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 ε 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]

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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 conjuguate 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, λ is a given quantum number and the Hamiltonian is defined by

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

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 μ. In [12], the model is shown to have a unique strong solution (ψ_λ, 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 ε ($\varepsilon := \hbar := \frac{\hbar}{\sqrt{m_e}}$ 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 φ^* denotes the complex conjugate of φ and d the dimension. If φ is solution to the time-dependent Schrödinger equation with potential $V(t,x)$, then its Wigner transform W^ε is solution to the Wigner equation, namely

$$\frac{\partial W^\varepsilon}{\partial t} + k \cdot \nabla_x W^\varepsilon + K *_k W^\varepsilon = 0,$$
$$K(t,x,k) = \frac{i}{(2\pi)^d} \int_{\mathbb{R}^d} e^{-ik\cdot y} \varepsilon^{-1} \left(V(t,x+\frac{\varepsilon}{2}y) - V(t,x-\frac{\varepsilon}{2}y) \right) dy.$$

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^ε in some sense. The Vlasov equation 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 ε 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 ε. This work thus provides uniform bounds in L^2_{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 this 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 Ω and its dimension by d. It is assumed in the sequel that $d=2$ or $d=3$. The domain Ω is then split into two zones, a *bounded active zone* denoted by Ω_0 and an *unbounded access zone*, consisting of n wave guides Ω_j, $j=1,\cdots,n$, see figure 2.1. The interfaces between Ω_0 and each Ω_j are supposed to be *flat* and are denoted by Γ_j. The waveguides Ω_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, η_j is basically the variable associated with the direction of propagation in the lead j. The outer boundaries of the Γ_j's are denoted by $\Gamma_{j,0}$. The remaining part of the boundary of Ω_0 is denoted by Γ_0 so that $\partial\Omega_0=\Gamma_0\bigcup\left(\cup_{j=1}^n\Gamma_j\right)$. We also introduce

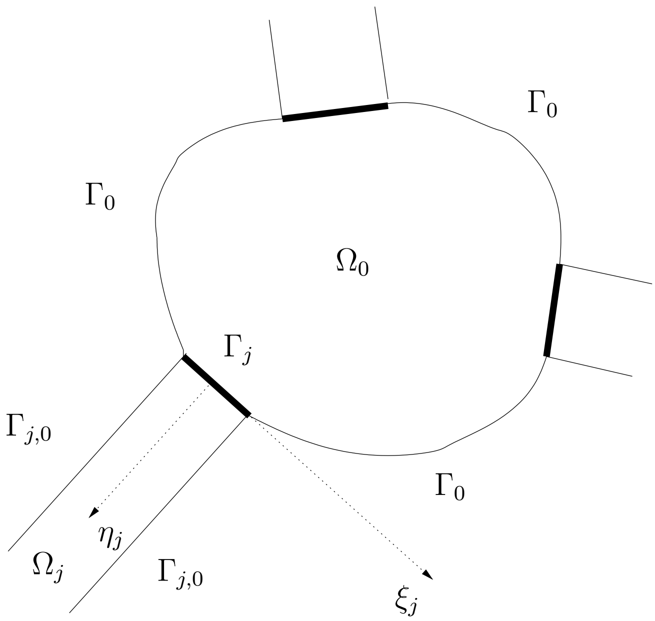

FIG. 2.1. *The domain* Ω

$(\mu_j)_{j=1,\cdots,n}$, a partition of unity of Ω, *i.e.* some $\mathcal{C}^\infty(\Omega)$ functions which satisfy

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

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 Ω_j, *i.e.*

$$V^0\in L^\infty(\Omega) \qquad ; \qquad V^0\big|_{\Omega_j}=V^0(\xi_j).$$

The fact that V^0 does not depend on η_j is necessary to be able to construct rather simple - though not obvious - boundary conditions on the interfaces Γ_j, $j\neq 0$. When V^0 is linear in η_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 $\mathcal{H}_j^0=-\frac{\varepsilon^2}{2}\Delta_{\xi_j}+V^0(\xi_j)$, 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*

$$\begin{cases} \mathcal{H}_j^0\chi_m^{0,j}=E_m^j\chi_m^{0,j}, & m\in\mathbb{N}^*, \quad j=1,\cdots,n, \\ \chi_m^{0,j}\in H_0^1(\Gamma_j), & \displaystyle\int_{\Gamma_j}\chi_m^{0,j}\overline{\chi_{m'}^{0,j}}\,d\sigma_j=\delta_{m,m'}, \end{cases} \tag{2.1}$$

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

$$\langle f,g\rangle_j:=\int_{\Gamma_j}f(\xi_j)\overline{g}(\xi_j)\,d\sigma_j, \qquad f_m^j:=\int_{\Gamma_j}f(\xi_j)\overline{\chi}_m^j(\xi_j)\,d\sigma_j.$$

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

We suppose without loss of generality that $E_m^j\geq 0$, $\forall m\geq 1$, $\forall j\geq 1$, it suffices in the sequel to multiply the time-dependent Schrödinger equation by the phase factor $e^{i\frac{t}{\varepsilon}\min_{j,m}E_m^j}$ to recover the general case where V_j 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 μ. μ is a non-negative measure on the state space Λ, and a pure state is denoted by λ. The wave functions are thus indexed by λ. Consider the following hypotheses for a family of function $\psi_\lambda^0\in H^1_{loc}(\Omega)$:

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

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

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

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

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

$$d\mu(\lambda)=\Phi(p,m_0,j_0)\,dp\,\delta(m_0)\,\delta(j_0),$$

where δ denotes the Dirac measure and the positive function $\Phi\in L^1(\mathbb{R}_+^*,\ell^1(\mathbb{N}^*\times\{1,\cdots,n\}))$ 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 $E_{m_0}^{j_0}$ is the transversal energy in the lead j_0. We add the following hypothesis on the measure μ,

$$\int_\Lambda (1+p^5)d\mu<+\infty, \tag{2.2}$$

and a local in λ version of (**H-2**):

(H-3) for any bounded set $K\subset\Omega$, there exists $C'_K>0$ finite and independent of λ such that

$$\Phi(\lambda)\|\psi_\lambda^0\|^2_{H^1(K)}\leq C'_K.$$

A family $\psi_\lambda^0\in H^1_{loc}(\Omega)$ 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 Γ_j, allowing for a simplification to a boundary value problem on the bounded domain Ω_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 ψ_λ^0 to Ω_j is projected on the transversal basis $(\chi_m^{0,j})_m$, *i.e.* $\psi_\lambda^0\big|_{\Omega_j}(\xi_j,\eta_j)=\sum_m\chi_m^{0,j}(\chi_j)f^j(\eta_j)$ so that f^j verifies, according to **(H-1)**,

$$-\frac{\varepsilon^2}{2}\frac{\partial^2 f^j}{\partial\eta_j^2}=(E(\lambda)-E_m^j)f^j,\qquad \eta_j\in\mathbb{R}^+,$$

and thus reads $f^j(\eta_j)=a_m^j\exp(-\frac{i\eta_j}{\varepsilon}\sqrt[+]{2(E(\lambda)-E_m^j)})+b_m^j\exp(\frac{i\eta_j}{\varepsilon}\sqrt[+]{2(E(\lambda)-E_m^j)})$. Above, $\sqrt[+]{\ }$ denotes the complex square root with a non-negative imaginary part, b_m^j is an unknown coefficient depending on the solution and a_m^j 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 momemtum p, on the transversal mode m_0 and with an amplitude one so that $a_m^j=\delta_j^{j_0}\delta_m^{m_0}$ and $E(\lambda)=\frac{1}{2}p^2+E_{m_0}^{j_0}$. The modes associated with $E_m^j<E(\lambda)$ are the propagating modes and the ones with $E_m^j>E(\lambda)$ are the evanescent modes. When $j=j_0$, b_m^j is a reflection coefficient, and when $j\neq j_0$, it is a transmission coefficient. The boundary conditions are obtained by eliminating b_m^j and formally read

$$\varepsilon\left.\frac{\partial\psi_\lambda^0}{\partial\eta_j}\right|_{\Gamma_j}=\mathbb{Z}_j[E(\lambda)](\psi_\lambda^0)+\mathbb{S}_j[E(\lambda)]. \tag{2.3}$$

These relations are impedance-like boundary conditions. The operator $\mathbb{Z}_j[E(\lambda)]$ corresponds to an homogeneous part while $\mathbb{S}_j[E(\lambda)]$ is a source term. They read

$$\mathbb{Z}_j[E(\lambda)](\psi_\lambda^0) = i\sum_{m=1}^{\infty} \sqrt[+]{2(E(\lambda)-E_m^j)}\,\psi_m^{0,j}\,\chi_m^{0,j}(\xi_j), \tag{2.4}$$

$$\mathbb{S}_j[E(\lambda)] = -2i\,\delta_j^{j_0}\,p\,\chi_{m_0}^{0,j}(\xi_j), \tag{2.5}$$

$$\psi_m^{0,j} = \left\langle \psi_\lambda^0(\eta_j=0,\cdot), \chi_m^{0,j} \right\rangle_j.$$

It is shown in [10] that these boundary conditions actually make sense in a weak formulation for every $\psi_\lambda^0 \in H^1(\Omega_0)$, 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 $\mathcal{V}$ if it satisfies:

1. $V \in \mathcal{C}^1([0,T], L^\infty(\Omega))$,
2. for any $j=1,\cdots,n$, 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

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

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

$$\psi_\lambda = 0 \quad ; \quad x\in \Gamma_0 \bigcup \left(\cup_{j=1}^n (\Gamma_{j,0}\times\mathbb{R}^+)\right), \tag{3.3}$$

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

where V_e belongs to the class of potentials $\mathcal{V}$ and ψ_λ^0 belongs to the class of initial conditions. Notice that the Schrödinger equation is set on the whole domain Ω 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 Ω_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

$$\chi_m^j(t,\xi_j) := \chi_m^{0,j}(\xi_j)\exp\left(-\frac{i}{\varepsilon}\int_0^t (V_j(\tau)+E_m^j)\,d\tau\right).$$

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

$$H^{1/2}(0,T) = \left\{ f\in L^2(0,T), \quad \textit{such that} \int_0^T\int_0^T \frac{|f(s)-f(\tau)|^2}{(s-\tau)^2}dsd\tau < \infty \right\}.$$

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

$$\mathbb{D}_j^{1/2} f(t,\xi_j) := \sqrt{2}\sum_{m\geq 1}\chi_m^j(t,\xi_j)\,\partial^{1/2}\left\langle f(t,\cdot),\chi_m^j(t,\cdot)\right\rangle_j. \tag{3.5}$$

Let now

$$\psi_\lambda^{pw} := \psi_\lambda^0\sum_{j=1}^n \mu_j\,\theta_\lambda^j, \tag{3.6}$$

$$\theta_\lambda^j(t) := \exp\left(-\frac{i}{\varepsilon}\int_0^t (E(\lambda)+V_j(s))\,ds\right), \tag{3.7}$$

where $(\mu_j)_j$ is the partition of unity introduced in section 2.1. Then, according to [12], the wave function ψ_λ satisfies the following boundary conditions,

$$\frac{\partial}{\partial\eta_j}(\psi_\lambda-\psi_\lambda^{pw}) = -\frac{e^{-i\pi/4}}{\sqrt{\varepsilon}}\,\mathbb{D}_j^{1/2}(\psi_\lambda-\psi_\lambda^{pw}) \quad ; \quad x\in\Gamma_j, \quad j=1,...,n.$$

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:

$$i\varepsilon\partial_t\psi_\lambda = \mathcal{H}(t)\psi_\lambda \quad ; \quad \psi_\lambda(0,\cdot)=\psi_\lambda^0 \quad ; \quad x\in\Omega_0 \quad ; \quad \lambda\in\Lambda, \tag{3.8}$$

$$\frac{\partial}{\partial\eta_j}(\psi_\lambda-\psi_\lambda^{pw}) = -\frac{e^{-i\pi/4}}{\sqrt{\varepsilon}}\,\mathbb{D}_j^{1/2}(\psi_\lambda-\psi_\lambda^{pw}) \quad ; \quad x\in\Gamma_j, \tag{3.9}$$

$$\psi_\lambda = 0 \quad ; \quad x\in\Gamma_0, \tag{3.10}$$

$$-\Delta V_s = \int_\Lambda |\psi_\lambda|^2 d\mu(\lambda) \quad ; \qquad x\in\Omega_0 \quad ; \quad V_s|_{\partial\Omega_0} = 0. \tag{3.11}$$

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 Ω_0 and on Γ_j, respectively. The exact statement is the following:

THEOREM 3.1. *[12]. Let $V_e \in \mathcal{V}$, ψ_λ^0 verifying hypothesis* **(H-1)**, *$d=2$ or $d=3$, and in addition*

$$\int_\Lambda \|\psi_\lambda^0\|_{H^2(K)}^2 d\mu(\lambda) < \infty \quad ; \quad \Phi \text{ has a compact support,}$$

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 (ψ_λ, V_s) to (3.1)–(3.4) such that

$$\psi_\lambda \in \psi_\lambda^{pw} + \mathcal{C}^0([0,T], H^2(\Omega)) \cap \mathcal{C}^1([0,T], L^2(\Omega)), \qquad \lambda \, a.e.,$$

$$V_s \in \mathcal{C}^0([0,T], H_0^1(\Omega)) \cap \mathcal{C}^0([0,T], H^4(\Omega)) \cap \mathcal{C}^1([0,T], H^2(\Omega)),$$

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 ε of the different bounds on ψ_λ 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 λ, $\psi_\lambda \in \mathcal{C}^\infty([0,T] \times \Omega)$ when $\psi_\lambda^0 \in \mathcal{C}^\infty(\Omega)$ and $V_e \in \mathcal{C}^\infty([0,T] \times \Omega)$. We will use this regularity further to use ψ_λ 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 ε-independent estimates. More precisely, the boundary condition (3.9) is split into homogeneous and inhomogeneous parts, that is

$$\frac{\partial \psi_\lambda}{\partial \eta_j} = -\frac{e^{-i\pi/4}}{\sqrt{\varepsilon}} \mathbb{D}_j^{1/2}(\psi_\lambda) + \mathbb{A}_j^\varepsilon(\psi_\lambda^{pw}),$$

where

$$\mathbb{A}_j^\varepsilon(\psi_\lambda^{pw}) := \left.\frac{\partial \psi_\lambda^{pw}}{\partial \eta_j}\right|_{\Gamma_j} + \frac{e^{-i\pi/4}}{\sqrt{\varepsilon}} \mathbb{D}_j^{1/2}(\psi_\lambda^{pw}),$$

$$= \frac{1}{\varepsilon}\left(\mathbb{Z}_j[E(\lambda)](\psi_\lambda^0) + \mathbb{S}_j[E(\lambda)]\right)\theta_\lambda^j + \frac{e^{-i\pi/4}}{\sqrt{\varepsilon}} \; \mathbb{D}_j^{1/2}(\psi_\lambda^{pw}). \tag{3.12}$$

Note here that we used the stationary open boundary conditions (2.3) to define $\mathbb{A}_j^\varepsilon(\psi_\lambda^{pw})$. The solutions to (3.8) are sought under the following weak form: let $u \in \mathcal{C}^1([0,T), H^1(\Omega_0))$ 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 λ a.e.,

$$-i\varepsilon \int_0^T (\psi_\lambda, \partial_s u) ds = i\varepsilon(\psi_\lambda^0, u(0,\cdot)) + \frac{1}{2}\varepsilon^2 \int_0^T (\nabla \psi_\lambda, \nabla u) ds + \int_0^T (V \psi_\lambda, u) ds$$

$$+\frac{1}{2}\sum_{j=1}^{n}\left[\varepsilon^{3/2}e^{-i\pi/4}\int_0^T\langle\mathbb{D}_j^{1/2}(\psi_\lambda),u\rangle_j\,ds-\varepsilon^2\int_0^T\langle\mathbb{A}_j^\varepsilon(\psi_\lambda^{pw}),u\rangle_j\,ds\right].\tag{3.13}$$

When the potential V_e belongs to the class $\mathcal{V}$, it is rather natural to consider wave-functions ψ_λ solution to (3.13) belonging to $L^2((0,T),H^1(\Omega_0))\cap\mathcal{C}^0([0,T],L^2(\Omega_0))$. 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 $f\in L^2((0,T),L^2(\Gamma_j))$, let

$$\mathcal{T}_j f(t,\xi_j):=\sum_{m\geq 1}e^{\frac{i}{\varepsilon}\int_0^t(E_m^j+V_j(s))ds}\left\langle f(t,\cdot),\chi_m^{0,j}\right\rangle_j\chi_m^{0,j}(\xi_j),\tag{3.14}$$

and let $(\mathcal{T}_j f)_m:=\langle\mathcal{T}_j f,\chi_m^{0,j}\rangle$. Consider now the functional space

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

and let E^0 be the space of functions belonging to E with a vanishing trace on Γ_0, *i.e.*

$$\mathsf{E}^0=\big\{\varphi\in\mathsf{E},\quad\text{such that}\quad\varphi_{|\Gamma_0}=0\big\}.$$

In the weak formulation (3.13), the boundary term $\int_0^T\langle\mathbb{D}_j^{1/2}(\psi_\lambda),u\rangle\,ds$ 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:

$$\int_0^T\langle\mathbb{D}_j^{1/2}(\psi_\lambda),u\rangle\,ds=\frac{e^{i\pi/4}}{2\pi}\sum_{m\geq 1}\int_{\mathbb{R}}\bar{\sqrt{\xi}}\,\mathcal{F}\big(\widetilde{\mathcal{T}_j\psi_\lambda}\big)_m\overline{\mathcal{F}\big(\widetilde{\mathcal{T}_j u}\big)_m}\,d\xi.\tag{3.15}$$

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

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 ε for the density n and energy $\mathcal{E}$ defined below:

THEOREM 3.2. *Let ψ_λ^0 belongs to the class of initial data, let $V_e\in\mathcal{V}$ and assume μ verifies* (2.2). *Let*

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

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

$$V_s\in L^2((0,T),W^{3,r}(\Omega_0))\cap H^1((0,T),W^{1,r}(\Omega_0))\qquad;\qquad\psi_\lambda\in E^0,$$

with $r<2$ *when* $d=2$ *and* $r=\frac{3}{2}$ *when* $d=3$*. Moreover, assuming that*

$$n(0)+\mathcal{E}(0)+\varepsilon\left|\sum_{j=1}^{n}\int_{\Lambda}\left\langle\mathbb{Z}_j[E(\lambda)](\psi_\lambda^0),\psi_\lambda^0\right\rangle_j d\mu\right|\leq C_0, \tag{3.16}$$

where C_0 *is independent of* ε*, there exists* C_1*, depending on* C_0*, on* $\|V_e\|_{\mathcal{C}^1([0,T],L^\infty(\Omega))}$*, on* $\|p\|_{L^5(\Lambda,d\mu)}$*, on* r*, and independent of* ε *as well such that,*

$$\|n\|_{L^\infty(0,T)}+\|\mathcal{E}\|_{L^1(0,T)}+\|\partial_t V_s\|_{L^2((0,T),L^r(\Omega_0))}\leq C_1, \tag{3.17}$$

where $r<2$ *when* $d=2$ *and* $r<\frac{3}{2}$ *when* $d=3$*.*

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 ε-independent estimates is more involved and requires a careful analysis of the boundary term $\mathbb{A}_j^\varepsilon(\psi_\lambda^{pw})$. Indeed, the term $\varepsilon\langle\mathbb{A}_j^\varepsilon(\psi_\lambda^{pw}),\psi_\lambda\rangle_j$ can be straightforwardly bounded by $C_0\|\psi_\lambda\|_{L^2(\Gamma_j)}\|\psi_\lambda^0\|_{H^{1/2}(\Gamma_j)}$ for some positive constant C_0 independent of ε ; by means of trace theorems, this bound turns into $\varepsilon^{-1/2}C_1\|\psi_\lambda\|^{1/2}_{L^2(\Omega_0)}\|\varepsilon\nabla\psi_\lambda\|^{1/2}_{H^1(\Omega_0)}\|\psi_\lambda^0\|_{H^{1/2}(\Gamma_j)}$ which has a wrong homogeneity in ε whatever the available bound on ψ_λ^0. We thus expect some compensations or averaging between the homogeneous stationary boundary conditions given by $\mathbb{Z}_j$ 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 ε-independent estimates rely as well on the verification of assumption (3.16). If the initial condition ψ_λ^0 is a solution to the Schrödinger equation not only in the leads but also in Ω_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 Γ_j's while they could have been set anywhere further in the guides. Doing so would have led to $L^2_{loc}(\Omega)$ estimates for the density and for the energy.

Proposition 3.3. *Let* $\mathbb{A}_j^\varepsilon$ *be defined in* (3.12), ψ_λ^{pw} *in* (3.6), $\mathbb{S}_j[E(\lambda)]$ *in* (2.5) *and* $\theta_\lambda^j(t)$ *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,* λ *a.e,*

$$\int_0^t\langle\mathbb{A}_j^\varepsilon(\psi_\lambda^{pw}),u\rangle_j\,ds=\frac{1}{\varepsilon}\int_0^t\langle\mathbb{S}_j[E(\lambda)]\theta_\lambda^j,u\rangle_j\,ds. \tag{3.18}$$

Proof. Setting

$$\mathbb{B}_j(\psi_\lambda^{pw})=\frac{1}{\varepsilon}\mathbb{Z}_j[E(\lambda)](\psi_\lambda^0)\theta_\lambda^j\quad;\quad\mathbb{C}_j(\psi_\lambda^{pw})=\frac{e^{-i\pi/4}}{\sqrt{\varepsilon}}\;\mathbb{D}_j^{1/2}(\psi_\lambda^{pw}),$$

(3.18) is equivalent to showing that $\int_0^t\langle\mathbb{B}_j(\psi_\lambda^{pw})+\mathbb{C}_j(\psi_\lambda^{pw}),u\rangle_j\,ds=0$. Let $u_m^j(t)$ be the projection $u_m^j(t)=\left\langle u(t,\cdot),\chi_m^{0,j}\right\rangle_j$. Then, plugging the definition of $\mathbb{Z}_j$ (2.4) into

$\mathbb{B}_j$ and denoting $\gamma_m^j = 2(E(\lambda) - E_m^j)$, it follows

$$\int_0^t \langle \mathbb{B}_j(\psi_\lambda^{pw}), u\rangle_j \, ds = \frac{i}{\varepsilon}\sum_m \sqrt[+]{\gamma_m^j}\,\psi_m^{0,j}\int_0^t e^{-\frac{i}{\varepsilon}\int_0^s (E(\lambda)+V_j(\tau))d\tau}\,\overline{u_m^j}(s)\,ds,$$

$$= \frac{i}{\varepsilon}\sum_m \sqrt[+]{\gamma_m^j}\,\psi_m^{0,j}\,\overline{\mathcal{F}U_m^j}(-\gamma_m^j/(2\varepsilon)).$$

Above, $\mathcal{F}$ denotes the Fourier transform with respect to time and U_m^j is defined as

$$U_m^j(s) = \begin{cases} u_m^j(s)\, e^{\frac{i}{\varepsilon}\int_0^s (E_m^j + V_j(\tau))d\tau} & \text{if} \quad s\in[0,t], \\ 0 \quad \text{if} \quad s\notin[0,t]. \end{cases}$$

Concerning $\mathbb{C}_j$, invoking (3.5) yields

$$\int_0^t \langle \mathbb{C}_j(\psi_\lambda^{pw}), u\rangle_j \, ds = \frac{\sqrt{2}e^{-i\pi/4}}{\sqrt{\varepsilon}}\sum_m \psi_m^{0,j}\int_0^t e^{-\frac{i}{\varepsilon}\int_0^s (E_m^j+V_j(\tau))d\tau}\,\overline{u_m^j}(s)\,\partial^{1/2}\left(e^{-\frac{i}{2\varepsilon}\gamma_m^j s}\right) ds,$$

$$= \frac{\sqrt{2}}{2\pi\sqrt{\varepsilon}}\sum_m \psi_m^{0,j}\int_{\mathbb{R}} \overline{\mathcal{F}U_m^j}(\xi)\ \sqrt[-]{\xi}\,\mathcal{F}\left[\mathbb{1}_{\mathbb{R}^+} e^{-\frac{i}{2\varepsilon}\gamma_m^j s}\right](\xi)\,d\xi,$$

where we used the Fourier-Plancherel equality and (4.17). Above, $\sqrt[-]{\ }$ is the complex square root with non-positive imaginary part. Actually, in the distribution sense,

$$\mathcal{F}\left[\mathbb{1}_{\mathbb{R}^+} e^{-\frac{i}{2\varepsilon}\gamma_m^j s}\right](\xi) = \pi\,\delta(\gamma_m^j/(2\varepsilon)+\xi) - \text{p.v.}\frac{i}{\gamma_m^j/(2\varepsilon)+\xi},$$

where p.v. stands for the principal value. Then,

$$\int_0^t \langle \mathbb{C}_j(\psi_\lambda^{pw}), u\rangle_j \, ds = \frac{1}{2\varepsilon}\sum_m \sqrt[-]{-\gamma_m^j}\,\psi_m^{0,j}\,\overline{\mathcal{F}U_m^j}(-\gamma_m^j/(2\varepsilon))$$

$$- \frac{i\sqrt{2}}{2\pi\sqrt{\varepsilon}}\sum_m \psi_m^{0,j}\,\text{p.v.}\int_{\mathbb{R}} \overline{\mathcal{F}U_m^j}(\xi)\,\frac{\sqrt[-]{\xi}}{\gamma_m^j/(2\varepsilon)+\xi}\,d\xi.$$

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 $\overline{\mathcal{F}U_m^j}$ can be extended to an holomorphic function for $z\in\mathbb{C}^+ = \{z\in\mathbb{C}, \quad \mathcal{I}m z \geq 0\}$. Besides, we have the estimates, for $z = re^{i\theta}\in\mathbb{C}^+$,

$$|\overline{\mathcal{F}U_m^j}(z)| \leq \frac{C(\delta)}{(r\sin\theta)^{\frac{1+\delta}{2+\delta}}}\|u_m^j\|_{L^{2+\delta}(0,t)}, \tag{3.19}$$

as well as

$$|\overline{\mathcal{F}U_m^j}(z)| \leq \|u_m^j\|_{L^1(0,t)}. \tag{3.20}$$

The function $\sqrt[-]{\xi}$ is also holomorphic on $\mathbb{C}^+ - \{0\}$ (provided we choose the convenient branch) so that, defining a convenient contour $\mathsf{C} = \mathsf{C}_R \cup \mathsf{C}_{\eta_1} \cup \mathsf{C}_{\eta_2} \cup \mathsf{C}_{R,\eta_1,\eta_2} \subset \mathbb{C}^+$, where C_R is the semi-circle centered at 0 of radius R, with $R > |\gamma_m^j|/(2\varepsilon)$, C_{η_1} the semi-circle centered at 0 of radius η_1, C_{η_2} the semi-circle centered at $-\gamma_m^j/(2\varepsilon)$ of radius η_2, and $\mathsf{C}_{R,\eta_1,\eta_2}$ connects the different semi-circles on $\mathbb{R}$, the Cauchy theorem yields

$$\int_{\mathsf{C}} \overline{\mathcal{F}U_m^j}(z) \frac{\sqrt[-]{z}}{\gamma_m^j/(2\varepsilon)+z} dz = 0. \tag{3.21}$$

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

$$\left| \int_{\mathsf{C}_R} \overline{\mathcal{F}U_m^j}(z) \frac{\sqrt[-]{z}}{\gamma_m^j/(2\varepsilon)+z} dz \right| \leq \frac{C}{R^{\delta/(2(2+\delta))}} \|u_m^j\|_{L^{2+\delta}(0,t)} \int_0^\pi \frac{d\theta}{|\sin\theta|^{\frac{1+\delta}{2+\delta}}},$$

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),

$$\left| \int_{\mathsf{C}_{\eta_1}} \overline{\mathcal{F}U_m^j}(z) \frac{\sqrt[-]{z}}{\gamma_m^j/(2\varepsilon)+z} dz \right| \leq C\eta_1^{3/2} \|u_m^j\|_{L^1(0,t)},$$

which vanishes in the limit $\eta_1 \to 0$. Concerning the integral on C_{η_2}, we have

$$\int_{\mathsf{C}_{\eta_2}} \overline{\mathcal{F}U_m^j}(z) \frac{\sqrt[-]{z}}{\gamma_m^j/(2\varepsilon)+z} dz = \int_\pi^0 \overline{\mathcal{F}U_m^j}\left(-\gamma_m^j/(2\varepsilon)+\eta_2 e^{i\theta}\right) \sqrt[-]{-\gamma_m^j/(2\varepsilon)+\eta_2 e^{i\theta}}\, i\, d\theta,$$

so that the Lebesgue dominated convergence theorem implies that the integral goes to $-i\pi \sqrt[-]{-\gamma_m^j/(2\varepsilon)}\, \overline{\mathcal{F}U_m^j}\left(-\gamma_m^j/(2\varepsilon)\right)$ as $\eta_2 \to 0$. Since the integral on $\mathsf{C}_{R,\eta_1,\eta_2}$ tends to

$$\text{p.v.} \int_{\mathbb{R}} \overline{\mathcal{F}U_m^j}(\xi) \frac{\sqrt[-]{\xi}}{\gamma_m^j/(2\varepsilon)+\xi} d\xi,$$

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

$$\text{p.v.} \int_{\mathbb{R}} \overline{\mathcal{F}U_m^j}(\xi) \frac{\sqrt[-]{\xi}}{\gamma_m^j/(2\varepsilon)+\xi} d\xi = i \frac{\pi}{\sqrt{2\varepsilon}} \sqrt[-]{-\gamma_m^j}\, \overline{\mathcal{F}U_m^j}(-\gamma_m^j/(2\varepsilon)).$$

Consequently,

$$\int_0^t \langle \mathbb{C}_j(\psi_\lambda^{pw}), u \rangle_j \, ds = \frac{1}{\varepsilon} \sum_m \sqrt[-]{-\gamma_m^j}\, \psi_m^{0,j}\, \overline{\mathcal{F}U_m^j}(-\gamma_m^j/(2\varepsilon)),$$

and it remains to notice that $\sqrt[-]{-\gamma_m^j} = -i \sqrt[+]{\gamma_m^j}$ to end the proof. $\square$

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 ψ_λ as a test function, we nevertheless need more regularity for ψ_λ than that given in the theorem, which is only $\psi_\lambda \in \psi_\lambda^{pw} + \mathcal{C}^0([0,T], H^2(\Omega)) \cap \mathcal{C}^1([0,T], L^2(\Omega))$. We thus consider a sequence of regular data $\psi_\lambda^{0,k} \in \mathcal{C}^\infty(\Omega)$ and $V_e^k \in \mathcal{C}^\infty([0,T] \times \Omega)$ such that (3.8)–(3.11) admits a unique solution ψ_λ^k verifying $\psi_\lambda^k \in \mathcal{C}^\infty([0,T] \times \Omega)$. 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 $1 \leq p < \infty$,

$$\psi_\lambda^{0,k} \to \psi_\lambda^0 \quad \text{strongly in} \quad H^1(K) \quad ; \quad V_e^k \to V_e \quad \text{strongly in} \quad \mathcal{C}^1([0,T], L^p(K)), \tag{4.1}$$

for any bounded set $K\subset\Omega$. This implies that, for any $u\in H^{1/4}((0,T),L^2(\Gamma_j))$,

$$\mathbb{D}^{1/2}_{j,k}(u)\to\mathbb{D}^{1/2}_{j}(u) \text{ strongly in } H^{-1/4}((0,T),L^2(\Gamma_j)), \tag{4.2}$$

$$\mathbb{A}^{\varepsilon}_{j,k}(\psi_\lambda^{pw,k})\to\mathbb{A}^{\varepsilon}_{j}(\psi_\lambda^{pw}) \text{ weakly in } L^2((0,T),L^2(\Gamma_j)). \tag{4.3}$$

In the same way, $\Phi(p,m,j)$ is localized so that the obtained $\Phi^k(p,m,j)$ has a compact support and Φ^k converges strongly to Φ 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 ε-independent estimates.

Density estimate. Consider this regular solution ψ_λ^k which is also obviously solution to (3.13). Multiplying (3.8) by ψ_λ^k, integrating in $[0,T]$ and taking the imaginary part, it follows

$$\|\psi_\lambda^k(T,\cdot)\|^2_{L^2(\Omega_0)}=\|\psi_\lambda^{0,k}\|^2_{L^2(\Omega_0)}+\sqrt{\varepsilon}\sum_{j=1}^{n}\mathcal{I}m\, e^{-i\pi/4}\int_0^T\left\langle\mathbb{D}^{1/2}_{j,k}(\psi_\lambda^k),\psi_\lambda^k\right\rangle_j ds$$

$$-\varepsilon\sum_{j=1}^{n}\mathcal{I}m\int_0^T\left\langle\mathbb{A}^{\varepsilon}_{j,k}(\psi_\lambda^{pw,k}),\psi_\lambda^k\right\rangle_j ds.$$

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 $s\in\mathbb{R}$,

$$\Phi^j_{m,T}(s)=\widetilde{(\mathcal{T}_j\psi_\lambda)}_m(s),$$

where $\mathcal{T}_j$ is the transformation previously introduced in (3.14), $(\mathcal{T}_j\psi_\lambda)_m(s)=\langle\mathcal{T}_j\psi_\lambda(s,\eta_j=0,\cdot),\chi_m^{0,j}\rangle_j$, and $\widetilde{\ }$ is the extension by 0 outside $[0,T]$. Then, according to (4.17) of Lemma 4.1,

$$\mathcal{I}m\, 2\pi e^{-i\pi/4}\int_0^T\left\langle\mathbb{D}^{1/2}_{j}(\psi_\lambda),\psi_\lambda\right\rangle_j ds=-\sqrt{2}\sum_m\int_{\mathbb{R}^-}\sqrt{-\xi}\,|\mathcal{F}\Phi^j_{m,T}(\xi)|^2\,d\xi, \tag{4.4}$$

The term involving $\mathbb{A}_j^\varepsilon$ is treated thanks to Lemma 3.3. Using the expression of $\mathbb{S}_j$ 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 $E(\lambda)=\frac{1}{2}p^2+E^{j_0}_{m_0}$ and therefore,

$$\int_0^T\langle\mathbb{A}^{\varepsilon}_{j}(\psi_\lambda^{pw}),\psi_\lambda\rangle_j\,ds=-\delta^j_{j_0}\frac{2ip}{\varepsilon}\int_0^T\theta_\lambda^{j_0}(s)\overline{\psi^{j_0}_{m_0}(s)}\,ds=-\delta^j_{j_0}\frac{2ip}{\varepsilon}\mathcal{F}\overline{\Phi^{j_0}_{m_0,T}}(p^2/2\varepsilon).$$

Gathering the previous estimates and integrating with respect to λ, we find

$$n(T)+\frac{\sqrt{2\varepsilon}}{2\pi}\sum_{j,m}\int_\Lambda\int_{\mathbb{R}_-}\sqrt{-\xi}\,|\mathcal{F}\Phi^j_{m,T}(\xi)|^2\,d\xi d\mu$$

$$\le n(0)+2\int_\Lambda p\left|\mathcal{F}\overline{\Phi^{j_0}_{m_0,T}}(p^2/2\varepsilon)\right|d\mu, \tag{4.5}$$

which gives after an integration in time,

$$\|n\|_{L^1(0,T^*)}+\frac{\sqrt{2\varepsilon}}{2\pi}\sum_{j,m}\int_0^{T^*}\int_\Lambda\int_{\mathbb{R}_-}\sqrt{-\xi}\,|\mathcal{F}\Phi^j_{m,T}(\xi)|^2\,d\xi d\mu dT$$
$$\leq T^*n(0)+2\int_0^{T^*}\int_\Lambda p\left|\mathcal{F}\overline{\Phi^{j_0}_{m_0,T}}(p^2/2\varepsilon)\right|d\mu dT. \tag{4.6}$$

Energy estimate. We multiply now (3.8) by $\partial_t\psi_\lambda$. Taking the real part and integrating in time yield,

$$\frac{\varepsilon^2}{2}\|\nabla\psi_\lambda(T,\cdot)\|^2_{L^2(\Omega_0)}=\frac{\varepsilon^2}{2}\|\nabla\psi^0_\lambda\|^2_{L^2(\Omega_0)}+\varepsilon^2\sum_{j=1}^n\mathcal{R}e\int_0^T\left\langle\frac{\partial\psi_\lambda}{\partial\eta_j},\partial_s\psi_\lambda\right\rangle_j ds$$
$$-\int_0^T\int_{\Omega_0}V(s,x)\partial_s|\psi_\lambda(s,x)|^2dxds.$$

We need to be a bit careful to extend $\partial_s\psi_\lambda$ by zero to $\mathbb{R}$ to use the Fourier tranform since ψ_λ does not vanish at 0 and at T. Let $\widetilde{\psi_\lambda}$ be this extension et let $\partial_s\widetilde{\psi_\lambda}$ be its derivative in the distribution sense so that

$$\frac{\partial\widetilde{\psi_\lambda}}{\partial s}(s,x)=\begin{cases}\dfrac{\partial\psi_\lambda}{\partial s}(s,x)-\psi_\lambda(T,x)\delta_T+\psi_\lambda(0,x)\delta_0, & s\in[0,T],\\ 0, \quad s\notin[0,T].\end{cases}$$

We then have

$$\int_0^T\left\langle\frac{\partial\psi_\lambda}{\partial\eta_j},\partial_s\psi_\lambda\right\rangle_j ds=\int_0^T\left\langle\frac{\partial\psi_\lambda}{\partial\eta_j},\partial_s\widetilde{\psi_\lambda}\right\rangle_j ds$$
$$+\left\langle\frac{\partial\psi_\lambda}{\partial\eta_j},\psi_\lambda\right\rangle_j(T)-\left\langle\frac{\partial\psi_\lambda}{\partial\eta_j},\psi_\lambda\right\rangle_j(0).$$

Using now the boundary conditions, both stationary and time-dependent, we find

$$\int_0^T\left\langle\frac{\partial\psi_\lambda}{\partial\eta_j},\partial_s\widetilde{\psi_\lambda}\right\rangle_j ds=-\frac{e^{-i\pi/4}}{\sqrt{\varepsilon}}\int_0^T\left\langle\mathbb{D}_j^{1/2}(\psi_\lambda),\partial_s\widetilde{\psi_\lambda}\right\rangle_j ds+\int_0^T\langle\mathbb{A}^\varepsilon_j(\psi^{pw}_\lambda),\partial_s\widetilde{\psi_\lambda}\rangle_j\,ds,$$

$$\left\langle\frac{\partial\psi_\lambda}{\partial\eta_j},\psi_\lambda\right\rangle_j(T)=-\frac{e^{-i\pi/4}}{\sqrt{\varepsilon}}\left\langle\mathbb{D}_j^{1/2}(\psi_\lambda),\psi_\lambda\right\rangle_j(T)+\langle\mathbb{A}^\varepsilon_j(\psi^{pw}_\lambda),\psi_\lambda\rangle_j(T),$$

$$\left\langle\frac{\partial\psi_\lambda}{\partial\eta_j},\psi_\lambda\right\rangle_j(0)=\frac{1}{\varepsilon}\left\langle\mathbb{Z}_j[E(\lambda)](\psi^0_\lambda),\psi^0_\lambda\right\rangle_j+\frac{1}{\varepsilon}\left\langle\mathbb{S}_j[E(\lambda)],\psi^0_\lambda\right\rangle_j,$$

and we recast the energy relation as

$$\frac{\varepsilon^2}{2}\|\nabla\psi_\lambda(T,\cdot)\|^2_{L^2(\Omega_0)}+L_1+L_2=\frac{\varepsilon^2}{2}\|\nabla\psi^0_\lambda\|^2_{L^2(\Omega_0)}+R_1+R_2+R_3$$
$$-\int_0^T\int_{\Omega_0}V(s,x)\partial_s|\psi_\lambda(s,x)|^2dxds, \tag{4.7}$$

where

$$L_1 = \varepsilon^{3/2} \sum_{j=1}^{n} \mathcal{R}e\, e^{-i\pi/4} \int_0^T \left\langle \mathbb{D}_j^{1/2}(\psi_\lambda), \partial_s \widetilde{\psi_\lambda} \right\rangle_j ds,$$

$$L_2 = \varepsilon^{3/2} \sum_{j=1}^{n} \mathcal{R}e\, e^{-i\pi/4} \left\langle \mathbb{D}_j^{1/2}(\psi_\lambda), \psi_\lambda \right\rangle_j (T),$$

$$R_1 = \varepsilon^2 \sum_{j=1}^{n} \mathcal{R}e \int_0^T \left\langle \mathbb{A}_j^\varepsilon(\psi_\lambda^{pw}), \partial_s \widetilde{\psi_\lambda} \right\rangle_j ds,$$

$$R_2 = \varepsilon^2 \sum_{j=1}^{n} \mathcal{R}e \left\langle \mathbb{A}_j^\varepsilon(\psi_\lambda^{pw}), \psi_\lambda \right\rangle_j (T),$$

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

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

$$\begin{aligned} \mathcal{R}e\, 2\pi e^{-i\pi/4} \int_0^T \left\langle \mathbb{D}_j^{1/2}(\psi_\lambda), \partial_s \widetilde{\psi_\lambda} \right\rangle_j ds &= \sqrt{2} \sum_m \int_{\mathbb{R}^+} \xi^{3/2} |\mathcal{F}\Phi_{m,T}^j(-\xi)|^2 d\xi \\ &- \frac{\sqrt{2}}{\varepsilon} \mathcal{I}m\, 2\pi e^{-i\pi/4} \sum_m \int_0^T (E_m^j + V_j) \partial^{1/2} (\mathcal{T}_j \psi_\lambda)_m \overline{(\mathcal{T}_j \psi_\lambda)_m} ds. \end{aligned}$$

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

$$\begin{aligned} \mathcal{I}m\, 2\pi e^{-i\pi/4} \sum_m E_m^j \int_0^T \partial^{1/2} (\mathcal{T}_j \psi_\lambda)_m \overline{(\mathcal{T}_j \psi_\lambda)_m} ds &= \\ -\sqrt{2} \sum_m E_m^j \int_{\mathbb{R}^-} \sqrt{-\xi} |\mathcal{F}\Phi_{m,T}^j(\xi)|^2 d\xi \leq 0. \end{aligned}$$

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

$$\begin{aligned} (g\psi_\lambda, \psi_\lambda)(T) = (g\psi_\lambda^0, \psi_\lambda^0) + \int_0^T (\partial_s g \psi_\lambda, \psi_\lambda)(s) ds + \mathcal{I}m \int_0^T (\nabla g, \overline{\psi_\lambda} \nabla \psi_\lambda)(s) ds \\ + \mathcal{I}m \sum_{j=1}^{n} \left[\varepsilon^{1/2} e^{-i\pi/4} \int_0^T \langle \mathbb{D}_j^{1/2}(\psi_\lambda), V_j \psi_\lambda \rangle_j ds - \varepsilon \int_0^T \langle \mathbb{A}_j^\varepsilon(\psi_\lambda^{pw}), V_j \psi_\lambda \rangle ds \right]. \end{aligned}$$

Applying (3.3) and using the expression of $\mathbb{S}_j$, we have

$$\varepsilon \left| \sum_{j=1}^{n} \int_0^T \int_\Lambda \langle \mathbb{A}_j^\varepsilon(\psi_\lambda^{pw}), V_j \psi_\lambda \rangle ds d\mu \right| \leq 2 \int_\Lambda p \left| \mathcal{F} V_{j_0} \overline{\Phi_{m_0,T}^{j_0}}(p^2/2\varepsilon) \right| d\mu.$$

This finally gives for L_1,

$$\frac{\sqrt{2}}{2\pi} \sum_{m,j} \int_\Lambda \int_{\mathbb{R}^+} \varepsilon^{3/2} \xi^{3/2} |\mathcal{F}\Phi_{m,T}^j(-\xi)|^2 d\xi d\mu + R_1^1 \leq \int_\Lambda L_1 d\mu, \tag{4.8}$$

where R_1^1 verifies, using (4.5):

$$|R_1^1| \leq C \int_\Lambda p \left| \mathcal{F} V_{j_0} \overline{\Phi^{j_0}_{m_0,T}} (p^2/2\varepsilon) \right| d\mu + C \left(n(0) + \|n\|_{L^1(0,T)} + \|\mathcal{E}\|_{L^1(0,T)} \right).$$

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

$$\begin{aligned} R_1 &= -\mathcal{R}e 2ip\varepsilon \int_0^T \theta_\lambda^{j_0}(s) \overline{\partial_t \widetilde{\psi^{j_0}_{m_0}}(s)} ds \\ &= -2p\mathcal{R}e \left[\frac{p^2}{2} \mathcal{F} \overline{\Phi^{j_0}_{m_0,T}} (p^2/2\varepsilon) + \mathcal{F} V_{j_0} \overline{\Phi^{j_0}_{m_0,T}} (p^2/2\varepsilon) \right]. \end{aligned} \tag{4.9}$$

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

$$\int_0^{T^*} L_2(T) dT = \frac{\sqrt{2}\varepsilon^{3/2}}{2\pi} \sum_{j,m} \int_{\mathbb{R}_+} \sqrt{\xi} |\mathcal{F} \Phi^j_{m,T^*}(\xi)|^2 d\xi, \tag{4.10}$$

and in the same way

$$\int_0^{T^*} R_2(T) dT = \varepsilon 2p \mathcal{I}m \mathcal{F} \overline{\Phi^{j_0}_{m_0,T^*}} (p^2/2\varepsilon). \tag{4.11}$$

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

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

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

$$\int_0^T \int_\Lambda \int_{\Omega_0} V_s \partial_s |\psi_\lambda|^2 dx ds d\mu = \frac{1}{2} \|\nabla V_s(T,\cdot)\|^2_{L^2(\Omega_0)} - \frac{1}{2} \|\nabla V_s(0,\cdot)\|^2_{L^2(\Omega_0)}.$$

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

$$\left| \int_\Lambda \int_0^T \int_{\Omega_0} V_e \partial_s |\psi_\lambda|^2 dx ds d\mu \right| \leq \|V_e\|_{\mathcal{C}^1([0,T], L^\infty(\Omega_0))} \left(n(T) + n(0) + \int_0^T n(s) ds \right).$$

The next step is to integrate (4.7) with respect to λ, 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,

$$\|\mathcal{E}\|_{L^1(0,T^*)} + \|n\|_{L^1(0,T^*)} + T_4 \leq C_1 + R_4 + C_2 \int_0^{T^*} \left(\|n\|_{L^1(0,T)} + \|\mathcal{E}\|_{L^1(0,T)} \right) dT, \tag{4.13}$$

where

$$\begin{aligned}
T_4 = & \frac{\sqrt{2}\varepsilon^{3/2}}{2\pi} \sum_{j,m} \int_0^{T^*} \int_\Lambda \int_{\mathbb{R}^+} \xi^{3/2} |\mathcal{F}\Phi^j_{m,T}(-\xi)|^2 \, d\xi d\mu dT \\
& + \frac{\sqrt{2\varepsilon}}{2\pi} \sum_{j,m} \int_0^{T^*} \int_\Lambda \int_{\mathbb{R}_-} \sqrt{-\xi} |\mathcal{F}\Phi^j_{m,T}(\xi)|^2 \, d\xi d\mu dT \\
& + \frac{\sqrt{2}\varepsilon^{3/2}}{2\pi} \sum_{j,m} \int_{\mathbb{R}_+} \sqrt{\xi} |\mathcal{F}\Phi^j_{m,T^*}(\xi)|^2 \, d\xi d\mu, \\
R_4 = & \int_0^{T^*} \int_\Lambda p^3 \left| \mathcal{F}\overline{\Phi^{j_0}_{m_0,T}}(p^2/2\varepsilon) \right| d\mu dT + C_3 \int_0^{T^*} \int_\Lambda p \left| \mathcal{F} V_{j_0} \overline{\Phi^{j_0}_{m_0,T}}(p^2/2\varepsilon) \right| d\mu dT \\
& + 2\varepsilon \int_\Lambda p \left| \mathcal{F}\overline{\Phi^{j_0}_{m_0,T^*}}(p^2/2\varepsilon) \right| d\mu + C_4 \int_0^{T^*} \int_\Lambda p \left| \mathcal{F}\overline{\Phi^{j_0}_{m_0,T}}(p^2/2\varepsilon) \right| d\mu dT.
\end{aligned}$$

The constants C_1, C_2, C_3 and C_4 depend on the constant C_0 of (3.16) and on $\|V_e\|_{\mathcal{C}^1([0,T],L^\infty(\Omega))}$. To end the proof we need now to bound R_4 and thus $\mathcal{F}\overline{\Phi^{j_0}_{m_0,t}}(p^2/\varepsilon)$, for $t = T, T^*$. A straightforward attempt by using trace theorems would fail again because of the homogeneity in ε. Indeed, we expect to estimate the trace with the help of the derivative of ψ_λ while the energy involves a derivative multiplied by ε. Nevertheless, it is expected that $\mathcal{F}\overline{\Phi^{j_0}_{m_0,t}}(p^2/\varepsilon)$ goes to zero as $\varepsilon \to 0$, and the rate of convergence is given by the regularity in time of ψ_λ which induces the decay of $\mathcal{F}\overline{\Phi^{j_0}_{m_0,t}}(\xi)$. This will allow to recover a correct homogeneity in ε to be able to use trace theorems. To this aim, we apply Lemma (4.2) which provides, for $p > 0$,

$$\left| \mathcal{F}\overline{\Phi^{j_0}_{m_0,t}}(p^2/2\varepsilon) \right| \le C \left(\frac{\varepsilon}{p^2} \right)^{1/4} \|\xi^{1/4} \mathcal{F}\overline{\Phi^{j_0}_{m_0,t}}\|_{L^2(\mathbb{R}^+)} + C \left(\frac{\varepsilon}{p^2} \right)^{1/2} \|\mathcal{F}\overline{\Phi^{j_0}_{m_0,t}}\|_{L^2(\mathbb{R})},$$

and Lemma (4.1) yields

$$\begin{aligned}
\|\mathcal{F}\overline{\Phi^{j_0}_{m_0,t}}\|_{L^2(\mathbb{R})} = 2\pi \|\psi^{j_0}_{m_0,t}\|_{L^2(0,t)} & \le 2\pi \|\psi_\lambda\|_{L^2((0,t),L^2(\Gamma_{j_0}))} \\
& \le C \|\psi_\lambda\|^{1/2}_{L^2((0,t),L^2(\Omega_0))} \|\nabla\psi_\lambda\|^{1/2}_{L^2((0,t),L^2(\Omega_0))}.
\end{aligned}$$

Notice here the fact that the L^2 norm of the trace is controlled by $\|\nabla\psi_\lambda\|^{1/2}_{L^2((0,t),L^2(\Omega_0))}$ while with non-flat interfaces the exponent would have been $1/2+\alpha$, with $\alpha > 0$. This would have led to a wrong homogeneity. We thus have, for $\beta = 1, 3$,

$$\begin{aligned}
\int_\Lambda p^\beta \left| \mathcal{F}\overline{\Phi^{j_0}_{m_0,t}}(p^2/2\varepsilon) \right| d\mu \le C \|n\|^{1/2}_{L^1(0,t)} + C \|\mathcal{E}\|^{1/2}_{L^1(0,t)} & \\
+ C\varepsilon^{1/4} \left(\int_\Lambda \|\xi^{1/4} \mathcal{F}\overline{\Phi^{j_0}_{m_0,t}}\|^2_{L^2(\mathbb{R}^+)} d\mu \right)^{1/2}, &
\end{aligned} \tag{4.14}$$

where the constant C depends on $\|p\|_{L^5(\Lambda,d\mu)}$. According to Remark 4.3, it can be easily shown that we have the same estimate as above for $\int_\Lambda p \left| \mathcal{F} V_{j_0} \overline{\Phi^{j_0}_{m_0,t}}(p^2/2\varepsilon) \right| d\mu$. We control now the last term of the above r.h.s, that is, for any $\eta > 0$,

$$\varepsilon^{1/4} \left(\int_\Lambda \|\xi^{1/4} \mathcal{F}\overline{\Phi^{j_0}_{m_0,t}}\|^2_{L^2(\mathbb{R}^+)} d\mu \right)^{1/2} \le \frac{1}{\eta} + \eta\sqrt{\varepsilon} \sum_{j,m} \int_\Lambda \int_{\mathbb{R}^-} \sqrt{-\xi} |\mathcal{F}\Phi^j_{m,t}(\xi)|^2 \, d\xi d\mu.$$

This allows to write

$$R_4 \leq C_\eta + C\eta\left(\|n\|_{L^1(0,T^*)} + \|\mathcal{E}\|_{L^1(0,T^*)} + T_4\right),$$

so that the Gronwall lemma and (4.13) imply that $\|n\|_{L^1(0,T^*)}$, $\|\mathcal{E}\|_{L^1(0,T^*)}$ are bounded independently of ε for any finite $T^*>0$ and in turn so do T_4 and $\|n\|_{L^\infty(0,T^*)}$ thanks to (4.5). In particular, we obtain that

$$\sqrt{\varepsilon}\sum_{j,m}\int_\Lambda\int_{\mathbb{R}} \sqrt{\xi}\,|\mathcal{F}\Phi^j_{m,T^*}(\xi)|^2 d\xi d\mu \leq C, \tag{4.15}$$

where C is independent of ε and of the regularization parameter k, and thus a bound in $H^{1/4}((0,T),L^2(\Gamma_j))$ for $\mathcal{T}_j\psi_\lambda$.

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 $V_s \in L^2((0,T),W^{3,r}(\Omega_0))$, thanks to standard elliptic regularity results. We estimate now $\partial_t V_s$ which is solution to

$$\Delta\partial_t V_s = \operatorname{div} J, \quad x\in\Omega_0, \qquad \partial_t V_s = 0, \quad x\in\partial\Omega_0,$$

where $J = \mathcal{I}m\,\varepsilon\int_\Lambda \overline{\psi}_\lambda\nabla\psi_\lambda d\mu(\lambda)$. 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 ε-independent bound on $\partial_t V_s$, we cannot use any Sobolev embeddings so that J is bounded independently of ε only in $L^2((0,T),L^1(\Omega_0))$, 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),

$$\psi^k_\lambda \in L^\infty((0,T),L^2(\Omega_0\times\Lambda;dxd\mu^k)) \qquad ; \qquad \nabla\psi^k_\lambda \in L^2((0,T),L^2(\Omega_0\times\Lambda;dxd\mu^k))),$$

with bounds independent of k, so that ψ^k_λ converges weakly-* to a limit $\psi_\lambda \in L^\infty((0,T),L^2(\Omega_0\times\Lambda;dxd\mu))$ as well as $\nabla\psi^k_\lambda$, up to the extraction of a subsequence. Remember that Φ^k converges strongly to Φ in $L^1(\mathbb{R}_+,\ell^1(\mathbb{N}^*\times\{1,\cdots,n\}))$ so that the weak-* limit of ψ^k_λ in $L^\infty((0,T),L^2(\Omega_0\times\Lambda;dxd\mu^k))$ is equal to that of ψ^k_λ in $L^\infty((0,T),L^2(\Omega_0\times\Lambda;dxd\mu))$. This implies that

$$\|\psi_\lambda\|_{L^\infty((0,T),L^2(\Omega_0\times\Lambda;dxd\mu))} \leq \liminf \|\psi^k_\lambda\|_{L^\infty((0,T),L^2(\Omega_0\times\Lambda;dxd\mu^k))},$$

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 ψ_λ and $\nabla\psi_\lambda$.

We pass now to the limit in the weak formulation (3.13). ψ^k_λ is obviously a solution to (3.13). Integrating with respect to Λ and choosing a test function u such that $u\in\mathcal{C}^1([0,T),L^2(\Omega_0\times\Lambda;dxd\mu))$ and $\nabla u\in\mathcal{C}^1([0,T),L^2(\Omega_0\times\Lambda;dxd\mu))$, 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 $d=3$,

$$V^k_s \in L^2((0,T),H^1_0(\Omega_0)) \qquad ; \qquad \partial_t V^k_s \in L^2((0,T),L^r(\Omega_0)),$$

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_s^k - such that V_s^k converges strongly to V_s 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, ψ_λ^k converges weakly - up to the extraction of a subsequence - to ψ_λ in $L^2((0,T),L^{r,2}(\Omega_0\times\Lambda;dxd\mu))$ (where $L^{r,2}(\Omega_0\times\Lambda;dxd\mu)$ is defined as the Banach space of functions f such that $\int_{\Omega_0}\|f(x,\cdot)\|^r_{L^2(\Lambda,d\mu)}dx<\infty$), 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

$$\int_0^T\int_\Lambda\int_{\Omega_0} V_s^k(s,x)\psi_\lambda^k(s,x)u(s,x,\lambda)dxdsd\mu.$$

It remains the boundary terms, namely

$$\frac{1}{2}\sum_{j=1}^n\left[\varepsilon^{1/2}e^{-i\pi/4}\int_0^T\langle\mathbb{D}^{1/2}_{j,k}(\psi_\lambda),u\rangle_j\,ds+\varepsilon\int_0^T\langle\mathbb{A}^\varepsilon_{j,k}(\psi_\lambda^{pw}),u\rangle\,ds\right].$$

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 $\mathcal{T}_j\psi_\lambda^k$ is bounded in $H^{1/4}((0,T),L^2(\Gamma_j))$, independently of k so that thanks to (4.2), $\int_0^T\langle\mathbb{D}^{1/2}_{j,k}(\psi_\lambda^k),u\rangle_j\,ds$ converges to $\int_0^T\langle\mathbb{D}^{1/2}_{j}(\psi_\lambda),u\rangle_j\,ds$.

We show now that the limit ψ_λ actually belongs to $\mathcal{C}^0([0,T],L^2(\Omega_0))$, λ a.e., so that the initial condition can be identified. Let us denote by ψ_λ^k and ψ_λ^l, k, $l\in\mathbb{N}^*$, two elements of the sequence of regularized solutions and define $w=\psi_\lambda^k-\psi_\lambda^l$. w verifies the following boundary conditions on Γ_j,

$$\frac{\partial w}{\partial\eta_j}=-\frac{e^{-i\pi/4}}{\sqrt{\varepsilon}}\mathbb{D}^{1/2}_{j,k}(w)+\frac{e^{-i\pi/4}}{\sqrt{\varepsilon}}\left[\mathbb{D}^{1/2}_{j,k}-\mathbb{D}^{1/2}_{j,l}\right](\psi_\lambda^l)+\left[\mathbb{A}^\varepsilon_{j,k}(\psi_\lambda^{pw,k})-\mathbb{A}^\varepsilon_{j,l}(\psi_\lambda^{pw,l})\right].$$

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

$$\begin{aligned}\|w(t,\cdot)\|^2_{L^2(\Omega_0)}&=\|w(t=0,\cdot)\|^2_{L^2(\Omega_0)}+\sqrt{\varepsilon}\sum_{j=1}^n\mathcal{I}m\,e^{-i\pi/4}\int_0^t\left\langle\mathbb{D}^{1/2}_{j,k}(w),w\right\rangle_j ds\\&\quad+\frac{2}{\varepsilon}\mathcal{I}m\int_0^t\int_{\Omega_0}(V^k-V^l)\psi_\lambda^l\,\overline{w}\,dxds+R_1+R_2,\\R_1&=-\sqrt{\varepsilon}\sum_{j=1}^n\mathcal{I}m\,e^{-i\pi/4}\int_0^t\left\langle\left[\mathbb{D}^{1/2}_{j,k}-\mathbb{D}^{1/2}_{j,l}\right](\psi_\lambda^l),w\right\rangle_j ds,\\R_2&=-\varepsilon\sum_{j=1}^n\mathcal{I}m\int_0^t\left\langle\mathbb{A}^\varepsilon_{j,k}(\psi_\lambda^{pw,k})-\mathbb{A}^\varepsilon_{j,l}(\psi_\lambda^{pw,l}),w\right\rangle_j ds.\end{aligned}$$

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

$$\begin{aligned}\|\left((V_s^k-V_s^l)\psi_\lambda^l\right)(t,\cdot)\|_{L^2(\Omega_0\times\Lambda;dxd\mu)}&\leq\|(V_s^k-V_s^l)(t,\cdot)\|_{L^3(\Omega_0)}\|\psi_\lambda^l(t,\cdot)\|_{L^6(\Omega_0,L^2(\Lambda,d\mu))}\\&\leq C\mathcal{E}(t)\|w(t,\cdot)\|_{L^2(\Omega_0\times\Lambda;dxd\mu)}.\end{aligned}\tag{4.16}$$

Moreover R_1, R_2 converge to zero as well thanks to (4.2), (4.3) and (4.15). $\psi_\lambda^k - \psi_\lambda^l$ is thus a Cauchy sequence in $\mathcal{C}^0([0,T], L^2(\Omega_0))$ so that the limit ψ_λ belongs as well to this space.

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

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

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

$$\|\psi_\lambda^1 - \psi_\lambda^2\|^2_{L^2(\Omega_0)} \leq \frac{2}{\varepsilon} \mathcal{I}m \int_0^t \int_{\Omega_0} (V_s^1 - V_s^2)\psi_\lambda^1 \left(\overline{\psi_\lambda^1} - \overline{\psi_\lambda^2}\right) dxds.$$

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

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

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:*

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

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

$$\begin{aligned} \partial^{1/2} f &= \frac{1}{\sqrt{\pi}} \frac{d}{dt} Ef * \left(\mathbb{1}_{\mathbb{R}^+} \frac{1}{\sqrt{\cdot}} \right), \qquad t \in \mathbb{R}, \\ \widehat{\partial^{1/2} f}(\xi) &= e^{i\pi/4} \sqrt[-]{\xi} \widehat{f}(\xi), \end{aligned} \tag{4.17}$$

where $\sqrt[-]{\ }$ *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 $\widehat{f}$ be the Fourier transform of Ef. Assuming $k^{1/4}\widehat{f}(k)\in L^2(\mathbb{R}^+)$, we have, for any $a>0$, for $\xi\geq a$,*

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

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

$$\widehat{f}(\xi)=\int_0^t f(s)e^{-i\xi s}ds=\widehat{\mathbb{1}_{[0,t]}Ef}=(H*\hat{f})(\xi)$$

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

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

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

$$\begin{aligned}\int_{\mathbb{R}}H(\xi-y)\widehat{f}(y)dy&=\int_{\mathbb{R}_-}+\int_0^{\xi-\beta}+\int_{\xi-\beta}^{\xi+\beta}+\int_{\xi+\beta}^{+\infty}\\&=I_1+I_2+I_3+I_4.\end{aligned}$$

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

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

Concerning I_2, we have

$$\begin{aligned}I_2&\leq\left(\int_0^{\xi-\beta}\frac{H(\xi-y)^2}{y^{1/2}}dy\right)^{1/2}\|y^{1/4}\widehat{f}(y)\|_{L^2(\mathbb{R}^+)},\\&\leq 2\left(\int_0^{\xi-\beta}\frac{dy}{|\xi-y|^2y^{1/2}}\right)^{1/2}\|y^{1/4}\widehat{f}(y)\|_{L^2(\mathbb{R}^+)}.\end{aligned}$$

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

$$\begin{aligned}\int_0^{\xi-\beta}\frac{dy}{|\xi-y|^2y^{1/2}}&=\frac{1}{\xi^{3/2}}\int_0^{1-\beta/\xi}\frac{dy}{|y-1|^2y^{1/2}},\\&=\int_0^{\alpha}+\int_{\alpha}^{1-\beta/\xi},\\&\leq\frac{1}{\xi^{3/2}}\frac{2\alpha^{1/2}}{(1-\alpha)^2}+\frac{1}{\xi^{3/2}}\frac{1}{\alpha^{1/2}}\left(\frac{\xi}{\beta}+\frac{1}{1-\alpha}\right),\\&=\mathcal{O}(\xi^{-1/2}).\end{aligned}$$

Proceeding analogously, I_3 is easily estimated thanks to (4.18),

$$
\begin{aligned}
I_3 &\leq t\left(\int_{\xi-\beta}^{\xi+\beta}\frac{dy}{\sqrt{y}}\right)^{1/2}\|y^{1/4}\widehat{f}(y)\|_{L^2(\mathbb{R}^+)},\\
&\leq \frac{\sqrt{2\beta}t}{(\xi-\beta)^{1/4}}\|y^{1/4}\widehat{f}(y)\|_{L^2(\mathbb{R}^+)}.
\end{aligned}
$$

In the same way,

$$
\begin{aligned}
I_4 &\leq 2\left(\int_{\xi+\beta}^{\infty}\frac{dy}{|\xi-y|^2y^{1/2}}\right)^{1/2}\|y^{1/4}\widehat{f}(y)\|_{L^2(\mathbb{R}^+)},\\
&\leq \frac{2}{\sqrt{\beta}(\xi+\beta)^{1/4}}\|y^{1/4}\widehat{f}(y)\|_{L^2(\mathbb{R}^+)}.
\end{aligned}
$$

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 $\mathcal{C}^1([0,t])$ function. Indeed, in this case the convolution kernel H verifies, instead of* (4.18),

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

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

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

where the constant C depends on $\|g\|_{\mathcal{C}^1([0,t])}$. 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

$$
\|\varphi\|_{L^2(\Gamma_j)}\leq C\|\varphi\|_{L^2(\Omega_0)}^{1/2-\alpha}\|\nabla\varphi\|_{L^2(\Omega_0)}^{1/2+\alpha},\qquad \alpha>0,\qquad j=1,\cdots,n,
$$

while we have the following Lemma:

LEMMA 4.1. *Let $\varphi\in H^1(\Omega_0)$ where Ω_0 is smooth (at least $\mathcal{C}^1$) and is defined in section 2. Assume that the trace of φ vanishes on Γ_0. Then there exists $C>0$ such that*

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

Proof. We assume that φ is regular proceed by density to conclude. Let us parametrize Ω_0 by an orthogonal set of coordinates $x=(x',\eta)$ such that if $\eta=0$, x belongs to the plane into which Γ_j is included. Such construction is possible since the interface Γ_j is plane. Thus $\varphi(x',0)$ is the trace of φ on Γ_j for $x'\in\Gamma_j$. We have

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

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 ineqality 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 ρ be a standard mollifier such that $0 \le \rho \le 1$, $\rho \in \mathcal{C}^\infty(\mathbb{R}^d)$, $\|\rho\|_{L^1} = 1$ 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 Ω to $\mathbb{R}^d$, see [1]. Let $V_e \in \mathcal{C}^1([0,T], L^\infty(\Omega))$ be in the class of potentials introduced in section 2.3, and define $V_e^\delta := \rho^\delta *_t \left(\rho^\delta *_x EV_e\right)$, where we use a one-dimensional mollifier for the time variable. Then $V_e^\delta \in \mathcal{C}^\infty(\mathbb{R}^{d+1})$ and V_e^δ converges strongly to V_e in $\mathcal{C}^1([0,T], L^p(K))$, $p < \infty$, for any bounded set $K \subset \Omega$. It is assumed in each wave guide Ω_j (equipped with the set of coordinates (ξ_j, η_j)) that V_e verifies $V_e(t,x) = V^0(\xi_j) + V_j(t)$, which is not true for V_e^δ. Nevertheless, as soon as $\eta_j \ge \delta$, V_e^δ shares a similar structure, that is $V_e^\delta(t,x) = V^{0,\delta}(\xi_j) + V_j^\delta(t)$, where $V^{0,\delta}(\xi_j) = \int_{\mathbb{R}^{d-1}} \int_{-\delta}^{\delta} EV^0(z)\rho(\xi_j - z, y)dzdy$ and $V_j^\delta = \rho *_t EV_j$. This suggests to define a fixed parameter δ_0, with $0 < \delta < \delta_0$, such that the transparent boundary conditions are prescribed on $\Gamma_j^{\delta_0} = \{(\eta_j, \xi_j) \in \Omega_j, \xi_j \in \Gamma_j, \eta_j = \delta_0)\}$. It is not possible to define them for $x \in \Omega_j$, $\eta_j \le \delta$, since V_e^δ does not satisfy the adequate decomposition.

In the same way, let $\psi_\lambda^{0,\delta} := \chi^\delta \rho^\delta *_x \left(E\psi_\lambda^0\right) \in \mathcal{C}^\infty(\Omega)$, where χ is a cut-off which ensures that $\psi_\lambda^{0,\delta}$ vanishes on the boundary $\partial\Omega$. $\psi_\lambda^{0,\delta}$ converges strongly to ψ_λ^0 in $H^1(K)$, for any bounded set $K \subset \Omega$. Let now $\chi_m^{0,j,\delta}$ be the solution to (2.1) with the regularized potential $V^{0,\delta}$ and $E_m^{j,\delta}$ be the associated eigenvalue. According to the regularity of the potential, $\chi_m^{0,j,\delta} \in \mathcal{C}^\infty(\Gamma_j)$. In each guide Ω_j, ψ_λ^0 reads:

$$\psi_\lambda^0(\xi_j, \eta_j) = \sum_m \left[\chi_m^{0,j}(\xi_j)\delta_m^{m_0}\delta_j^{j_0} \exp\left(\frac{-i\eta_j}{\varepsilon} \sqrt[+]{2(E(\lambda) - E_m^j)}\right) \right.$$
$$\left. + b_m^j \exp\left(\frac{i\eta_j}{\varepsilon} \sqrt[+]{2(E(\lambda) - E_m^j)}\right)\right].$$

This leads to the definition of

$$\varphi_\lambda^\delta(\xi_j, \eta_j) = \sum_m \left[\chi_m^{0,j,\delta}(\xi_j)\delta_m^{m_0}\delta_j^{j_0} \exp\left(\frac{-i\eta_j}{\varepsilon} \sqrt[+]{2(E(\lambda) - E_m^{j,\delta})}\right) \right.$$
$$\left. + b_m^j \exp\left(\frac{i\eta_j}{\varepsilon} \sqrt[+]{2(E(\lambda) - E_m^{j,\delta})}\right)\right],$$

so that $\varphi_\lambda^\delta \in \mathcal{C}^\infty(\Omega_j)$ and φ_λ^δ converges strongly to ψ_λ^0 in $H^1(K)$, for any bounded set $K \subset \Omega_j$. In each wave guide, we thus have, for $\eta_j \ge 0$,

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

Let χ be another smooth cut-off function equal to one on Ω_0 and whose support is included in the set $\{x \in \mathbb{R}^d, \eta_j \le \delta_0, j = 1, \cdots, n\}$ and let $\widetilde{\psi_\lambda^{0,\delta}} = \chi\psi_\lambda^{0,\delta} + (1-\chi)\varphi_\lambda^\delta$. We have $\widetilde{\psi_\lambda^{0,\delta}} \in \mathcal{C}^\infty(\Omega)$, and $\widetilde{\psi_\lambda^{0,\delta}}$ converges strongly to ψ_λ^0 in $H^1(K)$, for any bounded set $K \subset \Omega$.

Consider now the following regularized Schrödinger-Poisson problem:

$$i\varepsilon \frac{\partial \psi_\lambda^\delta}{\partial t} = -\frac{\varepsilon^2}{2}\Delta \psi_\lambda^\delta + \left(V_e^\delta + V_s^\delta\right)\psi_\lambda^\delta \quad ; \quad \psi_\lambda^\delta(t=0,\cdot) = \widetilde{\psi_\lambda^{0,\delta}} \quad ; \quad x \in \Omega,$$

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

Define as well:

$$\psi_\lambda^{pw,\delta} = \widetilde{\psi_\lambda^{0,\delta}} \sum_{j=1}^n \mu_j \, \theta_\lambda^{j,\delta} \qquad ; \qquad \theta_\lambda^{j,\delta}(t) = \exp\left(-\frac{i}{\varepsilon}\int_0^t (E(\lambda) + V_j^\delta(s))\, ds\right),$$

where $(\mu_j)_j$ is the partition of unity introduced in section 2.1. The previous construction of $\widetilde{\psi_\lambda^{0,\delta}}$ and V_e^δ insures that

$$i\varepsilon \frac{\partial \psi_\lambda^{pw,\delta}}{\partial t} = -\frac{\varepsilon^2}{2}\Delta \psi_\lambda^{pw,\delta} + \left(V_e^\delta + V_s^\delta\right)\psi_\lambda^{pw,\delta}, \quad x \in \Omega_j, \quad \eta_j \geq \delta_0,$$

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

$$\frac{\partial}{\partial \eta_j}(\psi_\lambda^\delta - \psi_\lambda^{pw,\delta}) = -\frac{e^{-i\pi/4}}{\sqrt{\varepsilon}}\, \mathbb{D}_{j,\delta}^{1/2}(\psi_\lambda^\delta - \psi_\lambda^{pw,\delta}) \quad ; \quad x \in \Gamma_j^{\delta_0}.$$

The definition of $\mathbb{D}_{j,\delta}^{1/2}$ 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 Γ_j instead of $\Gamma_j^{\delta_0}$.

Acknowledgments. The author would like to thank Naoufel Ben Abdallah for many discussions about the subject.

REFERENCES

[1] R. A. Adams, *Sobolev Spaces*, Academic Press, NY, San Francisco, London, 1975.

[2] D. Ahluwalia and J. Keller, *Exact and asymptotic representation of the sound field in a stratified ocean*, Wave propagation in underwater acoustics, Lecture Notes in Physics 70, Springer, (1977), pp. 14–85.

[3] X. Antoine and C. Besse, *Construction, structure and asymptotic approximations of a microdifferential transparent boundary condition for the linear Schrödinger equation*, J. Maths. Pures Appl., 9 (2001), pp. 701–738.

[4] A. Arnold, *Mathematical concept of open quantum boundary conditions*, Transp. Theory. Stat. Phys., 6 (2001), pp. 561–584.

[5] A. Arnold, M. Ehrhardt, and I. M. Sofronov, *Approximation, stability and fast calculations of non-local boundary conditions for the Schrödinger equstion*, Comm. in Math. Sciences, 1 (2003), pp. 501–556.

[6] G. Bal, G. Papanicolaou, and L. Ryzhik, *Radiative transport limit for the random Schrödinger equation*, Nonlinearity, 15 (2002), pp. 513–529.

[7] C. Bardos, F. Golse, and N. Mauser, *Weak coupling limit of the N-particle Schrödinger equation*, Methods Appl. Anal., 7 (2000), pp. 275–293.

[8] G. Bastard, *Wave mechanics applied to semiconductor heterostructures*, Halsted Press, 1988.

[9] N. Ben Abdallah, *A hybrid kinetic-quantum model for stationary electron transport in a resonant tunneling diode*, J. Stat. Phys., 90 (1998), pp. 627–662.

[10] ———, *On a muldidimensional Schrödinger-Poisson scattering model for semiconductors*, J. Math. Phys., 41 (2000), pp. 4241–4261.

[11] N. Ben Abdallah, P. Degond, and P. A. Markowich, *On a one-dimensional Schrödinger-Poisson scattering model*, ZAMP, 48 (1997), pp. 135–155.

[12] N. Ben Abdallah, F. Méhats, and O. Pinaud, *On a open transient Schrödinger-Poisson system*, Math. Meth. Mod. in App. Sci., 15 (2005), pp. 667–688.

[13] J. Benamou, F. Castella, T. Katsaounis, and B. Perthame, *High frequency limit in the Helmholtz equation*, Rev. Mat. Iberoamericana, 18 (2002), pp. 187–209.

[14] P. Degond and A. El Ayyadi, *A coupled Schrödinger drift-diffusion model for quantum semiconductor device simulations*, J. Comp. Phys., 181 (2002), pp. 222–259.

[15] M. Ehrhardt and R. E. Mickens, *Solutions to the Discrete Airy Equation: Application to Parabolic Equation Calculations*, J. Comput. Appl. Math., 172 (2004), pp. 183–206.

[16] B. Engquist and A. Majda, *Absorbing boundary conditions for the numerical simulation of waves*, Math. Comp., 31 (1971), pp. 629–651.

[17] L. Erdös and H. T. Yau, *Linear Boltzmann equation as the weak coupling limit of a random Schrödinger Equation*, Comm. Pure Appl. Math., 53(6) (2000), pp. 667–735.

[18] P. Gérard, P. A. Markowich, N. J. Mauser, and F. Poupaud, *Homogenization limits and Wigner transforms*, Comm. Pure Appl. Math., 50 (1997), pp. 323–380.

[19] J. Ginibre and G. Velo, *On a class of nonlinear Schrödinger equations with non-local interaction*, Math. Z., 170 (1980), pp. 109–136.

[20] R. Gorenflo and S. Vessela, *Abel Integral Equations*, Springer, NY, Berlin, 1991.

[21] P.-L. Lions and T. Paul, *Sur les mesures de Wigner*, Rev. Mat. Iberoamericana, 9 (1993), pp. 553–618.

[22] P. A. Markowich and N. J. Mauser, *The classical limit of a self-consistent quantum-Vlasov equation in 3-D*, Math. Meth. Mod. Appl. Sci., 3 (1993), pp. 109–124.

[23] F. Nier, *Schrödinger-Poisson systems in dimension $d \leq 3$: the whole space case*, Proc. Roy. Soc. Edinburgh Section A, 23 (1993), pp. 489–510.

[24] ———, *The dynamics of some open systems with short-range non-linearity*, Nonlinearity, 11 (1998), pp. 27–72.

[25] A. Pazy, *Semigroups of linear operators and applications to partial differential equations*, Springer, NY, Berlin, 1983.

[26] O. Pinaud, *In preparation.*

[27] E. Polizzi and N. Ben Abdallah, *Subband decomposition approach for the simulation of quantum electron transport in nanostructures*, J. Comput. Physics, 202 (2004), pp. 150–180.

[28] L. Ryzhik, G. Papanicolaou, and J. B. Keller, *Transport equations for elastic and other waves in random media*, Wave Motion, 24 (1996), pp. 327–370.

[29] S. Samko, A. Kilbas, and O. Marichev, *Fractional Integrals and Derivatives*, Gordon and Breach, 1993.

[30] F. Tappert, *The parabolic approximation method*, Wave propagation in underwater acoustics, Lecture Notes in Physics 70, Springer, (1977), pp. 224–287.

[31] R. Temam, *Navier-Stokes equations: theory and numerical analysis*, North Holland, 1984.

[32] E. Wigner, *On the quantum correction for thermodynamic equilibrium*, Phys. Rev. 40, (1932), pp. 742–749.