Quantum transport in RTD: asymptotic models and simulations of Schrödinger–Poisson systems.

"The unreasonable effectiveness of semiclassical analysis."

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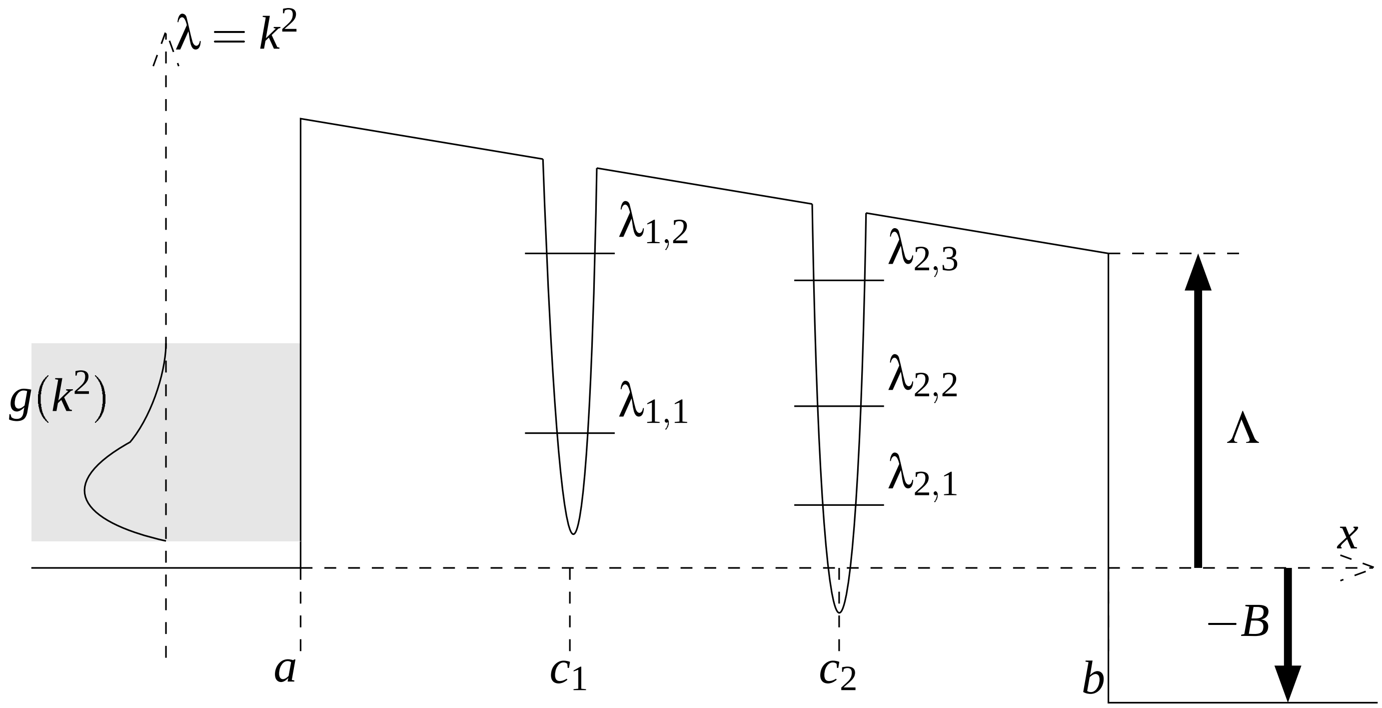
Joint work with V. Bonnaillie and A. Faraj.

Model

Quantum wells in a (semiclassical) island
Injection from the left (and right). Applied Bias B.



Model

$$H = -h^2\Delta + \tilde{V}_0(x) - W^h(x) + V_{NL}^h(x)$$

$$-W^h(x) = -\sum_{i=1}^{N} w_i \left(\frac{x - c_i}{h}\right)$$

$$[H, \varrho] = 0$$

ϱ F.F.E.S.S (Landauer-Büttiker)

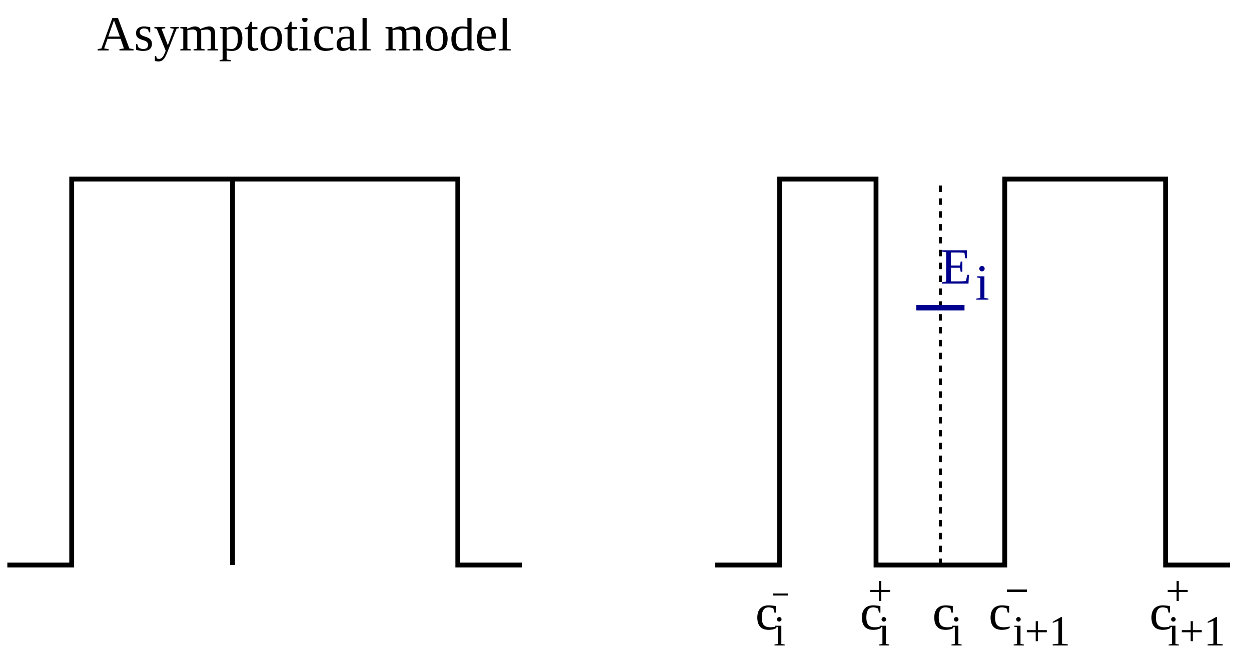
$$-\Delta V_{NL}^h = n$$

$$V(a) = V(b) = 0 \qquad \int n(x)\varphi(x) = \text{Tr } [\varrho\varphi]$$

$h = h_{eff}$ after rescaling

Model

Limit $h \to 0 \to$ finite dimensional system:
"The phenomena are governed by a finite number of resonant states"



Model

Limit $h \to 0 \to$ finite dimensional system:
Easy to solve numerically after some adaptations

$$h = h_{eff} \sim 0.1 \text{ or } 0.3$$

- Imaginary parts of resonances $e^{-\frac{d_{Ag}}{h}} \sim 0$ OK
- Comparison of tunnel effects: $e^{-\frac{A(h)}{h}} \overset{\geq}{\leq} e^{-\frac{B(h)}{h}}$
  $A(h \neq 0)$, $B(h \neq 0)$, $h = O(1)$.
- Charge in a well $\sim \delta_{c?}$. Feynmann-Hellman interpolation when V^h_{NL} small.

First results

Bonnaillie-Nier-Patel JCP-2006

- Fast numerical simulation (about 1 minute to solve 100 nonlinear problems) $->$ allows to study the effect of changing the values of the size of the barriers, the donnor density…

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First results

Bonnaillie-Nier-Patel JCP-2006

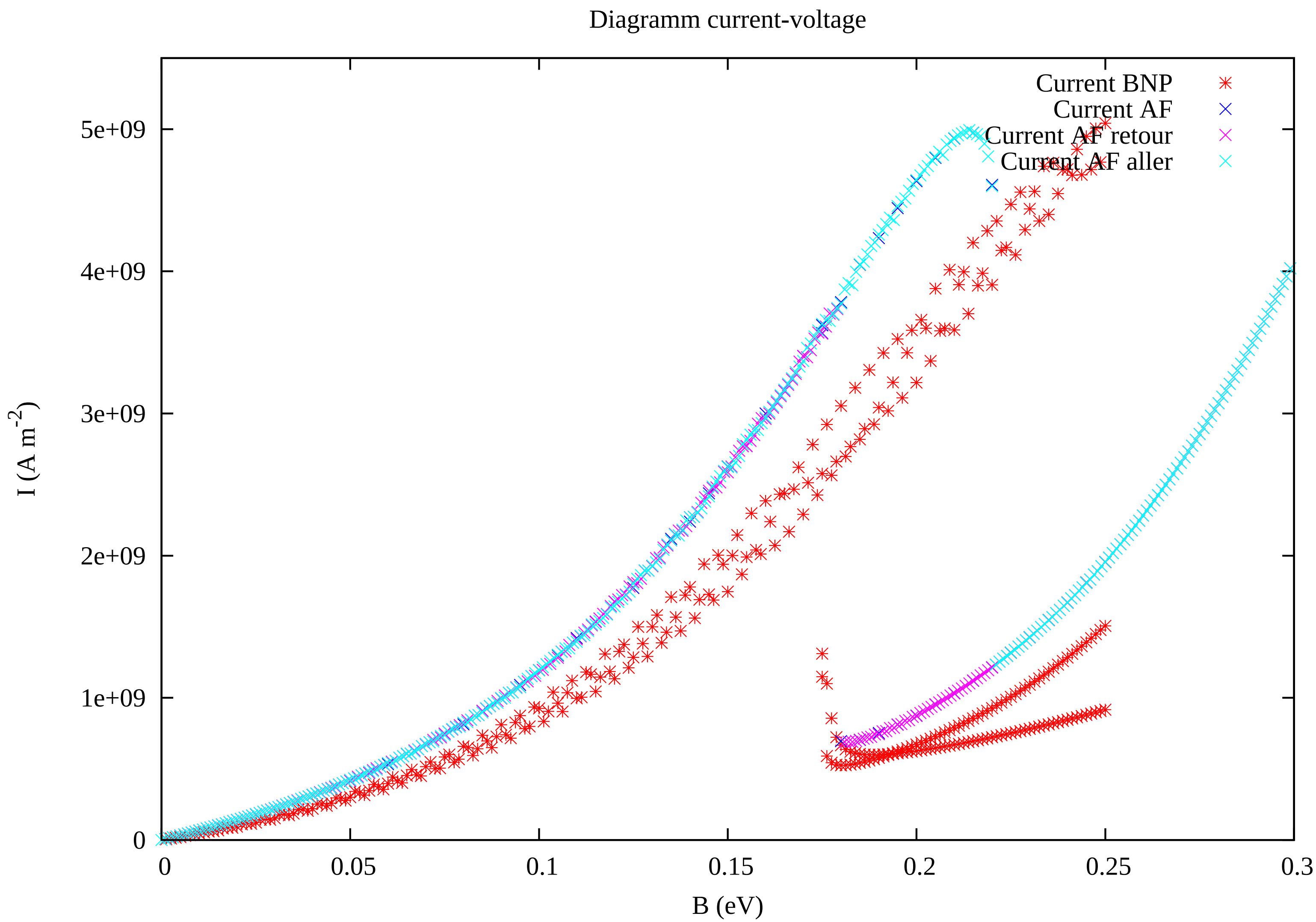
- Fast numerical simulation (about 1 minute to solve 100 nonlinear problems) $->$ allows to study the effect of changing the values of the size of the barriers, the donnor density. . .
- Provides complete bifurcation diagrams and explains the possibility of hysteresis effects.
- At first sight, good agreement with other numerical simulations (Pinaud for Ga-As and Kumar-Laux-Fischetti for Si-SiO2).

Comparison

- Full Schrödinger-Poisson and asymptotic model tested with the same numerical data.
- Check that the asymptotic model helps to guess all the possible nonlinear solutions.
- Check that the solutions with interaction of resonances detected with the asymptotic model make sense. Dynamics: beating effect?

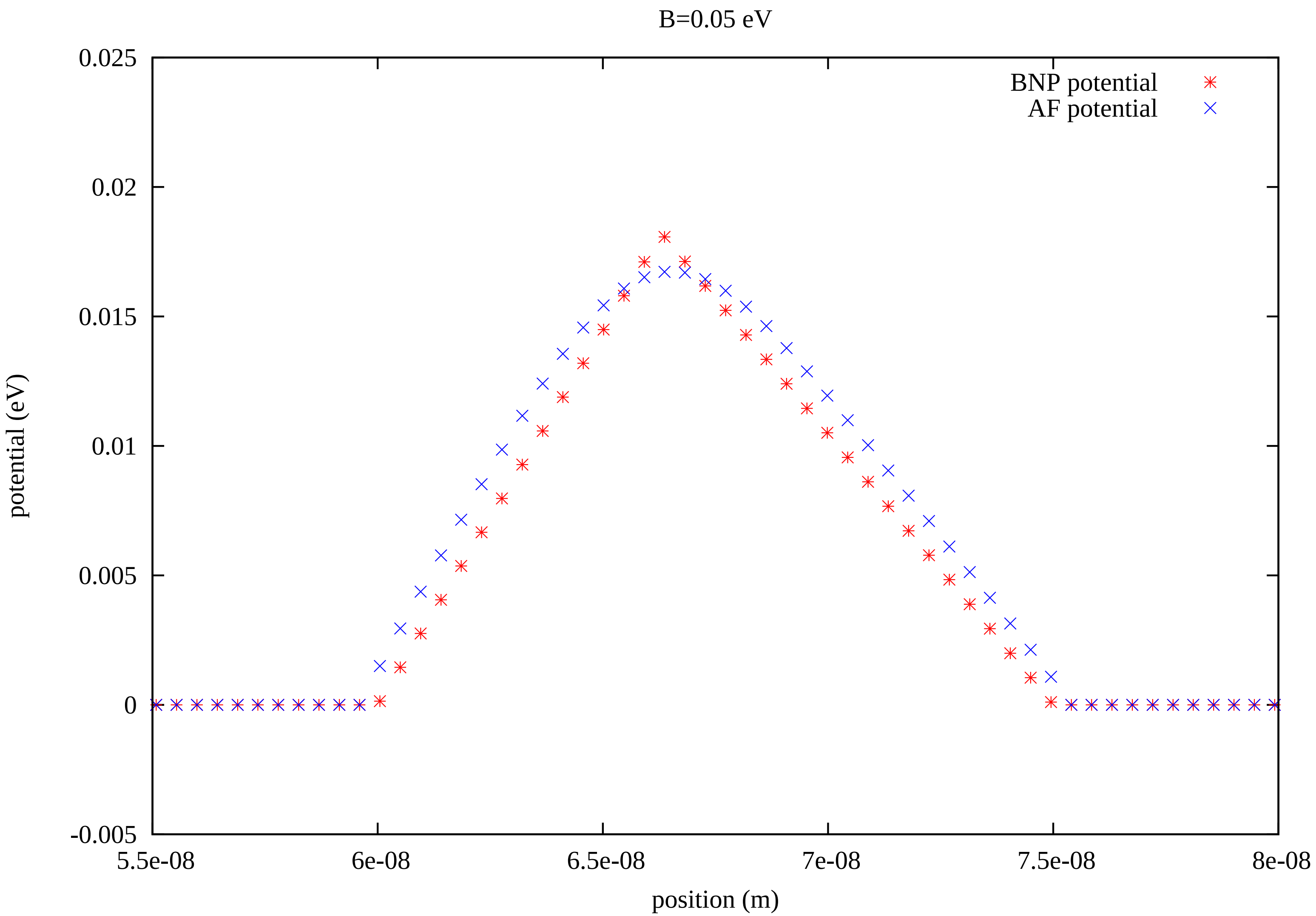
GaAs, 1 well, 1 resonance

I-V curve



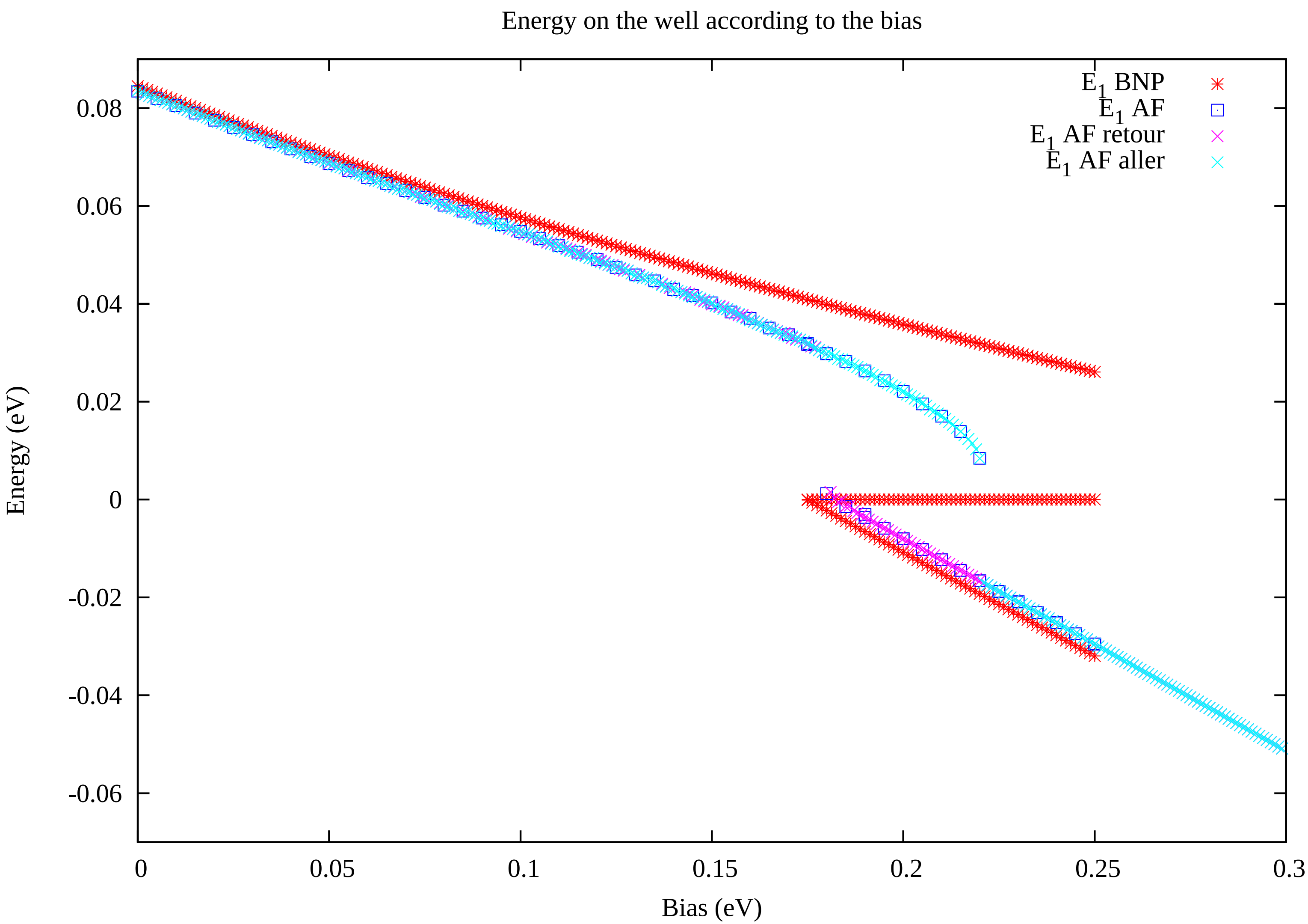
GaAs, 1 well, 1 resonance

Nonlinear potential



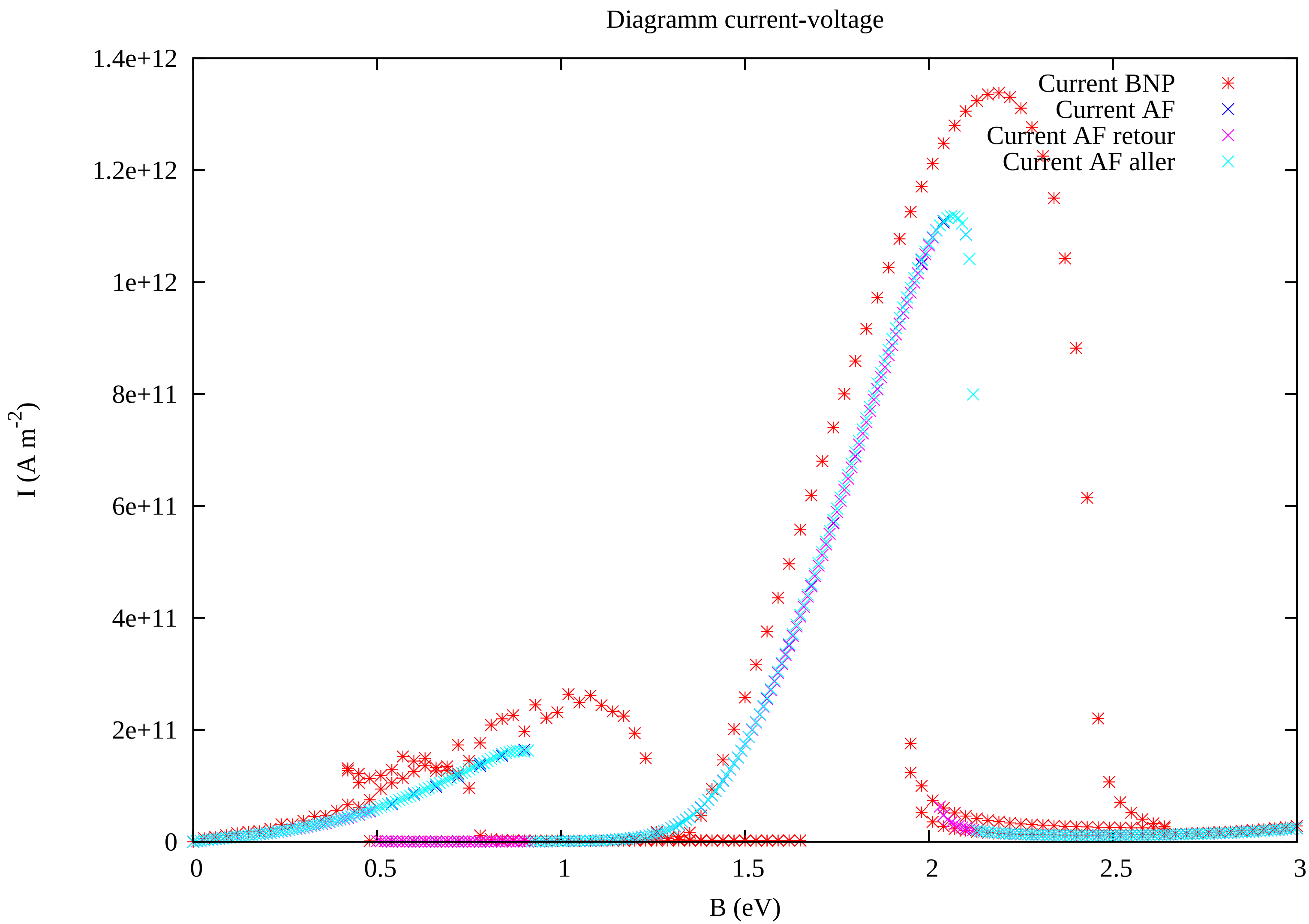
GaAs, 1 well, 1 resonance

$E_{res} - V$ curve



Si-SiO2, 1 well, 2 resonances

I-V curve



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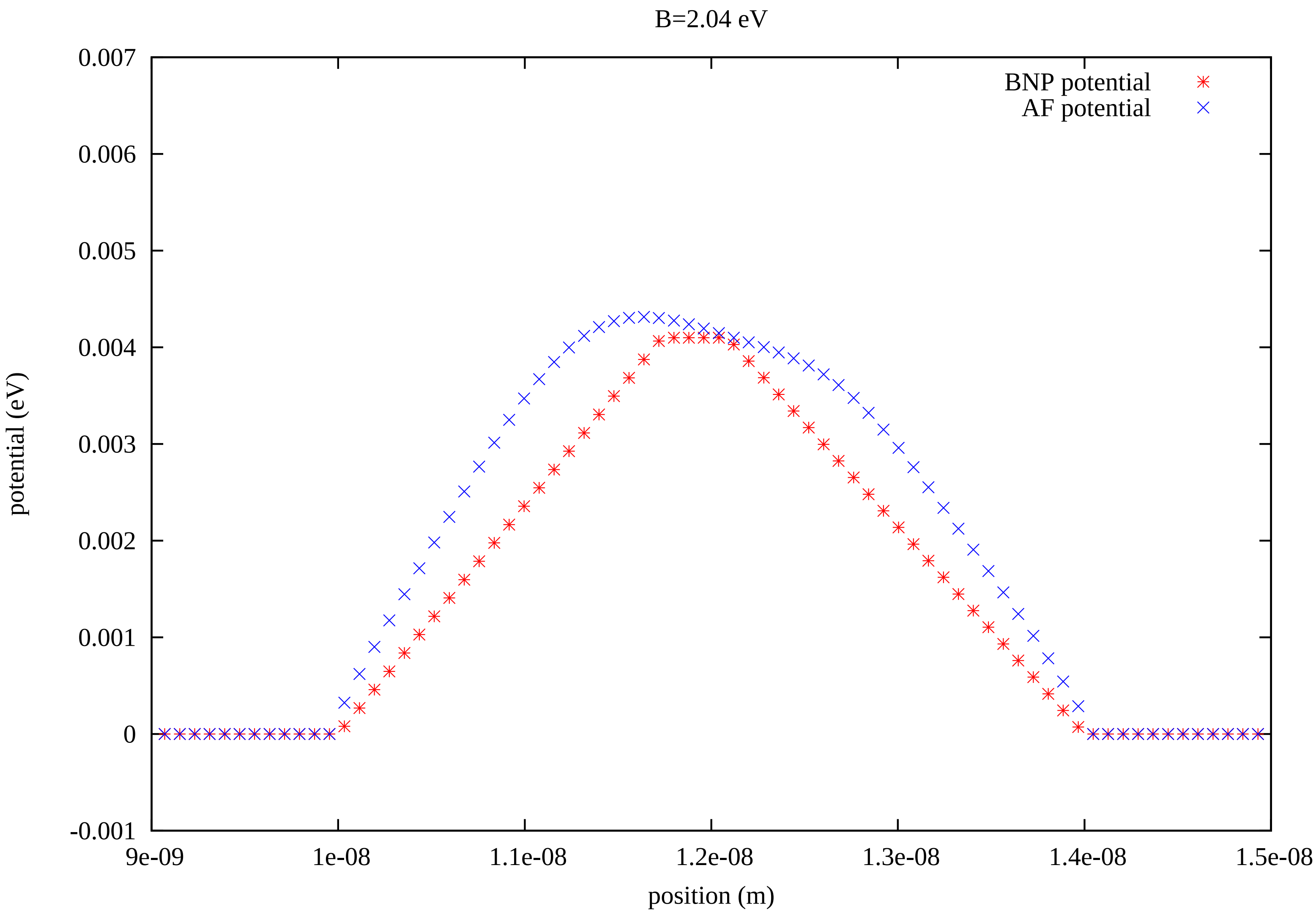

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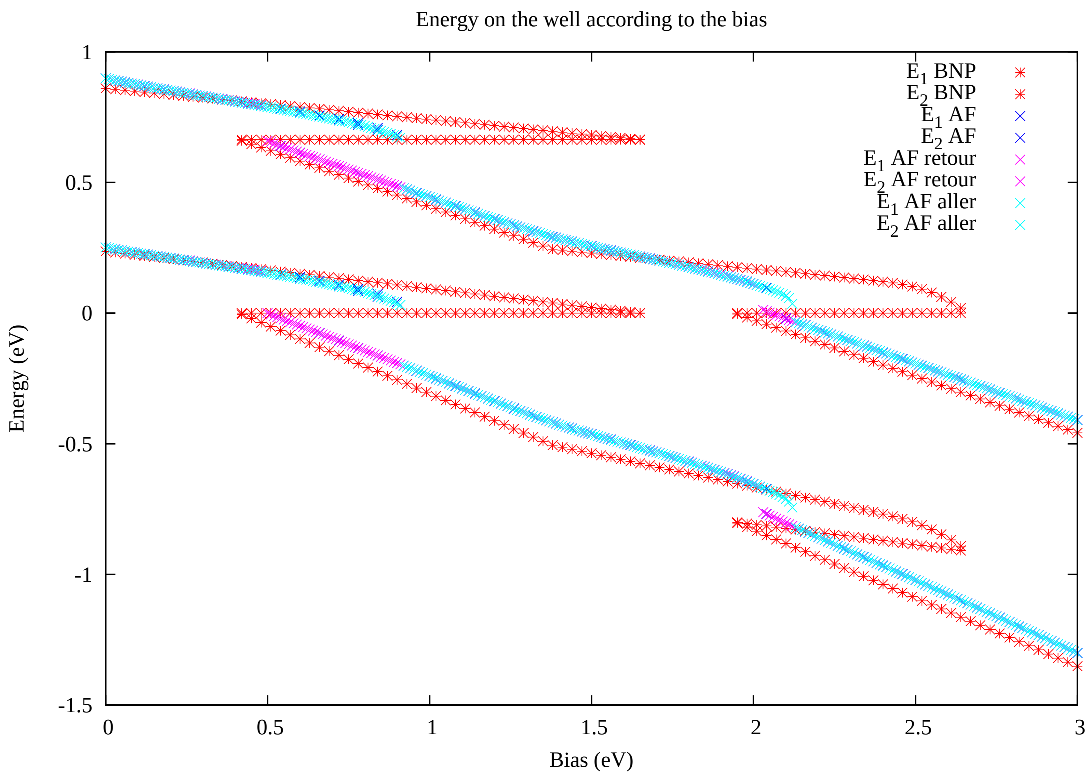
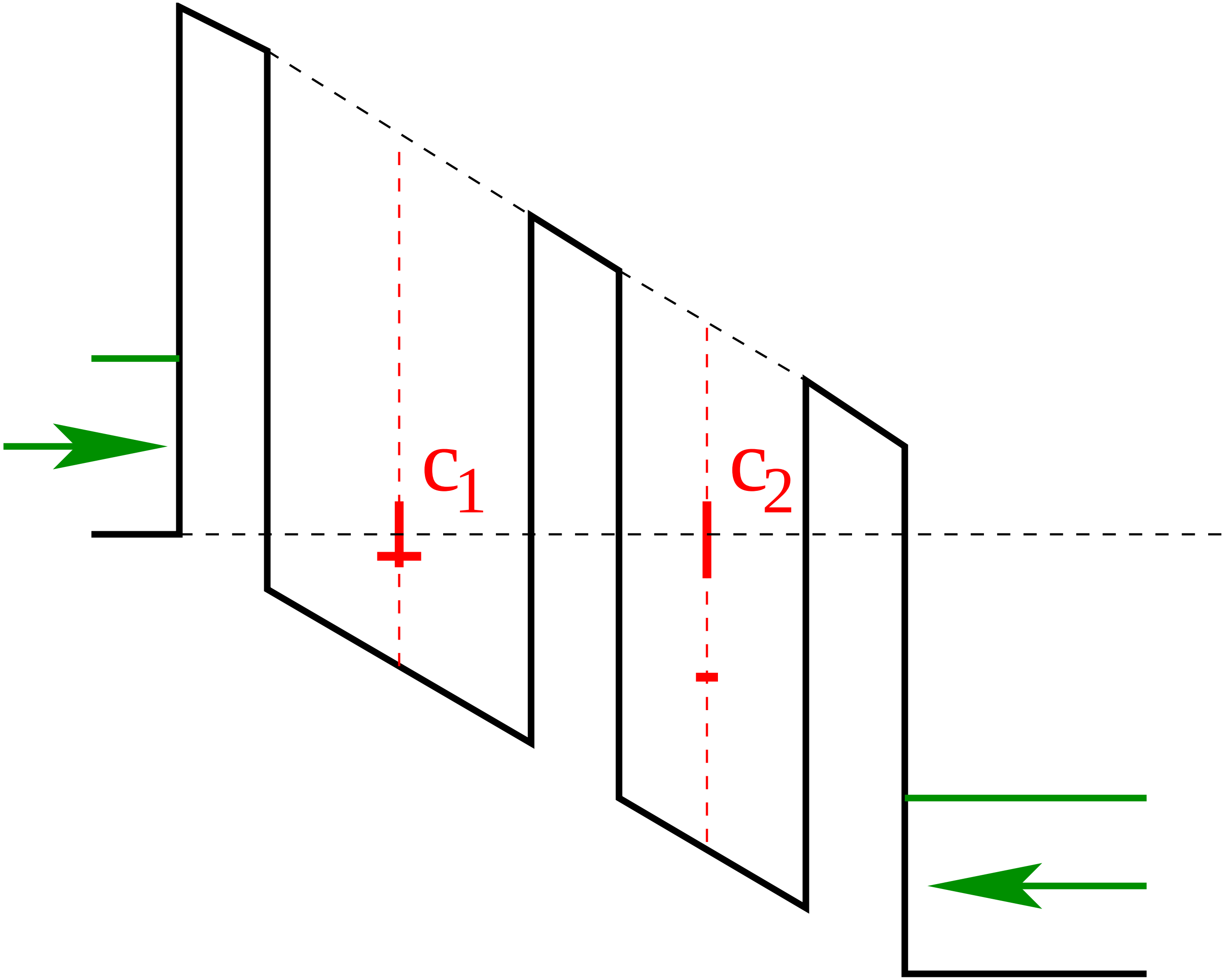


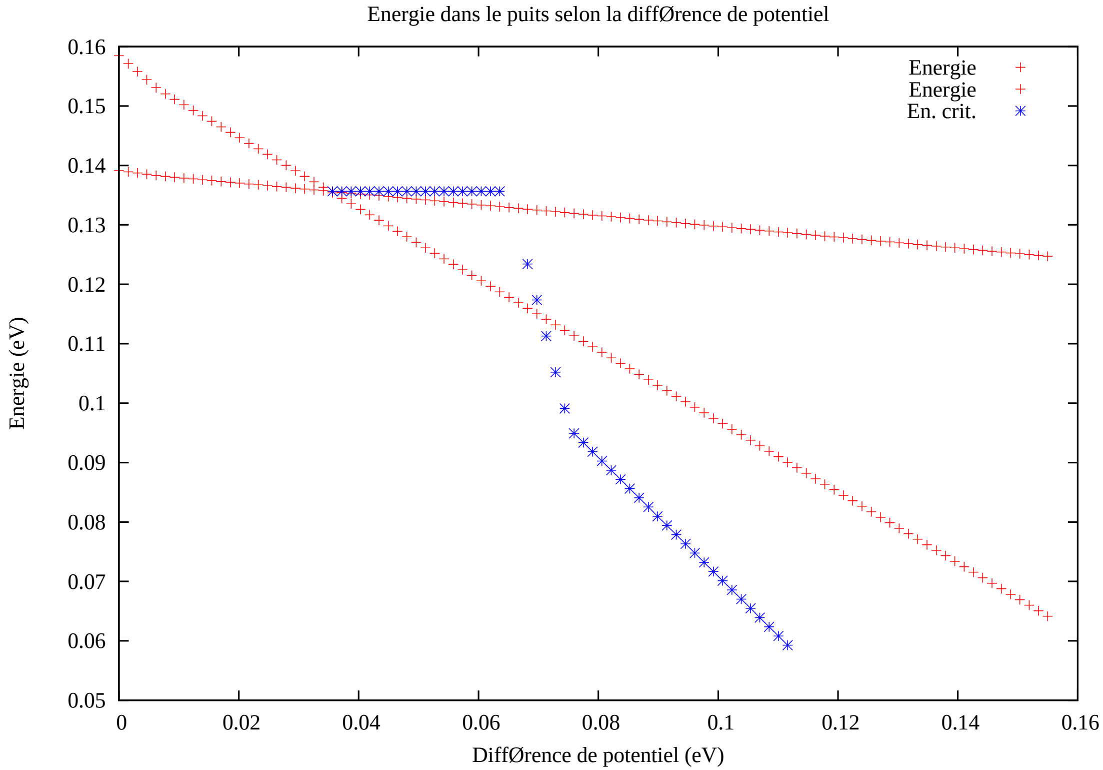
GaAs-2 Wells-2 resonances

Possible interaction of resonances



GaAs-2 Wells-2 resonances

Asymptotic model, $E_{res} - V$ curve



—: No nonlinear interaction. Energy crossing

—: The resonant energies are equal.

GaAs-2 Wells-2 resonances

Is it realistic ? Does it occur in the S.P. model ?

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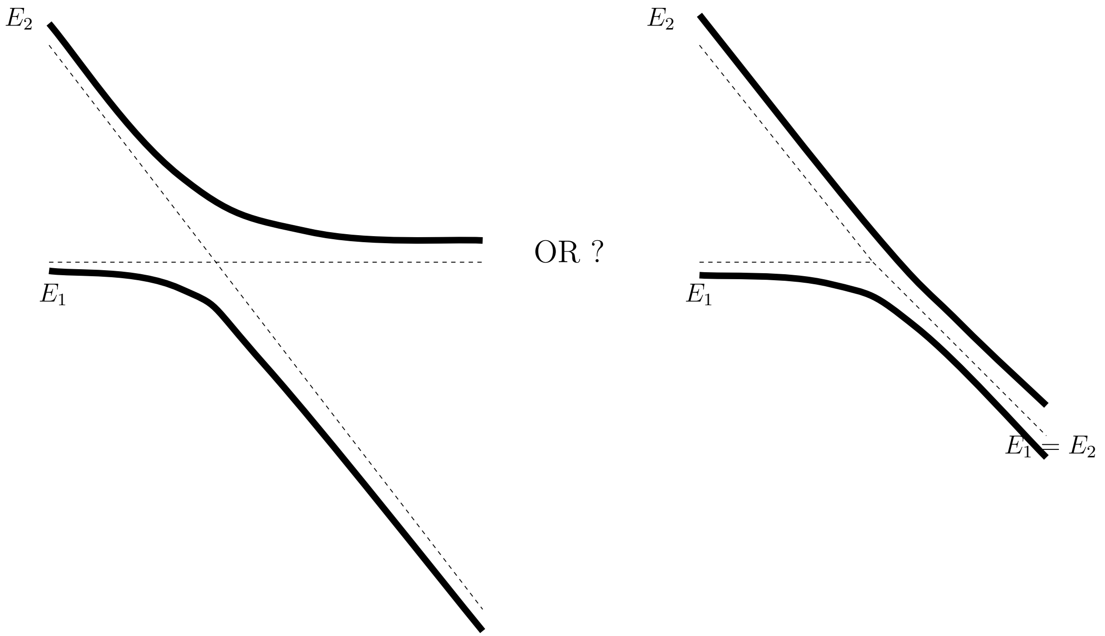
- Crossing or $E_1 = E_2 \overset{h>0}{\rightarrow}$ Avoided crossings



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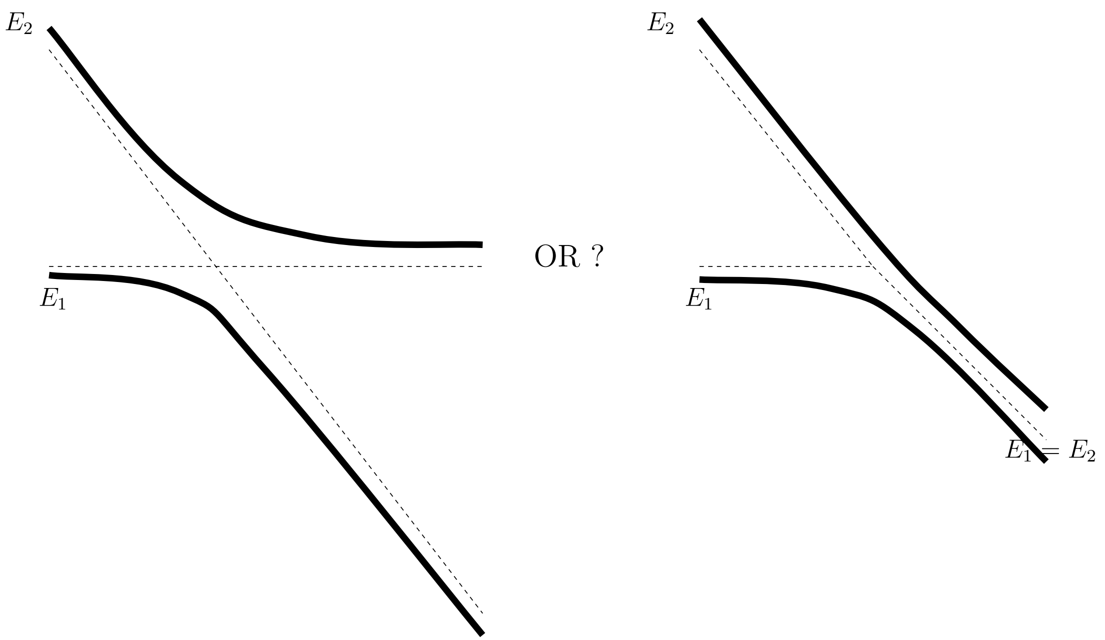
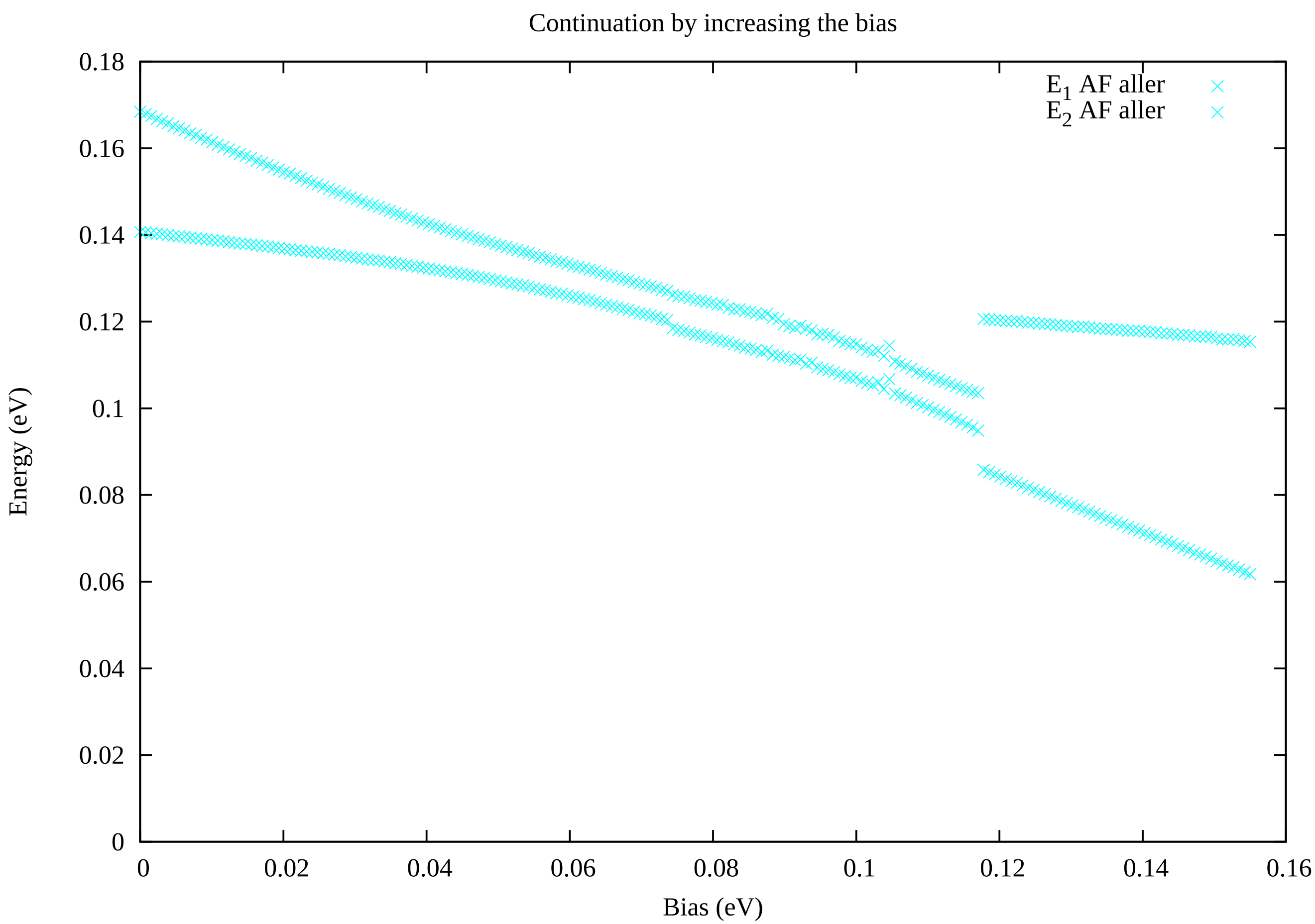


- Wells $[5nm, 3.5nm]$ Barriers $[5nm, 5nm, 6.5nm]$
  Previous bifurcation diagram sensitive to a a few Angström !!!.

2 Wells - 2 Resonances, comparison

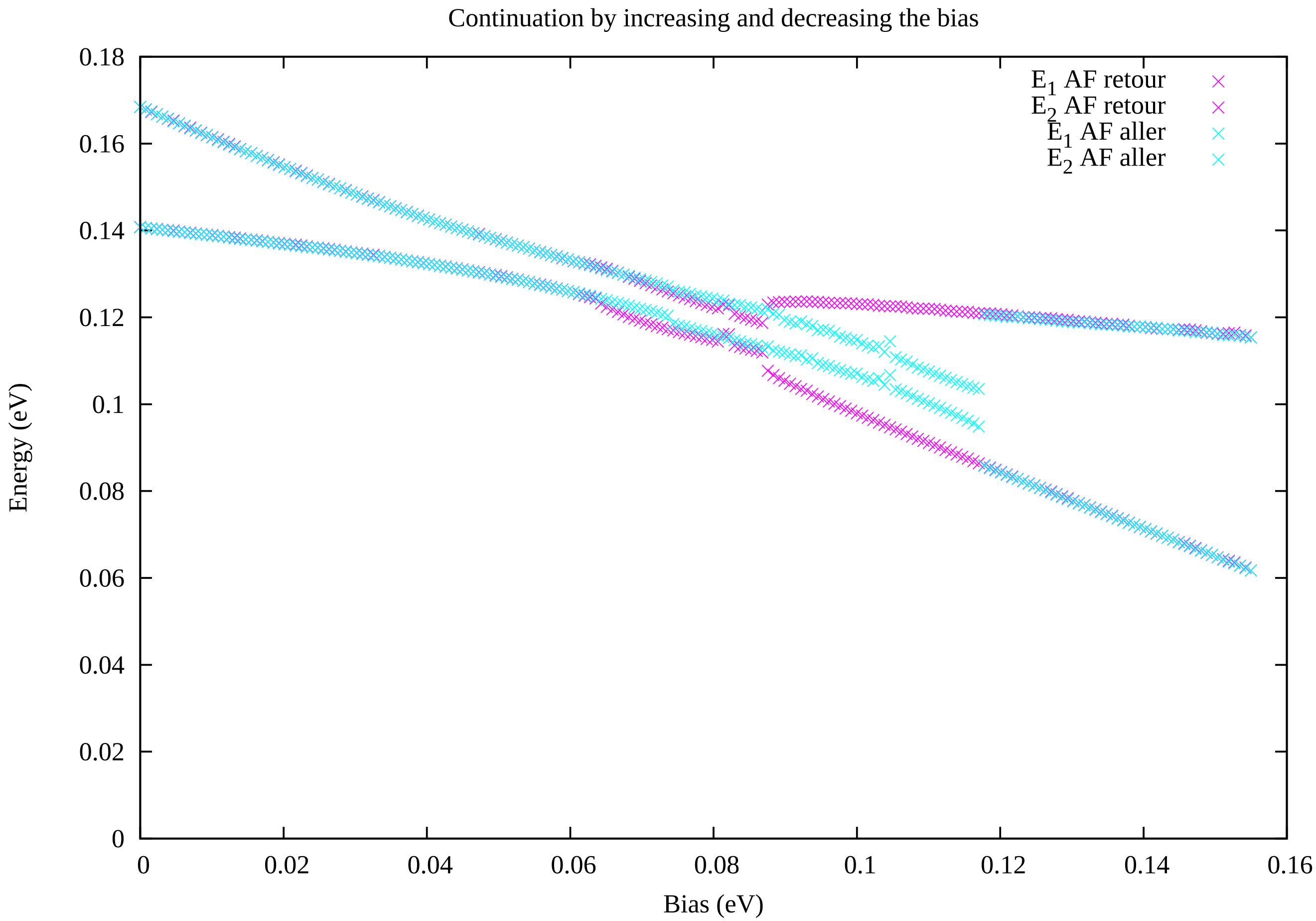
Continuation by increasing the bias



The second case is realized.

2 Wells - 2 Resonances, comparison

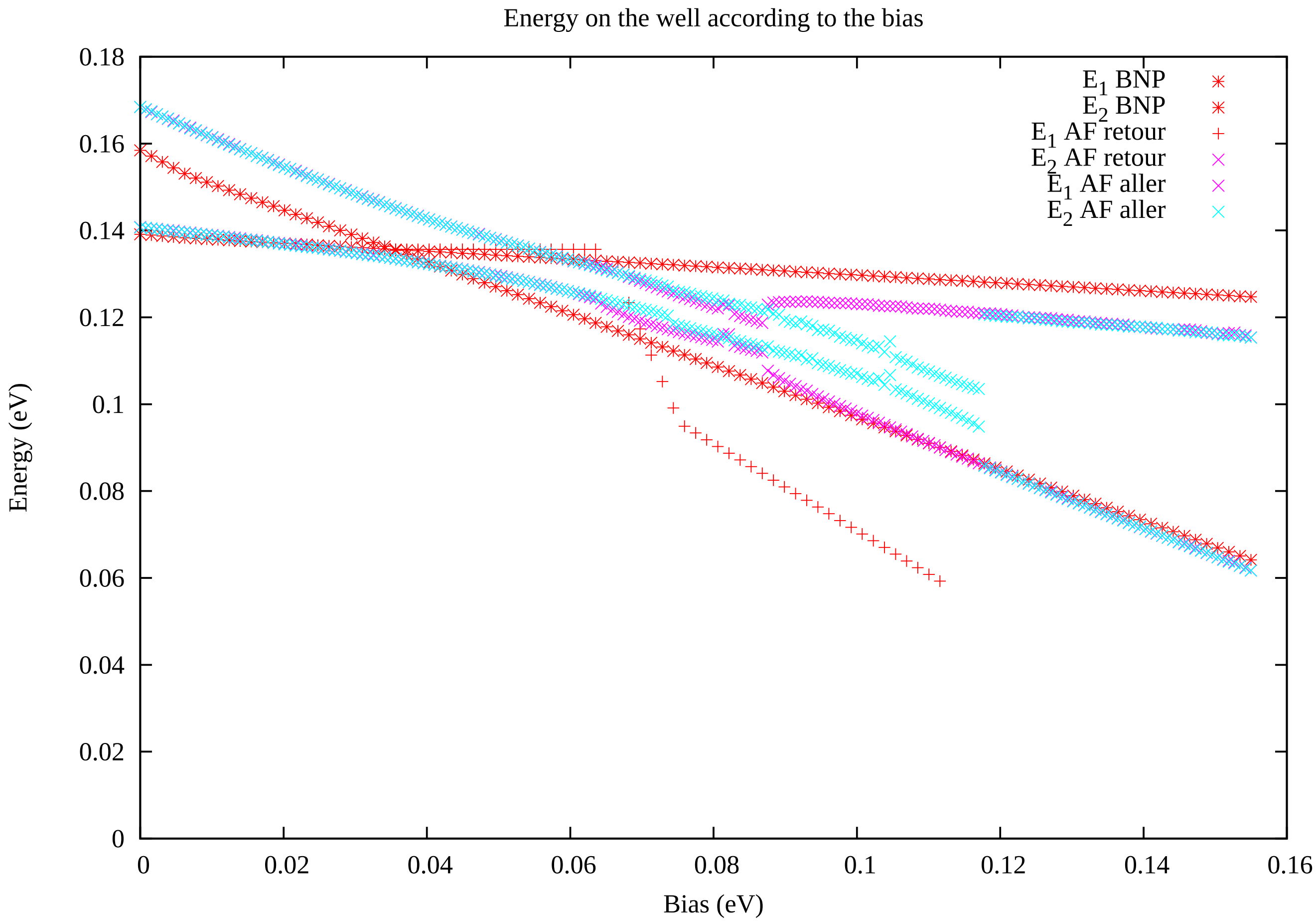
Continuation by in- and de-creasing the bias



For some bias, both solutions coexist !!

2 Wells - 2 Resonances, comparison

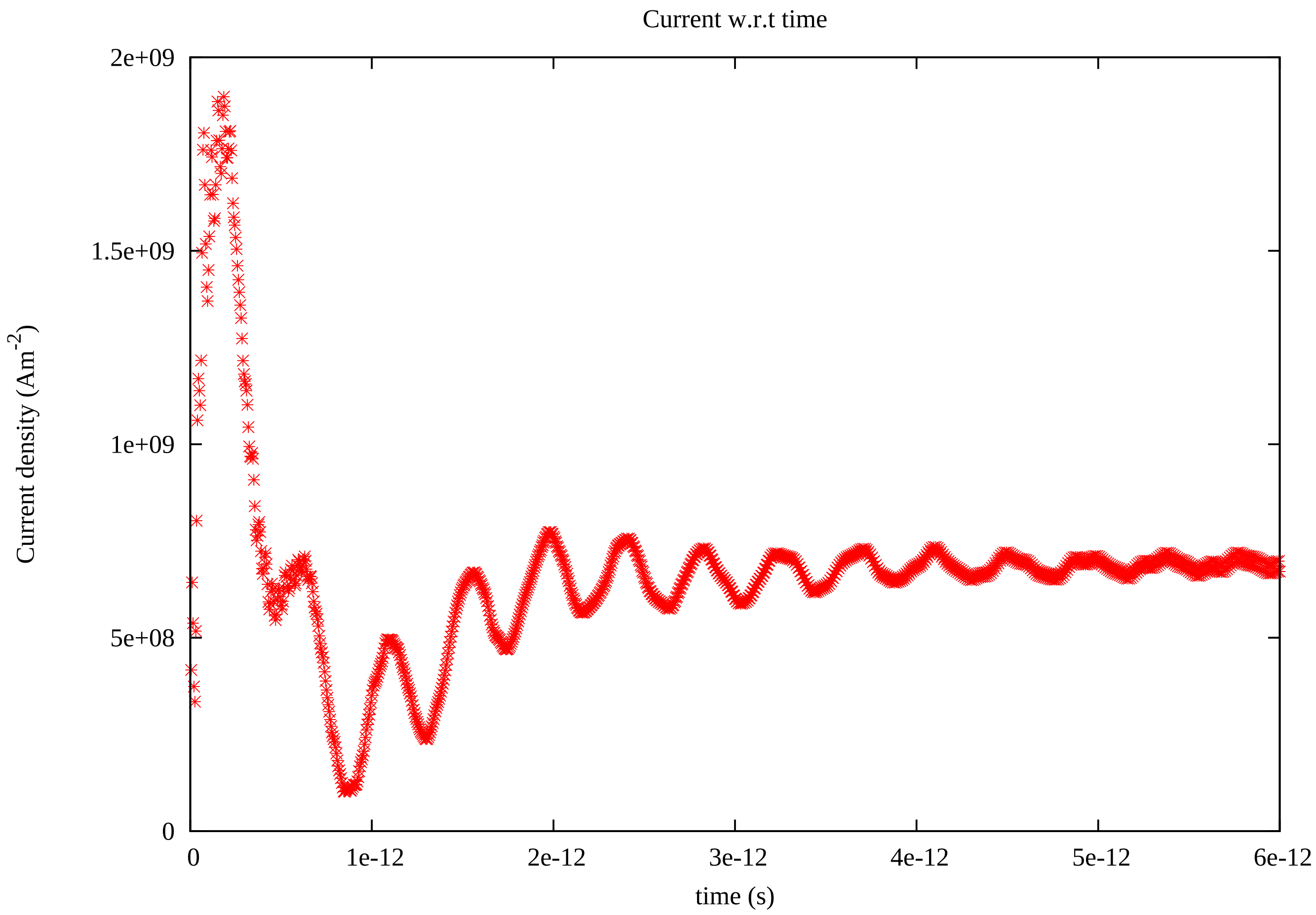
Comparison of the bifurcation diagrams



Remember the strong sensitivity to the data and all the approximation process.

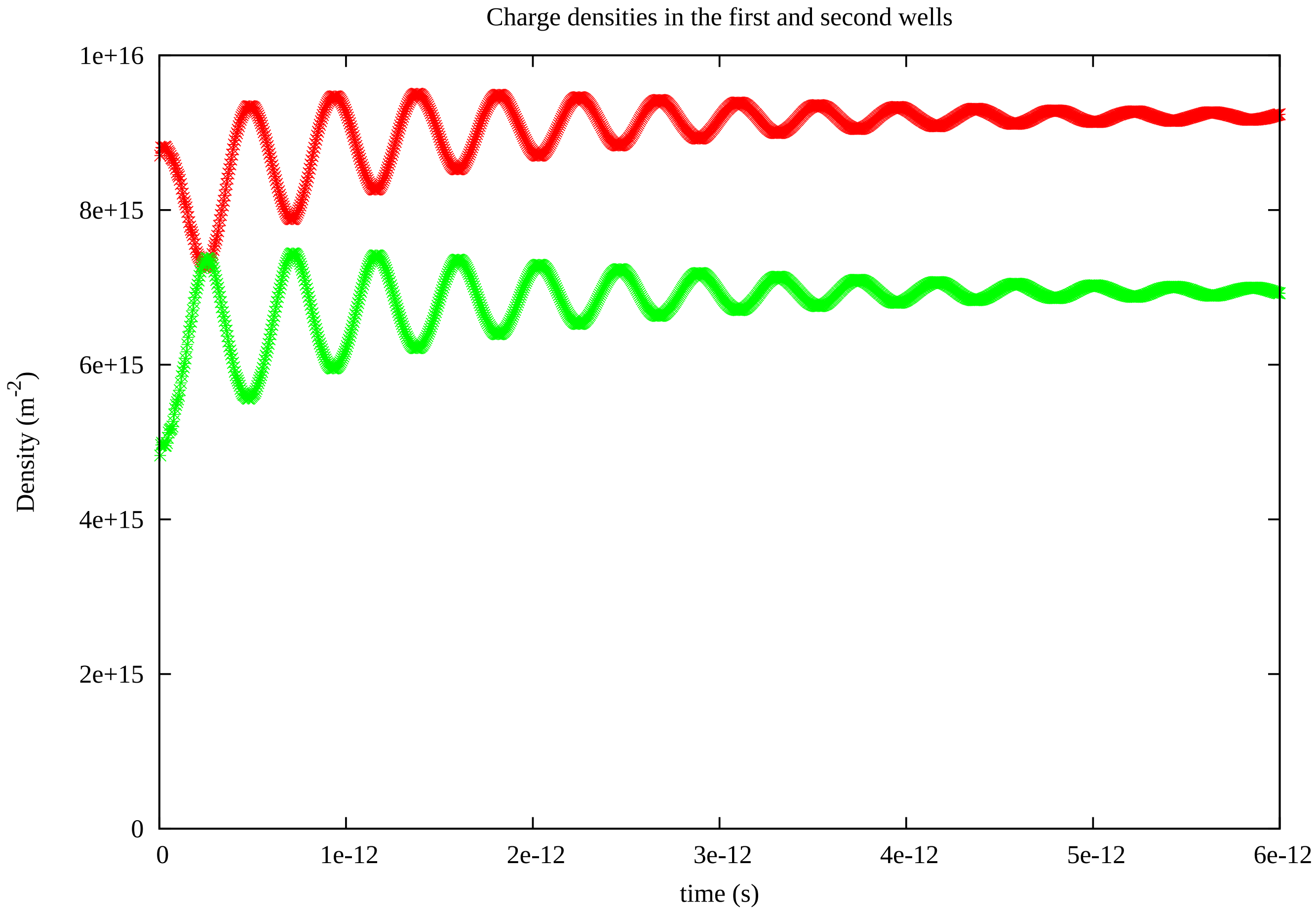
2 Wells - Beating effect

At time $t = 0$, the bias goes from $0V$ to $0.08V$



Is it a (damped) beating effect ?

2 Wells - Beating effect



And $T = \frac{h_{phys}}{\Delta E_{gap}}$ up to 10%.

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- All the semi-algebraic complexity of the bifurcation diagrams of the asymptotic model actually occurs in the Schrödinger-Poisson model.
- The faithful and fast computations of the asymptotic model allow to design interesting test cases for the Schrödinger-Poisson problem.