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Analysis of a Drift-Diffusion-Schrödinger-Poisson model

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Abstract. A Drift-Diffusion-Schrödinger-Poisson system is presented, which models the transport of a quasi bidimensional electron gas confined in a nanostructure. We prove the existence of a unique solution to this nonlinear system. The proof makes use of some *a priori* estimates due to the physical structure of the problem, and also involves the resolution of a quasistatic Schrödinger-Poisson system. © Académie des sciences/Éditions scientifiques et médicales Elsevier SAS

Analyse d'un modèle couplé Dérive-Diffusion-Schrödinger-Poisson

Résumé. *Nous présentons un système de Dérive-Diffusion-Schrödinger-Poisson qui décrit le transport d'un gaz d'électrons confiné dans une nanostructure. Nous montrons que ce système admet une unique solution. Cette preuve d'existence est obtenue à l'aide d'estimations* a priori *dues à la nature physique du problème et passe par la résolution d'un système quasistatique de Schrödinger-Poisson.* © Académie des sciences/Éditions scientifiques et médicales Elsevier SAS

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Nous présentons l'analyse mathématique d'un système couplé quantique-classique modélisant le transport d'électrons dans des nanostructures. Un gaz d'électrons est confiné selon une direction z, dimension dans laquelle le gaz présente un caractère quantique, et est transporté dans les deux autres directions spatiales notées x, où son comportement est de nature classique.

L'équation qui décrit ce transport est l'équation (1) de type Dérive-Diffusion instationnaire en dimension 2, que vérifie la densité surfacique du gaz $n_s(t,x)$. Le potentiel effectif $V_s(t,x)$ qui intervient dans le courant de dérive garde trace du caractère quantique du confinement du gaz d'électrons. En effet, étant donné un potentiel électrostatique $V(t,x,z)$, le potentiel V_s se calcule selon (4), où les $\epsilon_p(t,x)$ sont les niveaux d'énergies du Hamiltonien transverse, c'est-à-dire les solutions de l'équation de Schrödinger stationnaire (2). Enfin, le système complet étudié dans cette Note est entièrement couplé par le fait que le

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potentiel électrostatique V considéré est le potentiel autoconsistant généré par les électrons eux-mêmes et déterminé par l'équation de Poisson (3). Le modèle peut être obtenu, du moins formellement, comme une limite de diffusion d'un système de Boltzmann-Schrödinger-Poisson [2]. Signalons qu'un système Vlasov-Schrödinger-Poisson, présentant le même type de couplage quantique-classique, est analysé dans [1].

Ce problème est étudié sur un cylindre borné, c'est-à-dire $(x, z) \in \Omega = \omega \times (0, 1)$, avec les conditions aux limites "isolantes" (5). Le résultat principal de cette Note concerne l'existence et l'unicité de solutions faibles pour ce système Dérive-Diffusion-Schrödinger-Poisson :

THÉORÈME 0.1. – *Soit $T > 0$ arbitraire. Si la donnée initiale $n_s^0 \in L^2(\omega)$ vérifie $n_s \geq 0$ p.p., alors le système* (1)–(5) *admet une unique solution faible telle que*

$$n_s \in C([0, T], L^2(\omega)) \cap L^2((0, T), H^1(\omega)), \qquad V \in C([0, T], H^2(\Omega)).$$

Ce résultat est démontré à l'aide du théorème de point fixe de Banach. Nous présentons ici les deux outils principaux de cette preuve.

Une bonne façon de regarder le système (1)-(2)-(3) est de le considérer comme un couplage entre d'une part l'équation d'évolution (1) et d'autre part le système non linéaire quasistatique de Schrödinger-Poisson (2)-(3). Ce couplage se fait par l'intermédiaire de n_s et de V_s. Pour tirer parti de cette structure du système, il faut donc en particulier s'assurer que lorsque n_s est donnée, le système (2)-(3) est bien posé. C'est l'objet de la proposition suivante que nous démontrons par des méthodes variationnelles :

PROPOSITION 0.2. – *Soit $n_s \in L^2(\omega)$ telle que $n_s \geq 0$. Alors le système* (2)-(3) *admet une unique solution $(V, (\epsilon_p, \chi_p)_{p\geq 1})$. De plus l'application $n_s \mapsto V_s$ est localement Lipschitzienne de $L^2(\omega)$ vers $H^2(\omega)$.*

Ce résultat suffit à donner un résultat d'existence locale. Le caractère global de la solution provient des estimations *a priori* suivantes.

Notons $u = \frac{n_s}{\sum_p e^{-\epsilon_p}}$ et $\rho_p = u\, e^{-\epsilon_p}$. La fonction énergie libre dy système est définie par

$$W = \sum_p \int_\omega \rho_p \log \rho_p \, dx + \frac{1}{2} \sum_p \iint_\Omega |\partial_z \chi_p|^2 \rho_p \, dxdz + \frac{1}{2} \iint_\Omega |\nabla_{x,z} V|^2 \, dxdz.$$

LEMME 0.3. – *Toute solution de* (1)–(5) *telle que $W(0) < +\infty$ vérifie à tout instant $W(t) \leq W(0)$.*

LEMME 0.4. – *Soit $T > 0$. Toute solution du système* (1)–(5) *avec $n_s^0 \in L^2(\omega)$ vérifie : $n_s \in C([0, T], L^2(\omega)) \cap L^2((0, T), H^1(\omega))$. La norme de n_s dans ces espaces est majorée par une constante ne dépendant que de T and n_s^0.*

1. Introduction

This Note is devoted to the analysis of a coupled quantum-classical system, modeling the transport of a quasi bidimensional electron gas confined in a nanostructure. The coupling occurs in the momentum variable: the electrons are like point particles in the directions x parallel to the gas (classical transport) while they behave like waves in the transversal direction z (quantum description).

The transport of the gas is described by a 2D Drift-Diffusion equation, governing the evolution of a surfacic density n_s. The originality of this system is that the parameters of this equation keep a trace of the quantum confinement in the transversal direction. Indeed, the effective potential which gives the drift current is calculated with the *subband model* through the resolution of an adiabatic Schrödinger-Poisson system. It takes into account the selfconsistent electric potential generated by the electrons and the quantification of the energy in the z variable. The system can be obtained, at least formally, as the diffusion limit of a Boltzmann-Schrödinger-Poisson system [2]. A Vlasov-Schrödinger-Poisson system, which presents also a quantum-classical coupling, is analyzed in [1].

Let $\omega \subset \mathbb{R}^2$ be a regular and bounded domain and let $\Omega = \omega \times (0,1)$. The spatial variables are $(x,z) \in \Omega$. The model studied in this Note is the following coupled system:

$$\partial_t n_s - \mathrm{div}_x\,(\nabla_x n_s + n_s\,\nabla_x V_s) = 0, \tag{1}$$

$$\begin{cases} -\dfrac{1}{2}\,\partial_{zz}\chi_p + V\chi_p = \epsilon_p \chi_p & (p \geq 1), \\ \chi_p(t,x,\cdot) \in H_0^1(0,1), & \displaystyle\int_0^1 \chi_p\,\chi_q\,dz = \delta_{pq}\,, \end{cases} \tag{2}$$

$$-\Delta_{x,z} V = n, \tag{3}$$

where the unknowns are the surfacic density $n_s(t,x)$, the eigen-energies $\epsilon_p(t,x)$, the eigenfunctions $\chi_p(t,x;z)$, and the electrostatic potential $V(t,x,z)$. These equations are coupled through the density n and the effective potential V_s, which are defined by

$$n = n_s \sum_p \frac{e^{-\epsilon_p}}{\sum_q e^{-\epsilon_q}}\,|\chi_p|^2\,, \qquad V_s = -\log \sum_p e^{-\epsilon_p}. \tag{4}$$

This system (1)–(3) is completed with an initial condition $n_s(0,x) = n_s^0(x)$ and with the following conservative boundary conditions, where $\partial\omega$ is the boundary of ω and $\nu(x)$ denotes the unit outward normal vector at $x \in \partial\omega$:

$$\begin{cases} \partial_\nu n_s(t,x) = 0, \quad \partial_\nu V(t,x,z) = 0 & \text{for } x \in \partial\omega, \quad z \in (0,1), \\ V(t,x,0) = V(t,x,1) = 0 & \text{for } x \in \omega. \end{cases} \tag{5}$$

The main result of this Note is the following existence result:

THEOREM 1.1. – *Let $T > 0$. If $n_s^0 \in L^2(\omega)$ and $n_s \geq 0$ a.e., then the system* (1)–(5) *admits a unique weak solution such that*

$$n_s \in C([0,T], L^2(\omega)) \cap L^2((0,T), H^1(\omega)), \qquad V \in C([0,T], H^2(\Omega)).$$

This preliminary result will be developped and improved in a forthcoming paper [2], where more general boundary conditions and the addition of an external electric field will be considered.

Following [1], the system is viewed as the coupling between an evolution equation– the Drift-Diffusion equation (1)– and the quasistatic Schrödinger-Poisson system (2)-(3). This structure suggests to solve this system by using a fixed-point procedure for the unknown n_s, as for the standard Drift-Diffusion-Poisson problem [3, 5]. To this aim, we first exhibit some *a priori* estimates for the whole system. Then we show that for a given n_s the Schrödinger-Poisson system (2)-(3) is well-posed. Finally we sketch the existence proof, based on the Banach fixed-point theorem.

2. A priori estimates

Introducing the so-called Slotboom variable $u = n_s/(\sum_p e^{-\epsilon_p})$ and setting $j_s = -\sum_p e^{-\epsilon_p}\nabla_x u$, the Drift-Diffusion equation writes $\partial_t n_s + \mathrm{div}_x\, j_s$=0. The occupation factor of the pth subband is denoted by $\rho_p = u\,e^{-\epsilon_p}$, so that $n = \sum_p \rho_p\,|\chi_p|^2$ and $n_s = \sum_p \rho_p$. We define the total free energy of the system by

$$W = \sum_p \int_\omega \rho_p \log \rho_p\,dx + \frac{1}{2}\sum_p \iint_\Omega |\partial_z \chi_p|^2\,\rho_p\,dxdz + \frac{1}{2}\iint_\Omega |\nabla_{x,z} V|^2\,dxdz.$$

LEMMA 2.1. – *Any solution of* (1)–(5) *such that* $W(0) < +\infty$ *satisfies*

$$\forall t \geq 0 \qquad W(t) \;=\; W(0) - \int_0^t \int_\omega \left(\sum_p e^{-\epsilon_p} \right) \frac{|\nabla_x u|^2}{u}\, dxds \quad \leq\; W(0).$$

Proof. – We have

$$\frac{d}{dt} \sum_p \int_\omega \rho_p \log \rho_p \, dx = \int_\omega \partial_t n_s \log u \, dx - \sum_p \int_\omega \partial_t \rho_p \epsilon_p + \frac{d}{dt} \int_\omega n_s.$$

Since $\partial_\nu \epsilon_p = \left\langle |\chi_p|^2 \, \partial_\nu V \right\rangle$, the boundary conditions (5) imply $\partial_\nu u = 0$ on $\partial\omega$. Hence we have $j_s \cdot \nu = 0$ on $\partial\omega$ and the total charge $\int_\omega n_s$ is conserved. Besides, with the notation $\langle f \rangle = \int_0^1 f \, dz$, we have $\partial_t \epsilon_p = \left\langle |\chi_p|^2 \, \partial_t V \right\rangle$, which leads to

$$\frac{d}{dt} \sum_p \int_\omega \rho_p \log \rho_p \, dx = \int_\omega \mathrm{div}_x \, \left(\sum_p e^{-\epsilon_p} \nabla_x u \right) \log u \, dx - \frac{d}{dt} \int_\omega \sum_p \rho_p \, \epsilon_p \, dx + \iint_\Omega n \partial_t V \, dxdz.$$

Since $\langle \frac{1}{2} |\partial_z \chi_p|^2 \rangle - \epsilon_p = -\langle V |\chi_p|^2 \rangle$, we deduce

$$\frac{d}{dt} W = \int_\omega \mathrm{div}_x \, \left(\sum_p e^{-\epsilon_p} \nabla_x u \right) \log u \, dx - \iint_\Omega V \partial_t n \, dxdz + \frac{1}{2} \frac{d}{dt} \iint_\Omega |\nabla_{x,z} V|^2 \, dxdz.$$

The Poisson equation gives $- \iint V \, \partial_t n \, dxdz = -\frac{1}{2} \frac{d}{dt} \iint |\nabla_{x,z} V|^2 \, dxdz$. We conclude this proof after an integration by parts on the first term of the right-hand side. □

LEMMA 2.2. – *Let* $T > 0$. *Any solution of* (1)–(5) *such that* $n_s^0 \in L^2(\omega)$ *satisfies*

$$n_s \in C([0,T], L^2(\omega)) \cap L^2((0,T), H^1(\omega)),$$

for any $T > 0$, *with a bound depending only on* T *and on the data.*

Proof. – Multiply (1) by n_s and integrate on ω. After some integrations by parts we get

$$\frac{1}{2} \frac{d}{dt} \int_\omega n_s^2 \, dx + \int_\omega |\nabla_x n_s|^2 \, dx + \frac{1}{2} \int_\omega n_s^2 \, (-\Delta_x V_s) \, dx = 0.$$

Straightforward calculations lead to the following identity:

$$\begin{aligned} -n_s^2 \, \Delta_x V_s \quad = \quad & -4 n_s^2 \frac{\sum_p \epsilon_p^2 \, e^{-\epsilon_p}}{\sum_p e^{-\epsilon_p}} + n_s \left\langle n^2 + 4V^2 \, n \right\rangle + 2 n_s^2 \frac{\sum_p e^{-\epsilon_p} \left\langle (V + \epsilon_p) |\partial_z \chi_p|^2 \right\rangle}{\sum_p e^{-\epsilon_p}} \\ & - \frac{n_s^2}{\sum_p e^{-\epsilon_p}} \sum_p \sum_{q \neq p} \left(\frac{e^{-\epsilon_p} - e^{-\epsilon_q}}{\epsilon_p - \epsilon_q} \right) \left\langle \chi_p \chi_q \, \nabla_x V \right\rangle^2 \\ & + n_s^2 \frac{\sum_p e^{-\epsilon_p} \left\langle |\chi_p|^2 \, \nabla_x V \right\rangle^2}{\sum_p e^{-\epsilon_p}} - n_s^2 \left(\frac{\sum_p e^{-\epsilon_p} \left\langle |\chi_p|^2 \, \nabla_x V \right\rangle}{\sum_p e^{-\epsilon_p}} \right)^2 . \end{aligned}$$

By the Cauchy-Schwarz inequality the sum of the two terms in the third line is nonnegative. Moreover, except for the first one, the other terms are obviously nonnegative. We deduce

$$\frac{d}{dt} \int_\omega n_s^2 \, dx + \int_\omega |\nabla_x n_s|^2 \, dx \leq 4 \int_\omega n_s^2 \frac{\sum_p \epsilon_p^2 \, e^{-\epsilon_p}}{\sum_p e^{-\epsilon_p}} dx \leq 4 \|n_s\|_{L^4(\omega)}^2 \left\| \frac{\sum_p \epsilon_p^2 \, e^{-\epsilon_p}}{\sum_p e^{-\epsilon_p}} \right\|_{L^2(\omega)} .$$

By Proposition 3.1, the assumption $n_s^0 \in L^2(\omega)$ implies that $W(0) < +\infty$. Thus by Lemma 2.1 $W(t)$ is bounded for any t and, in particular, V is bounded in $L^\infty((0,T), H^1(\Omega))$ (thanks to Poincaré's inequality). Consequently, from the technical Lemma 2.3 below, we deduce that $(\sum_p \epsilon_p^2\, e^{-\epsilon_p})/(\sum_p e^{-\epsilon_p})$ is bounded in $L^\infty((0,T), L^2(\omega))$. We conclude the proof by using Gagliardo-Nirenberg's inequality to interpolate the L^4 norm of n_s between its L^2 and H^1 norms, then by applying Gronwall's lemma. □

LEMMA 2.3. – *Assume $V \in H^1(\Omega)$. Then the eigenvalues ϵ_p defined by* (2) *satisfy*

$$\frac{\sum_p |\epsilon_p|^\alpha\, e^{-\epsilon_p}}{\sum_p e^{-\epsilon_p}} \in L^q(\omega) \qquad \text{for any } \alpha \geq 0 \text{ and } q < +\infty.$$

Proof. – The eigenvalues and eigenvectors of (2) satisfy the (uniform in p) estimate [7]

$$\left|\epsilon_p(x) - \frac{\pi^2}{2}p^2\right| + \|\chi_p(x,\cdot)\|_{L_z^\infty} \leq C_1\, e^{C_2\|V(x,\cdot)\|_{L_z^2}}. \tag{6}$$

A lengthy but elementary computation gives $(\sum_p |\epsilon_p|^\alpha\ e^{-\epsilon_p})/\left(\sum_p e^{-\epsilon_p}\right) \leq C_3\, e^{\alpha C_2 \|V(x,\cdot)\|_{L_z^2}}$. Since $\|V(x,\cdot)\|_{L_z^2}$ is bounded in $H^1(\omega)$, Trudinger's inequality implies that $e^{\|V(x,\cdot)\|_{L_z^2}^2} \in L^1(\omega)$, which insures that $e^{\alpha C_2 \|V(x,\cdot)\|_{L_z^2}} \in L^q(\omega)$ for all $q < +\infty$. □

3. The quasistatic Schrödinger-Poisson system

In this section, the surfacic density n_s is assumed to be given and the system (2)-(3) is solved with the boundary conditions (5) on V. For the sake of simplicity the time parameter is omitted here and $n_s = n_s(x)$. In the sequel, we use the functional spaces $H_{01}^1 = \{V \in H^1(\Omega)\ : V(x,0) = V(x,1) = 0\}$ and $L^{p,q}(\Omega) = \{u \in L^1_{loc}(\Omega) \quad \text{such that} \quad \|u\|_{L^{p,q}(\Omega)} = \left(\int_\omega \|u(x,\cdot)\|^p_{L^q(0,1)}\, dx\right)^{1/p} < +\infty\}$.

PROPOSITION 3.1. – *Let $n_s \in L^2(\omega)$ such that $n_s \geq 0$. Then the system* (2)-(3) *admits a unique solution $(V, (\epsilon_p, \chi_p)_{p\geq 1})$, which satisfies the estimate $\|V\|_{H^2(\Omega)} \leq C(n_s)$, the constant $C(n_s)$ depending only on the $L^2(\omega)$ norm of n_s. Moreover if n_s and $\widetilde{n_s}$ are two data, the corresponding solutions satisfy : $\|V - \widetilde{V}\|_{H^2(\Omega} \leq C(n_s, \widetilde{n_s})\, \|n_s - \widetilde{n_s}\|_{L^2(\omega)}$.*

Proof. – Proceeding as in [1] and in the spirit of [6], we can show that a weak solution of (2)-(3) in H^1_{01} is a critical point with respect to V of the functional

$$J(V, n_s) = J_0(V) + J_1(V, n_s) = \frac{1}{2}\iint_\Omega |\nabla_{x,z} V|^2 + \int_\omega n_s\, \log \sum_p e^{-\epsilon_p[V]}\, dx,$$

where $(\epsilon_p[V])_{p\geq 1}$ are the eigenvalues of the Hamiltonian $-\frac{1}{2}\frac{d^2}{dz^2} + V$, *i.e.* satisfy (2). The functional J_0 is clearly continuous and strongly convex on H^1_{01}. The analysis of the functional $V \mapsto J_1(V, n_s)$ relies on the properties of $\epsilon_p[V]$, $\chi_p[V]$. From the inequality $|\epsilon_p[V] - \epsilon_p[\widetilde{V}]|(x) \leq \|V(x,\cdot) - \widetilde{V}(x,\cdot)\|_{L_z^\infty(0,1)}$, we deduce by straightforward computations that

$$|J_1(V, n_s) - J_1(\widetilde{V}, n_s)| \leq \int_\omega |n_s(x)|\, \sup_p \Big(|\epsilon_p[V] - \epsilon_p[\widetilde{V}]|(x)\Big)\, dx \leq \|n_s\|_{L^2(\omega)}\, \|V - \widetilde{V}\|_{L^{2,\infty}(\Omega)}.$$

The functional $J_1(\cdot, n_s)$ is globally Lipschitz on $L^{2,\infty}(\Omega)$, thus on $H^1(\Omega)$, since we have the embedding $H^1(\Omega) \subset L^{2,\infty}(\Omega)$ (see [1]).

Next we remark that $J_1(\cdot, n_s)$ is convex when n_s is nonnegative. Indeed, it is twice Gâteaux differentiable on $L^\infty(\Omega)$ and we have

$$\begin{aligned} d_V^2 J_1(V,n_s)W\cdot W &= -\int_\omega \frac{n_s}{\sum_p e^{-\epsilon_p}} \sum_p \sum_{q\neq p} \frac{e^{-\epsilon_p}-e^{-\epsilon_q}}{\epsilon_p-\epsilon_q} \left\langle \chi_p\chi_q W\right\rangle^2 \, dx \\ &\quad + \int_\omega n_s \left\{ \frac{\sum_p e^{-\epsilon_p}\langle|\chi_p|^2 W\rangle^2}{\sum_p e^{-\epsilon_p}} - \left(\frac{\sum_p e^{-\epsilon_p}\langle|\chi_p|^2 W\rangle}{\sum_p e^{-\epsilon_p}} \right)^2 \right\} dx. \end{aligned}$$

This quantity is nonnegative thanks to the Cauchy-Schwarz inequality. As a consequence, the functional $J(\cdot, n_s) = J_0 + J_1(\cdot, n_s)$ is continuous and strongly convex on H^1_{01}. Moreover using Poincaré's inequality on H^1_{01} we have

$$J(V,n_s) \geq C\|V\|^2_{H^1(\Omega)} - C\|n_s\|_{L^2(\Omega)}\|V\|_{H^1(\Omega)} + J(0,n_s),$$

thus $J(\cdot, n_s)$ is coercive and bounded from below on H^1_{01} : it admits a unique minimizer.

The H^2 estimate of V is obtained in several steps. Firstly, a H^1 estimate comes directly from $J(V,n_s) \leq J(0,n_s)$. Therefore, since the eigenfunctions satisfy (6), Trudinger's inequality implies that χ_p is bounded in any $L^{q,\infty}(\Omega)$, $q < +\infty$ (uniformly with respect to p). Hence the density n given by (4) is bounded in any $L^q(\Omega)$, $1 \leq q < 2$ and the elliptic regularity gives an estimate of V in $W^{2,q}$, $q < 2$. In particular we can choose a value $q > 3/2$: with a Sobolev embedding V is bounded in $L^\infty(\Omega)$. Then the last step is immediate: by (6) the χ_p's are bounded in $L^\infty(\Omega)$ and n is bounded in $L^2(\Omega)$, which gives $V \in H^2(\Omega)$.

The Lipschitz dependency of V with respect to n_s is also obtained with the same several steps as the H^2 estimate. We only give a sketch of the first one, the H^1 estimate. Let V and $\widetilde{V}$ denote the minimizers of $J(\cdot, n_s)$ and $J(\cdot, \widetilde{n_s})$. Using the linearity of J_1 with respect to n_s, its Lipschitz dependency with respect to V and its strong convexity, we get

$$\begin{aligned} \frac{1}{C}\|V-\widetilde{V}\|^2_{H^1(\Omega)} &\leq J(\widetilde{V},n_s) - J(V,n_s) = J_1(\widetilde{V}, n_s-\widetilde{n_s}) - J_1(V, n_s-\widetilde{n_s}) + J(\widetilde{V},\widetilde{n_s}) - J(V,\widetilde{n_s}) \\ &\leq C'\|V-\widetilde{V}\|_{H^1(\Omega)}\,\|n_s-\widetilde{n_s}\|_{L^2(\omega)}. \end{aligned}$$

□

4. The fixed-point procedure

The proof of existence and uniqueness relies on a contraction argument. Define the mapping $S : n_s \mapsto \widehat{n_s}$ on $X = C([0,T], L^2(\omega)) \cap L^2((0,T), H^1(\omega))$ as follows. The potential V is first defined in $C([0,T], H^2(\Omega))$ by solving the quasistatic Schrödinger-Poisson system (2)-(3) with the data $n_s(t,x)$. Next V_s is defined by (4): it has the same regularity as V, *i.e.* belongs to $C([0,T], H^2(\omega))$. Then $\widehat{n_s}$ is the solution of (1) with the effective force field $\nabla_x V_s \in C([0,T], H^1(\omega))$ and the initial data $n_s^0 \in L^2(\omega)$.

By Proposition 3.1 and the standard results on linear parabolic equations [4], the mapping S is well-defined. To prove that S is a contraction for small T, it suffices to write a Duhamel representation of n_s and to use the Lipschitz dependency of V with respect to n_s. The solution is global thanks to Lemma 2.2.

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