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Adiabatic approximation of the Schrödinger–Poisson system with a partial confinement: The stationary case

Olivier Pinaud[a)]
MIP, Laboratoire CNRS (UMR 5640), Université Paul Sabatier, 31062 Toulouse Cedex 04, France

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Asymptotic quantum transport models of a two-dimensional gas are presented. The models are the stationary versions of those introduced in a previous paper by Ben Abdallah, Méhats, Pinaud. The starting point is a singular perturbation of the three-dimensional stationary Schrödinger–Poisson system posed on bounded domain. The electron injection in the device is modeled thanks to open boundary conditions. Under a small density assumption, the asymptotics lead to a full two-dimensional first-order approximation of the initial model. An intermediate model, called the "2.5D adiabatic model" in Ben Abdallah, Méhats, Pinaud is then introduced. It shares the same structure as the limit but is shown to be a second-order approximation of the three-dimensional model. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1688432]

I. INTRODUCTION

The paper presents the stationary versions of the models previously analyzed in Ref. 11. These models, first introduced in Refs. 32 and 33 in a formal approach, were originally implemented in a stationary framework and with open boundary conditions. The objective of the paper is, as for Ref. 11, to prove rigorously the asymptotics derived in Refs. 32 and 33. Before going into the details, we recall the motivations of the introduction of open boundary conditions and confined systems.

In nanoscale semiconductor, the electronic transport can be described in various ways. Very often, like in resonant tunneling diodes,[15,22,29,31] the electrons are injected, through a wave guide or quantum wire, into an active device where all the important physical effects take place. Consequently, due to the ultrashort scale, a quantum description is needed into the device while in the leads, two situations are possible: the transport can be considered either as classical or as quantum. Then, the different descriptions have to be connected at the interface lead-active region. A quantum–quantum case was first treated in Ref. 26 thanks to the introduction of suitable boundary conditions and was analyzed in Ref. 6 while a classical–quantum one was studied in Ref. 5. Some other examples of such coupling can be found in Refs. 7, 8, 12, and 18.

Besides, the operation of many quantum devices relies on the formation of a bidimensional electron gas. Such a system is obtained by confining the electrons in one direction and allowing for transport in the two other directions, the confining appearing at some junctions between different layers. The reduced extension of the electron gas results, at low temperature, in an increase of the mobility and therefore to a ballistic transport.[2,25,30] Again, at this level, several strategies can be used: the transport along the nonconfined directions can be considered either as classical or as quantum. The classical–quantum description give rises to the theory of sub-bands which is widely used in the semiconductor physics literature.[2,3,17,38] Such a model has been rigourously derived in Ref. 9 and analyzed in Ref. 10.

The situation described in the paper is a fully quantum model: a heterostructure coupled to electrons reservoirs through wave guides is considered. The electrons behavior is assumed to be

[a)]Electronic mail: pinaud@mip.ups-tlse.fr

quantum both in the device and in the leads and the electrons gas is assumed to be confined in a particular direction. The initial model is a three-dimensional Schrödinger–Poisson system, where the electrons are described by a mixed state,

$$-\Delta\Psi_\lambda^\varepsilon+\frac{1}{\varepsilon^2}V_c\left(\frac{z}{\varepsilon}\right)\Psi_\lambda^\varepsilon+V^\varepsilon\Psi_\lambda^\varepsilon=E^\varepsilon\Psi_\lambda^\varepsilon, \tag{1.1}$$

$$-\Delta V^\varepsilon=n^\varepsilon, \tag{1.2}$$

$$n^\varepsilon=\int_\Lambda|\Psi_\lambda^\varepsilon|^2\,d\mu(\lambda)+\text{boundary conditions}, \tag{1.3}$$

where μ represents the statistics of the injected electrons and λ is a set of quantum numbers with values in Λ, and ε can be seen as the ratio between the kinetic and the confining energies of the electrons, see Ref. 11 for more details on the scaling. The external potential $(1/\varepsilon^2)\,V_c(z/\varepsilon)$ is a confining potential and the potential V^ε is the self-consistent potential due to space charge effects and is expected to be slowly varying in the z direction. Due to the strong confinement, the wave functions concentrate around the plane $\{z=0\}$ and the transport effects are almost two dimensional. In Ref. 11, in a time-dependent and whole space picture, the limit $\varepsilon\to 0$ was performed. The electronic density $n^\varepsilon(t,x,z)$ concentrates into a surface density $n_s(t,x)\,\delta(z)$ and the limit model was called *2D surface density model*. This model involves bidimensional Schrödinger equations, coupled to a bidimensional equation for the potential. An intermediate model, called the *2.5D adiabatic model*, first introduced in Refs. 32 and 33, was also derived and was shown to be a second order approximation of the initial model. This model couples 2D Schrödinger equations and a 3D equation for the potential. It has been shown numerically in Refs. 32 and 33, that the 2.5D model gives results in a very good agreement with those of the 3D model with a much lower computational cost. In this paper, we will develop a similar strategy to justify the asymptotics in the stationary framework. The differences in the analysis come from the boundedness of the transport domain and the stationary character of the problem. This requires to derive new estimates for the Poisson equation and to take particular care of the existence and uniqueness theory of the nonlinear stationary problem. More precisely, the results are proven under three main hypothesis: the first one states that the electrons are injected into the device on the ground state and is necessary in order to obtain ε-independent estimates. The two others hypothesis are directly related to uniqueness result concerning the solutions of the open Schrödinger–Poisson system stated in Ref. 6. In order to have uniqueness, one requires a weak coupling between the Schrödinger and the Poisson equations and also requires a statistics of injection avoiding the bound states of the device.

Within the time-dependent picture, quantum confining on very general surfaces have been previously investigated in Refs. 16, 23, and 28 for the linear Schrödinger equation. As pointed out in Ref. 37, the quantum constrained system can be related to the Born–Oppenheimer theory for molecular dynamics.[24,35] Even if these theories are mainly developed in a time-dependent and linear framework, they share similar properties with the problem presented in this paper. In the different cases, the electron dynamics is located on the eigenspaces of the confining (or transverse) Hamiltonian and is governed by an effective potential. In the present work, the main difficulty stems from the nonlinearity due to the Coulombian interaction.

The paper is organized as follows: in Sec. II we introduce the spectral elements of the confining operator, which enable to define the 2.5D adiabatic model; then we present in details the different models where special care is given to boundary conditions; the main results of the paper are presented in Sec. III; in Sec. IV we obtain some ε-independent estimates for (1.1)–(1.3) and we give existence and uniqueness results for the approximate models; in Sec. V, we prove that the 2.5D model is a second order approximation while in Sec. VI, the 2D model is proven to be only a first order approximation; Sec. VII is devoted to some extensions and comments; finally, an appendix contains some basic results on the Schrödinger equation and some regularity estimates for the Poisson equation which are used all along the paper.

II. NOTATIONS AND PRESENTATION OF THE MODELS

In the paper, Ω_0 denotes a regular domain of dimension 2. First, we define the following functional space.

Definition 2.1: Let $1 \leqslant p,\ q \leqslant +\infty$. *Then*

$$L_x^q L_z^p = \left\{ u \in L^1(\Omega_0 \times \mathbb{R}), \quad \|u\|_{L^{q,p}} = \left(\int_{\Omega_0} \|u(x,\cdot)\|_{L^p(\mathbb{R})}^q \, \mathrm{d}x \right)^{1/q} < +\infty \right\}$$

(*with an obvious generalization of this definition for* $q=+\infty$). In the sequel, $L^p(\Omega_0 \times \mathbb{R})$ will be more simply denoted L^p.

For a function $f=f(z)$ belonging to $L^1(\mathbb{R})$ we denote $\langle f \rangle = \int_{\mathbb{R}} f(z) \mathrm{d}z$. In particular, if $n(x,z)$ is the particle density, the surface density is defined by $n_s(x) = \langle n(x,\cdot) \rangle$.

A. Spectrum of the confinement operator

We introduce the properties of the confining potential V_c. We assume that it satisfies the

Assumption 2.2: The rescaled confining potential $V_c = V_c(z)$ *is a non-negative real-valued function in* $L^2_{loc}(\mathbb{R})$ *such that*

$$\lim_{|z| \to +\infty} V_c(z) = +\infty.$$

Under this assumption, the operator $A = -\frac{1}{2}(d^2/dz^2) + V_c$ defined on $X = L^2(\mathbb{R})$ with the domain

$$\mathcal{D}(A) = \{ u \in H^2(\mathbb{R}) \text{ such that } V_c\, u \in L^2(\mathbb{R}) \}$$

is self-adjoint, non-negative, and has a compact resolvent (see, e.g., Ref. 34). Hence, its spectrum is purely discrete and consists in a strictly increasing sequence of non-negative real numbers tending to infinity $(E_p)_{p \in \mathbb{N}^*}$. Moreover, the associated eigenfunctions $(\chi_p)_{p \in \mathbb{N}^*}$, chosen real-valued, form an orthonormal basis of $L^2(\mathbb{R})$ and verify

$$\forall a > 0, \quad \forall p \in \mathbb{N}^*, \quad \exists C_{a,p} > 0, \quad \text{such that}, \quad \forall z \in \mathbb{R}, \quad |\chi_p(z)| \leqslant C_{a,p}\, e^{-a|z|}. \tag{2.1}$$

The partial Hamiltonian involved in (1.1) is obtained by rescaling A:

$$A^\varepsilon = -\frac{1}{2} \frac{d^2}{dz^2} + V_c^\varepsilon = -\frac{1}{2} \frac{d^2}{dz^2} + \frac{1}{\varepsilon^2} V_c\left(\frac{z}{\varepsilon} \right).$$

This operator A^ε on $X = L^2(\mathbb{R})$ has the domain

$$\mathcal{D}(A^\varepsilon) = \{ u \in H^2(\mathbb{R}) \text{ such that } V_c^\varepsilon\, u \in L^2(\mathbb{R}) \}.$$

Its eigenfunctions $(\chi_p^\varepsilon)_{p \in \mathbb{N}^*}$ and eigenvalues $(E_p^\varepsilon)_{p \in \mathbb{N}^*}$ can be deduced by a simple rescaling from those of A:

$$\chi_p^\varepsilon(z) = \frac{1}{\sqrt{\varepsilon}} \chi_p\left(\frac{z}{\varepsilon} \right), \quad E_p^\varepsilon = \frac{E_p}{\varepsilon^2}.$$

We shall denote by Π_p^ε the orthogonal projector on $span(\chi_p^\varepsilon)$. The space $L^2(\mathbb{R}^2, span(\chi_p^\varepsilon))$ will be called the pth subband. With an abuse of notation, we shall also denote by Π_p^ε the orthogonal projector $\mathbb{I} \otimes \Pi_p^\varepsilon$ of $L^2(\mathbb{R}^3)$ on $L^2(\mathbb{R}^2, span(\chi_p^\varepsilon))$.

The following technical lemma, proved in Ref. 11, will be used several times in this paper.

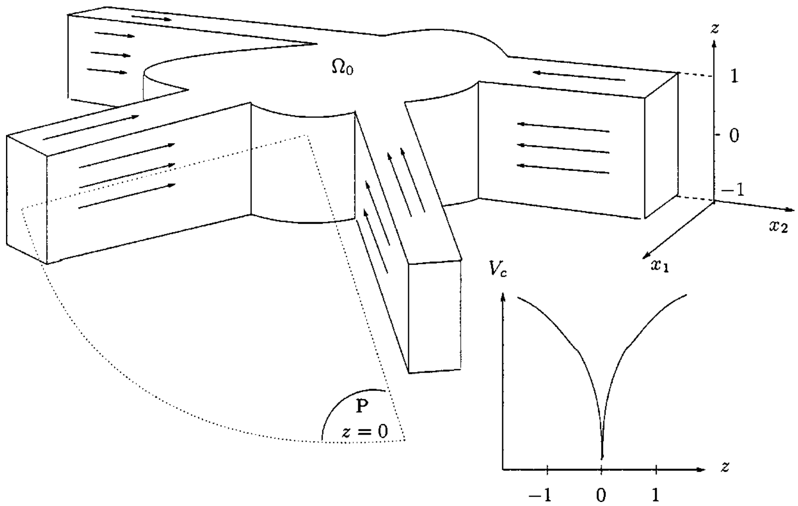

FIG. 1. The device projected in $\{z\in[-1,1]\}$.

Lemma 2.3: Let $V^\varepsilon\in W^{1,\alpha}(\mathbb{R})$ with $\alpha\in[1,+\infty]$. Then for any $p\in\mathbb{N}^*$ we have

$$\|[\Pi_p^\varepsilon,V^\varepsilon]\|_{\mathcal{L}(L^2(\mathbb{R}))}\leqslant C_p\,\varepsilon^{1-1/\alpha}\,\|\partial_z V^\varepsilon\|_{L^\alpha(\mathbb{R})},$$

where $[\cdot,\cdot]$ denotes the commutator of operators and C_p only depends on p.

Notice that this type of commutator estimates was already used in the semiclassical analysis of electrons motion in periodic crystals. In that case, the projector is the projector on the energy bands related to the Bloch decomposition, see Refs. 27 and 4.

B. Definition of the models

For the sake of completeness, the open boundary conditions introduced in Ref. 26 are derived step by step in Appendix A. We set now the geometry of the device.

The device domain consists in an active region, denoted by $\Omega_0\times\mathbb{R}$ connected to semi-infinite electrons reservoirs by n leads $\Omega_j\times\mathbb{R}$, $j=1,\ldots,n$, see Fig. 1 for a schematic drawing of the device in $\Omega_0\times[-1,1]$ and Fig. 2. The full domain of the device is $\Omega\times\mathbb{R}$, where $\Omega=\cup_{j=0}^n\Omega_j$. The boundary of Ω_0 is split into a part Γ_0 and n parts Γ_j, $j=1,\ldots,n$. We denote by ω_0 the boundary $(\Gamma_0\times\mathbb{R})\cup(\Omega_0\times\{z=\pm\infty\})$. The transport directions are denoted by $x:=(x_1,x_2)$ and the confined direction by z. The local coordinates of the lead j, $j\neq 0$ are denoted by η_j and ξ_j, see Fig. 2. The confining potential insures that the electrons stay around the plane $P=\{x\in\Omega,z=0\}$, see Figs. 1 and 2.

1. The 3D model

The 3D model is obtained by coupling the Poisson equation to a set of Schrödinger equations to be solved on the domain $\Omega_0\times\mathbb{R}$ with open boundary conditions. A single electron injected with an energy E^ε is represented by a wave function Ψ^ε solution of the Schrödinger equation

$$-\Delta\Psi^\varepsilon(x,z)+(V_c^\varepsilon(z)+V^\varepsilon(x,z))\Psi^\varepsilon(x,z)=E^\varepsilon\,\Psi^\varepsilon(x,z)\quad\text{in }\Omega_0\times\mathbb{R},\tag{2.2}$$

where V_c^ε is a confining potential and V^ε is, up to now, a given potential supported only in $\Omega_0\times\mathbb{R}$. Ψ^ε satisfies the nonhomogeneous open boundary conditions derived in Appendix A:

$$\left.\frac{\partial\Psi^\varepsilon}{\partial\eta_j}\right|_{\Gamma_j}=\mathbb{Z}_j^{3\mathrm{D}}[E^\varepsilon](\Psi^\varepsilon)+\mathbb{S}_j^{3\mathrm{D}}[E^\varepsilon],\tag{2.3}$$

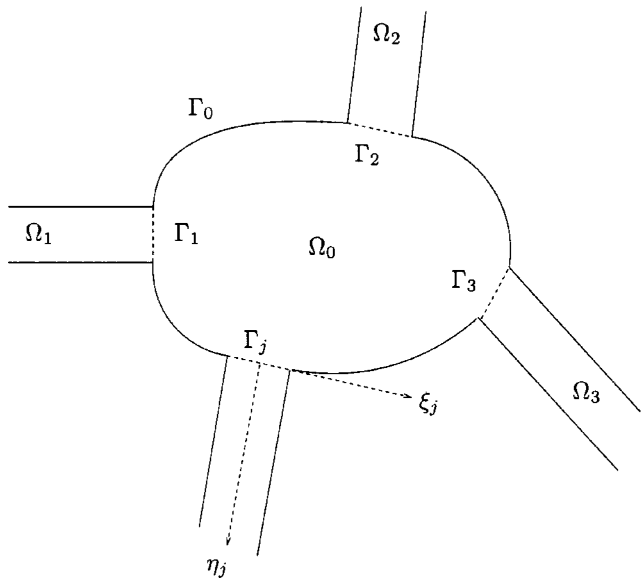

FIG. 2. The plane P.

$$\Psi^{\varepsilon}=0 \quad \text{on} \quad \omega_0. \tag{2.4}$$

The electrons populate the different sub-bands starting from the first sub-band. In Ref. 11, a model close to the one presented is analyzed in the time-dependent picture. Therein, the ε-independent estimates are obtained using crucially the Stricharz estimates introduced by Castella in Ref. 14 in order to solve the Schrödinger–Poisson system in L^2. This theory does not use H^1 energy estimates. Obviously, within the stationary framework, the Stricharz estimates are not available and one needs H^1 theory to obtain energy estimates. In the time-dependent picture, when the initial condition has a nonzero component on a sub-band with index $p \geqslant 2$, ε-independent *a priori* bounds in H^1 are only derived on a small time interval while the time interval can be made arbitrarily large for wave functions supported only on the first sub-band. Therefore, there is a little hope to obtain estimates for the stationary problem if the electrons populate the upper sub-bands. Consequently, we will only focus on the electrons injected on this first sub-band by assuming the following hypothesis.

Assumption 2.4: Let Θ_m^j and $\mathcal{E}_m^j$ be the eigenfunctions and eigenvalues of the jth transversal Schrödinger operator $-\partial_{\xi_j}^2$ with Dirichlet boundary conditions. Then, we suppose that the electrons are injected in the lead j_0, on the first sub-band, on the transversal mode m_0 and with a longitudinal kinetic energy k^2. This implies that $\mathbb{S}_j^{3D} = -2\,\delta_j^{j_0}\, ik\, \Theta_{m_0}^j \chi_1^{\varepsilon}$ and $E^{\varepsilon} = E_1^{\varepsilon} + \mathcal{E}_{m_0}^{j_0} + k^2$.

The wave functions Ψ^{ε} are thus parametrized by $\lambda = (m_0, j_0, k)$, $\Psi^{\varepsilon} := \Psi_{\lambda}^{\varepsilon}$ (the dependence on the parameter 1 of first sub-band is omitted). Notice that the assumption is compatible with some physical situations called electrical quantum limit, see for instance the numerical simulations in Refs. 32 and 33, where only the first sub-band is populated. This hypothesis is often verified in structures like T-stubs, quantum couplers, or various types of transistors. Indeed, in two-dimensional electron gases, the electron occupancy in the second sub-band is usually a small fraction (typically less than 10%) of the total electron density, see Refs. 36 and 20. Nervertheless, in parabolic quantum well structures, the electrons population in the sub-bands can be carefully controlled and the densities in two lowest sub-band can be similar to within 30%, see Refs. 19 and 21.

Assumption 2.4 thus implies that the boundary condition (2.3) reads

$$\left.\frac{\partial \Psi_\lambda^\varepsilon}{\partial \eta_j}\right|_{\Gamma_j} = \mathbb{Z}_j^{3\mathrm{D}}[E_1^\varepsilon + E_\lambda](\Psi_\lambda^\varepsilon) - 2\,\delta_j^{j_0}\, ik\,\Theta_{m_0}^j\,\chi_1^\varepsilon. \tag{2.5}$$

In order to take into account self-consistent effects, the electrons are supposed to be injected in the state λ by a source in the leads and the electronic density is assumed to be in a mixed state. It reads

$$n^\varepsilon(x,z) = \int_\Lambda |\Psi_\lambda^\varepsilon(x,z)|^2\,\mathrm{d}\mu(\lambda) = \sum_{j_0=1}^{n}\sum_{m_0=1}^{\infty}\int_{\mathbb{R}_+^\star}\Phi(j_0,m_0,k)|\Psi_{j_0,m_0,k}^\varepsilon(x,z)|^2\,\mathrm{d}k, \tag{2.6}$$

where $\Phi(j_0,m_0,k)$ is the statistics of injection and Λ is the set

$$\Lambda = [0,\ldots,n]\times\mathbb{N}^\star\times\mathbb{R}_+^\star.$$

The electrons being charged particles, they generate a self-consistent potential V^ε through the Poisson equation. It is assumed that the nonlinear interaction takes place only in the active region, the domain $\Omega_0\times\mathbb{R}$. Hence, V^ε solves

$$-\Delta V^\varepsilon = n^\varepsilon \quad \text{on} \quad \Omega_0\times\mathbb{R}, \tag{2.7}$$

$$V^\varepsilon = 0 \quad \text{on} \quad \partial\Omega_0\times\mathbb{R}, \tag{2.8}$$

$$V^\varepsilon \to 0 \quad \text{as} \quad |z|\to\infty. \tag{2.9}$$

The fact that the electrons are injected on the first sub-band does not imply that the wave function Ψ_λ^ε has only a contribution on this sub-band. Indeed, the different sub-bands are coupled through the z-dependence of V^ε. Nevertheless, it will be shown that the upper sub-bands are weakly populated since the potential V^ε is slowly varying with respect to the variable z. The 3D model finally read as follows.

The 3D model:

$$\begin{gathered}
-\Delta\Psi_\lambda^\varepsilon(x,z) + (V_c^\varepsilon(z) + V^\varepsilon(x,z))\Psi_\lambda^\varepsilon(x,z) = (E_1^\varepsilon + E_\lambda)\,\Psi_\lambda^\varepsilon(x,z) \quad \text{in} \quad \Omega_0\times\mathbb{R},\\
\Psi_\lambda^\varepsilon = 0 \quad \text{on} \quad \omega_0;\ \ \Psi_\lambda^\varepsilon \ \ \text{satisfies} \ \ (2.5) \quad \text{on} \quad \Gamma_j\times\mathbb{R}, \quad j\neq 0,\\
-\Delta V^\varepsilon = n^\varepsilon \quad \text{on} \quad \Omega_0\times\mathbb{R}, \quad n^\varepsilon(x,z) = \int_\Lambda |\Psi_\lambda^\varepsilon(x,z)|^2\,\mathrm{d}\mu(\lambda),\\
V^\varepsilon = 0 \quad \text{on} \quad \partial\Omega_0\times\mathbb{R};\ \ V^\varepsilon\to 0 \quad \text{as} \quad |z|\to\infty.
\end{gathered} \tag{2.10}$$

Existence and uniqueness: The model presented in Ref. 6 is slighty different from the 3D model but the results can be easily adapted. It is proven in Ref. 6 that, for a general μ satisfying an assumption of boundedness of the support, the 3D model admits a weak solution Ψ_λ^ε in $H^1(\Omega_0\times\mathbb{R})$. More precisely, the obtained density reads

$$n^\varepsilon = \int_\Lambda |\Psi_\lambda^\varepsilon|^2\,\mathrm{d}\mu(\lambda) + \quad \text{sum of bound states.}$$

This last statement means that the electrons having adequate energies are trapped into the active region. In other words, the bound states of the device can be excited by the injected beam of electrons (see Ref. 6 for more details). This implies, conjugated with the nonlinear character of the problem, the nonuniqueness of the solutions. Morever, the wave function satisfies estimates of the type

$$\|\Psi_\lambda^\varepsilon\|_{L^2} \leqslant \frac{C}{|\mathcal{E}^\varepsilon - E_\lambda|}, \tag{2.11}$$

where $\mathcal{E}^\varepsilon$ denotes an energy of the bound states. This leads to a nonintegrable singularity in the computation of the density. To derive the asymptotic models, the nonuniqueness property is not fundamental but in order to obtain error estimates, we need to recover uniqueness. This can be done thanks to the uniqueness result of Ref. 6: if the bound states are avoided by the statistics μ and if the nonlinearity is supposed to be weak enough the solutions are unique. Moreover, the fact that the bound states are avoided implies also, thanks to (2.11), some uniform bounds with respect to λ. This leads to the following definition.

Definition 2.5: Assume that V^ε is a given regular potential. Consider the operator $-\Delta + V_c^\varepsilon + V^\varepsilon - E_1^\varepsilon$ equipped with Dirichlet boundary conditions on ω_0 and with the homogeneous transparent boundary conditions (2.3) on $\Gamma_j \times \mathbb{R}$, $j=1,..,n$ with $\mathbb{S}_j^{3D}[E_1^\varepsilon + E_\lambda] := 0$. According to Ref. 6, this operator has a purely discrete spectrum and we will call "energies of the bound states" its eigenvalues $(\mathcal{E}_i^\varepsilon(V^\varepsilon))_{i \geqslant 1}$.

In order to simplify the analysis and to avoid additional technicalities, we set in the simplest way to make the electrons avoid the bound states, see Ref. 6. The requirement is given by the following

Assumption 2.6: The measure μ has a bounded support such that, for $\lambda \in supp\ \mu$, there exists $C > 0$, ε-independent such that

$$C \leqslant \mathcal{E}_1^\varepsilon(0) - E_\lambda .$$

This implies that the electrons avoid all the bound states. Indeed, by the maximum principle, V^ε is positive and then $\mathcal{E}_1^\varepsilon(0) \leqslant \mathcal{E}_1^\varepsilon(V^\varepsilon)$. Notice that above, this choice of μ is ε-independent since $\mathcal{E}_1^\varepsilon(0)$ is also ε-independent. This assumption is rather stringent in the general case and some ways to waive this restriction are proposed in Sec. VII. Nevertheless, in the case of confined devices at low temperatures, this hypothesis may nearly be verified. Indeed, in these structures, the typical statistics of injection is a Fermi–Dirac statistics. It reads

$$\Phi(E^\varepsilon) = \frac{1}{1 + \exp\left(\dfrac{E_F^\varepsilon - E^\varepsilon}{k_B T}\right)},$$

where k_B is the Boltzmann constant, T the temperature, and E_F^ε the rescaled Fermi level. In practical,

$$E_F^\varepsilon = E_1^\varepsilon + \mathcal{O}(1),$$

and the Fermi–Dirac reads

$$\Phi(E^\varepsilon) = \frac{1}{1 + \exp\left(\dfrac{E_\lambda + \mathcal{O}(1)}{k_B T}\right)},$$

which exhibits an exponential decay at low temperatures and also at high energies.

The theorem of Ref. 6 reads, for given ε, after a slight adaptation.

Theorem 2.7: *(Ref. 6) There exists $\delta(\varepsilon)$ positive, such that for every μ satisfying assumption 2.6 and*

$$\mu(\Lambda) < \delta(\varepsilon)$$

the 3D model admits a unique solution.

We shall see in the sequel that $\delta(\varepsilon)$ can be chosen ε-independent.

2. The 2D surface density model

The 2D surfacic density model is the coupling between many 2D Schrödinger equations and a 2D potential. When ε goes to zero, $|\chi_p^\varepsilon|^2$ concentrates around 0 and becomes then a Dirac measure. This leads to the definition of the limit model by replacing the self-consistent potential by its trace on the plane $\{x\in\Omega_0, z=0\}$ and by replacing the 3D density by a 2D density multiplied by a Delta measure. The boundary condition (2.5) becomes

$$\left.\frac{\partial\psi_\lambda}{\partial\eta_j}\right|_{\Gamma_j}=\mathbb{Z}_j^{2\mathrm{D}}[E_\lambda](\psi_\lambda)-2\,\delta_j^{j_0}\,ik\,\Theta_{m_0}^j, \tag{2.12}$$

where

$$\mathbb{Z}_j^{2\mathrm{D}}[E_\lambda](\psi_\lambda)=\sum_{m=1}^{N^j(E_\lambda)} ik_m^j(E_\lambda)\psi_{m,j}(0)\Theta_m^j(\xi_j)-\sum_{m=N^j(E_\lambda)+1}^{\infty} k_m^j(E_\lambda)\,\psi_{m,j}(0)\,\Theta_m^j(\xi_j).$$

The 2D surface density model then reads

$$\begin{gathered}-\Delta_x\psi_\lambda(x)+V(x,0)\psi_\lambda(x)=E_\lambda\,\psi_\lambda \quad \text{in } \Omega_0,\\ \psi_\lambda=0 \quad \text{on } \Gamma_0;\ \psi_\lambda \text{ satisfies (2.12) on } \Gamma_j, \quad j\neq 0,\\ -\Delta V(x,z)=n_s(x)\,\delta(z) \quad \text{on } \Omega_0\times\mathbb{R}, \quad n_s=\int_\Lambda|\psi_\lambda|^2\,\mathrm{d}\mu(\lambda),\\ V=0 \quad \text{on } \partial\Omega_0\times\mathbb{R};\ \lim_{|z|\to\infty}V=0 \quad \text{a.e. on } \Omega_0.\end{gathered} \tag{2.13}$$

Definition 2.8: Assume that V is a given regular potential. Consider the operator $-\Delta_x+V(\cdot,0)$ *equipped with Dirichlet boundary conditions on* Γ_0 *and with the homogeneous transparent boundary conditions (2.12) on* Γ_j, $j=1,..,n$ *without source term. According to Ref. 6, this operator has a purely discrete spectrum and we will call "energies of the 2D bound states" its eigenvalues* $(\mathcal{E}_i(V(\cdot,0)))_{i\geq 1}$.

3. The 2.5D model

The 2.5D adiabatic model is an intermediate model between the fully 3D model and the 2D surfacic density one. It takes into account the small thickness of the electron gas and consists in coupling a set of two-dimensional Schrödinger equations and the three-dimensional Poisson equation:

$$\begin{gathered}-\Delta_x\psi_\lambda^\varepsilon+\langle V^\varepsilon|\chi_1^\varepsilon|^2\rangle\,\psi_\lambda^\varepsilon(x)=E_\lambda\,\psi_\lambda^\varepsilon \quad \text{in } \Omega_0,\\ \psi_\lambda^\varepsilon=0 \quad \text{on } \Gamma_0;\ \psi_\lambda^\varepsilon \text{ satisfies (2.12) on } \Gamma_j, \quad j\neq 0,\\ -\Delta V^\varepsilon=n^\varepsilon|\chi_1^\varepsilon|^2 \quad \text{on } \Omega_0\times\mathbb{R}, \quad n^\varepsilon=\int_\Lambda|\psi_\lambda^\varepsilon|^2\,\mathrm{d}\mu(\lambda),\\ V^\varepsilon=0 \quad \text{on } \partial\Omega_0\times\mathbb{R};\ \lim_{|z|\to\infty}V^\varepsilon=0 \quad \text{a.e. on } \Omega_0.\end{gathered} \tag{2.14}$$

Remark 2.9: According to Definition 2.8, the energies of the bound states of the 2.5D model are naturaly denoted by $(\mathcal{E}_i(\langle V^\varepsilon|\chi_1^\varepsilon|^2\rangle))_{i\in\mathbb{N}^\star}$. *Morever, if V is a potential independent of the variable* z, *it comes easily that* $\mathcal{E}_i(V)=\mathcal{E}_i^\varepsilon(V)$.

III. MAIN RESULTS

In this paper, we will prove the following theorems.

Theorem 3.1: *Suppose that Assumptions 2.2, 2.4, and 2.6 are satisfied. Then, there exists* η *positive* ε*-independent such that, for every* μ *satisfying Assumption 2.6 and*

$$\mu(\Lambda) < \eta,$$

the 3D model (2.10) and the 2.5D adiabatic model (2.14) admit unique weak solutions, respectively, denoted by $(\Psi_\lambda^{3D}, V^{3D})$ *and by* $(\psi_\lambda^{2.5D}, V^{2.5D})$. *Moreover,* η *can be chosen such that we have the following error estimates, uniformly in* λ, for $\alpha > 0$, *for* $p \in [1,2)$,

$$\|\Psi_\lambda^{3D} - \psi_\lambda^{2.5D}\chi_1^\varepsilon\|_{W^{1,p}(\Omega_0, L^2(\mathbb{R}))} = \mathcal{O}(\varepsilon^{1-\alpha}), \tag{3.1}$$

$$\|V^{3D} - V^{2.5D}\|_{W^{1,p}(\Omega_0, L^\infty(\mathbb{R}))} = \mathcal{O}(\varepsilon^{2-\alpha}). \tag{3.2}$$

Furthermore the surfacic densities defined by $n_s^{3D} = \int_\Lambda \langle |\Psi_\lambda^{3D}|^2 \rangle \, \mathrm{d}\mu(\lambda)$ *and* $n_s^{2.5D} = \int_\Lambda |\psi_\lambda^{2.5D}|^2 \, \mathrm{d}\mu(\lambda)$ *satisfy*

$$\|n_s^{3D} - n_s^{2.5D}\|_{W^{1,p}(\Omega_0)} = \mathcal{O}(\varepsilon^{2-\alpha}) \quad \forall \alpha > 0, \quad \forall p \in [1,2). \tag{3.3}$$

Theorem 3.2: *Suppose that Assumptions 2.2, 2.4, and 2.6 are satisfied. Then, there exists* η *positive* ε*-independent such that, for every* μ *satisfying Assumption 2.6 and*

$$\mu(\Lambda) < \eta,$$

as $\varepsilon \to 0$, *the unique solution* $(\psi_\lambda^{2.5D}, n^{2.5D}, V^{2.5D})$ *of the 2.5D adiabatic model converges to the unique solution* $(\phi^{2D}, n_s^{2D}, V^{2D})$ *of the 2D surfacic density model (2.13) in the following sense: for* $\alpha > 0$, *for* $p \in [1,2)$,

$$\|\psi_\lambda^{2.5D} - \phi^{2D}\|_{W^{1,p}(\Omega_0)} = \mathcal{O}(\varepsilon^{1-\alpha}), \tag{3.4}$$

$$\|V^{2.5D} - V^{2D}\|_{W^{1,p}(\Omega_0, L^\infty(\mathbb{R}))} = \mathcal{O}(\varepsilon^{1-\alpha}), \tag{3.5}$$

$$\|n_s^{2.5D} - n_s^{2D}\|_{W^{1,p}(\Omega_0)} = \mathcal{O}(\varepsilon^{1-\alpha}), \tag{3.6}$$

where $n_s^{2D} = \int_\Lambda |\phi_\lambda^{2D}|^2 \, \mathrm{d}\mu(\lambda)$ *and* $n_s^{2.5D} = \int_\Lambda |\psi_\lambda^{2.5D}|^2 \, d\mu(\lambda)$. *Furthermore, we have the following bound from below:*

$$\|V^{2D} - V^{2.5D}\|_{L^2} + \|n_s^{2D} - n_s^{2.5D}\|_{L^2} \geqslant C\,\varepsilon, \tag{3.7}$$

where C *does not depend on* ε.

A straightforward consequence of these theorems is the following.

Corollary 3.3: Suppose that Assumptions 2.2, 2.4, and 2.6 are satisfied. Then, under the notations of Theorems 3.1 and 3.2, there exists η *positive* ε*-independent such that, for every* μ *satisfying Assumption 2.6 and*

$$\mu(\Lambda) < \eta,$$

the 3D model converges as $\varepsilon \to 0$ *to the 2D model. Furthermore, we have the estimate*

$$C_1\,\varepsilon \leqslant \|V^{2D} - V^{3D}\|_{L^2} + \|n_s^{2D} - n_s^{3D}\|_{L^2} \leqslant C_2\,\varepsilon^{1-\alpha}.$$

IV. ε-INDEPENDENT ESTIMATES AND WELL-POSEDNESS

In this section, we shall obtain some ε-independent estimates for the 3D and the 2.5D models. To this aim, we will use Proposition A.1 for both models. Besides, the well-posedness of the 2D and 2.5D models will also be studied.

Proposition 4.1: Let V^ε and Ψ_λ^ε be the solutions of the 3D model. Then, under assumption 2.2, 2.4, and 2.6 we have the following estimates, uniformly in λ,

$$\|\Psi_\lambda^\varepsilon\|_{H^1(\Omega_0,L^2(\mathbb{R}))}\leq C, \tag{4.1}$$

$$\|(\mathbb{I}-\Pi_1^\varepsilon)\Psi_\lambda^\varepsilon\|_{L^2}\leq C\,\varepsilon, \tag{4.2}$$

$$\|V^\varepsilon\|_{W^{1,p}(\Omega_0,H^s(\mathbb{R}))}\leq C \quad for \quad p\in(1,\infty),\quad s<\tfrac{3}{2},\quad p(1+2s)<8, \tag{4.3}$$

$$\|(\mathbb{I}-\Pi_1^\varepsilon)\Psi_\lambda^\varepsilon\|_{H^1(\Omega_0,L^2(\mathbb{R}))}\leq C\,\varepsilon^{1-\alpha},\quad \alpha>0, \tag{4.4}$$

where C is ε-independent.

Proof: The proof of (4.1) and (4.2) is a direct application of Proposition A.1 Indeed, according to the maximum principle V^ε is positive and according to hypothesis 2.4, Ψ_λ^ε satisfies the boundary condition (A10) with $a=1$. It suffices to apply (A12) and (A13) with $f=0$ to conclude.

The estimate (4.3) will be obtained by using the regularity properties of the Poisson equation given in Appendix B. To this aim, we first remark that $\int_\Lambda|\nabla_x\Psi_\lambda^\varepsilon|^2 d\mu(\lambda)\in L^1$ and $\int_\Lambda|\Psi_\lambda^\varepsilon|^2 d\mu(\lambda)\in L_x^pL_z^1$, for all $p\in[1,\infty)$, thanks to (4.1) and the embedding $H^1(\Omega_0)\hookrightarrow L^p(\Omega_0)$, $p<\infty$. This implies by interpolation, that for $r<2$,

$$\nabla_x n^\varepsilon=2\,\mathrm{Re}\int_\Lambda \overline{\Psi_\lambda^\varepsilon}\,\nabla_x\Psi_\lambda^\varepsilon\, d\mu(\lambda)\in L^{r,1}.$$

It suffices then to apply (B3) to conclude.

To prove (4.4), we form the quantity $w_\lambda^\varepsilon:=(\mathbb{I}-\Pi_1^\varepsilon)\Psi_\lambda^\varepsilon$. It can be easily seen that w_λ^ε solves

$$-\Delta w_\lambda^\varepsilon+(V_c^\varepsilon(z)+V^\varepsilon(x,z))w_\lambda^\varepsilon=(E_1^\varepsilon+E_\lambda)\,w_\lambda^\varepsilon+[\Pi_1^\varepsilon,V^\varepsilon]\Psi_\lambda^\varepsilon \tag{4.5}$$

with boundary conditions (A10) with $a=0$ and (A11). Hence, the estimate (A12) of Appendix A with $f=[\Pi_1^\varepsilon,V^\varepsilon]\Psi_\lambda^\varepsilon$ implies

$$\|w_\lambda^\varepsilon\|_{H^1(\Omega_0,L^2(\mathbb{R}))}\leq C\|[\Pi_1^\varepsilon,V^\varepsilon]\Psi_\lambda^\varepsilon\|_{L^2}\leq C\,\varepsilon^{1-1/p}\|\partial_z V^\varepsilon\|_{L_x^4L_z^p}\|\Psi_\lambda^\varepsilon\|_{L_x^4L_z^2}$$

thanks to Lemma 2.3. We conclude the proof by using (4.1) and by noticing that (4.3) implies that $\partial_z V^\varepsilon$ is bounded in $L_x^4L_z^p$ for any $p<\infty$, thanks to the embedding $H^{1/2-(1/p)}(\mathbb{R})\hookrightarrow L^p(\mathbb{R})$, for $p\in[2,\infty)$, see Ref. 1. □

Proposition 4.2: Let V^ε and ψ_λ^ε be the solutions of the 2.5D model. Then, under Assumptions 2.2, 2.4, and 2.6, we have the following estimates, uniformly in λ,

$$\|\psi_\lambda^\varepsilon\|_{H^1(\Omega_0)}\leq C, \tag{4.6}$$

$$\|V^\varepsilon\|_{W^{1,p}(\Omega_0,H^s(\mathbb{R}))}\leq C \quad for \quad p\in(1,\infty),\quad s<\tfrac{3}{2},\quad p(1+2s)<8, \tag{4.7}$$

where C is ε-independent.

Proof: To prove (4.6) and in order to apply Proposition A.1, we form artificially the function $\Phi_\lambda^\varepsilon(x,z):=\psi_\lambda^\varepsilon(x)\,\chi_1^\varepsilon(z)$ which solves

$$-\Delta\Phi_\lambda^\varepsilon+(V_c^\varepsilon+\langle V^\varepsilon|\chi_1^\varepsilon|^2\rangle)\Phi_\lambda^\varepsilon=(E_1^\varepsilon+E_\lambda)\,\Phi_\lambda^\varepsilon \quad \text{in } \Omega_0\times\mathbb{R}$$

equipped with boundary conditions (A10) with $a=1$ and (A11). (A12) concludes then the proof since V^ε is positive by the maximum principle.

The estimate (4.7) is proven analogously to (4.3) by using (4.6). □

The existence and uniqueness of solution for the 2.5D and the 2D models are direct applications of Theorem 7.2 of Ref. 6. The result is the following.

Theorem 4.3: *Let Assumptions 2.2, 2.4, and 2.6 be verified. Let $\Psi_\lambda^{3D}\in H^1(\Omega_0\times\mathbb{R})$ be a solution of the 3D model. Then, there exists an η positive such that, for every μ satisfying Assumption 2.6 and*

$$\mu(\Lambda)<\eta,$$

the 3D, the 2.5D, and the 2D models admit unique weak solutions. The solutions in $H^1(\Omega_0)$ of the 2.5D and the 2D models are, respectively, denoted by $\psi_\lambda^{2.5D}$ and ϕ_λ^{2D}. Moreover, we have the estimates, uniformly in λ,

$$\|\phi_\lambda^{2D}\|_{H^1(\Omega_0)}\leqslant C, \tag{4.8}$$

$$\|V^{2D}\|_{W^{1,p}(\Omega_0,H^s(\mathbb{R}))}\leqslant C \quad for \;\; p\in(1,\infty), \quad s<\tfrac{3}{2}, \quad p(1+2s)<8. \tag{4.9}$$

Sketch of the proof: The basic tools are the Leray–Schauder fixed point theorem and the regularity properties of the Poisson equation. The positivity of the potentials V^{2D} and $V^{2.5D}$ coupled to Assumption 2.6 imply direct bounds on the densities thanks to (A12) with $f=0$ and $a=1$. It follows, thanks to the Poisson equation, Lemmas B.1 and B.2, some compactness properties of the mapping and then to the existence result. The uniqueness is given by the fact that the fixed point procedures become contractions if the densities are small enough in L^1 norm. To this aim, we notice that, thanks to (4.1), (4.6) for n^{3D} and $n^{2.5D}$, and thanks to (A12) for n^{2D},

$$\|n^{3D}\|_{L^1}\leqslant C\mu(\Lambda),\;\; \|n^{2.5D}\|_{L^1}\leqslant C\mu(\Lambda), \quad \|n^{2D}\|_{L^1}\leqslant C\mu(\Lambda),$$

and then it suffices to choose η small enough such that each of the Leray–Schauder mappings are contractions. Equations (4.8) and (4.9) are direct applications of (A12) and Lemma B.2.

V. THE 2.5D MODEL IS A SECOND ORDER APPROXIMATION

In this section, we end the proof of Theorem 3.1 initiated in the preceding section. The used strategies are the same as Ref. 11. We assume that we are under the hypothesis of Theorem 4.3 which insure that the 3D and 2.5D models admit unique solutions. We denote respectively, by $(\Psi_\lambda^{3D},V^{3D})$ and $(\psi_\lambda^{2D},V^{2D})$, these solutions. We start by proving (3.2) by setting $V^{3D}-V^{2.5D}=V+R_1^\varepsilon+R_2^\varepsilon$ with

$$-\Delta V=|\chi_1^\varepsilon|^2(n_s^{3D}-n^{2.5D}), \quad -\Delta R_1^\varepsilon=r_1^\varepsilon, \quad -\Delta R_2^\varepsilon=r_2^\varepsilon$$

equipped with boundary conditions (B2) and where

$$n_s^{3D}=\int_\Lambda\int_{\mathbb{R}}|\Pi_1^\varepsilon\Psi_\lambda^{3D}|^2\,\mathrm{d}z\,\mathrm{d}\mu(\lambda), \quad r_1^\varepsilon=2\,\mathrm{Re}\int_\Lambda\overline{\Pi_1^\varepsilon\Psi_\lambda^{3D}}\;(\mathbb{I}-\Pi_1^\varepsilon)\Psi_\lambda^{3D}\,\mathrm{d}\mu(\lambda),$$

$$r_2^\varepsilon=\int_\Lambda|(\mathbb{I}-\Pi_1^\varepsilon)\Psi_\lambda^{3D}|^2\,\mathrm{d}\mu(\lambda).$$

Estimating the remainder terms R_1^ε and R_2^ε: Thanks to (4.1) and (4.4), we have directly, for $r<2$ and $\delta>0$,

$$\|r_1^\varepsilon\|_{W^{1,r}(\Omega_0,L^1(\mathbb{R}))}\leqslant C\,\varepsilon^{1-\delta},$$

$$\|r_2^\varepsilon\|_{W^{1,r}(\Omega_0,L^1(\mathbb{R}))}\leqslant C\,\varepsilon^{2-\delta},$$

$$\|z\,r_1^\varepsilon\|_{W^{1,r}(\Omega_0,L^1(\mathbb{R}))}\leqslant\|z\chi_1^\varepsilon\|_{L^2(\mathbb{R})}\,\varepsilon^{1-\alpha}\leqslant C\,\varepsilon^{2-\alpha}.$$

This implies that R_2^ε is almost of order two while R_1^ε is, up to now, almost of order one. To get one order more for R_1^ε, we will use (B5) of Appendix B. To this aim, we remark by orthogonality of $\Pi_1^\varepsilon\Psi_\lambda^{3D}$ and $(\mathbb{I}-\Pi_1^\varepsilon)\Psi_\lambda^{3D}$ that

$$\int_{\mathbb{R}} r_1^\varepsilon(x,z)\,\mathrm{d}z=0.$$

Thereby, (B5) applies. Choosing $s=\frac{1}{2}+\alpha$, $\beta=1-2\alpha$ with α positive and close to 0, we obtain, for all δ positive and $p<2$,

$$\|R_1^\varepsilon\|_{W^{1,p}(\Omega_0,H^{1/2+\alpha}(\mathbb{R}))}\leqslant C\,\varepsilon^{2-\delta},$$

$$\|R_2^\varepsilon\|_{W^{1,p}(\Omega_0,H^{1/2+\alpha}(\mathbb{R}))}\leqslant C\,\varepsilon^{2-\delta}$$

which leads to bounds in $W^{1,p}(\Omega_0,L^\infty(\mathbb{R}))$ thanks to the embedding $H^{1/2+\alpha}(\mathbb{R})\hookrightarrow L^\infty(\mathbb{R})$ for all α positive.

It remains now to treat V. In order to estimate $|\chi_1^\varepsilon|^2(n_s^{3D}-n^{2.5D})$, we use the Schrödinger equation solved by $w_\lambda^\varepsilon:=\Pi_1^\varepsilon\Psi_\lambda^{3D}-\chi_1^\varepsilon\,\psi_\lambda^{2.5D}$:

$$-\Delta w_\lambda^\varepsilon+V_c^\varepsilon w_\lambda^\varepsilon+\langle V^{3D}|\chi_1^\varepsilon|^2\rangle\,w_\lambda^\varepsilon=(E_1^\varepsilon+E_\lambda)w_\lambda^\varepsilon+f^\varepsilon+g^\varepsilon$$

equipped with the transparent homogeneous boundary conditions (A10) with $a=0$ and where

$$f^\varepsilon=-\Pi_1^\varepsilon\,V^{3D}(\mathbb{I}-\Pi_1^\varepsilon)\Psi_\lambda^{3D},\quad g^\varepsilon=\langle(V^{2.5D}-V^{3D})\,|\chi_1^\varepsilon|^2\rangle\chi_1^\varepsilon\psi_\lambda^{2.5D}.$$

Remarking that

$$\Pi_1^\varepsilon\,V^{3D}(\mathbb{I}-\Pi_1^\varepsilon)=\Pi_1^\varepsilon[\Pi_1^\varepsilon,V^{3D}],$$

we deduce from Lemma 2.3, (4.3) and (4.4) that, for δ strictly positive,

$$\|f^\varepsilon\|_{L^2}\leqslant C\,\varepsilon^{1-1/p}\|\partial_z V^{3D}\|_{L_x^4L_z^p}\|(\mathbb{I}-\Pi_1^\varepsilon)\Psi_\lambda^\varepsilon\|_{H^1(\Omega_0,L^2(\mathbb{R}))}=\mathcal{O}(\varepsilon^{2-\delta})$$

thanks to the embedding $H^{\frac{1}{2}-(1/p)}(\mathbb{R})\hookrightarrow L^p(\mathbb{R})$, for $p\in[2,\infty)$. Besides, according to (4.6), for $r>2$

$$\|g^\varepsilon\|_{L^2}\leqslant C\|V^{3D}-V^{2D}\|_{L_x^rL_z^\infty}$$

and we obtain finally, thanks to (A12), (4.22), and (4.6), that

$$\|w_\lambda^\varepsilon\|_{H^1(\Omega_0,L^2(\mathbb{R}))}\leqslant C\|f^\varepsilon\|_{L^2}+C\|g^\varepsilon\|_{L^2}\leqslant\mathcal{O}(\varepsilon^{2-\delta})+C\|V^{3D}-V^{2D}\|_{L_x^rL_z^\infty},$$

$$\|n_s^{3D}-n^{2.5D}\|_{W^{1,p}(\Omega_0)}\leqslant C\mu(\Lambda)^{1/2}\left(\int_\Lambda\|w_\lambda^\varepsilon\|^2_{H^1(\Omega_0,L^2(\mathbb{R}))}\,\mathrm{d}\mu(\lambda)\right)^{1/2}$$
$$\leqslant\mathcal{O}(\varepsilon^{2-\delta})+C\,\mu(\Lambda)\,\|V^{3D}-V^{2D}\|_{L_x^rL_z^\infty},$$

for $\delta>0$, $r>2$, and $p<2$. Applying (B3) in order to bound V, we find, according to the above estimate,

$$\|V\|_{W^{1,p}(\Omega_0,L^\infty(\mathbb{R}))} \leqslant C\,\varepsilon^{2-\delta} + C\,\mu(\Lambda)\,\|V^{3\mathrm{D}} - V^{2\mathrm{D}}\|_{L_x^r L_z^\infty}.$$

Gathering now the different estimates on R_1^ε, R_2^ε, and V leads to

$$\|V^{3\mathrm{D}} - V^{2\mathrm{D}}\|_{W^{1,p}(\Omega_0,L^\infty(\mathbb{R}))} \leqslant C\,\varepsilon^{2-\delta} + C\,\mu(\Lambda)\,\|V^{3\mathrm{D}} - V^{2\mathrm{D}}\|_{L_x^r L_z^\infty}.$$

Choosing $r \leqslant [2p/(2-p)]$ and $\mu(\Lambda)$ small enough end the proof thanks to the embedding $W^{1,p}(\Omega_0) \hookrightarrow L^r(\Omega_0)$.

VI. THE 2D MODEL IS A FIRST ORDER APPROXIMATION

In this section, we end the proof of Theorem 3.2. We first assume that we are under the hypothesis of Theorem 4.3 which insure that the 2D and 2.5D models admit unique solutions. We denote, respectively, by $(\psi_\lambda^{2.5\mathrm{D}}, V^{2.5\mathrm{D}})$ and $(\phi_\lambda^{2\mathrm{D}}, V^{2\mathrm{D}})$, these solutions. We start by proving (3.5) by writing

$$-\Delta(V^{2.5\mathrm{D}} - V^{2\mathrm{D}}) = |\chi_1^\varepsilon|^2 (n_s^{2.5\mathrm{D}} - n_s^{2\mathrm{D}}) + n_s^{2\mathrm{D}}(|\chi_1^\varepsilon|^2 - \delta(z)) \tag{6.1}$$

equipped with the boundary conditions (B2). In order to apply (B3) to (6.1), we first estimate the quantity $n_s^{2.5\mathrm{D}} - n_s^{2\mathrm{D}}$ by using the Schrödinger equation solved by $w_\lambda^\varepsilon := \chi_1^\varepsilon(\psi_\lambda^{2.5\mathrm{D}} - \phi_\lambda^{2\mathrm{D}})$:

$$-\Delta w_\lambda^\varepsilon + V_c^\varepsilon w_\lambda^\varepsilon + \langle V^{2.5\mathrm{D}} |\chi_1^\varepsilon|^2 \rangle\, w_\lambda^\varepsilon = (E_1^\varepsilon + E_\lambda) w_\lambda^\varepsilon + f^\varepsilon$$

equipped with the transparent homogeneous boundary conditions (A10) with $a=0$ and where

$$f^\varepsilon = (V^{2\mathrm{D}}(\cdot,0) - \langle V^{2.5\mathrm{D}} |\chi_1^\varepsilon|^2 \rangle)\chi_1^\varepsilon \phi_\lambda^{2\mathrm{D}}.$$

Estimating the source term f^ε: We have

$$\|f^\varepsilon\|_{L^2} \leqslant (\|V^{2\mathrm{D}} - V^{2.5\mathrm{D}}\|_{L_x^p L_z^\infty} + \|\langle (V^{2\mathrm{D}}(\cdot,0) - V^{2\mathrm{D}})\,|\chi_1^\varepsilon|^2 \rangle\|_{L^p(\Omega_0)})\|\phi_\lambda^{2\mathrm{D}}\|_{H^1(\Omega_0)}$$

$$\leqslant C\|V^{2\mathrm{D}} - V^{2.5\mathrm{D}}\|_{L_x^p L_z^\infty} + C\|\partial_z V^{2\mathrm{D}}\|_{L_x^p L_z^\alpha} \langle z^{1-1/\alpha} |\chi_1^\varepsilon|^2 \rangle,$$

$$p>2 \leqslant C\|V^{2\mathrm{D}} - V^{2.5\mathrm{D}}\|_{L_x^p L_z^\infty} + \mathcal{O}(\varepsilon^{1-\delta}), \quad \delta>0,$$

where we used the estimates (4.8), (4.9) and the embeddings $H^1(\Omega_0) \hookrightarrow L^q(\Omega_0)$, $q<\infty$ and $H^{1/2-(1/\alpha)}(\mathbb{R}) \hookrightarrow L^\alpha(\mathbb{R})$, $\alpha \in [2,\infty)$. Applying now (A12) in order to estimate w_λ^ε, we obtain uniformly in λ, thanks to the above estimate of the source term f^ε, for $p>2$, $\delta>0$, and $r<2$,

$$\|w_\lambda^\varepsilon\|_{H^1(\Omega_0,L^2(\mathbb{R}))} \leqslant C\|V^{2\mathrm{D}} - V^{2.5\mathrm{D}}\|_{L_x^p L_z^\infty} + \mathcal{O}(\varepsilon^{1-\delta}), \tag{6.2}$$

$$\|n_s^{2.5\mathrm{D}} - n_s^{2\mathrm{D}}\|_{W^{1,r}(\Omega_0)} \leqslant C\mu(\Lambda)\|V^{2\mathrm{D}} - V^{2.5\mathrm{D}}\|_{L_x^p L_z^\infty} + \mathcal{O}(\varepsilon^{1-\delta}). \tag{6.3}$$

It remains now to estimate the second part on the right-hand side of (B2). To this aim, we find, according to (B6), for $r<2$, $p(1+2(s+\beta)) \leqslant 4r$, $s+\beta<\frac{3}{2}$,

$$\|(-\Delta)^{-1}(n_s^{2\mathrm{D}}(|\chi_1^\varepsilon|^2 - \delta(z)))\|_{W^{1,p}(\Omega_0,H^s(\mathbb{R}))} \leqslant C\langle z|\chi_1^\varepsilon|^2\rangle^\beta \|n_s^{2\mathrm{D}}\|_{W^{1,r}(\Omega_0)}.$$

Since $\|n_s^{2\mathrm{D}}\|_{W^{1,r}(\Omega_0)}$ is bounded for $r\leqslant 2$ thanks to (4.8) and since $\langle z|\chi_1^\varepsilon|^2\rangle = \mathcal{O}(\varepsilon)$ thanks to 2.1, we have finally, by choosing $\beta = 1-\delta$, $s=\frac{1}{2}+(\delta/2)$,

$$\|(-\Delta)^{-1}(n_s^{2\mathrm{D}}(|\chi_1^\varepsilon|^2 - \delta(z)))\|_{W^{1,p}(\Omega_0,H^s(\mathbb{R}))} \leqslant \mathcal{O}(\varepsilon^{1-\delta}). \tag{6.4}$$

We are able now to estimate the difference $V^{2\mathrm{D}}-V^{2.5\mathrm{D}}$ by applying (B3). Gathering the bounds (6.1), (6.3), and (6.4) and thanks to the embedding $H^{1/2+\alpha}(\mathbb{R})\hookrightarrow L^{\infty}(\mathbb{R})$, $\alpha>0$, we find, for $\delta>0$, $q<2$, and $p>2$,

$$\|V^{2\mathrm{D}}-V^{2.5\mathrm{D}}\|_{W^{1,q}(\Omega_0,L^{\infty}(\mathbb{R}))}\leqslant C\mu(\Lambda)\|V^{2\mathrm{D}}-V^{2.5\mathrm{D}}\|_{L_x^pL_z^{\infty}}+\mathcal{O}(\varepsilon^{1-\delta}).$$

Choosing $p\leqslant 2q/(2-q)$ and $\mu(\Lambda)$ small enough end the proof of (3.5).

In order to prove (3.4) and (3.6), it suffices to apply (3.5), (6.2), and (6.3).

The estimate from below: For the proof of (3.7), we introduce $(e_i,\lambda_i)_{i\in\mathbb{N}^*}$, the Hilbertian decomposition of the x-Laplacian equipped with Dirichlet boundary condition on $\partial\Omega_0$. Let $g\in L^2(\Omega_0\times\mathbb{R})$ and let u be the solution of $-\Delta u=g$ on the domain $\Omega_0\times\mathbb{R}$ with Dirichlet boundary conditions on $\partial(\Omega_0\times\mathbb{R})$. It can be easily seen that the Fourier transform $\hat{u}$ of u reads

$$\hat{u}(x,\xi)=\sum_{i\geqslant 1}\frac{(\hat{g}(\cdot,\xi),e_i(\cdot))_{L_x^2}}{\lambda_i+\xi^2}e_i(x)$$

and thus, thanks to the Fourier–Plancherel equality

$$\|u\|_{L^2}^2=\|(-\Delta)^{-1}g\|_{L^2}^2=\sum_{i\geqslant 1}\int_{\mathbb{R}}\mathrm{d}\xi\left|\frac{(\hat{g},e_i)_{L_x^2}}{\lambda_i+\xi^2}\right|^2.$$

Hence, using the above equality, we find

$$\begin{aligned}\|(-\Delta)^{-1}(n_s^{2\mathrm{D}}(|\chi_1^{\varepsilon}|^2-\delta(z)))\|_{L^2}^2&=\sum_{i\geqslant 1}\int_{\mathbb{R}}\mathrm{d}\xi\left|\frac{(n_s^{2\mathrm{D}},e_i)_{L_x^2}}{\lambda_i+\xi^2}\right|^2\left|\int_{\mathbb{R}}|\chi_1^{\varepsilon}|^2(e^{-i\xi z}-1)\,\mathrm{dz}\right|^2\\&\geqslant\sum_{i\geqslant 1}\left|\frac{(n_s^{2\mathrm{D}},e_i)_{L_x^2}}{\lambda_i+1}\right|^2\int_0^1\mathrm{d}\xi\left|\int_{\mathbb{R}}|\chi_1^{\varepsilon}|^2(e^{-i\xi z}-1)\,\mathrm{dz}\right|^2\\&\geqslant C\,\|n_s^{2\mathrm{D}}\|_{H^{-1}(\Omega_0)}^2\int_0^1\mathrm{d}\xi\left|\int_{\mathbb{R}}|\chi_1|^2(e^{-i\varepsilon\xi z}-1)\,\mathrm{dz}\right|^2.\end{aligned}\tag{6.5}$$

Moreover, pointwise in ξz, as $\varepsilon\to 0$, we have

$$\frac{e^{-i\,\varepsilon\,\xi\,z}-1}{-i\,\varepsilon\,\xi\,z}\to 1.$$

Consequently, defining h by

$$\frac{h(\varepsilon)}{\varepsilon^2}=\frac{1}{\varepsilon^2}\int_0^1\mathrm{d}\xi\left|\int_{\mathbb{R}}|\chi_1|^2(e^{-i\varepsilon\xi z}-1)\,\mathrm{dz}\right|^2,$$

the Lebesgue dominated convergence theorem implies that

$$\frac{h(\varepsilon)}{\varepsilon^2}\to\frac{1}{3}\left|\int_{\mathbb{R}}z\,|\chi_1|^2\,\mathrm{dz}\right|^2=C.$$

To conclude, we come back to (6.1) and (6.5). By noticing that $\|n_s^{2\mathrm{D}}\|_{H^{-1}(\Omega_0)}=C$, there exists finally C_0 ε-independent such that

$$\|V^{2\mathrm{D}}-V^{2.5\mathrm{D}}\|_{L^2}^2+\|n_s^{2\mathrm{D}}-n_s^{2.5\mathrm{D}}\|_{L^2}^2\geqslant\|(-\Delta)^{-1}(n_s^{2\mathrm{D}}(|\chi_1^{\varepsilon}|^2-\delta(z)))\|_{L^2}^2\geqslant C_0\,\varepsilon^2.$$

This ends the proof.

VII. REMARKS

We considered here a model without exterior potential. The analysis still holds if a regular enough potential is added, for instance, a potential in $L^p(\Omega_0, W^{1,\infty}(\mathbb{R}))$, with $p>2$.

We also assumed that the open set Ω_0 is regular. This hypothesis can be weakened if the boundary conditions prescribed for the Poisson equation are modified: for instance, considering a square, we put Dirichlet boundary conditions in two parallel interfaces and Neumann conditions in the orthogonal ones.

All the analysis presented in the paper strongly relies on the Assumption 2.6 which is essential in order to obtain existence and uniqueness results. We conjecture that all the results still hold if this assumption is replaced by the

Assumption 7.1: The measure μ has a bounded support and there exists δ positive, ε-independent, such that, $\forall i \geqslant 1$,

$$\inf_{\lambda \in supp\ \mu} |E_\lambda - \mathcal{E}_i(0)| > \delta,$$

where the $\mathcal{E}_i$ are the energies of the bound states introduced in Definition 2.8.

This assumption means that the statistics avoids the bound states of the linear open Schrödinger equation, see Ref. 6 for more details. To prove the theorems under this framework, one has to show that the statistics still avoids the bound states when considering a nonzero self-consistent potential. This can be done by a careful analysis of the open Schrödinger equation and by setting a statistics whose total mass is weak enough such that there exists $\eta(\delta)$ such that, $\forall i \geqslant 1$,

$$\inf_{\lambda \in \text{supp}\ \mu} |E_\lambda - \mathcal{E}_i(V^\varepsilon)| > \eta(\delta).$$

On the other hand, following again,[6] a limit absorption procedure can be performed as well. One may add to the energy E^ε, a complex term $i\nu$ with $\nu>0$. Then all the results applies without Assumption 2.6. Then, the limit ν goes to zero has to be investigated and the difficulty in this step is to obtain ν-independent estimates. This will require a precise statement of the rate of convergence in ν in order to preserve the different errors estimates. To conclude, the Assumption 2.6 can be actually weakened but this improvment involves more technicalities than in the present analysis and not directly related to the purpose of this work.

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APPENDIX A: THE LINEAR SCHRÖDINGER EQUATION ON OPEN DOMAINS

In this section, we derive the open boundary conditions introduced in Ref. 6 and we give some estimates for the solution of the Schrödinger equation equipped with such conditions. More precisely, we seek a generalized eigenfunction Ψ^ε solution of the Schrödinger equation associated with the energy E^ε, this means

$$-\Delta\Psi^\varepsilon(x,z) + (V_c^\varepsilon(z) + V^\varepsilon(x,z))\Psi^\varepsilon(x,z) = E^\varepsilon\,\Psi^\varepsilon(x,z) \quad \text{in } \Omega\times\mathbb{R}, \tag{A1}$$

$$\Psi^\varepsilon \text{ is bounded}, \tag{A2}$$

$$\Psi^\varepsilon = 0 \quad \text{on } \partial(\Omega\times\mathbb{R}), \tag{A3}$$

where V_c^ε is a confining potential and was defined in Introduction and V^ε is a given regular potential, supported only in $\Omega_0 \times \mathbb{R}$. The equation (A1) is, in the lead j,

$$(-\partial_z^2 - \Delta_{\xi_j,\eta_j})\Psi^\varepsilon(\xi_j,\eta_j,z) + V_c^\varepsilon(z)\Psi^\varepsilon(\xi_j,\eta_j,z) = E^\varepsilon \Psi^\varepsilon(\xi_j,\eta_j,z), \quad j \neq 0, \tag{A4}$$

where ξ_j and η_j are the local coordinates of the lead j, see Fig. 2. The boundary conditions are obtained by explictly solving the Schrödinger equation in each lead. For this purpose, let Θ_m^j and $\mathcal{E}_m^j$, be the eigenfunctions and eigenvalues of the jth transversal Schrödinger operator $-\partial_{\xi_j}^2$ with Dirichlet boundary conditions. Ψ^ε can be written under the form, in the lead j,

$$\Psi^\varepsilon(\eta_j,\xi_j,z) = \sum_p \Pi_p^\varepsilon \Psi^\varepsilon = \sum_{p,m} \Psi_{p,m,j}^\varepsilon(\eta_j)\Theta_m^j(\xi_j)\chi_p^\varepsilon(z),$$

where $\Psi_{p,m,j}^\varepsilon$ is the component of Ψ^ε on the basis $(\Theta_m^j \otimes \chi_p^\varepsilon)_{p,m}$ and solves

$$-\frac{\partial^2 \Psi_{m,p,j}^\varepsilon}{\partial \eta_j^2} = (E^\varepsilon - E_p^\varepsilon - \mathcal{E}_m^j)\Psi_{m,p,j}^\varepsilon. \tag{A5}$$

Hence, setting

$$k_m^j(E^\varepsilon - E_p^\varepsilon) = \sqrt{|E^\varepsilon - E_p^\varepsilon - \mathcal{E}_m^j|},$$

$$N^j(E^\varepsilon - E_p^\varepsilon) = \sup\{m \geqslant 1,\ E^\varepsilon - E_p^\varepsilon > \mathcal{E}_m^j\},$$

we obtain

$$\Psi_{m,p,j}^\varepsilon(\eta_j) = a_{m,p}^j e^{-ik_m^j \eta_j} + b_{m,p}^j e^{ik_m^j \eta_j} \quad \text{if } m \leqslant N^j(E^\varepsilon - E_p^\varepsilon), \tag{A6}$$

$$\Psi_{m,p,j}^\varepsilon(\eta_j) = b_{m,p}^j e^{-k_m^j \eta_j} \quad \text{if } m > N^j(E^\varepsilon - E_p^\varepsilon). \tag{A7}$$

The modes associated with $m \leqslant N^j(E^\varepsilon - E_p^\varepsilon)$ are the propagating modes and the modes associated with $m > N^j(E^\varepsilon - E_p^\varepsilon)$ are the evanescent modes. The coefficients $a_{m,p}^j$ are known whereas the $b_{m,p}^j$ are the reflection–transmission coefficients and deduced from the solution. The boundary conditions on Γ_j are obtained by eliminating the $b_{m,p}^j$ coefficients and the result is,[6,26]

$$\left.\frac{\partial \Psi^\varepsilon}{\partial \eta_j}\right|_{\Gamma_j} = \mathbb{Z}_j^{3\mathrm{D}}[E^\varepsilon](\Psi^\varepsilon) + \mathbb{S}_j^{3\mathrm{D}}[E^\varepsilon], \tag{A8}$$

where

$$\mathbb{Z}_j^{3\mathrm{D}}[E^\varepsilon](\Psi^\varepsilon) = \sum_{p=1}^{\infty} \left(\sum_{m=1}^{N^j(E^\varepsilon - E_p^\varepsilon)} ik_m^j(E^\varepsilon - E_p^\varepsilon)\Psi_{p,m,j}^\varepsilon(0)\, \Theta_m^j(\xi_j) - \sum_{m=N^j(E^\varepsilon - E_p^\varepsilon)+1}^{\infty} k_m^j(E^\varepsilon - E_p^\varepsilon)\, \Psi_{p,m,j}^\varepsilon(0)\, \Theta_m^j(\xi_j) \right) \chi_p^\varepsilon,$$

$$\mathbb{S}_j^{3\mathrm{D}}[E^\varepsilon] = -2\sum_{p=1}^{\infty} \sum_{m=1}^{N^j(E^\varepsilon - E_p^\varepsilon)} ik_m^j(E^\varepsilon - E_p^\varepsilon)\, a_{m,p}^j\, \Theta_m^j(\xi_j)\, \chi_p^\varepsilon(z).$$

To summarize, the problem is solved only on the bounded domain $\Omega_0 \times \mathbb{R}$ with the boundary conditions (A8) and $\Psi = 0$ on ω_0.

We rewrite now these boundary conditions in the case of the nonlinear transport model of Sec. II B 1. According to Assumption 2.4, the energy E^ε is equal to $E_1^\varepsilon + E_\lambda$, where $E_\lambda = E_{m_0}^{j_0} + k^2$ and $a_{m,p}^j = \delta_p^1\, \delta_m^{m_0}\, \delta_j^{j_0}$. This implies that $\mathbb{S}_j^{3D}$ takes the simpler form

$$\mathbb{S}_j^{3D}[E_1^\varepsilon + E_\lambda] = -2\ \delta_j^{j_0}\, ik\, \Theta_{m_0}^j(\xi_j)\, \chi_1^\varepsilon(z).$$

Finally, in order to derive estimates for more general problems, we consider the following system:

$$-\Delta\Psi^\varepsilon(x,z) + (V_c^\varepsilon(z) + V^\varepsilon(x,z))\Psi^\varepsilon(x,z) = (E_1^\varepsilon + E_\lambda)\ \Psi^\varepsilon(x,z) + f(x,z) \quad \text{in } \Omega_0 \times \mathbb{R}, \tag{A9}$$

$$\left.\frac{\partial\Psi^\varepsilon}{\partial\eta_j}\right|_{\Gamma_j} = \mathbb{Z}_j^{3D}[E_1^\varepsilon + E_\lambda](\Psi^\varepsilon) - 2a\ \delta_j^{j_0}\, ik\, \Theta_{m_0}^j(\xi_j)\, \chi_1^\varepsilon(z), \tag{A10}$$

$$\Psi^\varepsilon = 0 \quad \text{on} \quad \omega_0, \tag{A11}$$

where a is a positive parameter and f a given source term. The well-poseness of this system has been studied in Ref. 6.

Proposition A.1: Let Ψ^ε be the solution of (A9)–(A11). Let $f \in L^2(\Omega_0 \times \mathbb{R})$, $V^\varepsilon \in L^\infty(\Omega_0 \times \mathbb{R})$ and V^ε non-negative a.e. Then, under Assumption 2.2, 2.4, and 2.6, we have, uniformly in λ,

$$\|\Psi^\varepsilon\|_{H^1(\Omega_0, L^2(\mathbb{R}))} \leq C\,(2a + \|f\|_{L^2}), \tag{A12}$$

$$\|(\mathbb{I} - \Pi_1^\varepsilon)\Psi^\varepsilon\|_{L^2} \leq C\,\varepsilon\,(2a + \|f\|_{L^2}), \tag{A13}$$

where C is a generic constant ε-independent.

Proof: Consider the kinetic energy along x and the kinetic energy along z defined by

$$\mathcal{E}_{\text{kin},x}^\varepsilon = \int_{\Omega_0 \times \mathbb{R}} |\nabla_x \Psi^\varepsilon|^2\, dx\, dz, \quad \mathcal{E}_{\text{kin},z}^\varepsilon = \int_{\Omega_0 \times \mathbb{R}} |\partial_z \Psi^\varepsilon|^2\, dx\, dz.$$

The potential energy and the external potential energy are, respectively, defined by

$$\mathcal{E}_{\text{pot}}^\varepsilon = \int_{\Omega_0 \times \mathbb{R}} V^\varepsilon |\Psi^\varepsilon|^2\, dx\, dz, \quad \mathcal{E}_{\text{ext}}^\varepsilon = \int_{\Omega_0 \times \mathbb{R}} V_c^\varepsilon\, |\Psi^\varepsilon|^2 dx\, dz.$$

We introduce also the energy coming from the boundary terms

$$\mathcal{E}_{BC}^\varepsilon = -\sum_{j=1}^{n} \int_{\Gamma_j \times \mathbb{R}} \left.\frac{\partial\Psi^\varepsilon}{\partial\eta_j}\right|_{\Gamma_j} \overline{\Psi^\varepsilon}\, d\xi_j\, dz.$$

A standard energy estimate for the Schrödinger equation, obtained after multiplication of (A9) by $\overline{\Psi_\lambda^\varepsilon}$ and some integration by parts, yields

$$\mathcal{E}_{\text{kin},x}^\varepsilon + \mathcal{E}_{\text{kin},z}^\varepsilon + \mathcal{E}_{\text{pot}}^\varepsilon + \mathcal{E}_{\text{ext}}^\varepsilon + \operatorname{Re} \mathcal{E}_{BC}^\varepsilon = (E_1^\varepsilon + E_\lambda)\|\Psi^\varepsilon\|_{L^2}^2 + \int_{\Omega_0 \times \mathbb{R}} f\, \overline{\Psi^\varepsilon} dx\, dz, \tag{A14}$$

$$\operatorname{Im} \mathcal{E}_{BC}^\varepsilon = 0. \tag{A15}$$

Besides, the boundary condition (A10) implies that

$$\operatorname{Re} \mathcal{E}_{BC}^{\varepsilon} = \sum_{j=1}^{n} \sum_{p=1}^{\infty} \sum_{m=N^j(E_\lambda+E_1^\varepsilon-E_p^\varepsilon)+1}^{\infty} k_m^j(E_\lambda+E_1^\varepsilon-E_p^\varepsilon)|\Psi_{p,m,j}^\varepsilon|^2 - 2a\,k\,\operatorname{Im}\Psi_{1,m_0,j_0}^\varepsilon, \tag{A16}$$

$$\operatorname{Im} \mathcal{E}_{BC}^{\varepsilon} = \sum_{j=1}^{n} \sum_{p=1}^{\infty} \sum_{m=1}^{N^j(E_\lambda+E_1^\varepsilon-E_p^\varepsilon)} k_m^j(E_\lambda+E_1^\varepsilon-E_p^\varepsilon)|\Psi_{p,m,j}^\varepsilon|^2 + 2a\,k\,\operatorname{Re}\Psi_{1,m_0,j_0}^\varepsilon = 0, \tag{A17}$$

and we first deduce from (A16) and (A17) that

$$|\Psi_{1,m_0,j_0}^\varepsilon| \leqslant 2a \tag{A18}$$

$$0 \leqslant \operatorname{Re}\mathcal{E}_{BC}^\varepsilon + 2a\,k\,\operatorname{Im}\Psi_{1,m_0,j_0}^\varepsilon. \tag{A19}$$

Moreover, according to Ref. 6, the operator $-\Delta + V_c^\varepsilon + V^\varepsilon - E_1^\varepsilon$ equipped with (A10) and (A11) with $a=0$, has a compact resolvent and denote $(\mathcal{E}_i^\varepsilon(V^\varepsilon))_{i\in\mathbb{N}^*}$ its spectrum and $(\Phi_i^\varepsilon)_{i\in\mathbb{N}^*}$ its associated eigenvectors. Since $V^\varepsilon \geqslant 0$, then $\mathcal{E}_1^\varepsilon(V^\varepsilon) \geqslant \mathcal{E}_1^\varepsilon(0)$ and it can be easily seen that $\mathcal{E}_1^\varepsilon(0)$ is ε-independent. It follows, after a projection of Ψ^ε on the basis $(\Phi_i^\varepsilon)_{i\in\mathbb{N}^*}$ that

$$\mathcal{E}_{\mathrm{kin},x}^\varepsilon + \mathcal{E}_{\mathrm{kin},z}^\varepsilon + \mathcal{E}_{\mathrm{pot}}^\varepsilon + \mathcal{E}_{\mathrm{ext}}^\varepsilon + \operatorname{Re}\mathcal{E}_{BC}^\varepsilon + 2a\,k\,\operatorname{Im}\Psi_{1,m_0,j_0}^\varepsilon - E_1^\varepsilon\|\Psi^\varepsilon\|_{L^2}^2 = \sum_{i\geqslant 1} \mathcal{E}_i^\varepsilon(V^\varepsilon)|(\Psi^\varepsilon,\Phi_i^\varepsilon)|^2.$$

Injecting this relation in (A14) leads to

$$(\mathcal{E}_1^\varepsilon(0)-E_\lambda)\|\Psi^\varepsilon\|_{L^2}^2 \leqslant \sum_{i\geqslant 1} (\mathcal{E}_i^\varepsilon(V^\varepsilon)-E_\lambda)|(\Psi^\varepsilon,\Phi_i^\varepsilon)|^2 \leqslant 4a^2 k + \|f\|_{L^2}\|\Psi^\varepsilon\|_{L^2},$$

where we used (A18) for the second inequality while the first inequality follows from the fact that $\mathcal{E}_i^\varepsilon(0) \leqslant \mathcal{E}_i^\varepsilon(V^\varepsilon)$ since V^ε is positive. We use now crucially Assumption 2.6 which implies that $\mathcal{E}_1^\varepsilon(0) - E_\lambda > C$, where C is ε-independent and this gives the L^2 estimate, uniform in λ,

$$\|\Psi^\varepsilon\|_{L^2} \leqslant C(2a\sqrt{k} + \|f\|_{L^2}). \tag{A20}$$

To conclude the proof, we come back to (A14) and by using (A19) and (A20), we obtain

$$\mathcal{E}_{\mathrm{kin},x}^\varepsilon + \mathcal{E}_{\mathrm{kin},z}^\varepsilon + \mathcal{E}_{\mathrm{pot}}^\varepsilon + \mathcal{E}_{\mathrm{ext}}^\varepsilon \leqslant E_1^\varepsilon\|\Psi^\varepsilon\|_{L^2}^2 + C(4a^2 + \|f\|_{L^2}^2),$$

where C depends on $\sup_{\lambda\in\operatorname{supp}\mu} E_\lambda$. Since

$$\mathcal{E}_{\mathrm{kin},z}^\varepsilon + \mathcal{E}_{\mathrm{ext}}^\varepsilon = \sum_{p=1}^{\infty} E_p^\varepsilon \|\Pi_p^\varepsilon \Psi^\varepsilon\|_{L^2}^2$$

and since V^ε is non-negative, we have $\mathcal{E}_{\mathrm{pot}}^\varepsilon \geqslant 0$ and finally

$$\mathcal{E}_{\mathrm{kin},x}^\varepsilon + \frac{1}{\varepsilon^2}(E_2 - E_1)\|(\mathbb{I} - \Pi_1^\varepsilon)\Psi^\varepsilon\|_{L^2}^2 \leqslant C(4a^2 + \|f\|_{L^2}^2)$$

which ends the proof. □

APPENDIX B: THE POISSON EQUATION WITH $L_x^r L_z^1$ DENSITIES

This section deals with the regularity of the solution of the Poisson equation

$$-\Delta V = n \quad \text{on} \quad \Omega_0 \times \mathbb{R}, \tag{B1}$$

$$V(\cdot,z)=0 \quad \text{on} \quad \partial\Omega_0, \qquad \lim_{|z|\to\infty} V(x,z)=0. \tag{B2}$$

In the whole section, $L_x^p L_z^q$ denotes the spaces introduced in Definition 2.1.

Lemma B.1: (i) Let V be the solution of (B1) and (B2), let $n\in L_x^r L_z^1$ *with* $r\in(1,\infty)$. *Then for* $s<\frac{3}{2}$ *and* $p(1+2s)\leqslant 4r$, *we have*

$$\|V\|_{L^p(\Omega_0,H^s(\mathbb{R}))}\leqslant C\|n\|_{L_x^r L_z^1}. \tag{B3}$$

(ii) Besides, for $s<\frac{1}{2}$ *and* $p(3+2s)\leqslant 4r$, *we have also*

$$\|\nabla_x V\|_{L^p(\Omega_0,H^s(\mathbb{R}))}\leqslant C\|n\|_{L_x^r L_z^1}. \tag{B4}$$

(iii) Let $n\in L_x^r L_z^1$ *such that* $z\,n\in L_x^r L_z^1$, *with* $r\in(1,+\infty)$ *and* $\int_{\mathbb{R}} n(\cdot,z)\mathrm{d}z=0$. *Then, for* $0\leqslant\beta\leqslant 1$, $p\in[2,+\infty)$, $s+\beta<\frac{3}{2}$ *and* $p(1+2(s+\beta)\leqslant 4r$, *we have*

$$\|V\|_{L^p(\Omega_0,H^s(\mathbb{R}))}\leqslant C\|z\,n\|_{L_x^r L_z^1}^{\beta}\,\|n\|_{L_x^r L_z^1}^{1-\beta}. \tag{B5}$$

(iv) Assume that $n(x,z)=n_s(x)\,(\rho(z)-\delta(z))$ *where* $n_s\in L^r(\Omega_0)$ *with* $r\in(1,+\infty)$, *where* $\rho\in L^1(\mathbb{R})$, *non-negative such that* $z\,\rho\in L^1(\mathbb{R})$ *and* $\|\rho\|_{L^1(\mathbb{R})}=1$. *Then, for* $0\leqslant\beta\leqslant 1$, $p\in[2,+\infty)$, $s+\beta<\frac{3}{2}$ *and* $p(1+2(s+\beta)\leqslant 4r$, *we have*

$$\|V\|_{L^p(\Omega_0,H^s(\mathbb{R}))}\leqslant C\|z\,\rho\|_{L^1}^{\beta}\,\|n_s\|_{L^r(\Omega_0)}. \tag{B6}$$

Proof: Taking the Fourier transform of (B1) with respect to z leads to

$$-\Delta_x\hat{V}(x,\xi)+\xi^2\,\hat{V}(x,\xi)=\hat{n}(x,\xi),$$

where

$$\hat{V}(x,\xi)=\int_{\mathbb{R}} V(x,z)\,e^{-i\,z\,\xi}\,\mathrm{d}z, \quad \hat{n}(x,\xi)=\int_{\mathbb{R}} n(x,z)\,e^{-i\,z\,\xi}\,\mathrm{d}z. \tag{B7}$$

Since $-\Delta_x$, equipped with Dirichlet boundary conditions on Ω_0, is a sectorial operator on $L^p(\Omega_0)$, for $p\in(1,+\infty)$, we have

$$\|\hat{V}(\cdot,\xi)\|_{L^p(\Omega_0)}\leqslant\frac{1}{\xi^2}\|-\Delta_x\hat{V}(\cdot,\xi)+\xi^2\hat{V}(\cdot,\xi)\|_{L^p(\Omega_0)}\leqslant\frac{1}{\xi^2}\|\hat{n}(\cdot,\xi)\|_{L^p(\Omega_0)}. \tag{B8}$$

Moreover, (B8), (B7), and standard elliptic estimates imply

$$\|\hat{V}(\cdot,\xi)\|_{W^{2,p}(\Omega_0)}\leqslant C\|\hat{n}(\cdot,\xi)\|_{L^p(\Omega_0)}, \tag{B9}$$

where C does not depend on ξ. Besides, for $p\geqslant 2$, we have thanks to the Hölder inequality,

$$\begin{aligned}\|V\|_{L^p(\Omega_0,H^s(\mathbb{R}))}^p&=\int_{\Omega_0}\left(\int_{\mathbb{R}}(1+\xi^{2s})\,|\hat{V}(x,\xi)|^2\,\mathrm{d}\xi\right)^{p/2}\mathrm{d}x\\&\leqslant\left\|\frac{1}{1+\xi^{\alpha}}\right\|_{L^{p/(p-2)}(\mathbb{R})}\int_{\Omega_0}\int_{\mathbb{R}}(1+\xi^{(2s+\alpha)p/2})\,|\hat{V}(x,\xi)|^p\,\mathrm{d}\xi\,\mathrm{d}x\\&\leqslant C\int_{\mathbb{R}}(1+\xi^{(2s+\alpha)p/2})\,\|\hat{V}(\cdot,\xi)\|_{L^r(\Omega_0)}^r\,\|\hat{V}(\cdot,\xi)\|_{L^\infty(\Omega_0)}^{p-r}\,\mathrm{d}\xi,\end{aligned} \tag{B10}$$

as soon as

$$0\leqslant 1-\frac{2}{p}<\alpha,\quad 1\leqslant r\leqslant p\leqslant\infty.$$

Coupling now (B8) and (B9) and using the embedding $W^{2,r}(\Omega_0)\hookrightarrow L^\infty(\Omega_0)$, for $r>1$, leads to

$$\begin{aligned}\|V\|^p_{L^p(\Omega_0,H^s(\mathbb{R}))}&\leqslant C\int_{\mathbb{R}}(1+\xi^{(2s+\alpha)p/2})\,\|\hat V(\cdot,\xi)\|^r_{L^r(\Omega_0)}\,\|\hat V(\cdot,\xi)\|^{p-r}_{W^{2,r}(\Omega_0)}\,\mathrm{d}\xi\\ &\leqslant C\int_{\mathbb{R}}(1+\xi^{2r-(2s+\alpha)p/2})^{-1}\,\|\hat n(\cdot,\xi)\|^p_{L^r(\Omega_0)}\,\mathrm{d}\xi\\ &\leqslant C\|n\|^p_{L^r_xL^1_z}\quad\text{if}\quad\frac{1}{\xi^{2r-(2s+\alpha)p/2}}\in L^1([1,+\infty)),\end{aligned}\tag{B11}$$

where we used the fact that $|\hat n(x,\xi)|\leqslant\|n(x,\cdot)\|_{L^1(\mathbb{R})}$. After some easy algebra, this gives the final conditions for (B3),

$$2\leqslant p<\infty,\quad s\leqslant\tfrac{3}{2},\quad p(1+2s)<4r.$$

For (B4), we use a classical interpolation equality in Ref. 13 which insures that

$$\|\nabla_x\hat V\|_{L^p(\Omega_0)}\leqslant C\|\Delta_x\hat V\|^{1/2}_{L^r(\Omega_0)}\;\|\hat V\|^{1/2}_{L^t(\Omega_0)}\leqslant C\|\Delta_x\hat V\|^{1/2}_{L^r(\Omega_0)}\;\|\hat V\|^{r/2r}_{L^r(\Omega_0)}\;\|\hat V\|^{1/2[1-(r/t)]}_{L^\infty(\Omega_0)}\tag{B12}$$

with $1/p=\frac{1}{2}[(1/t)+(1/r).]$ This inequality implies, together with (B8), (B9), for $t\geqslant r>1$,

$$\|\nabla_x\hat V\|_{L^p(\Omega_0)}\leqslant\frac{C}{\xi^{r/t}}\|\hat n\|_{L^r(\Omega_0)}.\tag{B13}$$

Replacing V by $\nabla_x V$ in (B11), using estimates (B9) and (B13), we obtain by proceeding as for (B11),

$$\begin{aligned}\|\nabla_x V\|^p_{L^p(\Omega_0,H^s(\mathbb{R}))}&\leqslant\left\|\frac{1}{1+\xi^\alpha}\right\|_{L^{p/(p-2)}(\mathbb{R})}\int_{\Omega_0}\int_{\mathbb{R}}(1+\xi^{(2s+\alpha)p/2})\,|\nabla_x\hat V(x,\xi)|^p\,\mathrm{d}\xi\,\mathrm{d}x\\ &\leqslant C\int_{\mathbb{R}}(1+\xi^{rp/t-(2s+\alpha)p/2})^{-1}\,\|\hat n(\cdot,\xi)\|^p_{L^r(\Omega_0)}\,\mathrm{d}\xi\leqslant C\|n\|^p_{L^r_xL^1_z}\end{aligned}$$

as soon as

$$0\leqslant 1-\frac{2}{p}<\alpha,\quad\frac{1}{p}=\frac{1}{2}\left(\frac{1}{t}+\frac{1}{r}\right),\quad r\leqslant t,\quad\frac{rp}{t}-\frac{1}{2}(2s+\alpha)p>1.$$

This concludes the proof of (B4) after some easy manipulations.

We end now the proof of Lemma B.1 by proving (B5). If $\int_{\mathbb{R}}n\,\mathrm{d}z=0$, it can easily remarked that

$$\left|\frac{\hat n(x,\xi)}{\xi}\right|=\left|\frac{1}{\xi}\int_{\mathbb{R}}(e^{-iz\xi}-1)n(x,z)\,\mathrm{d}z\right|\leqslant\|zn(x,.)\|_{L^1(\mathbb{R})},$$

since $|e^{-iz\xi}-1|\leqslant|z\,\xi|$, $\forall(k,\xi)\in\mathbb{R}^2$. This leads to, thanks to (B11),

$$\|V\|^p_{L^p(\Omega_0,H^s(\mathbb{R}))}\leqslant C\int_{\mathbb{R}}(1+\xi^{2r-(2s+\alpha)p/2-\beta p})^{-1}\left(\frac{\|\hat{n}(\cdot,\xi)\|^p_{L^r(\Omega_0)}}{\xi^p}\right)^{\beta}(\|\hat{n}(\cdot,\xi)\|^p_{L^r(\Omega_0)})^{1-\beta}\,\mathrm{d}\xi$$

$$\leqslant C\|z\,n\|^{\beta p}_{L^r_xL^1_z}\|n\|^{(1-\beta)p}_{L^r_xL^1_z}\quad\text{if}\quad\frac{1}{\xi^{2r-(2(s+\beta)+\alpha)p/2}}\in L^1([1,+\infty)),$$

which gives the result.

For (B6), we just remark that

$$\hat{n}(x,\xi)=n_s(x)\int_{\mathbb{R}}(e^{-iz\xi}-1)\rho(z)\,\mathrm{d}z$$

which is exactly the same form as above. □

In the same way, if n is given by $n(x,z)\coloneqq n_s(x)\,\delta(z)$, we have the following.

Lemma B.2: (i) Let V be the solution of (B1) and (B2) with $n(x,z)\coloneqq n_s(x)\,\delta(z)$, *where* $n_s\in L^r(\Omega_0)$ *with* $r\in(1,\infty)$. *Then, for* $s<\frac{3}{2}$ *and* $p(1+2s)\leqslant 4r$, *we have*

$$\|V\|_{L^p(\Omega_0,H^s(\mathbb{R}))}\leqslant C\|n\|_{L^r(\Omega_0)}. \tag{B14}$$

Besides, for $s<\frac{1}{2}$ *and* $p(3+2s)\leqslant 4r$, *we have also*

$$\|\nabla_x V\|_{L^p(\Omega_0,H^s(\mathbb{R}))}\leqslant C\|n\|_{L^r(\Omega_0)}. \tag{B15}$$

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