI}{dV} (< 0)$$

$$L = \frac{G}{\tau} (< 0) \rightarrow \quad \tau = \frac{\hbar}{\Gamma_L + \Gamma_R} \propto 1/T_{L,R}$$



$$C = C_Q + C_g \quad \begin{cases} C_Q = |G| \cdot \tau \\ C_g = \dfrac{A}{\dfrac{L_w}{\varepsilon_w} + \dfrac{2L_b}{\varepsilon_b} + \dfrac{L_d}{\varepsilon_d}} \end{cases}$$

Comparison

- **How computing frequency response?**

From current calculation, but in other methods:

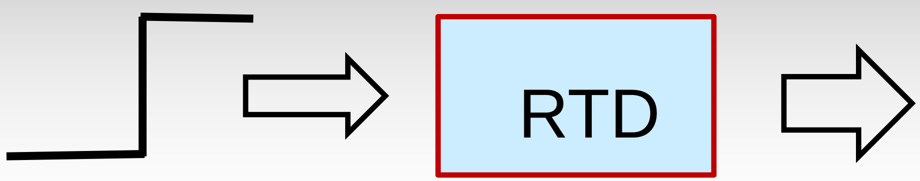
✓ By intrinsic NOT MEASURABLE parameters extraction (as life time in the well) [Zhao et al.2001]

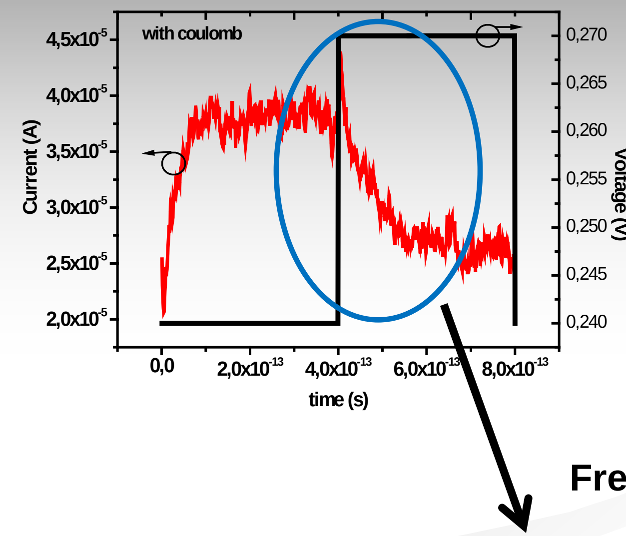
✓ From small signal equivalent circuit [Brown et al. 1989]

✓By DC characteristics but from not self consistent simulations

Intrinsic cut off frequency estimation : Two methods comparison

QMC

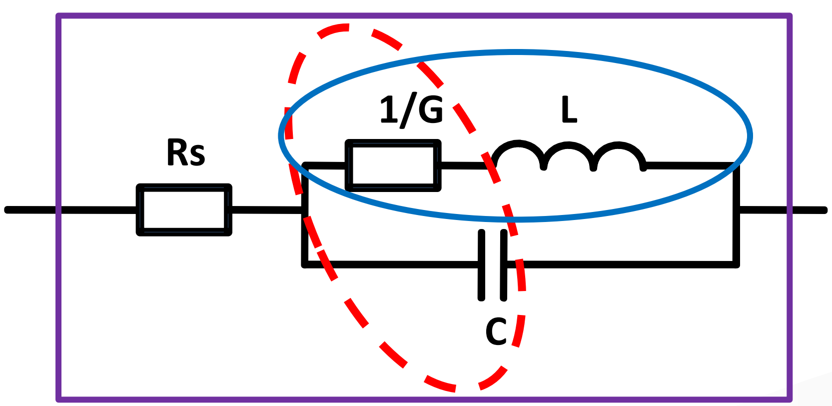




- ✓ (i)current conservation
- ✓ (ii)overall charge neutrality

Frequency=1/τ

SSEC



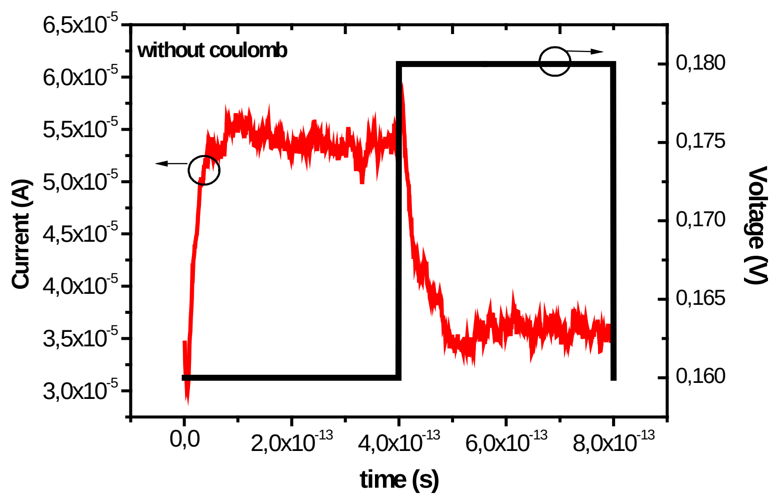
1. Without conditions (i) and (ii)
2. With condition (i)
3. With condition (i) and (ii)

1 . Without conditions (i) and (ii)

QMC

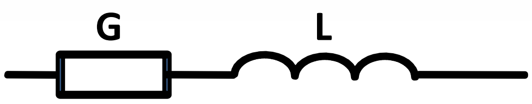
we remove self-consistency of the Coulomb interaction.

The current in the RTD follows the voltage step with an intrinsic delay of about *0,035* ps



SSEC

Can be simplified by connecting in series a negative conductance *G* and a negative inductance *L*



the time is assumed to be equal to the RTD dwell time $\tau_d = \hbar/\Gamma$

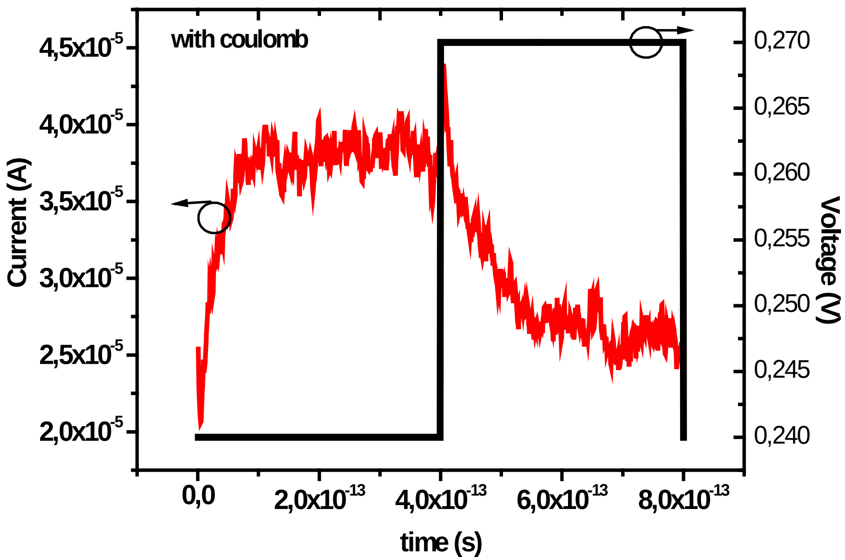
The value extracted for this structure is *0,03* ps in excellent agreement with QMC.

2. With condition (i):

QMC

The potential is computed by solving the Poisson equation self-consistently

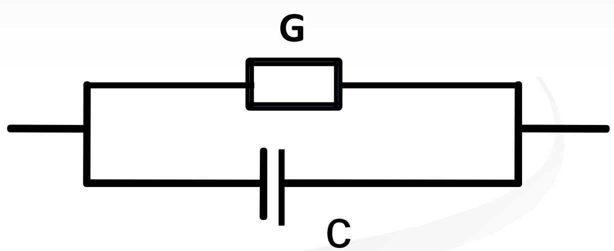
the "simulation box" is very small, thus leads are neglected.



τ~ 0,2 ps

SSEC

The Coulomb interaction can be modeled by a capacitance *C* in parallel to *G*

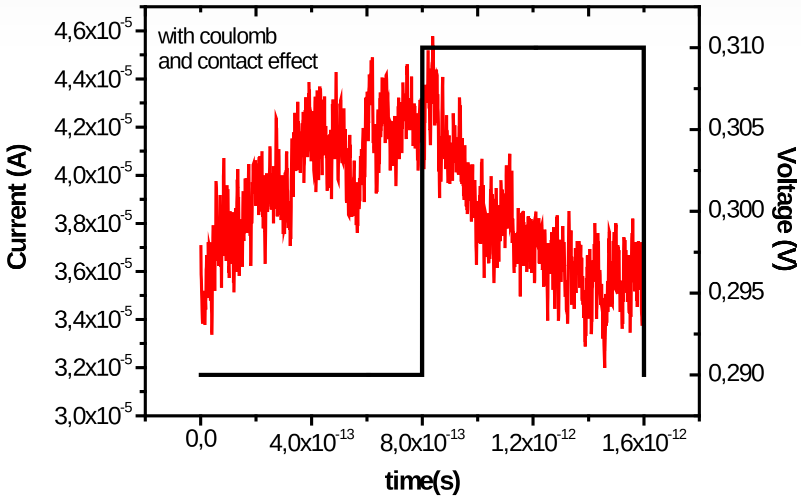


Cutoff frequency of SSEC results of *3.6* THz and it is consistent with the *0,25* ps characteristic time

3. With condition (i) and (ii):

QMC

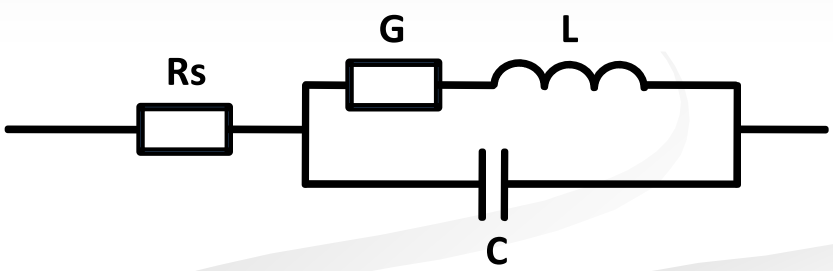
Leads have been introduced consistently with the Poisson equation



Intrinsic extracted frequency : 0,9 THz

SSEC

Contacts have been included by means of a series resistance



The cut off frequency is now *1,4* THz.

This value is in very good agreement with cutoff frequency reduction obtained with QMC .

Conclusions

- In investigation of RTD frequency response several limitations come to play:
  - The intrinsic tunneling process (life time in the well)
  - The transit time across the non-tunneling regions (leads, contacts…)
  - the total capacitance of the structure

- Two approaches have been evaluated and compared :

1. Quantum Monte Carlo simulations
2. Small Signal Equivalent Circuit

- Time-dependent simulation provides a rigorous picture of the physics that governs the frequency behavior of RTD. (simulation time 1 week)

- The equivalent small signal circuit is able to catch characteristic times, resulting a useful tool to design RTD. (simulation time 0 seconds! ☺)

Thank you for your attention !

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