Multiscale simulation of transport in an open quantum system: Resonances and WKB interpolation

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November 14, 2007

Introduction

- In nanoscale semiconductor structures, quantum effects arise and have to be taken into account in the modelling by means of the Schrödinger equation.
- The oscillatory behaviour of the solutions of such an equation induces serious numerical difficulties.
- We propose a method to reduce the simulation time for an RTD by both reducing the number of energy and position grid points.

The RTD(resonant tunneling diode) model

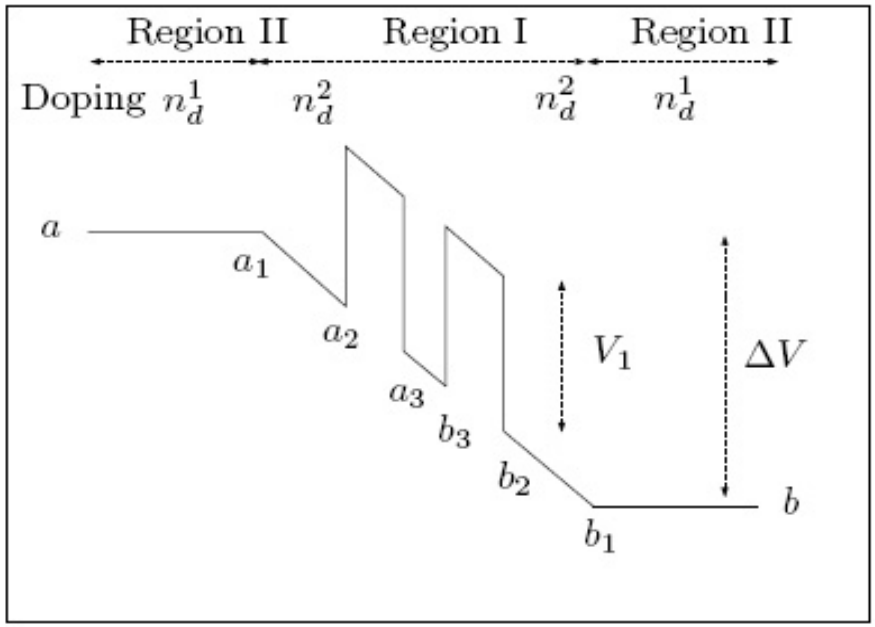

Figure 1: Schematics of the potential energy in an RTD

The Schrödinger-Poisson problem

The wave function of the electrons injected at $x = a$ with momentum $p \geq 0$ satisfies a stationary effective-mass Schrödinger equation with open boundary conditions:

$$\begin{cases} -\frac{\hbar}{2m}\varphi_p'' - qV\varphi_p = E_p^a\varphi_p, \ (p \geq 0) \\ \hbar\varphi_p'(a) + ip\varphi_p(a) = 2ip; \ \hbar\varphi_p'(b) = ip_b\varphi_p(b), \end{cases} \tag{1}$$

m: the effective mass (assumed to be constant in the device),
q: the elementary positive charge of the electron,
V is the total electrostatic potential in the device,

$$p_b = \sqrt{p^2 + 2qm(V_b - V_a)}; \ E_p^a = \frac{p^2}{2m} - qV_a$$

.

Similarly, electrons injected at $x = b$ with momentum $p \leq 0$

$$\begin{cases} -\frac{\hbar}{2m}\varphi_p'' - qV(x)\varphi_p = E_p^b\varphi_p, \ (p \leq 0) \\ \hbar\varphi_p'(b) + ip\varphi_p(b) = 2ip; \ \hbar\varphi_p'(a) = ip_b\varphi_p(a), \end{cases} \tag{2}$$

$$p_a = \sqrt{p^2 + 2qm(V_a - V_b)}; \ E_p^b = \frac{p^2}{2m} - qV_b$$

. The transmission coefficients are defined by

$$T(p) = \frac{\sqrt{(p^2 + 2qm(V_b - V_a))^+}}{|p|}|\varphi_p(b)|^2 \text{ for } p > 0 \tag{3}$$

$$T(p) = \frac{\sqrt{(p^2 + 2qm(V_b - V_a))^+}}{|p|}|\varphi_p(a)|^2 \text{ for } p < 0 \tag{4}$$

where $(a)^+ = \max(a, 0)$.

The electrons are assumed to be in a mixed state so that the electronic and current densities are given by

$$n(x) = \int_{-\infty}^{\infty} g(p)|\varphi_p(x)|^2 dp; \quad J = \frac{q}{m}\int_{-\infty}^{\infty} g(p)pT(p)dp \qquad (5)$$

where $g(p) := g_a(p)$ for $p > 0$, $g(p) := g_b(p)$ for $p < 0$(g_a being the statistics of the electrons injected at $x = a$).
$g(p)$ is a Fermi-Dirac integral given by

$$g(p) = \frac{mk_bT}{2\pi^2}\log\left(1 + \exp((-\frac{p^2}{2m} + E_F)/k_bT)\right). \qquad (6)$$

E_F: Fermi energy; k_b: Boltzmann constant.

The electrostatic potential V is split into two parts: $V = V_e + V_s$.
V_e is the external potential (including double barriers, applied voltage)
V_s is the self-consistent potential modeling the electron-electron interaction

$$\begin{cases} V_s''(x) = \frac{q}{\epsilon}(n(x) - n_D(x)) \\ v_s(a) = V_s(b) = 0 \end{cases} \tag{7}$$

where ϵ is the dielectric constant and n_D the doping density.

Reducing the number of spatial grid points

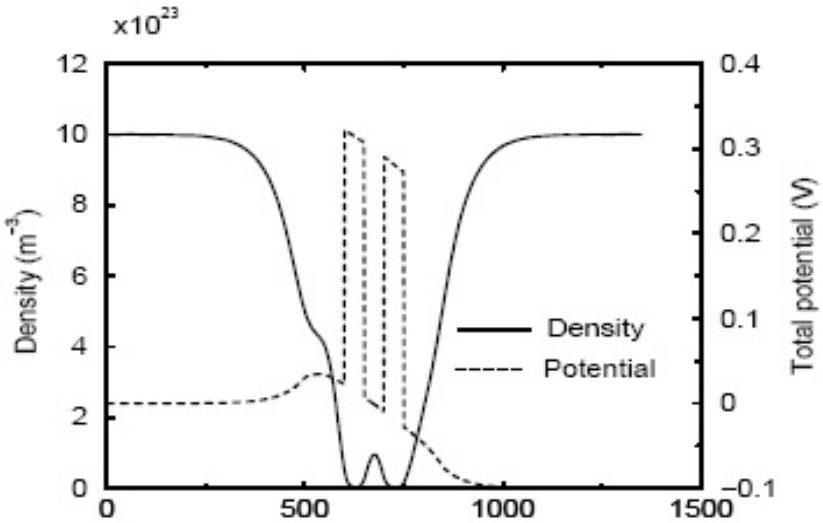

Figure 2: Density profile in an RTD : smooth variation

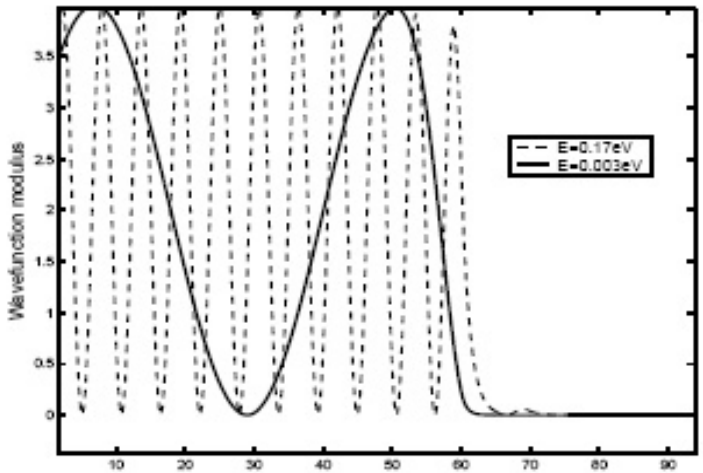

Figure 3: A low energy (slowly varying) and a high energy (strongly oscillating) wave functions

WKB method

- if the oscillation phase is known accurately, the phase factor could be used to interpolate the nodal values of the wave function and a coarser grid can be allowed.
- succeeds in 1d. WKB asymptotics provide us with an explicit formula for this phase factor.
- fails in 2d.

Reducing the number of energy grid points

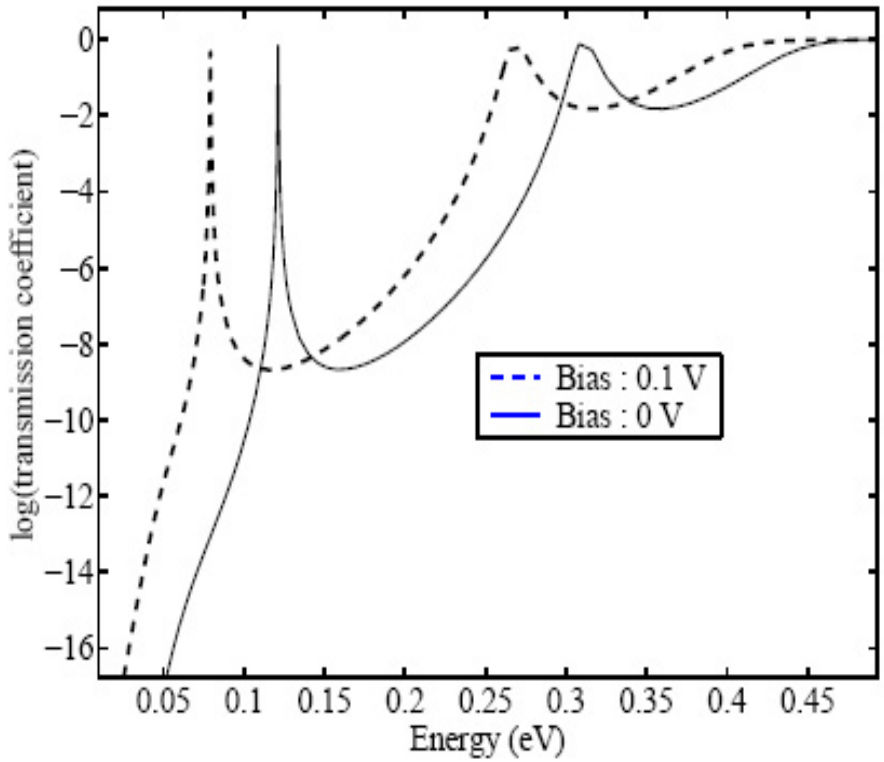

Figure 4: Transmission coefficient for an RTD at two different biases

The Presilla-Sjöstrand decomposition

- Some people detect the resonance peak first and only refine mesh around sharp resonance peak.
- Presilla and Sjöstrand split the wavefunction into an exterior and an interior wavefunction. The exterior solution does not exhibit any resonance. Only for the interior part, we need a refined energy grid.

The WKB-scheme

Consider a 1D stationary Schrödinger equation on the domain $[a, b]$,

$$-\frac{\hbar}{2m}\varphi''(x) + V(x)\varphi(x) = E\varphi(x), \tag{8}$$

$$\varphi(a) = \varphi_a\ ; \quad \varphi'(a) = \varphi'_a. \tag{9}$$

It can be written as a first order ODE, and then solved by Runge-Kutta method.

$$\Phi = \begin{pmatrix} \varphi \\ \varphi' \end{pmatrix}; \quad \Phi' = \begin{pmatrix} 0 & 1 \\ \frac{2m}{\hbar^2}(V - E) & 0 \end{pmatrix}\Phi; \quad \Phi(0) = \begin{pmatrix} \varphi_a \\ \varphi'_a \end{pmatrix}. \tag{10}$$

Remarks on solving Schrödinger

- the meshsize has to be small enough in order to resolve the oscillations of the wave function φ.
- need $\frac{\triangle x}{\lambda} \ll 1$, λ is the de Broglie wavelength of the particle.
- for $\frac{\triangle x}{\lambda} \gg 1$, the standard schemes fail, this actually happens for sufficiently high energy wavefunctions.

WKB approximation introduction

WKB (Wentzel-Kramers-Brillouin) approximation, is the most familiar example of a semiclassical calculation in quantum mechanics in which the wavefunction is recast as an exponential function, semiclassically expanded, and then either the amplitude or the phase is taken to be slowly changing.

1. We recast the wavefunction as the exponential of another function ψ, i.e. $\varphi = e^{\psi(x)}$.
2. 'Semiclassically expanded', each function is expanded as a power series in $\hbar$.

WKB for Schrödinger

For $E > V(x)$,

$$\varphi(x) \sim_{\hbar \to 0} \frac{A}{\sqrt[4]{2m(E - V(x))}} e^{iS(x)} + \frac{B}{\sqrt[4]{2m(E - V(x))}} e^{-iS(x)} \tag{11}$$

where A and B are constants and S(x) is the dimensionless action,

$$S(x) = \frac{\sqrt{2m}}{\hbar} \int_{x_0}^{x} \sqrt{E - V(s)} ds \tag{12}$$

There is an analogous formulation for $E < V(x)$.

Accuracy of WKB approximation

- accurate if
$$\frac{\hbar m|V'|}{[2m(E-V)]^{3/2}} \ll 1.$$
- exact if V is constant.
- breaks down close to turning point
$$\mathcal{T} = \{x \in [a,b], E = V(x)\}.$$

WKB-basis construction

Let $(x_n)_{0\leq n\leq N}$ be a subdivision of $[a, b]$ such that

$$x_0 = a < x_1 < ... < x_n < ... < x_N = b,$$

and let $\mathcal{I}_n = [x_n, x_{n+1}]$.
The WKB-interpolated function is given by

$$\widetilde{\varphi}(x) = \frac{A_n}{\sqrt[4]{2m(E - V(x))}} e^{iS(x)} + \frac{B_n}{\sqrt[4]{2m(E - V(x))}} e^{-iS(x)}, \quad x \in \mathcal{I}_n. \tag{13}$$

The constants A_n and B_n are computed by solving to the following 2×2 system

$$\begin{aligned}
\varphi_n &= \widetilde{\varphi}(x_n) := \frac{A_n}{\sqrt[4]{2m(E-V(x_n))}} e^{iS(x_n)} + \frac{B_n}{\sqrt[4]{2m(E-V(x_n))}} e^{-iS(x_n)}, \\
\varphi_{n+1} &= \widetilde{\varphi}(x_{n+1}) := \frac{A_n}{\sqrt[4]{2m(E-V(x_{n+1}))}} e^{iS(x_{n+1})} + \frac{B_n}{\sqrt[4]{2m(E-V(x_{n+1}))}} e^{-iS(x_n}
\end{aligned}$$

$$\widetilde{\varphi}(x) = \alpha_n(x) f_n(x) \varphi_n + \beta_n(x) f_{n+1}(x) \varphi_{n+1} \quad x \in \mathcal{I}_n \qquad (14)$$

where

$$f_n(x) = \sqrt[4]{\frac{E - V(x_n)}{E - V(x)}}; \quad \alpha_n(x) = -\frac{\sin S_{n+1}(x)}{\sin \gamma_n}; \quad \beta_n(x) = -\frac{\sin S_n(x)}{\sin \gamma_n}$$

$$S_n(x) = \frac{\sqrt{2m}}{\hbar} \int_{x_n}^{x} \sqrt[+]{E - V(s)} ds; \quad \gamma_n = \frac{\sqrt{2m}}{\hbar} \int_{x_n}^{x_{n+1}} \sqrt[+]{E - V(s)} ds$$

Remarks

If V is constant, $E > V$, $\lambda = \frac{\hbar}{\sqrt{2m(E-V)}}$, Then,

$$\alpha_n(x) = \frac{\sin(x_{n+1} - x)/\lambda}{\sin(x_{n+1} - x_n)/\lambda}; \quad \beta_n(x) = \frac{\sin(x - x_n)/\lambda}{\sin(x_{n+1} - x_n)/\lambda};$$

If $(x_{n+1} - x_n)/\lambda \ll 1$, we have asymptotic formulae

$$\alpha_n(x) \simeq \frac{x_{n+1} - x}{x_{n+1} - x_n}; \quad \beta_n(x) \simeq \frac{x - x_n}{x_{n+1} - x_n}$$

which is exactly the expressions of the P^1 basis functions!

small $|E - V(x)|$

When $|E - V(x)| < \delta$,

- $E - V$ has a constant sign in $\mathcal{I}_n$. We remove the singular prefactor $f_n(x)$ in the interpolation function.

$$\varphi(x) = \alpha_n(x)\varphi_n + \beta_n(x)\varphi_{n+1} \quad x \in \mathcal{I}_n \tag{15}$$

- When $E - V$ crosses zero in $E - V$, a turning point $\widetilde{x}$,and the WKB function are no longer suitable. In this case the Schrödinger equation implies $\varphi''(\widetilde{x}) = 0$ and then φ is almost a linear function. Therefore, we use a P^1 interpolation function

$$\varphi(x) = \frac{x_{n+1} - x}{x_{n+1} - x_n}\varphi_n + \frac{x - x_n}{x_{n+1} - x_n}\varphi_{n+1} \quad x \in \mathcal{I}_n$$

Discretization of the Schrödinger equation

We integrate the $1d$ Schrödinger equation between $x_{n+\frac{1}{2}}$ and $x_{n-\frac{1}{2}}$:

$$\varphi'_{n+\frac{1}{2}} - \varphi'_{n-\frac{1}{2}} = -\frac{2m}{\hbar}\int_{x_{n-\frac{1}{2}}}^{x_{n+\frac{1}{2}}}(E - V(x))\varphi(x)dx. \qquad (16)$$

Projecting φ onto different basis leads to the following three-point scheme for the Schrödinger equation

$$\varphi_{n+1} = \frac{1}{A_n}\left((B_n + \widetilde{B}_{n-1})\varphi_n + \widetilde{C}_{n-1}\varphi_{n-1}\right) \qquad (17)$$

the coefficients $A_n, B_n, \widetilde{B}_{n-1}, \widetilde{C}_{n-1}$ can be computed exactly.

algorithm summary

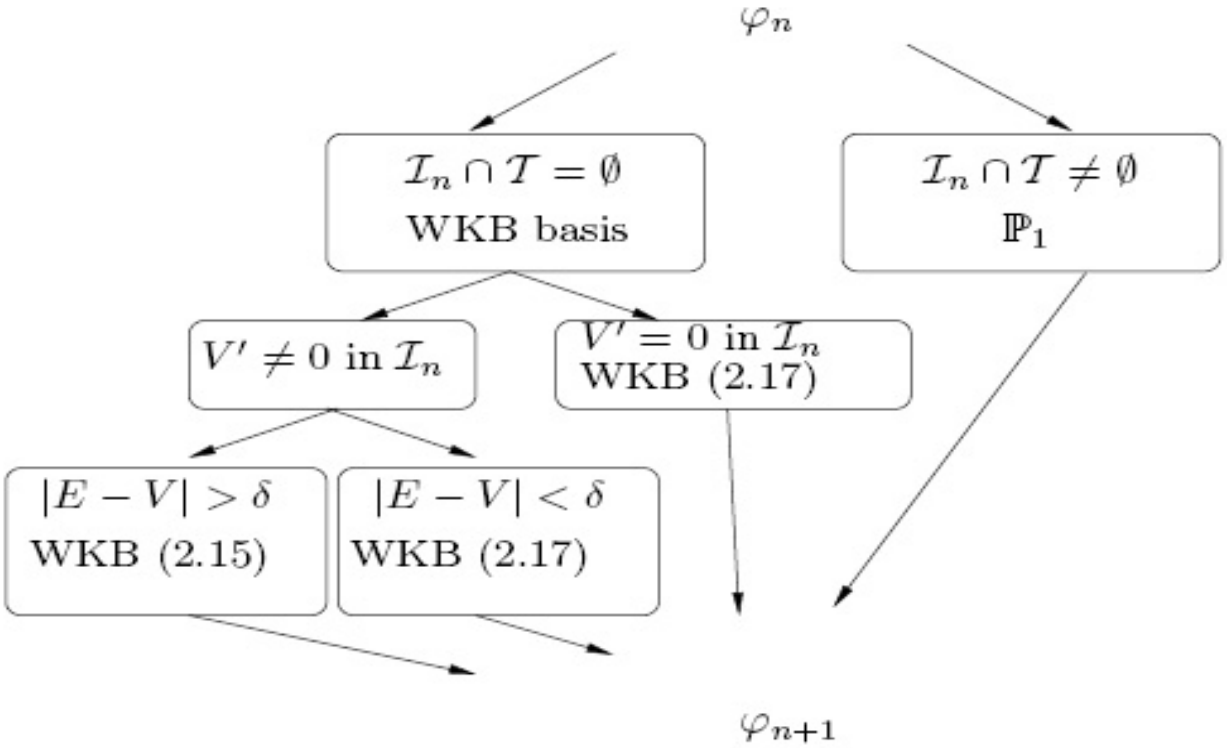

Figure 5: Choices for the WKB-interpolation

The Presilla-Sjöstrand decomposition

$$\varphi_p = \varphi_p^{ext} + \varphi_p^{int} \tag{18}$$

φ_p^{ext} essentially localized outside the barriers,
φ_p^{int} essentially localized in the well between the two barriers.
The exterior solution is defined as the solution of

$$\begin{cases} -\frac{\hbar}{2m}\frac{d^2\varphi_p^{ext}}{dx^2} - qV_{fill}\varphi_p^{ext} = E_p^a\varphi_p^{ext}, \ (p \geq 0) \\ \hbar\frac{d\varphi_p^{ext}}{dx}(a) + ip\varphi_p^{ext}(a) = 2ip; \ \hbar\frac{d\varphi_p^{ext}}{dx}(b) = ip_b\varphi_p^{ext}(b) \end{cases} \tag{19}$$

where V_{fill} is equal to the potential V with a filled well.

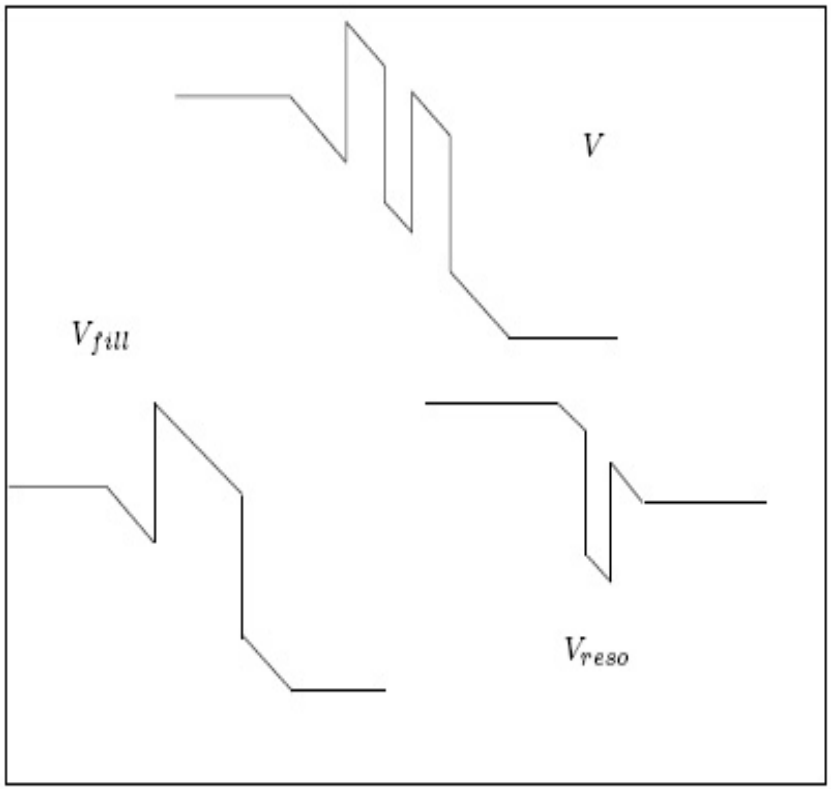

Figure 6: "True", "Filled" and "Resonant" potentialqThe different potentials

The interior solution is the solution of the nonhomogeneous Schrödinger equation

$$\begin{cases} -\frac{\hbar}{2m}\frac{d^2\varphi_p^{int}}{dx^2} - qV\varphi_p^{int} = E_p^a\varphi_p^{int} + q(V_{fill} - V)\varphi_p^{ext}, \ (p \geq 0) \\ \hbar\frac{d\varphi_p^{int}}{dx}(a) + ip\varphi_p^{int}(a) = 0; \ \hbar\frac{d\varphi_p^{int}}{dx}(b) = ip_b\varphi_p^{int}(b) \end{cases} \tag{20}$$

The source term is localized in the quantum well and has a non-zero contribution to φ_p^{int} when the energy E_p^a is close to resonant energies.

Resonant energies are defined as the non-trivial solutions of the eigenvalue problem

$$-\frac{\hbar}{2m}e_\lambda''(x) - qV(x)e_\lambda(x) = \lambda e_\lambda(x), \tag{21}$$

$$\hbar e_\lambda'(a) + i\sqrt[+]{2m(\lambda + qV_a)}e_\lambda(a) = 0;\ \hbar e_\lambda'(b) + i\sqrt[+]{2m(\lambda + qV_b)}e_\lambda(b) = 0 \tag{22}$$

where the eigenvalue $\lambda = E_R - i\Gamma/2$ has necessary a non-vanishing imaginary part.

- If λ is a real number, then Eqs (21) and (22) admits no solutions except the vanishing one.
- As soon as $\Gamma > 0$, Eqs (21) and (22) has several solutions.

Computing the resonant states.

Define the self-adjoint operator $\mathcal{H} = -d^2/dx^2 - qV_{reso}$ on $[c, d]$, with $c \in [a_1, a_2]$,$d \in [b_2, b_1]$, where

$$V_{reso} = \mathrm{I}_{[a_2,b_2]} V + \mathrm{I}_{[c,a_2]} V(a_2^+) + \mathrm{I}_{[b_2,d]} V(b_2^-). \tag{23}$$

The ground state of $\mathcal{H}$ is denoted by $\widetilde{e}$ and then solves

$$\begin{cases} \mathcal{H}\widetilde{e} = \widetilde{E}_R \widetilde{e} \\ \widetilde{e}(c) = \widetilde{e}(d) = 0. \end{cases} \tag{24}$$

The real part of the resonance E_R is approximated by $\widetilde{E}_R$ and the value of e inside the well is approximated by $\widetilde{e}$.

Extend $\widetilde{e}$ outside the double-barrier in order to recover an approximation of the full eigenstate e:

$$e(x,\Gamma) \approx \begin{cases} e_l(x,\Gamma) & \text{for} \quad x \in [a, a_3] \\ \widetilde{e}(x) & \text{for} \quad x \in [a_3, b_3] \\ e_r(x,\Gamma) & \text{for} \quad x \in [b_3, b] \end{cases}$$

$e_l(x,\Gamma)$ and $e_r(x,\Gamma)$ are the left and right extended functions given by

$$\begin{cases} -\frac{\hbar}{2m} e_l''(x) - qVe_l(x) = (E_R - i\Gamma/2)e_l(x) \quad \text{on } [a, a_3] \\ \hbar e_l'(a) + i \sqrt[+]{2m(E_R - i\Gamma/2 + qV_a)}\, e_l(a) = 0; \;\; e_l(a_3) = \widetilde{e}(a_3), \end{cases} \tag{25}$$

$$\begin{cases} -\frac{\hbar}{2m} e_r''(x) - qVe_r(x) = (E_R - i\Gamma/2)e_r(x) \quad \text{on } [b_3, b] \\ \hbar e_r'(a) + i \sqrt[+]{2m(E_R - i\Gamma/2 + qV_a)}\, e_r(a) = 0; \;\; e_r(b_3) = \widetilde{e}(b_3). \end{cases} \tag{26}$$

The resonance width is computed by multiplying Eq (21) by $\bar{e}$ then integrating it.

$$-\frac{\hbar}{2m}e_\lambda''(x) - qV(x)e_\lambda(x) = \lambda e_\lambda(x).$$

$$\Gamma \int_{a'}^{b'} |e(x,\Gamma)|^2 dx = \frac{\hbar}{m}\mathcal{I}m\left(\overline{e(x,\Gamma)}e'(x,\Gamma)\right)\Big|_{a'}^{b'} \qquad (27)$$

by iteration:

$$\Gamma_0 \int_{a'}^{b'} |e(x,0)|^2 dx = \frac{\hbar}{m}\mathcal{I}m\left(\overline{e(x,0)}e'(x,0)\right)\Big|_{a'}^{b'}$$

$$\Gamma_1 \int_{a'}^{b'} |e(x,\Gamma_0)|^2 dx = \frac{\hbar}{m}\mathcal{I}m\left(\overline{e(x,\Gamma_0)}e'(x,\Gamma_0)\right)\Big|_{a'}^{b'}$$

The amplitude factor.

Recall

$$-\frac{\hbar}{2m}\frac{d^2\varphi_p^{int}}{dx^2} - qV\varphi_p^{int} = E_p^a\varphi_p^{int} + q(V_{fill} - V)\varphi_p^{ext},\ (p \geq 0)$$

Taking the scalar product with e

$$\varphi_p^{int} = \theta^a(p)e(x)$$

with

$$\theta^a(p) = \frac{1}{E_p^a - \lambda}\frac{q\int_{a_3}^{b_3}(V_{fill} - V)\varphi_p^{ext}\bar{e}(x)dx}{\int_{a_3}^{b_3}|e(x)|^2dx} \tag{28}$$

Operations independent of p

- Step 1:computation of E_R and $\widetilde{e}$. Eq (24) is a generalized eigenvalue problem, which is solved with the inverse power method after a tridiagonal Househölder reduction.
- Step 2:computation of Γ and e. Eqs. (25) and (26) are solved using the WKB-scheme and then the solution are connected to $\widetilde{e}$ in order to form e. Γ is calculated by Eq. (27).

Operations depending on p

- Step 3: computation of φ_p^{ext}. The WKB-scheme is used to solve Eq. (19).
- Step 4: computation of φ_p^{int}. $\theta^a(p)$ is calculated by φ_p^{ext}, λ, e and (28).
- Final step : computation of n. n is given by formula (5). Let σ a given threshold. If $|p^2 - qV_a - E_R| > \sigma$, the energy meshsize is $\triangle E_{max}$. If $|p^2 - qV_a - E_R| < \sigma$, the meshsize is $\triangle E_{min}$. In the domain $|p^2 - qV_a - E_R| < \sigma$, one needs a very refined energy grid in order to compute $\theta^a(p)$ from (28). Hence, between two energy grid points, φ_p^{ext} is linearly interpolated with respect to p in N_{interp} points.

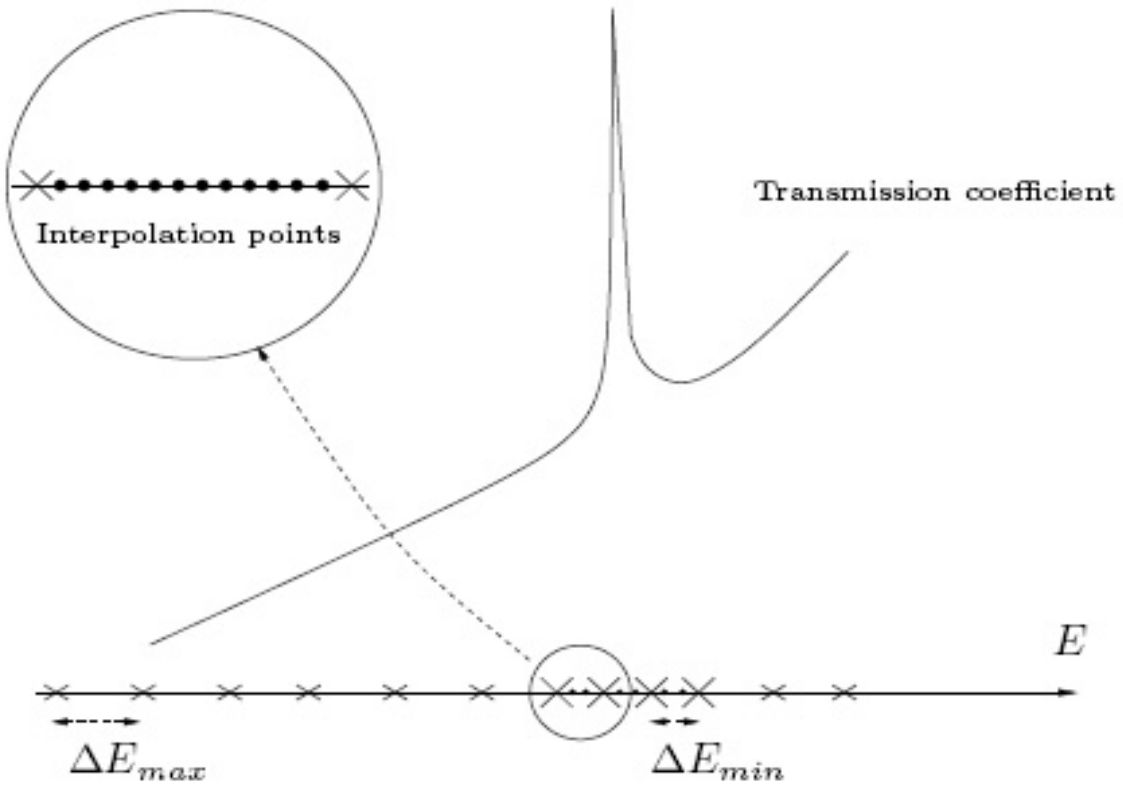

Figure 7: The energy mesh

Numerical results

- we concentrate on the WKB-scheme for linear Schrödinger equation.
- the Presilla-Sjöstrand decomposition is tested in a linear situation and then in the self-consistent case.

a	a_1	a_2	a_3	b_3	b_2	b_1	b	m_{eff}	V1
0nm	50nm	60nm	65nm	70nm	75 nm	85nm	1350nm	$0.067m_e$	-0.3V

Table 1: RTD parameters

Validation of the WKB-scheme

A simple case with $\triangle V = 0$. Since in this case V is piecewise constant, the Schrödinger equation can be explicitly solved.

- At the resonant energy, $E_p^a = 0.08958eV$.
- For an energy, $E_p^a = 0 : 046072eV$.

	E=0.08958eV			E=0.046072eV		
	N	error	time	N	error	time
WKB	13	4.10^{-14}	1	15	$2.2 * 10^{-15}$	1
RK	133	0.11	5	45	0.16	2
	193	0.025	11	85	0.015	3.3

Table 2: Results for the linear case

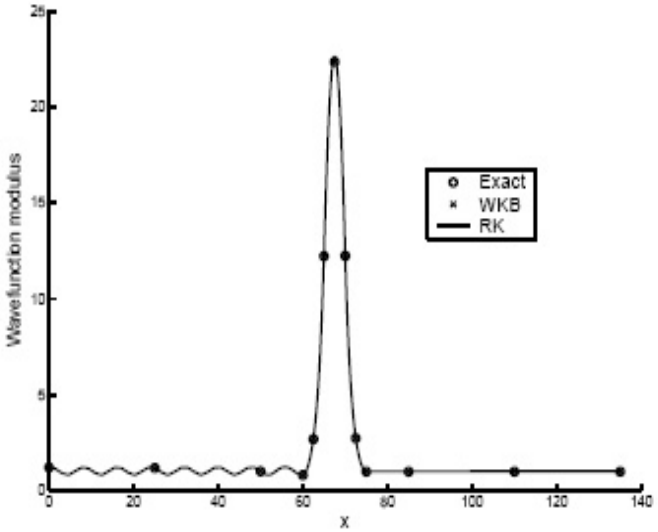

Figure 8: Comparison Exact-WKB-RK: resonant case with 15 points added

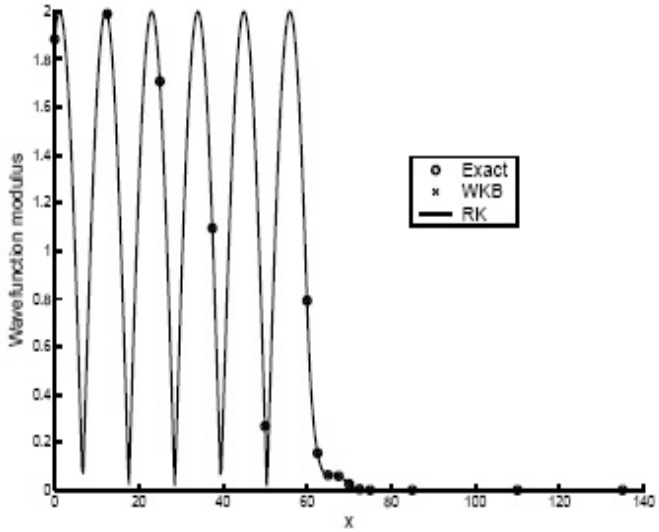

Figure 9: Comparison Exact-WKB-RK: non resonant case.

A case with turning points

A bias of 0.08 V is now applied at the edges of the device, and no explicit formula is provided for the solution. The reference solution is obtained by RK with a mesh $N = 1024$.

- For a small energy of 0.0039 eV
- For a higher energy with E = 0.17 eV

	E=0.0039eV			E=0.17eV		
	N	error	time	N	error	time
WKB	34	0.0064	1	34	0.001	1
RK	232	5e-5	2	298	0.011	3

Table 3: Results for the linear case with turning points

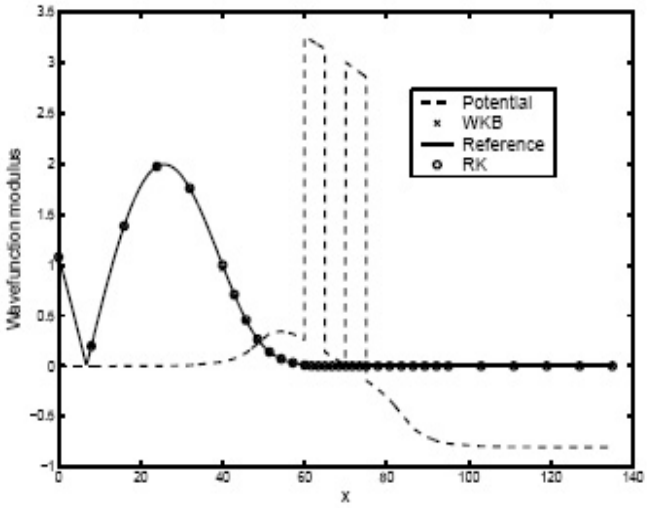

Figure 10: Comparison Reference-WKB-RK: small energy case with turning points

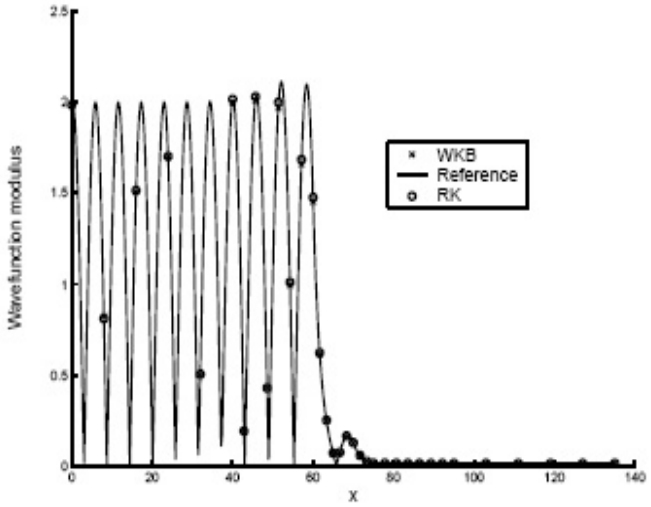

Figure 11: Comparison Reference-WKB-RK: high energy case

Validation of the Presilla-Sjöstrand decomposition

- the linear case where the exact solutions are available.
- the fully non-linear RTD model.

The electronic density is computed thanks to Eq. (5) and after an integration between $-k_{max}$ and k_{max}.

T	n_d^1	n_d^2	k_{max}	N_{GR}
300K	$1.10^{24} m^{-3}$	$1.10^{21} m^{-3}$	0.0626Å^{-1}	3

σ	Δk_{max}	Δk_{min}	N_{interp}
0.0026Å^{-1}	0.0008Å^{-1}	$0.0016\ \text{Å}^{-1}$	15

Table 4: Parameters for density computation

a linear case

The exact expressions of the density is compared to the results given by the Presilla-Sjöstrand decomposition and the method used in Pinaud (2002).

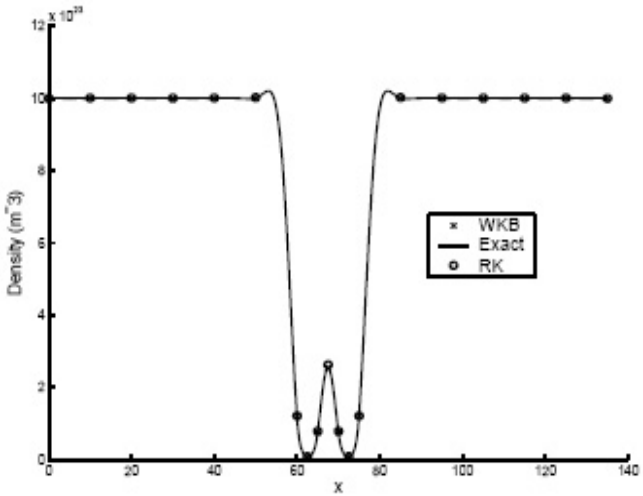

Figure 14: Reference-WKB-RK density in the linear case

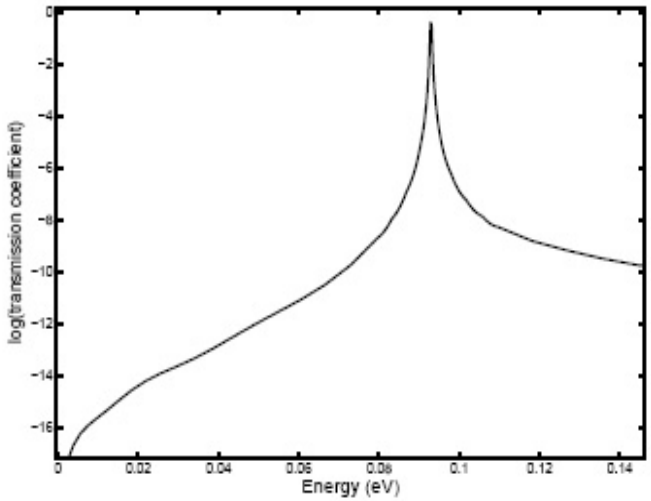

Figure 15: Transmission coefficient for the linear case

The fully non-linear problem

The self-consistent potential is computed thanks to the Gummel(1964) iterations. The reference potential and density are given by the method of Pinaud (2002) with an extremely refined mesh is chosen (1024).

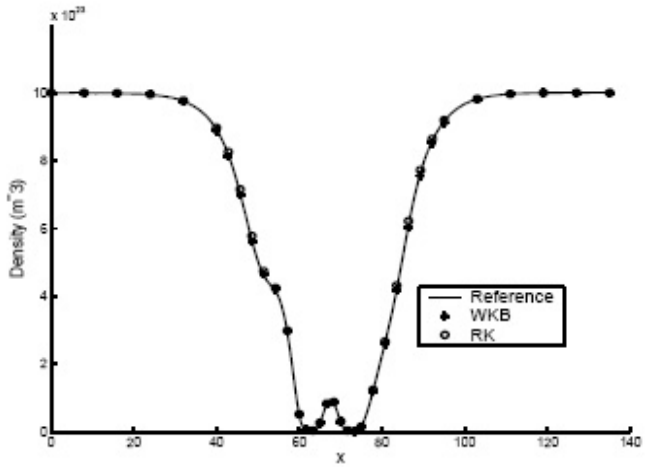

Figure 18: Comparison Reference-WKB-RK: density for the fully non-linear case

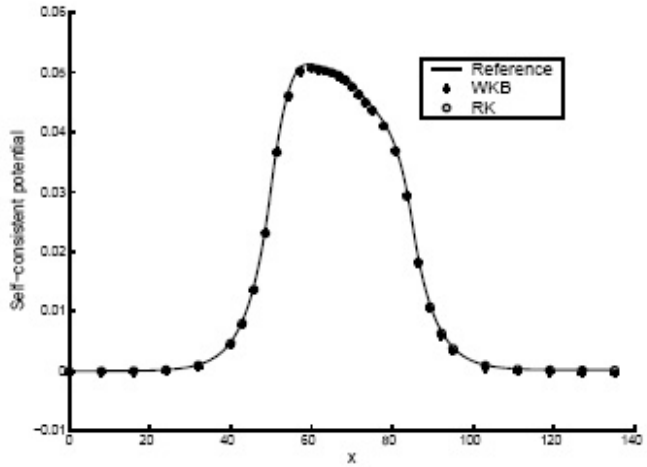

Figure 19: Self-consistent potential for the fully non-linear case

	Linear			Non-linear		
	N	error	time	N	error	time
WKB + One Mode	19	0.0010	1	34	0.0030	1
RK + Adaptative	232	0.0012	6	265	0.0040	5.5

Table 5: Results for the fully"' non-linear problem