On an open transient Schrödinger-Poisson system

Naoufel Ben Abdallah, Florian Méhats and Olivier Pinaud

MIP, Laboratoire CNRS (UMR 5640), Université Paul Sabatier, 118, route de Narbonne, 31062 Toulouse Cedex 04, France
nacufel@mip.ups-tlse.fr, mehats@mip.ups-tlse.fr, pinaud@mip.ups-tlse.fr

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.

1 Introduction
In nanoscale semiconductor devices, the typical length scale 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 \(\lambda\) is an index for the elementary states \(\psi_{\lambda}(t, x)\) and the integration is done with respect to a measure \(\mu\). Each state \(\psi_{\lambda}\) 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 have 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 gen-
eral 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 tech-
niques and functional calculus. Boundary conditions are not derived explicitly and
are taken into account implicitly thanks to the use of the notion of conjugate op-
erators. In the present paper, we use the Schrödinger picture and derive transparent
boundary conditions for them which makes it more suitable for numerical simulations
[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 \(\lambda\) 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 \(\psi_\rho\) corresponding
to electrons injected at the left boundary with a positive momentum \(p\) is a solution of the Schrödinger equation

\[-\frac{1}{2} \frac{d^2 \psi_\rho}{dx^2} + V \psi_\rho = \mathcal{E}(p) \psi_\rho\]

where \(\mathcal{E}(p) = \frac{\lambda^2}{2} + V(a)\). For \(x < a\), we have \(\psi_\rho(x) = e^{ipx} + r_p e^{-ipx}\) 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 \( p < 0 \), \( \psi_p \) 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 condition 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 restriction 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 settings 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 \( \Omega \) of \( \mathbb{R}^d \) (\( d = 2 \) or \( d = 3 \)) which is the union of a regular bounded domain \( \Omega_0 \) (the active region) and a finite number \( n \) of semi-infinite cylinders (leads) \( \Omega_j \) which represent the access zones (see Fig. 1). The interface between the active region \( \Omega_0 \) and the lead \( j \) (\( j = 1, \cdots, n \)) is denoted by \( \Gamma_j \). The remaining part of the boundary of \( \Omega_0 \) is denoted by \( \Gamma_0 \). The lead \( \Omega_j \) behaves as a waveguide, injecting electrons into the active region \( \Omega_0 \). It has a set of local coordinates \( \xi_j \in \Gamma_j, \eta_j \in \mathbb{R}^+ \) (see Fig. 1), where \( \xi_j \) is the transversal coordinate and \( \eta_j \) the longitudinal one. We introduce also \( (\mu_j(x))_{j=1, \cdots, n} \), a partition of unity of \( \Omega \), \( i.e. \) some \( C^\infty \) functions which satisfy for \( j = 1, \cdots, n \)

\[
\begin{align*}
0 \leq \mu_j \leq 1, & \sum_j \mu_j \equiv 1 \text{ on } \Omega \\
\mu_j \equiv 1 \text{ on } \Omega_j & \text{ and } \mu_j \equiv 0 \text{ on } \Omega_k \text{ for } k \neq 0, k \neq j
\end{align*}
\]

### Class of initial data

Let us define the operator

\[ \mathcal{H}^0 = -\Delta + V^0 \]
where $V^0$ is the exterior potential which is assumed to only depend on the transversal coordinate in the leads:

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

Let $(\Lambda, \mu)$ be a set equipped with a bounded nonnegative measure $\mu$ such that

$$\mu(\Lambda) = \int_\Lambda d\mu < +\infty. \quad (2.1)$$

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

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

$$\mathcal{H}^0\psi^0_\lambda = E(\lambda)\psi^0_\lambda \quad \text{on} \quad \Omega_j \quad (j = 1, \ldots, n).$$

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

**\textbf{(H-3)}** There exists $C > 0$ such that $\int_\Lambda \|\psi^0_\lambda\|_{H^2_{loc}(\Omega)}^2 d\mu(\lambda) \leq C$. 

---

Figure 1: The domain $\Omega$
Definition 2.1 The transversal eigenmodes and the eigenvalues of the guide $j$ are defined by

\[ \begin{align*}
-\Delta_{\xi j} \chi_m^{o,j} + V_j^0(\xi_j) \chi_m^{o,j} &= E_m^j \chi_m^{o,j}, \quad m \in \mathbb{N}^1 \\
\chi_m^{o,j} &\in H_0^1(\Gamma_j), \quad \int_{\Gamma_j} \chi_m^{o,j} \chi_m^{o,j} d\sigma(\xi_j) = \delta_{m,m'}
\end{align*} \tag{2.2} \]

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

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

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

where $\delta$ 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 $m_0$th mode in the lead $j_0$. The function $\Phi$ 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

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

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

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

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

\[ \varphi_m^j(\xi_j) = \chi_m^j(\xi_j) \langle \overline{\varphi} \chi_m^j \rangle_j \]

its projection on $\chi_m^j$. Thanks to (2.2), the relation $\varphi \mapsto \left( \sum_{m \geq 1} E_m^j \| \varphi_m^j \|_{L^2(\Gamma_j)} \right)^{1/2}$ 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 $V(t,x) = V_j^0(x) + V_j(t)$.

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 $\Omega_0$. We shall assume

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

5
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

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

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

$$i\partial_t \psi = \mathcal{H}(t) \psi, \quad \psi(0, \cdot) = \psi^0_\lambda, \quad x \in \Omega $$ \hspace{1cm} (2.3)

$$\mathcal{H}(t) = -\Delta + V_s(t, x) + V_s(t, x) \quad \text{supp}(V_s) \subset \Omega_0 $$ \hspace{1cm} (2.4)

$$-\Delta V_s = n = \int_{\Lambda} |\psi_\lambda|^2 d\mu(\lambda), \quad x \in \Omega_0 \quad V_s |_{\partial \Omega_0} \equiv 0. $$ \hspace{1cm} (2.5)

Notice that the Schrödinger equation is set on the hole domain $\Omega$ including the leads. We shall derive transparent boundary conditions allowing for it resolution on the domain $\Omega_0$ only. To this aim, we first remark that, according to (H-1) and (H-4) we have

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

Defining the phase factor

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

the plane wave function

$$\psi_{\lambda}^{\text{pw}}(t, x) = \psi^0_\lambda(x) \sum_{j=1}^n \mu_j(x) \theta^j_\lambda(t) $$ \hspace{1cm} (2.6)

satisfies

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

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

$$\chi_m^j(t, \xi_j) = \chi_m^{0j}(\xi_j) \exp \left( -i \int_0^t (V_j(\tau) + E_m^j) \, d\tau \right). $$ \hspace{1cm} (2.7)

At any time, $(\chi_m^j)$ is an orthonormal basis of $L^2(\Gamma_j)$.

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

$$I^{1/2} f = \frac{1}{\sqrt{\pi}} \int_0^t \frac{f(\tau)}{\sqrt{t - \tau}} \, d\tau$$
which verifies $\mathcal{I}^{1/2} f \in H^{1/2+\alpha}(0, T)$. Then, we define $\partial^{1/2} f := \frac{d}{dt} \mathcal{I}^{1/2} f$ by

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

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

$$\Pi_j^{1/2} f(t, \xi_j) = \sum_{m \geq 1} \chi_m^j(t, \xi_j) \mathcal{I}_{1/2} \left< f(t, \cdot) \chi_m^j(\cdot, \cdot) \right>_j$$

$$\Delta_j^{1/2} f(t, \xi_j) = \sum_{m \geq 1} \chi_m^j(t, \xi_j) \partial_{1/2} \left< f(t, \cdot) \chi_m^j(\cdot, \cdot) \right>_j.$$ 

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 such that

$$V_\lambda \in C^0([0, T], H^1(\Omega_0)) \cap C^0([0, T], H^4(\Omega_0)) \cap C^1([0, T], H^2(\Omega_0))$$

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

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

Moreover, the Schrödinger-Poisson system (2.3)–(2.5) on $\Omega$ is equivalent to the boundary value problem on $\Omega_0$ consisting in the Schrödinger-Poisson system (2.3)–(2.5) with a Dirichlet boundary condition on $\Gamma_0$ and one of the following equivalent boundary conditions on $\Gamma_j$, $j = 1, \ldots, n$:

$$\frac{\partial}{\partial \eta_j} (\psi_\lambda - \psi_\lambda^{pw}) = -e^{-i\pi/4} \Delta_j^{1/2} (\psi_\lambda - \psi_\lambda^{pw}) \quad \text{a.e.}$$

$$\psi_\lambda - \psi_\lambda^{pw} = -e^{i\pi/4} \Pi_j^{1/2} \left( \frac{\partial}{\partial \eta_j} (\psi_\lambda - \psi_\lambda^{pw}) \right) \quad \text{a.e.}$$

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

## 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 $\Gamma_j$, $j = 1, \ldots, n$. 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 $\Omega$, let us recall the standard result in the $L^2$ framework. Consider the Schrödinger equation

$$
\begin{align*}
  \left\{ \begin{array}{l}
    i\partial_t \Psi = -\Delta \Psi + V(t,x)\Psi + f(t,x) \quad \text{; } x \in \Omega \\
    \Psi(t=0,\cdot) = \Psi_0, \quad \Psi = 0 \text{ on } \mathbb{R}^+ \times \partial \Omega.
  \end{array} \right.
\end{align*}
$$

(3.1)

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

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

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

$$
\|\Psi(t)\|_{H^2(\Omega)} \leq C(1 + t^2) \left( \|\Psi_0\|_{H^2(\Omega)} + \|f\|_{C^1([0,T], L^2(\Omega))} \right) \left( 1 + \|V\|_{C^1([0,T], L^\infty(\Omega))} \right) \quad (3.4)
$$

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

$$
\Psi(t) = U(t,s)\Psi_0 + \int_s^t U(t,u)f(u)du \in L^2(\Omega). \quad (3.5)
$$

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

$$
u(t) = U(t,s)u_0 + \int_s^t U(t,u) (\partial_s V(s) \Psi(s) + \partial_s f(s))du \in L^2(\Omega) \quad (3.6)
$$

since

$$
u_0 = i\Delta \Psi_0 + V(0,x)\Psi_0 + f(0,x) \in L^2(\Omega)
$$

and

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

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

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 $\frac{\partial \Psi}{\partial n}$, integrate over $[0,t]$ and take the real part. Estimate (3.3) follows after straightforward integration by parts. 

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

$$
\| \psi_{\lambda}(t) - \psi^p_{\lambda}(t) \|_{L^2(\Omega)} \leq C t \| \psi^0_{\lambda} \|_{H^1(\Omega_0)} (1 + \| V \|_{C^0([0,t],L^\infty(\Omega))})
$$

(3.7)

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

(3.8)

(ii) Assume (H-1), (H-2) satisfied. Let $\psi_{\lambda} \in \psi^p_{\lambda} + \mathcal{E}$ be the unique solution of (2.3), with $V$ belonging to the class $\mathcal{V}$. Then $\psi_{\lambda}$ is the unique solution of the boundary value problem on $\Omega_0$ consisting in the Schrödinger equation (2.3) with the Dirichlet boundary condition on $\Gamma_0$ and one of the following equivalent boundary conditions a.e. on $\Gamma_j$, $j = 1, \cdots, n$:

$$
\frac{\partial}{\partial n_j}(\psi_{\lambda} - \psi^p_{\lambda}) = -e^{-i\pi/4} D_j^{1/2}(\psi_{\lambda} - \psi^p_{\lambda})
$$

(3.9)

$$
\psi_{\lambda} - \psi^p_{\lambda} = -e^{i\pi/4} P_j^{1/2}\left(\frac{\partial}{\partial n_j}(\psi_{\lambda} - \psi^p_{\lambda})\right).
$$

(3.10)

The following remark will be used all along the paper:

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

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

(3.11)

and then

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

(3.12)

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

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

(3.13)

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

$$
S_{\lambda}(V) = 2 \nabla \psi^0_{\lambda} \cdot \sum_{j \geq 1} \nabla \mu^j_{\lambda} \theta^j_{\lambda} + \psi^0_{\lambda} \sum_{j \geq 1} \left( \Delta \mu^j_{\lambda} + V_j \mu^j_{\lambda} \right) \theta^j_{\lambda}
$$

$$
+ \left[ (E(\lambda) - V) \psi^0_{\lambda} + \Delta \psi^0_{\lambda} \right] \sum_{j \geq 1} \mu^j_{\lambda} \theta^j_{\lambda}
$$

(3.14)
and satisfies
\[
\text{supp } S_\lambda(V) \subset \Omega_0.
\]  
(3.15)

Since \( \psi_\lambda^0 \in H^2_{\text{loc}}(\Omega) \) and \( V \in C^1([0, T], L^\infty(\Omega)) \), we have \( S_\lambda(V) \in C^1([0, T], L^2(\Omega)) \) and Lemma 3.1 applies: this gives the existence and uniqueness in \( \psi_\lambda^m + \mathcal{E} \). Estimates (3.7) and (3.8) are direct applications of (3.2) and (3.4) since
\[
\|S_\lambda(V)\|_{C^1([0, T], L^2(\Omega))} \leq C \|\psi_\lambda^0\|_{H^2(\Omega_0)} \left(1 + \|V\|_{C^1([0, T], L^\infty(\Omega))}\right).
\]  
(3.16)

In [3, 7, 14], some transparent boundary conditions were derived 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 \( \Omega_j \) and we extend them to the case of time-dependent external potentials. Consider the function \( \phi_\lambda \) defined hereabove. On each \( \Omega_j, j = 1, \cdots, n \), the wavefunction \( \phi_\lambda \) can be expanded on the basis \( (\chi_m^j(t, \cdot))_{m} \):
\[
\phi_\lambda(t, \xi_j, \eta_j) = \sum_{m \geq 1} \varphi_m(t, \eta_j) \chi_m^j(t, \xi_j).
\]

Since \( V \) belongs to the class \( \mathcal{V} \), it verifies
\[
V|_{\Omega_j} = V_j^0(\xi_j) + V_j(t) \quad j \neq 0
\]
and thanks to (3.13), \( \varphi_m(t, \eta_j) \) solves
\[
\begin{cases}
\frac{i}{\partial_t} \varphi_m(t, \eta_j) = -\frac{\partial^2 \varphi_m(t, \eta_j)}{\partial \eta_j^2} \quad (\eta_j \geq 0) \\
\varphi_m(0, \eta_j) = 0.
\end{cases}
\]  
(3.17)

Following now [3, 7, 14], \( \varphi_m \) verifies on \( \Gamma_j \) the scalar Dirichlet-to-Neumann boundary condition:
\[
\frac{\partial \varphi_m}{\partial \eta_j} = -e^{-i\pi/4} T^{1/2} (\varphi_m).
\]  
(3.18)

Similarly, \( \varphi_m \) satisfies the scalar Neumann-to-Dirichlet boundary condition:
\[
\varphi_m = -e^{i\pi/4} T^{1/2} \left( \frac{\partial \varphi_m}{\partial \eta_j} \right).
\]  
(3.19)

Finally, coming back to \( \phi_\lambda \), we obtain (3.9) and (3.10). Note 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 and then \( \phi_\lambda|_{\Gamma_j} \in H^{1/2}((0, T), L^2(\Gamma_j)) \) 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

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

(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

\[ \Upsilon^{1/2}(e^{-i \omega t}) = \frac{e^{-i \omega t}}{\sqrt{\omega}} \Upsilon(\omega t) \quad ; \quad \partial^{1/2}(e^{-i \omega t}) = \frac{1}{\sqrt{\pi \, t}} - i \sqrt{\omega} \, e^{-i \omega t} \Upsilon(\omega t). \]

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

**Lemma 3.5** Let \( \psi_{\lambda}^{pw} \in C^1([0,T], H_{loc}^2(\Omega)) \) be defined in (2.6), \( \Upsilon \) in (3.20) and \( D_j^{1/2} \) in (2.9). Then, we have the following formula

\[ D_j^{1/2}(\psi_{\lambda}^{pw}) = \sum_{m=1}^{+\infty} \left( \frac{1}{\sqrt{\pi \, t}} - i \sqrt{E(\lambda) - E_m^j} \, e^{-i (E(\lambda) - E_m^j) \, t} \right) \Upsilon(\lambda) \left( (E(\lambda) - E_m^j) \, t \right) \psi_m^j \chi_m^j \]

(3.21)

where \( \psi_m^j = \langle \psi_{\lambda}^{(0, \cdot)} \chi_m^j (\cdot) \rangle_j \). Furthermore, if \( |E(\lambda)| \leq M \) then we have

\[ ||D_j^{1/2}(\psi_{\lambda}^{pw})||_{L^2(\Gamma_j)} \leq C \sqrt{1 + \frac{1}{\pi \, t}} ||\psi_{\lambda}^{00}||_{H^2(\Omega_0)} \]

(3.22)

where \( C \) depends on \( M \), on \( M \) and on \( T \).

**Proof.** According to Lemma 3.4

\[ ||D_j^{1/2}(\psi_{\lambda}^{pw})||_{L^2(\Gamma_j)}^2 \leq \frac{1}{\pi \, t} ||\psi_{\lambda}^{00}||_{L^2(\Gamma_j)}^2 + M \sum_{m \geq 1} (M + E_m^j) ||\psi_m^j||^2 \]

and Remark 2.3 coupled to trace properties imply

\[ \sum_{m \geq 1} E_m^j ||\psi_m^j||^2 \leq C ||\psi_{\lambda}^{00}||_{H^1(\Gamma_j)} \leq C' ||\psi_{\lambda}^{00}||_{H^2(\Omega_0)}. \]

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
\[
S^{\pi/4} = \{ z \in \mathbb{C} : \text{Arg}(z) \in [-\pi/4, \pi/4] \},
\]
we have
\[
\int_0^T \langle \nabla(t) \mathbb{D}^{1/2}(f(t)) \rangle_j \, dt \in S^{\pi/4},
\]
and
\[
\int_0^T \langle \nabla(t) \mathbb{P}^{1/2}(g(t)) \rangle_j \, dt \in S^{\pi/4}.
\]

**Proof.** This lemma is a consequence of Definition 2.4 and of the Plancherel equality. Indeed, setting
\[
f^j_m(t) = \langle f(t), \overline{\chi_m^j} \rangle
\]
and denoting by \( P f^j_m \in H^{1/4}(\mathbb{R}) \) the function extended by zero outside \((0,T)\), we have
\[
\int_0^T \nabla(t) \mathbb{D}^{1/2} f^j_m \, dt = \frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} \sqrt{i\nu} \left| P \tilde{f}^j_m(i\nu) \right|^2 \, d\nu,
\]
where \( \sqrt{\cdot} \) denotes the square root with nonnegative real part. It is now enough to remark that for every real number \( \nu \) 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
\[
g^j_m(t) = \langle g(t), \overline{\chi_m^j} \rangle
\]
we have
\[
\int_0^T \nabla(t) \mathbb{D}^{1/2} g^j_m \, dt = \frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} \frac{1}{\sqrt{i\nu}} \left| P \tilde{g}^j_m(i\nu) \right|^2 \, d\nu \in S^{\pi/4}.
\]

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, \( \psi_\lambda \) satisfies the following estimates, for all \( T \) positive, for all \( t \in [0,T] \), \( \lambda \) a.e.,
\[
\| \psi_\lambda(t) \|_{L^2(\Omega_0)}^2 \leq \| \psi_\lambda^0 \|_{L^2(\Omega_0)}^2 + C \| \psi_\lambda^0 \|_{H^2(\Omega_0)} \int_0^t \left( 1 + \frac{1}{\sqrt{\pi s}} \right) \| \psi_\lambda(s) \|_{H^1(\Omega_0)} \, ds,
\]
\[
\| \psi_\lambda(t) \|_{H^1(\Omega_0)}^2 \leq C \| \psi_\lambda^0 \|_{H^2(\Omega_0)}^2 + C \int_0^t \left( 1 + \frac{1}{\sqrt{\pi s}} \right) \| \psi_\lambda(s) \|_{H^1(\Omega_0)}^2 \, ds - \int_0^t \int_{\Omega_0} \nabla V \cdot \psi_\lambda^2 \, ds
\]
\[
+ C \| \psi_\lambda^0 \|_{H^2(\Omega_0)} \int_0^t \| V(s) \|_{L^2(\Omega)} \left( \| \psi_\lambda^0 \|_{L^2(\Omega_0)} + \| \psi_\lambda(s) \|_{L^2(\Omega_0)} \right) \, ds.
\]
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 and integrating over $[0,t]$ leads to

$$\|\psi_\lambda(t)\|_{L^2(\Omega_0)}^2 = \|\psi_\lambda^0\|_{L^2(\Omega_0)}^2 - 2 \sum_{j=0}^n \mathcal{I}m \int_0^t \left< \frac{\partial \psi_\lambda}{\partial \eta_j} (s, \cdot) \overline{\psi_\lambda(s, \cdot)} \right> ds. \quad (3.28)$$

In order to estimate the non-linear boundary term, we first recast it into

$$\int_0^t \left< \frac{\partial \psi_\lambda}{\partial \eta_j} \overline{\psi_\lambda} \right> ds = - \int_0^t \left< e^{-i\pi/4} (\mathbb{D}^{1/2}_j \psi_\lambda) \overline{\psi_\lambda} \right> ds + \int_0^t \left< \frac{\partial \psi_{\lambda\text{pw}}}{\partial \eta_j} \overline{\psi_\lambda} \right> ds + \int_0^t \left< e^{-i\pi/4} (\mathbb{D}^{1/2}_j \psi_{\lambda\text{pw}}) \overline{\psi_\lambda} \right> ds. \quad (3.29)$$

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

$$\mathcal{I}m \int_0^t \left< e^{-i\pi/4} (\mathbb{D}^{1/2}_j \psi_\lambda) \overline{\psi_\lambda} \right> ds \leq 0$$

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

$$\int_0^t \left< \frac{\partial \psi_{\lambda\text{pw}}}{\partial \eta_j} \overline{\psi_\lambda} \right> ds \leq \int_0^t \|\psi_\lambda^0\|_{H^2(\Omega_0)} \|\psi_\lambda\|_{H^1(\Omega_0)} ds$$

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

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

This ends the proof of (3.26).

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

$$\|\nabla \psi_\lambda(t)\|_{L^2(\Omega_0)}^2 = \|\nabla \psi_\lambda^0\|_{L^2(\Omega_0)}^2 + 2 \sum_{j=0}^n \mathcal{R}e \int_0^t \left< \frac{\partial \psi_\lambda}{\partial \eta_j} \partial_t \overline{\psi_\lambda} \right> ds - \int_0^t \int_{\Omega_0} V \partial_t |\psi_\lambda|^2 ds. \quad (3.30)$$

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

$$\partial_t \phi_\lambda = - e^{i\pi/4} \mathbb{D}^{1/2}_j \left( \frac{\partial \phi_\lambda}{\partial \eta_j} \right) - i V_j \phi_\lambda + i e^{i\pi/4} \sum_{m \geq 1} E_m \chi_m \mathcal{T}_1 \left< \partial_t \phi_\lambda \overline{\chi_m} \right> \quad (3.31)$$
We then have
\[
\Re \sum_j \int_0^t \left\langle \frac{\partial \psi^\lambda}{\partial \eta_j} \overline{\partial_t \psi^\lambda} \right\rangle_j \, ds = -\Re \sum_j \int_0^t \left\langle \frac{\partial \phi^\lambda}{\partial \eta_j} \overline{\frac{D_{j/2}^{1/2} \left( \frac{\partial \phi^\lambda}{\partial \eta_j} \right)}{}} \right\rangle_j \, ds
\]
\[-\Im \sum_j \int_0^t V_j \left\langle \frac{\partial \phi^\lambda}{\partial \eta_j} \overline{\phi^\lambda} \right\rangle_j \, ds \]
\[-\Re i e^{-i\pi/4} \sum_{m \geq 1} E_m^j \int_0^t \left\langle \frac{\partial \phi^\lambda}{\partial \eta_j} \overline{\chi_m^j} \right\rangle_j \, I_{1/2} \left( \left\langle \frac{\partial \phi^\lambda}{\partial \eta_j} \chi_m^j \right\rangle_j \right) \, ds \leq 0.
\]

In the sequel of the proof we shall assume that \( \phi^\lambda \in C^1([0,T], H^1(\Omega_0)) \). If this is not the case, it is sufficient 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 \( \phi^\lambda \in H^{1/4}((0,T), H^{1/4}(\Omega_0)) \), 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 \( \phi^\lambda \in C^1([0,T], L^2(\Omega_0)) \) 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
\[
-\Re e^{-i\pi/4} \int_0^t \left\langle \frac{\partial \phi^\lambda}{\partial \eta_j} \overline{\frac{D_{j/2}^{1/2} \left( \frac{\partial \phi^\lambda}{\partial \eta_j} \right)}{}} \right\rangle_j \, ds \leq 0.
\]

Secondly, thanks to Remark (2.2) we notice that \( E_m^j \geq 0 \). Thus from (3.25) we obtain
\[
-\Re i e^{-i\pi/4} \sum_{m \geq 1} E_m^j \int_0^t \left\langle \frac{\partial \phi^\lambda}{\partial \eta_j} \overline{\chi_m^j} \right\rangle_j \, I_{1/2} \left( \left\langle \frac{\partial \phi^\lambda}{\partial \eta_j} \chi_m^j \right\rangle_j \right) \, ds \leq 0.
\]

Then we deduce that
\[
\Re \sum_j \int_0^t \left\langle \frac{\partial \psi^\lambda}{\partial \eta_j} \overline{\partial_t \psi^\lambda} \right\rangle_j \, ds \leq R_1 + R_2 + R_3,
\]
where
\[
R_1 = \Re \sum_j \int_0^t \left\langle \frac{\partial \psi_{\text{wav}}^\lambda}{\partial \eta_j} \overline{\partial_t \psi^\lambda} \right\rangle_j \, ds ; \quad R_2 = -\Im \sum_j \int_0^t V_j \left\langle \frac{\partial \phi^\lambda}{\partial \eta_j} \overline{\phi^\lambda} \right\rangle_j \, ds
\]
and
\[
R_3 = \Re \sum_j \int_0^t \left\langle \frac{\partial \phi^\lambda}{\partial \eta_j} \overline{\psi_{\text{wav}}^\lambda} \right\rangle_j \, ds.
\]
Let us estimate $R_1$, $R_2$ and $R_3$ separately. For $R_1$, an integration by parts and
standard trace estimates lead to
\[
R_1 \leq \| \psi_0^\lambda \|_{H^2(\Omega_0)} \left( \| \psi_0^\lambda \|_{H^1(\Omega_0)} + \| \psi_\lambda(t) \|_{H^1(\Omega_0)} + C \int_0^t \| \psi_\lambda(s) \|_{H^1(\Omega_0)} ds \right). \tag{3.32}
\]
In order to treat the term $R_2$, we set $\overline{V}(t, x) := \sum_j \mu_j(x) V_j(t)$ and remark that
\[
R_2 = -\text{Im} \int_0^t \int_{\Omega_0} \nabla \phi_\lambda \cdot \nabla (\overline{V} \phi_\lambda) \, dx \, ds - \text{Im} \int_0^t \int_{\Omega_0} \Delta \phi_\lambda \overline{\phi_\lambda} \, dx \, ds.
\]
Therefore (3.13) gives
\[
R_2 = \frac{1}{2} \int_0^t \int_{\Omega_0} \partial_t |\phi_\lambda|^2 \overline{V} \, dx \, ds - \text{Im} \int_0^t \int_{\Omega_0} S_\lambda \overline{\phi_\lambda} \overline{V} \, dx \, ds - \text{Im} \int_0^t \int_{\Omega_0} \nabla \phi_\lambda \cdot \nabla \overline{V} \phi_\lambda \, dx \, ds.
\]
Straightforward algebra leads to
\[
\text{Im} \int_0^t \int_{\Omega_0} S_\lambda \phi_\lambda \overline{\phi_\lambda} \, dx \, ds \leq C \| \phi_\lambda(t) \|_{L^2(\Omega_0)}^2 + C \int_0^t \| \phi_\lambda(s) \|_{L^2(\Omega_0)}^2 \, ds,
\]
\[
\text{Im} \int_0^t \int_{\Omega_0} \nabla \phi_\lambda \overline{\phi_\lambda} \nabla \overline{V} \, dx \, ds \leq C \int_0^t \| \phi_\lambda(s) \|_{H^1(\Omega_0)}^2 \, ds.
\]
Since
\[
\| \phi_\lambda(t) \|_{L^2(\Omega_0)} \leq \| \psi_0^\lambda \|_{L^2(\Omega_0)} + \| \psi_\lambda(t) \|_{L^2(\Omega_0)},
\]
we obtain, thanks to (3.26),
\[
R_2 \leq C \| \psi_0^\lambda \|^2_{H^2(\Omega_0)} + C \int_0^t \left( 1 + \frac{1}{\sqrt{\pi s}} \right) \| \psi_\lambda(s) \|^2_{H^1(\Omega_0)} \, ds
\]
\[+ C \| \psi_0^\lambda \|_{H^2(\Omega_0)} \int_0^t \| V(s) \|_{L^2(\Omega)} \left( \| \psi_0^\lambda \|_{L^2(\Omega_0)} + \| \psi_\lambda(s) \|_{L^2(\Omega_0)} \right) \, ds. \tag{3.33}
\]
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 $\partial_t \psi_\lambda^{pm}$ and integrating over $[0, t]$ leads to
\[
R_3 = -\text{Im} \int_0^t \int_{\Omega_0} \partial_t \phi_\lambda \partial_t \psi_\lambda^{pm} \, dx \, ds + \text{Re} \int_0^t \int_{\Omega_0} \nabla \phi_\lambda \cdot \nabla \overline{\psi_\lambda^{pm}} \, dx \, ds
\]
\[+ \text{Re} \int_0^t \int_{\Omega_0} V \phi_\lambda \partial_t \psi_\lambda^{pm} \, dx \, ds + \text{Re} \int_0^t \int_{\Omega_0} S_\lambda \partial_t \psi_\lambda^{pm} \, dx \, ds.
\]
Straightforward calculations coupled to (3.26) imply
\[
R_3 \leq C \| \psi_0^\lambda \|^2_{H^1(\Omega_0)} + C \| \psi_0^\lambda \|_{H^2(\Omega_0)} \int_0^t \left( 1 + \frac{1}{\sqrt{\pi s}} \right) \| \psi_\lambda(s) \|_{H^1(\Omega_0)} \, ds
\]
\[+ C \| \psi_0^\lambda \|_{H^2(\Omega_0)} \int_0^t \| V(s) \|_{L^2(\Omega)} \left( \| \psi_0^\lambda \|_{L^2(\Omega_0)} + \| \psi_\lambda(s) \|_{L^2(\Omega_0)} \right) \, ds. \tag{3.34}
\]
The proof is complete after gathering (3.33), (3.32) and (3.34).
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

$$-\Delta \mathcal{F}(V_s) = n [V_s] = \int_A |\psi^0\lambda [V_s]|^2 d\mu(\lambda) ; \quad x \in \Omega_0 ; \quad \mathcal{F}(V_s) |_{\partial \Omega_0} \equiv 0 \quad (4.35)$$

where $\psi^0\lambda [V_s]$ is given by

$$i \partial_t \psi^0\lambda = \mathcal{H}(t) \psi^0\lambda ; \quad \psi^0\lambda (0, \cdot) = \psi^0\lambda ; \quad x \in \Omega \quad (4.36)$$

$$\mathcal{H}(t) = -\Delta + V_c(t, x) + V_s(t, x) \quad (4.37)$$

with $V_c$ 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)-(H4), there exists a time $t_0$ such that the application $\mathcal{F}$ is contraction on $C^1([0, t_0], L^\infty(\Omega_0)) \cap C^0([0, t_0], H^1_0(\Omega_0))$.

**Proof.** For notational simplicity, let

$$X := C^1([0, t_0], L^\infty(\Omega_0)) \cap C^0([0, t_0], H^1_0(\Omega_0)).$$

We first check that $\mathcal{F}(X) \subset X$. It is straightforward to see that $V := V_c + V_s$ belongs to the class $\mathcal{V}$, so one can apply the results of Section 3. Since $\psi^0\lambda \in H^2_{\text{loc}}(\Omega)$, Proposition (3.2) (i) applies and (4.36)-(4.37) admits a unique solution $\psi^0\lambda [V_s] \in \mathcal{E} + \psi^0\lambda^0\nu$ such that, for all $t$ in $[0, t_0]$,

$$\int_X ||\psi^0\lambda (t) ||^2_{H^2_{\text{loc}}(\Omega)} d\mu(\lambda) \leq C(V_s).$$

Furthermore, the embedding $H^2(\Omega_0) \hookrightarrow L^\infty(\Omega_0)$, for $d \leq 3$, implies that $n [V_s] \in C^0([0, t_0], L^\infty(\Omega_0))$ and by (4.35), the elliptic regularity gives

$$\mathcal{F}(V_s) \in C^0([0, t_0], W^{2,q}(\Omega_0)) \cap C^0([0, t_0], H^1_0(\Omega_0)), \quad \forall q < \infty. $$

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

$$n_\lambda = |\psi^0\lambda|^2 ; \quad j_\lambda = \text{Im} (\psi^0\lambda \nabla \psi^0\lambda).$$

The charge conservation identity yields

$$\partial_t n_\lambda + \text{div} j_\lambda = 0. \quad (4.38)$$

By (4.35) and (4.38), $\partial_t \mathcal{F}(V_s)$ solves

$$\Delta \partial_t \mathcal{F}(V_s) = \text{div} J(V_s) ; \quad x \in \Omega_0 ; \quad \partial_t \mathcal{F}(V_s) |_{\partial \Omega_0} \equiv 0 \quad (4.39)$$

16
where
\[ J = \int_{\Omega} j_{\lambda} \, d\mu(\lambda). \]

Thanks to hypothesis (H-2) and the Jensen inequality, we have
\[ \| J(t) \|_{L^0(\Omega_0)} \leq C \left( \int_{\Lambda} \| \psi_{\lambda}(t) \|_{W^{1,0}(\Omega_0)}^2 \, d\mu(\lambda) \right)^{1/2} \left( \int_{\Lambda} \| \psi_{\lambda}(t) \|_{L^2(\Omega_0)}^2 \, d\mu(\lambda) \right)^{1/2} \]
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 \( d \leq 3 \), give a bound for \( J \) in \( C([0, t_0], L^0(\Omega_0)) \). This implies, together with (4.39) and standard elliptic regularity estimates, that \( \partial_t \mathcal{F}(V_s) \in C([0, t_0], W^{1,6}_0(\Omega_0)) \). Thanks to the embedding \( W^{1,6}(\Omega_0) \hookrightarrow L^\infty(\Omega_0) \), for \( d \leq 3 \), we deduce that
\[ \partial_t \mathcal{F}(V_s) \in C^0([0, t_0], L^\infty(\Omega_0)). \]

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 \( \widetilde{V}_s \), two potentials in an open ball of \( X \) with radius \( R \), let us denote by \( \psi_{\lambda} \) and \( \widetilde{\psi}_{\lambda} \) the associated wavefunctions, belonging to \( \mathcal{E} + \psi_{\lambda}^{\text{pr}} \). We have
\[ -\Delta \left( \mathcal{F}(V_s) - \mathcal{F}(\widetilde{V}_s) \right) = n(V_s) - n(\widetilde{V}_s) \quad (4.40) \]
\[ \Delta \partial_t \left( \mathcal{F}(V_s) - \mathcal{F}(\widetilde{V}_s) \right) = J(V_s) - J(\widetilde{V}_s). \quad (4.41) \]

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 (4.36). According to (4.36) and (4.37), \( w_{\lambda} \) solves
\[ i \partial_t w_{\lambda} = -\Delta w_{\lambda} + (V_s + \widetilde{V}_s) w_{\lambda} + (V_s - \widetilde{V}_s) \widetilde{\psi}_{\lambda} \quad ; \quad w_{\lambda}(0, \cdot) = 0. \quad (4.42) \]

Since \( V_s + \widetilde{V}_s \in C^1([0, t_0], L^\infty(\Omega)) \) and \( (V_s - \widetilde{V}_s) \widetilde{\psi}_{\lambda} \in C^1([0, t_0], L^2(\Omega)) \), Lemma (3.1) applies. Then (3.7), (3.8), (3.2) and (3.4) imply
\[ \| w_{\lambda}(t) \|_{L^2(\Omega)} \leq C R t_0 \| \psi_{\lambda}^0 \|_{H^1(\Omega)} \| V_s - \widetilde{V}_s \|_{C^0([0, t_0], L^\infty(\Omega_0))} \quad (4.43) \]
\[ \| w_{\lambda}(t) \|_{H^2(\Omega)} \leq C R \| \psi_{\lambda}^0 \|_{H^1(\Omega)} \| V_s - \widetilde{V}_s \|_{C^1([0, t_0], L^\infty(\Omega_0))} \quad (4.44) \]
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 (4.43), and obtain
\[ \| n(V_s) - n(\widetilde{V}_s) \|_{L^2(\Omega_0)}(t) \]
\[ \leq \left( \int_{\Omega} \| \psi_{\lambda} + \widetilde{\psi}_{\lambda} \|_{L^2(\Omega_0)}^2(\lambda) \, d\mu(\lambda) \right)^{1/2} \left( \int_{\Omega} \| w_{\lambda}(t) \|_{L^2(\Omega_0)}^2 \, d\mu(\lambda) \right)^{1/2} \quad (4.45) \]
\[ \leq C R \left( \int_{\Omega} \| \psi_{\lambda}^0 \|_{H^2(\Omega_0)}^2 \, d\mu(\lambda) \right)^{1/2} \left( \int_{\Omega} \| w_{\lambda}(t) \|_{L^2(\Omega_0)}^2 \, d\mu(\lambda) \right)^{1/2} \]
\[ \leq C R t_0 \| V_s - \widetilde{V}_s \|_{C^0([0, t_0], L^\infty(\Omega_0))} \]
Let us now treat the term $J(V_s) - J(\tilde{V}_s)$: after straightforward computations and 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

$$\|J(V_s) - J(\tilde{V}_s)\|_{L^1(\Omega_0)} \leq C \left( \int_{\Lambda} \|\psi_\lambda + \tilde{\psi}_\lambda\|_{H^2(\Omega_0)}^2(t) \ d\mu(\lambda) \right)^{1/2} \left( \int_{\Lambda} \|w_\lambda(t)\|_{W^{1,7/2}(\Omega_0)}^2 \ d\mu(\lambda) \right)^{1/2}.$$  

(4.46)

Then, a Gagliardo-Nirenberg interpolation inequality, together with (4.43) and (4.44), leads to

$$\|w_\lambda(t)\|_{W^{1,7/2}(\Omega_0)} \leq C \|w_\lambda(t)\|_{H^2(\Omega_0)}^{13/14} \|w_\lambda(t)\|_{L^2(\Omega_0)}^{1/14} \leq C_R t_0^{1/14} \|\tilde{\psi}_\lambda\|_{H^1(\Omega)} \|V_s - \tilde{V}_s\|_{C^1([0,t_0],L^\infty(\Omega_0))}.$$ 

Coming back to (4.46) and using (3.8), we have finally

$$\|J(V_s) - J(\tilde{V}_s)\|_{L^1(\Omega_0)} \leq C_R t_0^{1/14} \|V_s - V_s\|_{C^1([0,t_0],L^\infty(\Omega_0))}.$$  

(4.47)

We are able now to estimate the difference $\mathcal{F}(V_s) - \mathcal{F}(\tilde{V}_s)$ in $X$. Indeed, from (4.40) and (4.45) we deduce

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

Next, from (4.41), (4.46) and the embedding $W^{1,7/2}(\Omega_0) \hookrightarrow L^\infty(\Omega_0)$, we obtain

$$\|\partial_t \mathcal{F}(V_s) - \partial_t \mathcal{F}(\tilde{V}_s)\|_{C^0([0,t_0],L^\infty(\Omega_0))} \leq C \|\partial_t \mathcal{F}(V_s) - \partial_t \mathcal{F}(\tilde{V}_s)\|_{C^0([0,t_0],W^{1,7/2}(\Omega_0))} \leq C_R t_0^{1/14} \|V_s - \tilde{V}_s\|_{C^1([0,t_0],L^\infty(\Omega_0))}.$$ 

The proof is completed by choosing $t_0$ small enough. 

\[ \square \]

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 arbitrary large positive time. The proof crucially uses the sublinearity of the estimate (3.26).

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

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

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

$$\|n(t)\|_{L^1(\Omega_0)} \leq C + C \left( \int_0^t \left( 1 + \frac{1}{\sqrt{\pi s}} \right) \mathcal{E}(s) ds \right)^{1/2},$$  

(5.1)
\[ \epsilon(t) \leq C + C \int_0^t \left( 1 + \frac{1}{\sqrt{\pi s}} \right) \epsilon(s) ds + C \int_0^t \| V_s(s) \|_{L^2(\Omega)} \left( 1 + \|n(s)\|_{L^1(\Omega_0)}^{1/2} \right) ds + \frac{1}{2} \| \nabla V_s(t) \|_{L^2(\Omega_0)}^2 + \int_0^t \int_{\Omega_0} V_s \partial_n n \, dx \, ds - \int_0^t \int_{\Omega_0} V_s \partial_n n \, dx \, ds. \] 

(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

\[ \| V_s(t) \|_{W^{1,p}(\Omega_0)} \leq C \| n(t) \|_{L^1(\Omega_0)}, \quad 1 \leq p < 3/2. \]

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

\[ \| V_s \|_{L^2(\Omega_0)} \leq C \| n \|_{L^1(\Omega_0)}. \]

This implies in view of (5.1), that

\[ \int_0^t \| V_s(s) \|_{L^2(\Omega_0)} \left( 1 + \| n(s) \|_{L^1(\Omega_0)}^{1/2} \right) ds \leq C + C \left( \int_0^t \left( 1 + \frac{1}{\sqrt{\pi s}} \right) \epsilon(s) ds \right)^{3/4}. \]

(5.3)

Furthermore, the Poisson equation gives

\[ \frac{1}{2} \| \nabla V_s(t) \|_{L^2(\Omega_0)}^2 = \int_0^t \int_{\Omega_0} V_s \partial_n n \, dx \, ds = \frac{1}{2} \| \nabla V_s(0) \|_{L^2(\Omega_0)}^2, \]

(5.4)

and an integration by parts with respect to time gives

\[ \int_0^t \int_{\Omega_0} V_s \partial_n n \, dx \, ds \leq C + C \| n(t) \|_{L^1(\Omega_0)} + C \int_0^t \| n(s) \|_{L^1(\Omega_0)} ds \]

\[ \leq C + C \left( \int_0^t \left( 1 + \frac{1}{\sqrt{\pi s}} \right) \epsilon(s) ds \right)^{1/2}, \]

(5.5)

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

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

Since it is clear by (H-3) and the Poisson equation that \( \| \nabla V_s(0) \|_{L^2(\Omega_0)} \leq C \), a Gronwall argument leads to the a priori estimate

\[ \epsilon(t) \leq C_T, \quad \forall t \in [0, T]. \]

(5.6)

To show the regularity property announced in Theorem 2.5, we use again use 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

\[ n \in C^0([0, T], W^{1,3/2}(\Omega_0)) \quad ; \quad J \in C^0([0, T], L^{3/2}(\Omega_0)), \]

\[ V \in C^0([0, T], W^{3,3/2}(\Omega_0)) \quad ; \quad \partial_t V \in C^0([0, T], W^{1,3/2}(\Omega_0)). \]

(5.7)
Besides, according to (3.13), \( u_{\lambda} := \partial_t \phi_{\lambda} = \partial_t \psi_{\lambda} - \partial_t \psi^{\text{par}}_{\lambda} \) solves

\[
\begin{align*}
\begin{cases}
 i \frac{\partial u_{\lambda}}{\partial t} = -\Delta u_{\lambda} + V u_{\lambda} + \partial_t V \phi_{\lambda} - \partial_t S_{\lambda}(V) & \text{in } \Omega \\
\phi_{\lambda}(0, x) = iS_{\lambda}(V)(0, x)
\end{cases}
\end{align*}
\]

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

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

From the Schrödinger equation \( \Delta \phi_{\lambda} = -i \partial_t \phi_{\lambda} + V \phi_{\lambda} \) 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

\[ n \in C^0([0, T], H^2(\Omega_0)) ; \quad J \in C^0([0, T], H^1(\Omega_0)); \]

which yields, through elliptic estimates, to the regularity of \( V_{\ast} \) stated in Theorem 2.5.

**Acknowledgments**

The authors acknowledge support from the HYKE project, contract number HPRN-CT-2002-00282 and from the project CNRS MATH-STIC FMRX CT97 0157, "Simulation quantique des nanostructureslectroniques sur silicium".

**References**


