On an open transient Schrödinger-Poisson system

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Abstract

A mathematical model of quantum transient transport in dimension $d = 2, 3$ is derived and analyzed. The model describes the evolution of electrons injected into the device by reservoirs having a stationary statistics. The electrostatic potential in the device is modified by electron presence through electrostatic interaction. The wave functions are computed in the device region and satisfy non homogeneous open boundary conditions at the device edges. A priori estimates are deduced from the "dissipative properties" of the boundary conditions and from the repulsive character of the electrostatic interaction.

Key words : Quantum transport; transient Schrödinger-Poisson system; open boundary conditions.

1 Introduction

In nanoscale semiconductor devices, the typical lengthscale and the de Broglie wavelength of electrons are comparable. Therefore, quantum effects such as tunneling become important and have to be taken into account in the models. When the transport is ballistic (which means that electrons do not suffer any collision during their transit in the device), the Schrödinger picture is well adapted. The electrons are in a mixed state, each elementary state being a solution of the Schrödinger equation. More precisely, the density matrix can be written

$$\rho(t, x, x') = \int_\Lambda \psi_\lambda(t, x)\overline{\psi_\lambda}(t, x')\, d\mu(\lambda)$$

where λ is an index for the elementary states $\psi_\lambda(t, x)$ and the integration is done with respect to a measure μ. Each state ψ_λ is a solution of the Schrödinger equation

$$i\frac{\partial \psi_\lambda}{\partial t}(t, x) = -\Delta\psi_\lambda(t, x) + V(t, x)\psi_\lambda(t, x)$$

where V is the electrostatic potential. Since electrons are charged particles, they contribute to the electrostatic potential through the electrostatic interaction. The potential takes the form $V = V_e + V_s$ where V_e is a given (exterior) potential and

V_s is the self-consistent potential created by the electrons, which solves the Poisson equation

$$-\Delta V_s = n(t,x) := \rho(t,x,x) = \int_\Lambda |\psi_\lambda(t,x)|^2 \, d\mu(\lambda).$$

The so-obtained Schrödinger-Poisson system has been widely studied in the time dependent whole space setting in [11, 12, 16], and in the stationary case for bounded domains with Dirichlet boundary conditions in [21, 22] or the whole space case in [20]. In electronic devices, the nonlinear coupling effects take place in the middle of the structure. This active region is not a closed region but is connected to the exterior medium through access zones which can be considered at equilibrium and are modeled by waveguides. The access zones allow the injection of electrons into the active region which can be out of equilibrium. The Schrödinger-Poisson problem is then set on the active region; suitable transparent boundary conditions at the boundary between the access zones and the active zone have to be prescribed in order to model the continuous electron injection. In the stationary picture, transparent boundary conditions have been described in [17] and analyzed in [9] in the one dimensional case and in [8] for the multidimensional case. For the time dependent Schrödinger equation, transparent boundary conditions have been derived by several authors from different application fields [2, 3, 5, 7, 14] in the one dimensional case when the initial condition is compactly supported in the active region and their discretization has been studied in [4, 6].

Our aim here is to derive the boundary conditions for the transient Schrödinger equation in the case of continuous injection and to analyze the so-obtained Schrödinger-Poisson system. The one-dimensional case was already treated in [10] and we extend it to the dimension 2 or 3. F. Nier has already formulated and studied a more general version of this problem in [19]. He has used the density matrix formulation of quantum mechanics and analyzed the problem by means of scattering theory techniques and functional calculus. Boundary conditions are not derived explicitly and are taken into account implicitly thanks to the use of the notion of conjugate operators. In the present paper, we use the Schrödinger picture and derive transparent boundary conditions which are more suitable for numerical simulations (see [3, 23]).

To fix the ideas, let us briefly consider the stationary one dimensional model for a resonant tunneling diode. The device occupies a bounded interval $[a,b]$ where the electrostatic energy $V(x)$ varies. Outside this interval, the function V is a constant. The index λ of the statistical mixture is the momentum of incoming particles to the domain $[a,b]$ and shall be rather denoted by p. The wave function ψ_p corresponding to electrons injected at the left boundary with a positive momentum p is a solution of the Schrödinger equation

$$-\frac{1}{2}\frac{d^2\psi_p}{dx^2} + V\psi_p = \mathcal{E}(p)\psi_p$$

where $\mathcal{E}(p) = \frac{p^2}{2} + V(a)$. For $x < a$, we have $\psi_p(x) = e^{ipx} + r_p e^{-ipx}$ which expresses the fact that only the incoming wave e^{ipx} has a prescribed amplitude (equal to 1), the reflection amplitude r_p being an unknown of the problem. Transparent boundary conditions are obtained for $x = a$ by eliminating this unknown [8, 9]. The total charge density is then computed by the formula

$$n(x) = \int f(p)\, |\psi_p(x)|^2 \, dp,$$

where $f(p)$ is the given statistics of entering particles (for $p < 0$, ψ_p corresponds to electrons injected at $x = b$ with momentum p). The stationary problem has been studied in [8, 9] and in [19] in the density matrix formalism.

In the time dependent situation, we start from such a stationary solution and then abruptly change the applied voltage. The question is to model the evolution of the system. As mentioned above, a more general problem is dealt with in [19] by scattering theory techniques. We choose here another route to tackle the problem. Namely we shall derive inhomogeneous time dependent transparent boundary conditions for the Schrödinger equation (the derivation of homogeneous boundary conditions can be found in [3, 7, 2]). Then we take advantage of the repulsivity of the electrostatic interaction in order to derive a priori estimates for the Schrödinger-Poisson problem. By doing so, we remove the restiction needed in [19] that $f(p) = 0$ in the vicinity of those p's such that $\mathcal{E}(p) = V(a)$ or $V(b)$.

The outline of the paper is as follows: in section (2), we introduce the notations and the setting of the problem; the main results of the paper are presented at the end of this section; in section (3), the linear model is studied and the boundary conditions are defined; section (4) deals with the non-linear problem and local existence while in section (5) global behaviour and energy estimates are investigated.

2 Setting of the problem and main results

The charge carriers occupy a region Ω of $\mathbb{R}^d$ ($d = 2$ or $d = 3$) which is the union of a regular bounded domain Ω_0 (the active region) and a finite number n of semi-infinite cylinders (leads) Ω_j which represent the access zones (see Fig. 1). The interface between the active region Ω_0 and the lead j ($j = 1, \cdots, n$) is denoted by Γ_j. The remaining part of the boundary of Ω_0 is denoted by Γ_0. The lead Ω_j behaves as a waveguide, injecting electrons into the active region Ω_0. It has a set of local coordinates $\xi_j \in \Gamma_j, \eta_j \in \mathbb{R}^+$ (see Fig. 1), where ξ_j is the transversal coordinate and η_j the longitudinal one. We introduce also $(\mu_j(x))_{j=1,\cdots,n}$, a partition of unity of Ω, *i.e.* some C^∞ functions which satisfy for $j = 1, \cdots, n$

$$\begin{cases} 0 \le \mu_j \le 1, & \displaystyle\sum_j \mu_j \equiv 1 \quad \text{on } \Omega \\ \mu_j \equiv 1 \text{ on } \Omega_j & \text{and} \quad \mu_j \equiv 0 \text{ on } \Omega_k \quad \text{for } k \ne 0,\, k \ne j \end{cases}$$

Class of initial data

Let us define the operator

$$\mathcal{H}^0 = -\Delta + V^0$$

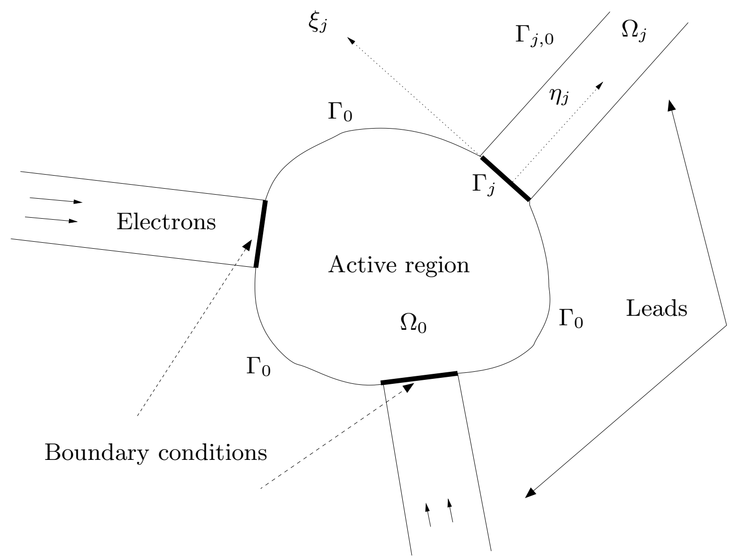

Figure 1: The domain Ω

where V^0 is the exterior potential which is assumed to only depend on the transversal coordinate in the leads:

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

Let (Λ, μ) be a set equipped with a bounded nonnegative measure μ such that

$$\mu(\Lambda) = \int_\Lambda d\mu < +\infty. \tag{2.1}$$

A family $\psi_\lambda^0 \in H_{loc}^2(\Omega)$ indexed by $\lambda \in \Lambda$ is said to belong to the class of initial data if the following hypotheses are satisfied:

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

$$\mathcal{H}^0\psi_\lambda^0 = E(\lambda)\psi_\lambda^0 \qquad \text{on } \Omega_j \quad (j = 1, \cdots, n).$$

(H-2) We have $\sup_{\lambda \in \operatorname{supp}\mu} |E(\lambda)| = M_E < +\infty$.

(H-3) For all bounded set $\mathcal{K} \subset \Omega$, there exists $C_\mathcal{K} > 0$ such that $\displaystyle\int_\Lambda \|\psi_\lambda^0\|_{H^2(\mathcal{K})}^2 d\mu(\lambda) \leq C_\mathcal{K}$.

The cut-off assumption **(H-2)** is introduced for technical simplicity and could be relaxed to

$$\int_\Lambda (E(\lambda))^p \|\psi_\lambda^0\|_{H^2(\mathcal{K})}^2 d\mu(\lambda) \leq C_\mathcal{K},$$

for p large enough and for all bounded set $\mathcal{K} \subset \Omega$.

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

$$\left\{\begin{array}{ll} -\Delta_{\xi_j}\,\chi_m^{0,j} + V_j^0(\xi_j)\,\chi_m^{0,j} = E_m^j\,\chi_m^{0,j}, & m \in \mathbb{N}^* \\ \chi_m^{0,j} \in H_0^1(\Gamma_j), \quad \displaystyle\int_{\Gamma_j} \chi_m^{0,j}\,\overline{\chi_{m'}^{0,j}}\,d\sigma(\xi_j) = \delta_{m,m'} & \end{array}\right. \tag{2.2}$$

where $d\sigma(\xi_j)$ is the surface measure on Γ_j. For any fixed j the sequence (E_m^j) tends to $+\infty$ as m tends to $+\infty$.

Typically in practice, $\lambda = \{k, m_0, j_0\}$, $\Lambda = \mathbb{R}^+ \times \mathbb{N}^* \times [1, n]$, $E(\lambda) = k^2 + E_{m_0}^{j_0}$ and

$$d\mu(\lambda) = \Phi(k, m_0, j_0)\,dk\,\delta_{m,m_0}\,\delta_{j,j_0}$$

where δ denotes the Kronecker symbol. The energy k^2 represents the kinetic energy of the electrons while $E_{m_0}^{j_0}$ is the transversal energy of the m_0th mode in the lead j_0. The function Φ is the statistics of the injected electrons.

Remark 2.2 *Without loss of generality, we assume $V_j^0 \geq 0$, a.e, $j = 1, \cdots, n$. Then*

$$E_m^j \geq 0 \quad \forall m \geq 1,\ j = 1, \cdots, n.$$

For a function g defined on Γ_j $(j \neq 0)$, we introduce the notation

$$\langle g\rangle_j := \int_{\Gamma_j} g(\xi_j)\,d\sigma(\xi_j).$$

Remark 2.3 *Let φ be an $L^2(\Gamma_j)$ function. We denote by*

$$\varphi_m^j(\xi_j) = \chi_m^j(\xi_j)\,\left\langle \varphi\overline{\chi_m^j}\right\rangle_j$$

its projection on χ_m^j. Thanks to (2.2), the relation $\varphi \mapsto \left(\displaystyle\sum_{m\geq 1} E_m^j\,\|\varphi_m^j\|^2_{L^2(\Gamma_j)}\right)^{1/2}$ defines a norm equivalent to the $H_0^1(\Gamma_j)$ norm.

Class $\mathcal{V}$ of potentials

We shall say that a potential W belongs to the class $\mathcal{V}$ if it satisfies:

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

In the Schrödinger-Poisson system presented in this paper, the potential V can be decomposed as the sum of a given external potential V_e and a selfconsistent potential V_s localized in the active zone, *i.e.* supported in Ω_0. We shall assume

(H-4) The external potential V_e belongs to the above defined class $\mathcal{V}$.

If $V_s \in C^1([0,T], L^\infty(\Omega))$, this assumption implies that V belongs to the class $\mathcal{V}$.

Let us now define the operator

$$\mathcal{H}(t) = -\Delta + V_e(t,x) + V_s(t,x).$$

The open Schrödinger-Poisson system consists in solving for $V_s(t,x)$ and $\psi_\lambda(t,x)$

$$i\partial_t \psi_\lambda = \mathcal{H}(t)\psi_\lambda \quad ; \quad \psi_\lambda(0,\cdot) = \psi_\lambda^0 \quad ; \quad x \in \Omega \tag{2.3}$$

$$\mathcal{H}(t) = -\Delta + V_e(t,x) + V_s(t,x) \quad ; \quad \mathrm{supp}(V_s) \subset \Omega_0 \tag{2.4}$$

$$-\Delta V_s = n = \int_\Lambda |\psi_\lambda|^2 d\mu(\lambda), \qquad x \in \Omega_0 \quad ; \quad V_s\,|_{\partial\Omega_0} \equiv 0. \tag{2.5}$$

Notice that the Schrödinger equation is set on the whole domain Ω including the leads. We shall derive transparent boundary conditions allowing for its resolution on the domain Ω_0 only. To this aim, we first remark that, according to **(H-1)** and **(H-4)** we have

$$\mathcal{H}(t)\psi_\lambda^0 = (E(\lambda) + V_j(t))\,\psi_\lambda^0 \qquad \text{on } \Omega_j \quad \text{ for } j = 1, \cdots, n.$$

Defining the phase factor

$$\theta_\lambda^j(t) = \exp\left(-i\int_0^t (E(\lambda) + V_j(s))\,ds\right),$$

the plane wave function

$$\psi_\lambda^{pw}(t,x) = \psi_\lambda^0(x)\sum_{j=1}^n \mu_j(x)\theta_\lambda^j(t) \tag{2.6}$$

satisfies

$$i\partial_t\psi_\lambda^{pw} = \mathcal{H}(t)\psi_\lambda^{pw} \qquad \text{on } \cup_{j=1,\cdots,n}\Omega_j \quad ; \quad \psi_\lambda^{pw}(0,x) = \psi_\lambda^0(x) \qquad \text{on } \Omega.$$

In order to define the boundary conditions, we introduce the following notation

$$\chi_m^j(t,\xi_j) = \chi_m^{0,j}(\xi_j)\,\exp\left(-i\int_0^t (V_j(\tau) + E_m^j)\,d\tau\right). \tag{2.7}$$

At any time, $(\chi_m^j)_{m\geq 1}(t,.)$ is an orthonormal basis of $L^2(\Gamma_j)$.

Definition 2.4 *For any given function $f \in H^\alpha(0,T)$, $\alpha \geq 0$, one defines - see [15]:*

$$\mathcal{I}^{1/2}f = \frac{1}{\sqrt{\pi}}\int_0^t \frac{f(\tau)}{\sqrt{t-\tau}}d\tau$$

which verifies $\mathcal{I}^{1/2} f \in H^{1/2+\alpha}(0,T)$. Then, we denote $\partial^{1/2} f$ as the distributional derivative of $\mathcal{I}^{1/2} f$:

$$\partial^{1/2} f = \frac{d}{dt}\mathcal{I}^{1/2} f = \frac{1}{\sqrt{\pi}}\frac{d}{dt}\int_0^t \frac{f(\tau)}{\sqrt{t-\tau}}d\tau.$$

For any $f \in H^{\alpha}((0,T),\, L^2(\Gamma_j))$, we set

$$\mathbb{I}_j^{1/2} f(t,\xi_j) = \sum_{m\geq 1} \chi_m^j(t,\xi_j)\, \mathcal{I}^{1/2} \left\langle f(t,\cdot)\, \overline{\chi_m^j(t,\cdot)} \right\rangle_j \tag{2.8}$$

$$\mathbb{D}_j^{1/2} f(t,\xi_j) = \sum_{m\geq 1} \chi_m^j(t,\xi_j)\, \partial^{1/2} \left\langle f(t,\cdot)\, \overline{\chi_m^j(t,\cdot)} \right\rangle_j . \tag{2.9}$$

The main results of this paper are summarized in the following theorem:

Theorem 2.5 *Assume $d = 2,3$. Under the hypotheses* **(H-1)**–**(H-4)** *above, the Schrödinger-Poisson system* (2.3)–(2.5) *admits a unique solution (ψ_λ, V_s) such that*

$$V_s \in \mathcal{C}^0([0,T], H_0^1(\Omega_0)) \cap \mathcal{C}^0([0,T], H^4(\Omega_0)) \cap \mathcal{C}^1([0,T], H^2(\Omega_0))$$

and $\psi_\lambda \in \psi_\lambda^{pw} + \mathcal{E}$ for $\lambda \in \Lambda$ a.e. with

$$\mathcal{E} = \mathcal{C}^0([0,T], H^2(\Omega)) \cap \mathcal{C}^1([0,T], L^2(\Omega)), \tag{2.10}$$

where T is arbitrary large. Moreover, the Schrödinger-Poisson system (2.3)–(2.5) *on Ω is equivalent to the boundary value problem on Ω_0 consisting in the Schrödinger-Poisson system* (2.3)–(2.5) *with a Dirichlet boundary condition on Γ_0 and one of the following equivalent boundary conditions on Γ_j, $j = 1,\cdots,n$:*

$$\frac{\partial}{\partial \eta_j}(\psi_\lambda - \psi_\lambda^{pw}) \;=\; -e^{-i\pi/4}\, \mathbb{D}_j^{1/2}(\psi_\lambda - \psi_\lambda^{pw}) \qquad a.e. \tag{2.11}$$

$$\psi_\lambda - \psi_\lambda^{pw} \;=\; -e^{i\pi/4}\, \mathbb{I}_j^{1/2}\left(\frac{\partial}{\partial \eta_j}(\psi_\lambda - \psi_\lambda^{pw})\right) \qquad a.e.. \tag{2.12}$$

In the whole paper, C will denote a generic constant, depending on μ_j, on $\|V_j\|_{\mathcal{C}^1([0,T])}$, on $\|V^0\|_{L^\infty}$, for $j = 1,\cdots,n$ and on M_E.

3 The linear equation

In this section, under hypothesis **(H-1)**–**(H-2)**, we study the linear Schrödinger equation (2.3) with

$$\mathcal{H}(t) = -\Delta + V(t,x)$$

and where V is given in the above defined class $\mathcal{V}$ of potentials. Firstly, we prove the well-posedness of this equation on $\psi_\lambda^{pw} + \mathcal{E}$. Notice that the classical L^2-theory does not apply since the initial data $\psi_\lambda^0 \notin L^2(\Omega)$. We also derive the boundary conditions satisfied by the wave function on each interface Γ_j, $j = 1,\cdots,n$. Finally, we give some estimates which will be crucial for the analysis of the non-linear problem.

3.1 Derivation of the boundary conditions

Before analyzing the Schrödinger equation in the open domain Ω, let us recall the standard result in the L^2 framework. Consider the Schrödinger equation

$$\begin{cases} i\partial_t \Psi = -\Delta\Psi + V(t,x)\Psi + f(t,x) \qquad ; \qquad x \in \Omega \\ \Psi(t=0,\cdot) = \Psi_0, \qquad \Psi = 0 \quad \text{on} \quad \mathbb{R}^+ \times \partial\Omega. \end{cases} \tag{3.1}$$

Lemma 3.1 *Let $V \in \mathcal{C}^1([0,T], L^\infty(\Omega))$, $f \in \mathcal{C}^1([0,T], L^2(\Omega))$ and $\Psi_0 \in H^2(\Omega)$. Then* (3.1) *admits a unique solution $\Psi \in \mathcal{C}^0([0,T], H^2(\Omega)) \cap \mathcal{C}^1([0,T], L^2(\Omega))$. Moreover Ψ satisfies the following estimates: $\forall T > 0$, $\forall t \in [0,T]$,*

$$\|\Psi(t)\|_{L^2(\Omega)} \leq \|\Psi_0\|_{L^2(\Omega)} + \|f\|_{L^1((0,t),L^2(\Omega))}, \tag{3.2}$$

$$\begin{aligned} \|\nabla\Psi(t)\|^2_{L^2(\Omega)} \quad &\leq \quad \|\nabla\Psi_0\|^2_{L^2(\Omega)} + C(1+t^3)\left(\|\Psi_0\|^2_{L^2(\Omega)} + \|f\|^2_{C^1([0,t],L^2(\Omega))}\right) \times \\ &\qquad \times \left(1 + \|V\|_{C^1([0,t],L^\infty(\Omega))}\right), \end{aligned} \tag{3.3}$$

$$\begin{aligned} \|\Psi(t)\|_{H^2(\Omega)} \quad &\leq \quad \left(\|\Psi_0\|_{H^2(\Omega)} + \|f\|_{C^1([0,t],L^2(\Omega))}\right) \times \\ &\qquad \times \left(1 + \|V\|_{C^1([0,t],L^\infty(\Omega))}\right). \end{aligned} \tag{3.4}$$

Proof. This proof is very standard. We shall however detail it for the sake of completeness. Since $V \in \mathcal{C}^1([0,T], L^\infty(\Omega))$, $i\Delta - iV$ generates a strongly differentiable unitary propagator $U(t,s)$ (see [24], theorem X.70) and then Ψ can be written

$$\Psi(t) = U(t,0)\Psi_0 + \int_0^t U(t,s)f(s)ds \in L^2(\Omega). \tag{3.5}$$

The regularity is obtained by noticing that $u := \partial_t\Psi$ verifies

$$u(t) = U(t,0)u_0 + \int_0^t U(t,s)\left(\partial_s V(s)\,\Psi(s) \ + \ \partial_s f(s)\right) ds \in L^2(\Omega) \tag{3.6}$$

since

$$u_0 = i\Delta\Psi_0 - iV(0,x)\Psi_0 - if(0,x) \in L^2(\Omega)$$

and

$$\partial_t V\,\Psi \ + \ \partial_t f \in C^0([0,T], L^2(\Omega)).$$

Finally, $\Psi \in \mathcal{C}^1([0,T], L^2(\Omega))$ and [13] (Remark 2.5.1 *(vi)*) gives $\Psi \in \mathcal{C}^0([0,T], H^2(\Omega)) \cap \mathcal{C}^1([0,T], L^2(\Omega))$.

To prove the estimate (3.4), we first notice from (3.5) that, $\forall T > 0$, $\forall t \in [0,T]$,

$$\|\Psi(t)\|_{L^2(\Omega)} \leq \|\Psi_0\|_{L^2(\Omega)} + \|f\|_{L^1((0,t),L^2(\Omega))}$$

and from (3.6) that

$$\|\partial_t\Psi(t)\|_{L^2(\Omega)} \leq C(1+t^2)\left(\|\Psi_0\|_{H^2(\Omega)} + \|f\|_{C^1([0,t],L^2(\Omega))}\right)\left(1 + \|V\|_{C^1([0,t],L^\infty(\Omega))}\right).$$

Finally, we estimate $\|\Delta\Psi(t)\|_{L^2(\Omega)}$ thanks to (3.1) to obtain (3.4). To obtain (3.3),we take the $L^2(\Omega)$ scalar product of (3.1) with $\partial_t\overline{\Psi}$, integrate over $[0,t]$ and take the real part. Estimate (3.3) follows after straightforward integration by parts. $\square$

Proposition 3.2 *(i) Assume $\psi_\lambda^0 \in H^2_{loc}(\Omega)$ such that* **(H-1)** *and* **(H-2)** *are satisfied. Then, the equation* (2.3)*, with V belonging to the class $\mathcal{V}$, admits a unique solution in $\psi_\lambda^{pw} + \mathcal{E}$, where ψ_λ^{pw} was defined in* (2.6)*. Moreover, this solution ψ_λ verifies the estimates, pointwise in t,*

$$\|\psi_\lambda(t) - \psi_\lambda^{pw}(t)\|_{L^2(\Omega)} \leq Ct\,\|\psi_\lambda^0\|_{H^2(\Omega_0)}\left(1 + \|V\|_{C^0([0,t],L^\infty(\Omega))}\right) \tag{3.7}$$

$$\|\psi_\lambda(t) - \psi_\lambda^{pw}(t)\|_{H^2(\Omega)} \leq C(1+t^2)\,\|\psi_\lambda^0\|_{H^2(\Omega_0)}\left(1 + \|V\|^2_{C^1([0,t],L^\infty(\Omega))}\right). \tag{3.8}$$

(ii) Assume **(H-1)**, **(H-2)** *satisfied. Let $\psi_\lambda \in \psi_\lambda^{pw} + \mathcal{E}$ be the unique solution of* (2.3)*, with V belonging to the class $\mathcal{V}$. Then ψ_λ is the unique solution of the boundary value problem on Ω_0 consisting in the Schrödinger equation* (2.3) *with the Dirichlet boundary condition on Γ_0 and one of the following equivalent boundary conditions a.e. on Γ_j, $j = 1,\cdots,n$:*

$$\begin{aligned}\frac{\partial}{\partial\eta_j}(\psi_\lambda - \psi_\lambda^{pw}) &= -e^{-i\pi/4}\,\mathbb{D}_j^{1/2}(\psi_\lambda - \psi_\lambda^{pw}) &(3.9)\\ \psi_\lambda - \psi_\lambda^{pw} &= -e^{i\pi/4}\,\mathbb{I}_j^{1/2}\left(\frac{\partial}{\partial\eta_j}(\psi_\lambda - \psi_\lambda^{pw})\right). &(3.10)\end{aligned}$$

The following remark will be used all along the paper:

Remark 3.3 *Standard interpolation results imply: for $0 \leq \sigma \leq 1$, $s \leq 1-\sigma$,*

$$\left[L^2((0,T),H^2(\Omega_0)),H^1((0,T),H^t(\Omega_0))\right]_\sigma = H^s((0,T),H^{2\sigma+(1-\sigma)t}(\Omega_0)), \tag{3.11}$$

see [1] for the definition of the interpolation brackets, and then

$$\mathcal{E} \subset H^s((0,T),H^{2\sigma}(\Omega_0)), \qquad 0 \leq \sigma \leq 1, \qquad s \leq 1-\sigma. \tag{3.12}$$

Proof. Let us first define the function $\phi_\lambda := \psi_\lambda - \psi_\lambda^{pw}$. Putting this expression into (2.3) and using **(H-1)**, we obtain

$$\begin{cases} i\dfrac{\partial\phi_\lambda}{\partial t} = -\Delta\phi_\lambda + V\,\phi_\lambda - S_\lambda(V) \quad \text{in } \Omega \\ \phi_\lambda(0,x) = 0, \end{cases} \tag{3.13}$$

where $S_\lambda(V)$ is defined by

$$\begin{aligned} S_\lambda(V) = {} & 2\,\nabla\psi_\lambda^0\cdot\sum_{j\geq 1}\nabla\mu^j\,\theta_\lambda^j + \psi_\lambda^0\sum_{j\geq1}\left(\Delta\mu^j + V_j\,\mu^j\right)\theta_\lambda^j \\ & + \left[(E(\lambda) - V)\psi_\lambda^0 + \Delta\psi_\lambda^0\right]\sum_{j\geq1}\mu^j\,\theta_\lambda^j \end{aligned} \tag{3.14}$$

and satisfies

$$\operatorname{supp} S_\lambda(V) \subset \Omega_0. \tag{3.15}$$

Since $\psi_\lambda^0 \in H^2_{loc}(\Omega)$ and $V \in \mathcal{C}^1([0,T], L^\infty(\Omega))$, we have $S_\lambda(V) \in \mathcal{C}^1([0,T], L^2(\Omega))$ and Lemma (3.1) applies: this gives the existence and uniqueness in $\psi_\lambda^{pw} + \mathcal{E}$. Estimates (3.7) and (3.8) are direct applications of (3.2) and (3.4) since

$$\|S_\lambda(V)\|_{\mathcal{C}^1([0,T],L^2(\Omega))} \le C\|\psi_\lambda^0\|_{H^2(\Omega_0)} \left(1 + \|V\|_{\mathcal{C}^1([0,T],L^\infty(\Omega))}\right). \tag{3.16}$$

The constant C above is λ-independent because of hypothesis **(H-2)**.

By using the approach developed in [14] for the wave equation, transparent boundary conditions were derived in [3, 7] for the 1D Schrödinger equation, in an homogeneous case and when the external potential is constant. In the present case, we apply the obtained results in each lead Ω_j and we extend them to the case of time-dependent external potentials. Consider the function ϕ_λ defined hereabove. On each Ω_j, $j = 1, \cdots, n$, the wavefunction ϕ_λ can be expanded on the basis $(\chi_m^j(t,\cdot))_m$:

$$\phi_\lambda(t, \xi_j, \eta_j) = \sum_{m\ge 1} \varphi_m(t, \eta_j)\, \chi_m^j(t, \xi_j).$$

Since V belongs to the class $\mathcal{V}$, it verifies

$$V\big|_{\Omega_j} = V_j^0(\xi_j) + V_j(t) \qquad j \ne 0$$

and thanks to (3.13), $\varphi_m(t, \eta_j)$ solves

$$\begin{cases} i\dfrac{\partial \varphi_m}{\partial t}(t,\eta_j) = -\dfrac{\partial^2 \varphi_m}{\partial \eta_j^2}(t,\eta_j) & (\eta_j \ge 0) \\ \\ \varphi_m(0,\eta_j) = 0. \end{cases} \tag{3.17}$$

Following now [3, 7], φ_m verifies on Γ_j the scalar Dirichlet-to-Neumann boundary condition:

$$\frac{\partial \varphi_m}{\partial \eta_j} = -e^{-i\pi/4}\, \partial^{1/2}\left(\varphi_m\right). \tag{3.18}$$

Similarly, φ_m satisfies the scalar Neumann-to-Dirichlet boundary condition:

$$\varphi_m = -e^{i\pi/4}\, \mathcal{I}^{1/2}\left(\frac{\partial \varphi_m}{\partial \eta_j}\right). \tag{3.19}$$

Finally, coming back to ϕ_λ, we obtain (3.9) and (3.10). Notice that (3.10) makes sense a.e. on $(0,T) \times \Gamma_j$ since $\phi_\lambda \in \mathcal{E}$ and then, by trace properties [18], $\frac{\partial}{\partial \eta_j}\phi_\lambda \in C^0([0,T], L^2(\Gamma_j))$. For (3.9), we deduce from (3.12) that $\mathcal{E} \subset H^{1/2}((0,T), H^1(\Omega_0))$. Therefore $\phi_\lambda|_{\Gamma_j} \in H^{1/2}((0,T), L^2(\Gamma_j))$ and (3.9) is verified a.e. on $(0,T) \times \Gamma_j$.

To complete the proof, it remains to remark that the solution of the boundary value problem (2.3) with (3.9) or (3.10) is unique. This property follows easily from estimate (3.26) that we shall prove in the next subsection. $\square$

3.2 Dissipation estimates

In this subsection, we first give some properties and dissipation relations of the boundary conditions (3.9) and (3.10). Then, we deduce some a priori estimates, leading in particular to uniqueness results.

Lemma 3.4 *Let the Fresnel integral be defined by*

$$\Upsilon(t) = \frac{1}{\sqrt{\pi}} \int_0^t \frac{e^{i\tau}}{\sqrt{\tau}}\, d\tau \quad ; \quad t \in \mathbb{R}. \tag{3.20}$$

There exists a positive constant M such that $|\Upsilon(t)| \leq M\sqrt{|t|}/(1+\sqrt{|t|})$ on $\mathbb{R}$. Moreover, we have the following identities

$$\mathcal{I}^{1/2}\left(e^{-i\omega t}\right) = \frac{e^{-i\omega t}}{\sqrt{\omega}}\, \Upsilon(\omega t) \qquad ; \qquad \partial^{1/2}\left(e^{-i\omega t}\right) = \frac{1}{\sqrt{\pi\, t}} - i\sqrt{\omega}\, e^{-i\omega t}\, \Upsilon(\omega t).$$

The proof of this lemma can be found in [15]. A direct consequence is

Lemma 3.5 *Let $\psi_\lambda^{pw} \in \mathcal{C}^1([0,T], H^2_{loc}(\Omega))$ be defined in (2.6), Υ in (3.20) and $\mathbb{D}_j^{1/2}$ in (2.9). Then, we have the following formula*

$$\mathbb{D}_j^{1/2}(\psi_\lambda^{pw}) = \sum_{m=1}^{+\infty} \Bigg(\frac{1}{\sqrt{\pi t}} - i\sqrt{E(\lambda) - E_m^j}\, e^{-i(E(\lambda)-E_m^j)\, t}\, \Upsilon\left(\left(E(\lambda) - E_m^j\right) t\right) \Bigg)\, \psi_m^{0,j} \chi_m^j \tag{3.21}$$

where $\psi_m^{0,j} = \langle \psi_\lambda^0(\eta_j = 0, \cdot)\, \overline{\chi_m^{0,j}} \rangle_j$. Here $(\chi_m^{0,j}, E_m^j)_{m\in\mathbb{N}^*}$ are the eigenvectors and eigenvalues of the guide j as expressed in (2.2) and χ_m^j is equal to $\chi_m^{0,j}$ modulated by a phase factor, see (2.7). Furthermore, if $|E(\lambda)| \leq M_E$ then we have

$$\|\mathbb{D}_j^{1/2}(\psi_\lambda^{pw})\|_{L^2(\Gamma_j)} \leq C\sqrt{1 + \frac{1}{\pi t}}\, \|\psi_\lambda^0\|_{H^2(\Omega_0)} \tag{3.22}$$

where C depends on M, on M_E and on T.

Proof. According to Lemma (3.4) and the estimate provided on Υ therein,

$$\|\mathbb{D}_j^{1/2}(\psi_\lambda^{pw})\|^2_{L^2(\Gamma_j)} \leq \frac{1}{\pi t} \|\psi_\lambda^0\|^2_{L^2(\Gamma_j)} + M \sum_{m\geq 1} \left(M_E + E_m^j\right) |\psi_m^{0,j}|^2$$

and Remark (2.3) coupled to trace properties imply

$$\sum_{m\geq 1} E_m^j |\psi_m^{0,j}|^2 \leq C\|\psi_\lambda^0\|^2_{H^1(\Gamma_j)} \leq C'\|\psi_\lambda^0\|^2_{H^2(\Omega_0)}.$$

□

The following technical lemma will enable to prove the dissipative properties of the homogeneous transparent boundary conditions:

Lemma 3.6 *Let $f \in H^{1/4}((0,T); L^2(\Gamma_j))$, $g \in L^2((0,T); L^2(\Gamma_j))$. Then, denoting by $S^{\pi/4}$ the cone*

$$S^{\pi/4} = \{z \in \mathbb{C} : \, Arg(z) \in [-\pi/4, \pi/4]\},$$

we have

$$\int_0^T \left\langle \overline{f}(t)\, \mathbb{D}^{1/2}(f(t)) \right\rangle_j \, dt \in S^{\pi/4}, \tag{3.23}$$

$$\int_0^T \left\langle \overline{g}(t)\, \mathbb{I}^{1/2}(g(t)) \right\rangle_j \, dt \in S^{\pi/4}. \tag{3.24}$$

As will be seen in the proof, Formula (3.23) is to be understood as a duality product of $H^{1/4}(0,T)$ and $H^{-1/4}(0,T)$. **Proof.** This lemma is a consequence of Definition (2.4) and of the Plancherel equality. Indeed, setting

$$f_m^j(t) = \left\langle f(t)\, \overline{\chi_m^{0,j}} \right\rangle_j$$

and denoting by $Pf_m^j \in H^{1/4}(\mathbb{R})$ the function extended by zero outside $(0,T)$, we have

$$\int_0^T \bar{f}_m^j \, \partial^{1/2} f_m^j \, dt = \frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} \sqrt[+]{i\nu} \left| \widehat{Pf_m^j}(i\nu) \right|^2 d\nu,$$

where $\sqrt[+]{}$ denotes the square root with nonnegative real part. It is now enough to remark that for every real number ν we have $\sqrt[+]{i\nu} \in S^{\pi/4}$ and that $S^{\pi/4}$ is stable by summations. Estimate (3.24) can be proved similarly. Indeed, denoting

$$g_m^j(t) = \left\langle g(t)\, \overline{\chi_m^{0,j}} \right\rangle_j$$

we have

$$\int_0^T \bar{g}_m^j \, \mathcal{I}^{1/2} g_m^j \, dt = \frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} \frac{1}{\sqrt[+]{i\nu}} \left| \widehat{Pg_m^j}(i\nu) \right|^2 d\nu \in S^{\pi/4}. \tag{3.25}$$

□

Let us now state the main result of this section:

Proposition 3.7 *Assume* **(H-1)**-**(H-2)** *satisfied and let V belong to the class $\mathcal{V}$. Let $\psi_\lambda \in \psi_\lambda^{pw} + \mathcal{E}$ be the unique solution of (2.3). Then, ψ_λ satisfies the following estimates, for all T positive, for all t in $]0,T]$, λ a.e.,*

$$\|\psi_\lambda(t)\|^2_{L^2(\Omega_0)} \leq \|\psi_\lambda^0\|^2_{L^2(\Omega_0)} + C\|\psi_\lambda^0\|_{H^2(\Omega_0)} \int_0^t \left(1 + \frac{1}{\sqrt{\pi s}}\right) \|\psi_\lambda(s)\|_{H^1(\Omega_0)} ds, \tag{3.26}$$

$$\begin{aligned} \|\psi_\lambda(t)\|^2_{H^1(\Omega_0)} \leq C\|\psi_\lambda^0\|^2_{H^2(\Omega_0)} &+ C \int_0^t \left(1 + \frac{1}{\sqrt{\pi s}}\right) \|\psi_\lambda(s)\|^2_{H^1(\Omega_0)} ds \\ &- \int_0^t \int_{\Omega_0} V \partial_t |\psi_\lambda|^2 ds \\ &+ C\|\psi_\lambda^0\|_{H^2(\Omega_0)} \int_0^t \|V(s)\|_{L^2(\Omega)} \left(\|\psi_\lambda^0\|_{L^2(\Omega_0)} + \|\psi_\lambda(s)\|_{L^2(\Omega_0)}\right) ds. \end{aligned} \tag{3.27}$$

Proof. This proof relies on the application of the dissipation relations (3.23)-(3.24). Taking the $L^2(\Omega_0)$ scalar product of (2.3) with $\psi_\lambda(t)$, taking the imaginary part (denoted by $\Im$) and integrating over $[0,t]$ leads to

$$\|\psi_\lambda(t)\|^2_{L^2(\Omega_0)} = \|\psi^0_\lambda\|^2_{L^2(\Omega_0)} - 2\sum_{j=0}^{n} \Im \int_0^t \left\langle \frac{\partial \psi_\lambda}{\partial \eta_j}(s,\cdot)\,\overline{\psi_\lambda}(s,\cdot)\right\rangle_j ds. \tag{3.28}$$

In order to estimate the non-linear boundary term, we first recast it into, using the boundary condition (2.11),

$$\begin{aligned}\int_0^t \left\langle \frac{\partial \psi_\lambda}{\partial \eta_j}\,\overline{\psi_\lambda}\right\rangle_j ds \;&=\; -\int_0^t \left\langle e^{-i\pi/4}\,\left(\mathbb{D}_j^{1/2}\psi_\lambda\right)\,\overline{\psi_\lambda}\right\rangle_j ds + \int_0^t \left\langle \frac{\partial \psi^{pw}_\lambda}{\partial \eta_j}\,\overline{\psi_\lambda}\right\rangle_j ds \\ &\quad + \int_0^t \left\langle e^{-i\pi/4}\,\left(\mathbb{D}_j^{1/2}\psi^{pw}_\lambda\right)\,\overline{\psi_\lambda}\right\rangle_j ds.\end{aligned} \tag{3.29}$$

Applying (3.23) to $\psi_\lambda \in \mathcal{E}$ implies

$$\Im \int_0^t \left\langle e^{-i\pi/4}\,\left(\mathbb{D}_j^{1/2}\psi_\lambda\right)\,\overline{\psi_\lambda}\right\rangle_j ds \le 0$$

and it remains to treat the linear terms of (3.29). The first one is estimated by

$$\int_0^t \left\langle \frac{\partial \psi^{pw}_\lambda}{\partial \eta_j}\,\overline{\psi_\lambda}\right\rangle_j ds \le \int_0^t \|\psi^0_\lambda\|_{H^2(\Omega_0)}\,\|\psi_\lambda\|_{H^1(\Omega_0)} ds$$

while, thanks to (3.22), we have for the second one

$$\int_0^t \left\langle e^{-i\pi/4}\,\left(\mathbb{D}_j^{1/2}\psi^{pw}_\lambda\right)\,\overline{\psi_\lambda}\right\rangle_j ds \le C\|\psi^0_\lambda\|_{H^2(\Omega_0)} \int_0^t \left(1+\frac{1}{\sqrt{\pi s}}\right)\|\psi_\lambda(s)\|_{H^1(\Omega_0)} ds.$$

This ends the proof of (3.26).

Let us now tackle (3.27). To this aim, we first take the real part (denoted by $\Re$) of the $L^2(\Omega_0)$ scalar product of (2.3) with $\partial_t\overline{\psi_\lambda}(t)$ and get

$$\begin{aligned}\|\nabla\psi_\lambda(t)\|^2_{L^2(\Omega_0)} = \|\nabla\psi^0_\lambda\|^2_{L^2(\Omega_0)} + 2\sum_{j=0}^{n} \Re \int_0^t \left\langle \frac{\partial \psi_\lambda}{\partial \eta_j}\,\overline{\partial_t\psi_\lambda}\right\rangle_j ds \\ - \int_0^t\int_{\Omega_0} V\partial_t|\psi_\lambda|^2 ds.\end{aligned} \tag{3.30}$$

In order to estimate the second term of the right hand side, we define $\phi_\lambda = \psi_\lambda - \psi^{pw}_\lambda$. This function satisfies the following equation on Γ_j (see (2.8) and (3.10))

$$\partial_t\phi_\lambda = -e^{i\pi/4}\,\mathbb{D}_j^{1/2}\left(\frac{\partial\phi_\lambda}{\partial\eta_j}\right) - i\,V_j\,\phi_\lambda + ie^{i\pi/4}\sum_{m\ge1} E^j_m\,\chi^j_m\,\mathcal{I}^{1/2}\left(\left\langle\frac{\partial\phi_\lambda}{\partial\eta_j}\,\overline{\chi^j_m}\right\rangle_j\right). \tag{3.31}$$

We then have

$$\begin{aligned}
\Re \sum_j \int_0^t \left\langle \frac{\partial \psi_\lambda}{\partial \eta_j}\, \partial_t \overline{\psi_\lambda} \right\rangle_j ds \;=\; & -\Re \sum_j e^{-i\pi/4} \int_0^t \left\langle \frac{\partial \phi_\lambda}{\partial \eta_j}\, \overline{\mathbb{D}_j^{1/2}\left(\frac{\partial \phi_\lambda}{\partial \eta_j}\right)} \right\rangle_j ds \\
& -\Im \sum_j \int_0^t V_j \left\langle \frac{\partial \phi_\lambda}{\partial \eta_j}\, \overline{\phi_\lambda} \right\rangle_j ds \\
-\Re\, i\, e^{-i\pi/4} \sum_{m\geq 1} E_m^j & \int_0^t \left\langle \frac{\partial \phi_\lambda}{\partial \eta_j}\, \overline{\chi_m^j} \right\rangle_j \mathcal{I}^{1/2}\left(\left\langle \frac{\partial \overline{\phi_\lambda}}{\partial \eta_j}\, \chi_m^j \right\rangle_j \right) ds \\
& +\Re \sum_j \int_0^t \left\langle \frac{\partial \psi_\lambda^{pw}}{\partial \eta_j}\, \partial_t \overline{\psi_\lambda} \right\rangle_j ds \\
& +\Re \sum_j \int_0^t \left\langle \frac{\partial \phi_\lambda}{\partial \eta_j}\, \partial_t \overline{\psi_\lambda^{pw}} \right\rangle_j ds.
\end{aligned}$$

In the sequel of the proof we shall assume that $\phi_\lambda \in \mathcal{C}^1([0,T], H^1(\Omega_0))$. If this is not the case, is suffices to regularize the data, then obtain the estimate for the regularized solution and pass to the limit in the regularization. We will use twice the dissipative properties stated in Lemma 3.6. Firstly, since by (3.11) we have $\phi_\lambda \in H^{1/4}((0,T), H^{7/4}(\Omega_0))$, some trace properties imply that $\frac{\partial}{\partial \eta_j}\phi_\lambda \in H^{1/4}((0,T), H^{1/4}(\Gamma_j))$ (notice that $\phi_\lambda \in \mathcal{C}^1([0,T], L^2(\Omega_0))$ would only lead to $\frac{\partial}{\partial \eta_j}\phi_\lambda$ in $H^{1/4-\alpha}((0,T), L^2(\Gamma_j))$, $\forall \alpha > 0$, which is not sufficient). Hence (3.23) applied to $\frac{\partial}{\partial \eta_j}\phi_\lambda$ gives

$$-\Re e^{-i\pi/4} \int_0^t \left\langle \frac{\partial \phi_\lambda}{\partial \eta_j}\, \overline{\mathbb{D}_j^{1/2}\left(\frac{\partial \phi_\lambda}{\partial \eta_j}\right)} \right\rangle_j ds \leq 0.$$

Secondly, thanks to Remark (2.2) we notice that $E_m^j \geq 0$. Thus from (3.25) we obtain

$$-\Re\, i\, e^{-i\pi/4} \sum_{m\geq 1} E_m^j \int_0^t \left\langle \frac{\partial \phi_\lambda}{\partial \eta_j}\, \overline{\chi_m^j} \right\rangle_j \mathcal{I}^{1/2}\left(\left\langle \frac{\partial \overline{\phi_\lambda}}{\partial \eta_j}\, \chi_m^j \right\rangle_j \right) ds \leq 0.$$

Then we deduce that

$$\Re \sum_j \int_0^t \left\langle \frac{\partial \psi_\lambda}{\partial \eta_j}\, \partial_t \overline{\psi_\lambda} \right\rangle_j ds \leq R_1 + R_2 + R_3,$$

where

$$R_1 = \Re \sum_j \int_0^t \left\langle \frac{\partial \psi_\lambda^{pw}}{\partial \eta_j}\, \partial_t \overline{\psi_\lambda} \right\rangle_j ds \quad ; \quad R_2 = -\Im \sum_j \int_0^t V_j \left\langle \frac{\partial \phi_\lambda}{\partial \eta_j}\, \overline{\phi_\lambda} \right\rangle_j ds$$

and

$$R_3 = \Re \sum_j \int_0^t \left\langle \frac{\partial \phi_\lambda}{\partial \eta_j}\, \partial_t \overline{\psi_\lambda^{pw}} \right\rangle_j ds.$$

Let us estimate R_1, R_2 and R_3 separately. For R_1, an integration by parts and standard trace estimates lead to

$$R_1 \leq \|\psi_\lambda^0\|_{H^2(\Omega_0)} \left(\|\psi_\lambda^0\|_{H^1(\Omega_0)} + \|\psi_\lambda(t)\|_{H^1(\Omega_0)} + C\int_0^t \|\psi_\lambda(s)\|_{H^1(\Omega_0)} ds \right). \quad (3.32)$$

In order to treat the term R_2, we set $\widetilde{V}(t,x) := \sum_j \mu_j(x) V_j(t)$ and remark that

$$R_2 = -\Im \int_0^t \int_{\Omega_0} \nabla\phi_\lambda \cdot \nabla(\widetilde{V}\overline{\phi_\lambda})\, dx\, ds + \Im \int_0^t \int_{\Omega_0} \Delta\phi_\lambda \widetilde{V}\overline{\phi_\lambda}\, dx\, ds.$$

Therefore (3.13) gives

$$R_2 = \frac{1}{2}\int_0^t \int_{\Omega_0} \partial_s|\phi_\lambda|^2\, \widetilde{V} dx\, ds - \Im \int_0^t \int_{\Omega_0} S_\lambda\, \overline{\phi_\lambda}\, \widetilde{V} dx\, ds - \Im \int_0^t \int_{\Omega_0} \nabla\phi_\lambda \cdot \nabla\widetilde{V}\, \overline{\phi_\lambda}\, dx\, ds.$$

Straightforward algebra leads to

$$\begin{aligned}
\int_0^t \int_{\Omega_0} \partial_s|\phi_\lambda|^2\, \widetilde{V} dx\, ds &\leq C\|\phi_\lambda(t)\|^2_{L^2(\Omega_0)} + C\int_0^t \|\phi_\lambda(s)\|^2_{L^2(\Omega_0)} ds, \\
\Im \int_0^t \int_{\Omega_0} S_\lambda\, \overline{\phi_\lambda}\, \widetilde{V} dx\, ds &\leq C\|\psi_\lambda^0\|_{H^2(\Omega_0)} \int_0^t \left(1 + \|V(s)\|_{L^2(\Omega)}\right) \|\phi_\lambda(s)\|_{L^2(\Omega_0)} ds, \\
\Im \int_0^t \int_{\Omega_0} \nabla\phi_\lambda\, \overline{\phi_\lambda}\, \nabla\widetilde{V}\, dx\, ds &\leq C\int_0^t \|\phi_\lambda(s)\|^2_{H^1(\Omega_0)} ds.
\end{aligned}$$

Since

$$\|\phi_\lambda(t)\|_{L^2(\Omega_0)} \leq \|\psi_\lambda^0\|_{L^2(\Omega_0)} + \|\psi_\lambda(t)\|_{L^2(\Omega_0)},$$

we obtain, thanks to (3.26),

$$\begin{aligned}
R_2 \leq{}& C\|\psi_\lambda^0\|^2_{H^2(\Omega_0)} + C\int_0^t \left(1 + \frac{1}{\sqrt{\pi s}}\right) \|\psi_\lambda(s)\|^2_{H^1(\Omega_0)} ds \\
&+ C\|\psi_\lambda^0\|_{H^2(\Omega_0)} \int_0^t \|V(s)\|_{L^2(\Omega)} \left(\|\psi_\lambda^0\|_{L^2(\Omega_0)} + \|\psi_\lambda(s)\|_{L^2(\Omega_0)}\right) ds. \quad (3.33)
\end{aligned}$$

To complete the proof of (3.27), it remains to treat the term R_3. For this purpose, we use again the Schrödinger equation (3.13). Taking the $L^2(\Omega_0)$ scalar product of (3.13) with $\partial_t\overline{\psi_\lambda^{pw}}$, taking the real part and integrating over $[0,t]$ leads to

$$\begin{aligned}
R_3 ={}& \Im \int_0^t \int_{\Omega_0} \partial_t\phi_\lambda\, \partial_t\overline{\psi_\lambda^{pw}}\, dxds + \Re \int_0^t \int_{\Omega_0} \nabla\phi_\lambda\, \nabla\partial_t\overline{\psi_\lambda^{pw}}\, dxds \quad (3.34) \\
&+ \Re \int_0^t \int_{\Omega_0} V\, \phi_\lambda\, \partial_t\overline{\psi_\lambda^{pw}}\, dxds - \Re \int_0^t \int_{\Omega_0} S_\lambda\, \partial_t\overline{\psi_\lambda^{pw}}\, dxds. \quad (3.35)
\end{aligned}$$

Straightforward calculations coupled to (3.26) imply

$$\begin{aligned}
R_3 \leq{}& C\|\psi_\lambda^0\|^2_{H^1(\Omega_0)} + C\|\psi_\lambda^0\|_{H^2(\Omega_0)} \int_0^t \left(1 + \frac{1}{\sqrt{\pi s}}\right) \|\psi_\lambda(s)\|_{H^1(\Omega_0)} ds \\
&+ C\|\psi_\lambda^0\|_{H^2(\Omega_0)} \int_0^t \|V(s)\|_{L^2(\Omega)} \left(\|\psi_\lambda^0\|_{L^2(\Omega_0)} + \|\psi_\lambda(s)\|_{L^2(\Omega_0)}\right) ds.
\end{aligned} \quad (3.36)$$

The proof is complete after gathering (3.33), (3.32) and (3.36). $\square$

4 Local-in-time existence and uniqueness

In this section, we prove that the system (2.3)-(2.5) has a unique local solution. We use a fixed point argument for the self-consistent V_s. Starting from a given potential V_s, we define the application $\mathcal{F}(V_s)$ by

$$-\Delta\mathcal{F}(V_s) = n\,[V_s] = \int_\Lambda |\psi_\lambda\,[V_s]\,|^2 d\mu(\lambda) \quad ; \quad x \in \Omega_0 \quad ; \quad \mathcal{F}(V_s)\,|_{\partial\Omega_0} \equiv 0 \tag{4.1}$$

where $\psi_\lambda\,[V_s]$ is given by

$$i\partial_t\psi_\lambda = \mathcal{H}(t)\psi_\lambda \quad ; \quad \psi_\lambda(0,\cdot) = \psi_\lambda^0 \quad ; \quad x \in \Omega \tag{4.2}$$

$$\mathcal{H}(t) = -\Delta + V_e(t,x) + V_s(t,x) \tag{4.3}$$

with V_e belonging to the class $\mathcal{V}$. The fact that $\mathcal{F}$ admits a unique fixed point for small times is a straightforward corollary of the following proposition:

Proposition 4.1 *Under hypothesis* **(H-1)**–**(H-4)***, there exists a time t_0 such that the application $\mathcal{F}$ is contraction on $\mathcal{C}^1([0,t_0],L^\infty(\Omega_0)) \cap \mathcal{C}^0([0,t_0],H_0^1(\Omega_0))$.*

Proof. For notational simplicity, let

$$X := \mathcal{C}^1([0,t_0],L^\infty(\Omega_0)) \cap \mathcal{C}^0([0,t_0],H_0^1(\Omega_0)).$$

We first check that $\mathcal{F}(X) \subset X$. It is straightforward to see that $V := V_e + V_s$ belongs to the class $\mathcal{V}$, so that one can apply the results of Section (3). Since $\psi_\lambda^0 \in H^2_{loc}(\Omega)$, Proposition (3.2) *(i)* applies and (4.2)-(4.3) admits a unique solution $\psi_\lambda\,[V_s] \in \mathcal{E} + \psi_\lambda^{pw}$ such that, for all t in $[0,t_0]$,

$$\int_\Lambda \|\psi_\lambda(t)\|^2_{H^2_{loc}(\Omega)}\, d\mu(\lambda) \le C(V_s).$$

Furthermore, the embedding $H^2(\Omega_0) \hookrightarrow L^\infty(\Omega_0)$, for $d \le 3$, implies that $n\,[V_s] \in \mathcal{C}^0([0,t_0],L^\infty(\Omega_0))$ and by (4.1), the elliptic regularity gives

$$\mathcal{F}(V_s) \in \mathcal{C}^0([0,t_0],W^{2,q}(\Omega_0)) \cap \mathcal{C}^0([0,t_0],H_0^1(\Omega_0)), \qquad \forall q < \infty.$$

Besides, in order to estimate $\partial_t\mathcal{F}(V_s)$, we introduce n_λ and j_λ defined by

$$n_\lambda = |\psi_\lambda|^2 \qquad ; \qquad j_\lambda = \Im(\overline{\psi_\lambda}\nabla\psi_\lambda).$$

The charge conservation identity yields

$$\partial_t n_\lambda + \operatorname{div} j_\lambda = 0. \tag{4.4}$$

By (4.1) and (4.4), $\partial_t \mathcal{F}(V_s)$ solves

$$\Delta\,\partial_t \mathcal{F}(V_s) = \mathrm{div} J(V_s) \quad ; \quad x \in \Omega_0 \quad ; \quad \partial_t \mathcal{F}(V_s)\,|_{\partial\Omega_0} \equiv 0 \tag{4.5}$$

where

$$J = \int_\Lambda j_\lambda \, d\mu(\lambda).$$

Thanks to hypothesis **(H-2)** and the Jensen inequality, we have

$$\|J(t)\|_{L^6(\Omega_0)} \le C \left(\int_\Lambda \|\psi_\lambda(t)\|^2_{W^{1,6}(\Omega_0)} \, d\mu(\lambda) \right)^{1/2} \left(\int_\Lambda \|\psi_\lambda(t)\|^2_{L^\infty(\Omega_0)} \, d\mu(\lambda) \right)^{1/2}$$

and the Sobolev embeddings $H^2(\Omega_0) \hookrightarrow L^\infty(\Omega_0)$ and $H^2(\Omega_0) \hookrightarrow W^{1,6}(\Omega_0)$, for $d \le 3$, give a bound for J in $\mathcal{C}([0,t_0], L^6(\Omega_0))$. This implies, together with (4.5) and standard elliptic regularity estimates , that $\partial_t \mathcal{F}(V_s) \in \mathcal{C}([0,t_0], W_0^{1,6}(\Omega_0))$. Thanks to the embedding $W^{1,6}(\Omega_0) \hookrightarrow L^\infty(\Omega_0)$, for $d \le 3$, we deduce that

$$\partial_t \mathcal{F}(V_s) \in \mathcal{C}^0([0,t_0], L^\infty(\Omega_0)).$$

This proves that $\mathcal{F}(V_s) \in X$.

We now prove that $\mathcal{F}$ is a contraction for t_0 small enough. Given two potentials V_s and $\widetilde{V}_s$ in an open ball of X with radius R, let us denote by ψ_λ and $\widetilde{\psi_\lambda}$ the associated wavefunctions, belonging to $\mathcal{E} + \psi_\lambda^{pw}$. We have

$$-\Delta \left(\mathcal{F}(V_s) - \mathcal{F}(\widetilde{V}_s) \right) = n(V_s) - n(\widetilde{V}_s) \tag{4.6}$$

$$\Delta\,\partial_t \left(\mathcal{F}(V_s) - \mathcal{F}(\widetilde{V}_s) \right) = J(V_s) - J(\widetilde{V}_s). \tag{4.7}$$

In order to control $n(V_s) - n(\widetilde{V}_s)$ and $J(V_s) - J(\widetilde{V}_s)$, we first estimate the quantity $w_\lambda := \psi_\lambda - \widetilde{\psi_\lambda}$ thanks to the Schrödinger equation (4.2). According to (4.2) and (4.3), w_λ solves

$$i\partial_t w_\lambda = -\Delta w_\lambda + (V_e + V_s) w_\lambda + (V_s - \widetilde{V}_s)\widetilde{\psi_\lambda} \qquad ; \qquad w_\lambda(0,\cdot) = 0. \tag{4.8}$$

Since $V_e + V_s \in \mathcal{C}^1([0,t_0], L^\infty(\Omega))$ and $(V_s - \widetilde{V}_s)\widetilde{\psi_\lambda} \in \mathcal{C}^1([0,t_0], L^2(\Omega))$, Lemma (3.1) applies. Then (3.7), (3.8), (3.2) and (3.4) imply

$$\|w_\lambda(t)\|_{L^2(\Omega)} \le C_R\, t_0\, \|\psi_\lambda^0\|_{H^1(\Omega)}\, \|V_s - \widetilde{V}_s\|_{C^0([0,t_0],L^\infty(\Omega_0))} \tag{4.9}$$

$$\|w_\lambda(t)\|_{H^2(\Omega)} \le C_R \|\psi_\lambda^0\|_{H^1(\Omega)} \|V_s - \widetilde{V}_s\|_{C^1([0,t_0],L^\infty(\Omega_0))} \tag{4.10}$$

To estimate the difference $n(V_s) - n(\widetilde{V}_s)$, we take advantage of (3.8) and of the embedding $H^2(\Omega_0) \hookrightarrow L^\infty(\Omega_0)$ as well as (4.9), and obtain

$$\begin{aligned}
&\|n(V_s) - n(\widetilde{V}_s)\|_{L^2(\Omega_0)}(t) \\
&\qquad \le \left(\int_\Lambda \|\psi_\lambda + \widetilde{\psi_\lambda}\|^2_{L^\infty(\Omega_0)}(t)\, d\mu(\lambda)\right)^{1/2} \left(\int_\Lambda \|w_\lambda(t)\|^2_{L^2(\Omega_0)}\, d\mu(\lambda)\right)^{1/2} \\
&\qquad \le C_R \left(\int_\Lambda \|\psi^0_\lambda\|^2_{H^2(\Omega_0)}\, d\mu(\lambda)\right)^{1/2} \left(\int_\Lambda \|w_\lambda(t)\|^2_{L^2(\Omega_0)}\, d\mu(\lambda)\right)^{1/2} \\
&\qquad \le C_R\, t_0\, \|V_s - \widetilde{V}_s\|_{C^0([0,t_0],L^\infty(\Omega_0))}
\end{aligned} \tag{4.11}$$

Let us now treat the term $J(V_s) - J(\widetilde{V}_s)$: after straightforward computations and the use of the embeddings $H^2(\Omega_0) \hookrightarrow L^\infty(\Omega_0)$, $W^{1,7/2}(\Omega_0) \hookrightarrow L^\infty(\Omega_0)$ and $H^2(\Omega_0) \hookrightarrow W^{1,7/2}(\Omega_0)$, we obtain

$$\begin{aligned}
&\|J(V_s) - J(\widetilde{V}_s)\|_{L^{7/2}(\Omega_0)}(t) \\
&\quad \le C \left(\int_\Lambda \|\psi_\lambda + \widetilde{\psi_\lambda}\|^2_{H^2(\Omega_0)}(t)\, d\mu(\lambda)\right)^{1/2} \left(\int_\Lambda \|w_\lambda(t)\|^2_{W^{1,7/2}(\Omega_0)}\, d\mu(\lambda)\right)^{1/2}.
\end{aligned} \tag{4.12}$$

Then, a Gagliardo-Nirenberg interpolation inequality, together with (4.9) and (4.10), leads to

$$\begin{aligned}
\|w_\lambda(t)\|_{W^{1,7/2}(\Omega_0)} &\le C\|w_\lambda(t)\|^{13/14}_{H^2(\Omega_0)}\, \|w_\lambda(t)\|^{1/14}_{L^2(\Omega_0)} & (4.13)\\
&\le C_R\, t_0^{1/14}\, \|\psi^0_\lambda\|_{H^1(\Omega)} \|V_s - \widetilde{V}_s\|_{C^1([0,t_0],L^\infty(\Omega_0))}. & (4.14)
\end{aligned}$$

Coming back to (4.12) and using (3.8), we have finally

$$\|J(V_s) - J(\widetilde{V}_s)\|_{L^{7/2}(\Omega_0)}(t) \le C_R\, t_0^{1/14}\, \|V_s - \widetilde{V}_s\|_{C^1([0,t_0],L^\infty(\Omega_0))}. \tag{4.15}$$

We are able now to estimate the difference $\mathcal{F}(V_s) - \mathcal{F}(\widetilde{V}_s)$ in X. Indeed, from (4.6) and (4.11) we deduce

$$\|\mathcal{F}(V_s) - \mathcal{F}(\widetilde{V}_s)\|_{C^0([0,t_0],H^2(\Omega_0))} \le C_R\, t_0\, \|V_s - \widetilde{V}_s\|_{C^0([0,t_0],L^\infty(\Omega_0))}.$$

Next, from (4.7), (4.12) and the embedding $W^{1,7/2}(\Omega_0) \hookrightarrow L^\infty(\Omega_0)$, we obtain

$$\begin{aligned}
\|\partial_t\mathcal{F}(V_s) - \partial_t\mathcal{F}(\widetilde{V}_s)\|_{C^0([0,t_0],L^\infty(\Omega_0))} &\le C\|\partial_t\mathcal{F}(V_s) - \partial_t\mathcal{F}(\widetilde{V}_s)\|_{C^0([0,t_0],W^{1,7/2}(\Omega_0))} \\
&\le C_R\, t_0^{1/14}\, \|V_s - \widetilde{V}_s\|_{C^1([0,t_0],L^\infty(\Omega_0))} \qquad (4.16)
\end{aligned}$$

The proof is completed by choosing t_0 small enough. □

5 Energy estimate and global existence result

In this section, we give the proof of Theorem (2.5). To this aim, we prove an energy estimate which allows to extend the local solution of the last section for any arbitrarily large positive time. The proof crucially uses the sublinearity of the estimate (3.26).

Consider the local solution ψ_λ constructed in the last section. This solution satisfies the estimates (3.26) and (3.27). Let us define the total energy by

$$\epsilon(t) = \int_\Lambda \|\psi_\lambda(t)\|^2_{H^1(\Omega_0)}\, d\mu(\lambda) + \frac{1}{2}\|\nabla V_s(t)\|^2_{L^2(\Omega_0)}.$$

By integrating (3.26) and (3.27) w.r.t. the measure $d\mu$ and by using **(H-3)**, we obtain the relations

$$\|n(t)\|_{L^1(\Omega_0)} \le C + C\left(\int_0^t \left(1+\frac{1}{\sqrt{\pi s}}\right)\epsilon(s)ds\right)^{1/2}, \tag{5.1}$$

$$\begin{aligned}
\epsilon(t) \;\le\; & C + C\int_0^t \left(1+\frac{1}{\sqrt{\pi s}}\right)\epsilon(s)ds \\
& +C\int_0^t \|V_s(s)\|_{L^2(\Omega)}\left(1+\|n(s)\|^{1/2}_{L^1(\Omega_0)}\right)ds \\
& +\frac{1}{2}\|\nabla V_s(t)\|^2_{L^2(\Omega_0)} - \int_0^t\int_{\Omega_0} V_s\,\partial_t n\,dx\,ds - \int_0^t\int_{\Omega_0} V_e\,\partial_t n\,dx\,ds.
\end{aligned} \tag{5.2}$$

To estimate the r.h.s. of (5.2), we need to control the L^2 norm of V_s. For this purpose, we deduce from elliptic regularity of the Poisson equation with an $L^1(\Omega_0)$ right hand side, that

$$\|V_s(t)\|_{W^{1,p}(\Omega_0)} \le C\|n(t)\|_{L^1(\Omega_0)}, \qquad 1 \le p < 3/2.$$

Next, from the Sobolev embedding $W^{1,p}(\Omega_0) \hookrightarrow L^q(\Omega_0)$ for $q \le \frac{3p}{3-p}$, we deduce that

$$\|V_s\|_{L^2(\Omega_0)} \le C\|n\|_{L^1(\Omega_0)}.$$

This implies in view of (5.1), that

$$\begin{aligned}
&\int_0^t \|V_s(s)\|_{L^2(\Omega_0)}\left(1+\|n(s)\|^{1/2}_{L^1(\Omega_0)}\right)ds \\
&\qquad\qquad \le C + C\left(\int_0^t\left(1+\frac{1}{\sqrt{\pi s}}\right)\epsilon(s)ds\right)^{3/4}.
\end{aligned} \tag{5.3}$$

Furthermore, the Poisson equation gives

$$\frac{1}{2}\|\nabla V_s(t)\|^2_{L^2(\Omega_0)} - \int_0^t\int_{\Omega_0} V_s\,\partial_t n\,dx\,ds = \frac{1}{2}\|\nabla V_s(0)\|^2_{L^2(\Omega_0)}, \tag{5.4}$$

and an integration by parts with respect to time gives

$$\begin{aligned}\int_0^t \int_{\Omega_0} V_e\, \partial_t n\, dx\, ds \quad &\leq C + C\|n(t)\|_{L^1(\Omega_0)} + C\int_0^t \|n(s)\|_{L^1(\Omega_0)} ds \\ &\leq C + C\left(\int_0^t \left(1 + \frac{1}{\sqrt{\pi s}}\right)\epsilon(s) ds\right)^{1/2},\end{aligned} \tag{5.5}$$

where we used **(H-4)**. Therefore, in view of (5.3), (5.4) and (5.5), (5.2) leads to

$$\epsilon(t) \leq C + \frac{1}{2}\|\nabla V_s(0)\|^2_{L^2(\Omega_0)} + C\int_0^t \left(1 + \frac{1}{\sqrt{\pi s}}\right)\epsilon(s) ds.$$

Since it is clear by **(H-4)** and the Poisson equation that $\|\nabla V_s(0)\|_{L^2(\Omega_0)} \leq C$, a Gronwall argument leads to the a priori estimate

$$\epsilon(t) \leq C_T, \qquad \forall t \in [0,T]. \tag{5.6}$$

To show the regularity property announced in Theorem (2.5), we use again the Poisson and Schrödinger equations. We first notice that, thanks to (5.6), the Poisson equation (2.5) and the embedding $H^1(\Omega_0) \hookrightarrow L^6(\Omega_0)$, we have

$$\begin{aligned} &n \in \mathcal{C}^0([0,T], W^{1,3/2}(\Omega_0)) \qquad ; \qquad J \in \mathcal{C}^0([0,T], L^{3/2}(\Omega_0)), \\ &V \in \mathcal{C}^0([0,T], W^{3,3/2}(\Omega_0)) \qquad ; \qquad \partial_t V \in \mathcal{C}^0([0,T], W^{1,3/2}(\Omega_0)).\end{aligned} \tag{5.7}$$

Besides, according to (3.13), $u_\lambda := \partial_t \phi_\lambda = \partial_t \psi_\lambda - \partial_t \psi_\lambda^{pw}$ solves

$$\begin{cases} i\dfrac{\partial u_\lambda}{\partial t} = -\Delta u_\lambda + V\, u_\lambda + \partial_t V \phi_\lambda - \partial_t S_\lambda(V) \quad \text{in } \Omega \\ u_\lambda(0,x) = iS_\lambda(V)(0,x) \end{cases}$$

and we obtain directly

$$\|\partial_t \phi_\lambda(t)\|_{L^2(\Omega_0)} \leq \|S_\lambda(V)(0,\cdot)\|_{L^2(\Omega_0)} + \|\partial_t V \phi_\lambda + \partial_t S_\lambda(V)\|_{L^1((0,T),L^2(\Omega_0))}.$$

The embeddings $W^{1,3/2}(\Omega_0) \hookrightarrow L^3(\Omega_0)$, $H^1(\Omega_0) \hookrightarrow L^6(\Omega_0)$ and (5.6) imply that

$$\int_\Lambda \|\partial_t V \phi_\lambda\|^2_{L^1((0,T),L^2(\Omega_0))} d\mu(\lambda) \leq C$$

and (3.16), (5.7) give

$$\|\partial_t S_\lambda(V)\|_{L^1((0,T),L^2(\Omega_0))} \leq C.$$

Finally, this leads to

$$\int_\Lambda \|\partial_t \phi_\lambda(t)\|^2_{L^2(\Omega_0)} d\mu(\lambda) \leq C, \qquad \forall t \in [0,T].$$

From the Schrödinger equation $\Delta\phi_\lambda = -i\partial_t\phi_\lambda + V\phi_\lambda - S_\lambda$ we deduce that

$$\int_\Lambda \|\psi_\lambda(t)\|^2_{H^2(\Omega_0)} d\mu(\lambda) \leq C.$$

The proof is completed after noticing that

$$n \in \mathcal{C}^0([0,T], H^2(\Omega_0)) \qquad ; \qquad J \in \mathcal{C}^0([0,T], H^1(\Omega_0));$$

which yields, through elliptic estimates, the regularity of V_s stated in Theorem (2.5).

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