UNIFORM BOUNDS AND WEAK SOLUTIONS TO AN OPEN SCHRÖDINGER-POISSON SYSTEM

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Abstract. This paper is concerned with the derivation of uniform bounds with respect to the scaled Planck constant $\varepsilon$ for solutions to the open transient Schrödinger-Poisson system introduced by Ben Abdallah and al in [On a open transient Schrödinger-Poisson system, Math. Meth. Mod. in App. Sci. 15, (2005), 667–688]. The uniform estimates stem from a careful analysis of the non-local in time transparent boundary conditions which allow to restrict the original problem posed on an unbounded domain to a bounded domain of interest. These bounds can be used to perform the semi-classical limit of the system. The paper also gives an existence and uniqueness result of weak solutions while they were previously defined in a strong sense.

Key words. semiconductors, non-linear Schrödinger equation, open boundary conditions, uniform estimates.

subject classifications. 35Q40, 35Q55.

1. Introduction

The modeling of semiconductors at the quantum level has become a very active area of research during the past decades. Indeed, the design of high-performance components requires the development of simulation tools that help the engineers in finding the best configurations. This in turn demands a compromise between the accuracy of the models and the computational cost, and thus to derive models as close to physics as possible with a relatively cheap cost of resolution. The particular geometry and physics of semiconductors allow for a wide variety of models, see for instance [8]. A semiconductor can roughly be decomposed into two zones: an access zone, through which the particles reach the active zone, where basically all the main physical effects take place. Whereas the access zone is generally not the most relevant part of the component, it has usually the largest dimensions (say some hundred of nanometers long) and thus a lot of computational time might be spent in there. On the other hand, the active zone, which could be roughly a few tens of nanometers long, represents the essential part of the semiconductor and then needs to be carefully treated. Indeed, the operation of the device is basically induced by the potential profile in the active region which presents some sharp variations - on the order of the De Broglie wavelength of the electrons - so that the dynamics requires a quantum description, more expensive than a kinetic one. It has then led to different strategies to lower the computational time spent in the access zones. One possible strategy is to prescribe adequate transparent boundary conditions at the interfaces access zone - active zone, so as to limit the resolution to the active zone ; another strategy is to model the two zones differently - which a relatively cheap treatment of the access zone - and to couple them at the interfaces. The first strategy has already received a great interest since it is related to many wave propagation problems in unbounded domains for which the aim is to restrict the resolution to a bounded zone of interest. Indeed, the Schrödinger equation governing the dynamics of the electrons can also be seen as a paraxial approximation of the Helmholtz equation, see [30] for one of the first derivation, so that some existing results apply. There is a very abundant literature about the subject, one could cite the pioneering work of [16], [3] for more recent advances, [4] in the context of semiconductors and [5]
uniform bounds and weak solutions to an open Schrödinger-Poisson system

for numerical considerations, and for instance [2, 30] for applications to underwater acoustics. Note that the concept of open systems at the quantum level cannot be straightforwardly defined as it is at the kinetic level where it suffices to prescribe the distribution function for incoming velocities. This requires the introduction of conjugate operators which dissociate ingoing from outgoing particles as it was done elegantly in a very general framework in [24]. The second strategy is also an active area of research. Typically, the active region is treated as fully quantum, with possibly some subband decomposition, see [27], while the access zone only requires a kinetic description. The two descriptions are then connected via adequate interfaces conditions, as it was done in [14, 9].

The description chosen in this paper is fully quantum, namely both in the access and active zones, and then falls into the first type of models. The dynamics of the electrons is then given by the Schrödinger equation everywhere in the semiconductor and it is assumed that their energy distribution is known. The electrons being charged particles, they self-interact. The non-linear effects are taken into account at Hartree level through a potential solution to the Poisson equation, given rise to the so-called Schrödinger-Poisson system. That system can be seen as a mean-field approximation of a system of many-interacting particles through a Coulomb potential [7]. There is as well an extensive literature about the subject, see for instance [19] for a general mathematical analysis, and [23, 24] in the context of open quantum system. In [12] a quantum transport model is introduced, and explicit boundary conditions at the interfaces access zone - active region are derived, and will be recalled further in the paper. The wavefunctions are solution to the Schrödinger equation

$$i\hbar \frac{\partial \psi_\lambda}{\partial t} = \mathcal{H}(t)\psi_\lambda,$$

where $\hbar$ is the Planck constant, $\lambda$ is a given quantum number and the Hamiltonian is defined by

$$\mathcal{H}(t) = -\frac{\hbar^2}{2m_e} \Delta + V_e(t,x) + V_s(t,x). \quad (1.1)$$

$m_e$ is the effective mass of the electron in the semiconductor (supposed to be constant to simplify), $V_e$ is an exterior potential, while $V_s$ is the self-consistent potential solution to the Poisson equation

$$-\Delta V_s = \int |\psi_\lambda|^2 d\mu,$$

for some measure $\mu$. In [12], the model is shown to have a unique strong solution $(\psi_\lambda, V_s)$ (in the sense that the Schrödinger equation is verified almost everywhere in time and space) provided the data are regular enough. A possible way to confirm that the introduced transparent boundary conditions correctly describe the physics of the device, is to perform the semi-classical limit of the above system, by letting the scaled Planck constant $\varepsilon$ ($\varepsilon := \hbar := \frac{\hbar}{\sqrt{m_e}}$ in the sequel) go to zero. This limit is performed by means of Wigner transforms [32] which relates the quantum dynamics to the classical one. It is thus expected that at the limit, the boundary conditions simply reduce to standard inflow boundary conditions, as it was done in [11] for a one-dimensional stationary model. The Wigner transform is defined by, for any $\varphi \in L^2(\mathbb{R}^d)$,

$$W^\varepsilon(x,k) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} e^{ix \cdot k} \varphi(x - \frac{\varepsilon}{2} y) \varphi^*(x + \frac{\varepsilon}{2} y) dy,$$
where \( \varphi^* \) denotes the complex conjugate of \( \varphi \) and \( d \) the dimension. If \( \varphi \) is solution to the time-dependent Schrödinger equation with potential \( V(t,x) \), then its Wigner transform \( W^\varepsilon \) is solution to the Wigner equation, namely

\[
\frac{\partial W^\varepsilon}{\partial t} + k \cdot \nabla_x W^\varepsilon + K * k W^\varepsilon = 0,
\]

\[
K(t,x,k) = \frac{i}{(2\pi)^d} \int_{\mathbb{R}^d} e^{-ik \cdot y} \varepsilon^{-1} \left( V(t,x+\varepsilon y) - V(t,x-\varepsilon y) \right) dy.
\]

Wigner transforms have found applications in many high-frequency asymptotic problems, see for instance [28] for a formal analysis of hyperbolic equations with random coefficients, [6, 17] for semi-classical limit of random Schrödinger equations, [21, 22] for Schrödinger-Poisson systems and [13] for the Helmholtz equation. Passing formally to the limit in the above equation leads to the Vlasov equation,

\[
\frac{\partial W}{\partial t} + k \cdot \nabla_x W - \nabla_x V \cdot \nabla_k W = 0,
\]

where \( W \) is the limit of \( W^\varepsilon \) in some sense. The Vlasov equation then has to be supplemented at the interfaces with inflow boundary conditions of the type \( W(t,x,k) = f(k) \) for entering wave vectors \( k \), which will be the classical analogue of the quantum transparent boundary conditions. Passing rigorously at the limit requires some uniform in \( \varepsilon \) bounds for the wavefunctions, which in turn provide estimates on the Wigner transform in some appropriate spaces, see [18, 21]. The purpose of the present paper is then to address the question of uniform bounds for the open Schrödinger-Poisson system introduced in [12]. While in standard Schrödinger equations with \( L^2 \) initial conditions those estimates are straightforward, it is not the case when considering open systems with transparent boundary conditions. The reference [12] gives some regularity results and estimates, without precising the dependence on \( \varepsilon \). This work thus provides uniform bounds in \( L^2_{\text{loc}} \) which stem from a careful analysis of the non-local in time boundary conditions imposed on the interfaces active zone - access zone. The semi-classical limit and the obtention of the inflow boundary conditions from the quantum transparent boundary conditions will be performed independently in a further work [26]. In addition to these estimates, we construct as well weak solutions to the open Schrödinger-Poisson model of [12] where the solutions were only defined in a strong sense. Those solutions verify the Schrödinger equation in a variational form which could be suitable for numerical simulations since it naturally incorporates the transparent boundary conditions in the formulation.

The paper is organized as follows: in section 2, we recall the transport model of [12] ; in section 3, we present the weak formulation and the main result, namely the uniform bounds ; in section 4, the proof of the theorem is given and finally one can find in Appendix A and B some technical results.

2. Setting of the problem. We recall in this section the transport model introduced in [12] in a time-dependent picture and in [10] in a stationary one. It consists of a Schrödinger-Poisson system posed on an unbounded domain, with non-vanishing conditions at the infinity modeling the electron injection in the structure. This system is then reduced to a problem posed on a bounded domain with suitable inhomogeneous transparent boundary conditions taking into account the injected particles.
2.1. Geometry. The unbounded domain is denoted by $\Omega$ and its dimension by $d$. It is assumed in the sequel that $d=2$ or $d=3$. The domain $\Omega$ is then split into two zones, a bounded active zone denoted by $\Omega_0$ and an unbounded access zone, consisting of $n$ wave guides $\Omega_j$, $j=1,\ldots,n$, see figure 2.1. The interfaces between $\Omega_0$ and each $\Omega_j$ are supposed to be flat and are denoted by $\Gamma_j$. The waveguides $\Omega_j$ have a cylinder-like structure and can thus be written as the cartesian product $\Gamma_j \times \mathbb{R}^+$. They are equipped with a local set of coordinates $(\xi_j,\eta_j) \in \Gamma_j \times \mathbb{R}^+$. Here, $\eta_j$ is basically the variable associated with the direction of propagation in the lead $j$. The outer boundaries of the $\Gamma_j$’s are denoted by $\Gamma_{j,0}$. The remaining part of the boundary of $\Omega_0$ is denoted by $\Gamma_0$ so that $\partial \Omega_0 = \Gamma_0 \bigcup \bigcup_{j=1}^n (\Gamma_{j,0} \Gamma_j)$. We also introduce $(\mu_j)_{j=1,\ldots,n}$, a partition of unity of $\Omega$, i.e. some $\mathcal{C}^\infty(\Omega)$ functions which satisfy

$$
\begin{cases}
0 \leq \mu_j \leq 1, & \sum_{j=1}^n \mu_j = 1 \quad \text{on } \Omega, \\
\mu_j = 1 \quad \text{on } \Omega_j, & j = 1,\ldots,n, \\
\mu_j = 0 \quad \text{on } \Omega_k \quad \text{for } k \neq 0, k \neq j.
\end{cases}
$$

2.2. Initial conditions. To model the electron injection, the initial conditions are supposed to be non-zero in the leads and to be scattering states of a given Hamiltonian $\mathcal{H}^0$ defined by

$$
\mathcal{H}^0 = -\frac{\varepsilon^2}{2} \Delta + V^0,
$$

where $V^0$ is an exterior potential which is assumed to depend only on the transversal coordinate in the leads $\Omega_j$, i.e.

$$
V^0 \in L^\infty(\Omega) ; \quad V^0|_{\Omega_j} = V^0(\xi_j).
$$
The fact that $V^0$ does not depend on $\eta_j$ is necessary to be able to construct rather simple - though not obvious - boundary conditions on the interfaces $\Gamma_j$, $j \neq 0$. When $V^0$ is linear in $\eta_j$, the analysis is more involved and the resulting boundary conditions are more complex, see for instance [15]. Moreover, $V^0$ does not belong to any $L^p(\Omega)$, $p < \infty$ since it supposedly does not vanish when $\eta_j \to \infty$. We then define the transversal Hamiltonian $H^0_j = -\frac{\epsilon^2}{2} \Delta \xi_j + V^0(\xi_j)$, equipped with Dirichlet boundary conditions on $\Gamma_{j,0}$. It admits a compact resolvent and this leads to the following definition:

**Definition 2.1.** The transversal eigenmodes and the eigenvalues of the guide $j$ are defined by

$$
\begin{cases}
H^0_j \lambda_m^{0,j} = E^0_m \lambda_m^{0,j}, & m \in \mathbb{N}^*, \quad j = 1, \ldots, n, \\
\lambda_m^{0,j} \in H^0_0(\Gamma_j), \quad \int_{\Gamma_j} \lambda_m^{0,j} \chi_m^j \, d\sigma_j = \delta_{m,m'},
\end{cases}
$$

where $\sigma_j$ is the surface measure on $\Gamma_j$. Notice that we do not write explicitly the dependence of $\lambda_m^{0,j}$ and $E^0_m$ on $\varepsilon$ for notational simplicity. For any fixed $j$ and $\varepsilon$, the sequence $(E^0_m)_m$ tends to $+\infty$ as $m$ tends to $+\infty$. For two functions $f$ and $g$ in $L^2(\Gamma_j)$, we define

$$
\langle f, g \rangle := \int_{\Gamma_j} f(\xi_j) \overline{g}(\xi_j) \, d\sigma_j, \quad f^j_m := \int_{\Gamma_j} f(\xi_j) \overline{\lambda}_m^j(\xi_j) \, d\sigma_j.
$$

**Remark 2.1.** Let $\varphi$ be an $L^2(\Gamma_j)$ function. The relation $\varphi \mapsto \left( \sum_{m \geq 1} (E^0_m)^{\alpha} |\varphi^j_m|^2 \right)^{1/2}$ defines a norm equivalent to the $H^\alpha(\Gamma_j)$ norm.

We suppose without loss of generality that $E^0_m \geq 0$, $\forall m \geq 1$, $\forall j \geq 1$, it suffices in the sequel to multiply the time-dependent Schrödinger equation by the phase factor $e^{i \frac{\varepsilon}{\hbar} \min_{j,m} E^0_m}$ to recover the general case where $V^0$ is negative and bounded from below.

The electrons are injected in the leads in given quantum states. These states follow a prescribed statistics denoted by $\mu$. $\mu$ is a non-negative measure on the state space $\Lambda$, and a pure state is denoted by $\lambda$. The wave functions are thus indexed by $\lambda$. Consider the following hypotheses for a family of function $\psi^j_\lambda \in H^{1,\text{loc}}(\Omega)$:

**H-1** For a.e. $\lambda \in \Lambda$, there exists a constant $E(\lambda)$ such that

$$
\mathcal{H}^0 \psi^0_\lambda = E(\lambda) \psi^0_\lambda \text{ on } \Omega_j, \quad \psi^0_\lambda = 0 \text{ on } \Gamma_{j,0} \times \mathbb{R}_+, \quad j \neq 0.
$$

**H-2** For any bounded set $K \subset \Omega$, there exists $C_K > 0$ finite such that

$$
\int_{\Lambda} \|\psi^0_\lambda\|^2_{H^1(\mathcal{K})} \, d\mu(\lambda) \leq C_K.
$$

In practice, the electrons are injected in the guide $j_0$, on the transversal mode $m_0$ and with a non-vanishing longitudinal momentum $p$. This implies that $\lambda = \{p,m_0,j_0\}$, $\Lambda = \mathbb{R}^+ \times \mathbb{N}^* \times \{1,\ldots,n\}$, $E(\lambda) = \frac{1}{2} p^2 + E_{m_0}$, and

$$
d\mu(\lambda) = \Phi(p,m_0,j_0) \, dp \delta(m_0) \delta(j_0),
$$
where $\delta$ denotes the Dirac measure and the positive function $\Phi \in L^1(\mathbb{R}_+, \mathcal{L}^1(\mathbb{N}^* \times \{1, \cdots, n\}))$ the statistics of the injected electrons, typically a Fermi-Dirac statistics. This is equivalent to writing, for any $\varphi \in L^1(\Lambda, d\mu)$,
\[
\int_{\Lambda} \varphi(\lambda) d\mu(\lambda) = \sum_{j_0=1}^{n} \sum_{m_0=1}^{\infty} \int_{\mathbb{R}^+} \varphi(p,m_0,j_0) \Phi(p,m_0,j_0) dp.
\]

The energy $\frac{1}{2}p^2$ represents the longitudinal kinetic energy of the electrons while $E_{j_0}^{m_0}$ is the transversal energy in the lead $j_0$. We add the following hypothesis on the measure $\mu$,
\[
\int_{\Lambda} (1+p^2) d\mu < +\infty,
\]
and a local in $\lambda$ version of (H-2):

(H-3) for any bounded set $K \subset \Omega$, there exists $C'_K > 0$ finite and independent of $\lambda$ such that
\[
\Phi(\lambda) ||\psi^0_\lambda||^2_{H^1(K)} \leq C'_K.
\]

A family $\psi^0_\lambda \in H^1_{loc}(\Omega)$ indexed by $\lambda \in \Lambda$ is then said to belong to the class of initial data if hypothesis (H-1)-(H-3) are satisfied.

Transparent boundary conditions for the initial conditions. It is proved in [10], that wave functions satisfying hypothesis (H-1) verify some boundary conditions on $\Gamma_j$, allowing for a simplification to a boundary value problem on the bounded domain $\Omega_0$. Same kind of boundary conditions have been obtained for the one-dimensional case in [11]. The explicit form of these stationary boundary conditions are needed in the sequel to carefully analyze their time-dependent version. We thus briefly describe their form and derivation now, the details can be found in [10].

The restriction of $\psi^0_\lambda$ to $\Omega_j$ is projected on the transversal basis $(\chi^0_m)^j_{m_1}$, i.e. $\psi^0_{\lambda|\Omega_j}(\xi_j, \eta_j) = \sum_m \chi^0_m(\xi_j)f^j(\eta_j)$ so that $f^j$ verifies, according to (H-1),
\[
-\frac{\varepsilon^2}{2} \frac{\partial^2 f^j}{\partial \eta_j^2} = (E(\lambda) - E^j_{m}) f^j, \quad \eta_j \in \mathbb{R}^+,
\]
and thus reads $f^j(\eta_j) = a^j_{m_0} \exp(-\frac{\varepsilon^{2m_0}}{2} \sqrt{2(E(\lambda) - E^j_{m_0})}) + b^j_{m_0} \exp(\frac{\varepsilon^{2m_0}}{2} \sqrt{2(E(\lambda) - E^j_{m_0})})$.

Above, $\sqrt{\cdot}$ denotes the complex square root with a non-negative imaginary part, $b^j_{m_0}$ is an unknown coefficient depending on the solution and $a^j_{m_0}$ is the amplitude of the injected electrons travelling towards the active region and is thus known. We suppose the electrons are injected in the lead $j_0$, with a momentum $p$, on the transversal mode $m_0$ and with an amplitude one so that $a^j_{m_0} = \delta_j^{m_0} \delta^{m_0}$ and $E(\lambda) = \frac{1}{2}p^2 + E^j_{m_0}$. The modes associated with $E^j_{m_0} < E(\lambda)$ are the propagating modes and the ones with $E^j_{m_0} > E(\lambda)$ are the evanescent modes. When $j = j_0$, $b^j_{m_0}$ is a reflection coefficient, and when $j \neq j_0$, it is a transmission coefficient. The boundary conditions are obtained by eliminating $b^j_{m_0}$ and formally read
\[
\varepsilon \left. \frac{\partial \psi^0_{\lambda}}{\partial \eta_j} \right|_{\Gamma_j} = S_j[E(\lambda)](\psi^0_{\lambda}) + Z_j[E(\lambda)].
\]
These relations are impedance-like boundary conditions. The operator $Z_j[E(\lambda)]$ corresponds to an homogeneous part while $S_j[E(\lambda)]$ is a source term. They read

$$Z_j[E(\lambda)](\psi^0_\lambda) = i \sum_{m=1}^{\infty} \sqrt{2(E(\lambda) - E_m^j)} \psi^0_m, \chi^0_m(\xi_j), \quad (2.4)$$

$$S_j[E(\lambda)] = -2i \delta_j^0 \chi^0_m(\xi_j), \quad (2.5)$$

$$\psi^0_m = \langle \psi^0_\lambda(\eta_j = 0, \cdot), \chi^0_m(\xi_j) \rangle.$$  

It is shown in [10] that these boundary conditions actually make sense in a weak formulation for every $\psi^0_\lambda \in H^1(\Omega_0)$, see therein for more details and a complete analysis of the related stationary open Schrödinger-Poisson system.

### 2.3. Potentials.

In [12], it is assumed that the exterior potential of the Hamiltonian (1.1) shares close properties to that of $V^0$. In order to solve exactly the Schrödinger equation in the leads for the derivation of the boundary conditions, it is supposed that the spatial dependence of the exterior potential $V_e$ is only transversal. The following class is then introduced in [12]: a given potential $V$ belongs to the class $V$ if it satisfies:

1. $V \in C^1([0,T], L^\infty(\Omega))$,
2. for any $j = 1, \ldots, n$, there exists a function $V_j(t)$ such that for $x \in \Omega_j$ we have $V(t,x) = V^0(x) + V_j(t)$.

The regularity in time is needed to obtain energy estimates, that is $H^1(\Omega_0)$ bounds for the wavefunction. One could also consider non-regular in time potentials with some Sobolev regularity in space but in the typical application we are interested in - namely quantum transport in nanostructures - the potentials present a barrier profile which is obviously not smooth.

### 3. The transient open Schrödinger-Poisson system.

It consists in solving for $V_s(t,x)$ and $\psi_\lambda(t,x)$ the following system

$$i \varepsilon \partial_t \psi_\lambda = \mathcal{H}(t)\psi_\lambda \quad ; \quad \psi_\lambda(0, \cdot) = \psi^0_\lambda \quad ; \quad x \in \Omega \quad ; \quad \lambda \in \Lambda, \quad (3.1)$$

$$\mathcal{H}(t) = -\frac{\varepsilon^2}{2} \Delta + V_e(t,x) + V_s(t,x), \quad (3.2)$$

$$\psi_\lambda = 0 \quad ; \quad x \in \Gamma \cup \bigcup_{j=1}^{n} (\Gamma_j \times \mathbb{R}^+), \quad (3.3)$$

$$-\Delta V_s = \int_\Lambda |\psi_\lambda|^2 d\mu(\lambda), \quad x \in \Omega_0 \quad ; \quad V_s|_{\partial\Omega_0} = 0, \quad (3.4)$$

where $V_e$ belongs to the class of potentials $V$ and $\psi^0_\lambda$ belongs to the class of initial conditions. Notice that the Schrödinger equation is set on the whole domain $\Omega$ including the leads. As it was done for the stationary case in [10] and in [11], it is proven in [12], thanks to the introduction of suitable boundary conditions, that this system is equivalent to the same Schrödinger-Poisson system posed only in the domain $\Omega_0$. In the next subsection, we recall the time-dependent transparent boundary conditions introduced in [12] and the theorem stating the existence and uniqueness of strong solutions to (3.1)–(3.4) in the sense of [25]. We then present the weak formulation of (3.1)–(3.4) and state the main result of the paper.
3.1. Transparent boundary conditions and strong solutions. We first introduce some notations. Let
\[ \chi_m^j(t,\xi_j) := \chi_m^0, j \exp \left( -\frac{i}{\varepsilon} \int_0^t (V_j(\tau) + E_j^m) d\tau \right). \]
At any time, \((\chi_m^j)_{m \geq 1}(t,.)\) is an orthonormal basis of \(L^2(\Gamma_j)\).

**Definition 3.1.** For any given function \(f \in H^{1/2}(0,T)\), one defines - see [20], or [29]:
\[ \partial^{1/2} f := \frac{1}{\sqrt{\pi}} \frac{d}{dt} \int_0^t \frac{f(\tau)}{\sqrt{t-\tau}} d\tau = \frac{1}{\sqrt{\pi}} \frac{d}{dt} \mathcal{I}^{1/2} f. \]

\(H^{1/2}(0,T)\), see [1], is the fractional Sobolev space of functions verifying
\[ H^{1/2}(0,T) = \left\{ f \in L^2(0,T), \text{ such that } \int_0^T \int_0^T \frac{|f(s) - f(\tau)|^2}{(s-\tau)^2} dsd\tau < \infty \right\}. \]

An alternative definition that will be used in the sequel defines \(H^{1/2}(0,T)\) as the restriction to \((0,T)\) of functions belonging to \(H^{1/2}(\mathbb{R})\). Then, for any \(f \in H^{1/2}((0,T),L^2(\Gamma_j))\), we set
\[ D^{1/2}_j f(t,\xi_j) := \sqrt{2} \sum_{m \geq 1} \chi_m^j(t,\xi_j) \partial^{1/2} \langle f(\cdot,\cdot), \chi_m^j(\cdot,\cdot) \rangle_j. \]

Let now
\[ \psi^{pw}_\lambda := \psi_0^\lambda \sum_{j=1}^n \mu_j \theta_\lambda^j, \]
\[ \theta_\lambda^j(t) := \exp \left( -\frac{i}{\varepsilon} \int_0^t (E(\lambda) + V_j(s)) ds \right), \]
where \((\mu_j)_j\) is the partition of unity introduced in section 2.1. Then, according to [12], the wave function \(\psi_\lambda\) satisfies the following boundary conditions,
\[ \frac{\partial}{\partial \eta_j} (\psi_\lambda - \psi^{pw}_\lambda) = -\frac{e^{-i\pi/4}}{\sqrt{\varepsilon}} D^{1/2}_j (\psi_\lambda - \psi^{pw}_\lambda) ; \quad x \in \Gamma_j, \quad j = 1, \ldots, n. \]

One can also write a boundary condition involving a half-integral \(\mathcal{I}^{1/2}\) rather than a half-derivative. The final system we will deal with in the sequel thereby couples many Schrödinger equations, posed on a bounded domain with open boundary conditions, to the Poisson equation. The complete system reads:
\[ i\varepsilon \partial_t \psi_\lambda = \mathcal{H}(t) \psi_\lambda ; \quad \psi_\lambda(0,\cdot) = \psi_0^\lambda \quad x \in \Omega_0 ; \quad \lambda \in \Lambda, \]
\[ \frac{\partial}{\partial \eta_j} (\psi_\lambda - \psi^{pw}_\lambda) = -\frac{e^{-i\pi/4}}{\sqrt{\varepsilon}} D^{1/2}_j (\psi_\lambda - \psi^{pw}_\lambda) ; \quad x \in \Gamma_j, \]
\[ \psi_\lambda = 0 \quad x \in \Gamma_0, \]
\[ -\Delta V_s = \int_{\Lambda} |\psi_\lambda|^2 d\mu(\lambda) \quad x \in \Omega_0 ; \quad V_s |_{\partial \Omega_0} = 0. \]
The existence result of [12] provides strong solutions to (3.8)–(3.11) in the sense that
the Schrödinger equation and the boundary conditions are verified almost everywhere
on Ω₀ and on Γ_j, respectively. The exact statement is the following:

**Theorem 3.1.** [12]. Let \( V_e \in V, \psi_0^\lambda \) verifying hypothesis \((H-1)\), \( d = 2 \) or \( d = 3 \), and in addition

\[
\int_\Lambda \| \psi_0^\lambda \|_{H^2(K)}^2 \, d\mu(\lambda) < \infty \quad ; \quad \Phi \text{ has a compact support},
\]

for any bounded set \( K \subset \Omega \). Then (3.8)–(3.11) is equivalent to (3.1)–(3.4) and there
exists a unique solution \((\psi_\lambda, V_s)\) to (3.1)–(3.4) such that

\[
\psi_\lambda \in \psi^{pw}_\lambda + C^0([0,T], H^2(\Omega)) \cap C^1([0,T], L^2(\Omega)), \quad \lambda \text{ a.e.,}
\]

\[
V_s \in C^0([0,T], H^0_0(\Omega)) \cap C^0([0,T], H^4(\Omega)) \cap C^1([0,T], H^2(\Omega)),
\]

for any positive arbitrary large \( T \) and so that (3.8) and (3.9) are verified almost
everywhere.

The above theorem does not provide any information about the dependence on \( \varepsilon \) of the different bounds on \( \psi_\lambda \) and \( V_s \), which is paramount for the semi-classical limit.

The proof can actually be adapted to yield more regularity of the solution when the
data are more regular, for instance we can get pointwise in \( \lambda \), \( \psi_\lambda \in C^\infty([0,T] \times \Omega) \)
when \( \psi_0^\lambda \in C^\infty(\Omega) \) and \( V_e \in C^\infty([0,T] \times \Omega) \). We will use this regularity further to use
\( \psi_\lambda \) as a test function in the weak formulation. Some details about the regularization
procedure are given in Appendix B.

### 3.2. Weak formulation and main result.

We present in this section the
weak formulation of (3.8)–(3.11) and the main result of the paper. The formulation
of the boundary terms requires a particular attention to obtain the \( \varepsilon \)-independent
estimates. More precisely, the boundary condition (3.9) is split into homogeneous and inhomogeneous parts, that is

\[
\frac{\partial \psi_\lambda}{\partial n_j} = -\frac{e^{-i\pi/4}}{\sqrt{\varepsilon}} D^{1/2}_j(\psi_\lambda) + A^\varepsilon_j(\psi^{pw}_\lambda),
\]

where

\[
A^\varepsilon_j(\psi^{pw}_\lambda) := \frac{\partial \psi^{pw}_\lambda}{\partial n_j} \bigg|_{\Gamma_j} + \frac{e^{-i\pi/4}}{\sqrt{\varepsilon}} D^{1/2}_j(\psi^{pw}_\lambda),
\]

\[
= \frac{1}{\varepsilon} (Z_j |E(\lambda)||\psi_0^\lambda| + S_j |E(\lambda)|) \theta^\lambda + e^{-i\pi/4} \sqrt{\varepsilon} D^{1/2}_j(\psi^{pw}_\lambda). \tag{3.12}
\]

Note here that we used the stationary open boundary conditions (2.3) to define
\( A^\varepsilon_j(\psi^{pw}_\lambda) \). The solutions to (3.8) are sought under the following weak form: let
\( u \in C^1([0,T), H^1(\Omega_0)) \) be a test function, where \( T \) is an arbitrary non-negative constant ; denoting by \( (\cdot, \cdot) \) the \( L^2(\Omega_0) \) inner product and using the Green formula, the boundary conditions (3.9) and (3.10), we find \( \lambda \) a.e.,

\[
-i \varepsilon \int_0^T (\psi_\lambda, \partial_t u) \, ds = i \varepsilon (\psi_0^\lambda, u(0, \cdot)) + \frac{1}{2} \varepsilon^2 \int_0^T (\nabla \psi_\lambda, \nabla u) \, ds + \int_0^T (V \psi_\lambda, u) \, ds
\]
When the potential $V_\varepsilon$ belongs to the class $\mathcal{V}$, it is rather natural to consider wave-functions $\psi_\lambda$ solution to (3.13) belonging to $L^2((0,T),H^1(\Omega_0)) \cap C^0([0,T],L^2(\Omega_0))$. Nevertheless, this regularity is not sufficient since the boundary terms need more integrability in time to make sense. To define the convenient functional space, we introduce the following family of unitary transformations: for any integrability in time to make sense. To define the convenient functional space, we introduce the following family of unitary transformations: for any $f \in L^2((0,T),L^2(\Gamma_j))$, let

$$T_j f(t,\xi_j) := \sum_{m \geq 1} \varepsilon^{j} f_j^m (E^0_{\varepsilon} + V_j(s)) ds \langle f(t,\cdot), \chi_{m}^{0,j} \rangle \chi_{m}^{0,j}(\xi_j),$$

(3.14)

and let $(T_j f)_m := \langle T_j f, \chi_{m}^{0,j} \rangle$. Consider now the functional space

$$E = \{ \varphi \in L^2((0,T),H^1(\Omega_0)) \cap C^0([0,T],L^2(\Omega_0)), \text{ such that } T_j \varphi \in H^{1/4}((0,T),L^2(\Gamma_j)), j = 1, \cdots, n \},$$

and let $E^0$ be the space of functions belonging to $E$ with a vanishing trace on $\Gamma_0$, i.e.

$$E^0 = \{ \varphi \in E, \text{ such that } \varphi|_{\Gamma_0} = 0 \}.$$

In the weak formulation (3.13), the boundary term $\int_0^T \langle D_j^{1/2} (\psi_\lambda), u \rangle ds$ has to be understood in the following weak sense, which uses the expression of the half-derivative in the Fourier space given in Lemma 4.1 of Appendix A:

$$\int_0^T \langle D_j^{1/2} (\psi_\lambda), u \rangle ds = \frac{i \varepsilon}{2\pi} \sum_{m \geq 1} \int_\mathbb{R} \sqrt{\xi} \mathcal{F}(\tilde{T}_j \mathcal{F}_{\psi_\lambda})_m \mathcal{F}(\tilde{T}_j u)_m d\xi.$$

(3.15)

Above, the $\tilde{\cdot}$ sign is the extension by 0 outside $[0,T]$. $\mathcal{F}$ stands for the Fourier transform with respect to time and $\sqrt{\cdot}$ is the complex square root with non-positive imaginary part. The dual variable of $t$ is denoted by $\xi$. This expression is well-defined for any $\psi_\lambda \in E$ and $u \in C^1([0,T],H^1(\Omega_0))$.

We state now the main result of the paper, which provides existence and uniqueness for the system (3.11)-(3.13) as well as uniform bounds in $\varepsilon$ for the density $n$ and energy $E$ defined below:

**Theorem 3.2.** Let $\psi_\lambda^i$ belongs to the class of initial data, let $V_\varepsilon \in \mathcal{V}$ and assume $\mu$ verifies (2.2). Let

$$n(t) := \int_{\Lambda} \|\psi_\lambda(t,\cdot)\|^2_{L^2(\Omega_0)} d\mu,$$

$$E(t) := \frac{\varepsilon^2}{2} \int_{\Lambda} \|\nabla \psi_\lambda(t,\cdot)\|^2_{L^2(\Omega_0)} d\mu + \frac{1}{2} \|\nabla V_\varepsilon(t,\cdot)\|^2_{L^2(\Omega_0)}.$$

Then, the Schrödinger-Poisson system (3.11)-(3.13) admits a unique solution, for $d = 2$ or $d = 3$, such that, $\lambda$ a.e.,

$$V_\varepsilon \in L^2((0,T),W^{3,r}(\Omega_0)) \cap H^4((0,T),W^{1,r}(\Omega_0)) \quad ; \quad \psi_\lambda \in E^0,$$
Proposition 3.3. Let \( \theta \) have led to \( \Gamma_j \) case in \([11]\). Schrödinger equation. This property has only been shown yet in the one-dimensional as it is in \([10]\), then (3.16) has to be verified by the solution to a stationary open \( \lambda \) we have, an argument. That property is shown in the next proposition. The averaging between the homogeneous stationary boundary conditions given by \( Z_j \) and the homogeneous time-dependent boundary conditions involving the half-derivative, which will allow to control the boundary terms in terms of other boundary terms with a sign argument. That property is shown in the next proposition. The \( \varepsilon \)-independent estimates rely as well on the verification of assumption (3.16). If the initial condition \( \psi^0_\lambda \) is a solution to the Schrödinger equation not only in the leads but also in \( \Omega_0 \), as it is in \([10]\), then (3.16) has to be verified by the solution to a stationary open Schrödinger equation. This property has only been shown yet in the one-dimensional case in \([11]\).

The proof of the theorem is the object of the next section. The existence and uniqueness part is very standard and is obtained after regularization of the problem in order to use Theorem 3.1. Some estimates give then some compactness results and allow to pass to the limit in weak formulation. The proof of the \( \varepsilon \)-independent estimates is more involved and requires a careful analysis of the boundary term \( A_j^\varepsilon(\psi^\text{pw}_\lambda) \). Indeed, the term \( \varepsilon \langle A_j^\varepsilon(\psi^\text{pw}_\lambda), \psi_\lambda \rangle \) can be straightforwardly bounded by \( C_0 \| \psi_\lambda \|_{L^2(\Gamma_j)} \| \psi^0_\lambda \|_{H^{1/2}(\Gamma_j)} \) for some positive constant \( C_0 \) independent of \( \varepsilon \); by means of trace theorems, this bound turns into \( \varepsilon^{-1/2} C_1 \| \psi_\lambda \|_{L^2(\Omega_0)} \| \varepsilon \nabla \psi_\lambda \|_{H^{1/2}(\Omega_0)} \| \psi^0_\lambda \|_{H^{1/2}(\Gamma_j)} \) which has no wrong homogeneity in \( \varepsilon \) whatever the available bound on \( \psi^0_\lambda \). We thus expect some compensations or averaging between the homogeneous stationary boundary conditions given by \( Z_j \) and the homogeneous time-dependent boundary conditions involving the half-derivative, which will allow to control the boundary terms in terms of other boundary terms with a sign argument. That property is shown in the next proposition. The \( \varepsilon \)-independent estimates rely as well on the verification of assumption (3.16). If the initial condition \( \psi^0_\lambda \) is a solution to the Schrödinger equation not only in the leads but also in \( \Omega_0 \), as it is in \([10]\), then (3.16) has to be verified by the solution to a stationary open Schrödinger equation. This property has only been shown yet in the one-dimensional case in \([11]\).

The proof of the theorem is the object of the next section. The existence and uniqueness part is very standard and is obtained after regularization of the problem in order to use Theorem 3.1. Some estimates give then some compactness results and allow to pass to the limit in weak formulation. The proof of the \( \varepsilon \)-independent estimates is more involved and requires a careful analysis of the boundary term \( A_j^\varepsilon(\psi^\text{pw}_\lambda) \). Indeed, the term \( \varepsilon \langle A_j^\varepsilon(\psi^\text{pw}_\lambda), \psi_\lambda \rangle \) can be straightforwardly bounded by \( C_0 \| \psi_\lambda \|_{L^2(\Gamma_j)} \| \psi^0_\lambda \|_{H^{1/2}(\Gamma_j)} \) for some positive constant \( C_0 \) independent of \( \varepsilon \); by means of trace theorems, this bound turns into \( \varepsilon^{-1/2} C_1 \| \psi_\lambda \|_{L^2(\Omega_0)} \| \varepsilon \nabla \psi_\lambda \|_{H^{1/2}(\Omega_0)} \| \psi^0_\lambda \|_{H^{1/2}(\Gamma_j)} \) which has no wrong homogeneity in \( \varepsilon \) whatever the available bound on \( \psi^0_\lambda \). We thus expect some compensations or averaging between the homogeneous stationary boundary conditions given by \( Z_j \) and the homogeneous time-dependent boundary conditions involving the half-derivative, which will allow to control the boundary terms in terms of other boundary terms with a sign argument. That property is shown in the next proposition. The \( \varepsilon \)-independent estimates rely as well on the verification of assumption (3.16). If the initial condition \( \psi^0_\lambda \) is a solution to the Schrödinger equation not only in the leads but also in \( \Omega_0 \), as it is in \([10]\), then (3.16) has to be verified by the solution to a stationary open Schrödinger equation. This property has only been shown yet in the one-dimensional case in \([11]\).

We decided in the theorem to set the transparent boundary conditions on the \( \Gamma_j \)'s while they could have been set anywhere further in the guides. Doing so would have led to \( L^2_{\text{loc}}(\Omega) \) estimates for the density and for the energy.

Proposition 3.3. Let \( A_j^\varepsilon \) be defined in (3.12), \( \psi^\text{pw}_\lambda \) in (3.6), \( B_j[E(\lambda)] \) in (2.5) and \( \theta_\lambda^0(t) \) in (3.7). Then, for any \( t > 0 \), for \( \psi_\lambda^0 \in H^{1/2}(\Gamma_j) \), \( u \in L^{2+\delta}((0,t),L^2(\Gamma_j)) \), \( \delta > 0 \), we have, \( \lambda \) a.e,

\[
\int_0^t \langle A_j^\varepsilon(\psi^\text{pw}_\lambda), u \rangle_j ds = \frac{1}{\varepsilon} \int_0^t \langle B_j[E(\lambda)] \theta_\lambda^0(t), u \rangle_j ds. \tag{3.18}
\]

Proof. Setting

\[
B_j(\psi^\text{pw}_\lambda) = \frac{1}{\varepsilon} Z_j[E(\lambda)](\psi^0_\lambda) \theta_\lambda^0; \quad C_j(\psi^\text{pw}_\lambda) = \frac{e^{-i\pi/4}}{\sqrt{\varepsilon}} D_j^{1/2}(\psi^\text{pw}_\lambda),
\]

(3.18) is equivalent to showing that \( \int_0^t \langle B_j(\psi^\text{pw}_\lambda) + C_j(\psi^\text{pw}_\lambda), u \rangle_j ds = 0 \). Let \( u^0_m(t) \) be the projection \( u^0_m(t) = \langle u(t, \cdot), \chi_m \rangle \). Then, plugging the definition of \( Z_j \) (2.4) into
and denoting $\gamma_m^j = 2(E(\lambda) - E_m^j)$, it follows
\[
\int_0^t \langle B_j(\psi^{p,w}_\lambda), u_j \rangle ds = \frac{i}{\varepsilon} \sum_m \sqrt{\gamma_m^j} \psi_0^{0,j} \int_0^t e^{-\frac{i}{\varepsilon} \int_0^s (E(\lambda) + V_j(\tau)) d\tau} \overline{u_m(s)} ds,
\]
\[
= \frac{i}{\varepsilon} \sum_m \sqrt{\gamma_m^j} \psi_0^{0,j} \mathcal{F} U_m^j(-\gamma_m^j/(2\varepsilon)).
\]

Above, $\mathcal{F}$ denotes the Fourier transform with respect to time and $U_m^j$ is defined as
\[
U_m^j(s) = \begin{cases} u_m^j(s) e^{\frac{i}{\varepsilon} \int_0^s (E_m^j + V_j(\tau)) d\tau} & \text{if } s \in [0,t], \\ 0 & \text{if } s \notin [0,t]. \end{cases}
\]

Concerning $C_j$, invoking (3.5) yields
\[
\int_0^t \langle C_j(\psi^{p,w}_\lambda), u_j \rangle ds = \sqrt{2} e^{-i \pi / 4} \sum_m \psi_0^{0,j} \int_0^t e^{-\frac{i}{\varepsilon} \int_0^s (E_m^j + V_j(\tau)) d\tau} \overline{u_m(s)} \partial^{1/2} \left( e^{-\frac{i}{\varepsilon} \gamma_m^j s} \right) ds,
\]
\[
= \frac{\sqrt{2}}{2\pi \sqrt{\varepsilon}} \sum_m \psi_0^{0,j} \int_{\mathbb{R}} \mathcal{F} U_m^j(\xi) \sqrt{\xi} \mathcal{F} \left[ \mathbb{I}_{\mathbb{R}} \cdot e^{-\frac{i}{\varepsilon} \gamma_m^j s} \right](\xi) d\xi,
\]
where we used the Fourier-Plancherel equality and (4.17). Above, $\sqrt{\cdot}$ is the complex square root with non-positive imaginary part. Actually, in the distribution sense,
\[
\mathcal{F} \left[ \mathbb{I}_{\mathbb{R}} \cdot e^{-\frac{i}{\varepsilon} \gamma_m^j s} \right](\xi) = \pi \delta(\gamma_m^j/(2\varepsilon) + \xi) - \text{p.v.} \frac{i}{\gamma_m^j/(2\varepsilon) + \xi},
\]
where p.v. stands for the principal value. Then,
\[
\int_0^t \langle C_j(\psi^{p,w}_\lambda), u_j \rangle ds = \frac{1}{2\varepsilon} \sum_m \sqrt{-\gamma_m^j} \psi_0^{0,j} \mathcal{F} U_m^j(-\gamma_m^j/(2\varepsilon))
\]
\[
- \frac{i \sqrt{2}}{2\pi \sqrt{\varepsilon}} \sum_m \psi_0^{0,j} \text{p.v.} \int_{\mathbb{R}} \mathcal{F} U_m^j(\xi) \frac{\sqrt{\xi}}{\gamma_m^j/(2\varepsilon) + \xi} d\xi.
\]

To conclude the proof, it remains to evaluate the integral of second term of the r.h.s. of the above equation. To this aim, we use standard complex analysis. Let us first notice that $\mathcal{F} U_m^j$ can be extended to an holomorphic function for $z \in \mathbb{C}^+ = \{ z \in \mathbb{C}, \ Im z \geq 0 \}$. Besides, we have the estimates, for $z = re^{i\theta} \in \mathbb{C}^+$,
\[
|\mathcal{F} U_m^j(z)| \leq \frac{C(\delta)}{(r \sin \theta)^{2+\delta}} \| u_m^j \|_{L^{2+\delta}(0,t)},
\]
\[
(3.19)
\]
as well as
\[
|\mathcal{F} U_m^j(z)| \leq \| u_m^j \|_{L^1(0,t)}.
\]
\[
(3.20)
\]
The function $\sqrt{\xi}$ is also holomorphic on $\mathbb{C}^+ - \{0\}$ (provided we choose the convenient branch) so that, defining a convenient contour $\mathcal{C} = \mathcal{C}_R \cup \mathcal{C}_{r_1} \cup \mathcal{C}_{r_2} \cup \mathcal{C}_{R,r_1}, r_2 \subset \mathbb{C}^+$,
where $C_R$ is the semi-circle centered at 0 of radius $R$, with $R > |\gamma_m^j|/(2\epsilon)$, $C_{\eta_1}$ the semi-circle centered at 0 of radius $\eta_1$, $C_{\eta_2}$ the semi-circle centered at $-\gamma_m^j/(2\epsilon)$ of radius $\eta_2$, and $C_{R,\eta_1,\eta_2}$ connects the different semi-circles on $\mathbb{R}$, the Cauchy theorem yields

$$\int_C \frac{\nabla U_m^\dagger(z)}{\gamma_m^j/(2\epsilon) + z} \, dz = 0.$$  \hfill(3.21)

We evaluate now the integral on each contour. We have, according to (3.19),

$$\left| \int_{C_R} \frac{\nabla U_m^\dagger(z)}{\gamma_m^j/(2\epsilon) + z} \, dz \right| \leq \frac{C}{R^{5/(2(2+\delta))}} \| u_m^j \|_{L^2(0, t)} \frac{\pi}{\sin \theta \sqrt{|z|}} \, d\theta,$$

so that the integral on $C_R$ goes to zero as $R$ goes to the infinity as soon as $\delta > 0$. In the same way, according to (3.20),

$$\left| \int_{C_{\eta_1}} \frac{\nabla U_m^\dagger(z)}{\gamma_m^j/(2\epsilon) + z} \, dz \right| \leq C \eta_1^{3/2} \| u_m^j \|_{L^1(0, t)},$$

which vanishes in the limit $\eta_1 \to 0$. Concerning the integral on $C_{\eta_2}$, we have

$$\int_{C_{\eta_2}} \frac{\nabla U_m^\dagger(z)}{\gamma_m^j/(2\epsilon) + z} \, dz = \int_0^\pi \nabla U_m^\dagger \left( -\gamma_m^j/(2\epsilon) + \eta_2 e^{i\theta} \right) \sqrt{-\gamma_m^j/(2\epsilon) + \eta_2 e^{i\theta} i} \, d\theta,$$

so that the Lebesgue dominated convergence theorem implies that the integral goes to $-i\pi \sqrt{-\gamma_m^j/(2\epsilon)} \nabla U_m^\dagger \left( -\gamma_m^j/(2\epsilon) \right)$ as $\eta_2 \to 0$. Since the integral on $C_{R,\eta_1,\eta_2}$ tends to

$$\text{p.v.} \int_R \frac{\nabla U_m^\dagger(\xi)}{\gamma_m^j/(2\epsilon) + \xi} \, d\xi,$$

as $R \to \infty$, $\eta_1 \to 0$ and $\eta_2 \to 0$, we finally get, using (3.21),

$$\text{p.v.} \int_R \frac{\nabla U_m^\dagger(\xi)}{\gamma_m^j/(2\epsilon) + \xi} \, d\xi = \frac{i\pi}{\sqrt{2\epsilon}} \sqrt{-\gamma_m^j \nabla U_m^\dagger \left( -\gamma_m^j/(2\epsilon) \right)}.$$

Consequently,

$$\int_0^t \langle C_j(\psi_\lambda^\text{pw}), u_j \rangle \, ds = \frac{1}{\epsilon} \sum_m \sqrt{-\gamma_m^j \psi_m^0 \nabla U_m^\dagger \left( -\gamma_m^j/(2\epsilon) \right)},$$

and it remains to notice that $\sqrt{-\gamma_m^j} = -i \sqrt{\gamma_m^j}$ to end the proof. \hfill\Box

4. Proof of the theorem. We start by regularizing the problem to apply the previous existence result of [12] given in Theorem 3.1 where the initial condition is more regular. To be able to use $\psi_\lambda$ as a test function, we nevertheless need more regularity for $\psi_\lambda$ than that given in the theorem, which is only $\psi_\lambda \in \mathcal{C}^0([0, T], H^2(\Omega)) \cap \mathcal{C}^1([0, T], L^2(\Omega))$. We thus consider a sequence of regular data $\psi^0_\lambda, V^0_e \in C^\infty(\Omega)$ and $V^k_e \in C^\infty([0, T] \times \Omega)$ such that (3.8)–(3.11) admits a unique solution $\psi^k_\lambda$ verifying $\psi^k_\lambda \in C^\infty([0, T] \times \Omega)$. All the manipulations that will follow further are then justified. The regularization procedure is not direct and is sketched in Appendix B. The regularized data verify, for $1 \leq p < \infty$,

$$\psi^0_\lambda \rightharpoonup \psi^0_\lambda \text{ strongly in } H^1(K) ; \quad V^k_e \to V_e \text{ strongly in } C^1([0, T], L^p(K)),$$

(4.1)
for any bounded set $K \subset \Omega$. This implies that, for any $u \in H^{1/2}((0,T),L^2(\Gamma_j))$,
\begin{align}
\mathcal{D}_{1,k}^{1/2}(u) &\to \mathcal{D}_j^{1/2}(u) \text{ strongly in } H^{-1/2}((0,T),L^2(\Gamma_j)), \\
\mathcal{A}_{j,k}^{\epsilon}(\psi_{\lambda}^{pw,k}) &\to \mathcal{A}_j^{\epsilon}(\psi_{\lambda}^{pw}) \text{ weakly in } L^2((0,T),L^2(\Gamma_j)).
\end{align}
(4.2) (4.3)
In the same way, $\Phi(p,m,j)$ is localized so that the obtained $\Phi^k(p,m,j)$ has a compact support and $\Phi^k$ converges strongly to $\Phi$ in $L^1(\mathbb{R}_+^*, \ell^1(\mathbb{N}^* \times \{1, \cdots, n\}))$.

We prove now the bounds that will allow to pass to the limit. They will also provide the $\epsilon$-independent estimates.

**Density estimate.** Consider this regular solution $\psi_{\lambda}^{\epsilon}$ which is also obviously solution to (3.13). Multiplying (3.8) by $\psi_{\lambda}^{\epsilon}$, integrating in $[0,T]$ and taking the imaginary part, it follows
\[
\|\psi_{\lambda}^{\epsilon}(T)\|^2_{L^2(\Omega)} = \|\psi_{\lambda}^{0,k}\|^2_{L^2(\Omega)} + \sqrt{\varepsilon} \sum_{j=1}^n \mathcal{I}_m e^{-i\pi/4} \int_0^T \left\langle \mathcal{D}_{j,k}^{1/2}(\psi_{\lambda}^{k}), \psi_{\lambda}^{\epsilon} \right\rangle_j ds
\]
\[
- \varepsilon \sum_{j=1}^n \mathcal{I}_m \int_0^T \left\langle \mathcal{A}_{j,k}^{\epsilon}(\psi_{\lambda}^{pw,k}), \psi_{\lambda}^{\epsilon} \right\rangle_j ds.
\]
We drop in the sequel the $k$ superscript to clarify the notations, keeping in mind until further notice that the wavefunctions we are manipulating are the regular solutions. Define now for any $s \in \mathbb{R}$,
\[
\Phi_{m,T}^j(s) = (T_j \psi_{\lambda})_m(s),
\]
where $T_j$ is the transformation previously introduced in (3.14), $(T_j \psi_{\lambda})_m(s) = (T_j \psi_{\lambda}(s, n_j = 0, \lambda m_j))_1$, and $\sim$ is the extension by 0 outside $[0,T]$. Then, according to (4.17) of Lemma 4.1,
\[
\mathcal{I}_m 2 \pi e^{-i\pi/4} \int_0^T \left\langle \mathcal{D}_{j}^{1/2}(\psi_{\lambda}), \psi_{\lambda} \right\rangle_j ds = - \sqrt{2} \sum_m \int_{\mathbb{R}} \sqrt{-\xi} |\mathcal{F}_{\Phi_{m,T}}^j(\xi)|^2 d\xi,
\]
(4.4)
The term involving $A_j^{\epsilon}$ is treated thanks to Lemma 3.3. Using the expression of $S_j$ given by (2.5) and since the electrons are injected with a momentum $p$, in the lead $j_0$ and in the transversal mode $m_0$, we have $E(\lambda) = \frac{p^2}{2} + E_{m_0}$ and therefore,
\[
\int_0^T \left\langle A_j^{\epsilon}(\psi_{\lambda}^{pw}), \psi_{\lambda} \right\rangle ds = - \delta_{j_0}^j \frac{2ip}{\varepsilon} \int_0^T \theta_{m_0}(s) \overline{\psi_{m_0}^{\epsilon}(s)} ds = - \delta_{j_0}^j \frac{2ip}{\varepsilon} \mathcal{F}_{\Phi_{m_0,T}}(p^2/2\varepsilon).
\]
Gathering the previous estimates and integrating with respect to $\lambda$, we find
\[
n(T) + \frac{\sqrt{2}}{2\pi} \sum_{j,m} \int_{\lambda} \int_{\mathbb{R}} \sqrt{-\xi} |\mathcal{F}_{\Phi_{m,T}}^j(\xi)|^2 d\xi d\mu
\]
\[
\leq n(0) + 2 \int_{\lambda} p \left| \mathcal{F}_{\Phi_{m_0,T}}(p^2/2\varepsilon) \right| d\mu,
\]
(4.5)
which gives after an integration in time,
\[
\|n\|_{L^1(0,T^\ast)} + \frac{\sqrt{2\varepsilon}}{2\pi} \sum_{j,m} \int_{t=0}^{T^\ast} \int_{\Lambda} \int_{\mathbb{R}} \sqrt{-\xi} |\mathcal{F} \Phi_{m,T}^n(\xi)|^2 d\xi d\mu dT
\]
\[
\leq T^\ast n(0) + 2 \int_{0}^{T^\ast} \int_{\Lambda} \left| \mathcal{F} \Phi_{m,T}^n(p^2/2\varepsilon) \right| d\mu dT.
\]

(4.6)

**Energy estimate.** We multiply now (3.8) by \( \partial_t \psi_\lambda \). Taking the real part and integrating in time yield,
\[
\frac{\varepsilon^2}{2} \| \nabla \psi_\lambda(T,\cdot) \|_{L^2(\Omega_0)}^2 = \frac{\varepsilon^2}{2} \| \nabla \psi_\lambda^0 \|_{L^2(\Omega_0)}^2 + \varepsilon^2 \sum_{j=1}^{n} \Re \int_{0}^{T} \left\langle \frac{\partial \psi_\lambda}{\partial \eta_j}, \partial_s \psi_\lambda \right\rangle_j \, ds
\]
\[
- \int_{0}^{T} \int_{\Omega_0} V(s,x) \partial_s |\psi_\lambda(s,x)|^2 \, dx ds.
\]

We need to be a bit careful to extend \( \partial_s \psi_\lambda \) by zero to \( \mathbb{R} \) to use the Fourier transform since \( \psi_\lambda \) does not vanish at 0 and at \( T \). Let \( \tilde{\psi}_\lambda \) be this extension and let \( \partial_s \tilde{\psi}_\lambda \) be its derivative in the distribution sense so that
\[
\frac{\partial \tilde{\psi}_\lambda}{\partial s}(s,x) = \begin{cases} \frac{\partial \psi_\lambda}{\partial s}(s,x) & \text{if } s \in [0,T], \\ 0 & \text{if } s \notin [0,T]. \end{cases}
\]

We then have
\[
\int_{0}^{T} \left\langle \frac{\partial \tilde{\psi}_\lambda}{\partial \eta_j}, \partial_s \tilde{\psi}_\lambda \right\rangle_j \, ds = \int_{0}^{T} \left\langle \frac{\partial \tilde{\psi}_\lambda}{\partial \eta_j}, \partial_s \tilde{\psi}_\lambda \right\rangle_j \, ds
\]
\[
+ \left\langle \frac{\partial \tilde{\psi}_\lambda}{\partial \eta_j}, \psi_\lambda \right\rangle_j(T) - \left\langle \frac{\partial \tilde{\psi}_\lambda}{\partial \eta_j}, \psi_\lambda \right\rangle_j(0).
\]

Using now the boundary conditions, both stationary and time-dependent, we find
\[
\int_{0}^{T} \left\langle \frac{\partial \psi_\lambda}{\partial \eta_j}, \partial_s \tilde{\psi}_\lambda \right\rangle_j \, ds = -\frac{e^{-i\pi/4}}{\sqrt{\varepsilon}} \int_{0}^{T} \left\langle D_j^{1/2}(\psi_\lambda), \partial_s \tilde{\psi}_\lambda \right\rangle_j \, ds + \int_{0}^{T} \left\langle A_j^{(\varepsilon)}(\psi_\lambda^w), \partial_s \tilde{\psi}_\lambda \right\rangle_j \, ds,
\]
\[
\left\langle \frac{\partial \tilde{\psi}_\lambda}{\partial \eta_j}, \psi_\lambda \right\rangle_j(T) = -\frac{e^{-i\pi/4}}{\sqrt{\varepsilon}} \left\langle D_j^{1/2}(\psi_\lambda), \psi_\lambda \right\rangle_j(T) + \left\langle A_j^{(\varepsilon)}(\psi_\lambda^w), \psi_\lambda \right\rangle_j(T),
\]
\[
\left\langle \frac{\partial \tilde{\psi}_\lambda}{\partial \eta_j}, \psi_\lambda \right\rangle_j(0) = \frac{1}{\varepsilon} \left\langle Z_j[E(\lambda)](\psi_\lambda^0), \psi_\lambda^0 \right\rangle_j + \frac{1}{\varepsilon} \left\langle S_j[E(\lambda)], \psi_\lambda^0 \right\rangle_j,
\]
and we recast the energy relation as
\[
\frac{\varepsilon^2}{2} \| \nabla \psi_\lambda(T,\cdot) \|_{L^2(\Omega_0)}^2 + L_1 + L_2 = \frac{\varepsilon^2}{2} \| \nabla \psi_\lambda^0 \|_{L^2(\Omega_0)}^2 + R_1 + R_2 + R_3
\]
\[
- \int_{0}^{T} \int_{\Omega_0} V(s,x) \partial_s |\psi_\lambda(s,x)|^2 \, dx ds,
\]

(4.7)
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where

\[
L_1 = \varepsilon^{3/2} \sum_{j=1}^{n} \text{Re} e^{-i\pi/4} \int_0^T \left\langle D_j^{1/2} (\psi_\lambda), \partial_s \bar{\psi}_\lambda \right\rangle_j ds,
\]

\[
L_2 = \varepsilon^{3/2} \sum_{j=1}^{n} \text{Re} e^{-i\pi/4} \left\langle D_j^{1/2} (\psi_\lambda), \psi_\lambda \right\rangle_j (T),
\]

\[
R_1 = \varepsilon^2 \sum_{j=1}^{n} \text{Re} \int_0^T \left\langle \mathcal{A}_j^\varepsilon (\psi_\lambda^{\text{per}}), \partial_s \bar{\psi}_\lambda \right\rangle_j ds,
\]

\[
R_2 = \varepsilon^2 \sum_{j=1}^{n} \text{Re} \left\langle \mathcal{A}_j^\varepsilon (\psi_\lambda^{\text{per}}), \psi_\lambda \right\rangle_j (T),
\]

\[
R_3 = -\varepsilon \sum_{j=1}^{n} \text{Re} \left[ \langle \mathcal{S}_j [E(\lambda) [\psi_\lambda^0]], \psi_\lambda^0 \rangle_j + \langle \mathcal{S}_j [E(\lambda)], \psi_\lambda^0 \rangle_j \right].
\]

We treat now each term separately. For the non-linear boundary term \(L_1\), we have thanks to the Fourier-Plancherel equality:

\[
\text{Re} 2\pi e^{-i\pi/4} \int_0^T \left\langle D_j^{1/2} (\psi_\lambda), \partial_s \bar{\psi}_\lambda \right\rangle_j ds = \sqrt{2} \sum_{m,j} \int_{\mathbb{R}^+} \xi^{3/2} |\mathcal{F} \phi_{m,T}^j (-\xi)|^2 d\xi
\]

\[
- \frac{\sqrt{2}}{\varepsilon} \text{Im} 2\pi e^{-i\pi/4} \sum_{m,j} \int_0^T (E_m + V_j) \partial^{1/2} (T_j \psi_\lambda) m \langle T_j \psi_\lambda \rangle m ds.
\]

Using (4.4) and the fact that we assumed \(E^j_m \geq 0, m \geq 1, j \geq 1\), we have

\[
\text{Im} 2\pi e^{-i\pi/4} \sum_{m,j} E_m^j \int_0^T \partial^{1/2} (T_j \psi_\lambda) m \langle T_j \psi_\lambda \rangle m ds = \frac{-\sqrt{2}}{\varepsilon} \sum_{m,j} E_m^j \int_{\mathbb{R}^+} \sqrt{-\xi} |\mathcal{F} \phi_{m,T}^j (\xi)|^2 d\xi \leq 0.
\]

The last term of \(L_1\) is treated by multiplying the Schrödinger equation by \(\sum_j \mu_j V_j \psi_\lambda := g \psi_\lambda\), by integrating in time and taking the imaginary part, which yield

\[
(g \psi_\lambda, \psi_\lambda)(T) = \langle g \psi_\lambda^0, \psi_\lambda^0 \rangle + \int_0^T (\partial_s g \psi_\lambda, \psi_\lambda)(s) ds + \text{Im} \int_0^T (\nabla g, \bar{\psi}_\lambda \nabla \psi_\lambda)(s) ds
\]

\[
+ \text{Im} \sum_{j=1}^{n} \left[ \varepsilon^{1/2} e^{-i\pi/4} \int_0^T \langle D_j^{1/2} (\psi_\lambda), V_j \psi_\lambda \rangle_j ds - \varepsilon \int_0^T \langle \mathcal{A}_j^\varepsilon (\psi_\lambda^{\text{per}}), V_j \psi_\lambda \rangle ds \right].
\]

Applying (3.3) and using the expression of \(S_j\), we have

\[
\varepsilon \left| \sum_{j=1}^{n} \int_0^T \langle \mathcal{A}_j^\varepsilon (\psi_\lambda^{\text{per}}), V_j \psi_\lambda \rangle ds \right| \leq 2 \int_\Lambda p \left| \mathcal{F} V_{\mu,T} \Phi_{m_{\text{per}} T}^j (p^2 / 2\varepsilon) \right| d\mu.
\]

This finally gives for \(L_1\),

\[
\frac{\sqrt{2}}{2\pi} \sum_{m,j} \int_{\mathbb{R}^+} \xi^{3/2} e^{i\pi/4} |\mathcal{F} \phi_{m,T}^j (-\xi)|^2 d\xi d\mu + R_1^1 \leq \int_\Lambda L_1 d\mu,
\]

(4.8)
where $R_1^1$ verifies, using (4.5):

$$|R_1^1| \leq C \int_{\Lambda} p \left| \mathcal{F} V_j \Phi_{m_0,T}^j(p^2/2\epsilon) \right| d\mu + C \left( n(0) + \|n\|_{L^1(0,T)} + \|\mathcal{E}\|_{L^1(0,T)} \right).$$

The generic constant $C$ above depends on $\|V_j\|_{C^1([0,T])}$. For the boundary term $R_1$, an integration by part and (3.3) give

$$R_1 = -2p \text{Re} \left[ \frac{p^2}{2} \mathcal{F} \Phi_{m_0,T}^j(p^2/2\epsilon) + \mathcal{F} V_j \Phi_{m_0,T}^j(p^2/2\epsilon) \right]. \quad (4.9)$$

The term $L_2$ is integrated in time to be able to use similar arguments as those of the density estimate. It yields,

$$\int_0^{T^*} L_2(T) dT = \sqrt{\frac{2\epsilon^3}{3\pi}} \sum_{j,m} \int_{\mathbb{R}^+} \sqrt{\xi} |\mathcal{F} \Phi_{m,T}^j(\xi)|^2 d\xi, \quad (4.10)$$

and in the same way

$$\int_0^{T^*} R_2(T) dT = \epsilon \text{Re} \left[ \frac{p^2}{2} \mathcal{F} \Phi_{m_0,T}^j(p^2/2\epsilon) \right]. \quad (4.11)$$

The last term $R_3$ is straightforwardly bounded thanks to hypothesis (3.16) and Lemma 4.1,

$$\left| \int_{\Lambda} R_3 d\mu \right| \leq C_0 + C \|p\|_{L^2(\Lambda; d\mu)}^{1/2} n^{1/4}(0) \mathcal{E}^{1/4}(0). \quad (4.12)$$

It remains to tackle the term involving the potential $V = V_e + V_s$. Using the Poisson equation (3.11), we find

$$\int_0^{T} \int_{\Omega_0} V_s \partial_s |\psi| dxd\mu = \frac{1}{2} \|\nabla V_s(T, \cdot)\|_{L^2(\Omega_0)}^2 - \frac{1}{2} \|\nabla V_s(0, \cdot)\|_{L^2(\Omega_0)}^2.$$

The term including the exterior potential $V_e$ is easily handled after an integration by part,

$$\left| \int_{\Omega_0} \int_0^{T} V_e \partial_s |\psi| dxd\mu \right| \leq \|V_e\|_{C^1([0,T], L^\infty(\Omega_0))} \left( n(T) + n(0) + \int_0^{T} n(s) ds \right).$$

The next step is to integrate (4.7) with respect to $\lambda$, to add (4.6) to it and to use (4.8), (4.10), (4.9), (4.11), (4.12) and hypothesis (3.16). Gathering the different estimates, we find,

$$\|\mathcal{E}\|_{L^1(0,T^*)} + \|n\|_{L^1(0,T^*)} + T_4 \leq C_1 + R_4 + C_2 \int_0^{T^*} \left( \|n\|_{L^1(0,T)} + \|\mathcal{E}\|_{L^1(0,T)} \right) dT, \quad (4.13)$$
easily shown that we have the same estimate as above for

\[ F_{\rho m, T}(\xi) = \int_{\mathbb{R}^+} \xi |F_{\rho m, T}(\xi)|^2 d\xi d\mu dT \]

and Lemma (4.1) yields

\[ \|F_{\rho m, T}^n\|_{L^2(\mathbb{R})} \leq C \left( \frac{\varepsilon}{p^2} \right)^{1/4} \|\xi^{1/4} F_{\rho m, T}^n\|_{L^2(\mathbb{R}^+)} + C \left( \frac{\varepsilon}{p^2} \right)^{1/2} \|F_{\rho m, T}^n\|_{L^2(\mathbb{R})}, \]

and Lemma (4.1) yields

\[ \|F_{\rho m, T}^n\|_{L^2(\mathbb{R})} = 2\pi \|\psi_{\rho m, T}^n\|_{L^2(0, T)} \leq 2\pi \|\psi_{\lambda}\|_{L^2(0, T), L^2(\Gamma_0)} \leq C \|\psi_{\lambda}\|_{L^2(0, T), L^2(\Gamma_0)} \|\nabla \psi_{\lambda}\|_{L^2(0, T), L^2(\Gamma_0)} \]
This allows to write
\[ R_4 \leq C_q + C_\eta \left( \|n\|_{L^1(0,T^\ast)} + \|\mathcal{E}\|_{L^1(0,T^\ast)} + T_4 \right), \]
so that the Gronwall lemma and (4.13) imply that \( \|n\|_{L^1(0,T^\ast)}, \|\mathcal{E}\|_{L^1(0,T^\ast)} \) are bounded independently of \( \varepsilon \) for any finite \( T^\ast > 0 \) and in turn so do \( T_4 \) and \( \|n\|_{L^\infty(0,T^\ast)} \) thanks to (4.5). In particular, we obtain that
\[ \sqrt{\varepsilon} \sum_{j,m} \int_\Lambda \sqrt{\varepsilon} \mathcal{F} \Phi_{j,m,T}^\varepsilon(\xi) d\mu \leq C, \quad (4.15) \]
where \( C \) is independent of \( \varepsilon \) and of the regularization parameter \( k \), and thus a bound in \( H^{1/4}((0,T),L^2(T_j)) \) for \( T_j \psi_A \).

To conclude the derivation of the different bounds, it remains to estimate \( V_s \). The fact that \( \|n\|_{L^\infty(0,T)} \) and \( \|\mathcal{E}\|_{L^1(0,T)} \) are bounded imply \( \int_\Lambda |\psi_\lambda|^2 d\mu(\lambda) \in L^2((0,T),W^{1,r}(\Omega_0)) \), with \( r < 2 \) for \( d = 2 \) and \( r = \frac{3}{2} \) for \( d = 3 \) which in turn gives \( V_s \in L^2((0,T),W^{3,4}(\Omega_0)) \), thanks to standard elliptic regularity results. We estimate now \( \partial_t V_s \) which is solution to
\[ \Delta \partial_t V_s = \text{div} \, J, \quad x \in \Omega_0, \quad \partial_t V_s = 0, \quad x \in \partial \Omega_0, \]
where \( J = 2n \varepsilon \int_\Lambda \overline{\psi}_\lambda \nabla \psi_\lambda d\mu(\lambda) \). \( J \) belongs to \( L^2((0,T),L^r(\Omega_0)) \), with same \( r \) as above. Elliptic regularity then implies that \( \partial_t V_s \) is in \( L^2((0,T),W^{1,r}(\Omega_0)) \). To get the \( \varepsilon \)-independent bound on \( \partial_t V_s \), we cannot use any Sobolev embeddings so that \( J \) is bounded independently of \( \varepsilon \) only in \( L^2((0,T),L^{1/4}(\Omega_0)) \), which implies the \( L^2((0,T),L^{r}(\Omega_0)) \) estimate announced in (3.17).

End of the proof of existence. So far, estimate (3.17) has been proved for regular data. It remains true at the limit for unregularized data as we will see in the sequel using standard compactness results. Thanks to (3.17),
\[ \psi_\lambda^k \in L^\infty((0,T),L^2(\Omega_0 \times \Lambda; dx dm)) \quad ; \quad \nabla \psi_\lambda^k \in L^2((0,T),L^2(\Omega_0 \times \Lambda; dx dm)), \]
with bounds independent of \( k \), so that \( \psi_\lambda^k \) converges weakly-* to a limit \( \psi_\lambda \in L^\infty((0,T),L^2(\Omega_0 \times \Lambda; dx dm)) \) as well as \( \nabla \psi_\lambda^k \), up to the extraction of a subsequence. Remember that \( \Phi^k \) converges strongly to \( \Phi \) in \( L^1(\mathbb{R}^+; L^1([0,n] \times \{1,\ldots,n\})) \) so that the weak-* limit of \( \psi_\lambda^k \) in \( L^\infty((0,T),L^2(\Omega_0 \times \Lambda; dx dm)) \) is equal to that of \( \psi_\lambda^k \) in \( L^\infty((0,T),L^2(\Omega_0 \times \Lambda; dx dm)) \). This implies that
\[ \|\psi_\lambda\|_{L^\infty((0,T),L^2(\Omega_0 \times \Lambda; dx dm))} \leq \liminf\|\psi_\lambda^k\|_{L^\infty((0,T),L^2(\Omega_0 \times \Lambda; dx dm))}, \]
with same relation for \( \nabla \psi_\lambda \) with an \( L^2 \) norm in time. Hence, estimate (3.17) is also verified at the limit by \( \psi_\lambda \) and \( \nabla \psi_\lambda \).

We pass now to the limit in the weak formulation (3.13). \( \psi_\lambda^k \) is obviously a solution to (3.13). Integrating with respect to \( \Lambda \) and choosing a test function \( u \) such that \( u \in C^1([0,T),L^2(\Omega_0 \times \Lambda; dx dm)) \) and \( \forall u \in C^1([0,T),L^2(\Omega_0 \times \Lambda; dx dm)) \), the non-boundary linear terms pass to the limit readily, only the boundary terms and the non-linear one require some attention. Thanks to the previously obtained bounds, we have for \( d = 2 \) or \( d = 3 \),
\[ V_s^k \in L^2((0,T),H^1_0(\Omega_0)) \quad ; \quad \partial_t V_s^k \in L^2((0,T),L^r(\Omega_0)), \]
where \( r < 2 \) when \( d = 2 \) and \( r < \frac{3}{2} \) when \( d = 3 \) with bounds independent of \( k \), so that there exists a subsequence still - denoted by \( V^k \) - such that \( V^k \) converges strongly to \( V^\star \) in \( L^2((0,T),L^r(\Omega_0)) \), for any \( 1 \leq r \leq 6 \), in three dimensions and \( 1 \leq r < \infty \), in two dimensions. See [31] for a standard compactness result. In the same way, thanks to standard Sobolev embeddings, \( \psi^k \) converges weakly - up to the extraction of a subsequence - to \( \psi_\lambda \) in \( L^2((0,T),L^{r/2}(\Omega_0 \times \Lambda;dxdu)) \) (where \( L^{r/2}(\Omega_0 \times \Lambda;dxdu) \) is defined as the Banach space of functions \( f \) such that \( \int_{\Omega_0} \| f(x,\cdot) \|_{L^{r/2}(\Lambda,d\mu)}(dx < \infty) \), for any \( 1 \leq r \leq 6 \), in three dimensions and \( 1 \leq r < \infty \), in two dimensions. This thus allows to pass to the limit in the non-linear term

\[
\int_0^T \int_{\Lambda} \int_{\Omega_0} V^k(s,x)\psi^k(s,x)u(s,x,\lambda)dxdsd\mu.
\]

It remains the boundary terms, namely

\[
\frac{1}{2} \sum_{j=1}^n \left[ \frac{e^{1/2}e^{-\nu/4}}{\varepsilon} \int_0^T \langle \mathcal{D}_{j,k}^{1/2}(\psi^\lambda),u \rangle_j ds + \varepsilon \int_0^T \langle \mathcal{A}_{j,k}(\psi^\lambda),w \rangle ds \right].
\]

The second one converges straightforwardly because of (4.3). The first one is treated thanks to its weak formulation (3.15). We know from (4.15) that \( T^1_{\psi^\lambda} \) is bounded in \( H^{1/4}((0,T),L^2(\Gamma_j)) \), independently of \( k \) so that thanks to (4.2),

\[
\int_0^T \langle \mathcal{D}_{j,k}^{1/2}(\psi^\lambda),u \rangle_j ds \to \int_0^T \langle \mathcal{D}_{j,k}^{1/2}(\psi^\lambda),u \rangle_j ds.
\]

Proceeding as in the proof of estimate (4.5), we obtain

\[
\| w(t,\cdot) \|_{L^2(\Omega_0)}^2 = \| w(t=0,\cdot) \|_{L^2(\Omega_0)}^2 + \sqrt{\varepsilon} \sum_{j=1}^n \int_0^t \langle \mathcal{D}_{j,k}(w),w \rangle_j ds + R_1 + R_2,
\]

where

\[
R_1 = -\varepsilon \sum_{j=1}^n \int_0^t \left( \int \left( \mathcal{D}_{j,k}^{1/2} - \mathcal{D}_{j,l}^{1/2} \right) (\psi^\lambda_j),w \right) \cdot ds,
\]

\[
R_2 = -\varepsilon \sum_{j=1}^n \int_0^t \left( \int \left( \mathcal{D}_{j,k}^{1/2} - \mathcal{D}_{j,l}^{1/2} \right) (\psi^\lambda_j),w \right) \cdot ds.
\]

The first term of the r.h.s goes to zero as \( k,l \to \infty \) thanks to (4.1), the second one is negative, the third one is treated using the Gronwall Lemma and that

\[
\| (V^k - V^\star) \psi^\lambda(t,\cdot) \|_{L^2(\Omega_0 \times \Lambda;dxdu)} \leq \| (V^k - V^\star) (t,\cdot) \|_{L^2(\Omega_0)} \| \psi^\lambda(t,\cdot) \|_{L^2(\Omega_0 \times \Lambda;dxdu)} \leq C\| w(t,\cdot) \|_{L^2(\Omega_0 \times \Lambda;dxdu)}.
\]
Moreover $R_1, R_2$ converge to zero as well thanks to (4.2), (4.3) and (4.15). \( \psi^k - \psi^l \) is thus a Cauchy sequence in $C^0([0,T], L^2(\Omega_0))$ so that the limit $\psi_\lambda$ belongs as well to this space.

It just remains to show that (3.13) is indeed verified almost everywhere in $\lambda$ and to treat the Poisson equation. For the first claim, it suffices to take a test function of the form $u(t,x)\phi(\lambda)$, with $u \in C^1([0,T), H^1(\Omega_0))$, $f \in L^2(\Lambda)$. For the Poisson equation, using a weak formulation, $V_\lambda^k$ passes straightforwardly to the limit, as well as $\int_{\lambda} |\psi^k_\lambda|^2 d\mu$. We only need to show that its limit equals $\int_{\lambda} |\psi_\lambda|^2 d\mu$. This requires some local estimates with respect to $\lambda$. Using the fact that the non-linear potential $V_\lambda^k$ is bounded, the density and energy estimates can be rewritten in local in $\lambda$ versions so as to obtain

$$\|\psi^k_\lambda\|_{L^2((0,T), H^1(\Omega_0))} \leq C(T) \left(1 + p^5 + \|\psi^0_\lambda\|_{L^2(\Omega_0)}^2 + \varepsilon^2 \|\nabla \psi^0_\lambda\|_{L^2(\Omega_0)}^2\right),$$

for some constant $C$ independent of $k$. Multiplying by $\Phi$, using (2.2) and hypothesis (H-3), we get a uniform in $\lambda$ bound for $\Phi \|\psi^k_\lambda\|_{L^2((0,T), H^1(\Omega_0))}$. We thus have that $\sqrt{\Phi} \psi^k_\lambda$ converges weakly - up to the extraction of a subsequence - in $L^2((0,T), L^2(\Omega_0))$ to $\sqrt{\Phi} \psi_\lambda$, $\lambda$ a.e., where $r \leq 6$ in three dimensions and $r < \infty$ in two dimensions. This allows then to identify the limit of $\int_{\lambda} |\psi^k|^2 d\mu$ with $\int_{\lambda} |\psi_\lambda|^2 d\mu$ and concludes the proof of existence.

**Uniqueness.** We claim that two solutions to (3.13) in $E^0$, $\psi_\lambda^i$, $i = 1,2$, with same initial condition verify the relation

$$\|\psi_\lambda^1 - \psi_\lambda^2\|_{L^2(\Omega_0)}^2 \leq \frac{2}{\varepsilon} \Im \int_{\Omega_0} \int_0^t (V^1_s - V^2_s) \psi_\lambda^1 \left(\overline{\psi_\lambda^2} - \psi_\lambda^2\right) dxds.$$

Such an estimate is proved in the same manner as the density estimate (4.6): by first deriving it with regular solutions, and then by passing to the limit. Following (4.16), it comes

$$\|(\psi_\lambda^1 - \psi_\lambda^2)(t,\cdot)\|_{L^2(\Omega_0 \times \Lambda, dx d\mu)} \leq C \int_0^t \mathcal{E}(s) \|(\psi_\lambda^1 - \psi_\lambda^2)(s,\cdot)\|_{L^2(\Omega_0 \times \Lambda, dx d\mu)} ds,$$

so that the Gronwall Lemma yields $\psi_\lambda^1 = \psi_\lambda^2$ since $\mathcal{E}$ is bounded in $L^1(0,T)$.

**Appendix A: some technical Lemmas.** We state first the following Lemma. The (easy) proof is left to the reader.

**Lemma 4.1.** Let $f \in H^{1/2}(0,T)$, and define:

$$\partial^{1/2} f := \frac{1}{\sqrt{\pi}} \frac{d}{dt} \int_0^t \frac{f(\tau)}{\sqrt{t-\tau}} d\tau, \quad 0 \leq t \leq T.$$

Denoting by $Ef$ the extension by zero outside $(0,T)$ and by $\widehat{f}$ its Fourier transform, we have the identities

$$\partial^{1/2} f = \frac{1}{\sqrt{\pi}} \frac{d}{dt} Ef * \left(\mathbb{1}_{\mathbb{R}_+} \frac{1}{\sqrt{\xi}}\right), \quad t \in \mathbb{R},$$

$$\widehat{\partial^{1/2} f}(\xi) = e^{\pi/4} \sqrt{\xi} \widehat{f}(\xi),$$

(4.17)
where $\sqrt{\cdot}$ stands for the complex square root with non-positive imaginary part and $\mathbb{1}_{\mathbb{R}^+}$ for the indicatrix function of $\mathbb{R}^+$.

The second Lemma basically states that if a function $g(x)$ belong to $L^2(\mathbb{R})$, as well as $|x|^{1/4}g(x)$, and if $g$ is the Fourier transform of a function with a bounded support, then $g$ decays as $|x|^{-1/4}$.

**Lemma 4.2.** Let $f$ be a function in $L^2(0,t)$. Denote by $Ef$ its extension by zero outside $(0,t)$ and let $\hat{f}$ be the Fourier transform of $Ef$. Assuming $k^{1/4}\,\hat{f}(k) \in L^2(\mathbb{R}^+)$, we have, for any $a > 0$, for $\xi \geq a$,

$$|\hat{f}(\xi)| \leq C \left( (1 + t) \xi^{-1/4} \|k^{1/4}\hat{f}\|_{L^2(\mathbb{R}^+)} + \xi^{-1/2} \|\hat{f}\|_{L^2(\mathbb{R})} \right),$$

where $C$ depends on $a$.

**Proof.** The proof strongly relies on the fact that we compute the Fourier transform of a function with bounded support. From the definition, we have

$$\hat{f}(\xi) = \int_{[-t,t]} f(s)e^{-i\xi s}ds = \mathbb{1}_{[0,t]}Ef = (H \ast \hat{f})(\xi)$$

where $H(\xi) = \mathbb{1}_{[0,t]} = (-i\xi)^{-1}(e^{-it\xi} - 1)$. $H$ verifies

$$|H(\xi)| \leq t, \quad \forall \xi \in \mathbb{R}; \quad |H(\xi)| \leq \frac{2}{|\xi|}, \quad \forall |\xi| > 0. \quad (4.18)$$

We assume that $\xi \geq a > 0$. The convolution $H \ast \hat{f}$ is then split into four terms, with $0 < \beta < a$:

$$\int_{\mathbb{R}} H(\xi - y) \hat{f}(y)dy = \int_{\mathbb{R}^+} + \int_{0}^{\xi - \beta} + \int_{\xi - \beta}^{\xi + \beta} + \int_{\xi + \beta}^{+\infty} = I_1 + I_2 + I_3 + I_4.$$

Having in mind that $\xi \geq a > 0$, if follows readily from (4.18) that

$$I_1 \leq \|H(\xi + \cdot)\|_{L^2(\mathbb{R}^+)} \|\hat{f}\|_{L^2(\mathbb{R})} \leq 2 \xi^{-1/2} \|\hat{f}\|_{L^2(\mathbb{R})}.$$

Concerning $I_2$, we have

$$I_2 \leq \left( \int_{0}^{\xi - \beta} \frac{H(\xi - y)^2}{y^{1/2}} \frac{dy}{y^{1/2}} \right)^{1/2} \|\hat{f}(y)\|_{L^2(\mathbb{R}^+)},$$

$$\leq 2 \left( \int_{0}^{\xi - \beta} \frac{dy}{|\xi - y|^2 y^{1/2}} \right)^{1/2} \|\hat{f}(y)\|_{L^2(\mathbb{R}^+)}. $$

Consider now an $\alpha$ such that $0 < \alpha < 1 - \beta/a < 1 - \beta/\xi$ and $\alpha < a$. Then

$$\int_{0}^{\xi - \beta} \frac{dy}{|\xi - y|^2 y^{1/2}} = \frac{1}{\xi^{3/2}} \int_{0}^{1-\beta/\xi} \frac{dy}{|y-1|^2 y^{1/2}},$$

$$= \int_{0}^{\alpha} + \int_{\alpha}^{1-\beta/\xi},$$

$$\leq \frac{1}{\xi^{3/2}} \frac{2\alpha^{1/2}}{(1-\alpha)^2} + \frac{1}{\xi^{3/2}} \frac{1}{\alpha^{1/2}} \left( \frac{\xi}{\beta} + \frac{1}{1-\alpha} \right),$$

$$= O(\xi^{-1/2}).$$
Proceeding analogously, $I_3$ is easily estimated thanks to (4.18),

$$I_3 \leq \frac{t}{\sqrt{9}} \left[ \int_0^{1/3} \frac{dy}{y^{1/2}} \right]^{1/2} \|y^{1/4} \hat{f}(y)\|_{L^2(\mathbb{R}^+)}.$$

In the same way,

$$I_4 \leq \frac{2}{\sqrt{3 \beta}} \|y^{1/4} \hat{f}(y)\|_{L^2(\mathbb{R}^+)}.$$

The proof is then ended by gathering the different estimates on $I_1$, $I_2$, $I_3$ and $I_4$. □

**Remark 4.3.** The previous lemma can be generalized to functions of the form $g(s)f(s)$ where $f$ satisfies the hypothesis of the lemma and $g$ is a $C^1([0,t])$ function. Indeed, in this case the convolution kernel $H$ verifies, instead of (4.18),

$$|H(\xi)| \leq C_1, \quad \forall \xi \in \mathbb{R} ; \quad |H(\xi)| \leq \frac{C_2}{|\xi|}, \quad \forall |\xi| > 0,$$

for two positive constants $C_1$ and $C_2$, so that the proof of the lemma still applies. The result is thus

$$|\hat{f}g(\xi)| \leq C \left( 1 + t \right) \xi^{-1/2} \|k^{1/4} \hat{f}\|_{L^2(\mathbb{R}^+)} + \xi^{-1/2} \|\hat{f}\|_{L^2(\mathbb{R})},$$

where the constant $C$ depends on $\|g\|_{C^1([0,t])}$. That relation is used at the end of the proof of the energy estimate.

The last Lemma is a reformulation of a standard trace theorem when considering flat boundaries. Notice that applying straightforwardly the existing results would have given

$$\|\varphi\|_{L^2(\Gamma_j)} \leq C\|\varphi\|_{L^2(\Omega_0)} \|\nabla \varphi\|_{L^2(\Omega_0)}, \quad j = 1, \ldots, n,$$

while we have the following Lemma:

**Lemma 4.1.** Let $\varphi \in H^1(\Omega_0)$ where $\Omega_0$ is smooth (at least $C^1$) and is defined in section 2. Assume that the trace of $\varphi$ vanishes on $\Gamma_0$. Then there exists $C > 0$ such that

$$\|\varphi\|_{L^2(\Gamma_j)} \leq C\|\varphi\|_{L^2(\Omega_0)} \|\nabla \varphi\|_{L^2(\Omega_0)}, \quad j = 1, \ldots, n.$$

**Proof.** We assume that $\varphi$ is regular proceed by density to conclude. Let us parametrize $\Omega_0$ by an orthogonal set of coordinates $x = (x', \eta)$ such that if $\eta = 0$, $x$ belongs to the plane into which $\Gamma_j$ is included. Such construction is possible since the interface $\Gamma_j$ is plane. Thus $\varphi(x',0)$ is the trace of $\varphi$ on $\Gamma_j$ for $x' \in \Gamma_j$. We have

$$|\varphi(x',\eta)|^2 = |\varphi(x',0)|^2 + 2Re \int_0^\eta \varphi(x',y) \frac{\partial \varphi(x',y)}{\partial y} dy.$$

Then, the Cauchy-Schwarz inequality implies

$$\|\varphi\|_{L^2(\Gamma_j)}^2 \leq \|\varphi\|_{L^2(\Omega_0)}^2 + 2\|\varphi\|_{L^2(\Omega_0)} \|\nabla \varphi\|_{L^2(\Omega_0)}.$$

Finally, the Poincaré inequality allows to control $\|\varphi\|_{L^2(\Omega_0)}$ in terms of $\|\nabla \varphi\|_{L^2(\Omega_0)}$ and this concludes the proof. □
Appendix B: sketch the regularization. The particular geometry and the different assumptions made on the data render the problem not straightforward to regularize. Indeed, the initial wave function is supposed to crucially solve a Schrödinger equation in each wave guide and the potentials have as well some important properties. We give here the main ideas about how this procedure can be pursued.

Let \( \rho \) be a standard mollifier such that \( 0 \leq \rho \leq 1, \rho \in C^\infty(\mathbb{R}^d), \| \rho \|_{L^1} = 1 \) and whose support is included in the unit ball centered at zero. We denote by \( \rho^\delta := \rho(\frac{x}{\delta}) \) and by \( E \) either an extension operator from \((0,T) \times \Omega \) to \( \mathbb{R}^{d+1} \) or from \( \Omega \) to \( \mathbb{R}^d \), see [1]. Let \( V_\varepsilon \in C^1([0,T],L^\infty(\Omega)) \) be in the class of potentials introduced in section 2.3, and define \( V^\varepsilon := \rho^\delta * (\rho^\delta * E V_\varepsilon) \), where we use a one-dimensional mollifier for the time variable. Then \( V_\varepsilon \in C^\infty(\mathbb{R}^{d+1}) \) and \( V_\varepsilon \) converges strongly to \( V_\varepsilon \) in \( C^1([0,T],L^p(K)) \), \( p < \infty \), for any bounded set \( K \subset \Omega \). It is assumed in each wave guide \( \Omega_j \) (equipped with the set of coordinates \( (\xi_j, \eta_j) \)) that \( V_\varepsilon \) satisfies \( V_\varepsilon(t,x) = V_0^\varepsilon(\xi_j) + V_j(t) \), which is not true for \( V^\varepsilon \).

Nevertheless, as soon as \( \eta_j \geq \delta \), \( V^\varepsilon \) shares a similar structure, that is \( V^\varepsilon(t,x) = \rho^\delta(\xi_j) + V^\varepsilon(t) \), where \( V^\delta(\xi_j) := \int_{\varepsilon-\delta}^{\varepsilon+\delta} E V_\varepsilon(z) \rho(\xi_j - z,y) \) \( dz \, dy \) and \( V_j^\varepsilon = \rho \ast E V_j \). This suggests to define a fixed parameter \( \delta_0 \), with \( 0 < \delta < \delta_0 \), such that the transparent boundary conditions are prescribed on \( \Gamma^\delta_j = \{ (\eta_j, \xi_j) \in \Omega_j, \xi_j \in \Gamma_j, \eta_j = \eta_0 \} \). It is not possible to define them for \( x \in \Omega_j, \eta_j < \delta \), since \( V^\varepsilon \) does not satisfy the adequate decomposition.

In the same way, let \( \psi^0,\delta := \chi^\delta \rho^\delta \ast E (\psi^0) \in C^\infty(\Omega) \), where \( \chi \) is a cut-off which ensures that \( \psi^0,\delta \) vanishes on the boundary \( \partial \Omega \). \( \psi^0,\delta \) converges strongly to \( \psi^0 \) in \( H^1(K) \), for any bounded set \( K \subset \Omega \). Let now \( \chi_{m,j} \) be the solution to (2.1) with the regularized potential \( V^0,\delta \) and \( E_j \) be the associated eigenvalue. According to the regularity of the potential, \( \chi_{m,j} \) \( \in C^\infty(\Gamma_j) \). In each guide \( \Omega_j \), \( \psi^0 \) reads:

\[
\psi^0,\delta(\xi_j, \eta_j) = \sum_m \left[ \chi^0,\delta(\xi_j) \delta_m \varphi^0,\delta \exp\left( \frac{-i \eta_j}{\varepsilon} \sqrt{2(E(\lambda) - E_m^\delta)} \right) 
+ b_m \exp\left( \frac{i \eta_j}{\varepsilon} \sqrt{2(E(\lambda) - E_m^\delta)} \right) \right].
\]

This leads to the definition of

\[
\varphi^0,\delta(\xi_j, \eta_j) = \sum_m \left[ \chi^0,\delta(\xi_j) \delta_m \varphi^0,\delta \exp\left( \frac{-i \eta_j}{\varepsilon} \sqrt{2(E(\lambda) - E_m^\delta)} \right) 
+ b_m \exp\left( \frac{i \eta_j}{\varepsilon} \sqrt{2(E(\lambda) - E_m^\delta)} \right) \right],
\]

so that \( \varphi^0 \in C^\infty(\Omega_j) \) and \( \varphi^0 \) converges strongly to \( \psi^0 \) in \( H^1(K) \), for any bounded set \( K \subset \Omega_j \). In each wave guide, we thus have, for \( \eta_j \geq 0, \)

\[
-\frac{\varepsilon^2}{2} \Delta \varphi^0,\delta + V^0,\delta \varphi^0,\delta = E(\lambda) \varphi^0,\delta.
\]

Let \( \chi \) be another smooth cut-off function equal to one on \( \Omega_0 \) and whose support is included in the set \( \{ x \in \mathbb{R}^d, \eta_j \leq \delta_0, j = 1, \ldots, n \} \) and let \( \psi^0,\delta = \chi \psi^0,\delta + (1 - \chi) \varphi^0,\delta \). We have \( \psi^0,\delta \in C^\infty(\Omega), \) and \( \psi^0,\delta \) converges strongly to \( \psi^0 \) in \( H^1(K) \), for any bounded set \( K \subset \Omega \).
Consider now the following regularized Schrödinger-Poisson problem:

\[
\frac{i\varepsilon}{\partial \psi_{\lambda}^{\delta}} = -\frac{\varepsilon^2}{2} \Delta \psi_{\lambda}^{\delta} + (V_{\delta}^{e} + V_{\delta}^{s}) \psi_{\lambda}^{\delta}; \quad \psi_{\lambda}^{\delta}(t = 0, \cdot) = \overline{\psi_{\lambda}^{\delta}}; \quad x \in \Omega,
\]

\[-\Delta V_{\delta}^{s} = \int_{\Lambda} |\psi_{\lambda}^{\delta}|^2 d\mu(\lambda); \quad x \in \Omega_0; \quad V_{\delta}^{s}|_{\partial \Omega_0} = 0.
\]

Define as well:

\[
\psi_{\lambda}^{pw,\delta} = \overline{\psi_{\lambda}^{\delta}} \sum_{j=1}^{n} \mu_j \theta_{j,\delta}^{\lambda}; \quad \theta_{j,\delta}^{\lambda}(t) = \exp \left( -\frac{i}{\varepsilon} \int_{0}^{t} (E(\lambda) + V_{j}^{\delta}(s)) ds \right),
\]

where \((\mu_j)\) is the partition of unity introduced in section 2.1. The previous construction of \(\overline{\psi_{\lambda}^{\delta}}\) and \(V_{\delta}^{e}\) insures that

\[
\frac{i\varepsilon}{\partial \psi_{\lambda}^{pw,\delta}} = -\frac{\varepsilon^2}{2} \Delta \psi_{\lambda}^{pw,\delta} + (V_{\delta}^{e} + V_{\delta}^{s}) \psi_{\lambda}^{pw,\delta}; \quad x \in \Omega_j, \quad \eta_j \geq \delta_0,
\]

so that Theorem 3.1 applies and provides a unique strong solution \((\psi_{\lambda}^{\delta}, V_{\delta}^{s})\), the \(C^\infty\) regularity is easily deduced from that of the data. Moreover, \(\psi_{\lambda}^{\delta}\) verifies:

\[
\frac{\partial}{\partial \eta_j} (\psi_{\lambda}^{\delta} - \psi_{\lambda}^{pw,\delta}) = -\frac{e^{-i\pi/4}}{\sqrt{\varepsilon}} D_{j,\delta}^{1/2} (\psi_{\lambda}^{\delta} - \psi_{\lambda}^{pw,\delta}); \quad x \in \Gamma_{j_0}^{\delta}.
\]

The definition of \(D_{j,\delta}^{1/2}\) is the same as (3.5), \(\chi_{m}^{0,j}\) being replaced by \(\chi_{m}^{0,j,\delta}\) so that we have (4.1)–(4.3).

For the sake of clarity of the paper and without loss of generality, we abusively decided to set the boundary conditions in the proof of theorem on the interfaces \(\Gamma_j\) instead of \(\Gamma_{j_0}^{\delta}\).

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REFERENCES

Uniform bounds and weak solutions to an open Schrödinger-Poisson system