

Diffusive transport of partially quantized particles: existence, uniqueness and long time behaviour.

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Abstract

A self-consistent model for charged particles, accounting for quantum confinement, diffusive transport and electrostatic interaction is considered. The electrostatic potential is a solution of a three dimensional Poisson equation with the particle density as the source term. This density is the product of a two dimensional surface density and that of a one dimensional mixed quantum state. The surface density is the solution of a drift-diffusion equation with an effective surface potential deduced from the fully three dimensional one and which involves the diagonalization of a one dimensional Schrödinger operator. The overall problem is viewed as a two dimensional drift-diffusion equation coupled to a Schrödinger-Poisson system. The latter is proven to be well posed by a convex minimization technique. A relative entropy and an *a priori* L^2 estimate provide enough bounds to prove existence and uniqueness of a global in time solution. In the case of thermodynamic equilibrium boundary data, a unique stationary solution is proven to exist. The relative entropy allows to prove the convergence of the transient solution towards it as time grows to infinity. Finally, the low order approximation of the relative entropy is used to prove that this convergence is exponential in time.

Key words: Schrödinger equation, drift-diffusion system, Poisson equation, relative entropy, long-time behavior, subband method, convex minimization.

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1 Introduction and main result

The drift-diffusion equation is one of the most used models for charged particle transport in various areas such as gas discharges, plasmas or semiconductors. It consists in a conservation equation for the particle density, in which the current density is the sum of two terms. One is proportional to the particle density and to the electrostatic forces. This term is referred to as the drift current. The second

term is the diffusion current and is proportional to the gradient of the particle density [28, 29, 19, 20, 10, 11].

The drift-diffusion model can be derived from kinetic theory when the mean free path related to particle interactions with a thermal bath is small compared to the system length-scale. In semiconductors, one of the most important mechanism driving the electrons towards a diffusive regime is collisions with phonons (vibrations of the semiconductor crystal lattice) which drive the electrons towards a local equilibrium at the lattice temperature [28, 36]. We refer to [34, 25] for a rigorous derivation from the Boltzmann equation and to [19, 28, 29, 20] and references therein for the analysis of this system when coupled to the Poisson equation for the electrostatic potential.

Quantum systems at global thermodynamic equilibrium can be described as a statistical mixture of eigenstates of the Schrödinger operator. The occupation number of each state is given by a thermodynamic equilibrium statistic function. Typically, it is given by $\exp(\frac{E_F - E}{k_B T})$ for Boltzmann statistics, or $1/(1 + \exp(\frac{E - E_F}{k_B T}))$ for Fermi-Dirac statistics, where E is the energy of the considered state, k_B is the Boltzmann constant, T is the temperature and E_F is the so-called Fermi energy which, at zero temperature, represents the threshold between occupied and unoccupied states [30, 31, 32, 38].

In nanoscale semiconductor devices like ultrashort channel double gate MOSFETs (DGMOS), electrons might be extremely confined in one or several directions that we shall refer to as the confining directions. This leads to a partial quantization of the energy. In the non-confined direction(s), that we shall also refer to as the transport direction(s), following the length and energy scales, transport might have a quantum nature or be purely classical in the kinetic or diffusive regimes. In the present work, we are interested in the last regime. Namely, we consider a particle system which is partially quantized in one direction (denoted by z) and which, in the transport direction denoted by x , has a diffusive motion. The system is at equilibrium in the confined direction with a local Fermi level ϵ_F which depends on the transport variable x . The variable x is assumed to lie in a bounded regular domain $\omega \in \mathbb{R}^2$ while z belongs to the interval $(0, 1)$. The spatial domain is then $\Omega = \omega \times (0, 1)$. At a time t and a position (x, z) , the particle density $N(t, x, z)$ is given by

$$N(t, x, z) = \sum_{k=1}^{+\infty} e^{\epsilon_F(t,x) - \epsilon_k(t,x)} |\chi_k(t, x, z)|^2, \quad (1.1)$$

where ϵ_F is the Fermi Level and (χ_k, ϵ_k) is the complete set of eigenfunctions and eigenvalues of the Schrödinger operator in the z variable

$$\begin{cases} -\frac{1}{2} \partial_z^2 \chi_k + V \chi_k = \epsilon_k \chi_k & (k \geq 1), \\ \chi_k(t, x, \cdot) \in H_0^1(0, 1), & \int_0^1 \chi_k \chi_\ell dz = \delta_{k\ell}. \end{cases} \quad (1.2)$$

The electrostatic potential V is a solution of the Poisson equation

$$-\Delta_{x,z} V = N. \quad (1.3)$$

The surface density

$$N_s(t, x) = \int_0^1 N(t, x, z) dz = e^{\epsilon_F} \sum_{k=1}^{+\infty} e^{-\epsilon_k(t, x)} \quad (1.4)$$

satisfies the drift-diffusion equation

$$\partial_t N_s - \operatorname{div}_x (\nabla_x N_s + N_s \nabla_x V_s) = 0, \quad (1.5)$$

where the effective potential V_s is given by

$$V_s = -\log \sum_k e^{-\epsilon_k}. \quad (1.6)$$

Remark also that N can be rewritten

$$N(t, x, z) = \frac{N_s(t, x)}{\mathcal{Z}(t, x)} \sum_{k=1}^{+\infty} e^{-\epsilon_k(t, x)} |\chi_k(t, x, z)|^2, \quad (1.7)$$

where the repartition function \mathcal{Z} is given by

$$\mathcal{Z}(t, x) = \sum_{k=1}^{+\infty} e^{-\epsilon_k(t, x)}. \quad (1.8)$$

The unknowns of the overall system are the surface density $N_s(t, x)$, the eigenenergies $\epsilon_k(t, x)$, the eigenfunctions $\chi_k(t, x, z)$ and the electrostatic potential $V(t, x, z)$. The Fermi level ϵ_F is determined by :

$$\epsilon_F(t, x) = \log \frac{N_s(t, x)}{\mathcal{Z}(t, x)}. \quad (1.9)$$

This will be useful for the study of global equilibria. The system (1.2)–(1.8) is completed with the initial condition

$$N_s(0, x) = N_s^0(x) \quad (1.10)$$

and with the following boundary conditions :

$$\begin{cases} N_s(t, x) = N_b(x), & V(t, x, z) = V_b(x, z), & \text{for } x \in \partial\omega, \quad z \in (0, 1), \\ \partial_z V(t, x, 0) = \partial_z V(t, x, 1) = 0, & & \text{for } x \in \omega. \end{cases} \quad (1.11)$$

In application like the Double-Gate transistor [4], the frontier $\partial\omega \times [0, 1]$ includes the source and the drain contacts as well as insulating or artificial boundary. On the other hand $\omega \times \{0\}$ and $\omega \times \{1\}$ represent the gate contacts (in addition to possible insulating boundaries). Mixed type boundary conditions are then to be prescribed. The boundary conditions (1.11) do not take into account this complexity and are chosen for the mathematical convenience : elliptic regularity properties of the Poisson equation (1.3) are needed in our proofs.

1.1 Main Results

Assumption 1.1

- The initial condition satisfies $N_s^0 \in L^2(\omega)$ and $N_s^0 \geq 0$, a.e.
- The boundary data for the surface density satisfy $0 < N_1 \leq N_b \leq N_2$ a.e., where N_1 and N_2 are positive constants, $N_b \in C^2(\partial\omega)$.
- The Dirichlet datum for the potential satisfies $V_b \in C^2(\partial\omega \times [0, 1])$ and the compatibility condition

$$\frac{\partial V_b}{\partial z}(x, 0) = \frac{\partial V_b}{\partial z}(x, 1) = 0, \quad \forall x \in \partial\omega.$$

The first result of this paper is the following existence and uniqueness theorem:

Theorem 1.2 *Let $T > 0$ be fixed. Under Assumption 1.1, the system (1.2)–(1.11) admits a unique weak solution such that*

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

The second result concerns the asymptotic behaviour of the solution as times tends to $+\infty$. To this aim, we shall first define the notion of global equilibrium for boundary data, under which we show that there exists a unique stationary solution, and finally prove that the time dependent solution converges exponentially fast to this stationary solution.

Assumption 1.3 *The boundary is said to be at global equilibrium if there exists a real number $u^\infty > 0$ such that $\forall x \in \partial\omega$, $N_b(x) = u^\infty e^{-V_s^\infty(x)}$, where V_s^∞ is defined by*

$$V_s^\infty(x) = -\log\left(\sum_k e^{-\epsilon_k[V_b](x)}\right).$$

In view of (1.9), it means that the Fermi level at the boundary is constant.

In this assumption, as well as in the sequel of the paper, for each potential V , the notation $\epsilon_k[V]$ stands for the k th eigenvalue of the Hamiltonian $-\frac{1}{2}\partial_z^2 + V$ and $\chi_k[V]$ denotes the corresponding eigenfunction (solving (1.2)).

The stationary problem reads

$$\left\{ \begin{array}{l} -\operatorname{div}_x (\nabla_x N_s^\infty + N_s^\infty \nabla_x V_s^\infty) = 0, \\ -\frac{1}{2}\partial_z^2 \chi_k^\infty + V^\infty \chi_k^\infty = \epsilon_k^\infty \chi_k^\infty, \\ -\Delta_{x,z} V^\infty = N^\infty = \frac{N_s^\infty}{\mathcal{Z}^\infty} \sum_{k=1}^{+\infty} |\chi_k^\infty|^2 e^{-\epsilon_k^\infty}, \\ \mathcal{Z}^\infty = \sum_{\ell=1}^{+\infty} e^{-\epsilon_\ell^\infty}, \end{array} \right. \quad (1.12)$$

with the boundary conditions

$$\begin{cases} N_s^\infty(x) = N_b(x), & V^\infty(x, z) = V_b(x, z) & \text{for } x \in \partial\omega, \quad z \in (0, 1), \\ \partial_z V^\infty(x, 0) = \partial_z V^\infty(x, 1) = 0 & & \text{for } x \in \omega, \end{cases} \quad (1.13)$$

where we have used the short notation ϵ_k^∞ for $\epsilon_k[V^\infty]$ and χ_k^∞ for $\chi_k[V^\infty]$.

Proposition 1.4 *Under Assumptions 1.1 and 1.3, the stationary problem (1.12)–(1.13) admits a unique solution such that $N_s^\infty \in C^2(\bar{\omega})$ and $V^\infty \in C^2(\bar{\Omega})$.*

The following theorem proves the exponential convergence of the time dependent solution towards the stationary one.

Theorem 1.5 *Let Assumptions 1.1 and 1.3 hold. Let N_s, V and N_s^∞, V^∞ be respectively the time dependent and the stationary solutions defined respectively in Theorem 1.2 and Proposition 1.4. There exist two constants $\lambda > 0$ and $C > 0$ such that for all $t \geq 0$,*

$$\|N_s - N_s^\infty\|_{L^2(\omega)}(t) + \|V - V^\infty\|_{H^1(\omega)}(t) \leq Ce^{-\lambda t}.$$

The outline of the paper is as follows. In the next subsection, we briefly explain how the drift-diffusion-Schrödinger system can be derived as a diffusion limit of a Boltzmann type model. In Section 2, we prove Theorem 1.2. The strategy of the proof as well as various notations are detailed in Subsection 2.1. Let us just mention that two essential ingredients are used : the first is a relative entropy inequality which provides preliminary estimates on the solution, which are then completed with an L^2 estimate on the surface density. The second ingredient is the analysis of the Schrödinger-Poisson system (1.2)–(1.3) which is shown to be uniquely solvable by convex minimization techniques in the spirit of [30, 31, 32]. Section 3 is devoted to the proof of Theorem 1.5 which uses a quadratic approximation of the relative entropy given in Section 2, and which is a Lyapunov functional for the linearized system around the stationary solution. The Appendix is devoted to some technical lemmata and to classical results for Sturm-Liouville operators.

1.2 Formal derivation from kinetic theory

The drift-diffusion-Schrödinger system (1.2), (1.5), (1.6) can be derived as a diffusion limit of a kinetic system for partially quantized particles, called the kinetic subband system. More precisely, for a partially quantized system, the particle density can be written

$$N(t, x, z) = \sum_{k=1}^{+\infty} \rho_k(t, x) |\chi_k(t, x, z)|^2$$

where χ_k is given by (1.2). In the physics terminology [5, 18, 13], the wave function χ_k is called the wave function of the k th subband and ϵ_k its energy. The surface

densities $\rho_k(t, x)$ are the occupation numbers of the subbands and are given in the kinetic framework by

$$\rho_k(t, x) = \int_{\mathbb{R}^2} f_k(t, x, v) dv$$

where f_k are solutions of kinetic equations, in which the electrostatic potential energy V is replaced by the subband energy ϵ_k . In the collision-less case, such a model, which in quantum chemistry is related to the so-called Born-Oppenheimer approximation [37, 35, 23], has been obtained by the first two authors in [6] by a partial semiclassical limit of the Schrödinger equation and analyzed in [7, 8]. In order to obtain the diffusive regime, we introduce intersubband collisions [5, 1] in the Fermi golden rule approximation

$$\partial_t f_k^\eta + \frac{1}{\eta} \{\mathcal{H}_k, f_k^\eta\} = \frac{1}{\eta^2} Q(f^\eta)_k, \quad (1.14)$$

where η is the scaled mean free path assumed to be small and $\{\cdot, \cdot\}$ is the Poisson bracket $\{g, h\} = \nabla_x h \cdot \nabla_v g - \nabla_v h \cdot \nabla_x g$, Moreover \mathcal{H}_p is the energy of the system in the k th subband

$$\mathcal{H}_k(t, x, v) = \frac{1}{2}v^2 + \epsilon_k(t, x),$$

where we recall that ϵ_k is the subband energy. The collision operator Q is defined by

$$Q(f)_p = \sum_{k'} \int_{\mathbb{R}^2} \alpha_{k,k'}(v, v') (\mathcal{M}_k(v) f_{k'}(v') - \mathcal{M}_{k'}(v') f_k(v)) dv',$$

where α depends on the system and the function \mathcal{M}_k is the Maxwellian :

$$\mathcal{M}_k(t, x, v) = \frac{1}{2\pi \mathcal{Z}} e^{-\mathcal{H}_k(t, x, v)}.$$

The diffusion limit consists in letting η going to 0 (a rigorous study of this limit will be the object of a future work). Admitting that f_k^η converges as η tends to zero towards a limit f_k^0 , then $f_k^0 \in \text{Ker } Q$ which can be shown to be equal to

$$\text{Ker } Q = \{f \text{ such that } \exists \rho \in \mathbb{R} : f_k = \rho \mathcal{M}_k, \quad \forall k \geq 1\}.$$

Therefore

$$f_k^0(t, x, v) = N_s(t, x) \mathcal{M}_k(t, x, v).$$

We remark that $N_s(t, x) = \sum_k \int_{\mathbb{R}^2} f_k^0(t, x, v) dv$ is the surface density of particles.

Identifying the terms in (1.14) and letting η goes to 0, one can prove in the same spirit as in previous works on diffusion approximation [25, 34] that N_s satisfies the drift-diffusion equation :

$$\partial_t N_s - \text{div}_x (\mathbb{D}(\nabla_x N_s + N_s \nabla_x V_s)) = 0,$$

where V_s is the effective potential defined by (1.6) and \mathbb{D} is a diffusion matrix (symmetric positive definite) depending on the choice of the transition rates $\alpha_{k,k'}$. In this paper, we consider for simplicity the case $\mathbb{D} = \mathbb{I}$ where \mathbb{I} is the identity matrix in \mathbb{R}^2 .

2 Existence and uniqueness (Proof of Theorem 1.2)

2.1 Notations and strategy of the proof

As done in [7], we view the system as a two dimensional drift-diffusion equation (1.5) for the surface density coupled to the quasistatic Schrödinger-Poisson system (1.2), (1.3). The drift-diffusion equation determines the value of the surface density in terms of the electrostatic potential, while the Schrödinger-Poisson systems allows to compute the potential as a function of the surface density.

The overall problem is then solved by a fixed-point procedure for the unknown N_s , as for the standard drift-diffusion-Poisson problem [19, 28, 29]. The global in time existence heavily relies on an entropy estimate.

The first block now in the proof is to consider the quasistatic Schrodinger-Poisson system which consists, for any given nonnegative function $N_s(x)$ defined on ω , in finding a potential $V(x, z)$ defined on Ω and satisfying

$$\left\{ \begin{array}{l} -\Delta_{x,z}V = N(x, z); \quad (x, z) \in \Omega \\ N(x, z) = N_s(x) \sum_{k=1}^{+\infty} \frac{e^{-\epsilon_k(x)}}{\mathcal{Z}(x)} |\chi_k(x, z)|^2; \quad \mathcal{Z}(x) = \sum_{\ell=1}^{+\infty} e^{-\epsilon_\ell(x)} \\ \left\{ \begin{array}{l} -\frac{1}{2} \partial_z^2 \chi_k + V \chi_k = \epsilon_k \chi_k \quad (k \geq 1), \\ \chi_k(t, x, \cdot) \in H_0^1(0, 1), \quad \int_0^1 \chi_k \chi_\ell dz = \delta_{k\ell}, \\ V = V_b \text{ on } \partial\omega \times (0, 1), \quad \partial_z V(x, 0) = \partial_z V(x, 1) = 0 \quad \text{for } x \in \omega. \end{array} \right. \end{array} \right. \quad (2.1)$$

For this problem, we have the following result whose proof is postponed.

Proposition 2.1 *Let $N_s \in L^2(\omega)$ such that $N_s \geq 0$. Then the system (2.1) admits a unique solution $(V, (\epsilon_k, \chi_k)_{k \geq 1})$, which satisfies the estimates $\|V\|_{H^2(\Omega)} \leq C(N_s)$, the constant $C(N_s)$ depending only on the $L^2(\omega)$ norm of N_s . Moreover, for two arbitrary data N_s and \widetilde{N}_s , the corresponding solutions satisfy :*

$$\|V - \widetilde{V}\|_{H^2(\Omega)} \leq C(N_s, \widetilde{N}_s) \|N_s - \widetilde{N}_s\|_{L^2(\omega)}.$$

In order to prove existence of solutions of the overall problem, we need to show some *a priori* estimates for the solution. We shall begin with a relative entropy inequality (see e.g. [2, 3, 17] for classical counterparts), then show a uniform L^p estimate for the surface density. In order to do so, we proceed like in the standard drift-diffusion case [19] and define the slotboom variable

$$u = e^{\epsilon_F} = \frac{N_s}{\mathcal{Z}}. \quad (2.2)$$

We also define the surface current density

$$J_s = -\nabla_x N_s - N_s \nabla_x V_s = - \sum_k e^{-\epsilon_k} \nabla_x u, \quad (2.3)$$

in such a way that the drift-diffusion equation is written

$$\partial_t N_s + \operatorname{div}_x J_s = 0.$$

We denote by ρ_k the occupation factor of the k th subband

$$\rho_k = u e^{-\epsilon_k} \quad (2.4)$$

so that

$$N = \sum_k \rho_k |\chi_k|^2 \quad ; \quad N_s = \sum_k \rho_k.$$

Now we introduce two extensions \underline{N}_s and \underline{V} of the boundary data. These extensions are respectively defined on ω and Ω and chosen in such a way that

- $\underline{N}_s \in C^2(\bar{\omega})$, $0 < \underline{N}_1 \leq \underline{N}_s \leq \underline{N}_2$ with two nonnegative constants N_1 and N_2 , and $\underline{N}_s|_{\partial\omega} = N_b$.
- $\underline{V} \in C^2(\bar{\Omega})$ and satisfies the boundary conditions: $\underline{V}|_{\partial\omega \times (0,1)} = V_b$ and for all $x \in \omega$, $\partial_z \underline{V}(x, 0) = \partial_z \underline{V}(x, 1) = 0$.

It is clear that for regular enough domains such functions exist. Solving (1.2) with \underline{V} instead of V , we find two sequences $\epsilon_k[\underline{V}](x)$ and $\chi_k[\underline{V}](x, z)$, that we shall shortly denote by $\underline{\epsilon}_k$ and $\underline{\chi}_k$. We then define \underline{u} , $\underline{\epsilon}_F$, \underline{z} and $\underline{\rho}_k$ by

$$\underline{u} = \frac{N_s}{\underline{z}} \quad ; \quad \underline{z} = \sum_k e^{-\epsilon_k} \quad ; \quad \underline{\epsilon}_F = \log \underline{u} \quad ; \quad \underline{\rho}_k = \underline{u} e^{-\epsilon_k} = e^{\underline{\epsilon}_F - \epsilon_k},$$

as well as the density

$$\underline{N}(x, z) = \sum_k \underline{\rho}_k(x) |\underline{\chi}_k(x, z)|^2.$$

It is readily seen that

$$\|\nabla_x \underline{u} / \underline{u}\|_{L^\infty(\omega)} < \infty. \quad (2.5)$$

The relative entropy of (ρ_k, V) with respect to $(\underline{\rho}_k, \underline{V})$ is defined by:

$$\begin{aligned} W = & \sum_k \int_\omega (\rho_k \log(\rho_k / \underline{\rho}_k) - \rho_k + \underline{\rho}_k) dx + \frac{1}{2} \iint_\Omega |\nabla_{x,z}(V - \underline{V})|^2 dx dz \\ & + \int_\omega \sum_k u e^{-\epsilon_k} (\epsilon_k[V] - \epsilon_k[\underline{V}] - \langle |\chi_k|^2 (V - \underline{V}) \rangle) dx, \end{aligned} \quad (2.6)$$

where we use the notation $\langle f \rangle = \int_0^1 f dz$. As will be shown later on, the three terms of right hand side of the above identity are nonnegative. Besides, W has the following compact form

$$W = \iint_{\Omega} (N(\epsilon_F - V - (\underline{\epsilon}_F - \underline{V})) - N + \underline{N}) dx dz + \frac{1}{2} \iint_{\Omega} |\nabla_{x,z}(V - \underline{V})|^2 dx dz.$$

Let us comment on this formula. One can note that the familiar form of the relative entropy for classical drift-diffusion systems is recovered here. The main difference is that, in the classical case, the relation between the Fermi level, the electrostatic potential and the density is local: $\epsilon_F - V = \log N$ (see e.g. [2, 10, 19]), while here this relation is non local in space. This form is also similar to the one recently obtained in [21] for a fully quantum drift-diffusion model (QDD). This model was derived in [14] by following the strategy of quantum moments developed in [16] (see also the review paper [15]). It consists of a 3D drift-diffusion equation involving a quantum chemical potential which depends on the density in a non local way, *via* the resolution of a quasistatic auxiliary quantum problem. In the QDD model, the quantum chemical potential is the generalization of the term $\epsilon_F - V$ of the present model.

The following two propositions provide some *a priori* estimates needed for the resolution of the coupled system:

Proposition 2.2 *Let $T \geq 0$. Let (N_s, V) be a weak solution of (1.5), (1.2), (1.3), (1.11) such that $N_s \in C([0, T], L^2(\omega)) \cap L^2([0, T], H^1(\omega))$ and $V \in C([0, T], H^2(\Omega))$. Then we have*

$$\forall t \in [0, T], \quad 0 \leq W(t) < C_T,$$

where C_T is a constant only depending on T , $W(0)$ and \underline{u} .

Proposition 2.3 *Let $T > 0$ and assume $N_s^0 \in L^p(\omega)$ for some $p \in [2, +\infty]$ and let (N_s, V) be weak solution of (1.5), (1.2), (1.3), (1.11) such that $N_s \in C([0, T], L^2(\omega)) \cap L^2([0, T], H^1(\omega))$ and $V \in C([0, T], H^2(\Omega))$. Then*

$$N_s \in C([0, T], L^p(\omega)),$$

for any $T > 0$, with a bound depending only on T , N_b , V_b and $\|N_s^0\|_{L^p(\omega)}$.

2.2 Proof of the entropy inequality

The aim of this subsection is the proof of Proposition 2.2. Let (N_s, V) be a weak solution of (1.5), (1.2), (1.3). Since $V \in C([0, T], H^2(\Omega))$, by Lemma A.6, we deduce that $V_s \in C([0, T], H^2(\Omega))$. This is enough to ensure that $N_s \geq 0$, thanks to the maximum principle for parabolic equations (see for instance [27]).

The relative entropy is the sum of three positive terms.

Let us now show that the relative entropy W defined by (2.6) is nonnegative. This

is obviously the case for the two first terms. In order to deal with the third one, let us denote $\epsilon_k^s := \epsilon_k[sV + (1-s)\underline{V}]$, and $\chi_k^s = \chi_k[sV + (1-s)\underline{V}]$. Straightforward computations using Lemma A.3 of the Appendix lead to

$$\begin{aligned} & \sum_k u e^{-\epsilon_k} (\epsilon_k[V] - \epsilon_k[\underline{V}] - \langle |\chi_k|^2 (V - \underline{V}) \rangle) = \\ & = \int_0^1 \int_1^s \sum_{k, \ell \neq k} u \frac{e^{-\epsilon_k} - e^{-\epsilon_\ell}}{\epsilon_k^\sigma - \epsilon_\ell^\sigma} \langle \chi_k^\sigma (V - \underline{V}) \chi_\ell^\sigma \rangle^2 d\sigma ds \geq 0, \end{aligned}$$

since the sequence $(\epsilon_k = \epsilon_k[V])_{k \geq 1}$ is increasing. This is enough to conclude that $W \geq 0$, as the sum of three nonnegative terms.

The initial relative entropy is finite.

Since $N_s^0 \in L^2(\omega)$, then by Proposition 2.1 we have $V \in H^2(\Omega) \subset L^\infty(\Omega)$. From Lemma A.1 we deduce that

$$\|\epsilon_k - \frac{1}{2}\pi^2 k^2\|_{L^\infty(\omega)} \leq \|V\|_{L^\infty(\Omega)}.$$

This is enough to deduce that $W(0) < +\infty$.

Relative entropy dissipation.

Let us now compute dW/dt . We first remark that

$$\frac{d}{dt} \sum_k \int_\omega (\rho_k \log(\rho_k/\underline{\rho}_k) - \rho_k + \underline{\rho}_k) dx = \sum_k \int_\omega \partial_t \rho_k \log(\rho_k/\underline{\rho}_k) dx.$$

Taking advantage from the identity $N_s = \sum \rho_k$ and from $\log \rho_k = \log u - \epsilon_k$, the right hand side is equal to

$$\int_\omega \partial_t N_s \log(u/\underline{u}) dx - \sum_k \int_\omega \partial_t \rho_k (\epsilon_k - \underline{\epsilon}_k) dx.$$

With the identity $\partial_t \epsilon_k = \langle |\chi_k|^2 \partial_t V \rangle$ (see Lemma (A.3)) and (1.5) we obtain

$$\begin{aligned} \frac{d}{dt} \sum_k \int_\omega (\rho_k \log(\rho_k/\underline{\rho}_k) - \rho_k + \underline{\rho}_k) dx &= \int_\omega \operatorname{div}_x \left(\sum_k e^{-\epsilon_k} \nabla_x u \right) \log \frac{u}{\underline{u}} dx \\ &\quad - \frac{d}{dt} \int_\omega \sum_k \rho_k (\epsilon_k - \underline{\epsilon}_k) dx \\ &\quad + \iint_\Omega \sum_k \rho_k |\chi_k|^2 \partial_t V dx dz. \end{aligned}$$

The Poisson equation and the fact that $V = \underline{V}$ on $\partial\omega \times (0, 1)$ give

$$\begin{aligned} \frac{d}{dt} \frac{1}{2} \iint_\Omega |\nabla_{x,z}(V - \underline{V})|^2 dx dz &= \iint_\Omega \partial_t N (V - \underline{V}) dx dz \\ &= \frac{d}{dt} \iint_\Omega N (V - \underline{V}) dx dz - \iint_\Omega N \partial_t V dx dz. \end{aligned}$$

By using (1.6) and the expression of ρ_k , we obtain

$$\frac{d}{dt}W = \int_{\omega} \operatorname{div}_x \left(\sum_k e^{-\epsilon_k} \nabla_x u \right) \log(u/\underline{u}) dx.$$

After an integration by parts, we deduce thanks to $u = \underline{u}$ on $\partial\omega$ that

$$\frac{d}{dt}W = - \int_{\omega} \sum_k e^{-\epsilon_k} \frac{|\nabla_x u|^2}{u} dx + \int_{\omega} \sum_k e^{-\epsilon_k} \frac{\nabla_x u \cdot \nabla_x \underline{u}}{\underline{u}} dx. \quad (2.7)$$

In the sequel, we shall use the notation

$$D(t) = \int_{\omega} \sum_k e^{-\epsilon_k} \frac{|\nabla_x u|^2}{u} dx \quad (2.8)$$

and shall refer to this term as the entropy dissipation rate. Let now define $\beta = \|\nabla_x \underline{u}/\underline{u}\|_{L^\infty(\omega)} < +\infty$ (from (2.5)). A straightforward Cauchy-Schwarz inequality leads to:

$$\frac{d}{dt}W + D \leq \beta \sqrt{D} \sqrt{\|N_s\|_{L^1(\omega)}}.$$

Using the inequality $2ab \leq \varepsilon^2 a^2 + 1/\varepsilon^2 b^2$ for $\varepsilon > 0$ small enough, we get

$$\frac{d}{dt}W \leq C \|N_s\|_{L^1(\omega)}$$

Since the function $F(t) = t \log(t) - t + 1$, satisfies $F(t) \geq t + (1 - e)$, we obtain

$$\begin{aligned} W &\geq \sum_k \int_{\omega} \underline{\rho}_k F(\rho_k/\underline{\rho}_k) dx \geq \sum_k \int_{\omega} \underline{\rho}_k (\rho_k/\underline{\rho}_k + 1 - e) dx \\ &\geq \int_{\omega} N_s dx - (e - 1) \int_{\omega} \underline{N}_s dx, \end{aligned}$$

which leads to the differential inequality

$$\frac{d}{dt}W \leq C \int_{\omega} N_s dx \leq C(W + C_0),$$

where C_0 only depends on the data of the problem (and not on the considered solution). The Gronwall lemma implies $W(t) \leq C_T$ for all $t \in [0, T]$, where C_T only depends on T , $W(0)$ and data ($W(0) < +\infty$ if $N_s^0 \in L^2(\omega)$).

Remark 2.4 The above manipulations are formal for weak solutions (defined such that $N_s \in C([0, T], L^2(\omega))$). To make the argument rigorous, it is enough to regularize the data, obtain a regular solution for which the result holds, then pass to the limit in the regularization parameter and use the uniqueness of the weak solution (proved in Section 2.5).

2.3 Proof of the L^p estimate

The aim of this subsection is the proof of Proposition 2.3. We have seen in Section 2.2 that $W(0) < C(\|N_s^0\|_{L^2(\omega)})$. Hence Proposition 2.2 implies

$$\forall t \leq T, \quad \|V(t)\|_{H^1(\Omega)} + \|N_s(t)\|_{L^1(\omega)} \leq C_T. \quad (2.9)$$

Thanks to the Trudinger inequality (A.8) and to (A.6), as well as Lemma A.5 the functions

$$S_1(t, x) = \sup_{k \geq 1} \|\chi_k(t, x, \cdot)\|_{L^\infty}^2 \quad ; \quad S_2(t, x) = \sum_{k \geq 1} \frac{e^{-\epsilon_k(t, x)}}{\mathcal{Z}(t, x)} (\epsilon_k(t, x))^2 \quad (2.10)$$

are in $L^\infty((0, T), L^p(\omega))$ for any finite p and satisfy the bound

$$\forall p < +\infty, \quad \|S_1(t, \cdot)\|_{L^p(\omega)} + \|S_2(t, \cdot)\|_{L^p(\omega)} \leq C_p, \quad (2.11)$$

where C_p is a constant only depending on $\|V(t)\|_{H^1(\Omega)}$. From now on, we denote

$$n_s = N_s - \underline{N}_s \quad ; \quad n = N - \underline{N} \quad ; \quad v_s = V_s - \underline{V}_s \quad ; \quad v = V - \underline{V}. \quad (2.12)$$

Proof of Proposition 2.3 for $p \in [2, +\infty)$.

Multiply (1.5) by $n_s|n_s|^{p-2}$ and integrate on ω . After an integration by parts, we get

$$\begin{aligned} \frac{1}{p} \frac{d}{dt} \int_{\omega} |n_s|^p dx + (p-1) \int_{\omega} |\nabla_x n_s|^2 |n_s|^{p-2} dx + \frac{p-1}{p} \int_{\omega} \nabla_x |n_s|^p \cdot \nabla_x V_s dx = \\ = \int_{\omega} \Delta_x \underline{N}_s n_s |n_s|^{p-2} dx + \int_{\omega} \operatorname{div}_x (\underline{N}_s \nabla_x V_s) n_s |n_s|^{p-2} dx. \end{aligned}$$

The last term of the left hand side can be written after an integration by parts

$$-\frac{p-1}{p} \int_{\omega} |n_s|^p \Delta_x V_s dx.$$

The above computations follow closely the standard drift-diffusion Poisson system for which the above term is nonnegative. In our case however, $-\Delta_x V_s \neq N_s$ which induces additional difficulties. Indeed, with the Poisson equation (1.3), we have: $-\Delta_x V = \partial_z^2 V + N$. And, after some integrations by parts,

$$\langle \partial_z^2 V | \chi_k|^2 \rangle = 2 \langle V \chi_k \partial_z^2 \chi_k \rangle + 2 \langle V | \partial_z \chi_k|^2 \rangle.$$

Thanks to the Schrödinger equation (1.2), we have:

$$\partial_z^2 \chi_k = 2(V - \epsilon_k) \chi_k \quad \text{and} \quad 2 \langle V | \chi_k|^2 \rangle + |\partial_z \chi_k|^2 = 2\epsilon_k.$$

Thus,

$$\langle \partial_z^2 V | \chi_k|^2 \rangle = 4 \langle V^2 | \chi_k|^2 \rangle + 2 \langle (V + \epsilon_k) | \partial_z \chi_k|^2 \rangle - 4\epsilon_k^2.$$

These remarks lead to the following identity :

$$\begin{aligned}
-\Delta_x V_s &= -4S_2(t, x) + \frac{\langle N^2 + 4V^2 N \rangle}{N_s} + 2 \sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}} \langle (V + \epsilon_k) |\partial_z \chi_k|^2 \rangle \\
&\quad - \frac{1}{\mathcal{Z}} \sum_k \sum_{\ell \neq k} \left(\frac{e^{-\epsilon_k} - e^{-\epsilon_\ell}}{\epsilon_k - \epsilon_\ell} \right) \langle \chi_k \chi_\ell \nabla_x V \rangle^2 \\
&\quad + \sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}} \langle |\chi_k|^2 \nabla_x V \rangle^2 - \left(\sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}} \langle |\chi_k|^2 \nabla_x V \rangle \right)^2,
\end{aligned} \tag{2.13}$$

where S_2 is defined in (2.10). By the Cauchy-Schwarz inequality, the sum of the last two terms of the right hand side is nonnegative. Moreover, except for the first one, the other terms are obviously nonnegative. By an integration by parts, we deduce

$$\frac{1}{p} \frac{d}{dt} \int_\omega |n_s|^p dx + (p-1) \int_\omega |\nabla_x n_s|^2 |n_s|^{p-2} dx \leq I + II + III \tag{2.14}$$

where

$$\begin{aligned}
I &= 4 \frac{p-1}{p} \int_\omega |n_s|^p S_2 dx, \\
II &= \int_\omega \Delta_x \underline{N_s} n_s |n_s|^{p-2} dx, \\
III &= \int_\omega \operatorname{div}_x (\underline{N_s} \nabla_x V_s) n_s |n_s|^{p-2} dx.
\end{aligned}$$

Let us now analyze each term separately.

Estimating I.

Thanks to the Hölder inequality, for all $r > 1$ and $r' = r/(r-1)$ we have :

$$I = 4 \frac{p-1}{p} \int_\omega |n_s|^p S_2 dx \leq C \| |n_s|^{\frac{p}{2}} \|_{L^{2r}}^2 \| S_2 \|_{L^{r'}}.$$

By applying Gagliardo-Nirenberg and Young inequalities we have for $r > 1$

$$\left\| |n_s|^{\frac{p}{2}} \right\|_{L^{2r}(\omega)}^2 \leq C \left\| |n_s|^{\frac{p}{2}} \right\|_{L^2(\omega)}^{2/r} \left\| |n_s|^{\frac{p}{2}} \right\|_{H^1(\omega)}^{2(1-1/r)} \leq C \left(\frac{1}{\varepsilon^r} \|n_s\|_{L^p}^p + \varepsilon^{\frac{r}{r-1}} \left\| |n_s|^{\frac{p}{2}} \right\|_{H^1(\omega)}^2 \right).$$

By using the estimate (2.11) and Poincaré inequality we obtain

$$I \leq C_\varepsilon \|n_s\|_{L^p}^p + C\varepsilon \int_\omega |\nabla_x |n_s|^{p/2}|^2 dx. \tag{2.15}$$

Estimating II.

This is an easy task. By a straightforward Hölder inequality, we have

$$|II| = \left| \int_\omega \Delta_x \underline{N_s} n_s |n_s|^{p-2} dx \right| \leq \|n_s\|_{L^p(\omega)}^{p-1} \|\Delta_x \underline{N_s}\|_{L^p(\omega)}. \tag{2.16}$$

Estimating III.

This term needs more work. We first begin by an integration by parts and obtain

$$III = -(p-1) \iint_{\Omega} \frac{N_s}{\mathcal{Z}} \sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}} |\chi_k|^2 \nabla_x V \cdot \nabla_x n_s |n_s|^{p-2} dx dz.$$

This leads to the inequality

$$|III| \leq (p-1) \|\underline{N}_s\|_{L^\infty} \iint_{\Omega} |S_1(t, x)| |\nabla_x V| |\nabla_x n_s| |n_s|^{p-2} dx dz,$$

where S_1 is defined in (2.10). Taking advantage of (2.11), we find after a Hölder inequality

$$|III| \leq C_{q,r} \|\underline{N}_s\|_{L^\infty} \|\nabla_x V\|_{L^q} \|\nabla_x n_s |n_s|^{p-2}\|_{L^r} \quad (2.17)$$

for any (q, r) such that $q < +\infty$ and $r > q'$, where $q' = q/(q-1)$. By choosing $r = \frac{p}{p-1}$, we have by a Hölder inequality

$$\|\nabla_x n_s |n_s|^{p-2}\|_{L^r} \leq \|\nabla_x n_s |n_s|^{\frac{p-2}{2}}\|_{L^2} \|n_s\|_{L^p}^{\frac{p-2}{2}}.$$

Now one can apply (2.17) with any $q > p$. By choosing q close enough to p , the following Sobolev inequality holds

$$\|\nabla_x V\|_{L^q} \leq C_1 \|V\|_{W^{2,s}} \leq C_2 \|N\|_{L^s} + C_3$$

for some $s < p$. Using again the inequality

$$N \leq N_s S_1, \quad (2.18)$$

where S_1 is defined by (2.10) and satisfies the uniform bound (2.11), we immediately obtain $\|N\|_{L^s} \leq C \|N_s\|_{L^p} \leq C (\|\underline{N}_s\|_{L^p} + \|n_s\|_{L^p})$. Besides, we have

$$\int_{\omega} |\nabla_x n_s|^2 |n_s|^{p-2} dx = \frac{4}{p^2} \int_{\omega} |\nabla_x (|n_s|^{p/2})|^2 dx. \quad (2.19)$$

All in all, (2.17) becomes

$$|III| \leq C \|\nabla_x (|n_s|^{p/2})\|_{L^2(\omega)} \|n_s\|_{L^p(\omega)}^{(p-2)/2} (\|n_s\|_{L^p(\omega)} + \|\underline{N}_s\|_{L^p(\omega)} + 1),$$

which leads, after a Young inequality to

$$|III| \leq C_1 \varepsilon^2 \int_{\omega} |\nabla_x (|n_s|^{p/2})|^2 dx + \frac{C_2}{\varepsilon^2} \|n_s\|_{L^p(\omega)}^p + \frac{C_3}{\varepsilon^2} \|n_s\|_{L^p(\omega)}^{p-2}, \quad (2.20)$$

where ε is an arbitrarily small constant and C_1, C_2, C_3 are independent from ε .

Consider now the inequality (2.14). Inserting the inequalities (2.19), (2.16), (2.15) and (2.20) in (2.14) and fixing ε small enough, there exists $A > 0$ and nonnegative constants still denoted by C_1, C_2 and C_3 such that

$$\begin{aligned} & \frac{1}{p} \frac{d}{dt} \int_{\omega} |n_s|^p dx + A \int_{\omega} |\nabla_x (|n_s|^{p/2})|^2 dx \\ & \leq C_1 \int_{\omega} |n_s|^p dx + C_2 \|n_s\|_{L^p(\omega)}^{p-1} + C_3 \|n_s\|_{L^p(\omega)}^{p-2}. \end{aligned}$$

A Gronwall argument leads to the boundedness on $[0, T]$ of $\|n_s(t)\|_{L^p(\omega)}$.

Proof of Proposition 2.3 for $p = +\infty$.

Since $N_s \in L^p(\omega)$ for all $1 \leq p < +\infty$, then by (2.18) and (2.11), $n \in L^r(\Omega)$ for all $1 \leq r < +\infty$. Therefore the Poisson equation (1.3) leads to $V \in W^{2,r}(\Omega)$. By Sobolev embeddings, the potential V lies in $L^\infty([0, T] \times \Omega)$. Hence from (2.13) and (A.2) we deduce that there exists a nonnegative constant a such that $\Delta_x V_s \leq a$. We use the standard notation f_+ for the positive part of f :

$$f_+ = \begin{cases} f & \text{if } f \geq 0, \\ 0 & \text{else.} \end{cases}$$

Let us define

$$A(t) = \lambda e^{at}, \quad \text{where } \lambda \geq \max(\|N_s^0\|_{L^\infty(\omega)}, \|N_b\|_{L^\infty(\partial\omega)}). \quad (2.21)$$

Then, from (1.5) and the choice of a ,

$$\partial_t(N_s - A(t)) - \operatorname{div}_x(\nabla_x(N_s - A(t))) + (N_s - A(t))\nabla_x V_s \leq 0.$$

Multiplying this equation by $(N_s - A(t))_+$ and integrating over ω , we get after an integration by part

$$\frac{1}{2} \frac{d}{dt} \int_{\omega} (N_s - A(t))_+^2 dx + \int_{\omega} |\nabla_x(N_s - A(t))_+|^2 dx + \frac{1}{2} \int_{\omega} \nabla_x(N_s - A(t))_+^2 \nabla_x V_s dx \leq 0.$$

After another integration by parts and since $\Delta_x V_s \leq a$,

$$\frac{d}{dt} \int_{\omega} (N_s - A(t))_+^2 dx - a \int_{\omega} (N_s - A(t))_+^2 dx \leq 0.$$

We deduce from this inequality and the choice of λ in (2.21) that for all $t \in [0, T]$, $N_s \leq A(t)$ thus $N_s \leq \lambda e^{aT}$.

2.4 Analysis of the Schrödinger-Poisson system

In this subsection, we prove Proposition 2.1. We use the functional spaces

$$H_\omega^1 = \{V \in H^1(\Omega) : \forall x \in \partial\omega, z \in [0, 1], V(x, z) = 0\}$$

and

$$L_x^p L_z^q(\Omega) = \{u \in L_{loc}^1(\Omega) \text{ such that } \|u\|_{L_x^p L_z^q(\Omega)} = \left(\int_{\omega} \|u(x, \cdot)\|_{L^q(0,1)}^p dx \right)^{1/p} < +\infty\}.$$

Thanks to Gagliardo-Nirenberg inequalities and interpolation estimates, one can prove the

Lemma 2.5 *We have the Sobolev imbedding of $H^1(\Omega)$ into $L_x^2 L_z^\infty(\Omega)$.*

Let $V_0 \in H^2(\Omega)$ be such that $V_0 = V_b$ on $\partial\omega \times (0, 1)$ and $\partial_z V_0(x, 0) = \partial_z V_0(x, 1) = 0$ for all $x \in \omega$ (for instance we can take $V_0 = \underline{V}$). Proceeding as in [7] and in the spirit of [30] we can show that a weak solution of (2.1) in the affine space $V_0 + H_\omega^1$ is a critical point with respect to V of the functional

$$\begin{aligned} J(V, N_s) &= J_0(V) + J_1(V, N_s) \\ &= \frac{1}{2} \iint_{\Omega} |\nabla_{x,z} V|^2 + \int_{\omega} N_s \log \sum_k e^{-\epsilon_k[V]} dx, \end{aligned}$$

where we recall that $(\epsilon_k[V])_{k \geq 1}$ denote the eigenvalues of the Hamiltonian $-\frac{1}{2} \frac{d^2}{dz^2} + V$, *i.e.* satisfy (1.2).

The functional J_0 is clearly continuous and strongly convex on $H^1(\Omega)$. The analysis of the functional $V \mapsto J_1(V, N_s)$ relies on the properties of $\epsilon_k[V]$. From the inequality (see Lemma A.1)

$$|\epsilon_k[V] - \epsilon_k[\tilde{V}]|(x) \leq \|V(x, \cdot) - \tilde{V}(x, \cdot)\|_{L_z^\infty(0,1)}$$

and

$$\log \frac{\sum_k e^{-\epsilon_k[V]}}{\sum_k e^{-\epsilon_k[\tilde{V}]}} \leq \log \frac{\sum_k e^{-\epsilon_k[\tilde{V}] + \sup_\ell (|\epsilon_\ell[V] - \epsilon_\ell[\tilde{V}]|)}}{\sum_k e^{-\epsilon_k[\tilde{V}]}}$$

we deduce

$$\begin{aligned} |J_1(V, N_s) - J_1(\tilde{V}, N_s)| &\leq \int_{\omega} |N_s(x)| \sup_k (|\epsilon_k[V] - \epsilon_k[\tilde{V}]|(x)) dx \\ &\leq \|N_s\|_{L^2(\omega)} \|V - \tilde{V}\|_{L_x^2 L_z^\infty(\Omega)}. \end{aligned} \quad (2.22)$$

The functional $J_1(\cdot, N_s)$ is globally Lipschitz continuous on $L_x^2 L_z^\infty(\Omega)$, thus on $H^1(\Omega)$, thanks to Lemma 2.5.

Next, $J_1(\cdot, N_s)$ is twice Gâteaux differentiable on $L^\infty(\Omega)$ and

$$\begin{aligned} d_V^2 J_1(V, N_s) W \cdot W &= - \int_{\omega} \frac{N_s}{\mathcal{Z}} \sum_k \sum_{\ell \neq k} \frac{e^{-\epsilon_k} - e^{-\epsilon_\ell}}{\epsilon_k - \epsilon_\ell} \langle \chi_k \chi_\ell W \rangle^2 dx \\ &\quad + \int_{\omega} N_s \left\{ \sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}} \langle |\chi_k|^2 W \rangle^2 - \left(\frac{\sum_k e^{-\epsilon_k} \langle |\chi_k|^2 W \rangle}{\mathcal{Z}} \right)^2 \right\} dx. \end{aligned}$$

When N_s is nonnegative, this quantity is nonnegative thanks to the Cauchy-Schwarz inequality. Thus $J_1(\cdot, N_s)$ is convex. As a consequence, the functional $J(\cdot, N_s) = J_0 + J_1(\cdot, N_s)$ is continuous and strongly convex on $V_0 + H_\omega^1$. Moreover, using the Poincaré inequality on H_ω^1 and (2.22) with $\tilde{V} = 0$, we have

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

thus $J(\cdot, N_s)$ is coercive and bounded from below on H_ω^1 : it admits a unique minimizer, denoted by V , which is then solution of our problem with the boundary conditions (1.11).

Now we prove the H^2 estimate of V . Since V is a minimizer of $J(\cdot, N_s)$ we have $J(V, N_s) \leq J(0, N_s)$. Thus,

$$\frac{1}{2} \iint_{\Omega} |\nabla_{x,z} V|^2 dx dz \leq J_1(0, N_s) - J_1(V, N_s).$$

Applying (2.22), we deduce that V is bounded in $H^1(\Omega)$, with a bound only depending on the L^2 norm of N_s . Therefore the function S_1 defined in (2.10) satisfies the bound (2.11). Since $N \leq N_s S_1$, we deduce that the density N lies in $L^r(\Omega)$ for any $r < 2$, which implies by elliptic regularity that $V \in W^{2,r}(\Omega)$. This implies that V actually lies in L^∞ which leads, in view of (A.6), to $S_1 \in L^\infty$. Therefore, N is bounded in $L^2(\Omega)$, which gives $V \in H^2(\Omega)$ thanks to the elliptic regularity.

Let us now prove the Lipschitz dependence of V with respect to N_s in $H^2(\Omega)$. Let V and \tilde{V} denote the minimizers of $J(\cdot, N_s)$ and $J(\cdot, \tilde{N}_s)$. Using the linearity of J_1 with respect to N_s , its Lipschitz dependence with respect to V from (2.22), the strong convexity of J and the fact that \tilde{V} minimizes $J(\cdot, \tilde{N}_s)$, we get

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

Thus, we have first the Lipschitz dependence of V in $H^1(\Omega)$. The Poisson equation gives $-\Delta(V - \tilde{V}) = N - \tilde{N}$, and

$$\begin{aligned} N - \tilde{N} &= (N_s - \tilde{N}_s) \sum_k \frac{e^{-\epsilon_k} |\chi_k|^2}{\mathcal{Z}} + \tilde{N}_s \sum_k \left(\frac{e^{-\epsilon_k}}{\mathcal{Z}} - \frac{e^{-\tilde{\epsilon}_k}}{\tilde{\mathcal{Z}}} \right) |\chi_k|^2 \\ &\quad + \tilde{N}_s \sum_k \frac{e^{-\tilde{\epsilon}_k}}{\tilde{\mathcal{Z}}} (|\chi_k|^2 - |\tilde{\chi}_k|^2) \end{aligned}$$

(we denote $\tilde{\epsilon}_k$ instead of $\epsilon_k[\tilde{V}]$ and $\tilde{\chi}_k$ instead of $\chi_k[\tilde{V}]$). With Lemma A.4,

$$\|\chi_k - \tilde{\chi}_k\|_{L_z^\infty} \leq C_1 e^{C_2(\|V\|_{L_z^2} + \|\tilde{V}\|_{L_z^2})} \|V - \tilde{V}\|_{L_z^1}. \quad (2.23)$$

Denoting $\chi_k^s = \chi_k[\tilde{V} + s(V - \tilde{V})]$ and $\epsilon_k^s = \epsilon_k[\tilde{V} + s(V - \tilde{V})]$, we have with Lemma A.3,

$$\begin{aligned} \sum_k \left(\frac{e^{-\epsilon_k}}{\mathcal{Z}} - \frac{e^{-\tilde{\epsilon}_k}}{\tilde{\mathcal{Z}}} \right) |\chi_k|^2 &= \int_0^1 \frac{\sum_k \langle |\chi_k^s|^2 (V - \tilde{V}) \rangle e^{-\epsilon_k^s}}{\sum_\ell e^{-\epsilon_\ell^s}} \frac{\sum_k |\chi_k|^2 e^{-\epsilon_k^s}}{\sum_\ell e^{-\epsilon_\ell^s}} ds - \\ &\quad \int_0^1 \sum_k \frac{\langle |\chi_k^s|^2 (V - \tilde{V}) \rangle e^{-\epsilon_k^s}}{\sum_\ell e^{-\epsilon_\ell^s}} |\chi_k|^2 ds. \end{aligned}$$

Thus, since we have proved that $\chi_k^s \in L^\infty(\Omega)$, $\forall s \in [0, 1]$, we deduce

$$\left| \sum_k \left(\frac{e^{-\epsilon_k}}{\mathcal{Z}} - \frac{e^{-\tilde{\epsilon}_k}}{\tilde{\mathcal{Z}}} \right) |\chi_k|^2 \right| \leq C \|V - \tilde{V}\|_{L_z^1}. \quad (2.24)$$

Hence, from (2.23) and (2.24), it yields,

$$\|N - \tilde{N}\|_{L^2(\Omega)} \leq C\|N_s - \tilde{N}_s\|_{L^2(\omega)} + C\|V - \tilde{V}\|_{L^2(\Omega)}.$$

Finally, from the Lipschitz dependence of V with respect to N_s in $H^1(\Omega)$, we have locally $\|V - \tilde{V}\|_{L^2(\Omega)} \leq C\|N_s - \tilde{N}_s\|_{L^2(\omega)}$. Thus, $\|N - \tilde{N}\|_{L^2(\Omega)} \leq C\|N_s - \tilde{N}_s\|_{L^2(\omega)}$ with a constant C depending on $\|N_s\|_{L^2(\omega)}$ and $\|\tilde{N}_s\|_{L^2(\omega)}$. Applying the elliptic regularity, we conclude $\|V - \tilde{V}\|_{H^2(\Omega)} \leq C(\|N_s\|_{L^2(\omega)}, \|\tilde{N}_s\|_{L^2(\omega)})\|N_s - \tilde{N}_s\|_{L^2(\omega)}$. \square

Remark 2.6 We can also solve this problem by assuming that $u \in L^2(\omega)$ is given such that $u \geq 0$. More precisely, the system (1.2), (1.3) is now written

$$\begin{cases} \frac{1}{2} \partial_z^2 \chi_k + V \chi_k = \epsilon_k \\ -\Delta_{x,z} V = u \sum_k |\chi_k|^2 e^{-\epsilon_k}. \end{cases}$$

Following the same idea as above, a weak solution of this system in the affine space $V_0 + H^1(\Omega)$ is the unique minimizer with respect to V of the convex functional:

$$J(V) = \frac{1}{2} \iint_{\Omega} |\nabla_x V|^2 dx dz + \int_{\omega} u \sum_k e^{-\epsilon_k [V]} dx,$$

(in fact, for H^1 potentials, it is not guaranteed that this functional takes finite values; to circumvent this difficulty, one can instead solve an auxiliary problem where the exponential is truncated for negative arguments, then estimate its solution and show that it is nonnegative). As before, we have $V \in H^2(\Omega)$ for $u \in L^2(\omega)$.

Proof of Proposition 1.4. We consider the stationary problem (1.12)–(1.13). First, we remark that the stationary drift-diffusion equation and the boundary conditions gives

$$\begin{cases} -\operatorname{div} \left(\sum_k e^{-\epsilon_k^\infty} \nabla_x u \right) = 0 & \text{for } x \in \omega, \\ u = u^\infty & \text{for } x \in \partial\omega, \end{cases}$$

Thus $u = u^\infty$. Then (1.12) can be written

$$\begin{cases} -\frac{1}{2} \partial_z^2 \chi_k^\infty + V^\infty \chi_k^\infty = \epsilon_k^\infty \chi_k^\infty, \\ -\Delta_{x,z} V^\infty = u^\infty \sum_k |\chi_k^\infty|^2 e^{-\epsilon_k^\infty}. \end{cases}$$

And the solution of this Schrödinger-Poisson system is the minimum of the convex functional (see Remark 2.6):

$$J(V) = \frac{1}{2} \iint_{\Omega} |\nabla_{x,z} V|^2 dx dz + \int_{\omega} u^\infty \sum_k e^{-\epsilon_k [V]} dx,$$

where $(\epsilon_k [V])_{p \geq 1}$ are the eigenvalues of the Hamiltonian, i.e. satisfy (1.2). \square

2.5 Proof of Theorem 1.2

The proof of existence and uniqueness relies on a contraction argument in the spirit of [28]. We first define the map $F : N_s \mapsto \widehat{N}_s$ as follows :

Step 1. For a given $N_s \geq 0$, solve the Schrödinger-Poisson system (2.1) as in Section 2.4. From the obtained $V \in C([0, T], H^2(\Omega))$ (see Proposition 2.1), define V_s by (1.6). Thanks to Lemma A.6, V_s belongs to $C([0, T], H^2(\omega))$.

Step 2. The surface potential V_s being known, solve the following parabolic equation for the unknown \widehat{N}_s :

$$\partial_t \widehat{N}_s - \operatorname{div}_x (\nabla_x \widehat{N}_s + \widehat{N}_s \nabla_x V_s) = 0, \quad (2.25)$$

with the boundary condition :

$$\widehat{N}_s(t, x) = N_b(x) \quad \text{for } x \in \partial\omega, \quad (2.26)$$

and the initial value :

$$\widehat{N}_s(0, x) = N_s^0(x) \quad \text{for } x \in \partial\omega.$$

Standard results on parabolic equations ([27]) leads to the existence and uniqueness of the solution \widehat{N}_s of (2.25), (2.26). Of course, $\widehat{N}_s \geq 0$. The map F is then defined after these two steps by $F(N_s) := \widehat{N}_s$.

Let us now show that F is a contraction on the space $M_{a,T}$ defined by $M_{a,T} = \{n : \|n\|_T \leq a\}$, where the norm is :

$$\|n\|_T = \left[\max_{0 \leq t \leq T} \|n(t)\|_{L^2(\omega)}^2 + \int_0^T \|n(t)\|_{H^1(\omega)}^2 dt \right]^{1/2}. \quad (2.27)$$

These two parameters T and a will be specified later on. Let N_s and \widetilde{N}_s be two elements of $M_{a,T}$. The difference $\delta F = F(\widetilde{N}_s) - F(N_s)$ verify

$$\partial_t \delta F - \operatorname{div}_x (\nabla_x \delta F + \delta F \nabla_x V_s + F(\widetilde{N}_s) \nabla_x \delta V_s) = 0, \quad (2.28)$$

with the notation $\delta V_s = V_s - \widetilde{V}_s$. The boundary conditions become :

$$\delta F(0, x) = 0, \quad \forall x \in \omega; \quad \delta F(t, x) = 0, \quad \forall x \in \partial\omega, \quad \forall t \in [0, T].$$

Multiplying (2.28) by δF and integrating on ω , we get after an integration by parts

$$\frac{1}{2} \frac{d}{dt} \int_{\omega} |\delta F|^2 dx + \int_{\omega} |\nabla_x(\delta F)|^2 dx + \int_{\omega} \nabla_x(\delta F) (\delta F \nabla_x V_s + F(\widetilde{N}_s) \nabla_x(\delta V_s)) dx = 0.$$

The Cauchy-Schwarz inequality applied to the third term leads to :

$$\frac{1}{2} \frac{d}{dt} \|\delta F\|_{L^2}^2 + \|\nabla_x(\delta F)\|_{L^2}^2 \leq \|\nabla_x(\delta F)\|_{L^2} \left(\|\delta F \nabla_x V_s\|_{L^2} + \|F(\widetilde{N}_s) \nabla_x(\delta V_s)\|_{L^2} \right).$$

Thus,

$$\begin{aligned} \frac{d}{dt} \|\delta F\|_{L^2}^2 + \|\nabla_x(\delta F)\|_{L^2}^2 &\leq 2\|\delta F \nabla_x V_s\|_{L^2}^2 + 2\|F(\widetilde{N}_s) \nabla_x(\delta V_s)\|_{L^2}^2 \\ &\leq 2\|\delta F\|_{L^4}^2 \|\nabla_x V_s\|_{L^4}^2 + 2\|F(\widetilde{N}_s)\|_{L^4}^2 \|\nabla_x(\delta V_s)\|_{L^4}^2. \end{aligned} \quad (2.29)$$

Besides, we have

$$|\nabla_x V_s| = \frac{|\sum_k \int_0^1 |\chi_k|^2 \nabla_x V e^{-\epsilon_k} dz|}{\sum_k e^{-\epsilon_k}} \leq |S_2(t, x)| \int_0^1 |\nabla_x V| dz,$$

where S_2 is defined by (2.10). From Proposition 2.1 and the fact that $N_s \in M_{a,T}$, we deduce that

$$\max_{0 \leq t \leq T} \|V(t)\|_{H^2(\Omega)} \leq C_1(a),$$

where $C_1(a)$ is a constant only depending on a . From Lemma A.6 and the imbedding $H^2(\Omega) \hookrightarrow L^\infty(\Omega)$, we deduce the pointwise in time inequalities

$$\max_{0 \leq t \leq T} (\|S_2(t)\|_{L^\infty} + \|V_s(t)\|_{H^2(\omega)}) \leq C_2(a).$$

From Lemma A.6 and Proposition 2.1, we know that there exists a constant $C_2(a)$ such that,

$$\|\nabla_x(\delta V_s)\|_{L^4} \leq C \|\delta V_s\|_{H^2(\omega)} \leq C_2(a) \|\delta N_s\|_{L^2(\omega)}.$$

Inserting the above inequalities in (2.29), we obtain the inequality

$$\frac{d}{dt} \|\delta F\|_{L^2}^2 + \|\nabla_x(\delta F)\|_{L^2}^2 \leq C_3(a) \left(\|\delta F\|_{L^4}^2 + \|F(\widetilde{N}_s)\|_{L^4}^2 \|\delta N_s\|_{L^2}^2 \right).$$

The Gagliardo Nirenberg inequality leads to

$$\frac{d}{dt} \|\delta F\|_{L^2}^2 + \frac{1}{2} \|\nabla_x(\delta F)\|_{L^2}^2 \leq C_4(a) \left(\|\delta F\|_{L^2}^2 + \|F(\widetilde{N}_s)\|_{L^4}^2 \|\delta N_s\|_{L^2}^2 \right). \quad (2.30)$$

Taking $\widetilde{N}_s = 0$ in the above inequality leads to

$$\begin{aligned} \frac{d}{dt} \|F(N_s) - F(0)\|_{L^2}^2 + \frac{1}{2} \|\nabla_x(F(N_s) - F(0))\|_{L^2}^2 &\leq \\ &C_4(a) \left(\|F(N_s) - F(0)\|_{L^2}^2 + \|F(0)\|_{L^4}^2 \|N_s\|_{L^2}^2 \right), \end{aligned}$$

which implies

$$\begin{aligned} \|F(N_s)(t) - F(0)(t)\|_{L^2}^2 &\leq \|F(N_s)(0) - F(0)(0)\|_{L^2}^2 e^{C_4(a)t} \\ &+ C_4(a) \|F(0)\|_{L^4}^2 \int_0^t \|N_s(\tau)\|_{L^2}^2 e^{C_4(a)(t-\tau)} d\tau. \end{aligned}$$

We then obtain

$$\|F(N_s)\|_T \leq C_5(a) e^{C_5(a)T},$$

where $\|\cdot\|_T$ is defined in (2.27) and C_5 only depends on a . Of course, since N_s and \widetilde{N}_s play the same role, we obviously have

$$\|F(\widetilde{N}_s)\|_T \leq C_5(a) e^{C_5(a)T}. \quad (2.31)$$

Let us now go back to (2.30), which after a Gronwall inequality yields

$$\begin{aligned} \|\delta F(t)\|_{L^2}^2 &\leq C_4(a) \|\delta N_s\|_T^2 \int_0^t e^{C_4(a)(t-\tau)} \|F(\widetilde{N}_s)(\tau)\|_{L^4}^2 d\tau \\ &\leq C_4(a) e^{C_4(a)t} \|\delta N_s\|_T^2 \int_0^t \|F(\widetilde{N}_s)(\tau)\|_{L^2} \|\nabla_x F(\widetilde{N}_s)(\tau)\|_{L^2} d\tau \\ &\leq C_4(a) e^{C_4(a)t} \|\delta N_s\|_T^2 \sqrt{T} \|F(\widetilde{N}_s)\|_T^2. \end{aligned}$$

We then deduce from (2.31) that

$$\|\delta F(t)\|_T \leq C_6(a) T^{1/4} e^{C_6(a)T} \|\delta N_s\|_T.$$

Let us now take $a = 2\|F(0)\|_1$ and choose the parameter $T \leq 1$ small enough so that $C_6(a) T^{1/4} e^{C_6(a)T} \leq 1/2$. Since $\|\cdot\|_T$ is increasing with respect to T , it is readily seen that F leaves $M_{a,T}$ invariant and is a contraction on this set. We have then constructed a unique solution on a time interval T_0 which only depends on the L^2 norm of the initial datum and on the $H^{1/2}(\partial\omega)$ norm of the boundary values for N_s and V_s . In order to construct a global solution, we take T_0 as the origin and prove as above the existence and uniqueness of the solution on $[T_0, 2T_0]$. This is made possible thanks to the locally uniform in time L^2 *a priori* estimate on the self-consistent solution, given in Proposition 2.3. Proceeding analogously we construct the solution $[2T_0, 3T_0]$ until covering completely the interval $[0, T]$.

3 Long time behaviour

The study of the exponential convergence to the equilibrium is established in two steps. First we prove the convergence towards 0 as t goes to $+\infty$ and the decreasing of the relative entropy defined by

$$\begin{aligned} W(t) &= \sum_k \int_{\omega} (\rho_k \log(\rho_k/\rho_k^\infty) - \rho_k + \rho_k^\infty) dx + \frac{1}{2} \iint_{\Omega} |\nabla_{x,z}(V - V^\infty)|^2 dx dz \\ &\quad + \int_{\omega} \sum_k u e^{-\epsilon_k} \left(\epsilon_k[V] - \epsilon_k[V^\infty] - \int_0^1 |\chi_k|^2 (V - V^\infty) dz \right) dx, \end{aligned} \quad (3.1)$$

where we define $\rho_k^\infty = u^\infty e^{-\epsilon_k^\infty}$. We denote

$$n = N - N^\infty, \quad v = V - V^\infty, \quad v_s = V_s - V_s^\infty, \quad n_s = N_s - N_s^\infty. \quad (3.2)$$

We deduce:

$$\begin{cases} \partial_t n_s - \operatorname{div}_x (\nabla_x n_s + N_s^\infty \nabla_x v_s + n_s \nabla_x V_s^\infty + n_s \nabla_x v_s) = 0, \\ -\Delta_{x,z} v = n. \end{cases} \quad (3.3)$$

Next we consider a quadratic approximation of the relative entropy and prove its exponential convergence to 0 as t goes to $+\infty$.

In the sequel, the letter C stands for a positive constant depending only on the data and ε stands for an arbitrarily small positive constant.

3.1 Convergence of the relative entropy

This section is devoted to the following preliminary result:

Proposition 3.1 *Under Assumption 1.1 and 1.3, the solution of the drift-diffusion-Schrödinger-Poisson system (1.1)–(1.11) is such that:*

(i) *The relative entropy W defined by (3.1) is decreasing and*

$$\lim_{t \rightarrow +\infty} W(t) = 0.$$

(ii) *We have $n_s \rightarrow 0$ in $L^1(\omega)$ and $v \rightarrow 0$ in $H^1(\omega)$ as t goes to $+\infty$.*

Proof. This proof is based on an idea developed in [19]. Let (N_s^∞, V^∞) solve the stationary problem (1.12). We deduce from (2.7) that the relative entropy satisfies:

$$\frac{d}{dt} W(t) = -D(t),$$

where D is given by (2.8). Then, for all $t \geq 0$, we have

$$W(t) + \int_0^t D(\tau) d\tau = W(0), \quad (3.4)$$

which implies that there exists a sequence $t_j \rightarrow +\infty$ such that

$$D(t_j) \rightarrow 0 \quad \text{as } j \rightarrow +\infty. \quad (3.5)$$

Now, straightforward calculations using $N_s = ue^{-V_s}$ give

$$D = \int_\omega (4|\nabla_x \sqrt{N_s}|^2 + 2\nabla_x N_s \cdot \nabla_x V_s + N_s |\nabla_x V_s|^2) dx. \quad (3.6)$$

After an integration by parts, we get

$$\int_\omega \nabla_x N_s \cdot \nabla_x V_s dx = - \int_\omega N_s \Delta_x V_s dx + \int_{\partial\omega} N_s \partial_\nu V_s d\sigma,$$

where $\nu(x)$ denotes the outward unitary normal vector at $x \in \partial\omega$ and $d\sigma$ the surface measure on $\partial\omega$ induced by the Lebesgue measure. Therefore we deduce from (3.6) that

$$\begin{aligned} 4\|\nabla_x \sqrt{N_s}\|_{L^2}^2 &\leq D + 2 \int_\omega N_s \Delta_x V_s dx - 2 \int_{\partial\omega} N_s \partial_\nu V_s d\sigma \\ &\leq D + 8 \int_\omega N_s S_2 dx - 2 \int_{\partial\omega \times (0,1)} N \partial_\nu V d\sigma dz \\ &\leq D + 8\|N_s\|_{L^4} \|S_2\|_{L^{4/3}} + 2\|N_b\|_{L^\infty} \|V\|_{H^2} \\ &\leq D + C\|N_s\|_{L^4} + C\|N\|_{L^2} + C, \end{aligned}$$

where we recall that S_2 is given by (2.10) and satisfies (2.11). Besides, it is readily seen that $N \leq N_s S_1$ where S_1 is given in (2.10) and satisfies (2.11). Therefore $\|N\|_{L^2} \leq C\|N_s\|_{L^4}$. We conclude from the above inequality that

$$4\|\nabla_x \sqrt{N_s}\|_{L^2}^2 \leq D + C\|N_s\|_{L^4} + C.$$

Applying a Gagliardo-Nirenberg inequality to the function $\sqrt{N_s}$ in the right-hand side, we obtain (for any $\varepsilon > 0$)

$$4\|\nabla_x \sqrt{N_s}\|_{L^2}^2 \leq D + C\|N_s\|_{L^1}^{1/2} \|\sqrt{N_s}\|_{H^1} + C \leq D + C_\varepsilon\|N_s\|_{L^1} + \varepsilon\|\nabla_x \sqrt{N_s}\|_{L^2}^2 + C,$$

which leads, in view of (2.9), to the inequality

$$\|\nabla_x \sqrt{N_s}\|_{L^2}^2(t) \leq C(D(t) + 1). \quad (3.7)$$

By evaluating (3.5) and (3.7) at $t = t_j$, we deduce the boundedness in $H^1(\omega)$ of the sequence $(\sqrt{N_s(t_j)})_j$. Because of the compactness embedding of $H^1(\omega)$ into $L^4(\omega)$, we can assume without loss of generality that there exists $\overline{N_s}$ belonging to $L^2(\omega)$ such that $\sqrt{\overline{N_s}} \in H^1(\omega)$ and

$$N_s(t_j) \longrightarrow \overline{N_s} \text{ in } L^2(\omega). \quad (3.8)$$

Thanks to the properties of the trace of $H^1(\omega)$ functions and the compact embedding $H^{1/2}(\partial\omega) \hookrightarrow L^4(\partial\omega)$, we have $\overline{N_s}|_{\partial\omega} = N_b$. From Proposition 2.1, we know that the mapping $N_s \mapsto V$ defined by

$$\begin{cases} -\frac{1}{2}\partial_z^2 \chi_k + V\chi_k = \epsilon_k \chi_k & (k \geq 1), \\ -\Delta_{x,z} V = N = N_s \sum_k \frac{|\chi_k|^2 e^{-\epsilon_k}}{\mathcal{Z}}, \end{cases}$$

(with the boundary conditions of V in (1.11)) is well-posed for $N_s \in L^2(\omega)$ such that $N_s \geq 0$ a.e. and is continuous from $L^2(\omega)$ into $H^2(\Omega)$. Moreover, by Lemma A.6 we also know that the mapping $V \mapsto V_s$ defined by

$$\begin{cases} V_s = -\log\left(\sum_k e^{-\epsilon_k}\right) \\ -\frac{1}{2}\partial_z^2 \chi_k + V\chi_k = \epsilon_k \chi_k \end{cases}$$

is continuous from $H^2(\Omega)$ to $H^2(\omega)$. It follows that

$$\exists \overline{V_s} \in H^2(\omega) \text{ such that } V_s(t_j) \longrightarrow \overline{V_s} \text{ in } H^2(\omega) \subset C(\overline{\omega}).$$

Hence,

$$u(t_j) = N_s(t_j) e^{V_s(t_j)} \longrightarrow \overline{N_s} e^{\overline{V_s}} \text{ in } L^2(\omega). \quad (3.9)$$

Now (3.5) and (3.8) imply that, for any $h \in (L^4(\omega))^2$, we have

$$\begin{aligned} \left| \int_{\omega} \nabla_x (N_s(t_j) e^{V_s(t_j)}) h \, dx \right| &= \left| \int_{\omega} \nabla_x u(t_j) h \, dx \right| \\ &\leq \left(\int_{\omega} e^{-V_s(t_j)} \frac{|\nabla_x u(t_j)|^2}{u(t_j)} \, dx \right) \|N_s(t_j) e^{2V_s(t_j)}\|_{L^2(\omega)}^{1/2} \|h\|_{L^4(\omega)} \\ &\longrightarrow 0 \text{ as } j \rightarrow +\infty. \end{aligned}$$

Taking into account (3.9), we deduce that $\overline{N_s} e^{\overline{V_s}}$ is constant in ω . Since $\overline{N_s}|_{\partial\omega} = N_b$ and $\overline{V_s}|_{\partial\omega} = V_s^\infty$, Assumption 1.3 implies $\overline{N_s} e^{\overline{V_s}} = u^\infty$. Thus, $(\overline{N_s}, \overline{V_s})$ can be identified as the unique solution of the stationary Schrödinger-Poisson system (see Remark 2.6):

$$\overline{N_s} = N_s^\infty, \quad \overline{V_s} = V_s^\infty \text{ and analogously } V(t_j) \longrightarrow V^\infty \text{ as } j \rightarrow +\infty.$$

Since the function W is decreasing, we have

$$\lim_{t \rightarrow +\infty} W(t) = \lim_{j \rightarrow +\infty} W(t_j) = 0.$$

Consequently, $\|v(t)\|_{H^1(\Omega)} \rightarrow 0$ and $\|n_s\|_{L^1(\omega)} \rightarrow 0$ as $t \rightarrow +\infty$ by a Poincaré inequality and the following Csiszár-Kullback inequality [3], [12], [26]: for all $n_1, n_2 \in L^1(\omega)$, $n_1 \geq 0$ a.e., $n_2 \geq 0$ a.e. with $\int_{\omega} n_1 \, dx = \int_{\omega} n_2 \, dx = N_0$, we have

$$\|n_1 - n_2\|_{L^1(\omega)}^2 \leq 2N_0 \int_{\omega} n_1 \log \frac{n_1}{n_2} \, dx.$$

□

3.2 Exponential convergence

This section is devoted to the proof of the main result of this paper, i.e. the exponential convergence of the surface density N_s and the electrostatic potential V to the equilibrium functions. We will consider the differences n, n_s, v, v_s defined in (3.2) and introduce the quadratic approximation of the relative entropy:

$$L(t) = \frac{1}{2} \int_{\omega} \frac{(n_s)^2}{N_s^\infty} \, dx + \int_{\omega} n_s v_s \, dx - \frac{1}{2} \iint_{\Omega} |\nabla v|^2 \, dx dz + \int_{\omega} N_s^\infty v_s \, dx - \iint_{\Omega} N^\infty v \, dx dz. \quad (3.10)$$

Since the Poisson equation gives $\iint_{\Omega} n v \, dx dz = \iint_{\Omega} |\nabla v|^2 \, dx dz$, we can rewrite

$$L(t) = \frac{1}{2} \int_{\omega} \frac{(n_s)^2}{N_s^\infty} \, dx + \frac{1}{2} \iint_{\Omega} |\nabla v|^2 \, dx dz + \int_{\omega} N_s v_s \, dx - \iint_{\Omega} N v \, dx dz. \quad (3.11)$$

In order to prove Theorem 1.5, we need three technical lemmata that we prove further in subsection 3.2.2:

Lemma 3.2 Consider a weak solution of (1.2)–(1.11). Then for all $t \geq 0$, we have

$$\frac{1}{2} \int_{\omega} \frac{(n_s)^2}{N_s^{\infty}} dx + \frac{1}{2} \iint_{\Omega} |\nabla v|^2 dx dz \leq L(t) \leq \frac{1}{2} \int_{\omega} \frac{(n_s)^2}{N_s^{\infty}} dx + \int_{\omega} n_s v_s dx.$$

Lemma 3.3 Let V and \underline{V} belong to $L^2(0, 1)$ and V_s, \underline{V}_s be defined by

$$V_s = -\log \sum_k \exp(-\epsilon_k[V]) \quad ; \quad \underline{V}_s = -\log \sum_k \exp(-\epsilon_k[\underline{V}]).$$

Then, by setting $v = V - \underline{V}$ and $v_s = V_s - \underline{V}_s$, we have

$$|\nabla_x v_s|^2 \leq C_1 e^{C_2(\|\underline{V}\|_{L^2(0,1)} + \|v\|_{L^2(0,1)})} (\langle |\nabla_x v|^2 \rangle + \langle |v|^2 \rangle \langle |\nabla_x \underline{V}|^2 \rangle), \quad (3.12)$$

where C_1 and C_2 are two positive constants.

Lemma 3.4 Consider a weak solution of (1.2)–(1.11). Then there exist two non-negative constants C_1 and C_2 such that for all $t \geq 0$,

$$\int_{\omega} \frac{(n_s)^2}{N_s^{\infty}} |\nabla_x v_s|^2 dx \leq \frac{1}{2} \int_{\omega} N_s^{\infty} \left| \nabla_x \left(\frac{n_s}{N_s^{\infty}} + v_s \right) \right|^2 dx + C_1 L(t)^4 + C_2 L(t) \|v\|_{H^1(\Omega)},$$

where L is defined in (3.11). Moreover, we have

$$\|v_s\|_{L^6(\Omega)} \leq C \|v\|_{H^1(\Omega)}, \quad (3.13)$$

for a nonnegative constant C .

3.2.1 Proof of Theorem 1.5

From (3.10) and the Poisson equation, we deduce that

$$\frac{d}{dt} L(t) = \int_{\omega} \partial_t n_s \left(\frac{n_s}{N_s^{\infty}} + v_s \right) dx + \int_{\omega} N_s \partial_t v_s dx - \iint_{\Omega} N \partial_t v dx dz.$$

Furthermore, $e^{-V_s} = \sum_k e^{-\epsilon_k} = \mathcal{Z}$ and $\partial_t \epsilon_k = \langle |\chi_k|^2 \partial_t v \rangle$ imply

$$\partial_t v_s = \frac{1}{\mathcal{Z}} \sum_k \langle |\chi_k|^2 \partial_t v \rangle e^{-\epsilon_k}.$$

Hence $\int_{\omega} N_s \partial_t v_s dx = \iint_{\Omega} N \partial_t v dx dz$. With (3.3) and after an integration by parts, we get

$$\frac{d}{dt} L(t) = - \int_{\omega} (\nabla_x n_s + N_s^{\infty} \nabla_x v_s + n_s \nabla_x V_s^{\infty} + n_s \nabla_x v_s) \cdot \nabla_x \left(\frac{n_s}{N_s^{\infty}} + v_s \right) dx.$$

Since $\nabla_x N_s^{\infty} + N_s^{\infty} \nabla_x V_s^{\infty} = 0$, we deduce that

$$\frac{d}{dt} L(t) = - \int_{\omega} N_s^{\infty} \left| \nabla_x \left(\frac{n_s}{N_s^{\infty}} + v_s \right) \right|^2 dx - \int_{\omega} n_s \nabla_x v_s \cdot \nabla_x \left(\frac{n_s}{N_s^{\infty}} + v_s \right) dx. \quad (3.14)$$

Now we will show that the second term of the right-hand side of can be controlled by the first one for long time. From Lemma 3.4, we deduce

$$\begin{aligned}
& - \int_{\omega} n_s \nabla_x v_s \cdot \nabla_x \left(\frac{n_s}{N_s^\infty} + v_s \right) dx \\
& \leq \frac{1}{2} \int_{\omega} \frac{(n_s)^2}{N_s^\infty} |\nabla_x v_s|^2 dx + \frac{1}{2} \int_{\omega} N_s^\infty \left| \nabla_x \left(\frac{n_s}{N_s^\infty} + v_s \right) \right|^2 dx \\
& \leq \frac{3}{4} \int_{\omega} N_s^\infty \left| \nabla_x \left(\frac{n_s}{N_s^\infty} + v_s \right) \right|^2 dx + C_1 L(t)^4 + C_2 \|v\|_{H^1(\Omega)} L(t).
\end{aligned}$$

Thanks to the Poincaré inequality and Lemma 3.2, we have

$$\begin{aligned}
-\frac{1}{4} \int_{\omega} N_s^\infty \left| \nabla_x \left(\frac{n_s}{N_s^\infty} + v_s \right) \right|^2 dx & \leq -\frac{C}{4} \int_{\omega} N_s^\infty \left(\frac{n_s}{N_s^\infty} + v_s \right)^2 dx \\
& \leq -\frac{C}{2} \int_{\omega} \left(\frac{1}{2} \frac{(n_s)^2}{N_s^\infty} + n_s v_s \right) dx \leq -\frac{C}{2} L(t).
\end{aligned}$$

Hence, we have obtained from (3.14)

$$\frac{d}{dt} L(t) \leq -C_0 L(t) + C_1 L(t)^4 + C_2 \|v\|_{H^1(\Omega)} L(t). \quad (3.15)$$

By Proposition 3.1 (ii), there exists $T > 0$ such that, for all $t \geq T$, $C_2 \|v\|_{H^1(\omega)}(t) \leq C_0/2$. Thus, for all $t \geq T$,

$$\frac{d}{dt} L(t) \leq -\frac{C_0}{2} L(t) + C_1 L(t)^4. \quad (3.16)$$

From (3.5) and (3.7), there exists a sequence $t_j \rightarrow +\infty$ as $j \rightarrow +\infty$ such that the sequence $(\sqrt{N_s(t_j)})_{j \in \mathbb{N}}$ is bounded in $H^1(\omega)$. Up to a renumbering, we can suppose that for all $j \in \mathbb{N}$, $t_j \geq T$. Moreover, by interpolation, we have

$$\left\| \frac{n_s}{\sqrt{N_s^\infty}} \right\|_{L^2(\omega)} \leq C \|n_s\|_{L^1(\omega)}^{1/4} \|n_s\|_{L^3(\omega)}^{3/4}.$$

By the Sobolev embedding of $H^1(\omega)$ into $L^6(\omega)$, we deduce that $\|n_s\|_{L^3(\omega)}(t_j)$ is bounded. Since we have proved in Proposition 3.1 (ii) that $n_s \rightarrow 0$ in $L^1(\omega)$ as t goes to $+\infty$, this insures the convergence towards 0 of $\|n_s/\sqrt{N_s^\infty}\|_{L^2(\omega)}(t_j)$ as j goes to $+\infty$. Moreover, with the bound of L in Lemma 3.2 we deduce

$$L(t) \leq \frac{1}{2} \left\| \frac{n_s}{\sqrt{N_s^\infty}} \right\|_{L^2(\omega)}^2 + C \|n_s\|_{L^2(\omega)} \|v_s\|_{L^6(\omega)}.$$

And (3.13) provides a bound of $\|v_s\|_{L^6(\omega)}$ by $\|v\|_{H^1(\Omega)}$ which converges towards 0 as t goes to $+\infty$ thanks to Proposition 3.1. We can conclude now that $\lim_{j \rightarrow +\infty} L(t_j) = 0$. Hence,

$$\exists t_* > 0 \text{ such that } C_1 L(t_*)^3 \leq \frac{C_0}{4}. \quad (3.17)$$

Now we define the set

$$\mathcal{A} := \left\{ t \in [t_*, +\infty) \text{ such that } \forall s \in [t_*, t], C_1 L(s)^3 \leq \frac{C_0}{4} \right\}.$$

By continuity of L , \mathcal{A} is a closed set which contains t_* from (3.17). Moreover, if $t_0 \in \mathcal{A}$, from (3.16) we deduce that L is decreasing near t_0 . By continuity of L , it yields that \mathcal{A} is open. Thus, $\mathcal{A} = [t_*, +\infty)$, i.e.

$$\forall t \in [t_*, +\infty), \frac{d}{dt} L(t) \leq -\frac{C_0}{4} L(t).$$

We obtain the announced result by integrating this last inequality.

3.2.2 Proofs of the technical lemmata

Proof of Lemma 3.2. The concavity of the function $x \mapsto \log x$ leads to the inequality

$$v_s = \log \left(\frac{\sum_k e^{-\epsilon_k^\infty}}{\sum_k e^{-\epsilon_k}} \right) = \log \left(\sum_k \frac{e^{-\epsilon_k}}{\sum_\ell e^{-\epsilon_\ell}} e^{\epsilon_k - \epsilon_k^\infty} \right) \geq \sum_k \frac{e^{-\epsilon_k}}{\sum_\ell e^{-\epsilon_\ell}} (\epsilon_k - \epsilon_k^\infty). \quad (3.18)$$

Therefore

$$\begin{aligned} N_s v_s - \langle Nv \rangle &= N_s \left(v_s - \sum_k \frac{e^{-\epsilon_k}}{\sum_\ell e^{-\epsilon_\ell}} \langle |\chi_k|^2 v \rangle \right) \\ &\geq \frac{N_s}{\sum_\ell e^{-\epsilon_\ell}} \sum_k e^{-\epsilon_k} (\epsilon_k - \epsilon_k^\infty - \langle |\chi_k[V]|^2 v \rangle). \end{aligned}$$

The right hand side of this inequality is exactly the third term of (2.6) which is positive. Therefore

$$\int_\omega N_s v_s dx - \iint_\Omega Nv dx dz \geq 0. \quad (3.19)$$

By exchanging the roles of (N, N^∞) and (V, V^∞) , we find

$$\iint_\Omega N^\infty v dx dz - \int_\omega N_s^\infty v_s dx \geq 0 \quad (3.20)$$

which leads, by (3.11) and for all $t \geq 0$, to

$$0 \leq \frac{1}{2} \int_\omega \frac{(n_s)^2}{N_s^\infty} dx + \frac{1}{2} \iint_\Omega |\nabla v|^2 dx dz \leq L(t).$$

This ends the proof of Lemma 3.2. Remark that the sum of (3.19) and (3.20) leads to the inequality

$$\int_\omega n_s v_s dx \geq \iint_\Omega nv dx dz = \iint_\Omega |\nabla v|^2 \geq 0.$$

□

Proof of Lemma 3.3. We have

$$\nabla_x v_s = \sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}} (\partial_x \epsilon_k - \partial_x \underline{\epsilon}_k) + \sum_k \left(\frac{e^{-\epsilon_k}}{\mathcal{Z}} - \frac{e^{-\underline{\epsilon}_k}}{\underline{\mathcal{Z}}} \right) \partial_x \underline{\epsilon}_k, \quad (3.21)$$

with the notation $\underline{\mathcal{Z}} = \sum_\ell e^{-\underline{\epsilon}_\ell}$. Thus, by a Jensen inequality,

$$|\nabla_x v_s|^2 \leq 2 \sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}} |\partial_x \epsilon_k - \partial_x \underline{\epsilon}_k|^2 + 2 \left| \sum_k \left(\frac{e^{-\epsilon_k}}{\mathcal{Z}} - \frac{e^{-\underline{\epsilon}_k}}{\underline{\mathcal{Z}}} \right) \partial_x \underline{\epsilon}_k \right|^2. \quad (3.22)$$

For the first term of the right hand side, we use the results stated in Lemma A.2 and A.4:

$$\begin{aligned} & \sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}} |\partial_x \epsilon_k - \partial_x \underline{\epsilon}_k|^2 \\ & \leq 2 \sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}} \langle |\chi_k|^2 \nabla_x v \rangle^2 + 2 \sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}} \langle (|\chi_k|^2 - |\underline{\chi}_k|^2) \nabla_x \underline{V} \rangle^2 \\ & \leq C_1 e^{C_2 \|V(x, \cdot)\|_{L^2(0,1)}} \langle |\nabla_x v|^2 \rangle + \int_0^1 C_1 e^{C_2 \|\underline{V}(x, \cdot) + sv(x, \cdot)\|_{L^2(0,1)}} \langle |v|^2 \rangle \langle |\nabla_x \underline{V}|^2 \rangle ds. \end{aligned}$$

Consequently, we have

$$\sum_k \frac{e^{-\epsilon_k}}{\mathcal{Z}} |\partial_x \epsilon_k - \partial_x \underline{\epsilon}_k|^2 \leq C_1 e^{C_2 (\|\underline{V}\|_{L^2(0,1)} + \|v\|_{L^2(0,1)})} (\langle |\nabla_x v|^2 \rangle + \langle |v|^2 \rangle \langle |\nabla_x \underline{V}|^2 \rangle). \quad (3.23)$$

We can write the second term of the right hand side of (3.22) as follows:

$$\begin{aligned} \sum_k \left(\frac{e^{-\epsilon_k}}{\mathcal{Z}} - \frac{e^{-\underline{\epsilon}_k}}{\underline{\mathcal{Z}}} \right) \partial_x \underline{\epsilon}_k &= \int_0^1 \frac{\sum_k \langle |\chi_k^s|^2 v \rangle e^{-\epsilon_k^s}}{\sum_\ell e^{-\epsilon_\ell^s}} \frac{\sum_k \langle |\chi_k|^2 \nabla_x \underline{V} \rangle e^{-\epsilon_k^s}}{\sum_\ell e^{-\epsilon_\ell^s}} ds \\ &\quad - \int_0^1 \sum_k \frac{\langle |\chi_k^s|^2 v \rangle e^{-\epsilon_k^s}}{\sum_\ell e^{-\epsilon_\ell^s}} \langle |\chi_k|^2 \nabla_x \underline{V} \rangle ds, \end{aligned}$$

where we use the notation $\epsilon_k^s = \epsilon_k[\underline{V} + sv]$ and $\chi_k^s = \chi_k[\underline{V} + sv]$. Thus, by applying the L^∞ bound in the z direction for χ_k^s and $\underline{\chi}_k$ stated in Lemma A.2, we obtain

$$\left| \sum_k \left(\frac{e^{-\epsilon_k}}{\mathcal{Z}} - \frac{e^{-\underline{\epsilon}_k}}{\underline{\mathcal{Z}}} \right) \partial_x \underline{\epsilon}_k \right|^2 \leq C_1 e^{C_2 (\|\underline{V}\|_{L^2(0,1)} + \|v\|_{L^2(0,1)})} \langle |v|^2 \rangle \langle |\nabla_x \underline{V}|^2 \rangle. \quad (3.24)$$

By combining (3.23) and (3.24) in (3.22), we obtain (3.12). □

Proof of Lemma 3.4. From (3.12), we deduce

$$\begin{aligned} \int_{\omega} \frac{(n_s)^2}{N_s^\infty} |\nabla_x v_s|^2 dx \\ \leq C_1 \int_{\omega} \frac{(n_s)^2}{N_s^\infty} e^{C_2(\|V^\infty\|_{L^2_\sharp(0,1)} + \|v\|_{L^2_\sharp(0,1)})} (\langle |\nabla_x v|^2 \rangle + \langle |v|^2 \rangle \langle |\nabla_x V^\infty|^2 \rangle) dx. \end{aligned} \quad (3.25)$$

Throughout the proof, C , C_1 and C_2 stand for universal constants. Since V is bounded in $H^1(\Omega)$ uniformly in time, the Trudinger inequality implies

$$\exp(C_2(\|V^\infty\|_{L^2_\sharp(0,1)} + \|v\|_{L^2_\sharp(0,1)})) \in L^p(\omega), \quad \forall p \in [1, \infty). \quad (3.26)$$

Thus a Hölder inequality gives

$$\int_{\omega} \frac{(n_s)^2}{N_s^\infty} e^{C_2(\|V^\infty\|_{L^2_\sharp(0,1)} + \|v\|_{L^2_\sharp(0,1)})} \langle |\nabla_x v|^2 \rangle dx \leq C \left\| \frac{n_s}{\sqrt{N_s^\infty}} \right\|_{L^3(\omega)}^2 \|\langle |\nabla_x v|^2 \rangle\|_{L^8(\omega)}. \quad (3.27)$$

Using the expression given in (1.7) for $n = N - N^\infty$, we deduce

$$n = n_s \sum_k \frac{|\chi_k|^2 e^{-\epsilon_k}}{\mathcal{Z}} + N_s^\infty \sum_k \left[(|\chi_k|^2 - |\chi_k^\infty|^2) \frac{e^{-\epsilon_k}}{\mathcal{Z}} + |\chi_k^\infty|^2 \left(\frac{e^{-\epsilon_k}}{\mathcal{Z}} - \frac{e^{-\epsilon_k^\infty}}{\mathcal{Z}^\infty} \right) \right].$$

As we saw before, denoting $\epsilon_k^s = \epsilon_k[V + sv]$, and $\chi_k^s = \chi_k[V + sv]$ we can rewrite with Lemma A.3 the third term as follow :

$$\begin{aligned} \sum_k |\chi_k^\infty|^2 \left(\frac{e^{-\epsilon_k}}{\mathcal{Z}} - \frac{e^{-\epsilon_k^\infty}}{\mathcal{Z}^\infty} \right) &= \int_0^1 \frac{\sum_k \langle |\chi_k^s|^2 v \rangle e^{-\epsilon_k^s}}{\sum_\ell e^{-\epsilon_\ell^s}} \frac{\sum_k |\chi_k^\infty|^2 e^{-\epsilon_k^s}}{\sum_\ell e^{-\epsilon_\ell^s}} ds - \\ &\int_0^1 \sum_k \frac{\langle |\chi_k^s|^2 v \rangle e^{-\epsilon_k^s}}{\sum_\ell e^{-\epsilon_\ell^s}} |\chi_k^\infty|^2 ds. \end{aligned}$$

Since Lemma A.2 provides a bound of the eigenvectors of the Hamiltonian χ_k uniformly in k , we deduce, thanks to Lemma A.2 and Lemma A.4,

$$|n|(x, z) \leq C_1 e^{C_2(\|V^\infty\|_{L^2_\sharp(0,1)} + \|v\|_{L^2_\sharp(0,1)})} (|n_s|(x) + N_s^\infty \|v\|_{L^1_\sharp(0,1)}(x)).$$

Therefore, using interpolation inequalities, (3.26) and $N_s^\infty \in L^\infty(\omega)$, ones deduces from elliptic regularity for the Poisson equation (1.3) that :

$$\|v\|_{H^2(\Omega)} \leq C \|n\|_{L^2(\Omega)} \leq C (\|n_s\|_{L^{18/7}(\omega)} + \|v\|_{H^1(\Omega)}). \quad (3.28)$$

With a Gagliardo-Nirenberg inequality and (3.28), we have

$$\begin{aligned} \|\langle |\nabla_x v|^2 \rangle\|_{L^8(\omega)} &\leq C \|\langle |\nabla_x v|^2 \rangle\|_{L^2(\omega)}^{1/4} \|\langle |\nabla_x v|^2 \rangle\|_{H^1(\omega)}^{3/4} \\ &\leq C \|v\|_{H^1(\Omega)}^{1/4} (\|n_s\|_{L^{18/7}(\omega)}^{3/4} + \|v\|_{H^1(\Omega)}^{3/4}). \end{aligned} \quad (3.29)$$

By interpolation inequalities, we get

$$\left\| \frac{n_s}{\sqrt{N_s^\infty}} \right\|_{L^3(\omega)}^2 \leq \left\| \frac{n_s}{\sqrt{N_s^\infty}} \right\|_{L^2(\omega)} \left\| \frac{n_s}{\sqrt{N_s^\infty}} \right\|_{L^6(\omega)} \quad (3.30)$$

and

$$\|n_s\|_{L^{18/7}(\omega)} \leq \|n_s\|_{L^2(\omega)}^{2/3} \|n_s\|_{L^6(\omega)}^{1/3}. \quad (3.31)$$

Thus by (3.27), (3.29), (3.30) and (3.31), we obtain

$$\begin{aligned} & \int_{\omega} \frac{(n_s)^2}{N_s^\infty} e^{C_2(\|V^\infty\|_{L_z^2(0,1)} + \|v\|_{L_z^2(0,1)})} \langle |\nabla_x v| \rangle^2 dx \\ & \leq C \left\| \frac{n_s}{\sqrt{N_s^\infty}} \right\|_{L^2(\omega)} \left\| \frac{n_s}{\sqrt{N_s^\infty}} \right\|_{L^6(\omega)} \|v\|_{H^1(\Omega)}^{1/2} (\|n_s\|_{L^2(\omega)} \|n_s\|_{L^6(\omega)}^{1/2} + \|v\|_{H^1(\Omega)}^{3/2}). \end{aligned}$$

Finally, using $N_s^\infty \geq C > 0$ and Lemma 3.2, we have

$$\begin{aligned} & \int_{\omega} \frac{(n_s)^2}{N_s^\infty} e^{C_2(\|V^\infty\|_{L_z^2(0,1)} + \|v\|_{L_z^2(0,1)})} \langle |\nabla_x v| \rangle^2 dx \\ & \leq C_1 L(t) \|n_s\|_{L^6(\omega)}^{3/2} \|v\|_{H^1(\Omega)}^{1/2} + C_2 L(t)^{1/2} \|n_s\|_{L^6(\omega)} \|v\|_{H^1(\Omega)}^2. \end{aligned} \quad (3.32)$$

Now, to handle the term $\|n_s\|_{L^6(\omega)}$, we decompose $\|n_s\|_{L^6(\omega)} \leq C(\|n_s/N_s^\infty + v_s\|_{L^6(\omega)} + \|v_s\|_{L^6(\omega)})$. By (3.18) we have:

$$|v_s| \leq \max \left\{ \sum_k \frac{e^{-\epsilon_k}}{\sum_\ell e^{-\epsilon_\ell}} |\epsilon_k - \epsilon_k^\infty|, \sum_k \frac{e^{-\epsilon_k^\infty}}{\sum_\ell e^{-\epsilon_\ell^\infty}} |\epsilon_k^\infty - \epsilon_k| \right\}.$$

Hence, with Lemma A.4 and (3.26), we deduce

$$\|v_s\|_{L^6(\omega)} \leq C \|v\|_{L_x^8 L_z^1(\Omega)} \leq C \|v\|_{H^1(\Omega)},$$

thanks to the Sobolev embedding of $H^1(\Omega)$ into $L_x^8 L_z^1(\Omega)$, which proves the inequality (3.13) in Lemma 3.4. Moreover Proposition 3.1 provides a uniform bound on $\|v\|_{H^1(\Omega)}$ which, with the inequality (3.32) and Lemma 3.2, leads to

$$\begin{aligned} & \int_{\omega} \frac{(n_s)^2}{N_s^\infty} e^{C_2(\|V^\infty\|_{L_z^2(0,1)} + \|v\|_{L_z^2(0,1)})} \langle |\nabla_x v| \rangle^2 dx \\ & \leq C_1 L(t) \left\| \frac{n_s}{N_s^\infty} + v_s \right\|_{L^6(\omega)}^{3/2} + C_2 L(t)^{1/2} \left\| \frac{n_s}{N_s^\infty} + v_s \right\|_{L^6(\omega)} \|v\|_{H^1(\Omega)} + C_3 L(t) \|v\|_{H^1(\Omega)}. \end{aligned} \quad (3.33)$$

Finally, using $x^{1/4} y^{3/4} \leq \frac{1}{4\varepsilon^3} x + \frac{3}{4} \varepsilon y$, we have

$$\begin{aligned} L(t) \left\| \frac{n_s}{N_s^\infty} + v_s \right\|_{L^6(\omega)}^{3/2} & \leq \frac{1}{4\varepsilon^3} L(t)^4 + \frac{3}{4} \varepsilon \left\| \frac{n_s}{N_s^\infty} + v_s \right\|_{L^6(\omega)}^2 \\ & \leq \frac{1}{4\varepsilon^3} L(t)^4 + C\varepsilon \left\| \nabla_x \left(\frac{n_s}{N_s^\infty} + v_s \right) \right\|_{L^2(\omega)}^2, \end{aligned}$$

where the Sobolev embedding $H^1 \hookrightarrow L^6(\omega)$ and the Poincaré inequality are used. Proceeding analogously for the second term in (3.33), we obtain the desired inequality for ε fixed small enough.

In order to estimate the second term in (3.25), we first use the Sobolev embedding $H^1(\Omega) \hookrightarrow L_x^8 L_z^1(\Omega)$ and (3.26), we have

$$\int_{\omega} \frac{(n_s)^2}{N_s^\infty} e^{C_2(\|V^\infty\|_{L_z^2(0,1)} + \|v\|_{L_z^2(0,1)})} \langle |v| \rangle^2 \langle |\nabla_x V^\infty| \rangle^2 dx \leq C \|v\|_{H^1(\Omega)}^2 \left\| \frac{n_s}{\sqrt{N_s^\infty}} \right\|_{L^3(\omega)}^2.$$

With (3.30) and Lemma 3.2, it yields

$$\begin{aligned} & \int_{\omega} \frac{(n_s)^2}{N_s^\infty} e^{C_2(\|V^\infty\|_{L_z^2(0,1)} + \|v\|_{L_z^2(0,1)})} \langle |v| \rangle^2 \langle |\nabla_x V^\infty| \rangle^2 dx \\ & \leq CL(t)^{1/2} \|v\|_{H^1(\Omega)}^2 \left(\left\| \frac{n_s}{N_s^\infty} + v_s \right\|_{L^6(\omega)} + \|v_s\|_{L^6(\omega)} \right). \end{aligned} \quad (3.34)$$

By proceeding as above, we obtain the desired inequality for the second term, which concludes the proof. \square

Appendix

Spectral properties of the Hamiltonian

In this appendix, we first list some basic properties of eigenfunctions and eigenvalues of the Schrödinger operator in the z variable. Most of these properties, which are used along the paper are either proved or can be proved by straightforwardly adapting the techniques of the book of Pöschel and Trubowitz [33]. Therefore, very few proofs are provided in this appendix.

For a given real valued function U in $L^2(0, 1)$, let $H[U]$ be the Schrödinger operator

$$H[U] := -\frac{1}{2} \frac{d^2}{dz^2} + U(z)$$

defined on the domain $D(H[U]) = H^2(0, 1) \cap H_0^1(0, 1)$.

This operator admits a strictly increasing sequence of real eigenvalues $(\epsilon_k[U])_{k \geq 1}$ going to $+\infty$. The corresponding eigenvectors, denoted by $(\chi_k[U](z))_{k \geq 1}$ (chosen such that $\chi_k'(0) > 0$), form an orthonormal basis of $L^2(0, 1)$. They satisfy of course

$$\begin{cases} -\frac{1}{2} \frac{d^2}{dz^2} \chi_k + U \chi_k = \epsilon_k \chi_k, \\ \chi_k \in H_0^1(0, 1), \quad \int_0^1 \chi_k \chi_\ell dz = \delta_{kl}. \end{cases} \quad (\text{A.1})$$

Obviously, for $U = 0$, we have $\epsilon_k[0] = \frac{1}{2} \pi^2 k^2$ and $\chi_k[0](z) = \sqrt{2} \sin(\pi k z)$.

Lemma A.1 *Let U and V be two real-valued functions in $L^2(0, 1)$ such that $U - V \in L^\infty(0, 1)$. Then the corresponding eigenvalues verify*

$$|\epsilon_k[U] - \epsilon_k[V]| \leq \|U - V\|_{L^\infty(0,1)}. \quad (\text{A.2})$$

In particular, the case $V = 0$ gives $|\epsilon_k[U] - \frac{1}{2} \pi^2 k^2| \leq \|U\|_{L^\infty(0,1)}$.

Moreover, following the study of the spectral properties of $H[U]$ in Chapter 2 of [33], we have the following lemma :

Lemma A.2 *There exists a positive constant C_U depending only on $\|U\|_{L^2(0,1)}$ such that*

$$|\epsilon_k[U] - \frac{1}{2} \pi^2 k^2| \leq C_U \quad ; \quad \|\chi_k[U] - \sqrt{2} \sin(\pi k z)\|_{L^\infty(0,1)} \leq C_U.$$

Moreover the constant C_U can be chosen such that $C_U \leq C_1 \exp(C_2 \|U\|_{L^2(0,1)})$, where the constants C_1 and C_2 are independent of U and k .

Lemma A.3 Let $V = V(\lambda, z) \in L_{loc}^\infty(\lambda, L_z^2(0, 1))$ where λ is a real parameter (typically $\lambda = t$ or $\lambda = x_i$). Let us shortly denote ϵ_k instead of $\epsilon_k[V(\lambda, \cdot)]$ and χ_k instead of $\chi_k[V(\lambda, \cdot)]$. Assume that $\partial_\lambda V \in L_{loc}^1(\lambda, L_z^2(0, 1))$. Then

(i) $\partial_\lambda \epsilon_k \in L_{loc}^1$ and

$$\partial_\lambda \epsilon_k = \langle |\chi_k|^2 \partial_\lambda V \rangle.$$

(ii) $\partial_\lambda \chi_k \in L_{loc}^1(\lambda, L_z^\infty(0, 1))$ and we have

$$\partial_\lambda \chi_k = \sum_{\ell \neq k} \frac{\langle \chi_k \chi_\ell \partial_\lambda V \rangle}{\epsilon_k - \epsilon_\ell} \chi_\ell.$$

Lemma A.4 Let V and \tilde{V} be two real-valued functions in $L^2(0, 1)$. Then there exist two positive constants C_1 and C_2 independent of p , V and \tilde{V} such that

$$|\epsilon_k[V] - \epsilon_k[\tilde{V}]| \leq C_1 \exp(C_2(\|V\|_{L^2(0,1)} + \|\tilde{V}\|_{L^2(0,1)})) \|V - \tilde{V}\|_{L^1(0,1)}. \quad (\text{A.3})$$

And,

$$\|\chi_k[V] - \chi_k[\tilde{V}]\|_{L^\infty(0,1)} \leq C_1 \exp(C_2(\|V\|_{L^2(0,1)} + \|\tilde{V}\|_{L^2(0,1)})) \|V - \tilde{V}\|_{L^1(0,1)}. \quad (\text{A.4})$$

Proof. The estimate (A.3) is an easy consequence of Lemmata A.2 and A.3.

Let us prove (A.4). Without loss of generality, we assume that $\epsilon_k[V] > 0$ (by shifting V and \tilde{V} by the same constant). Let us denote

$$u_k = \frac{\chi_k[\tilde{V}]'(0)}{\chi_k[V]'(0)} \chi_k[V] \quad ; \quad \tilde{u}_k = \chi_k[\tilde{V}], \quad (\text{A.5})$$

so that $u_k'(0) = \tilde{u}_k'(0)$. Writing the equation satisfied by $u_k - \tilde{u}_k$ and proceeding like in the proof of Lemma 1, Chapter 1 of [33], we have

$$\begin{aligned} u_k(z) - \tilde{u}_k(z) &= 2 \int_0^z s(z-t) V(t) (u_k - \tilde{u}_k)(t) dt \\ &\quad + 2 \int_0^z s(z-t) \tilde{u}_k(t) ((V - \tilde{V})(t) - (\epsilon_k[V] - \epsilon_k[\tilde{V}])) dt, \end{aligned}$$

where,

$$s(t) = \frac{\sin(\sqrt{2\epsilon_k[V]} t)}{\sqrt{2\epsilon_k[V]}}.$$

By a Gronwall argument, we prove (A.4) for the difference $u_k - \tilde{u}_k$. We finally deduce the result for $\chi_k[V] - \chi_k[\tilde{V}]$ by using the property $\int_0^1 |\chi_k|^2 dz = 1$. \square

Now, we give two technical lemmata, where the potential is defined on Ω . We recall that $(x, z) \in \Omega = \omega \times (0, 1)$ where ω is a bounded regular domain of \mathbb{R}^2 .

Lemma A.5 Assume that $V \in H^1(\Omega)$ and let ϵ_k be the eigenvalues defined by (1.2). Then, for all $\alpha \geq 0$ and $q \in [1, +\infty)$, we have

$$I_\alpha := \frac{1}{\mathcal{Z}} \sum_k |\epsilon_k|^\alpha e^{-\epsilon_k} \in L^q(\omega),$$

where $\mathcal{Z} = \sum_k e^{-\epsilon_k}$. The L^q norm of I_α is bounded by a constant only depending on α, q and $\|V\|_{H^1}$.

Proof. Lemma A.2 states that the eigenvalues and eigenvectors of (1.2) satisfy the (uniform in p) estimate

$$\left| \epsilon_k(x) - \frac{\pi^2}{2} k^2 \right| + \|\chi_k(x, \cdot)\|_{L^\infty} \leq C_1 e^{C_2 \|V(x, \cdot)\|_{L^2_\mathbb{Z}}}. \quad (\text{A.6})$$

It is enough to show that

$$I_\alpha(x) \leq C_3 e^{\alpha C_2 \|V(x, \cdot)\|_{L^2_\mathbb{Z}}}. \quad (\text{A.7})$$

Indeed, since $\|V(x, \cdot)\|_{L^2_\mathbb{Z}}$ is bounded in $H^1(\omega)$, the Trudinger inequality,

$$\int_{\mathcal{O}} \exp(|u|^{N/(N-1)}) < +\infty, \quad \forall u \in W^{1,N}(\mathcal{O}), \quad \mathcal{O} \subset \mathbb{R}^N \quad (\text{A.8})$$

implies that $e^{\|V(x, \cdot)\|_{L^2_\mathbb{Z}}^2} \in L^1(\omega)$, which ensures that $e^{\alpha C_2 \|V(x, \cdot)\|_{L^2_\mathbb{Z}}} \in L^q(\omega)$ for all $q < +\infty$ thus leading to the result.

Let us now prove (A.7). To this aim, we treat differently low and high energies. More precisely, we have

$$\begin{aligned} I_\alpha &= \frac{1}{\mathcal{Z}} \sum_{|\epsilon_k| \leq KA} |\epsilon_k|^\alpha e^{-\epsilon_k} + \frac{1}{\mathcal{Z}} \sum_{|\epsilon_k| \geq KA} |\epsilon_k|^\alpha e^{-\epsilon_k} \\ &\leq (KA)^\alpha + \frac{1}{\mathcal{Z}} \sum_{|\epsilon_k| \geq KA} |\epsilon_k|^\alpha e^{-\epsilon_k} \end{aligned} \quad (\text{A.9})$$

where K is chosen larger than 2 ($K > 2$) and A is such that $|\epsilon_k - \frac{1}{2}\pi^2 k^2| < A$. This choice implies that

$$\frac{1}{2}k^2\pi^2 - A < \epsilon_k < \frac{1}{2}k^2\pi^2 + A$$

and, for high energies ($|\epsilon_k| \geq KA$), that we have

$$A < \frac{1}{2(K-1)} k^2 \pi^2.$$

Hence, the high energy contribution can be estimated as follows:

$$\begin{aligned}
\sum_{|\epsilon_k| \geq KA} |\epsilon_k|^\alpha e^{-\epsilon_k} &\leq \sum_{k > \sqrt{2(K-1)A}/\pi} \left(\frac{1}{2} k^2 \pi^2 + A \right)^\alpha e^{-k^2 \pi^2 / 2} e^A \\
&\leq \left(1 + \frac{1}{K-1} \right)^\alpha e^A \sum_{k > \sqrt{2(K-1)A}/\pi} \left(\frac{1}{2} k^2 \pi^2 \right)^\alpha e^{-k^2 \pi^2 / 2} \\
&\leq C_\alpha \left(1 + \frac{1}{K-1} \right)^\alpha e^A \int_{\sqrt{2(K-1)A}/\pi}^{\infty} \left(\frac{1}{2} \pi^2 x^2 \right)^\alpha e^{-\pi^2 x^2 / 2} dx,
\end{aligned}$$

where we used the elementary property:

$$\lim_{n \rightarrow +\infty} \frac{\sum_{k \geq n} f(k)}{\int_n^{+\infty} f(x) dx} = 1,$$

for any nonnegative function decaying at infinity and such that the following integral $\int_0^{+\infty} f(x) dx$ converges. Assuming that $\alpha \neq 0$ (the case $\alpha = 0$ is trivial), an integration by parts leads to the estimate

$$\int_{\sqrt{2(K-1)A}/\pi}^{\infty} \left(\frac{1}{2} \pi^2 x^2 \right)^\alpha e^{-\pi^2 x^2 / 2} e^A dx \leq C((K-1)A)^{\alpha-1/2} e^{-(K-1)A} e^A,$$

which leads to

$$\sum_{|\epsilon_k| \geq KA} |\epsilon_k|^\alpha e^{-\epsilon_k} \leq C_\alpha A^{\alpha-1/2} e^{-(K-1)A} e^A.$$

Besides, thanks to the choice of A , we obviously have

$$\sum_k e^{-\epsilon_k} \geq C e^{-A}.$$

Therefore, going back to (A.9), we have

$$I_\alpha \leq (KA)^\alpha + C_\alpha A^{\alpha-1/2} e^{(3-K)A}.$$

Setting $K = 4$, we have a bound on $A^{-1/2} e^{(3-K)A}$ for large A . Thus we proved that $I \leq C_\alpha A^\alpha$ and (A.7) follows thanks to (A.6) by taking $A = C_1 \exp(C_2 \|V(x, \cdot)\|_{L^2_\omega})$. \square

Lemma A.6 *The map $V \mapsto V_s = -\log(\sum_k e^{-\epsilon_k[V]})$ is locally Lipschitz continuous from $H^2(\Omega)$ to $H^2(\omega)$, where $(\epsilon_k[V])_k$ denotes the whole set of eigenvalues of the Hamiltonian $-\frac{1}{2} \frac{d^2}{dz^2} + V$.*

Proof. Since the summation over k can be done easily, it is enough to show the result for the map $V \mapsto \epsilon_k[V]$. Let U, V be two bounded potentials of $H^2(\Omega)$. From Lemma A.1, we deduce easily that $\|\epsilon_k[U] - \epsilon_k[V]\|_{L^2(\omega)} \leq C\|U - V\|_{H^2(\Omega)}$. For the first derivative, we write with Lemma A.3:

$$\begin{aligned} \int_{\omega} |\nabla_x \epsilon_k[U] - \nabla_x \epsilon_k[V]|^2 dx &\leq 2 \int_{\Omega} |\nabla_x(U - V)|^2 |\chi_k[U]|^4 dx dz \\ &\quad + 2 \int_{\Omega} |\nabla_x V|^2 (|\chi_k[U]|^2 - |\chi_k[V]|^2)^2 dx dz. \end{aligned}$$

The Sobolev embedding of $H^2(\Omega)$ into $L^\infty(\Omega)$ implies that for all nonnegative constant C_2 ,

$$\exp(C_2(\|U\|_{L^2_\sharp(0,1)} + \|V\|_{L^2_\sharp(0,1)})) \in L^\infty(\omega).$$

Thus, with Lemma A.2 we have a bound of $\chi_k[U]$ in $L^\infty(\Omega)$ and with Lemma A.4,

$$\|\chi_k[U] - \chi_k[V]\|_{L^\infty(\Omega)} \leq C\|U - V\|_{H^2(\Omega)}. \quad (\text{A.10})$$

We deduce,

$$\int_{\omega} |\nabla_x \epsilon_k[U] - \nabla_x \epsilon_k[V]|^2 dx \leq C\|U - V\|_{H^1(\Omega)}^2 + C\|U - V\|_{H^2(\Omega)}^2.$$

Now it remains to estimate the difference of the second derivative of $\epsilon_k[U] - \epsilon_k[V]$. We recall that from Lemma A.1, we deduce easily

$$\|\epsilon_k[U] - \epsilon_k[V]\|_{L^\infty(\omega)} \leq C\|U - V\|_{H^2(\Omega)}. \quad (\text{A.11})$$

If $i = 1$ or 2 , $j = 1$ or 2 , by the expression of the derivatives stated in Lemma A.3, we have

$$\partial_{x_i x_j} \epsilon_k[V] = \int_0^1 \partial_{x_i x_j} V |\chi_k[V]|^2 dz + 2 \int_0^1 \chi_k[V] \partial_{x_i} \chi_k[V] \partial_{x_j} V dz.$$

As before, we can show the Lipschitz dependency in $V \in H^2(\Omega)$ of the first term of the right hand side. For the second one, we need the following result, which is proved below : there exists a positive constant δ_V depending only on $\|V\|_{H^2(\Omega)}$ such that

$$\forall (k, l) \in (\mathbb{N}^*)^2 \quad |\epsilon_k[V] - \epsilon_l[V]| \geq \delta_V |k - l|^2. \quad (\text{A.12})$$

Since $\chi_k[V]$ is bounded in $L^\infty(\Omega)$, using the expression of $\partial_{x_i} \chi_k[V]$ in Lemma A.3 and (A.12), we have $|\partial_{x_i} \chi_k[V]| \leq C \langle |\partial_{x_i} V| \rangle$. Therefore,

$$\begin{aligned} |\chi_k[U] \partial_{x_i} \chi_k[U] \partial_{x_j} U - \chi_k[V] \partial_{x_i} \chi_k[V] \partial_{x_j} V| &\leq C |\chi_k[U] - \chi_k[V]| \langle |\partial_{x_i} U| \rangle |\partial_{x_i} U| + \\ &\quad + C |\partial_{x_i} U| |\partial_{x_i} \chi_k[U] - \partial_{x_i} \chi_k[V]| + C \langle |\partial_{x_i} V| \rangle |\partial_{x_i}(U - V)|. \end{aligned}$$

Thus, it remains to see the Lipschitz dependency in V of $\partial_{x_i}\chi_k[V]$. We have

$$\begin{aligned}
\partial_{x_i}(\chi_k[U] - \chi_k[V]) &= \sum_{\ell \neq k} \left(\frac{\langle \chi_k[U] \chi_\ell[U] \partial_{x_i} U \rangle}{\epsilon_k[U] - \epsilon_\ell[U]} \chi_\ell[U] - \frac{\langle \chi_k[V] \chi_\ell[V] \partial_{x_i} V \rangle}{\epsilon_k[V] - \epsilon_\ell[V]} \chi_\ell[V] \right) \\
&= \sum_{\ell \neq k} \frac{\langle \chi_k[U] \chi_\ell[U] \partial_{x_i} U - \chi_k[V] \chi_\ell[V] \partial_{x_i} V \rangle}{\epsilon_k[U] - \epsilon_\ell[U]} \chi_\ell[U] \\
&\quad + \sum_{\ell \neq k} \frac{\langle \chi_k[V] \chi_\ell[V] \partial_{x_i} V \rangle}{\epsilon_k[V] - \epsilon_\ell[V]} (\chi_\ell[U] - \chi_\ell[V]) \\
&\quad + \sum_{\ell \neq k} \langle \chi_k[V] \chi_\ell[V] \partial_{x_i} V \rangle \chi_\ell[V] \frac{\epsilon_k[V] - \epsilon_k[U] + \epsilon_\ell[U] - \epsilon_\ell[V]}{(\epsilon_k[U] - \epsilon_\ell[U])(\epsilon_k[V] - \epsilon_\ell[V])}.
\end{aligned}$$

From (A.10), (A.11) and (A.12), we deduce that :

$$\|\partial_{x_i}\chi_k[U] - \partial_{x_i}\chi_k[V]\|_{L^2(\Omega)} \leq C(1 + \|\partial_{x_i}U\|_{L^2(\Omega)} + \|\partial_{x_i}V\|_{L^2(\Omega)})\|U - V\|_{H^2(\Omega)}.$$

With the Sobolev embedding of $H^1(\Omega)$ into $L^2(\Omega)$, $\|\partial_{x_i}V\|_{L^2(\Omega)} \leq C\|V\|_{H^2(\Omega)}$. This concludes the proof of the Lipschitz dependency with respect to V of the second derivative.

Proof of (A.12). If $k = \ell$, this inequality is obvious. Let us first prove that there exists a constant δ_V depending only on $\|V\|_{H^2(\Omega)}$, such that

$$\min_{k \neq \ell} |\epsilon_k[V] - \epsilon_\ell[V]| \geq \delta_V. \quad (\text{A.13})$$

If not, by the compact embedding of $H^2(\Omega)$ into $L^\infty(\Omega)$ it would be possible to find a sequence (V^n) converging to V in the L^∞ strong topology and a sequence k^n of integers such that $\epsilon_{k^n+1}[V^n] - \epsilon_{k^n}[V^n]$ converges to zero as n tends to $+\infty$. The asymptotic behaviour of the ϵ_k 's deduced from Lemma A.1 implies that the sequence (k^n) is bounded, thus, up to an extraction, it is stationary: $k^n = k$. Besides, (A.2) implies that $\epsilon_k[V^n]$ converges to $\epsilon_k[V]$ and $\epsilon_{k+1}[V^n]$ to $\epsilon_{k+1}[V]$. Hence $\epsilon_k[V] = \epsilon_{k+1}[V]$, which is a contradiction with the fact that the eigenvalues are strictly increasing. Moreover, by (A.2), we have

$$\frac{\pi^2}{2}k^2 - \|V\|_{L^\infty(\Omega)} \leq \epsilon_k[V] \leq \frac{\pi^2}{2}k^2 + \|V\|_{L^\infty(\Omega)}.$$

Therefore, for any (k, l) :

$$|\epsilon_k[V] - \epsilon_\ell[V]| \geq \frac{\pi^2}{2}|k - \ell|^2 + \pi^2|k - \ell| - 2\|V\|_{L^\infty(\Omega)}.$$

Hence, if $\pi^2|k - \ell| \geq 2\|V\|_{L^\infty(\Omega)}$, then $|\epsilon_k[V] - \epsilon_\ell[V]| \geq \frac{\pi^2}{2}|k - \ell|^2$. From this inequality and (A.13) we deduce easily (A.12) (up to a change of δ_V). \square

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