Modélisation d'une diode à effet tunnel résonant en régime transitoire

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Résumé. *Un modèle de transport quantique transitoire est dérivé et analysé. Il décrit l'évolution des fonctions d'onde d'un système d'électrons injectés dans une zone active à partir de réservoirs selon une statistique stationnaire. Le potentiel électrostatique est modifié, dans la région active, par l'interaction électrostatique due à la présence des électrons. Les équations de Schrödinger sont résolues uniquement dans la zone active et sont munies de conditions aux limites transparentes non homogènes aux extrémités de cette même zone. Les estimations a priori sont déduites des "propriétés dissipatives" des conditions aux limites et de la repulsivité de l'interaction électrostatique.*

A mathematical model for the transcient evolution of a resonant tunneling diode

Abstract. *A mathematical model of quantum transient transport is derived and analyzed. The model describes the evolution of electrons injected into the "device" by reservoirs having a stationary statistics. The electrostatic potential in the device is modified by electron presence through electrostatic interaction. The wave functions are computed in the device region and satisfy non homogeneous open boundary conditions at the device edges. A priori estimates are deduced from the "dissipative properies" of the boundary conditions and from the repulsive character of the electrostatic interaction.*

Version française abrégée

L'objet de cette note est la dérivation et l'analyse d'un modèle pour le transport quantique d'électrons dans une diode a effet tunnel résonant en régime transitoire. Le modèle prend en compte l'injection d'électrons à partir des contacts suivant une statistique stationnaire. La diode est représentée par l'intervalle $[a, b]$. Les contacts a, b sont reliés à des reservoirs injectant les électrons selon une statistique $g_a(p)$ et $g_b(p)$ où p est l'impulsion des électrons. En régime stationnaire, les électrons injectés en $x = a$ avec une impulsion $p \geq 0$ sont représentés par la fonction d'onde ϕ_p solution de (les constantes physiques sont choisies égales à 1 et $2m = 1$)

$$\begin{cases} -\phi_p'' - V^-\phi_p = (p^2 - V_a^-)\phi_p \quad (p \geq 0) \\ \\ \phi_p'(a) + ip\phi_p(a) = 2ip \qquad \phi_p'(b) = i\sqrt[+]{p^2 + (V_b^- - V_a^-)}\phi_p(b) \end{cases}$$

où V^- est le potential électrostatique ($V_{a,b}^- = V^-(a, b)$). Les électrons injectés en $x = b$ avec une impulsion $p \leq 0$ sont représentés par une fonction d'onde ϕ_p solution de (5). Le potentiel V^- est supposé constant en dehors de l'intervalle $[a, b]$ de telle façon que les fonctions d'ondes satisfont (6) et (7). Le potentiel électrostatique V^- est la somme d'un potentiel extérieur $V_e{}^-$ incluant la double barrière, la tension appliquée et l'effet de la densité de dopage et d'un potentiel V_s^- solution de l'équation de Poisson (9) où la densité électronique est $n(x) = \int_{\mathbb{R}} g(p)|\phi_p(x)|^2\,dx$ et $g(p) := g_a(p)$ pour $p > 0$ et $g(p) := g_b(p)$ pour $p < 0$. En utilisant les techniques de [4], il est facile de montrer le

THÉORÈME 1 *Supposons que g_a, g_b sont dans L^1, positives et à support compact et $V_e^- \in L^\infty$. Alors, le système (4)–(9) admet une solution $V_s^- \in W^{2,\infty}(a,b)$, $\phi_p \in H^2(a,b)$, uniformément pour p dans le support de g_a, g_b.*

On suppose maintenant qu'à l'instant $t = 0$ la tension appliquée en $x = b$ est soudainement changée de la valeur V_b^- à une valeur V_b. Ainsi la nouvelle valeur du potentiel extérieur est V_e donnée par (10). Nous modélisons l'évolution des fonctions d'onde et du potentiel par

$$V(t,x) = V_e(x) + V_s(t,x) \quad ; \quad \frac{d^2 V_s}{dx^2} = n, \quad x \in [a,b] \quad ; \quad V_s(t,a) = V_s(t,b) = 0. \tag{1}$$

$$n(t,x) = \int_{-\infty}^{+\infty} g(p) |\psi_p(t,x)|^2 \, dp \quad ; \quad x \in [a,b] \tag{2}$$

et les ψ_p's sont les solutions de

$$i \frac{d\psi_p}{dt}(t,x) = -\frac{d^2\psi_p}{dx^2}(t,x) - V(t,x)\psi_p(t,x) \qquad (x \in \mathbb{R}) \qquad ; \quad \psi_p(0,x) = \phi_p(x) \tag{3}$$

Les ϕ_p étant les fonctions d'onde stationnaires associées au potentiel V^- (solutions de (4) and (5)). Le premier résultat de cette note est

PROPOSITION 1 *Supposons que $V \in L^\infty_x(\mathbb{R}) + C(\mathbb{R}_+, W^{2,\infty}(\mathbb{R}))$. La solution ψ_p de (3) satisfait les conditions aux limites transparentes non homogènes (14)-(15).*

Pour prouver cette proposition, on écrit $\psi_p = u_p + v_p$ où v_p est donné par (16) pour $p > 0$. Il est alors aisé de voir que u_p est solution de (17)-(18). En remarquant que $G(V)$ est nul en dehors de $[a,b]$, le même calcul que dans [1] montre que si les traces en a et b de u_p et u_p' sont continues, alors u_p satisfait des conditions transparentes homogènes, qui, écrites en termes de ψ_p, donnent (14)-(15). Sur le problème couplé, nous avons le théorème suivant

THÉORÈME 2 *Sous les hypotheses du théorème 1, le problème (1)-(2)-(3) admet une unique solution telle que $V_s \in C(\mathbb{R}_+, W^{2,\infty}([a,b])) \cap C^1(\mathbb{R}_+, L^\infty([a,b]))$.*

La preuve de ce théorème repose sur une procédure de point fixe. Les estimations a priori sont obtenues en multipliant l'équation de Schrödinger par $\overline{\psi_p}$ ou $\partial_t \overline{\psi_p}$ et en utilisant les propriétés "dissipatives" des conditions aux limites transparentes et le caractère répulsif de l'interaction Coulombienne. (Pour les détails, voir [7]).

1 Introduction

In this note, we consider a one dimensional quantum device (e.g. a resonant tuneling diode), represented by the interval $[a,b]$. The contacts a, b are linked to electron reservoirs, injecting electrons following some given profiles $g_a(p),\ p \geq 0,\ g_b(p),\ p \leq 0$, where p is the momentum of the injected electron (typically, the profiles g_a and g_b correspond to Fermi-Dirac Statistics). At negative times, the electrostatic potential is equal to V_a^- at the source contact a and V_b^- at the drain contact b. A stationary regime is assumed to build up. At time t=0, the applied voltages are suddenly changed to V_a and V_b (we shall assume, without loss of generality, that $V_a^- = V_a$). The aim of this note is to derive a mathematical model for the self-consistent evolution of the device under these conditions and to give and existence and uniqueness reslut of solutions for this model. The note is organized as follows : in section 2, we recall the stationary model (treated in [6], [4], [3]) and the existence result related to it. Section 3 is devoted to the construction of the time-dependent model. It relies on the open boundary conditions ([1, 9, 8]). In particular, we prove that the wave functions satisfy non homogeneous open boundary conditions at the boundary a,b, including the case where the electrostatic potential V is time-dependent in $[a,b]$. This allows the construction of a self-consistent evolution model for this problem. We prove in section 4 that the self-consistent model has a unique solution.

Another formulation of the problem treated in this paper has been proposed and analyzed in [10]. It relies on a density matrix representation of electrons. Boundary conditions are taken into account implicitly thanks to the use the notion of conjugate operators and the analysis is done in an abstract setting thanks to functional calculus and commutator estimates for the Schrödinger operator. This note puts somehow the work done in [10] in a setting suitable for numerical computations. Besides, although the results of [10] are more general than ours, they require the functions g_a and g_b be equal to zero for energies approaching the applied voltages. We remove this hypothesis, in the specific case we are dealing with in this note, by using the fact that the electrostatic interaction is repulsive which leads to additional a priori bounds.

We have been recently awared that Anton Arnold proposed the non homogeneous boundary conditions without rigorous justification and developed a strategy to discretize them ([2]). In [5], another model for electron injection is proposed and covers the case where the inflow data g_a and g_b depend on time (while the potential is stationary).

2 The stationary model

We assume that electrons are injected at both contacts with given profiles $g_a(p)$ and $g_b(p)$. For electrons injected at $x=a$ with momentum $p \geq 0$, the wave function ϕ_p satisfies (the physical constants are set to 1 and $2m=1$)

$$\begin{cases} -\phi_p'' - V^-\phi_p = (p^2 - V_a^-)\phi_p = E_p^a\phi_p \quad (p \geq 0) \\ \\ \phi_p'(a) + ip\phi_p(a) = 2ip \qquad \phi_p'(b) = i\sqrt[+]{p^2 + (V_b^- - V_a^-)}\phi_p(b) \end{cases} \tag{4}$$

where V^- is the electrostatic potential which builds up in the device. In the same way, electrons injected at $x=b$ with momentum $p \leq 0$ are represented by the wave function ϕ_p satisfying

$$\begin{cases} -\phi_p'' - V^-\phi_p = (p^2 - V_b^-)\phi_p = E_p^b\phi_p \quad (p \leq 0) \\ \\ \phi_p'(b) + ip\phi_p(b) = 2ip \qquad \phi_p'(a) = i\sqrt[+]{p^2 + (V_a^- - V_b^-)}\phi_p(a) \end{cases} \tag{5}$$

where $\sqrt[+]{\alpha}$ is the complex square of the real number α root having a positive real part ($\alpha \geq 0$) or positive imaginary part ($\alpha \leq 0$). Since we assume $V^- = V_a^-$ for $x<a$ and V_b^- for $x>b$, we have for $p>0$

$$\phi_p(x) = e^{ip(x-a)} + r_p e^{-ip(x-a)} \quad (x<a) \qquad ; \qquad \phi_p(x) = t_p e^{i\sqrt[+]{p^2+(V_b^- - V_a^-)}(x-b)} \quad (x>b) \tag{6}$$

and for $p<0$

$$\phi_p(x) = e^{ip(x-b)} + r_p e^{-ip(x-b)} \quad (x>b) \qquad ; \qquad \phi_p(x) = t_p e^{i\sqrt[+]{p^2-(V_b^- - V_a^-)}(x-a)} \quad (x<a) \tag{7}$$

The electron density can be computed as follows :

$$n(x) = \int_{-\infty}^{+\infty} g(p)|\phi_p(x)|^2\,dp \tag{8}$$

where $g(p) = g_a(p)$ for $p>0$, $g(p) = g_b(p)$, $p<0$ and g_a g_b are the statistics of electrons injected at $x=a$ (respectively $x=b$). Since electrons are charged particles, they contribute to the electrostatic potential V^- through Coulomb interaction. Therefore, the electrostatic potential V^- splits in two parts : $V^- = V_e^- + V_s^-$, where V_e^- is the external potential (including double barriers, applied voltage and doping effects) and V_s^- is the self-consistent potential satisfying

$$\frac{d^2 V_s^-}{dx^2} = n, \quad V_s^-(a) = V_s^-(b) = 0 \tag{9}$$

THEOREM 1 *Assume that g_a, g_b are nonnegative compactly supported L^1 functions and $V_e^- \in L^\infty$. Then, the system (4)–(9) admits a solution such that $V_s^- \in W^{2,\infty}(a,b)$, $\phi_p \in H^2(a,b)$, uniformly for p in the support of g_a, g_b.*

The proof of this theorem is readily seen from the multidimensional problem treated in [4].

3 The time-dependent model

At time $t = 0$, the electrostatic potential in the drain ($x = b$) is changed from V_b^- to V_b so that the external potential changes from V_e^- to V_e where

$$V_e = V_e^- + (V_b - V_b^-)\,\frac{x-a}{b-a}\,\mathbb{1}_{a \le x \le b} + (V_b - V_b^-)\,\mathbb{1}_{b \le x}. \tag{10}$$

We assume that the electrostatic interaction takes place in the device $[a,b]$, while the electrostatic potential stays stationary in the contacts. Therefore, the total electrostatic potential is

$$V(t,x) = V_e(x) + V_s(t,x) \quad ; \quad \frac{d^2 V_s}{\partial x^2} = n, \quad x \in [a,b] \quad ; \quad V_s(t,a) = V_s(t,b) = 0. \tag{11}$$

where the density $n(t,x)$ is defined by

$$n(t,x) = \int_{-\infty}^{+\infty} g(p) |\psi_p(t,x)|^2 \, dp \quad ; \quad x \in [a,b] \tag{12}$$

and the ψ_p's are solutions of

$$i\frac{d\psi_p}{dt}(t,x) = -\frac{d^2\psi_p}{dx^2}(t,x) - V(t,x)\psi_p(t,x) \qquad (x \in \mathbb{R}) \qquad ; \quad \psi_p(0,x) = \phi_p(x) \tag{13}$$

and ϕ_p are the stationary wave functions associated to the potential V^- (solutions of (4) and (5)).

PROPOSITION 2 *Let ψ_p be a solution of (13) and assume $V = V_e + V_s \in L_x^\infty(\mathbb{R}) + C(\mathbb{R}_+, W^{2,\infty}([a,b]) \cap C^1(\mathbb{R}_+, L^\infty([a,b]))$ with supp $V_s \in [a,b]$, then ψ_p satisfies the following non homogeneous open boundary conditions*

$$\frac{d\psi_p}{dx}(a,t) - \frac{d\phi_p}{dx}(a) e^{-iE_p^+ t} = \mathcal{D}_{1/2}^a \left(\psi_p(a,.) - \phi_p(a) e^{-iE_p^+ t}\right) \tag{14}$$

$$\frac{d\psi_p}{dx}(b,t) - \frac{d\phi_p}{dx}(b) e^{-iE_p^- t} = \mathcal{D}_{1/2}^b \left(\psi_p(b,.) - \phi_p(b) e^{-iE_p^- t}\right) \tag{15}$$

with

$$\mathcal{D}_{1/2}^\alpha(f(.)) = \sqrt{\frac{1}{\pi}} e^{-\frac{\pi}{4} i} e^{iV^\alpha t} \frac{d}{dt} \int_0^t \frac{f(\tau) e^{-iV^\alpha \tau}}{\sqrt{t-\tau}} d\tau$$

$$V^\alpha = \begin{cases} V_a^- & if \quad \alpha = a \\ V_b & if \quad \alpha = b \end{cases} \qquad E_p^+ = \begin{cases} E_p^a & if \quad p > 0 \\ E_p^b & if \quad p < 0 \end{cases} \qquad E_p^- = \begin{cases} E_p^a - (V_b - V_b^-) & if \quad p > 0 \\ E_p^b - (V_b - V_b^-) & if \quad p < 0 \end{cases}$$

Proof. We shall only sketch the proof for the case $p > 0$. The $p < 0$ case follows by analogy. We make the following change of unknown function $\psi_p(t,x) = u_p(t,x) + v_p(t,x)$ where

$$v_p(t,x) \equiv \chi(x)\varphi_1(t,x) + (1-\chi(x))\varphi_2(t,x) \tag{16}$$

$$\varphi_1(t,x) = \phi_p(x)\, e^{-i\left(p^2 - V_a^-\right)t} \quad ; \quad \varphi_2(t,x) = \phi_p(x) e^{-i\left(p^2 - (V_a^- - V_b^- + V_b)\right)t}$$

and χ is a C^∞ function satisfying $0 \le \chi \le 1$, $\chi = 1$ on $(-\infty, a]$ and $\chi = 0$ on $[b, +\infty)$. A simple algebraic manipulation shows that the function u_p satisfies

$$i\frac{du_p}{dt} = -\frac{d^2u_p}{dx^2} - Vu_p + G(V) \qquad ; \qquad u_p(0,x) = 0 \tag{17}$$

where

$$G(V) = (V_a^- - V)\chi\varphi_1 + (V_b - V_b^- + V^- - V)(1-\chi)\varphi_2 + (\varphi_1 - \varphi_2)\partial_{xx}\chi + 2\partial_x\chi\partial_x(\varphi_1 - \varphi_2) \tag{18}$$

Since $V_a^- = V(t,x)$ for $x \le a$, $V_b = V(t,x)$ for $x \ge b$ and $\partial_x \chi = 0$, $x \ge b,\ x \le a$, then u_p is a solution of a non homogeneous Schrödinger equation with a source term supported in $[a,b]$ and a vanishing initial condition. The derivation of homogeneous open boundary conditions can be done for u_p without any difficulty (see [1, 8] for example). Indeed, the boundary conditions are obtained by first Laplace transforming the Schrödinger equation in the reservoir regions ($x < a$ and $x > b$) and then by connecting the obtained result to the interior solution ($x \in [a,b]$). This can be done rigorously since u_p is regular enough (it is easy to see using the regularity of V and standard semigroup arguments that u_p is in $C(\mathbb{R}^+, H^2(\mathbb{R}))$. Consequently,$u_p$ satisfies the homogeneous open boundary condition at $x = a$ and $x = b$ (see [1]). Going back to ψ_p, and taking advantage of (6) and (7), the boundary conditions (14)-(15) are obtained afeter some algebra. ∎

4 Existence and uniqueness of solutions

THEOREM 2 *Under the hypotheses of theorem 1, the evolution problem (11)-(12)-(13) has a unique solution such that* $V_s \in C(\mathbb{R}_+, W^{2,\infty}([a,b])) \cap C^1(\mathbb{R}_+, L^\infty([a,b]))$.

The regularity result of the electrostatic potential V_s is not optimal. The proof relies on a fixed point argument for V_s. We only sketch the proof of the a priori estimates. Let V, $(\psi_p)_{p\in\mathbb{R}}$ be a solution of the self consistent problem. the wave functions ψ_p satisfy boundary conditions of the following form

$$\frac{d\psi_p}{dx}(a,t) = \mathcal{D}^a_{1/2}(\psi_p(a,.)) + f_a(t)$$

where f_a is a regular function and $\mathcal{D}^a_{1/2}$ satisfies $\Im\left(\int_0^t \overline{\phi}(s)\mathcal{D}^a_{1/2}(\phi)(s)ds\right) \le 0$ ($\Im$ is the imaginary part) and an analogous boundary condition at $x = b$ (see [1]). Multiplying the Schrödinger equation by $\overline{\psi_p}$ integrating w.r.t. the time variable between 0 and t and w.r.t. $x \in [a,b]$, and taking the imaginary part leads to

$$\|\psi_p(t,.)\|^2_{L^2(a,b)} \le C(1 + \int_0^t \|\psi_p(s,.)\|_{L^\infty} ds) \tag{19}$$

On the other hand, multiplying the Schrödinger equation (17) by $g(p)\dfrac{\partial \overline{u}_p}{\partial t}$, taking the real part and integrating with respect to t, p, x, we find the following energy Identity

$$\mathcal{E}(t) = \mathcal{E}(0) + \int_0^t \int_p g(p) \int_a^b \Re\left(\overline{u}_p \frac{dG(V^+)}{dt}\right) dxdpds - \frac{1}{2}\int_0^t \int_p g(p) \int_a^b \frac{dV_s}{dt}|u_p|^2 dxdpds \tag{20}$$

$$\mathcal{E}(t) := \frac{1}{4}\int_{\mathbb{R}}\int_p g(p)|\partial_x u_p|^2 dpdx - \frac{1}{2}\int_{\mathbb{R}}\int_p V(t,x)g(p)|u_p|^2 dpdx, + \int_{\mathbb{R}}\int_p \Re\left(g(p)G(V)\overline{u}_p\right)\, dpdx.$$

Since V is negative up to a constant independent of time, replacing the integrals w.r.t. the x variable by integrals over $[a,b]$ leads to a smaller quantity than $\mathcal{E}(t)$. Next, we replace in (20) u_p by $\psi_p - v_p$ and use the identities

$$-\int_a^b \frac{dV_s}{dt}(t,x)\int_p g(p)|\psi_p(t,x)|^2\, dp\, dx = \frac{1}{2}\frac{d}{dt}\int_a^b |\frac{dV_s}{dx}(t,x)|^2 dx$$

$$\frac{d^2}{dx^2}\frac{dV_s}{dt} = -\frac{dJ}{dx} \quad ; \quad J = \Im\int_p g(p)\overline{\psi_p}\frac{d\psi_p}{dx}\, dp.$$

Introducing the notation $K = \int_a^b\int_p g(p)|\partial_x\psi_p|^2 dpdx$, the above coputations lead to the following estimate

$$K(t) + C\|V_s'(t,.)\|_{L^2}^2 \le C + \|n(t,.)\|_{L^1} + K(t)^{\frac{1}{2}} + \int_0^t \|n(s,.)\|_{L^1}\left(1 + \|n(s,.)\|_{L^1}^{\frac{1}{2}} + K(s)^{\frac{1}{2}}\right) ds$$

Using (19), the Sobolev embedding $H^1(a,b) \hookrightarrow L^\infty(a,b)$ and a Gronwall argument, is it easy to show that

$$\|n(t,.)\|_{L^1} \le C + C\int_0^t K^{\frac{1}{2}}(s)ds$$

After some algebra, the following estimate is obtained

$$C_0K(t) + C_1\int_a^b |\frac{dV_s}{dx}(t,x)|^2 dx \le C_2(1 + \int_0^t K(s)\, ds) \quad ; \quad t \in [0,T]$$

where T is an arbitrary positive time on which depend the positive constant $C_{0,1,2}$. This shows the boundedness of the left hand side of the above inequality and this result is used to prove existence of solutions (see [7]). ■

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