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High Density Limit of the Stationary One Dimensional Schrödinger–Poisson System*

Raymond El Hajj[†] Naoufel Ben Abdallah[‡]

Abstract

The stationary one dimensional Schrödinger–Poisson system on a bounded interval is considered in the limit of a small Debye length (or small temperature). Electrons are supposed to be in a mixed state with the Boltzmann statistics. Using various reformulations of the system as convex minimization problems, we show that only the first energy level is asymptotically occupied. The electrostatic potential is shown to converge towards a boundary layer potential with a profile computed by means of a half space Schrödinger–Poisson system.

Key words. convex minimization, min-max theorem, concentration-compactness principle, boundary layer

AMS. 35A15, 35J10, 35Q40, 46N50, 75G65, 81Q10

1 Introduction and main results

1.1 Introduction

The Schrödinger–Poisson system is one of the most used models for quantum transport of charged particles in semiconductors as well as for quantum chemistry problems [3, 5, 8, 13, 14, 15, 18, 19, 20, 21, 22, 23, 30]. It describes the quantum motion of an ensemble of electrons submitted to and interacting with an electrostatic potential. The electron ensemble might be completely confined or in interaction with reservoirs. In the latter case, one speaks about open systems for which the particles are described by means of the scattering states of the Schrödinger Hamiltonian corresponding to the electrostatic potential which is in turn coupled to electron particle density through the electrostatic interaction. This leads to nonlinear partial differential equations whose analysis involves scattering theory techniques and limiting absorption theorems [23, 4, 3] and in which the

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repulsive character of the electrostatic interaction plays an important role in the analysis (it provides the necessary a priori estimates for solving the problem).

For closed systems, the particles are described thanks to the eigenstates and eigenenergies of the Schrödinger Hamiltonian. The electron density is the superposition of the densities of the eigenstates with an occupation number decreasingly depending on their eigenenergy. The coupling is again obtained through the Poisson equation modeling the electrostatic interaction. This problem was reformulated by Nier [20, 21, 22] as a minimization of a convex function (whose unknown is the electrostatic potential) which allows us to prove existence and uniqueness results. In [15], one can find generalizations including local contributions to the potential and which can be included in the functional to be minimized. This short review partially covers stationary problems. For evolution problems, an extended bibliography is available, and we refer the reader to the books of Markowich, Ringhofer, and Schmeiser [19] and Cazenave [10] for references.

In this paper we are interested in a singularly perturbed version of the Schrödinger–Poisson system which arises from the description of the so-called two dimensional electron gases [1, 11]. The electrons, in such systems, are strongly confined in one direction, at the interface between two material, and are free to move in the two remaining ones. In [6], the analysis of the Schrödinger equation of strongly confined electrons in one direction is performed. The confined direction is called z and the confining potential is assumed to be given and scaled as $\frac{1}{\varepsilon^2}V_c(\frac{z}{\varepsilon})$, where ε is a small parameter. Approximate models for the transport direction (orthogonal to z) derived heuristically in the previous works [25, 26, 27] are then analyzed in [6, 24]. The aim of the present work is to somehow justify the scaling $\frac{1}{\varepsilon^2}V_c(\frac{z}{\varepsilon})$ by the analysis of the self-consistent Schrödinger–Poisson system in the z direction. This is why we shall forget about the transport issues in the orthogonal direction and assume that the considered system is invariant with respect to it. The parameter ε in the present work is linked to the scaled Debye length as shall be explained later. The analysis relies on the minimization formulation of the problem leading to a singularly perturbed functional. After a rescaling argument, we are led to the analysis of a half space Schrödinger–Poisson system in which only the first eigenstate is occupied. Additional estimates are obtained thanks to reformulation of the single state Schrödinger–Poisson system as another minimization problem whose unknown is the first eigenfunction (and not the potential). This formulation is used in quantum chemistry [9].

Let us now come to the precise description of the problem and the results. The system is one dimensional and occupies the interval $[0, 1]$. The electrostatic energy is given by $V_\varepsilon(z)$. It satisfies the following one dimensional stationary Schrödinger–Poisson system:

$$\left\{ \begin{array}{l} -\frac{d^2\varphi_p}{dz^2} + V\varphi_p = \mathcal{E}_p\varphi_p, \quad z \in [0, 1], \\ \varphi_p \in H^1(0, 1), \quad \varphi_p(0) = 0, \quad \varphi_p(1) = 0, \quad \int_0^1 \varphi_p\varphi_q = \delta_{pq}, \\ -\varepsilon^3\frac{d^2V}{dz^2} = \frac{1}{\mathcal{Z}} \sum_{p=1}^{+\infty} e^{-\mathcal{E}_p}|\varphi_p|^2, \quad \mathcal{Z} = \sum_{p=1}^{+\infty} e^{-\mathcal{E}_p}, \\ V(0) = 0, \quad \frac{dV}{dz}(1) = 0. \end{array} \right. \quad (1)$$

The dimensionless parameter ε is a small parameter which is devoted to tending to zero. The choice of the third power is done for notational convenience as shall be understood

later. This parameter is related to the Debye length and shall be explicitly given by the rescaling of the Schrödinger–Poisson system (19) (see subsection 1.3). The eigenvalues of the Schrödinger operator $(\mathcal{E}_p)_p$ are the energy levels in the potential well. The sum in the right-hand side of the Poisson equation includes all eigenvalues of the Schrödinger operator. In the limit $\varepsilon \rightarrow 0$, one expects that the wave functions concentrate at $z = 0$. The boundary condition for the potential at $z = 1$ is physically justified in some physical situations such as in bulk materials. However, a Dirichlet condition is more commonly used in such problems. The analysis can be carried out in that case with the cost of technical complexity since a new boundary layer at $z = 1$ will appear and the eigenvalues will have asymptotically a double multiplicity. For simplicity, we do not consider this case. Since the density is very high in the limit $\varepsilon \rightarrow 0^+$, the Boltzmann statistics should be replaced by the Fermi–Dirac ones. The analysis can be done in this case with the cost of technical complications. More detailed comments about this are given in the last section of this paper. In order to analyze the boundary layer, we make the change of variables

$$\varphi_p(z) = \frac{1}{\sqrt{\varepsilon}} \psi_p\left(\frac{z}{\varepsilon}\right), \quad \mathcal{E}_p = \frac{1}{\varepsilon^2} E_p, \quad V(z) = \frac{1}{\varepsilon^2} U\left(\frac{z}{\varepsilon}\right), \quad \xi = \frac{z}{\varepsilon}. \quad (2)$$

Then, U verifies $-\frac{d^2 U}{d\xi^2} = \frac{1}{\tilde{Z}} \sum_{p=1}^{+\infty} e^{-\frac{E_p}{\varepsilon^2}} |\psi_p|^2$ with $\tilde{Z} = \sum_{p=1}^{+\infty} e^{-\frac{E_p}{\varepsilon^2}}$. Since there is a uniform gap with respect to ε between E_1 and E_p for $p \geq 2$ (see Lemma 4.2), the terms $e^{-\frac{E_p}{\varepsilon^2}}$ with $p \geq 2$ are expected to be negligible when compared to the first one ($p = 1$). Therefore, it is natural to expect the solution of (1) to be asymptotically close to the solution of the following Schrödinger–Poisson system in which only the first energy level is taken into account:

$$\left\{ \begin{array}{l} -\frac{d^2 \tilde{\varphi}_1}{dz^2} + \tilde{V} \tilde{\varphi}_1 = \tilde{\mathcal{E}}_1 \tilde{\varphi}_1, \quad z \in [0, 1], \\ \tilde{\mathcal{E}}_1 = \inf_{\varphi \in H_0^1(0,1), \|\varphi\|_{L^2}=1} \left\{ \int_0^1 |\varphi'|^2 + \int_0^1 \tilde{V} \varphi^2 \right\}, \\ -\varepsilon^3 \frac{d^2 \tilde{V}}{dz^2} = |\tilde{\varphi}_1|^2, \\ \tilde{V}(0) = 0, \quad \frac{d\tilde{V}}{dz}(1) = 0. \end{array} \right. \quad (3)$$

Moreover, when ε goes to zero, we will prove that the electrostatic potential, \tilde{V}_ε , solution of (3) converges towards a boundary layer potential with profile, U_0 , solution of the following half line problem:

$$\left\{ \begin{array}{l} -\frac{d^2 \psi_1}{d\xi^2} + U \psi_1 = E_1 \psi_1, \quad \xi \in [0, +\infty[, \\ E_1 = \inf_{\psi \in H_0^1(\mathbb{R}^+), \|\psi\|_{L^2}=1} \left\{ \int_0^{+\infty} |\psi'|^2 + \int_0^{+\infty} U \psi^2 \right\}, \\ -\frac{d^2 U}{d\xi^2} = |\psi_1|^2, \\ U(0) = 0, \quad \frac{dU}{d\xi} \in L^2(\mathbb{R}^+). \end{array} \right. \quad (4)$$

1.2 Main results

In this paper, a rigorous analysis and comparison of the systems presented above will be provided. Namely, (1) and (3) are posed on a bounded domain. The one dimensional Schrödinger–Poisson system on a bounded interval was studied by Nier in [20]. Each of these systems can be reformulated as a minimization problem (see section 2 for details). However, the limit problem (4) is posed on an unbounded domain. Our first result deals with the study of (4). We also prove that it can be formulated as a minimization problem.

Theorem 1.1. *Let $J_0(\cdot)$ be the energy functional defined on $\dot{H}_0^1(\mathbb{R}^+)$ (given by (22)) by*

$$J_0(U) = \frac{1}{2} \int_0^{+\infty} |U'|^2 - E_1^\infty[U], \quad (5)$$

where $E_1^\infty[U]$ is the fundamental mode of the Schrödinger operator given by (33). The limit problem (4) has a unique solution $(U_0, E_{1,0}, \psi_{1,0})$, and U_0 satisfies the following minimization problem:

$$J_0(U_0) = \inf_{U \in \dot{H}_0^1(\mathbb{R}^+)} J_0(U). \quad (6)$$

The comparison of the systems presented above is established by our second main theorem.

Theorem 1.2. *Let V_ε , \tilde{V}_ε , and U_0 be the potentials satisfying problems (1), (3), and (4), respectively. Then the following estimates hold:*

$$\|V_\varepsilon - \tilde{V}_\varepsilon\|_{H^1(0,1)} = \mathcal{O}(e^{-\frac{c}{\varepsilon^2}}) \quad (7)$$

and

$$\left\| \tilde{V}_\varepsilon - \frac{1}{\varepsilon^2} U_0 \left(\frac{\cdot}{\varepsilon} \right) \right\|_{H^1(0,1)} = \mathcal{O}(e^{-\frac{c}{\varepsilon}}), \quad (8)$$

where c is a general strictly positive constant independent of ε .

The paper is organized as follows. In the next subsection, we present some remarks on the scaling giving model (1), and we end this section by fixing some notation and definitions. In section 2, we recall the spectral properties of the Schrödinger operator on a bounded domain and state the optimization problems corresponding to (1) and (3) (or more precisely to the intermediate systems (10) and (11)). Section 3 is devoted to the analysis of the limit problem (4) posed on the half line (proof of Theorem 1.1). We will first study the properties of the fundamental mode of the Schrödinger operator (Proposition 3.1). The limit problem leads us to the study of a minimization problem posed on an unbounded domain. This will be done by means of the concentration-compactness principle introduced by Lions in [17]. Estimates (7) and (8) are proved in section 4. Some comments concerning the Fermi–Dirac statistics, the choice of the boundary conditions, and the problems of the multidimensional case are given in section 5. Finally, Appendix A is devoted to the proof of Lemma 3.1.

First, let us make this remark.

Remark 1.1. *To prove (7)–(8), we use the scaled versions of (1) and (3) when applying the changes of variables (2) and*

$$\tilde{\varphi}_1(z) = \frac{1}{\sqrt{\varepsilon}} \tilde{\psi}_1 \left(\frac{z}{\varepsilon} \right), \quad \tilde{\mathcal{E}}_1 = \frac{1}{\varepsilon^2} \tilde{E}_1, \quad \tilde{V}(z) = \frac{1}{\varepsilon^2} \tilde{U} \left(\frac{z}{\varepsilon} \right), \quad \xi = \frac{z}{\varepsilon}. \quad (9)$$

Then the intermediate Schrödinger–Poisson models write

$$\left\{ \begin{array}{l} -\frac{d^2\psi_p}{d\xi^2} + U\psi_p = E_p\psi_p, \quad \xi \in \left[0, \frac{1}{\varepsilon}\right], \\ \psi_p \in H^1\left(0, \frac{1}{\varepsilon}\right), \quad \psi_p(0) = 0, \quad \psi_p\left(\frac{1}{\varepsilon}\right) = 0, \quad \int_0^{\frac{1}{\varepsilon}} \psi_p\psi_q = \delta_{pq}, \\ -\frac{d^2U}{d\xi^2} = \frac{1}{\tilde{\mathcal{Z}}} \sum_{p=1}^{+\infty} e^{-\frac{E_p}{\varepsilon^2}} |\psi_p|^2, \quad \tilde{\mathcal{Z}} = \sum_{p=1}^{+\infty} e^{-\frac{E_p}{\varepsilon^2}}, \\ U(0) = 0, \quad \frac{dU}{d\xi}\left(\frac{1}{\varepsilon}\right) = 0 \end{array} \right. \quad (10)$$

and

$$\left\{ \begin{array}{l} -\frac{d^2\tilde{\psi}_1}{d\xi^2} + \tilde{U}\tilde{\psi}_1 = \tilde{E}_1\tilde{\psi}_1, \quad \xi \in \left[0, \frac{1}{\varepsilon}\right], \\ \tilde{E}_1 = \inf_{\psi \in H_0^1(0, \frac{1}{\varepsilon}), \|\psi\|_{L^2}=1} \left\{ \int_0^{\frac{1}{\varepsilon}} |\psi'|^2 + \int_0^{\frac{1}{\varepsilon}} \tilde{U}\psi^2 \right\}, \\ -\frac{d^2\tilde{U}}{d\xi^2} = |\tilde{\psi}_1|^2, \\ \tilde{U}(0) = 0, \quad \frac{d\tilde{U}}{d\xi}\left(\frac{1}{\varepsilon}\right) = 0. \end{array} \right. \quad (11)$$

Remark that it is natural to expect (11) to be close, when ε goes to zero, to the limit problem (4) posed on $[0, +\infty)$.

1.3 Remark on the scaling

Here we show how the system (1) can be obtained by a rescaling of the Schrödinger–Poisson system written with the physical dimensional variables. Indeed, let $(\chi_p(Z), \Lambda_p)$ be the eigenfunctions and the eigenenergies of the one dimensional Schrödinger operator (the confinement operator) $-\frac{\hbar^2}{2m} \frac{d^2}{dZ^2} + W$ with homogeneous Dirichlet data:

$$-\frac{\hbar^2}{2m} \frac{d^2\chi_p}{dZ^2} + W\chi_p = \Lambda_p\chi_p, \quad (12)$$

where \hbar is the Planck constant and m denotes the effective mass of the electrons in the crystal. The $(\chi_p)_p$ is an orthonormal basis of $L^2(0, L)$. The variable Z belongs to $[0, L]$, where L is the typical length of the confinement. Denoting by n the electronic density, this can be written

$$n(Z) = \sum_{p=1}^{+\infty} n_p |\chi_p(Z)|^2. \quad (13)$$

In this formula, $|\chi_p(Z)|^2$ is the probability of presence at point Z of an electron in the p th state. Using Boltzmann statistics, the occupation factor n_p is given by

$$n_p = \frac{N_s}{\mathcal{Z}} \exp\left(-\frac{\Lambda_p}{k_B T}\right), \quad \mathcal{Z} = \sum_{q=1}^{+\infty} \exp\left(-\frac{\Lambda_q}{k_B T}\right), \quad (14)$$

where k_B is the Boltzmann constant, T denotes the temperature, and N_s is the surface density assumed to be given. With this notation we have $\int_0^L n(Z) dZ = N_s$, which means that the total number of electrons in the interval $[0, L]$ (per unit surface in the two remaining spatial directions) is given. The electrostatic potential W and the electron density n are coupled through the Poisson equation:

$$-\frac{d^2W}{dZ^2} = \frac{q^2}{\varepsilon_0\varepsilon_r}n \quad (15)$$

with boundary conditions

$$W(0) = 0, \quad \frac{dW}{dZ}(L) = 0. \quad (16)$$

In (15), the constant q is the elementary electric charge and $\varepsilon_0, \varepsilon_r$ are, respectively, the permittivity of the vacuum and the relative permittivity of the material.

Let us rescale the problem (12)–(16) by noticing that

$$z = \frac{Z}{L} \in [0, 1], \quad W(Z) = (k_B T)V\left(\frac{Z}{L}\right), \quad \Lambda_p = (k_B T)\mathcal{E}_p, \quad \chi_p(Z) = \frac{1}{\sqrt{L}}\varphi_p\left(\frac{Z}{L}\right). \quad (17)$$

We assume that $\frac{\hbar^2}{2mL^2}$ is of the same order of the thermal energy ($k_B T$). In order to simplify the mathematical presentation, we suppose that

$$\frac{\hbar^2}{2mL^2} = k_B T. \quad (18)$$

By inserting (17) into the system (12)–(16), we obtain, after straightforward computation, the system (1) in which ε is related to the scaled Debye length:

$$\varepsilon^3 = \left(\frac{\lambda_D}{L}\right)^2, \quad \lambda_D = \sqrt{\frac{k_B T \varepsilon_0 \varepsilon_r}{q^2 N}}, \quad (19)$$

where $N = \frac{N_s}{L}$ is the average volume density of electrons.

1.4 Notation and definitions

We summarize in this subsection the different variables and notation used in this paper.

- For the Schrödinger–Poisson problems posed on $[0, 1]$, z denotes the space variable, V denotes the potential variable, and (\mathcal{E}, φ) represents any eigenvalue and the corresponding eigenfunction of the Schrödinger operator. For systems posed on $[0, \frac{1}{\varepsilon}]$ or on \mathbb{R}^+ , we use ξ, U , and (E, ψ) as variables. The same notation with $\tilde{\cdot}$, i.e., $(\tilde{V}, \tilde{\mathcal{E}}, \tilde{\varphi})$ or $(\tilde{U}, \tilde{E}, \tilde{\psi})$, is used for the variables of Schrödinger–Poisson systems in which only the first eigenstate is taken into account.
- For any real valued function $V \in L^2(0, L)$, where $L > 0$ is given ($L = 1$ or $\frac{1}{\varepsilon}$ here), we denote by $H[V]$ the Dirichlet–Schrödinger operator

$$H[V] = -\frac{d^2}{dx^2} + V(x) \quad (x = z \text{ or } \xi \text{ here}) \quad (20)$$

defined on the domain $D(H[V]) = H^2(0, L) \cap H_0^1(0, L)$. In addition, the sequence of eigenenergies and eigenfunctions of $H[V]$ will be denoted by $(E_p[V], \psi_p[V])_{p \in \mathbb{N}^*}$. We give in the next section the main properties satisfied by the functions $V \mapsto E_p[V]$ and $V \mapsto \psi_p[V]$ for any $p \in \mathbb{N}^*$.

- The potentials satisfying (1) and (3) are denoted by V_ε and \tilde{V}_ε . In addition, $(\mathcal{E}_{p,\varepsilon}, \varphi_{p,\varepsilon})$ and $(\tilde{\mathcal{E}}_{p,\varepsilon}, \tilde{\varphi}_{p,\varepsilon})$, with $p \in \mathbb{N}^*$, represent the corresponding energy couples of $H[V_\varepsilon]$ and $H[\tilde{V}_\varepsilon]$, respectively. In other words, $\mathcal{E}_{p,\varepsilon} := E_p[V_\varepsilon]$, $\varphi_{p,\varepsilon} := \psi_p[V_\varepsilon]$, $\tilde{\mathcal{E}}_{p,\varepsilon} := E_p[\tilde{V}_\varepsilon]$, and $\tilde{\varphi}_{p,\varepsilon} := \psi_p[\tilde{V}_\varepsilon]$. Similarly, the solutions of (10) and (11) will be denoted, respectively, by $(U_\varepsilon, E_{p,\varepsilon}, \psi_{p,\varepsilon})$ and $(\tilde{U}_\varepsilon, \tilde{E}_{p,\varepsilon}, \tilde{\psi}_{p,\varepsilon})$. Finally, we fix $(U_0, E_{1,0}, \psi_{1,0})$ to denote the solution of the limit problem (4).

Let us now define some spaces which will be used throughout this paper.

Definition 1.1. (i) For $L > 0$, we define

$$H^{1,0}(0, L) = \{U \in H^1(0, L), U(0) = 0\}. \quad (21)$$

(ii) The space $\dot{H}_0^1(\mathbb{R}^+)$ is defined as follows:

$$\dot{H}_0^1(\mathbb{R}^+) = \{U \in L_{loc}^2(\mathbb{R}^+), U' \in L^2(\mathbb{R}^+), U(0) = 0, \text{ and } U \geq 0\}. \quad (22)$$

(iii) For any $0 < L \leq +\infty$, we shall denote by S_L the set of normalized functions of $H_0^1(0, L)$ with respect to the L^2 -norm

$$S_L = \left\{ \varphi \in H_0^1(0, L), \int_0^L \varphi^2 = 1 \right\}. \quad (23)$$

Here $H_0^1(0, L)$ is the space of H^1 -functions vanishing on 0 and L , and when $L = +\infty$

$$H_0^1(\mathbb{R}^+) = \{\psi \in H^1(\mathbb{R}^+), \psi(0) = 0\}.$$

2 Schrödinger–Poisson system on a bounded domain

We begin this part by recalling some basic properties satisfied by the eigenvalues and the eigenfunctions of the one dimensional Schrödinger operator (20). These properties are standard and can be found in [16, 20, 28, 29]. The operator $H[V]$ is self-adjoint, is bounded from below, and has compact resolvent. There exists a strictly increasing sequence $(E_p[V])_p$ of real numbers tending to $+\infty$ and an orthonormal basis of $L^2(0, L)$, $(\psi_p[V])_p$, such that $\psi_p[V] \in D(H[V])$ and

$$H[V]\psi_p[V] = E_p[V]\psi_p[V]. \quad (24)$$

For $V = 0$, we have by a simple calculation

$$E_p[0] = \frac{\pi^2 p^2}{L^2}, \quad \psi_p[0](x) = \sqrt{\frac{2}{L}} \sin\left(\frac{p\pi x}{L}\right). \quad (25)$$

The eigenvalues $E_p[V]$ are simple and satisfy the following characterization (min-max principle) [29]:

$$E_p[V] = \min_{V_p \in \mathbb{V}_p(D(H[V]))} \max_{\varphi \in V_p, \varphi \neq 0} \frac{(H[V]\varphi, \varphi)_{L^2}}{\|\varphi\|_{L^2}^2}, \quad (26)$$

where $\mathbb{V}_p(D(H[V]))$ is the set of the subspaces of $D(H[V])$ with dimension equal to p , and (\cdot, \cdot) denotes the scalar product in L^2 . In view of the min-max formula (26), one can verify that for any $p \in \mathbb{N}^*$, $E_p[\cdot]$ is an increasing function, which means that

$$E_p[V] \leq E_p[W] \quad \text{if } V \leq W \text{ a.e.}$$

Moreover, we have the Lipschitz property, for any real valued functions V, W in $L^\infty(0, L)$,

$$|E_p[V] - E_p[W]| \leq \|V - W\|_{L^\infty(0, L)}. \quad (27)$$

Besides, one can prove the following lemma [20].

Lemma 2.1. *For any $p \in \mathbb{N}^*$, the maps*

$$E_p[\cdot] : L^2(0, L) \longrightarrow \mathbb{R}, \quad \psi_p[\cdot] : L^\infty(0, L) \longrightarrow L^1(0, L)$$

are Gâteaux differentiable, and their derivatives are given, respectively, by

$$\begin{aligned} dE_p[V].W &= \int_0^L |\psi_p[V]|^2 W dx \quad \text{and} \\ d\psi_p[V].W &= \sum_{q \neq p} \frac{1}{E_p[V] - E_q[V]} \left(\int_0^L W \psi_p \psi_q dx \right) \psi_q \end{aligned} \quad (28)$$

for any $V, W \in L^\infty(0, L)$.

Using the spectral properties of the Schrödinger operator, one can prove the following proposition. For details on the proof see [20].

Proposition 2.1. *The systems (10) and (11) are well posed. They are equivalent, respectively, to the following minimization problems:*

$$J_\varepsilon(U_\varepsilon) = \inf_{U \in H^{1,0}(0, M_\varepsilon)} J_\varepsilon(U) \quad (29)$$

and

$$\tilde{J}_\varepsilon(\tilde{U}_\varepsilon) = \inf_{U \in H^{1,0}(0, M_\varepsilon)} \tilde{J}_\varepsilon(U), \quad (30)$$

where $M_\varepsilon = \frac{1}{\varepsilon}$. The energy functionals J_ε and \tilde{J}_ε are given by

$$J_\varepsilon(U) = \frac{1}{2} \int_0^{M_\varepsilon} |U'|^2 + \varepsilon^2 \log \left(\sum_{p=1}^{+\infty} e^{-\frac{E_p[U]}{\varepsilon^2}} \right) \quad (31)$$

and

$$\tilde{J}_\varepsilon(U) = \frac{1}{2} \int_0^{M_\varepsilon} |U'|^2 - E_1[U]. \quad (32)$$

Each one of problems (29) and (30) admits a unique solution.

Remark 2.1. *One can similarly study the systems (1) and (3) and prove that each one is equivalent to an optimization problem.*

3 Analysis of the limit problem (4)

The aim of this part is to study the well-posedness of the limit problem (4) posed on the half line. Namely, this part is concerned with the proof of Theorem 1.1. We begin with the study of the fundamental mode, $E_1^\infty[\cdot]$, of the Schrödinger operator. Its main properties are listed in Proposition 3.1.

3.1 Properties of the fundamental mode of the Schrödinger operator on $[0, +\infty)$

We begin by defining the fundamental mode.

Definition 3.1. *For any real and positive function $U \in L_{loc}^1(\mathbb{R}^+)$, the fundamental mode of the Schrödinger operator is*

$$E_1^\infty[U] = \inf_{\psi \in S_\infty} J_U(\psi), \quad (33)$$

where for any $\psi \in S_\infty$ (defined by (23)) we have

$$J_U(\psi) = \int_0^{+\infty} |\psi'|^2 + \int_0^{+\infty} U\psi^2. \quad (34)$$

One difficulty due to the unboundedness of the interval $[0, +\infty)$ is that $E_1^\infty[\cdot]$ might not be an eigenvalue but only the lower bound of the essential spectrum. The following proposition gives some properties of $E_1^\infty[\cdot]$ and some sufficient conditions on the potential for which $E_1^\infty[\cdot]$ is an eigenvalue.

Proposition 3.1. 1. *The map $U \mapsto E_1^\infty[U]$ is a continuous, concave, and increasing function with values in $\overline{\mathbb{R}^+} := [0, +\infty]$ satisfying*

$$E_1^\infty[U] \leq \limsup_{\xi \rightarrow +\infty} U(\xi). \quad (35)$$

2. *If $U \in L_{loc}^1(\mathbb{R}^+)$, $U \geq 0$ such that $E_1^\infty[U] < \liminf_{\xi \rightarrow +\infty} U(\xi)$, then $E_1^\infty[U]$ is reached by a unique positive function $\psi_1[U]$, which means that there exists a unique positive function $\psi_1[U] \in S_\infty$ such that $E_1^\infty[U] = J_U(\psi_1[U])$. In addition, we have*

$$\frac{dE_1^\infty}{dU}[U].W = \int_0^{+\infty} |\psi_1[U]|^2 W d\xi \quad (36)$$

for any function W in $L_0^\infty(\mathbb{R}^+)$, the space of bounded functions with compact support on \mathbb{R}^+ .

3. *Let $U \in L_{loc}^1(\mathbb{R}^+)$ be a positive function such that $\lim_{\xi \rightarrow +\infty} U(\xi)$ exists, $U \leq \lim_{\xi \rightarrow +\infty} U(\xi)$, and $E_1^\infty[U] = \lim_{\xi \rightarrow +\infty} U(\xi)$. Then we have*

$$\frac{dE_1^\infty}{dU}[U].W = 0$$

for any $W \in L_0^\infty(\mathbb{R}^+)$.

4. Let α be an arbitrary positive constant. Then we have

$$E_1^\infty[\alpha\sqrt{\xi}] = \alpha^{\frac{4}{5}} E_1^\infty[\sqrt{\xi}]. \quad (37)$$

Remark 3.1. There is quite a difference between the third case of this proposition, where $E_1^\infty[U] = \lim_{\xi \rightarrow +\infty} U(\xi)$, and the second case, which includes $E_1^\infty[U] < \lim_{\xi \rightarrow +\infty} U(\xi)$. This result is natural and can be interpreted as follows. The classically allowed region for a particle with energy E is the set $\mathcal{A} = \{\xi \in [0, +\infty); U(\xi) \leq E\}$. In the case $E \geq U(\xi)$ on $[0, +\infty)$, the set \mathcal{A} extends to $+\infty$ so that there is no bound state, while in the case $E < \lim_{\xi \rightarrow +\infty} U(\xi)$ the set \mathcal{A} is bounded and E is a bounded state energy.

Lemma 3.1. Let $U \in \dot{H}_0^1(\mathbb{R}^+)$ such that $E_1^\infty[U] < \liminf_{+\infty} U$. Then all minimizing sequences $(\psi_n)_n$ of problem (33) are relatively compact in $L^2(\mathbb{R}^+)$.

This lemma is needed for the proof of the second point of Proposition 3.1. It is proved in Appendix A. The proof is based on the concentration-compactness principle.

Proof of Proposition 3.1. 1. Remark first that for any positive function U , $E_1^\infty[U]$ exists and belongs to $\overline{\mathbb{R}^+}$. It is easy to check, from the definition of $E_1^\infty[\cdot]$, that it is a continuous, concave, and increasing function. To prove inequality (35), let $\psi \in S_\infty$ be fixed and set $\psi_\delta = \sqrt{\delta}\psi(\delta\xi)$ for any real positive δ . Then $\psi_\delta \in S_\infty$, and since $E_1^\infty[U]$ verifies (33), we have

$$E_1^\infty[U] \leq J_U(\psi_\delta). \quad (38)$$

Moreover, we have $J_U(\psi_\delta) = \delta^2 \int_0^{+\infty} |\psi'(\xi)|^2 d\xi + \int_0^{+\infty} U(\frac{\xi}{\delta}) \psi^2(\xi) d\xi$. Then

$$\limsup_{\delta \rightarrow 0} J_U(\psi_\delta) \leq \int_0^{+\infty} \limsup_{\delta \rightarrow 0} U\left(\frac{\xi}{\delta}\right) \psi^2(\xi) d\xi \leq \limsup_{\xi \rightarrow +\infty} U(\xi).$$

Taking the $\limsup_{\delta \rightarrow 0}$ of (38), one obtains inequality (35).

2. Let $(\psi_n)_n$ be a minimizing sequence of $E_1^\infty[U]$; i.e., $\psi_n \in S_\infty$ for any $n \in \mathbb{N}^*$ and $J_U(\psi_n) \rightarrow_{n \rightarrow +\infty} E_1^\infty[U]$. The sequence $(\psi_n)_n$ is bounded in $H_0^1(\mathbb{R}^+)$, there exist a function $\psi \in H_0^1(\mathbb{R}^+)$ and a subsequence also denoted (ψ_n) such that (ψ_n) converges weakly to ψ in $H_0^1(\mathbb{R}^+)$, and since $J_U(\cdot)$ is weakly lower semicontinuous (it is strictly convex and lower semicontinuous) we have $J_U(\psi) \leq \liminf_{n \rightarrow +\infty} J_U(\psi_n)$. Then

$$J_U(\psi) \leq E_1^\infty[U]. \quad (39)$$

Besides, the hypothesis $E_1^\infty[U] < \liminf_{+\infty} U$ implies that the sequence $(\psi_n)_n$ is relatively compact in $L^2(\mathbb{R}^+)$ (see Lemma 3.1). Then, up to an extraction of subsequence, $(\psi_n)_n$ converges strongly to ψ in $L^2(\mathbb{R}^+)$. Since $\|\psi_n\|_{L^2(\mathbb{R}^+)}^2 = 1$, for all n , we have $\|\psi\|_{L^2(\mathbb{R}^+)}^2 = 1$, and then ψ belongs to S_∞ . Therefore, in view of the definition of $E_1^\infty[U]$ (33), $E_1^\infty[U] \leq J_U(\psi)$ and with (39) we have $E_1^\infty[U] = J_U(\psi)$. Let us now show that $E_1^\infty[U]$ is a simple eigenvalue and the corresponding eigenfunction has a constant sign. Indeed, let ψ_1 and ψ_2 be two minimizers of $J_U(\cdot)$ on S_∞ , i.e., $\psi_1, \psi_2 \in S_\infty$, such that $E_1^\infty[U] = J_U(\psi_1) = J_U(\psi_2)$, and let $\phi = \sqrt{\frac{\psi_1^2}{2} + \frac{\psi_2^2}{2}}$. The function ϕ belongs to S_∞ , and we have

$$J_U(\phi) = \frac{1}{2} J_U(\psi_1) + \frac{1}{2} J_U(\psi_2) - \int_0^{+\infty} \left| \frac{\psi_1 \psi_2' - \psi_2 \psi_1'}{2\phi} \right|^2 = E_1^\infty[U] - \int_0^{+\infty} \left| \frac{\psi_1 \psi_2' - \psi_2 \psi_1'}{2\phi} \right|^2.$$

Since $E_1^\infty[U] \leq J_U(\phi)$ ($\phi \in S_\infty$), we get $\int_0^{+\infty} \left| \frac{\psi_1 \psi_2' - \psi_2 \psi_1'}{2\phi} \right|^2 = 0$, which implies that ψ_1 and ψ_2 are proportional, and so $E_1^\infty[U]$ is simple. In particular, ψ and $|\psi|$ are two minimizers of $E_1^\infty[U]$; they are then proportional, and since $\int_0^{+\infty} |\psi|^2 = 1$ we conclude that $\psi = \pm |\psi|$. We then choose $\psi_1[U] = |\psi|$, which is positive. This is the unique positive eigenfunction corresponding to $E_1^\infty[U]$. To end the proof of the second point of Proposition 3.1, let W be a compactly supported bounded function ($W \in L_0^\infty(\mathbb{R}^+)$) and remark that for a small real t we have $E_1^\infty[U + tW] \leq E_1^\infty[U] + |t| \|W\|_\infty < \liminf_{\xi \rightarrow +\infty} U(\xi)$. In addition, since $W \in L_0^\infty$, we have $\liminf_{\xi \rightarrow +\infty} U = \liminf_{\xi \rightarrow +\infty} (U(\xi) + tW(\xi))$. Then, for any small real t , we have $E_1^\infty[U + tW] < \lim_{\xi \rightarrow +\infty} (U(\xi) + tW(\xi))$. Therefore, for all bounded and compactly supported functions W and for all $t \in \mathbb{R}$ small, $E_1^\infty[U + tW]$ is an eigenvalue. Let ψ_t be the corresponding positive eigenfunction. We have

$$E_1^\infty[U + tW] = \int_0^{+\infty} |\psi_t'|^2 d\xi + \int_0^{+\infty} (U + tW) |\psi_t|^2 d\xi \geq E_1^\infty[U] + t \int_0^{+\infty} W |\psi_t|^2 d\xi.$$

Similarly, one has

$$E_1^\infty[U] \geq E_1^\infty[U + tW] - t \int_0^{+\infty} W |\psi_1[U]|^2 d\xi.$$

Then, if t is a small nonnegative real (without loss of generality), one can write

$$\int_0^{+\infty} W |\psi_t|^2 d\xi \leq \frac{E_1^\infty[U + tW] - E_1^\infty[U]}{t} \leq \int_0^{+\infty} W |\psi_1[U]|^2 d\xi. \quad (40)$$

Besides, since $(\psi_t)_t$ is bounded in $H_0^1(\mathbb{R}^+)$, there exists a positive function $\psi_0 \in H_0^1$ such that ψ_t converges weakly to ψ_0 , when $t \rightarrow 0^+$, in $H_{loc}^1(\mathbb{R}^+)$ and strongly in $L_{loc}^2(\mathbb{R}^+)$. By passing to the limit $t \rightarrow 0^+$ in

$$-\psi_t'' + (U + tW)\psi_t = E_1^\infty[U + tW]\psi_t$$

we obtain

$$-\psi_0'' + U\psi_0 = E_1^\infty[U]\psi_0 \quad \text{in } \mathcal{D}'(0, +\infty).$$

Since ψ_0 is positive, we deduce that $\psi_0 = \psi_1[U]$. Finally, to obtain (36) we just have to take the limit $t \rightarrow 0^+$ of (40).

3. Remark first that, since $E_1^\infty[\cdot]$ is a nondecreasing real function, we have for $t \geq 0$

$$\frac{E_1^\infty[U - t|W|] - E_1^\infty[U]}{t} \leq \frac{E_1^\infty[U + tW] - E_1^\infty[U]}{t} \leq \frac{E_1^\infty[U + t|W|] - E_1^\infty[U]}{t}.$$

Therefore, it is sufficient to prove $\frac{dE_1^\infty}{dU}[U].W = 0$ for $W \geq 0$ and $W \leq 0$ (the general case can be deduced by passing to the limit $t \rightarrow 0^+$ in the above inequalities).

(i) Let $W \in L_0^\infty(\mathbb{R}^+)$ and $W \geq 0$. Then we have $E_1^\infty[U] \leq E_1^\infty[U + tW]$. Besides, by (35), we have $E_1^\infty[U + tW] \leq \lim_{\xi \rightarrow +\infty} (U(\xi) + tW(\xi)) = \lim_{\xi \rightarrow +\infty} U(\xi) = E_1^\infty[U]$. Then, for all $W \geq 0$ in L_0^∞ , $E_1^\infty[U + tW] = E_1^\infty[U]$, and the result is proved in this case.

(ii) Let $W \in L_0^\infty(\mathbb{R}^+)$, let $W \leq 0$, and let $(t_n)_{n \in \mathbb{N}}$ be a sequence decreasing towards 0^+ . The sequence $(E_1^\infty[U + t_n W])_n$ is increasing and satisfies $E_1^\infty[U + t_n W] \leq \lim_{+\infty} U = E_1^\infty[U]$ for all $n \in \mathbb{N}$. Therefore, either it is stationary in the vicinity of $+\infty$ and in that case $\frac{dE_1^\infty}{dU}[U].W = 0$, or it satisfies

$$E_1^\infty[U + t_n W] < \lim_{+\infty} U \quad \forall n \in \mathbb{N}. \quad (41)$$

In the latter case, $E_1^\infty[U + t_n W]$ is an eigenvalue and there exists a sequence $(\psi_n) \in S_\infty$, $\psi_n \geq 0$, such that

$$E_1^\infty[U + t_n W] = J_{U+t_n W}(\psi_n) = \inf_{\psi \in S_\infty} J_{U+t_n W}(\psi).$$

Besides, we have $E_1^\infty[U + t_n W] \geq E_1^\infty[U] + t_n \int_0^{+\infty} W \psi_n^2 d\xi$ and

$$\left| \frac{E_1^\infty[U + t_n W] - E_1^\infty[U]}{t_n} \right| \leq - \int_0^{+\infty} W \psi_n^2 d\xi. \quad (42)$$

The sequence $(\psi_n)_n$ being bounded in $H_0^1(\mathbb{R}^+)$, one can find a positive function $\psi \in H_0^1(\mathbb{R}^+)$ and a subsequence of $(\psi_n)_n$ also denoted by $(\psi_n)_n$ such that ψ_n converges weakly to ψ in $H_{loc}^1(\mathbb{R}^+)$ and strongly in $L_{loc}^2(\mathbb{R}^+)$. In addition ψ satisfies, in the sense of distributions,

$$-\psi'' + U\psi = E_1^\infty[U]\psi = \lim_{+\infty} (U)\psi.$$

This implies that $\psi'' = (U - \lim_{+\infty} U)\psi \leq 0$ with $\psi \in H_0^1(\mathbb{R}^+)$. We deduce that $\psi = 0$ a.e., and we get the result by passing to the limit in (42), W being compactly supported.

4. Let us now verify the identity (37). Since the potential $(\alpha\sqrt{\xi})$ tends to $+\infty$ when ξ goes to $+\infty$, $E_1^\infty[\alpha\sqrt{\xi}]$ is reached by a positive function $\psi \in S_\infty$:

$$-\psi''(\xi) + (\alpha\sqrt{\xi})\psi = E_1^\infty[\alpha\sqrt{\xi}]\psi.$$

Setting $\xi = \alpha^\beta \zeta$ and $\bar{\psi}(\zeta) = \sqrt{\alpha^\beta} \psi(\alpha^\beta \zeta)$ for an arbitrary constant β , we get

$$-\frac{1}{\alpha^{2\beta}} \bar{\psi}''(\zeta) + \alpha^{1+\frac{\beta}{2}} \sqrt{\zeta} \bar{\psi}(\zeta) = E_1^\infty[\alpha\sqrt{\xi}] \bar{\psi}(\zeta).$$

By choosing β such that $-2\beta = 1 + \frac{\beta}{2}$, so that $\beta = \frac{-2}{5}$, we obtain

$$-\bar{\psi}''(\zeta) + \sqrt{\zeta} \bar{\psi}(\zeta) = \alpha^{\frac{-4}{5}} E_1^\infty[\alpha\sqrt{\xi}] \bar{\psi}(\zeta),$$

which implies that $E_1^\infty[\alpha\sqrt{\xi}] = \alpha^{\frac{4}{5}} E_1^\infty[\sqrt{\xi}]$. The proof of Proposition 3.1 is achieved.

3.2 Proof of Theorem 1.1

In what follows, we will show that (6) admits a unique solution verifying (4). Indeed, the functional $J_0(\cdot)$ is obviously continuous and strictly convex on $\dot{H}_0^1(\mathbb{R}^+)$. To prove the existence of a unique $U_0 \in \dot{H}_0^1(\mathbb{R}^+)$ satisfying (6), it remains to verify that $J_0(\cdot)$ is coercive on $\dot{H}_0^1(\mathbb{R}^+)$. For this let $U \in \dot{H}_0^1(\mathbb{R}^+)$ and write $U(\xi) = \int_0^\xi U'(t) dt$. This implies that $U(\xi) \leq \|U'\|_{L^2} \sqrt{\xi}$, and since $E_1^\infty[\cdot]$ is an increasing function one has $E_1^\infty[U] \leq E_1^\infty[\|U'\|_{L^2} \sqrt{\xi}]$. Applying (37) with $\alpha = \|U'\|_{L^2}$ we get $E_1^\infty[U] \leq \|U'\|_{L^2}^{\frac{4}{5}} E_1^\infty[\sqrt{\xi}]$, and finally we have

$$J_0(U) \geq \frac{1}{2} \|U'\|_{L^2}^2 - E_1^\infty[\sqrt{\xi}] \cdot \|U'\|_{L^2}^{\frac{4}{5}} \xrightarrow{\|U'\|_{L^2} \rightarrow +\infty} +\infty.$$

Let us now prove that U_0 is a solution of the limit problem (4). Namely, we have to check that $E_1^\infty[U_0]$ is an eigenvalue. To this aim, we first write the Euler–Lagrange equation for U_0 :

$$-U_0'' = \frac{dE_1^\infty}{dU}[U_0] \geq 0. \quad (43)$$

Therefore, U_0 is a concave function belonging to $\dot{H}_0^1(\mathbb{R}^+)$. It is thus a continuous, increasing, and positive function on \mathbb{R}^+ , and $\lim_{+\infty} U_0$ exists in $\overline{\mathbb{R}}$. It now remains to check that $E_1^\infty[U_0] < \lim_{+\infty} U_0$, which will ensure that $E_1^\infty[U_0] := E_{1,0}$ is an eigenvalue with unique positive eigenfunction $\psi_{1,0} \in S_\infty$ (see point two of Proposition 3.1). We proceed by contradiction and assume that $E_1^\infty[U_0] = \lim_{+\infty} U_0$. Applying the third point of Proposition 3.1, one obtains $\frac{dE_1^\infty}{dU}[U_0] = 0$. In view of (43) and the fact that U_0 is a concave positive function in $\dot{H}_0^1(\mathbb{R}^+)$, we deduce that $U_0 = 0$ and $\min_{U \in \dot{H}_0^1(\mathbb{R}^+)} J_0(U) = 0$. But a simple rescaling argument shows that J_0 takes negative values, and so its minimum is negative. To prove this claim, we fix a potential U in $\dot{H}_0^1(\mathbb{R}^+)$ such that $\int_0^{+\infty} |U'|^2 = 1$, $\lim_{+\infty} U = +\infty$ and let $\psi_1 \in S_\infty$ be the eigenfunction corresponding to $E_1^\infty[U]$. For $\varepsilon > 0$, setting $U^\varepsilon(\xi) = \varepsilon^2 U(\varepsilon\xi)$ and $\psi_1^\varepsilon(\xi) = \sqrt{\varepsilon} \psi_1(\varepsilon\xi)$, we have

$$-\frac{d^2\psi_1^\varepsilon}{d\xi^2} + U^\varepsilon\psi_1^\varepsilon(\xi) = \varepsilon^2 E_1^\infty[U]\psi_1^\varepsilon(\xi),$$

which implies that $E_1^\infty[U^\varepsilon] = \varepsilon^2 E_1^\infty[U]$. After straightforward computations, we finally obtain

$$\begin{aligned} J_0(U^\varepsilon) &= \frac{1}{2} \int_0^{+\infty} \left| \frac{dU^\varepsilon}{d\xi} \right|^2 d\xi - E_1^\infty[U^\varepsilon] = \frac{\varepsilon^5}{2} \int_0^{+\infty} |U'|^2 d\xi - \varepsilon^2 E_1^\infty[U] \\ &= -\varepsilon^2 E_1^\infty[U] \left(1 - \frac{\varepsilon^3}{2E_1^\infty[U]} \right), \end{aligned}$$

which is negative for ε small enough. The proof of Theorem 1.1 is complete.

4 Convergence analysis

The various models presented in the first section of this work are all well posed. In this section, we shall estimate the difference between their solutions in terms of ε . Namely, we have to prove estimates (7) and (8). The following lemma will be useful.

Lemma 4.1. *Let $(U_0, E_{1,0}, \psi_{1,0})$ be the solution of the limit problem (4). There exist $a, b \in \mathbb{R}^+$ independent of ε such that for all ε small we have*

$$\|\psi_{1,0}\|_{L^2(M_\varepsilon, +\infty)} \leq a e^{-bM_\varepsilon} \quad (44)$$

with $M_\varepsilon = \frac{1}{\varepsilon}$.

Proof. We have $-\psi_{1,0}'' + U_0\psi_{1,0} = E_{1,0}\psi_{1,0}$ such that $\psi_{1,0} \geq 0$, $\psi_{1,0}(\xi) \rightarrow_{\xi \rightarrow +\infty} 0$ ($\psi_{1,0} \in H_0^1(\mathbb{R}^+)$), $E_{1,0} < \lim_{+\infty} U_0$, and U_0 increases to its limit at $+\infty$. Then one can find two nonnegative constants c and δ independent of ε such that for all ε small enough we have

$$-\psi_{1,0}''(\xi) \leq -\delta\psi_{1,0}(\xi) \quad \text{for } \xi \in [M_\varepsilon, +\infty[$$

and $\psi_{1,0}(M_\varepsilon) \leq c e^{-\sqrt{\delta}M_\varepsilon}$. Let $S(\xi) = c e^{-\sqrt{\delta}\xi}$ and $\psi = \psi_{1,0} - S$. Then we have $S'' = \delta S$ and

$$-\psi''(\xi) + \delta\psi(\xi) \leq 0, \quad \xi \in [M_\varepsilon, +\infty[\quad (45)$$

with

$$\psi(M_\varepsilon) \leq 0 \quad \text{and} \quad \psi(+\infty) = 0.$$

By the maximum principle, one deduces that $\psi \leq 0$ on $[M_\varepsilon, +\infty[$. Thus

$$\psi_{1,0}(\xi) \leq ce^{-\sqrt{\delta}\xi} \quad \text{on } [M_\varepsilon, +\infty[,$$

which yields estimate (44). \square

We begin by proving the second estimate (8) of Theorem 1.2. For this we will compare (see Proposition 4.1) the potentials U_0 and \tilde{U}_ε solutions of (6) and (30), respectively. This will be done thanks to an idea consisting of the reformulation of the problems (4) and (11) as minimization problems whose unknown is the first eigenfunction. This is the subject of the following remark.

Remark 4.1. For $\phi \in S_{M_\varepsilon}$ (see Definition 1.1), where $M_\varepsilon = \frac{1}{\varepsilon}$, let us set

$$A_\varepsilon(\phi) = \int_0^{M_\varepsilon} |\phi'(\xi)|^2 d\xi + \frac{1}{2} \int_0^{M_\varepsilon} \int_0^{M_\varepsilon} \phi^2(\xi)\phi^2(\zeta) \min(\xi, \zeta) d\xi d\zeta \quad (46)$$

and for $\phi \in S_\infty$

$$A_0(\phi) = \int_0^{+\infty} |\phi'(\xi)|^2 d\xi + \frac{1}{2} \int_0^{+\infty} \int_0^{+\infty} \phi^2(\xi)\phi^2(\zeta) \min(\xi, \zeta) d\xi d\zeta. \quad (47)$$

The functional A_ε satisfies $A_\varepsilon(|\phi|) = A_\varepsilon(\phi)$ and the convexity property

$$A_\varepsilon \left(\sqrt{t\phi_1^2 + (1-t)\phi_2^2} \right) \leq tA_\varepsilon(\phi_1) + (1-t)A_\varepsilon(\phi_2)$$

for $t \in (0, 1)$, the inequality being strict if $|\phi_1|$ and $|\phi_2|$ are not proportional (these properties are also satisfied by A_0). The functionals are obvious weakly lower semicontinuous on their domain of definition, in such a way that the minimization problems

$$A_\varepsilon(\phi_\varepsilon) = \min_{\phi \in H_0^1(0, M_\varepsilon), \|\phi\|_{L^2} = 1} A_\varepsilon(\phi) \quad (48)$$

and

$$A_0(\phi_0) = \min_{\phi \in H_0^1(\mathbb{R}^+), \|\phi\|_{L^2} = 1} A_0(\phi) \quad (49)$$

have unique positive solutions. The problems (48) and (49) are equivalent, respectively, to (11) and (4). Indeed, the functions ϕ_ε and ϕ_0 satisfy

$$-\phi_\varepsilon'' + U(\phi_\varepsilon)\phi_\varepsilon = \mu_\varepsilon\phi_\varepsilon \quad \text{on } [0, M_\varepsilon],$$

$$-\phi_0'' + U(\phi_0)\phi_0 = \mu_0\phi_0 \quad \text{on } \mathbb{R}^+,$$

where μ_ε (respectively, μ_0) is the Lagrange multiplier associated with the constraint $\|\phi\|_{L^2} = 1$ and $U(\phi_\varepsilon)$, $U(\phi_0)$ denote, respectively,

$$U(\phi_\varepsilon)(\xi) = \int_0^{M_\varepsilon} |\phi_\varepsilon(\zeta)|^2 \min(\xi, \zeta) d\zeta, \quad U(\phi_0)(\xi) = \int_0^{+\infty} |\phi_0(\zeta)|^2 \min(\xi, \zeta) d\zeta.$$

In addition, since ϕ_ε and ϕ_0 are positive and the function $K(\xi, \zeta) = \min(\xi, \zeta)$ is the kernel corresponding to the Laplacian in dimension one, we have

$$(U(\phi_\varepsilon), \mu_\varepsilon, \phi_\varepsilon) = (\tilde{U}_\varepsilon, \tilde{E}_{1,\varepsilon}, \tilde{\psi}_{1,\varepsilon}) \quad \text{and} \quad (U(\phi_0), \mu_0, \phi_0) = (U_0, E_{1,0}, \psi_{1,0}).$$

Proposition 4.1. *The solutions U_0 and \tilde{U}_ε of (6) and (30), respectively, verify the following estimate:*

$$\left\| \frac{d}{d\xi} (\tilde{U}_\varepsilon - U_0) \right\|_{L^2(0, M_\varepsilon)}^2 = \mathcal{O}(e^{-\frac{c}{\varepsilon}}), \quad (50)$$

where c is a strictly positive constant independent of ε and $M_\varepsilon = \frac{1}{\varepsilon}$. This yields estimate (8).

Proof. We start by comparing $A_0(\psi_{1,0})$ and $A_\varepsilon(\tilde{\psi}_{1,\varepsilon})$. Let $\chi_\varepsilon \in \mathcal{D}(0, +\infty)$ be such that $\chi_\varepsilon(\xi) = 1$ on $[0, M_\varepsilon - 1]$, $\chi_\varepsilon(\xi) = 0$ on $[M_\varepsilon, +\infty[$, and $0 \leq \chi_\varepsilon \leq 1$. The function $\chi_\varepsilon \cdot \psi_{1,0}|_{(0, M_\varepsilon)}$ belongs to $H_0^1(0, M_\varepsilon)$, and for ε small we have $\|\chi_\varepsilon \cdot \psi_{1,0}\|_{L^2(0, M_\varepsilon)} \neq 0$. Let $\beta_\varepsilon = \|\chi_\varepsilon \cdot \psi_{1,0}\|_{L^2(0, M_\varepsilon)}$. Then we have $\frac{1}{\beta_\varepsilon} \chi_\varepsilon \cdot \psi_{1,0} \in S_{M_\varepsilon}$ and, with (44), $\beta_\varepsilon = 1 + \mathcal{O}(e^{-\frac{c}{\varepsilon}})$. Then, in view of Remark 4.1, the following inequalities can be straightforwardly justified:

$$A_\varepsilon(\tilde{\psi}_{1,\varepsilon}) \leq A_\varepsilon\left(\frac{1}{\beta_\varepsilon} \chi_\varepsilon \cdot \psi_{1,0}\right) \leq A_\varepsilon(\psi_{1,0}) + \mathcal{O}(e^{-\frac{c}{\varepsilon}}) \leq A_0(\psi_{1,0}) + \mathcal{O}(e^{-\frac{c}{\varepsilon}}),$$

where c is a strictly positive constant independent of ε . Besides, we have

$$A_0(\psi_{1,0}) \leq A_0(\tilde{\psi}_{1,\varepsilon}) = A_\varepsilon(\tilde{\psi}_{1,\varepsilon}).$$

Here and in what follows, we still denote by $\tilde{\psi}_{1,\varepsilon}$ the extension of $\tilde{\psi}_{1,\varepsilon}$ by zero on $[M_\varepsilon, +\infty[$ when it is taken as a function on \mathbb{R}^+ . Consequently, we have

$$|A_\varepsilon(\tilde{\psi}_{1,\varepsilon}) - A_0(\psi_{1,0})| = A_\varepsilon(\tilde{\psi}_{1,\varepsilon}) - A_0(\psi_{1,0}) = \mathcal{O}(e^{-\frac{c}{\varepsilon}}). \quad (51)$$

Furthermore, A_0 is uniformly convex on S_∞ and $\psi_{1,0}$ realizes its minimum. Then one can find a constant $c_0 > 0$ independent of ε such that

$$\|\psi_{1,0} - \tilde{\psi}_{1,\varepsilon}\|_{H^1(\mathbb{R}^+)}^2 \leq c_0 |A_0(\psi_{1,0}) - A_0(\tilde{\psi}_{1,\varepsilon})|.$$

In addition, since $A_0(\tilde{\psi}_{1,\varepsilon}) = A_\varepsilon(\tilde{\psi}_{1,\varepsilon})$ and with (51), one deduces that

$$\|\psi_{1,0} - \tilde{\psi}_{1,\varepsilon}\|_{H^1(\mathbb{R}^+)}^2 = \mathcal{O}(e^{-\frac{c}{\varepsilon}}). \quad (52)$$

The potential $U_0 - \tilde{U}_\varepsilon$ satisfies

$$-\frac{d^2}{d\xi^2} (U_0 - \tilde{U}_\varepsilon)(\xi) = |\psi_{1,0}(\xi)|^2 - |\tilde{\psi}_{1,\varepsilon}(\xi)|^2 \quad \text{on } [0, M_\varepsilon].$$

Then, multiplying this equation by $U_0 - \tilde{U}_\varepsilon$, one obtains after integration by parts

$$\begin{aligned} \left\| \frac{d}{d\xi} (U_0 - \tilde{U}_\varepsilon) \right\|_{L^2(0, M_\varepsilon)}^2 &\leq \frac{dU_0}{d\xi}(M_\varepsilon)(U_0(M_\varepsilon) - \tilde{U}_\varepsilon(M_\varepsilon)) \\ &\quad + \sup_{\xi \in [0, M_\varepsilon]} (|U_0(\xi) - \tilde{U}_\varepsilon(\xi)|) \int_0^{M_\varepsilon} (|\psi_{1,0}|^2 - |\tilde{\psi}_{1,\varepsilon}|^2) d\xi. \end{aligned}$$

Moreover, in view of Remark 4.1, we have, for every $\xi \in [0, M_\varepsilon]$,

$$\begin{aligned} (U_0 - \tilde{U}_\varepsilon)(\xi) &= \int_0^{M_\varepsilon} (|\psi_{1,0}|^2 - |\tilde{\psi}_{1,\varepsilon}|^2)(\zeta) \min(\xi, \zeta) d\zeta + \int_{M_\varepsilon}^{+\infty} |\psi_{1,0}|^2 \min(\xi, \zeta) d\zeta \\ &\leq M_\varepsilon \left(\int_0^{M_\varepsilon} (|\psi_{1,0}|^2 - |\tilde{\psi}_{1,\varepsilon}|^2)(\zeta) d\zeta + \int_{M_\varepsilon}^{+\infty} |\psi_{1,0}|^2(\zeta) d\zeta \right) \end{aligned}$$

and $\frac{dU_0}{d\xi}(M_\varepsilon) = - \int_{M_\varepsilon}^{+\infty} \frac{d^2 U_0}{d\xi^2}(\xi) d\xi = \int_{M_\varepsilon}^{+\infty} |\psi_{1,0}|^2 d\xi$. Then

$$\begin{aligned} \left\| \frac{d}{d\xi}(U_0 - \tilde{U}_\varepsilon) \right\|_{L^2(0, M_\varepsilon)}^2 &\leq M_\varepsilon \left(\int_0^{M_\varepsilon} (|\psi_{1,0}|^2 - |\tilde{\psi}_{1,\varepsilon}|^2)(\zeta) d\zeta + \int_{M_\varepsilon}^{+\infty} |\psi_{1,0}|^2(\zeta) d\zeta \right)^2 \\ &\leq 2M_\varepsilon \left(\|\psi_{1,0} - \tilde{\psi}_{1,\varepsilon}\|_{L^2(0, M_\varepsilon)}^2 + \|\psi_{1,0}\|_{L^2(M_\varepsilon, +\infty)}^4 \right), \end{aligned}$$

and with (52) and (44) one obtains (50). Moreover, with the change of variable $\tilde{V}_\varepsilon(\cdot) = \frac{1}{\varepsilon^2} \tilde{U}_\varepsilon(\frac{\cdot}{\varepsilon})$ one deduces that

$$\left\| \frac{d}{d\xi} \left(\tilde{V}_\varepsilon - \frac{1}{\varepsilon^2} \tilde{U}_0 \left(\frac{\cdot}{\varepsilon} \right) \right) \right\|_{L^2(0,1)}^2 = \frac{1}{\varepsilon^5} \left\| \frac{d}{d\xi} (\tilde{U}_\varepsilon - U_0) \right\|_{L^2(0, M_\varepsilon)}^2 = \mathcal{O}(e^{-\frac{\varepsilon}{\varepsilon}}),$$

and then estimate (8) holds. \square

Let us now give the following result, which shows the existence of a uniform gap between the first eigenvalue $\tilde{E}_{1,\varepsilon} := E_1[\tilde{U}_\varepsilon]$ and the others $E_p[\tilde{U}_\varepsilon]$.

Lemma 4.2. *There exists a constant $G > 0$, independent of ε , such that*

$$E_p[\tilde{U}_\varepsilon] - \tilde{E}_{1,\varepsilon} \geq G \quad \forall p \geq 2. \quad (53)$$

Proof. Since $(E_p[\tilde{U}_\varepsilon])_{p \geq 1}$ is an increasing sequence, it is sufficient to show (53) only for $p = 2$. We argue by contradiction and suppose that $|E_2[\tilde{U}_\varepsilon] - \tilde{E}_{1,\varepsilon}| \rightarrow 0$ as ε goes to zero. In view of Remark 4.1, we have $\tilde{E}_{1,\varepsilon} = A_\varepsilon(\tilde{\psi}_{1,\varepsilon})$ and $E_{1,0} = A_0(\psi_{1,0})$. Then, with (51), $|\tilde{E}_{1,\varepsilon} - E_{1,0}| = \mathcal{O}(e^{-\frac{\varepsilon}{\varepsilon}})$. We deduce that $E_2[\tilde{U}_\varepsilon]$ and $\tilde{E}_{1,\varepsilon}$ converge to $E_{1,0}$ when $\varepsilon \rightarrow 0$. Then the eigenfunctions $\psi_2[\tilde{U}_\varepsilon]$ and $\tilde{\psi}_{1,\varepsilon}$, corresponding, respectively, to $E_2[\tilde{U}_\varepsilon]$ and $\tilde{E}_{1,\varepsilon}$, prolonged by zero on $[\frac{1}{\varepsilon}, +\infty)$, are bounded in $H_0^1(\mathbb{R}^+)$ with respect to ε . There exists ψ_1 (respectively, ψ_2) $\in H_0^1(\mathbb{R}^+)$ such that $\tilde{\psi}_{1,\varepsilon}$ (respectively, $\psi_2[\tilde{U}_\varepsilon]$) converges weakly in $H_{loc}^1(\mathbb{R}^+)$ to ψ_1 (respectively, ψ_2). By passing to the limit $\varepsilon \rightarrow 0^+$ in $\mathcal{D}'(0, +\infty)$, in the equations

$$\begin{aligned} -\tilde{\psi}_{1,\varepsilon}'' + \tilde{U}_\varepsilon \tilde{\psi}_{1,\varepsilon} &= \tilde{E}_{1,\varepsilon} \tilde{\psi}_{1,\varepsilon}, \\ -(\psi_2[\tilde{U}_\varepsilon])'' + \tilde{U}_\varepsilon \psi_2[\tilde{U}_\varepsilon] &= E_2[\tilde{U}_\varepsilon] \psi_2[\tilde{U}_\varepsilon] \end{aligned}$$

one deduces that ψ_1 and ψ_2 are two eigenfunctions corresponding to $E_{1,0}$. In addition, we have

$$\begin{aligned} |J_{U_0}(\tilde{\psi}_{1,\varepsilon}) - E_{1,0}| &= \left| \int_0^{+\infty} |\tilde{\psi}'_{1,\varepsilon}|^2 + \int_0^{+\infty} U_0 |\tilde{\psi}_{1,\varepsilon}|^2 - E_{1,0} \right| \\ &= \left| \int_0^{M_\varepsilon} |\tilde{\psi}'_{1,\varepsilon}|^2 + \int_0^{M_\varepsilon} \tilde{U}_\varepsilon |\tilde{\psi}_{1,\varepsilon}|^2 - E_{1,0} + \int_0^{+\infty} (U_0 - \tilde{U}_\varepsilon) |\tilde{\psi}_{1,\varepsilon}|^2 \right| \\ &\leq |\tilde{E}_{1,\varepsilon} - E_{1,0}| + \sup_{[0, M_\varepsilon]} (|U_0 - \tilde{U}_\varepsilon|) \xrightarrow{\varepsilon \rightarrow 0} 0. \end{aligned}$$

Then $(\tilde{\psi}_{1,\varepsilon})$ (and similarly $(\psi_2[\tilde{U}_\varepsilon])$) is a minimizing sequence of “ $E_{1,0} = \inf_{\psi \in S_\infty} J_{U_0}(\psi)$.” Moreover, since $E_{1,0} < \lim_{+\infty} U_0$ (see the proof of Theorem 1.1) and applying Lemma 3.1, $(\tilde{\psi}_{1,\varepsilon})$ and $(\psi_2[\tilde{U}_\varepsilon])$ (up to extraction of subsequences) converge strongly in $L^2(\mathbb{R}^+)$. Thus, since $\tilde{\psi}_{1,\varepsilon}$ and $\psi_2[\tilde{U}_\varepsilon]$ are two normalized and orthogonal functions in $L^2(\mathbb{R}^+)$ for any $\varepsilon > 0$, we deduce that their limits when $\varepsilon \rightarrow 0$, ψ_1 and ψ_2 , which are two eigenfunctions of $E_{1,0}$, are also normalized and orthogonal in $L^2(\mathbb{R}^+)$. This contradicts the fact that $E_{1,0}$ is a simple eigenvalue. \square

Proposition 4.2. *The potentials U_ε and \tilde{U}_ε solutions of (10) and (11) verify that*

$$\|U_\varepsilon - \tilde{U}_\varepsilon\|_{H^1(0, M_\varepsilon)} = \mathcal{O}(e^{-\frac{c}{\varepsilon^2}}), \quad (54)$$

where c is a strictly positive constant independent of ε . This gives estimate (7).

Proof. Recall first that U_ε and \tilde{U}_ε verify, respectively, (29) and (30). To prove estimate (54), it is sufficient to compare the energies $J_\varepsilon(U_\varepsilon)$ and $J_\varepsilon(\tilde{U}_\varepsilon)$ because we have

$$\|U_\varepsilon - \tilde{U}_\varepsilon\|_{H^1(0, M_\varepsilon)}^2 \leq c_0 |J_\varepsilon(U_\varepsilon) - J_\varepsilon(\tilde{U}_\varepsilon)|, \quad (55)$$

where c_0 is independent of ε . A straightforward comparison gives the following inequalities:

$$\tilde{J}_\varepsilon(\tilde{U}_\varepsilon) \leq \tilde{J}_\varepsilon(U_\varepsilon) \leq J_\varepsilon(U_\varepsilon) \leq J_\varepsilon(\tilde{U}_\varepsilon). \quad (56)$$

Besides, we have $\tilde{U}_\varepsilon \geq 0$, and $E_p[\cdot]$ is an increasing function; then $E_p[\tilde{U}_\varepsilon] \geq E_p[0] = \varepsilon^2 p^2 \pi^2$. Moreover, since $\tilde{E}_{1,\varepsilon}$ converges to $E_{1,0}$, which is then finite, there exists a constant $c_1 > 0$ independent of ε such that

$$E_p[\tilde{U}_\varepsilon] - \tilde{E}_{1,\varepsilon} \geq \varepsilon^2 p^2 \pi^2 - c_1. \quad (57)$$

Combining (53) and (57), one finds $c_2 > 0$ and $c_3 > 0$ independent of ε such that

$$E_p[\tilde{U}_\varepsilon] - \tilde{E}_{1,\varepsilon} \geq c_2 \varepsilon^2 p^2 \pi^2 + c_3 \quad \forall p \geq 2.$$

This implies that

$$\sum_{p \geq 2} e^{-\frac{E_p[\tilde{U}_\varepsilon] - E_1[\tilde{U}_\varepsilon]}{\varepsilon^2}} = \mathcal{O}(e^{-\frac{c_3}{\varepsilon^2}}),$$

and since

$$J_\varepsilon(\tilde{U}_\varepsilon) = \tilde{J}_\varepsilon(\tilde{U}_\varepsilon) + \varepsilon^2 \log \left(1 + \sum_{p \geq 2} e^{-\frac{E_p[\tilde{U}_\varepsilon] - E_1[\tilde{U}_\varepsilon]}{\varepsilon^2}} \right),$$

we obtain

$$J_\varepsilon(\tilde{U}_\varepsilon) = \tilde{J}_\varepsilon(\tilde{U}_\varepsilon) + \mathcal{O}(\varepsilon^2 e^{-\frac{c_3}{\varepsilon^2}}),$$

which leads to (54) in view of (55) and (56). \square

5 Comments

5.1 Fermi–Dirac statistics

It is more natural to consider Fermi–Dirac statistics in the high density limit ($\varepsilon \rightarrow 0$). Here we give some remarks and elements on the limit in this case. The scaled occupation factor of the p th state with Fermi–Dirac statistics is given by

$$n_p^{FD} = f_{FD}(\mathcal{E}_p - \mathcal{E}_F),$$

where \mathcal{E}_F is the Fermi level and f_{FD} is the Fermi–Dirac distribution

$$f_{FD}(u) = \log(1 + e^{-u}), \quad (58)$$

The scaled Boltzmann distribution function, however, is given by $f_B(u) = e^{-u}$. The Poisson equation in model (1) can be written as follows:

$$-\frac{d^2V}{d\xi^2} = \sum_{p=1}^{+\infty} f_{B(FD)}(\mathcal{E}_p - \mathcal{E}_F) |\varphi_p|^2$$

under the following constraint on the Fermi energy:

$$\sum_{p=1}^{+\infty} f_{B(FD)}(\mathcal{E}_p - \mathcal{E}_F) = \frac{1}{\varepsilon^3}. \quad (59)$$

In the Boltzmann case, one can explicitly solve (59) with respect to \mathcal{E}_F , and we have

$$e^{\mathcal{E}_F} = \frac{1}{\varepsilon^3 \sum_{p=1}^{+\infty} e^{-\mathcal{E}_p}},$$

which yields (1). The first remark we give in the Fermi–Dirac case is that $e^{\mathcal{E}_F}$ cannot be expressed explicitly in terms of $e^{-\mathcal{E}_p}$. The analysis of the limit can, however, be extended to this case but with technical complications that we have avoided in the Boltzmann statistics case. When applying the change of variables (2) and $\mathcal{E}_F = \frac{1}{\varepsilon^2} \epsilon_F$ the intermediate problem (10) becomes in the Fermi–Dirac statistics case

$$\left\{ \begin{array}{l} -\frac{d^2\psi_p}{d\xi^2} + U\psi_p = E_p\psi_p, \quad \xi \in \left[0, \frac{1}{\varepsilon}\right], \\ \psi_p \in H^1\left(0, \frac{1}{\varepsilon}\right), \quad \psi_p(0) = 0, \quad \psi_p\left(\frac{1}{\varepsilon}\right) = 0, \quad \int_0^{\frac{1}{\varepsilon}} \psi_p\psi_q = \delta_{pq}, \\ -\frac{d^2U}{d\xi^2} = \varepsilon^3 \sum_{p=1}^{+\infty} f_{FD}\left(\frac{E_p - \epsilon_F}{\varepsilon^2}\right) |\psi_p|^2, \quad \sum_{p=1}^{+\infty} f_{FD}\left(\frac{E_p - \epsilon_F}{\varepsilon^2}\right) = \frac{1}{\varepsilon^3}, \\ U(0) = 0, \quad \frac{dU}{d\xi}\left(\frac{1}{\varepsilon}\right) = 0. \end{array} \right. \quad (60)$$

Since f_{FD} is a regular, positive, and decreasing function on \mathbb{R} , the Schrödinger–Poisson system in a bounded domain in the Fermi–Dirac case is well posed and can also be expressed as an optimization problem; see the work of Nier [20] in the unidimensional case and [22] in higher dimensions. More precisely, (60) is equivalent to

$$J_\varepsilon(U_\varepsilon) = \inf_{U \in H^{1,0}\left(0, \frac{1}{\varepsilon}\right)} J_\varepsilon(U), \quad (61)$$

where

$$J_\varepsilon(U) = \frac{1}{2} \int_0^{\frac{1}{\varepsilon}} |U'|^2 - \varepsilon^3 \sum_{p=1}^{+\infty} \left[f_{FD}\left(\frac{E_p[U] - \epsilon_F[U]}{\varepsilon^2}\right) \epsilon_F[U] - \varepsilon^2 \int_{\frac{E_p[U] - \epsilon_F[U]}{\varepsilon^2}}^{+\infty} f_{FD}(u) du \right]. \quad (62)$$

Replacing $f_{FD}(\cdot)$ by $f_B(u) = e^{-u}$, $J_\varepsilon(\cdot)$ is nothing else but the functional (31) modulo a constant independent of the variable U . The uniform gap showed in Lemma 4.2 remains

correct. Then, as in the proof of Proposition 4.2, there are two constants $c_1 > 0$ and $c_2 > 0$ such that

$$(E_p - \epsilon_F) - (E_1 - \epsilon_F) \geq c_1 \varepsilon^2 p^2 \pi^2 + c_2 \quad \forall p \geq 2.$$

Since f_{FD} is a decreasing function and $\log(1 + u) \sim u$ when $u \rightarrow 0^+$, then for all $p \geq 2$

$$\begin{aligned} \log \left(1 + e^{-\frac{E_p - \epsilon_F}{\varepsilon^2}} \right) &\leq \log \left(1 + e^{-\frac{c_2}{\varepsilon^2}} e^{-c_1 p^2 \pi^2} e^{-\frac{E_1 - \epsilon_F}{\varepsilon^2}} \right) \leq c e^{-\frac{c_2}{\varepsilon^2}} e^{-c_1 p^2 \pi^2} e^{-\frac{E_1 - \epsilon_F}{\varepsilon^2}} \\ &\leq c e^{-\frac{c_2}{\varepsilon^2}} e^{-c_1 p^2 \pi^2} \log \left(1 + e^{-\frac{E_1 - \epsilon_F}{\varepsilon^2}} \right), \end{aligned}$$

where $c > 0$ is a general constant independent of ε . This implies that

$$\frac{\sum_{p \geq 2} \log \left(1 + e^{-\frac{E_p - \epsilon_F}{\varepsilon^2}} \right)}{\log \left(1 + e^{-\frac{E_1 - \epsilon_F}{\varepsilon^2}} \right)} \leq c \left(\sum_{p \geq 2} e^{-c_1 p^2 \pi^2} \right) e^{-\frac{c_2}{\varepsilon^2}}.$$

Thus, a formal analysis shows that, asymptotically when $\varepsilon \rightarrow 0$, (60) is close to a Schrödinger–Poisson system with only the first energy level. However, the rigorous analysis of the limit, $\varepsilon \rightarrow 0$, of (61)–(62) is more technically complicated than the Boltzmann case for which the functional J_ε has an explicit expression given by (31).

5.2 Boundary conditions and higher dimension

The choice of Neumann boundary condition at $z = 1$ can be justified for modulation doping devices (see [2]) for which $z = 1$ is in the bulk of the semiconductor and the hypothesis of a vanishing electric field is justified. This hypothesis also makes the analysis simple because the boundary layer in the limit $\varepsilon \rightarrow 0^+$ is located at $z = 0$. If V satisfies Dirichlet boundary conditions, then another boundary layer takes place at $z = 1$. The analysis can probably be extended to this case, but the first eigenvalue will have asymptotically a multiplicity 2. The multidimensional problem is more complicated, where the location of the electrons in the boundary layer may depend on the geometry of the boundary. Such problems have been noticed for the Schrödinger equation with a magnetic field by [7, 12] and are beyond the scope of our work.

A Proof of Lemma 3.1

This appendix is devoted to the proof of Lemma 3.1. We will use the concentration-compactness principle. This principle is a general method introduced by Lions [17] to solve various minimizing problems posed on unbounded domains. It is shown that all minimizing sequences are relatively compact if and only if some strict subadditivity inequalities hold. The proof is based upon a lemma called the concentration-compactness lemma. For more details on the principle, we refer the reader to [17]. Let us begin by recalling the concentration-compactness lemma.

Lemma A.1 (concentration-compactness lemma). *1. Let $(\rho_n)_{n \geq 1}$ be a sequence in $L^1(\mathbb{R})$ satisfying $\rho_n \geq 0$ in \mathbb{R} and $\int_{\mathbb{R}} \rho_n dx = \lambda$ for a fixed $\lambda > 0$. Then there exists a subsequence $(\rho_{n_k})_{k \geq 1}$ satisfying one of the three following possibilities:*

(i) (Compactness): there exists $y_k \in \mathbb{R}$ such that

$$\forall \varepsilon > 0, \quad \exists R < +\infty, \quad \int_{y_k + B_R} \rho_{n_k}(x) dx \geq \lambda - \varepsilon,$$

where $B_R = \{x \in \mathbb{R}; |x| \leq R\}$.

(ii) (Vanishing):

$$\lim_{k \rightarrow +\infty} \sup_{y \in \mathbb{R}} \int_{y + B_R} \rho_{n_k}(x) dx = 0.$$

(iii) (Dichotomy): There exists $\alpha \in]0, \lambda[$ such that for all $\varepsilon > 0$, there exist $k_0 \geq 1$ and $\rho_k^1, \rho_k^2 \in L^1_+(\mathbb{R})$ such that for $k \geq k_0$

$$\|\rho_{n_k} - (\rho_k^1 + \rho_k^2)\|_{L^1} \leq \varepsilon, \quad \left| \int_{\mathbb{R}} \rho_k^1 dx - \alpha \right| \leq \varepsilon, \quad \left| \int_{\mathbb{R}} \rho_k^2 dx - (\lambda - \alpha) \right| \leq \varepsilon,$$

where ρ_k^1 has compact support and $\text{dist}(\text{supp}(\rho_k^1), \text{supp}(\rho_k^2)) \rightarrow_k +\infty$.

2. If $\rho_n = |u_n|^2$ with u_n bounded in $H^1(\mathbb{R})$, there exists a subsequence (ρ_{n_k}) such that either compactness (i), vanishing (ii), or dichotomy (iii) occurs as follows: there exists $\alpha \in]0, \lambda[$ such that for all $\varepsilon > 0$ there exist $k_0 \geq 1$, u_k^1, u_k^2 bounded in $H^1(\mathbb{R})$ satisfying for $k \geq k_0$

$$\left\{ \begin{array}{l} \|u_{n_k} - (u_k^1 + u_k^2)\|_{L^2} \leq \delta(\varepsilon) \xrightarrow{\varepsilon \rightarrow 0} 0, \\ \left| \int_{\mathbb{R}} |u_k^1|^2 dx - \alpha \right| \leq \varepsilon, \quad \left| \int_{\mathbb{R}} |u_k^2|^2 dx - (\lambda - \alpha) \right| \leq \varepsilon, \\ \text{dist}(\text{supp}(u_k^1), \text{supp}(u_k^2)) \xrightarrow{k \rightarrow +\infty} +\infty, \\ \liminf_k \int_{\mathbb{R}} \{|\nabla u_{n_k}|^2 - |\nabla u_k^1|^2 - |\nabla u_k^2|^2\} dx \geq 0. \end{array} \right.$$

First, we need to give some notation. For $V \in \dot{H}_0^1(\mathbb{R}^+)$ and $\varepsilon \in \mathbb{R}^+$, we define

$$I_\varepsilon = \inf \left\{ J_V(\varphi), \quad \varphi \in H_0^1(\mathbb{R}^+), \quad \int_0^{+\infty} \varphi^2 = \varepsilon \right\}, \quad (63)$$

where $J_V(\varphi) = \int_0^{+\infty} |\varphi'|^2 + \int_0^{+\infty} V \varphi^2$, and

$$I_\varepsilon^\infty = \inf \left\{ J_\infty(\varphi), \quad \varphi \in H_0^1(\mathbb{R}^+), \quad \int_0^{+\infty} \varphi^2 = \varepsilon \right\}, \quad (64)$$

where $J_\infty(\varphi) = \int_0^{+\infty} |\varphi'|^2 + V^\infty \int_0^{+\infty} \varphi^2$ and $V^\infty = \liminf_{+\infty} V$.

Lemma A.2. Let $V \in \dot{H}_0^1(\mathbb{R}^+)$ such that $E_1^\infty[V] < \liminf_{+\infty} V$. Then the following strict subadditivity inequality holds:

$$I_\varepsilon < I_\alpha + I_{\varepsilon-\alpha}^\infty \quad \forall 0 < \alpha < \varepsilon. \quad (65)$$

Proof. Take $\varphi \in H_0^1(\mathbb{R}^+)$ such that $\int_0^{+\infty} \varphi^2 = \varepsilon$ and let $\psi = \frac{\sqrt{\alpha}}{\sqrt{\varepsilon}}\varphi$. Then $\psi \in H_0^1(\mathbb{R}^+)$, $\int_0^{+\infty} \psi^2 = \alpha$, and $J_V(\psi) = \frac{\alpha}{\varepsilon}J_V(\varphi)$. This implies that $\varepsilon I_\alpha \leq \alpha I_\varepsilon$ for any arbitrary $\alpha > 0$ and $\varepsilon > 0$. We also deduce that $\varepsilon I_\alpha = \alpha I_\varepsilon$ (and similarly $\varepsilon I_\alpha^\infty = \alpha I_\varepsilon^\infty$) for any $\varepsilon, \alpha > 0$. In particular, if $\alpha = 1$, $\varepsilon I_1 = I_\varepsilon$ (or $\varepsilon I_1^\infty = I_\varepsilon^\infty$) for any $\varepsilon > 0$. Moreover, by definition we have $I_1 = E_1^\infty[V] < V^\infty$. Then, for all $\varphi \in H_0^1(\mathbb{R}^+)$ such that $\int_0^{+\infty} \varphi^2 = 1$, we have $I_1 < \int_0^{+\infty} |\varphi'|^2 + V^\infty$. This implies that $I_1 < I_1^\infty$, and by multiplying by $(\varepsilon - \alpha)$, which is positive if $0 < \alpha < \varepsilon$, one obtains $\varepsilon I_1 - \alpha I_1 < (\varepsilon - \alpha)I_1^\infty$ and inequality (65) holds. \square

Proof of Lemma 3.1. Applying the concentration-compactness lemma for $(\rho_n)_n$: $\rho_n(x) = |\psi_n(x)|^2$ on \mathbb{R}^+ and zero elsewhere, there exists a subsequence $(\rho_{n_k})_k$ satisfying one of the three cases given by Lemma A.1. If vanishing (ii) occurs, i.e., if

$$\lim_{k \rightarrow +\infty} \sup_{y \in \mathbb{R}} \int_{y+B_R} \rho_{n_k}(x) dx = 0 \quad \forall R \geq 0,$$

which implies that

$$\lim_{k \rightarrow +\infty} \sup_{y \in \mathbb{R}^+} \int_y^{y+R} |\psi_{n_k}(x)|^2 dx = 0 \quad \forall R \geq 0,$$

then, for all $\varepsilon > 0$ small enough, one can find a sequence $(R_k)_k$ of increasing positive real such that $\int_0^{R_k} |\psi_{n_k}(x)|^2 dx \leq \varepsilon$ for all k . We have

$$\begin{aligned} \int_0^{+\infty} |\psi'_{n_k}|^2 dx + \int_0^{+\infty} V \psi_{n_k}^2 dx &= \int_0^{+\infty} |\psi'_{n_k}|^2 dx + \int_0^{R_k} V \psi_{n_k}^2 dx + \int_{R_k}^{+\infty} V \psi_{n_k}^2 dx \\ &\geq \int_0^{+\infty} |\psi'_{n_k}|^2 dx - \|V\|_\infty \cdot \varepsilon + (V^\infty - \varepsilon) \int_{R_k}^{+\infty} \psi_{n_k}^2 dx. \end{aligned}$$

This implies that there exists $\delta(\varepsilon)$, tending to zero when $\varepsilon \rightarrow 0$, such that

$$J_V(\psi_{n_k}) \geq J_\infty(\psi_{n_k}) - \delta(\varepsilon) \geq I_1^\infty - \delta(\varepsilon).$$

Now let k go to $+\infty$ and ε to zero. Then we obtain

$$I_1 \geq I_1^\infty,$$

which contradicts the strict subadditivity inequality (65).

Now we assume that $(\rho_{n_k})_k$ verifies the dichotomy case; i.e., there exists $\alpha \in]0, 1[$ such that for all $\varepsilon > 0$ there exist $k_0 \geq 1$, ψ_k^1, ψ_k^2 bounded in $H^1(\mathbb{R}^+)$ satisfying for $k \geq k_0$

$$\left\{ \begin{array}{l} \|\psi_{n_k} - (\psi_k^1 + \psi_k^2)\|_{L^2} \xrightarrow{\varepsilon \rightarrow 0} 0, \\ \left| \int_0^{+\infty} |\psi_k^1(x)|^2 dx - \alpha \right| \leq \varepsilon, \quad \left| \int_0^{+\infty} |\psi_k^2(x)|^2 dx - (1 - \alpha) \right| \leq \varepsilon, \\ \text{dist}(\text{supp}(\psi_k^1), \text{supp}(\psi_k^2)) \xrightarrow{k \rightarrow +\infty} +\infty, \\ \liminf_k \int_{\mathbb{R}^+} \underbrace{\{|\nabla \psi_{n_k}|^2 - |\nabla \psi_k^1|^2 - |\nabla \psi_k^2|^2\}}_{\gamma_k} dx \geq 0. \end{array} \right.$$

One can write (see [17])

$$\psi_{n_k} = \psi_k^1 + \psi_k^2 + \varphi_k, \quad \text{where} \quad \psi_k^1 \psi_k^2 = \psi_k^1 \varphi_k = \psi_k^2 \varphi_k = 0 \quad \text{a.e.,}$$

and without loss of generality, we suppose that $\text{supp}(\psi_k^2) \subset [R_k, +\infty[$, where R_k tends to $+\infty$ with k . This implies that

$$\begin{aligned} \int_0^{+\infty} V \psi_{n_k}^2 &= \int_0^{+\infty} V |\psi_k^1|^2 + \int_0^{+\infty} V |\psi_k^2|^2 + \int_0^{+\infty} V |\varphi_k|^2 \\ &\geq \int_0^{+\infty} V |\psi_k^1|^2 + (V^\infty - \varepsilon) \int_0^{+\infty} |\psi_k^2|^2 - \|V\|_\infty \cdot \delta(\varepsilon) \end{aligned}$$

and

$$\int_0^{+\infty} |\psi'_{n_k}|^2 + \int_0^{+\infty} V \psi_{n_k}^2 \geq \int_0^{+\infty} |\psi'_{n_k}|^2 + \int_0^{+\infty} V |\psi_k^1|^2 + V^\infty \int_0^{+\infty} |\psi_k^2|^2 - \delta(\varepsilon).$$

Hence,

$$J_V(\psi_{n_k}) \geq \gamma_k + J_V(\psi_k^1) + J_\infty(\psi_k^2) - \delta(\varepsilon). \quad (66)$$

Besides, let $\alpha_k = \int_0^{+\infty} |\psi_k^1(x)|^2 dx$, $\beta_k = \int_0^{+\infty} |\psi_k^2(x)|^2 dx$. For all fixed $\varepsilon > 0$, the sequences $(\alpha_k)_k$ and $(\beta_k)_k$ are bounded in \mathbb{R}^+ . There are subsequences, still denoted by $(\alpha_k)_k$ and $(\beta_k)_k$, which converge in \mathbb{R}^+ to α_ε and β_ε , respectively, where α_ε and β_ε belong to \mathbb{R}^+ such that

$$|\alpha_\varepsilon - \alpha| \leq \varepsilon \quad \text{and} \quad |\beta_\varepsilon - (1 - \alpha)| \leq \varepsilon. \quad (67)$$

Inequality (66) yields

$$J_V(\psi_{n_k}) \geq \gamma_k + I_{\alpha_k} + I_{\beta_k}^\infty - \delta(\varepsilon).$$

Taking the \liminf_k of the last inequality and letting ε tend to zero, we obtain in view of (67) and the fact that $\liminf_k \gamma_k \geq 0$

$$I_1 \geq I_\alpha + I_{1-\alpha}^\infty,$$

which contradicts the strict subadditivity inequality (65).

Consequently, the sequence $(\rho_{n_k})_k$ verifies the compactness case of the concentration-compactness lemma which yields straightforwardly that the minimizing sequence $(\psi_n)_n$ is relatively compact in $L^2(\mathbb{R}^+)$.

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