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Far from equilibrium steady states of 1D-Schrödinger-Poisson systems with quantum wells I

V. Bonnaillie-Noël*, F. Nier†, Y. Patel

Abstract

We describe the asymptotic of the steady states of the out-of equilibrium Schrödinger-Poisson system, in the regime of quantum wells in a semiclassical island. After establishing uniform estimates on the nonlinearity, we show that the nonlinear steady states lie asymptotically in a finite-dimensional subspace of functions and that the involved spectral quantities are reduced to a finite number of so-called asymptotic resonant energies. The asymptotic finite dimensional nonlinear system is written in a general setting with only a partial information on its coefficients. After this first part, a complete derivation of the asymptotic nonlinear system will be done for some specific cases in a forthcoming article [BNP2].

MSC (2000): 34L25; 34L30; 34L40; 65L10; 65Z05; 81Q20; 82D37.

Keywords: Schrödinger-Poisson system; Asymptotic analysis; Multiscale problems.

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1 Introduction

1.1 Motivation

This analysis is motivated by the study of quantum electronic transport in semiconductor heterostructures, like resonant tunneling diodes. It is modelled on the basis of a mean field Hartree type description of the electrostatic interaction of particles, known as the Schrödinger-Poisson system. The modelling of resonant tunneling diodes includes the following characteristic features:

1. Steady electronic currents are observed. This can be achieved only within the modelling of out-of-equilibrium quantum systems.

2. The $I-V$ curves of such devices present negative differential resistance. We are in a far from equilibrium regime, for which the linear response theory is questionnable.

3. A very rich nonlinear phenomenology can be observed in such devices, with hysteresis phenomena (see [JLPS], [PrSj]) and even steadily oscillating currents (see [KKetal]).

4. The general wisdom about these systems says that the nonlinear effects are governed by little number of resonant states.

This article is a part of a larger program, namely the understanding of the nonlinear dynamics of these out-of-equilibrium quantum systems. One issue is to prove rigorously that a simple Schrödinger-Poisson system in a far from equilibrium regime, that is when the steady states show a strong anisotropy in the momentum variable at the quantum scale, can lead to multiple solutions to the nonlinear stationary problem with non trivial bifurcation diagrams. A first check was provided by Jona-Lasinio, Presilla and Sjöstrand in [JLPS], [PrSj]. A second issue which goes definitely further than those previous works is the explanation of the production of complex bifurcation diagrams in terms of the geometry of the potential, which requires an accurate analysis of tunnel effects.
The present work was achieved on the basis of former works by the second author and of the ph-D thesis of the third author. This analysis lead the three authors to the introduction of some reduced model which happens to be very efficient in the numerical simulation of realistic devices (see [BNP]). Only the first part of the mathematical analysis is provided here and complements will be presented in a forthcoming article [BNP2].

The points 1) and 2) above are now well understood. A presentation can be done within a Landauer-Büttiker approach [BuLa], [Lan], [ChVi] and [BDM] which involves the scattering states. This modelling allows a strong anisotropy of the occupation number with respect to the momentum and it definitely differs from all the approach where the density matrix looks like a function of the Hamiltonian [BKNR1], [BKNR2]. This latter modelling (and probably the entropy maximizing approach of [DMR] as well) better suits the situation of little variations from the thermodynamical equilibrium, ends with corrected drift-diffusion models and cannot produce multiple solutions due to monotonicity properties. It should be noted that all these modelling consider the reservoirs as fixed objects which only provide some kind of inhomogeneous boundary conditions, in comparison with the theoretical analysis of non equilibrium steady states widely studied within the framework of the von Neumann algebraic approach of statistical physics and which concerns the evolution of the full system, small system plus reservoirs (see for example [JaPi]).
For our model, a complete general functional framework which catches the proper nonlinear steady states and provides a well defined nonlinear dynamics was provided in [Ni3], after using a phase-space approach with some specific tools of the time dependent approach in scattering theory.

Besides the building of a proper functional framework, those models became even more interesting after the articles of Jona-Lasinio, Presilla and Sjöstrand [JLPS], [PrSj] where convincing heuristic arguments and calculations on those simple nonlinear systems were provided as an explanation for observed hysteresis phenomena, in agreement with point 3). Then the question arose whether a complete explanation from an asymptotic analysis on the Schrödinger-Poisson system or whether new nonlinear phenomena could be predicted in some more complex geometric setting like a multiple wells problem. For instance, no real explanation is provided in [JLPS], [PrSj] for the presence or the absence of hysteresis phenomena according to the geometry of the barrier potentials. Our reduced model (see [NiPa], [BNP] and forthcoming article [BNP2]) provides such an explanation, with additional results.

Finally point 4) provides the relevant asymptotic. Resonant states are effective when the imaginary part of resonances are small. Such a behavior can be achieved when the potential barrier are high or large and it is well formulated within a semiclassical asymptotic (small parameter $h \to 0$, imaginary part of resonances of order $\mathcal{O}(e^{-c/h})$). Nevertheless a full semiclassical asymptotic with $\mathcal{O}(1)$ large wells would lead to a large number of resonant states within a fixed energy interval. Point 4) can be fulfilled by considering quantum wells in a semiclassical island. The introduction of the small parameter $h > 0$ as a rescaled Fermi-length as well as a full justification of this asymptotic regime within the presentation of realistic devices has been done in [BNP].

From a mathematical point of view, this problem presents two specific difficulties.

- A non usual multiple wells problem has to be considered: it is not exactly a semiclassical problem and it is nonlinear.
- The introduction of resonances requires the implementation of a complex deformation and the study of non self-adjoint operators.

Fortunately, the one-dimensional framework provides some simplifications or accurate estimates which allow a complete analysis. First a uniform control on the nonlinear potential with the help of some monotony principles can be obtained in $W^{1,\infty}$. Hence the nonlinear potential can be replaced by an h-dependent potential, with uniform bounds in $W^{1,\infty}$. Some standard arguments of the semiclassical analysis for resonances (see [HeSj1]), for multiple wells (see [HeSj2], [HeSj3]), or for the Breit-Wigner formula (see [GeMa]) have to be adapted. Again the weak regularity is partly compensated by the fact that we work on a 1D problem. This article is almost self-contained in the sense that the proofs which are exactly the same as in the usual semiclassical setting were

not reproduced. Precise references are given for these technical parts. Nevertheless some details have to be checked in order to ensure that these techniques can be adapted with the quantum wells and the limited regularity of the nonlinear semiclassical potential. The 1D Schrödinger-Poisson system studied here admits natural *a priori* regularity estimates, uniform with respect to the small parameter $h \to 0$. This leads asymptotically to a perfect splitting of the quantum and classical scales.

1.2 Quantum framework

In the whole study, the framework is the following: $h > 0$ denotes the semiclassical parameter obtained in realistic cases as a rescaled Fermi length (see [BNP]) and $I := [a, b]$ is a given compact interval of the real line. Let P_B^h the Schrödinger operator on the real line:

$$P_B^h := -h^2 \frac{d^2}{dx^2} + \mathcal{B}, \quad \mathcal{B} \equiv \mathcal{B}_I + \mathcal{B}_\infty, \tag{1.1}$$

where

$$\mathcal{B}_I(x) := -B\,\frac{x-a}{b-a}\,\mathbf{1}_{[a,b]}(x), \quad \mathcal{B}_\infty(x) := -B \cdot \mathbf{1}_{[b,+\infty)}(x), \tag{1.2}$$

and B is a non negative constant. The potential $\mathcal{B}$ simply describes the applied bias. The reference Hamiltonian is the self-adjoint realization in the Hilbert space $L^2(\mathbb{R})$ of P_B^h:

$$D(H_B^h) = H^2(\mathbb{R}), \quad \forall u \in D(H_B^h), \quad H_B^h u := P_B^h u. \tag{1.3}$$

Since several self-adjoint (or non self-adjoint) closure of the same differential operator will be considered, the notation P refers to the differential operators acting on $\mathcal{C}_0^\infty$, while H will be used for its realization as an unbounded operator on L^2.
We restrict our analysis in this work to operators in the form

$$P^h[V] := P_B^h + V, \quad V \in L^\infty(I), \tag{1.4}$$

and denote by $H^h[V]$ the self-adjoint realization in $L^2(\mathbb{R})$ of $P^h[V]$:

$$D(H^h[V]) = H^2(\mathbb{R}), \quad \forall u \in D(H^h[V]), \quad H^h[V]u := P^h[V]u, \tag{1.5}$$

after identifying $V \in L^\infty(I)$ with $V(x)1_I(x) \in L^\infty(\mathbb{R})$.

Of particular interest is the case where the potential $V = V^h$ depends on the small parameter h and describes quantum wells in an island with cliffs. It splits into

$$V^h := V_0 + V_{NL}^h, \quad V_0 := \tilde{V}_0 - W^h, \quad \tilde{V}_0,\ V_{NL}^h \in W^{1,\infty}(I). \tag{1.6}$$

The function $\tilde{V}_0$, which models the island potential, can be any non negative Lipschitz function independent of h. Practically it is simply a constant potential on I, $\tilde{V}_0(x) = V_0\, 1_I(x)$ with $V_0 \in \mathbb{R}_+$. The function W^h, which described the quantum wells, is defined by

$$W^h(x) := \sum_{i=1}^{N} w_i \left(\frac{x - c_i}{h} \right). \tag{1.7}$$

In this definition of W^h, the positions $(c_i)_{i=1}^N$ are N given points in (a, b) and w_i are non negative L^∞-functions supported in the interval $[-\kappa, \kappa]$, with $\kappa > 0$ fixed. We denote by U^h the support of the function W^h and $U := \cup_{i=1}^N \{c_i\}$ the region where the quantum wells concentrate, and set $c_0 := a$, $c_{N+1} := b$ (see Figure 1).

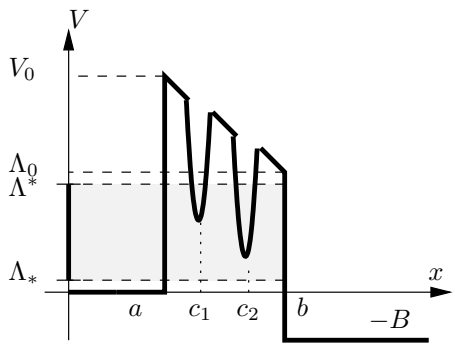


Figure 1: Total potential $\mathcal{B} + V^h - W^h$.

Assumption 1 *Suppose that*

$$\Lambda_0 := \inf_{x \in I} \tilde{V}_0(x) + \mathcal{B}(x) > 0\,, \tag{1.8}$$

and fix the parameters Λ_* and Λ^* so that $0 < \Lambda_* < \Lambda^* < \Lambda_0$.

We will focus on the energy range $\lambda \in [\Lambda_*, \Lambda^*]$.

Finally the function V_{NL}^h describes the mean field nonlinear potential which takes into account the repulsive electrostatic interaction. It will be given as a solution to the Poisson equation on $I = [a, b]$ and will satisfy

$$\forall h > 0, \quad V_{NL}^h \in W^{1,\infty}(I), \quad V_{NL}^h \geq 0. \tag{1.9}$$

Such Hamiltonians are used in the modelling of quantum electronic transport in mesoscopic structures like resonant tunelling diodes (RTD) or super-lattices. The nonlinear steady states can be studied within a Landauer-Büttiker approach: see [BuLa], [Lan], [ChVi] and [BDM] or [Ni3] for possible functional frameworks concerned with the extension to the nonlinear analysis including the nonlinear dynamics. This approach involves the scattering wave functions and requires the analysis of the continuous spectrum of $H^h[V]$. Since for any potential $V \in L^\infty(I)$, $H^h[V]$ is a compactly supported L^∞-perturbation of the reference Hamiltonian H_B^h or the Hamiltonian with step potential $-h^2\Delta + \mathcal{B}_\infty$, the limiting absorption principle holds. By standard arguments ([Ya2], [Pat]) one even gets the absence of imbedded eigenvalues

$$\forall h > 0, \quad \sigma_{\rm ess}(H^h[V]) = \sigma_{\rm ac}(H^h[V]) = [-B; \infty), \tag{1.10}$$

and the scattering states of $H^h[V]$ are indeed well defined for any $V \in L^\infty(I)$.

Remark 1 *Under the non necessary additional assumption*

$$\forall i \in \{1, \ldots, N\}\,, \quad \tilde{V}_0(c_i) + \inf \sigma\left(-\Delta - w_i\right) > 0\,, \tag{1.11}$$

one can even check like in Theorem 3.4 or Theorem 3.6 that there is no eigenvalue at all for $h > 0$ small enough (and $V_{NL}^h \geq 0$) ;

$$\sigma(H^h[V]) = \sigma_{ac}(H^h[V]) = [-B, +\infty)\,.$$

We focus on the energies $\lambda \in [\Lambda_*, \Lambda^*]$.
We consider the incoming scattering states $\psi_-^h(k,\cdot)$ of the Hamiltonian $H^h[V]$ parameterized by the wave vector k (we omit to write the dependence with respect to the potential for scattering states). They provide a diagonalization of $H^h[V]$ over the continuous spectrum (see formula (1.19)). Precisely, introduce first the dispersion relation associated with the reference Hamiltonian $H_{\mathcal{B}}^h$

Definition 1.1 *Set for* $k \in \mathbb{R}^*$

$$\lambda_k := \left| \begin{array}{ll} k^2 & \text{if } k > 0, \\ k^2 - B & \text{if } k < 0. \end{array} \right. \tag{1.12}$$

This dispersion relation (1.12) gives, for the wave vector k, the energy λ_k of the incoming plane wave represented by $\psi_-^h(k,\cdot)$. Again, we are mostly interested in the k's such that $\lambda_k \in [\Lambda_*, \Lambda^*]$.

By definition, the incoming generalized eigenfunction $\psi_-^h(k,\cdot)$ defined for $k \in \mathbb{R}$ solves the differential equation:

$$P^h \psi_-^h(k,\cdot) = \lambda_k \psi_-^h(k,\cdot), \tag{1.13}$$

with the normalization (of incoming plane waves)

$$\text{for } k > 0 \qquad \psi_-(k,x) = \left\{ \begin{array}{ll} e^{i\frac{kx}{h}} + r_k\, e^{-i\frac{kx}{h}} & \text{for} \quad x < a \\ t_k\, e^{i\frac{(\lambda_k+B)^{1/2}x}{h}} & \text{for} \quad x > b\,, \end{array} \right. \tag{1.14}$$

$$\text{for } k < 0 \qquad \psi_-(k,x) = \left\{ \begin{array}{ll} t_k\, e^{-i\frac{(\lambda_k)^{1/2}x}{h}} & \text{for} \quad x < a \\ e^{i\frac{kx}{h}} + r_k\, e^{-i\frac{kx}{h}} & \text{for} \quad x > b\,. \end{array} \right. \tag{1.15}$$

The square root $z^{1/2}$ is chosen with the ramification along the half-line $i\mathbb{R}_-$ in order to ensure that $e^{-i(\lambda_k)^{1/2}x}$ decays exponentially as $x \to -\infty$ when $\lambda_k \in (-B, 0)$.
These coefficients determine the scattering matrix (r_k, t_k) for positive energies $\lambda_k > 0$. They are linked for $\lambda_k > 0$ by the relation

$$|r_k|^2 + \sqrt{\frac{\lambda_k}{\lambda_k + B}}|t_k|^2 = 1, \quad \lambda_k > 0\,. \tag{1.16}$$

Since the wave vector k is a log-derivative, this normalization of the wave functions can be written in terms of boundary conditions at $x = a$ and $x = b$, in this specific one-dimensional case fitting with realistic problems:

$$\begin{aligned} &\left[h\partial_x + i\lambda_k^{1/2}\right]_{|x=a} u = 2ike^{i\frac{ka}{h}}, \\ &\left[h\partial_x - i(\lambda_k + B)^{1/2}\right]_{|x=b} u = 0, \qquad \text{for } k > 0 \end{aligned} \tag{1.17}$$

$$\begin{aligned} \text{and} \qquad &\left[h\partial_x + i\lambda_k^{1/2}\right]_{|x=a} u = 0, \\ &\left[h\partial_x - i(\lambda_k + B)^{1/2}\right]_{|x=b} u = 2ike^{i\frac{kb}{h}}, \qquad \text{for } k < 0\,. \end{aligned} \tag{1.18}$$

Thus the problem over the real line is reduced to a boundary problem on I with boundary conditions depending on the spectral parameter (1.17)-(1.18). These boundary conditions are exact transparent boundary conditions. This setting makes rather easy the complex deformation argument used in the analysis of resonances (see [BaCo], [HeSj1] or [HiSi] for a more general introduction). Here considering a complex λ_k around any positive value is easily implemented because the coefficients on the boundary conditions at $x = a$ and $x = b$ depend holomorphically on λ_k (or k).
We end this section with three elementary properties :

1. With this normalization, it appears that for any non negative continuous function θ on $[\Lambda_*, \Lambda^*]$, the operator $\mathbf{1}_I\theta(H^h[V])\mathbf{1}_I$ is an integral operator. Moreover the kernel is given by

$$\mathbf{1}_I\theta(H^h[V])\mathbf{1}_I[x,y] = \int_k \theta(\lambda_k)\psi_-^h(k,x)\overline{\psi_-^h(k,y)}\frac{dk}{2\pi h}, \quad (x,y) \in I \times I. \tag{1.19}$$

2. Note that because of the regularity of ψ_-^h, it follows by Mercer's theorem (see [Si, Thm 3.5]) that this operator is trace-class, with a trace equal to the diagonal integral.

3. Note also that because the solutions to the ODE (1.13) in the interval I is a 2-dimensional linear subspace, say $\mathcal{S}_{\lambda_k} \subset H^2(a,b)$, conditions (1.17)-(1.18) form an affine system in $\mathcal{S}_{\lambda_k}$. Resonances around positive energies correspond to the exceptional complex values of $\lambda_k = z$ for which the continuous linear functionals defining this system are proportional.

1.3 Schrödinger-Poisson system

Here we are interested in the study of the stationary case. We first fix the profile of the incoming beam of electrons over the structure between a and b.

Notation 1 *Fix a continuous non negative function $k \mapsto g(k)$ such that $g(k) = 0$ if $\lambda_k \notin (\Lambda_*, \Lambda^*)$, see (1.12).*

A beam of electrons corresponds to a superposition of scattering states with density g. The electronic density is then described by the measure $dn_g[V]$ defined by

$$dn_g[V](x) := \int_{\mathbb{R}} g(k)|\psi_-^h(k,x)|^2 \frac{dk}{2\pi h}\,. \tag{1.20}$$

It is convenient to introduce the function $g(K_-^h)$ of the asymptotic momentum operator defined (see [DeGe], [Ni3] for a more general presentation) according to:

$$g(K_-^h)[x,y] = \int_{\mathbb{R}} g(k)\psi_-^h(k,x)\overline{\psi_-^h(k,y)}\frac{dk}{2\pi h}\,.$$

Its localized version $\mathbf{1}_I g(K_-^h)\mathbf{1}_I$ has the integral kernel

$$\mathbf{1}_I g(K_-^h)\mathbf{1}_I[x,y] = \int_{\mathbb{R}} g(k)\mathbf{1}_I(x)\psi_-^h(k,x)\overline{\psi_-^h(k,y)}\mathbf{1}_I(y)\frac{dk}{2\pi h}. \tag{1.21}$$

The operator $g(K_-^h)$ is a density matrix and the density fulfills the weak formulation

$$\forall \varphi \in \mathcal{C}^0(I), \quad \int_I \varphi(x)dn_g[V](x) = \mathrm{Tr}\,[\mathbf{1}_I g(K_-^h)\mathbf{1}_I\varphi]. \tag{1.22}$$

Note that in the particular case where $g(k)$ is a function of the energy, *i.e.* $g(k) \equiv \theta(\lambda_k)$, $g(K_-^h)$ is a function of the Hamiltonian

$$g(K_-^h) = \theta(H^h)\,. \tag{1.23}$$

Functions of the Hamiltonian can be viewed as equilibrium states (and even thermodynamical equilibrium states when θ is decreasing). For such states, the current through the device is null. Hence out-of-equilibrium steady states with a non vanishing current have to be described with a function $g(k)$ which is not a function of the energy. In order to make this situation clear, we assume the next possibly extendible assumption (see [BNP] for an easy generalization towards more realistic problems).

Assumption 2 *Fix a non negative function $\theta \in \mathcal{C}_c^0((\Lambda_*, \Lambda^*))$ and assume that*

$$g(k) = 1_{k>0} \cdot \theta(\lambda_k). \text{ In particular, } \quad 0 \leq g(k) \leq \theta(\lambda_k). \tag{1.24}$$

The Schrödinger-Poisson system is an Hartree model which includes the self-consistent electrostatic potential within the device ($a \leq x \leq b$). Hence the nonlinear potential V_{NL}^h is a solution to

$$\begin{cases} H^h[V^h] = H_B^h + \tilde{V}_0 - W^h + V_{NL}^h, \\ -\Delta V_{NL}^h = dn_g[V^h], \quad V_{NL}^h = (a) = V_{NL}^h(b) = 0. \end{cases} \tag{1.25}$$

Note that the assumption $g \geq 0$ yields $dn_g[V^h] \geq 0$ and $V_{NL}^h \geq 0$.
It is known, (see [BDM], [Ni3]) , that the system (1.25) admits solutions, for fixed $h > 0$. Furthermore with the absence of negative eigenvalues provided by the condition (1.11), it is easily checked that the solutions to (1.25) are the only steady states of the nonlinear dynamics studied in [Ni3]. Yet, uniform estimates with respect to h are not given in [Ni3]. We are now interested in the structure of the set of asymptotic solutions as $h \to 0$. A first step consists in getting *a priori* estimates on the semi-linear problem. This is performed in Section 2. Since for a given $h > 0$ the density $dn_g[V^h]$ is a bounded positive measure, we introduce the following spaces:

Definition 1.2 *Call $(\mathcal{M}_b(I), \|\cdot\|_b)$ the Banach space of bounded complex measures on $[a, b]$ and let*

$$BV_0^2(I) := \left\{ V \in \mathcal{C}^0(I) \,|\, V'' \in \mathcal{M}_b(I), \quad V(a) = 0 = V(b) \right\}, \tag{1.26}$$

normed by $\|V\| := \|V\|_\infty + \|V''\|_b$.

With this norm , $BV_0^2(I)$ is a Banach space continuously embedded in $W^{1,\infty}(I)$ and compactly embedded in the Hölder spaces $\mathcal{C}^{0,\alpha}(I)$ for $\alpha \in (0, 1)$.

1.4 Results

Theorem 1.3 *Consider problem (1.25). Then for $h > 0$ sufficiently small:*
i) The family of potentials $(V_{NL}^h)_{h>0}$ is uniformly bounded in $L^\infty(I)$.
ii) The family of measures $(dn_g[V^h])_{h>0}$ is bounded in $\mathcal{M}_b(I)$ and the family $(V_{NL}^h)_{h>0}$ is bounded in $BV_0^2(I)$.
iii) Consequently, the family of potentials $(V_{NL}^h)_{h>0}$ is bounded in $W^{1,\infty}(I)$ and relatively compact in the Hölder space $\mathcal{C}^{0,\alpha}(I)$ for any $\alpha \in (0, 1)$.

We then try to identify the weak* possible limits dn_g^0 of the measure $dn_g[V^h]$. Owing to the boundedness stated in Theorem 1.3 *ii)*, we shall make the next simplifying assumption which makes sense after possibly extracting a subsequence $(h_n)_{n\in\mathbb{N}}$.

Assumption 3 *The convergence*

$$dn_g[V^h] \overset{h\to 0}{\rightharpoonup} dn_g^0$$

holds for the weak topology of $\mathcal{M}_b(I) = \mathcal{C}^0(I)'$.

The following notations for the total potential

$$\mathcal{V}^h := V^h + \mathcal{B} = \tilde{V}_0 + V_{NL}^h - W^h + \mathcal{B}, \tag{1.27}$$

and for the total potential with filled wells

$$\tilde{\mathcal{V}}^h := \mathcal{V}^h + W^h = \tilde{V}_0 + V_{NL}^h + \mathcal{B}, \tag{1.28}$$

are convenient. The solution to

$$-\Delta V = dn_g^0\,, \quad V(a) = V(b) = 0 \tag{1.29}$$

is denoted V_{NL}^0 and we set

$$\tilde{\mathcal{V}}^0 := \tilde{V}_0 + V_{NL}^0 + \mathcal{B}\,. \tag{1.30}$$

Theorem 1.3 has the next consequence.

Corollary 1.4 *Make the Assumption 3. Then the filled potential $\tilde{\mathcal{V}}^h$ is uniformly bounded in $W^{1,\infty}(I)$ and converges in $\mathcal{C}^{0,\alpha}(I)$ to $\tilde{\mathcal{V}}^0$ as $h \to 0$ for any $\alpha < 1$. Moreover if the second derivative $\partial_x^2 \tilde{V}_0$ is a bounded measure, the weak convergence*

$$\partial_x^2 \tilde{\mathcal{V}}^h \overset{h\to 0}{\rightharpoonup} \partial_x^2 \tilde{\mathcal{V}}^0 = \partial_x^2 \tilde{V}_0 - dn_g^0$$

also holds in $\mathcal{M}_b(I)$.

Remark 2 *Note that the solution of the asymptotic Poisson equation does not depend on the possible mass of dn_g^0 concentrated on $x = a$ or $x = b$. Indeed the asymptotic potential V_{NL}^0 forgets any boundary layer and the boundary value problem* (1.29) *is equivalently written with the restricted measure $dn_g^0\big|_{(a,b)}$.*

The idea leading to an accurate description of the the asymptotic density dn_g^0 is the following: suppose in a first step that the wells are filled, that is $W^h = 0$ and $\mathcal{V}^h = \tilde{\mathcal{V}}^h$. In the classical picture, the incoming particles of energy $\lambda_k \leq \Lambda^*$ are reflected by the cliffs, so one expects that $dn_g^0 \equiv 0$ in (a, b). Now, the introduction of the wells W^h generates trapped quantum states transformed into resonant states after the interaction with the continuous spectrum. The tunnel effect allows these states to be occupied in a stationary setting. Besides, the quantum wells with an $\mathcal{O}(h)$-diameter produce two interesting effects. Firstly the density will asymptotically concentrate like delta-functions in positions around the c_i's. Secondly the resonant energies attached to one well are separated by $\mathcal{O}(1)$ gaps (see Remark 3 below). With a finite number of wells, this asymptotic implements the general wisdom that the nonlinear system is essentially governed by *finite* number of resonant states of the system (point 4 of our introduction). The relevancy of this asymptotic, with quantum wells in a semiclassical island, has been carefully checked in [BNP] with numerical data fitting with realistic situations.

To state our results we need the notion of asymptotic resonant energy.

Notation 2 *Denote, for $i = 1, \ldots, N$, by σ_i the set of the eigenvalues of the Hamiltonian $-\Delta - w_i$ on the real line*

$$\sigma_i := \left\{e_k^i\right\}_{k\in K_i} \subset (-\infty, 0), \quad K_i \subset \mathbb{N}, \quad i = 1, \ldots, N. \tag{1.31}$$

Definition 1.5 *We will say that $\lambda \in \mathbb{R}$ is an asymptotic resonant energy for the potential $\mathcal{V}^h$ if and only if*

$$\lambda \in \mathcal{E}_0 := \bigcup_{i=1}^N \mathcal{E}_i, \quad \mathcal{E}_i := \sigma_i + \tilde{\mathcal{V}}^0(c_i). \tag{1.32}$$

Moreover, we define the multiplicity m_λ of the asymptotic resonant energy λ as

$$m_\lambda := \#J_\lambda, \quad \textit{where} \quad J_\lambda := \{i \in \{1, \ldots, N\} \ \textit{s.t.} \ \lambda \in \mathcal{E}_i\}\,. \tag{1.33}$$

Finally, for $i = 1, \ldots, N$, we will say that the well c_i is resonant at the energy λ (or λ-resonant) if and only if $i \in J_\lambda$.

Remark 3 *The set $\sigma_i + \tilde{\mathcal{V}}^0(c_i)$ is nothing but the set of the eigenvalues of the Hamiltonian $\hat{H}_i^1 := -\Delta - w_i + \tilde{\mathcal{V}}^0(c_i)$ on $\mathbb{R}$, which is unitarily equivalent to the Hamiltonian $\hat{H}_i^h := -h^2\Delta - w_i(\cdot/h) + \tilde{\mathcal{V}}^0(c_i)$.*

Theorem 1.6 *Make the Assumptions 1 and 3 and fix a non negative function $\theta \in \mathcal{C}_c^0((\Lambda_*, \Lambda^*))$ and assume the convergence of $\tilde{\mathcal{V}}^h$ stated in Corollary 1.4. Let $dn_g[V^h]$ be the density defined according to* (1.20) *and Assumption 2 or by taking $g(k) = \theta(\lambda_k)$. Then the weak limit dn_g^0 satisfies*

$$dn_g^0\big|_{(a,b)} = \sum_{\lambda \in \mathcal{E}_0} \sum_{i \in J_\lambda} t_i^\lambda \, \theta(\lambda) \, \delta_{x=c_i}, \tag{1.34}$$

with the following specifications:
i) In the case of a function of the Hamiltonian, that is $g(k) = \theta(\lambda_k)$, all the t_i^λ's are equal to 1 for every $\lambda \in \mathcal{E}_0$ and $i \in J_\lambda$.
ii) If $g(k) = 1_{k>0} \cdot \theta(\lambda_k)$, then for every $\lambda \in \mathcal{E}_0$ and $i \in J_\lambda$, t_i^λ lie in the interval $[0,1]$.
Finally, the asymptotic nonlinear potential V_{NL}^0 which solves (1.29) *is an affine function on each interval $[c_i, c_{i+1}]$, $i = 0, \dots, N$.*

Note that the sum is a finite sum, since the set $\mathcal{E}_0 \cap \operatorname{supp}\theta$ is finite. Observe immediately that point *ii*) follows from *i*) because if one denotes

$$\theta_\lambda(k) := \theta(\lambda_k) \tag{1.35}$$

one has $0 \le dn_g[V^h] \le dn_{\theta_\lambda}[V^h]$, and *ii*) is obtained by Theorem 1.3 and Poisson's equation (1.25). Moreover, the nonlinearity asymptotically lies in a finite dimensional subspace $\mathcal{A}$ of $\mathcal{C}^0(I)$:

$$\mathcal{A} := \left\{ V \in \mathcal{C}^0(I) \ \text{ s.t. } V_{|\partial I} = 0 \text{ and } V_{|[c_i, c_{i+1}]} \text{ is affine, } i = 0, \dots, N \right\}. \tag{1.36}$$

In this finite dimensional space, the asymptotic nonlinear system can be written either with the coordinate system $= (V(c_i))_{i=1,\dots,N} \in \mathbb{R}^N$ or with the more convenient one $(-V'(c_i+0) + V'(c_i - 0))_{i=1,\dots,N}$ proportionnal to the collection of total charges in the wells.

Theorem 1.6-*i)* gives a mean to compute the potential V_{NL}^0 in the particular case where g is a function of the Hamiltonian. In the anisotropic case *ii)* the determination of the t_i^λ's relies on a discussion on the Agmon distance between the wells. A forthcoming paper [BNP2] will be dedicated to the analysis of these coefficients.

In order to prove the results, we adopt the following strategy: as the problem is a semi-linear problem, we get *a priori* estimates for the nonlinear potential (Section 2), and then reduce the analysis to the linear analysis of the Hamiltonian $H^h[V^h]$ with uniform estimates on the potential $(V^h)_{h>0}$. Useful results on the Dirichlet problem in the interval I with accurate estimates of the resolvent kernel are reviewed in Section 3. The analysis of resonances starts in Section 4 and Section 5 and ends in Section 6 with a version of the Breit-Wigner formula for the local density of states.

2 A priori Estimates

We first prove some estimates for self-adjoint realizations of P^h on $\Omega = \mathbb{R}$ or Ω an open sub-interval of I.
Consider the differential operator P^h defined by (1.4), for any $B \ge 0$ with (1.6)-(1.9), and let $\tilde{P}^h$ be defined by

$$\tilde{P}^h[V^h] := P^h[V^h] + W^h \equiv -h^2 \frac{d^2}{dx^2} + \tilde{\mathcal{V}}^h .$$

Remark 4 *The ˜ symbol recurrently refers to the situation where the wells are filled. According to our general convention the letter P refers to the differential operator while H refers to some closed realization as an unbounded operator.*

Proposition 2.1 *Fix a non negative smooth function $\hat{\theta} \in \mathcal{C}_0^\infty(\mathbb{R})$, and call H_Ω^h (resp. $\tilde{H}_\Omega^h$) the self-adjoint realization on $L^2(\Omega)$ of P^h (resp. $\tilde{P}^h$) with domain $H_0^1(\Omega) \cap H^2(\Omega)$. Then, for any given compact subset $K \subset \mathbb{R}$, and $h > 0$, the operators $\mathbf{1}_K \hat{\theta}(H_\Omega^h)\mathbf{1}_K$ and $\mathbf{1}_K \hat{\theta}(\tilde{H}_\Omega^h)\mathbf{1}_K$ are trace-class. Moreover the estimate*

$$Tr\,[\mathbf{1}_K \hat{\theta}(H_\Omega^h)\mathbf{1}_K] - Tr\,[\mathbf{1}_K \hat{\theta}(\tilde{H}_\Omega^h)\mathbf{1}_K] \leq C_K \left(1 + \left\|\tilde{\mathcal{V}}^h\right\|_{L^\infty}\right)$$

holds with a constant C_K independent of $h \in (0, h_0)$.

Proof: In dimension 1 and for any fixed $h > 0$, these operators are trace class (see [Si]). For the comparison, we use the Dynkin-Helffer-Sjöstrand formula (see [Dav], [HeSj4], [Ni1]):

$$\hat{\theta}(H_\Omega^h) = \frac{1}{2i\pi} \int_{\mathbb{C}} \frac{\partial \tilde{\hat{\theta}}}{\partial \bar{z}}(z)(z - H_\Omega^h)^{-1} dz \wedge d\bar{z}, \tag{2.1}$$

where $\tilde{\hat{\theta}}$ is a compactly supported almost-analytic extension of $\hat{\theta}$. Apply then the second resolvent formula for $z \notin \mathbb{R}$ and write with $\tilde{P}^h - P^h = W^h$:

$$\mathbf{1}_K (z - H_\Omega^h)^{-1} \mathbf{1}_K - \mathbf{1}_K (z - \tilde{H}_\Omega^h)^{-1} \mathbf{1}_K = -\mathbf{1}_K (z - H_\Omega^h)^{-1} W^h (z - \tilde{H}_\Omega^h)^{-1} \mathbf{1}_K. \tag{2.2}$$

Introduce then a smooth cut-off function χ, equal to 1 on a fixed neighborhood of U^h if $\Omega \neq \mathbb{R}$, and take $\chi \equiv 1$ if $\Omega = \mathbb{R}$. Write the r.h.s of eq. (2.2)

$$[\mathbf{1}_K (z - H_\Omega^h)^{-1} \chi][W^h (i + h^2\Delta)^{-1}][(i + h^2\Delta)\chi(z - \tilde{H}_\Omega^h)^{-1} \mathbf{1}_K], \tag{2.3}$$

where $-\Delta$ denotes the free Laplacian on $\mathbb{R}$. By the spectral theorem, the first factor of (2.3) is a bounded operator with norm $\mathcal{O}(|\mathrm{Im}(z)|^{-1})$ uniformly w.r.t. $h > 0$. Since the operator $[W^h(i + h^2\Delta)^{-1}]$ is unitarily equivalent to $W^{h=1}(i + \Delta)^{-1}$, it is trace class uniformly with respect to h, z. Indeed the latter writes $f(x)g(-i\nabla)$ whose symbol is L^1 (see [ReSi3, Thm XI. 20, p. 47]).
For the last factor, the decomposition

$$(i + h^2\Delta)\chi(z - \tilde{H}_\Omega^h)^{-1} = (i + h^2\Delta)\chi(i + h^2\Delta_\Omega)^{-1} \left[1 + (i - z + \tilde{\mathcal{V}}^h)(z - \tilde{H}_\Omega^h)^{-1}\right],$$

leads to

$$\left\|(i + h^2\Delta)\chi(z - \tilde{H}_\Omega^h)^{-1}\right\| \leq C_K \frac{\langle z \rangle}{|\mathrm{Im}(z)|} \left(1 + \left\|\tilde{\mathcal{V}}^h\right\|_{L^\infty}\right).$$

□

Proposition 2.1 says that the quantum wells can be forgotten for a uniform global estimate of the density of states. Thanks to a monotony principle shown in [Ni2], one can prove the following result:

Proposition 2.2 *Consider the Schrödinger-Poisson system (1.20)-(1.25). Then the family of potentials $(V_{NL}^h)_{h>0}$ is uniformly bounded in L^∞.*

Proof: For a given function F, we will denote by F_λ the function $k \mapsto F(\lambda_k)$ (see (1.12) for the definition of λ_k). By assumption on the shape of the incoming beam of electrons, one has:

$$0 \leq g(k) \leq \theta_\lambda(k), \tag{2.4}$$

so we will first study the density of particles corresponding to the equilibrium state described by θ_λ, that is the measure $dn_{\theta_\lambda}[V^h]$. The proof consists in controlling the total mass of the measures by similar quantities relative to other Hamiltonians. In dimension 1, the regularity provided by the Poisson equation with bounded measure as a right-hand side allows the integration by parts

$$\frac{1}{2}\int_a^b \left(\frac{dV_{NL}^h}{dx}\right)^2 dx = \int_a^b V_{NL}^h dn_g[V^h](x) \leq \int_a^b V_{NL}^h dn_{\theta_\lambda}[V^h](x)\,. \tag{2.5}$$

Now, chose a non negative smooth compactly supported function $\hat{\theta} \in \mathcal{C}_0^\infty(\mathbb{R})$ decreasing over $(-B, \Lambda^*)$ and with support included in $(-\infty, \Lambda^*)$ such that

$$0 \leq \theta \leq \hat{\theta}. \tag{2.6}$$

We then get by positivity of V_{NL}^h and the expression of the measure in (1.20)

$$\frac{1}{2}\int_a^b \left(\frac{dV_{NL}^h}{dx}\right)^2 dx \leq \int_a^b V_{NL}^h dn_{\theta_\lambda}[V^h](x) \leq \int_a^b V_{NL}^h dn_{\hat{\theta}_\lambda}[V^h](x). \tag{2.7}$$

Set then

$$V_2^h := V^h - V_{NL}^h \equiv \tilde{V}_0 - W^h, \tag{2.8}$$

and consider now the Hamiltonian $H_2^h := H_B^h + V_2^h$. Apply then the monotony principle (see Appendix B) with $H_1 = H_2^h = H_B^h + V_2^h$ and $H_2 = H_B^h + V^h$: the last term of (2.7) is bounded by

$$\begin{aligned} \int_a^b V_{NL}^h dn_{\hat{\theta}_\lambda}[V^h](x) &\leq \int_a^b V_{NL}^h dn_{\hat{\theta}_\lambda}[V_2^h](x) \\ &\leq \|V_{NL}^h\|_{L^\infty(I)} \int_a^b dn_{\hat{\theta}_\lambda}[V_2^h](x). \end{aligned} \tag{2.9}$$

Applying Proposition 2.1 gives, coming back to (2.8)

$$\int_a^b dn_{\hat{\theta}_\lambda}[\tilde{V}_0 - W^h](x) \leq C + \int_a^b dn_{\hat{\theta}_\lambda}[\tilde{V}_0](x)\,, \tag{2.10}$$

the constant C being independent of h since the potential $\tilde{V}_0$ does not depend on h. Finally, we need an upper bound for the density of particles in the island I in the case of the potential $\tilde{V}_0 + \mathcal{B}$. For this, we reduce the problem to the case of the constant potential on I and equal to Λ^*. Apply again the monotony principle with $H_1 = H_B^h - \mathcal{B} + \Lambda^*$ and $H_2 = H_B^h + \tilde{V}_0$. Since $H_2 - H_1 = \tilde{V}_0 + \mathcal{B} - \Lambda^* =: \delta V$ is larger than $\Lambda_0 - \Lambda^* > 0$ according to (1.8), one has uniformly on I

$$\delta V(x) > \inf_I(\tilde{V}_0 + \mathcal{B}) - \Lambda^* \geq \Lambda_0 - \Lambda^* =: \alpha > 0, \quad \text{and} \quad \delta V(x) \leq \|\tilde{V}_0\|_{L^\infty}. \tag{2.11}$$

By writing $dn_{\hat{\theta}_\lambda}^*$ for the measure $dn_{\hat{\theta}_\lambda}[\Lambda^* - \mathcal{B}_I]$, the inequality

$$\alpha \int_a^b dn_{\hat{\theta_\lambda}}[\tilde{V}_0] \leq \int_a^b \delta V \cdot dn_{\hat{\theta_\lambda}}[\tilde{V}_0] \leq \int_a^b \delta V \cdot dn_{\hat{\theta}_\lambda}^* \leq \|\tilde{V}_0\|_{L^\infty} \int_a^b dn_{\hat{\theta}_\lambda}^*\,,$$

implies

$$0 \leq \int_a^b dn_{\hat{\theta}_\lambda}[\tilde{V}_0] \leq \frac{\|\tilde{V}_0\|_{L^\infty}}{\alpha} \int_a^b dn^*_{\hat{\theta}_\lambda}. \tag{2.12}$$

Since $\int_a^b dn^*_{\hat{\theta}}$ is a constant not depending on h (see Appendix D for explicit formulas), we get, combining (2.7), (2.10) and (2.12)

$$\frac{1}{2}\|V^h_{NL}\|^2_{H^1_0} \leq \left(C + \frac{\|\tilde{V}_0\|_{L^\infty}}{\alpha} \int_a^b dn^*_{\hat{\theta}} \right) \|V^h_{NL}\|_{L^\infty}. \tag{2.13}$$

We conclude with the standard imbedding of H^1_0 in L^∞. □

Theorem 1.3 gathers the results of Proposition 2.2 with the next result.

Proposition 2.3 *The family of measures $(dn_g[V^h])_h$ is uniformly bounded in $\mathcal{M}_b(I)$. It follows that the family of potentials (V^h_{NL}) is bounded in $BV^2_0(I)$. In particular it is a relatively compact family in every Hölder space $\mathcal{C}^{0,\alpha}(I)$, $\alpha \in (0,1)$.*

Proof: By definition of dn_{θ_λ} and simple comparison, one gets

$$\int_I dn_g[V^h] \leq \int_I dn_{\theta_\lambda}[V^h] = \mathrm{Tr}\,[\mathbf{1}_I \theta(H^h)\mathbf{1}_I] \leq \mathrm{Tr}\,[\mathbf{1}_I \hat{\theta}(H^h)\mathbf{1}_I].$$

Apply again Proposition 2.1, since now the family of potentials is uniformly bounded in L^∞. Again the uniform boundedness of the right-hand side with respect to $h > 0$ comes from (2.9), (2.10), (2.12) and Appendix D. □

3 Results on the Dirichlet Problem

From now, we systematically make Assumption 3 and reduce the analysis to a linear analysis of $H^h[V^h]$.

For the contribution of the resonances in the evaluation of spectral quantities, the idea consists in considering the non-self adjoint boundary value problem with complex coefficients in the boundary conditions (1.17)(1.18) as a perturbartion of the homogeneous Dirichlet problem.

3.1 Some notations

In order to measure the error, we shall use several standard tools:
1) The h-dependent H^s-norms:

$$\|u\|^2_{s,h} := \sum_{k \leq s} \|h^k \partial^k_x u\|^2_{L^2(I)}, \quad (u \in H^s(I)) \tag{3.1}$$

will be used mainly with $s = 0, 1, 2$.
2) The Agmon distance is defined for any potential $V \in L^\infty(I)$ according to

Definition 3.1 *For an energy $\lambda \in \mathbb{R}$ and a potential V, we define the Agmon distance by :*

$$\forall x, y \in I, \quad d(x, y; V, \lambda) = \left| \int_x^y \sqrt{(V(t) - \lambda)_+}\, dt \right|. \tag{3.2}$$

For our estimates, we should take $V = \mathcal{V}^h$. Yet, it is equivalent to work with the distance relative to the potential $\tilde{\mathcal{V}}^h$ since the support of W^h is included in a finite union of intervals with diameter $2\kappa h$.
Moreover owing to the lower bound

$$\forall \lambda \in [\Lambda_*, \Lambda^*], \quad \forall x \in I, \quad \inf_{h>0,\, x\in I} \tilde{\mathcal{V}}^h(x) - \lambda \geq \Lambda_0 - \Lambda^* =: \delta > 0, \tag{3.3}$$

all the Agmon distances (depending on $\tilde{\mathcal{V}}^h$) are uniformly equivalent to the usual Euclidean distance.
3) Finally in the analysis of the tunnel effect, it is usual to introduce the estimates within the next setting.

Definition 3.2 *For an h-dependent vector $f(h)$ in a normed space E with norm $\| \, \|_E$ and a positive real valued function $g(h)$, we write*

$$f(h) = \tilde{\mathcal{O}}\left(g(h)\right), \quad (\textit{as } h \to 0) \tag{3.4}$$

if there exists $\eta_0 > 0$ such that

$$\forall \eta \in (0, \eta_0), \quad \exists C_\eta > 0, \quad \forall h \in (0, h_0), \quad \|f(h)\|_E \leq C_\eta e^{\frac{\eta}{h}} g(h)\,.$$

3.2 Decay estimate

Like in Proposition 2.1, Ω denotes an open interval in I and H^h_Ω the self-adjoint Dirichlet realization of $P^h[V^h]$ with domain $H^1_0(\Omega) \cap H^2(\Omega)$.

We shall use the following result about the decay of the eigenfunctions of H^h_Ω.

Proposition 3.3 *Suppose that $U_\Omega := \{c_1, \ldots, c_N\} \cap \Omega$ is not empty. For every $h > 0$ sufficiently small, let $\lambda^h \in (\Lambda_*, \Lambda^*)$ be an eigenvalue of H^h_Ω and ϕ^h an L^2-normalized corresponding eigenfunction:*

$$(H^h_\Omega - \lambda^h)\phi^h = 0.$$

Then, the estimate

$$\forall x \in \Omega, \quad \left| \frac{d^j}{dx^j} \phi^h(x) \right| \leq C h^{-2j-1} e^{-\frac{\tilde{d}_h(x, U_\Omega)}{h}}, \quad j \in \{0, 1\}\,,$$

holds with $C > 0$ uniform w.r.t $h \in (0, h_0)$ if $\tilde{d}_h$ stands for the Agmon distance for the potential $\tilde{\mathcal{V}}^h$ at the energy λ^h.

Remark 5 *Note that contrary to the general use, we do not introduce at this level the $\tilde{\mathcal{O}}$ but an accurate estimate made possible in this simple one-dimensional case. This accurate estimate will be combined in the proof of Theorem 3.4 with the uniform Lipschitz estimate on $\tilde{\mathcal{V}}^h$ (see especially* (3.11), (3.12), (3.13)*). This provides a complete splitting between the semiclassical and quantum scale in spite of a limited regularity assumption.*

Proof: Set $\Omega = [\alpha, \beta]$. 1) Let us begin with the estimate of $\phi^h(x)$.
Apply the Agmon identity of Appendix A with $P = P^h$, $z = \lambda^h$, $u_1 = u_2 = \phi^h$ and $\varphi(x) = \tilde{d}_h(x, U_\Omega)$ where ϕ^h is an eigenfunction of H^h_Ω with eigenvalue λ^h. Since $\mathcal{V}^h - \lambda^h - \varphi'^2 = -W^h$, the inequalities $\varphi = \mathcal{O}(h)$ in U^h and $\|\phi^h\|_{L^2} = 1$ imply

$$e^{\pm\frac{\varphi}{h}} = \mathcal{O}(1) \text{ in } U^h \quad \text{and} \quad \int (\mathcal{V}^h - \lambda^h - \varphi'^2)\, |v^h|^2 = \mathcal{O}(1).$$

From the Agmon identity, we deduce an estimate for $v^h = e^{\varphi/h}\phi^h$:

$$\left\| h\frac{dv^h}{dx} \right\|_{L^2} = \mathcal{O}(1).$$

Since $v^h(\alpha) = v^h(\beta) = 0$, it follows

$$\left\| v^h \right\|_{L^2} + \left\| \frac{dv^h}{dx} \right\|_{L^2} = \mathcal{O}\left(\frac{1}{h}\right).$$

This implies

$$\|v^h\|_{L^\infty} = \mathcal{O}\left(\frac{1}{h}\right),$$

and then

$$\forall x \in \Omega, |\phi^h(x)| \leq \frac{C}{h} e^{-\tilde{d}_h(x,U_\Omega)}.$$

2) For the estimate of $d\phi^h/dx$, we use the equation

$$\begin{cases} -h^2\dfrac{d^2\phi^h}{dx^2} + \mathcal{V}^h\phi^h = \lambda^h\phi^h, \\ \phi^h(\alpha) = \phi^h(\beta) = 0. \end{cases}$$

As $\phi^h \in \mathcal{C}^1([\alpha,\beta])$, there exists $c \in (\alpha,\beta)$ such that $\frac{d\phi^h}{dx}(c) = 0$. The function g defined by $g = e^{\varphi/h}\, d\phi^h/dx$ satisfies

$$\begin{cases} h^2 g' = h\varphi' e^{\frac{\varphi}{h}} \dfrac{d\phi^h}{dx} + h^2 e^{\frac{\varphi}{h}} \dfrac{d^2\phi^h}{dx^2}, \\ h^2 g(c) = 0. \end{cases}$$

Using the equation satisfies by ϕ^h, we deduce

$$\begin{aligned} h^2 g' &= h\varphi' \left(e^{\frac{\varphi}{h}}\phi^h\right)' - |\varphi'|^2 e^{\frac{\varphi}{h}}\phi^h + (\mathcal{V}^h - \lambda^h)\, e^{\frac{\varphi}{h}}\phi^h \\ &= h\varphi' \frac{dv^h}{dx} - |\varphi'|^2 v^h + (\mathcal{V}^h - \lambda^h) v^h. \end{aligned}$$

Then $\|h^2 g'\|_{L^2} = \mathcal{O}(1/h)$. Cauchy-Schwarz inequality gives the L^∞-estimate for g : $|g(x)| \leq C/h^3$ for any $x \in [\alpha,\beta]$ and also of $d\phi^h/dx$:

$$\forall x \in \Omega = [\alpha,\beta], \quad \left| \frac{d\phi^h}{dx}(x) \right| \leq \frac{C}{h^3}\, e^{-\tilde{d}_h(x,U_\Omega)}.$$

□

Remark. When the potential is regular, a better estimate like

$$\forall x \in \Omega, \quad \left|\phi^h(x)\right| \leq C h^{-\frac{1}{2}} e^{-\tilde{d}_h(x,U_\Omega)/h},$$

holds and even a complete WKB expansion is possible. Here the low regularity and the concentration of the quantum wells prevent from such an accurate result.

3.3 Spectrum for one single well

From the spectral viewpoint, we are interested in localizing the eigenvalues of H^h_Ω in the limit $h \to 0$. The first result concerns the problem with one well.

Theorem 3.4 *Let Ω be a sub-interval of (a,b) containing exactly one well c_i, $i \in \{1,\dots,N\}$. Then :*
i) Every eigenvalue of H^h_Ω in (Λ_*,Λ^*) converges, and the limit belongs to the set $\mathcal{E}_i$ (see (1.32)).
ii) For every $\lambda_0 \in (\Lambda_*,\Lambda^*) \cap \mathcal{E}_i$ and any fixed small enough $\varepsilon > 0$, the Dirichlet Hamiltonian H^h_Ω has exactly one eigenvalue in $[\lambda_0 - \varepsilon, \lambda_0 + \varepsilon]$ for $h \in (0, h_\varepsilon)$.

Proof: Call $\{\lambda^h_1,\dots,\lambda^h_r\}$ the eigenvalues of H^h_Ω in the interval $[\Lambda_*,\Lambda^*]$, and $\phi^h_1,\dots,\phi^h_r$ an orthonormal system of corresponding eigenfunctions. Because of Proposition 2.1, since the rank of the spectral projections are given by traces of functions of H^h_Ω one has:

$$r = \mathcal{O}(1), \quad h \to 0$$

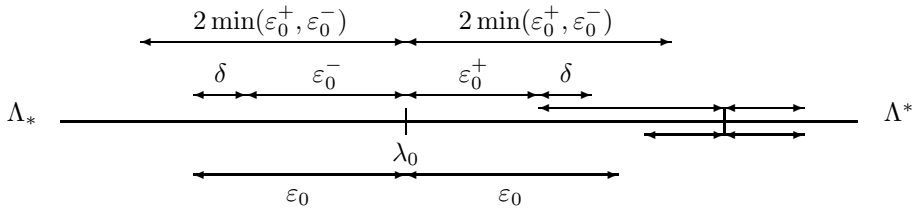
(take for θ a smooth version of the function $\mathbf{1}_{[\varepsilon,\Lambda_0]}$, $\varepsilon > 0$ small). The idea is to use the ellipticity of the problem, and the scaling of the wells in order to replace the potential $\tilde{\mathcal{V}}^h$ near a well by a constant one. Let $\hat{H}^h$ the Hamiltonian with domain $H^2(\mathbb{R})$ given by:

$$\forall u \in D(\hat{H}^h), \quad \hat{H}^h u := \hat{P}^h u, \quad \hat{P}^h := -h^2 \frac{d^2}{dx^2} + \tilde{\mathcal{V}}^h(c_i) \cdot \mathbf{1} - w_i\left(\frac{x - c_i}{h}\right). \tag{3.5}$$

This Hamiltonian is unitarily equivalent to $-\Delta + \tilde{\mathcal{V}}^h(c_i) - w_i(\cdot - c_i)$, whose eigenvalues is the set

$$\mathcal{E}^h_i := \mathcal{E}_i + \alpha^h_i, \quad \alpha^h_i = \tilde{\mathcal{V}}^h(c_i) - \tilde{\mathcal{V}}^0(c_i) \to 0, \quad h \to 0. \tag{3.6}$$

Since $\|\tilde{\mathcal{V}}^h - \tilde{\mathcal{V}}^0\|_{\mathcal{C}^0} \to 0$ when $h \to 0$, for any $\lambda_0 \in [\Lambda_*,\Lambda^*] \cap \mathcal{E}_i$ there exists $\varepsilon_0 > 0$ such that $\hat{H}^h$ has exactly one eigenvalue in $(\lambda_0 - \varepsilon_0, \lambda_0 + \varepsilon_0)$. To analyze the spectrum of H^h in the whole set $[\Lambda_*,\Lambda^*]$, we then choose, for each λ_0, two numbers $\varepsilon^+_0 > 0$, $\varepsilon^-_0 > 0$ such that the intervals $(\lambda_0 - \varepsilon^-_0, \lambda_0 + \varepsilon^+_0)$ are disjoint and their union covers a compact neighborhood of $[\Lambda_*,\Lambda^*]$ and such that $\hat{H}^h$ has no eigenvalues in each annulus $\{\varepsilon_0 < |\lambda - \lambda_0| < 2\min\{\varepsilon^+_0, \varepsilon^-_0\}\}$.



Let now $\eta > 0$, and χ a smooth cut-off function supported in Ω such that $\chi = 1$ if $d(x,\partial\Omega) \geq 2\eta$ and $\chi = 0$ if $d(x,\partial\Omega) \leq \eta$. Owing to the exponential decay of the ϕ^h_j's stated in Proposition 3.3, the estimate

$$\langle \chi\phi^h_j, \chi\phi^h_k \rangle_{L^2(\Omega)} = \delta_{jk} + \mathcal{O}\left(e^{-\frac{c_0}{h}}\right), \quad j,k \in \{1,\dots,r\}, \tag{3.7}$$

for some $c_0 > 0$ independent on $h > 0$ and $\eta > 0$.
For any $j \in \{1,\dots,r\}$, the function $\chi\phi^h_j$ belongs to the domain of $\hat{H}^h$ with the identity

$$\hat{P}^h \chi\phi^h_j = \lambda^h_j \chi\phi^h_j + [P^h,\chi]\phi^h_j + (\tilde{\mathcal{V}}^h(c_i) - \tilde{\mathcal{V}}^h(x))\chi\phi^h_j. \tag{3.8}$$

Owing to the exponential decay of ϕ_j^h, the commutator term satisfies:

$$\|[P^h,\chi]\phi_j^h\|_{L^2(\Omega)} = \mathcal{O}\left(h^{-1}e^{-\frac{\tilde{d}_h(c_i,\partial\Omega)-2\eta}{h}}\right), \tag{3.9}$$

where $\tilde{d}_h$ is the Agmon distance for $\tilde{\mathcal{V}}^h$ at the energy λ_i^h. Because the potential $\tilde{\mathcal{V}}^h$ is greater than Λ_0 and $\lambda_i^h \leq \Lambda^* < \Lambda_0$, the r.h.s in (3.9) is of order $O(e^{-c'/h})$ with c' independent of the potential and the energy.
For the last term of the r.h.s. of (3.8), just write for $\varepsilon > 0$

$$\begin{aligned}[\tilde{\mathcal{V}}^h(c_i)-\tilde{\mathcal{V}}^h(x)]\chi\phi_j^h &= \mathbf{1}_{|x-c_i|\leq\varepsilon}\cdot[\tilde{\mathcal{V}}^h(c_i)-\tilde{\mathcal{V}}^h(x)]\chi\phi_j^h \\ &+ \mathbf{1}_{|x-c_i|>\varepsilon}\cdot[\tilde{\mathcal{V}}^h(c_i)-\tilde{\mathcal{V}}^h(x)]\chi\phi_j^h.\end{aligned} \tag{3.10}$$

Since the family of potentials $(\tilde{\mathcal{V}}^h)_{h>0}$ is $W^{1,\infty}(I)$-bounded, the first term is treated by writing

$$\left\|\mathbf{1}_{|x-c_i|\leq\varepsilon}\cdot[\tilde{\mathcal{V}}^h(c_i)-\tilde{\mathcal{V}}^h(x)]\chi\phi_j^h\right\|_{L^2(\Omega)} \leq \varepsilon\sup\|\tilde{\mathcal{V}}^h\|_{W^{1,\infty}}\|\chi\phi_j^h\|_{L^2(\Omega)} = \mathcal{O}(\varepsilon), \tag{3.11}$$

and again by the accurate decay estimates of Proposition 3.3, the second term is estimated by

$$\left\|\mathbf{1}_{|x-c_i|>\varepsilon}\cdot(\tilde{\mathcal{V}}^h(c_i)-\tilde{\mathcal{V}}^h(x))\chi\phi_j^h\right\|_{L^2(\Omega)} = \mathcal{O}\left(e^{-\frac{c_0'\varepsilon}{h}}\right). \tag{3.12}$$

We then choose

$$\varepsilon := h^\alpha, \quad \alpha\in(0,1), \tag{3.13}$$

and we obtain by combining (3.12), (3.11), (3.9), (3.8)

$$\forall j=1,\dots,r, \quad \hat{P}^h\chi\phi_j^h = \lambda_j^h\chi\phi_j^h + \mathcal{O}(h^\alpha) \quad \text{in } L^2(\Omega). \tag{3.14}$$

Now, fix $\delta>0$ such that $\hat{H}^h$ has no eigenvalue in $\{\varepsilon_0^+ < \lambda-\lambda_0 < \varepsilon_0^+ + \delta\}\cup\{-\varepsilon_0^- - \delta < \lambda-\lambda_0 < -\varepsilon_0^+\}$ and apply Proposition C.1 (see Appendix C) to $A=\hat{H}^h$, $[\lambda_-,\lambda^+] = [\lambda_0-\varepsilon_0^-,\lambda_0+\varepsilon_0^+]$, $N=r$, $a=\delta>0$, $\mu_j=\lambda_j^h$, $\psi_j=\chi\phi_j^h$, from which we conclude

$$\vec{d}\Big(\text{span}\,\{\chi\phi_1^h,\dots,\chi\phi_r^h\},\mathbf{1}_{[\lambda_0-\varepsilon_0^-,\lambda_0+\varepsilon_0^+]}(\hat{H}^h)\Big) \leq \left(\frac{r}{1+o(1)}\right)^{1/2}\frac{\varepsilon}{a} = \mathcal{O}(h^\alpha). \tag{3.15}$$

This last estimate forces H^h to have at most one eigenvalue in $[\lambda_0-\varepsilon_0^-,\lambda_0+\varepsilon_0^+]$, $r\leq 1$, when $h>0$ is small enough.

We finish by proving $i)$ and $ii)$. For this, let $\hat{\phi}_0^h$ be a normalized eigenvector for the eigenvalue λ_0 of the Hamiltonian $\hat{H}^h = -h^2d^2/dx^2+\tilde{\mathcal{V}}^0(c_i)-w_i((\cdot-c_i)/h)$, unitarily equivalent to $-d^2/dx^2+\tilde{\mathcal{V}}^0(c_i)-w_i$ Then $\hat{\phi}_0^h$ is an eigenvector of $\hat{H}^h$ for the eigenvalue $\lambda_0+\alpha_i^h$ (see (3.6)). Estimates similar to (3.9), (3.11), (3.12) lead to

$$P^h\hat{\phi}_0^h = (\lambda_0+\alpha_i^h)\hat{\chi}\hat{\phi}_0^h + \mathcal{O}(h^\alpha) \quad \text{in } L^2(\Omega). \tag{3.16}$$

Apply again Proposition C.1 in a small interval centered around $\lambda_0+\alpha_i^h$ in the following way: since $\hat{H}^h$ has at most one eigenvalue in $[\lambda_0-\varepsilon_0^-,\lambda_0+\varepsilon_0^+]$, it is easy to choose a convenient parameter a in Proposition C.1 (Appendix C) by a simple argument of counting: set $L_j := [jh^{\alpha/2},(j+1)h^{\alpha/2}[$, and $K_j := -L_j\cup L_j$. If $\{\lambda_0+\alpha_i^h\}+K_1$ contains the eigenvalue, one defines $I_h = [\lambda_0+\alpha_i^h - 2h^{\alpha/2},\lambda_0+\alpha_i^h+2h^{\alpha/2}]$, else $I_h = [\lambda_0+\alpha_i^h-h^{\alpha/2},\lambda_0+\alpha_i^h+h^{\alpha/2}]$. This furnishes an interval I_h

of diameter $\mathcal{O}(h^{\alpha/2})$ around $\lambda_0 + \alpha_i^h$ and a real $a = a(h) > 0$ of order $h^{\alpha/2}$ leading again with Proposition C.1 to

$$\vec{d}\big(\mathrm{span}\,(\chi\hat{\phi}_0^h), \mathbf{1}_{I_h}(H_\Omega^h)\big) = \mathcal{O}(h^{\alpha/2})\,. \tag{3.17}$$

This yields $r = 1$ and the convergence of the eigenvalue to λ_0. □

Remark 6 *It follows that the well c_i is λ-resonant if and only if there exists a domain Ω containing c_i such that for any open set $\omega \subset \Omega$ the Dirichlet operator H_ω^h has an eigenvalue converging to λ as h goes to 0.*

3.4 Spectrum in the multiple wells case

A way of studying the spectral properties of the multiple wells Dirichlet problem consists in decoupling it into N one-well problems. Following [Hel] or [HeSj3], a good choice of open sets is the following: fix $\lambda \in [\Lambda_*, \Lambda^*]$, and if $\tilde{d}_h$ (resp. $\tilde{d}_0$) denotes the Agmon distance at the energy λ for the potential $\tilde{\mathcal{V}}^h$ (resp. $\tilde{\mathcal{V}}^0$), we define

$$S_1 := \min_{j\neq k} \tilde{d}_h(c_j, c_k) \quad (= S_1(h)) \tag{3.18}$$

and for a fixed small enough $\eta > 0$,

$$\Omega_i := I \setminus \bigcup_{k\neq i} \{x \in I, \tilde{d}_0(x, c_k) \leq \eta\}, \quad i = 1, \ldots, N\,. \tag{3.19}$$

The h-dependance of S_1 recalled between the parentheses of (3.18) is omitted in the sequel.

Note that these open sets are not disjoint and Ω_i contains only the well c_i. The use of the distance $\tilde{d}_0$ makes sure that they do not depend on h although the h-dependence would be well controlled.
We first eliminate the non resonant wells before giving a result similar to Theorem 3.4.

Proposition 3.5 *Let λ be an asymptotic resonant energy and suppose that the well c_i is not λ-resonant. Then there exists a positive constant c such that for any eigenvalue $\lambda^h \in (\lambda - c, \lambda + c)$, one has*

$$\forall x \in (c_i - c, c_i + c), \quad |\phi^h(x)| \leq e^{-\frac{c}{h}}, \quad h \to 0$$

where ϕ^h is an L^2-normalized eigenfunction of H_I^h for the eigenvalue λ^h.

In plain words, eigenfunctions for eigenvalues converging to λ are exponentially small in the non λ-resonant wells.
Proof: Since λ is not a resonant energy for the well c_i, we can choose the open set ω containing the only well c_i and the compact energy interval $\Lambda \ni \lambda$ such that for $h > 0$ sufficiently small, the Dirichlet operator H_ω^h has no spectrum in Λ (see Remark 6). For a smooth cut-off function θ supported in ω and equal to 1 on a δ-neighborhood of c_i ($\delta > 0$ small), one has

$$P^h\theta\phi^h = \lambda^h\theta\phi^h + [P^h, \theta]\phi^h. \tag{3.20}$$

The residual term satisfies by Proposition 3.3 the decay estimate

$$\|[P^h, \theta]\phi^h\|_{L^2(I)} \leq C_\delta e^{-\frac{c_\delta}{h}}, \quad c_\delta > 0, \quad h \to 0.$$

Note that the vector $\theta\phi^h$ is not zero.

Apply again Proposition C.1 in a compact interval strictly contained in Λ and $a > 0$ not depending on $h > 0$. If we denote by F the spectral subspace for H^h_ω associated to this compact interval, it follows

$$\vec{d}(\mathrm{span}\{\theta\phi^h\}, F) \leq \frac{1}{\|\theta\phi^h\|}\frac{C_\delta e^{-\frac{c_\delta}{h}}}{a}. \tag{3.21}$$

Since F is null by choice of Λ, it follows by properties of the distance $\vec{d}$ that the l.h.s. of (3.21) is greater than 1. This provides an L^2-estimate of $\theta\phi^h$. The H^2 regularity of a solution to (3.20) provides the pointwise estimate in $(c_i-\delta, c_i+\delta)$. Finally choose the constant $c > 0$ small enough. □

The analogous to Theorem 3.4 writes

Theorem 3.6 *Recall that H^h_ω denotes the Dirichlet realization of P^h to the open set ω. Then, for $h > 0$ sufficiently small :*
i) After ordering, every eigenvalue of H^h_I in (Λ_*, Λ^*) converges as $h \to 0$ and the limit belongs to the set $\mathcal{E}_0$ (see (1.32)).
ii) For every $\lambda \in (\Lambda_*, \Lambda^*) \cap \mathcal{E}_0$ and any small enough $\varepsilon > 0$, the operators H^h_I has exactly m_λ eigenvalue(s) in $[\lambda - \varepsilon, \lambda + \varepsilon]$ as soon as $h < h_\varepsilon$.
Call them λ^h_i $(i \in J_\lambda)$.
iii) Fix such a λ. Let $(\Omega_i)_{i\in J_\lambda}$ the subdomains of I defined in (3.19). Call $(\psi^h_i)_{i\in J_\lambda}$ normalized eigenvectors associated to the unique eigenvalue of $H^h_{\Omega_i}$ converging to λ. There exists a unitary matrix $(p^h_{i,j})_{1\leq i,j\leq m_\lambda}$ such that in $L^2(I)$

$$\forall i \in J_\lambda, \quad \phi^h_i - \sum_{j\in J_\lambda} p^h_{i,j}\psi^h_j = \tilde{\mathcal{O}}\left(e^{-\frac{S_1}{h}}\right),$$

with S_1 defined according to (3.18).

Proof: It suffices to follow the proof in [Hel, pp. 34-35], while Proposition 3.5 guarantees that the non resonant wells are negligible in the decay estimates (see also [Pat, p. 148] for details). □

3.5 Resolvent estimates

Let us briefly recall the decay results of the kernel of the resolvents. Fix $\eta > 0$ (η small) and for a point $p \in (a, b)$, let χ_p denote a smooth cut-off function supported in the set $\{|x - p| \leq \eta\}$.

Like in [HeSj3, p. 143] (see also [DiSj] or [Pat, p. 135] for this specific case), the combination of the Agmon estimate (see Appendix A) with the spectral theorem provides in the one well-case ($N = 1$) the following estimates

$$\forall z \notin \sigma(H^h_I), \quad \left\|\chi_x(H^h_I - z)^{-1}\chi_y\right\| \leq C_\eta \frac{e^{\frac{-\tilde{d}_h(x,y)+C\eta}{h}}}{\min(r_h, 1)}, \tag{3.22}$$

where $r_h = \mathrm{dist}(z, \sigma(H^h_I))$, and $\tilde{d}_h$ is the Agmon distance for the potential $\tilde{\mathcal{V}}^h$ at the energy $\lambda := \mathrm{Re}(z)$.

A straightforward adaptation of the analysis of the multiple wells Dirichlet problem carried out in [HeSj2], [HeSj3, p. 147] or [Pat, p. 151] provides the same estimate for $N > 1$.

Proposition 3.7 *For h in $(0, h_0)$, h_0 small enough, consider $z_h \in \mathbb{C} \setminus \sigma(H^h_I)$ such that there exists $\lambda_0 \in [\Lambda_*, \Lambda^*]$ with $z_h \to \lambda_0$ as $h \to 0$ and set $\lambda_h = Re(z_h)$ and $r_h = dist(z_h, \sigma(H^h_I))$. If*

$r_h \geq e^{-S_1/2h}$ with $S_1 := \min_{k\neq l} \tilde{d}_h(c_k, c_l)$, then the kernel of the resolvent $(H_I^h - z_h)^{-1}$ satisfies

$$\left|(H_I^h - z_h)^{-1}[x,y]\right| = \frac{\tilde{\mathcal{O}}\left(e^{-\frac{\tilde{d}_h(x,y)}{h}}\right)}{\min(r_h, 1)},$$

with uniform constants with respect to $x, y \in I$ and where $\tilde{d}_h$ is the Agmon distance for the potential $\tilde{\mathcal{V}}^h$ at the energy $\lambda_h := Re(z_h)$.

Proof: Let θ be a $\mathcal{C}^\infty$ even function supported in a neigborhood $[-3\eta, 3\eta]$ and equal to 1 on $[-\eta, \eta]$ where η and Ω_i are linked by relation (3.19). We define

$$\theta_i(x) := \theta(x - c_i), \quad \chi_i(x) = 1 - \sum_{j\neq i} \theta_j(x), \quad \forall i = 1, \ldots, N. \tag{3.23}$$

Let $\tilde{\chi}_i$ $\mathcal{C}^\infty$ functions with support in Ω_i defined in (3.19) such that

$$\sum_{i=1}^N \tilde{\chi}_i = 1.$$

We define

$$T_i(z) := (H_{\Omega_i}^h - z)^{-1} \quad \text{and} \quad R_0 := \sum_{i=1}^N \chi_i T_i(z) \tilde{\chi}_i.$$

Then we have

$$\begin{aligned}
(H_I^h - z)R_0 &= \sum_{i=1}^N \chi_i \tilde{\chi}_i + \sum_{i=1}^N [P^h, \chi_i] T_i(z) \tilde{\chi}_i \\
&= 1 + \sum_{i=1}^N [P^h, \chi_i] T_i(z) \tilde{\chi}_i \\
&= 1 - \sum_{i=1}^N \sum_{k\neq i} [P^h, \theta_k] T_i(z) \tilde{\chi}_i,
\end{aligned}$$

since $\chi_i \tilde{\chi}_i = \tilde{\chi}_i$ and using (3.23). We have to study the convergence of the serie $\sum_{n\geq 0} R_0 \varepsilon^n$ with $\varepsilon = \sum_{i=1}^N \sum_{k\neq i} [P^h, \theta_k] T_i(z) \tilde{\chi}_i$. We notice that $\tilde{\chi}_i [P^h, \theta_k]$ is equal to 0 as soon $k \neq i$ and if $k = i$, this term is $[P^h, \theta_k]$. Then,

$$R_0 \varepsilon^n = \sum_{i_0=1}^N \sum_{i_1\neq i_0}^N \cdots \sum_{i_{n-1}\neq i_n}^N \chi_{i_0} T_{i_0} [P^h, \theta_{i_1}] T_{i_1} [P^h, \theta_{i_2}] T_{i_2}, \ldots, [P^h, \theta_{i_n}] T_{i_n} \tilde{\chi}_{i_n}.$$

Since the function θ_k is localized in a neighborhood of the well c_k, we can write for $s = 0, 1, \ldots, N-1$

$$[P^h, \theta_{i_s}] T_{i_s}(z) [P^h, \theta_{i_{s+1}}] = [P^h, \theta_{i_s}] \chi_{i_s} T_{i_s}(z) \chi_{i_{s+1}} [P^h, \theta_{i_{s+1}}].$$

This last relation allows to use results on the one-well problem (3.22), then

$$\left\|\chi_{i_s} T_{i_s}(z) \chi_{i_{s+1}}\right\| \leq C_\eta \frac{e^{-\frac{\tilde{d}_h(x,y) - C\eta}{h}}}{\min(r_h, 1)}.$$

This leads to the following estimate

$$\|\chi_{x_0} R_0 \varepsilon^n \chi_{y_0}\| \leq C_\eta^{n+1} \frac{e^{-\frac{\varphi_n(x_0,y_0)-nC\eta}{h}}}{\min(r_h,1)^{n+1}},$$

where $\varphi_n(x_0,y_0) = \min_{i_0,\ldots,i_n} d(y_0,c_{i_n}) + d(c_{i_n},c_{i_{n-1}}) + \ldots + d(c_{i_1},c_{i_0}) + d(c_{i_0},x_0)$. In fact, the function φ_n is the length of the the shortest way from y to x going through n different wells. We can bound from below φ_n by

$$\varphi_n(x_0,y_0) \geq d(x_0,y_0) + nS_1.$$

Then the serie is convergent under the assumption $r_h \geq e^{-S_1/2h}$ and we can write

$$\chi_{x_0}(H_I^h - z)^{-1}\chi_{y_0} = \sum_{n\geq 0} \chi_{x_0} R_0 \varepsilon^n \chi_{y_0}.$$

Appendix E provides the pointwise estimates. □

Corollary 3.8 *If $r_h \geq C^{-1}h^C$ for some $C > 0$, then*

$$\left|(z - H_I^h)^{-1}[x,y]\right| = \tilde{\mathcal{O}}\left(e^{-\tilde{d}_h(x,y)}\right).$$

Another consequence is the improved pointwise estimate for the eigenfunctions of the Dirichlet problem ([HeSj3, p.138] or [Pat, p. 153]):

Proposition 3.9 *For every $h > 0$ sufficiently small, let $\lambda^h \in (\Lambda_*, \Lambda^*)$ and ϕ^h an L^2-normalized corresponding eigenfunction of H_Ω^h. Suppose that $\lambda^h \to \lambda_0 \in \mathcal{E}_0 \cap (\Lambda_*, \Lambda^*)$. Then the estimates*

$$\forall x \in \Omega, \quad \left|\frac{d^j}{dx^j}\phi^h(x)\right| = \tilde{\mathcal{O}}\left(e^{-\frac{\tilde{d}_0(x,U_0)}{h}}\right), \quad j \in \{0,1\},$$

hold when $\tilde{d}_0$ stands for the Agmon distance for the potential $\tilde{\mathcal{V}}^0$ at the energy λ_0 and $U_0 = \cup_{i\in J_{\lambda_0}} \{c_i\}$ for the set of λ_0-resonant wells.

Remark 7 *Here the $\tilde{\mathcal{O}}$-writing of the estimates allows to replace the h-dependent quantities, $\tilde{\mathcal{V}}^h$, $\tilde{d}_h$ and λ_h by their asymptotic values $\tilde{\mathcal{V}}^0$, $\tilde{d}_0$ and λ_0.*

4 Complex deformation

4.1 A reduced Stone's formula

The results of Theorem 1.6 are derived from a good information about the asymptotic local density of states associated with functions of the Hamiltonian. According to Stone's formula and the limiting absorption principle, a possible method is the computing of a quite precise expression of the resolvent, since for $\lambda \in [\Lambda_*, \Lambda^*] \subset \sigma_{\rm ac}(H^h)$ ($H^h = H^h[V^h]$):

$$\frac{1}{2i\pi}\mathbf{1}_I\left[(H^h - (\lambda + i0))^{-1} - (H^h - (\lambda - i0))^{-1}\right]\mathbf{1}_I = \mathbf{1}_I \frac{\partial E}{\partial \lambda}(\lambda)\mathbf{1}_I\,, \tag{4.1}$$

and of its meromorphic extension through the spectral half-line $(0,\infty) \subset [-B,\infty)$, in order to take into account the contribution of resonant states.
We will focus on this meromorphic extension from the upper-half plane while the corresponding

results for the extension from the lower-half plane are easily carried over after changing i into $-i$.
Resolvent. Fix $z \in \mathbb{C}$, $\mathrm{Im}(z) > 0$ and consider the problem with unknown $u \in H^2(\mathbb{R})$:

$$(P^h - z)u = f, \quad f \in L^2(I), \quad z \in \mathbb{C}, \quad \mathrm{Im}(z) > 0, \quad \mathrm{Re}(z) \in (\Lambda_*, \Lambda^*). \tag{4.2}$$

Again because the potential is constant on both sides of the interval I, the problem with unknown $u \in H^2(\mathbb{R})$:

$$(P^h - z)u = f, \quad f \in L^2(I)\,,$$

can be explicitly solved outside I, and the condition $u \in L^2$ eliminates exponentially growing modes. It is easy to check that this condition is exactly given by (1.17)-(1.18) when $\mathrm{Im}(z) > 0$. Precisely, we can write the next statement.

Proposition 4.1 *Let $z \in \mathbb{C}$, $Im(z) > 0$, $Re(z) \in (\Lambda_*, \Lambda^*)$. Consider the linear functionals $T_a(z)$, $T_b(z)$ on $H^2(I)$ given by :*

$$T_a(z)u := \left[h\partial_x + iz^{1/2}\right]_{|x=a} u, \quad T_b(z)u := \left[h\partial_x - i(z+B)^{1/2}\right]_{|x=b} u,$$

and the closed unbounded operator H_z^h defined by

$$D(H_z^h) := \left\{u \in H^2(I) \text{ s.t. } T_a(z)u = T_b(z)u = 0\right\},$$

$$\forall u \in D(H_z^h), \quad H_z^h u := P^h u.$$

Then the restriction on I of the solution to equation (4.2) is $(H_z^h - z)^{-1} f$. In other words :

$$\mathbf{1}_I (H^h - z)^{-1} \mathbf{1}_I = (H_z^h - z)^{-1}, \quad Im(z) > 0, \quad Re(z) \in (\Lambda_*, \Lambda^*).$$

Remark 8

1. *We will check that for such $z's$, operator $H_z^h - z$ is invertible (see Proposition 4.2 and Proposition 5.2 below).*
2. *Note that since the solutions on I of the homogeneous equation associated with (4.2) make a linear 2-dimensional subspace of $H^2(I)$, the injectivity of operator $(H_z^h - z)$ is equivalent to the independence of the functionals $T_a(z)$, $T_b(z)$.*
3. *By replacing i by $-i$ in the definitions of the functionals $T_a(z)$ and $T_b(z)$, one obtains the corresponding boundary conditions for $Im(z) < 0$.*

4.2 Resonances

In our one-dimensional situation, it is quite simple to detect the resonances as poles of the scattering matrix. According to the end of Subsection 4.1, one states

Proposition 4.2 *Let z a complex number such that $Re(z) > 0$. Then z is a resonance of the operator P if and only if $H_z^h - z$ is not injective.*

Indeed, the non-injectivity of $H_z^h - z$ is equivalent to the fact that the linear functionals are proportional, so the normalization given in (1.14)-(1.15) is not performable.

Remark 9 *The anti-resonances are defined similarly after considering the meromorphic extension from the lower half-plane $\{Im(z) < 0\}$ while changing i into $-i$ in the transparent boundary conditions (see Remark 8).*

4.3 Analysis of the resolvent

Recall that since we are interested in getting the spectral density inside the island I, Proposition 4.1 allows to work with $H_z^h - z$ in place of $H^h - z$. Moreover, because Theorem 3.6 ensures that the set $\mathcal{E}^0$ of asymptotic resonant energies is discrete, we will make the following reduction:

Assumption 4 *Suppose that the set $[\Lambda_*, \Lambda^*]$ contains exactly one asymptotic resonant energy $\lambda_0 \in (\Lambda_*, \Lambda^*)$. Recall that m_{λ_0} denotes its multiplicity according to (1.33) and that $(\lambda_j^h)_{1\le j\le m_{\lambda_0}}$ are the ordered eigenvalues of H_I^h lying in $[\Lambda_*, \Lambda^*]$ (and converging to λ_0).*

Introduce

$$\Omega_h := \{z \in \mathbb{C} \quad \text{s.t.} \quad \mathrm{Re}(z) \in K_h, \quad \mathrm{Im}(z) \in [-4h, 4h]\}\,, \tag{4.3}$$

$$\text{with} \qquad K_h := [\lambda_0 - \alpha^h, \lambda_0 + \alpha^h]\,, \tag{4.4}$$

$$\text{and} \qquad \alpha^h := 4\max\left\{h, |\lambda_0 - \lambda_j^h|,\, j = 1, \dots, m_{\lambda_0}\right\}\,. \tag{4.5}$$

The parameter z is assumed to satisfy

$$z \in \Omega_h\,.$$

Proposition 3.9 indicates that from the spectral viewpoint, around a resonant energy the non resonant wells do not matter. We adapt to this remark the filled well Hamiltonians

$$\tilde{H}_I^h = H_I^h + W^h \quad \text{and} \quad \tilde{H}_z^h = H_z^h + W^h\,. \tag{4.6}$$

Set then for given $\lambda \in (\Lambda_*, \Lambda^*)$

$$W_\lambda^h := \sum_{i\in J_\lambda} w_i\left(\frac{\cdot - c_i}{h}\right), \quad U_\lambda^h := \mathrm{supp}\, W_\lambda^h. \tag{4.7}$$

Define then

$$\tilde{H}_I^h(\lambda) := H_I^h + W_\lambda^h \quad \text{and} \quad \tilde{H}_z^h(\lambda) := H_z^h + W_\lambda^h\,, \tag{4.8}$$

the operators associated to respectively the Dirichlet and transparent problems with the λ-resonant wells filled. The parameter λ remains fixed as $h \to 0$ and those definitions lead to

$$\tilde{H}_\bullet^h(\lambda) = H_\bullet^h$$

when $\lambda \neq \lambda_0$ and

$$\tilde{H}_\bullet^h(\lambda_0) = H_\bullet^h + W_{\lambda_0}^h\,.$$

In particular, $\tilde{H}_I^h(\lambda_0)$ has no eigenvalue in $[\Lambda_*, \Lambda^*]$.

An accurate analysis of the resolvent $(H_z^h - z)^{-1}$ starts with essentially two steps :

1. Eliminate the non resonant wells : we show that $\tilde{H}_z^h(\lambda_0) - z$ is invertible for all $z \in \Omega_h$.
2. Check that for z far from λ_0, $H_z^h - z = \tilde{H}_z^h(\lambda) - z$, $\lambda \neq \lambda_0$, is invertible.

Hence the notation $\tilde{H}_z^h(\lambda)$ is convenient for a compact formulation of different results.

Proposition 4.3 *Make the Assumption 4 and fix any $\lambda \in [\Lambda_*, \Lambda^*]$.*
i) For any $z \in \Omega_h$ if $\lambda = \lambda_0$ (resp. $z \in [\Lambda_*, \Lambda^*] \times [-4h, 4h]$ and $\mathrm{dist}(z, \lambda_0) > \alpha^h/2$ or $|Im(z)| \ge 2h$ if $\lambda \neq \lambda_0$), the operator $\tilde{H}_z^h(\lambda) - z$ is invertible. The kernel of the resolvent is estimated by

$$\left|(\tilde{H}_z^h(\lambda) - z)^{-1}[x, y]\right| = \tilde{\mathcal{O}}\left(e^{-\frac{\tilde{d}(x,y)}{h}}\right)\,,$$

where $\tilde{d}$ stands for the Agmon distance for the potential $\tilde{\mathcal{V}}^h$ at the energy $Re(z)$. Moreover the constants can be chosen uniform with respect to $x, y \in I$ and z.
ii) For any function $\varphi \in \mathcal{C}_c^0((a,b))$, $(\tilde{H}_z^h(\lambda) - z)^{-1}\varphi$ belongs to the space $\mathcal{L}^1$ of trace-class operators for $z \in \Omega_h$ if $\lambda = \lambda_0$ (resp. $z \in [\Lambda_*, \Lambda^*] \times [-4h, 4h]$ and $\mathrm{dist}(z, \lambda_0) > \alpha^h/2$ or $|Im(z)| \geq 2h$ if $\lambda \neq \lambda_0$), with the estimate

$$\left\|(\tilde{H}_z^h(\lambda) - z)^{-1}\varphi\right\|_{\mathcal{L}^1} \leq C_\varphi h^{-2}\,.$$

Remark 10 *In particular, applying i) with $\lambda = \lambda_0$, gives, since $H_z^h(\lambda) = H_z^h$ and using Prop. 4.2 that P^h has no resonance in the set*

$$\left\{z \in \Omega_h,\ |Im(z)| > 2h \text{ or } dist(z, \lambda_0) \geq \frac{\alpha_h}{2}\right\}\,.$$

Proof: The first statement will be proved in three steps a) b) and c) where the last two ones are very similar.
i)-a) We start with the strongly elliptic problem: suppose that $\lambda = \lambda_0$, $z \in \Omega_h$ and $J_{\lambda_0} = \{1, \ldots, N\}$, that is $\tilde{H}_z^h(\lambda_0) = \tilde{H}_z^h$ (every well is filled). We use the Agmon identity of Appendix A where φ is a $\mathcal{C}^1(I)$-function satisfying the eiconal condition:

$$\inf_{h>0, x\in I} \tilde{\mathcal{V}}^h(x) - \mathrm{Re}(z) - \varphi'^2(x) \geq m > 0\,,$$

and we take the real part of both sides. Since $z \in \Omega_h$ is possibly complex, there are boundary terms in the Agmon estimates (see Appendix A) but their coefficients are $\mathcal{O}(h^3)$. For $z \in \Omega_h$ and with the condition $\Lambda_0 - \Lambda^* > 0$ according Assumption 1, the coercivity of the variational formulation with the transparent conditions (see Proposition 4.1) is easily checked when $h > 0$ is small enough: Taking $\varphi \equiv 0$ provides the existence of the resolvent and uniform bounds.
Taking φ with the above eiconal condition provide the weighted estimate

$$\forall f \in L^2(I), \quad \left\|e^{\frac{\varphi}{h}}(\tilde{H}_z^h - z)^{-1} f\right\|_{1,h} \leq C \left\|e^{\frac{\varphi}{h}} f\right\|_{L^2}\,.$$

The case $\varphi \equiv (1-\eta)\tilde{d}(\cdot, y)$ for fixed $y \in (a,b)$ (which satisfies the eiconal condition) implies i) in this specific case. The pointwise estimate of the Schwartz kernel of the resolvent is obtained after Appendix E
i)-b) In the weaker case, $\lambda = \lambda_0$, $z \in \Omega_h$, $J_{\lambda_0} \neq \{1, \ldots, N\}$, the problem is neither self-adjoint nor strongly elliptic. Only the wells in $U_{\lambda_0}^h = \mathrm{supp}\, W_{\lambda_0}^h$ according to (4.7) are filled and the other non resonant wells are left. We use an approximation argument with the latter estimate. Set

$$S_0^z := \tilde{d}(U^h \setminus U_{\lambda_0}^h, \partial I) \tag{4.9}$$

where $\tilde{d}$ is the Agmon distance for the potential $\tilde{\mathcal{V}}^h$ and the energy $\mathrm{Re}(z)$. Introduce, for $\eta > 0$ small, the cut-off functions $\chi, \tilde{\psi}$ such that $0 \leq \chi, \tilde{\psi} \leq 1$, $\chi \equiv 1$ in the set $\{x \in I, \tilde{d}(x, U^h \setminus U_{\lambda_0}^h) \leq S_0^z - \eta\}$, $\tilde{\psi} \equiv 1$ in the set $\{\tilde{d}(x, \tilde{U}^h \setminus U_{\lambda_0}^h) \leq (S_0^z - \eta)/2\}$, $\chi \equiv 0$ in $\left\{\tilde{d}(x, U^h \setminus U_{\lambda_0}^h) \geq S_0^z - \eta/2\right\}$ and $\tilde{\psi} \equiv 0$ in the set $\{\tilde{d}(x, \tilde{U}_\lambda^h \setminus U_{\lambda_0}^h) \geq (S_0^z + \eta)/2\}$.
Choose

$$R(\lambda_0) := (\tilde{H}_z^h - z)^{-1}(1 - \tilde{\psi}) + \chi(\tilde{H}_I^h(\lambda_0) - z)^{-1}\tilde{\psi}. \tag{4.10}$$

as an approximate right inverse for $\tilde{H}_z^h(\lambda_0) - z$: Actually $\tilde{H}_z^h(\lambda_0)$ is replaced by the corresponding Dirichlet Hamiltonian around the remaining non λ_0-resonant wells. Note that $R(\lambda_0)$ is well defined since for $z \in \Omega_h$, z is uniformly far away from the spectrum of $\tilde{H}_I^h(\lambda_0)$.
A straightforward computation using $\tilde{H}_z^h(\lambda_0)\chi = \tilde{H}_I^h(\lambda_0)\chi$ and $\chi\tilde{\psi} = \tilde{\psi}$ gives

$$(\tilde{H}_z^h(\lambda_0) - z)R(\lambda_0) = 1 - \varepsilon, \quad \varepsilon := \varepsilon_0 + \varepsilon_1, \tag{4.11}$$

where

$$\varepsilon_0 := \tilde{W}_\lambda^h(\tilde{H}_z^h - z)^{-1}(1-\tilde{\psi}), \quad \varepsilon_1 := -[P^h,\chi](\tilde{H}_I^h(\lambda_0)-z)^{-1}\tilde{\psi}. \tag{4.12}$$

With the estimate about $(\tilde{H}_z^h - z)^{-1}$ and the control of the resolvent $(\tilde{H}_I^h(\lambda_0)-z)^{-1}$ of the Dirichlet Hamiltonian provided by Proposition 3.7 with the uniform lower bound $\mathrm{dist}(z,\sigma(H_I^h(\lambda_0))) \geq c > 0$, one deduces the inequality

$$\|\varepsilon_0\| + \|\varepsilon_1\| \leq C_\eta e^{\frac{-S_0^z + c\eta}{2h}}, \tag{4.13}$$

in the operator norm.
The relation

$$(\tilde{H}_z^h(\lambda_0) - z)R(\lambda_0) = 1 - \varepsilon, \quad \|\varepsilon\| \leq C_\eta e^{\frac{-S_0^z + c\eta}{2h}} \tag{4.14}$$

ensures the injectivity of $(\tilde{H}_z^h(\lambda_0) - z)$ and provides a right inverse after using the Neumann series for $(1-\varepsilon)^{-1}$.
Similarly, setting

$$L(\lambda_0) := (1-\tilde{\psi})(\tilde{H}_z^h - z)^{-1} + \tilde{\psi}(\tilde{H}_I^h(\lambda_0) - z)^{-1}, \tag{4.15}$$

leads to

$$L(\lambda_0)(\tilde{H}_z^h(\lambda_0) - z) = 1 + \varepsilon', \quad \|\varepsilon'\| \leq C_\eta e^{\frac{-S_0^z + c\eta}{2h}}, \tag{4.16}$$

and provides a left inverse for $\tilde{H}_z^h(\lambda_0) - z$.
The estimate of the kernel of the resolvent is now obtained after considering the first terms in the expansion series defining the inverse

$$\chi_x \cdot R(\lambda_0) \sum_{k=0}^{\infty} \varepsilon^k \cdot \chi_y.$$

The estimate for $k=0$ is clear according to the estimates of the kernels (part a) and Proposition 3.7) appearing in the definition of $R(\lambda_0)$. For $k \geq 1$, note first, since $\tilde{\psi}[P^h,\chi] = 0$ and $(1-\tilde{\psi})\tilde{W}_\lambda^h = 0$ that by computing the terms corresponding to $k=1$, $k=2$ and then by induction, the general term splits for any $k \geq 1$ into two terms, namely

$$\chi_x R(\lambda)\varepsilon^k \chi_y = \chi_x(\tilde{H}_z^h - z)^{-1}\left(\prod_{j=1}^{k} \varepsilon_{[j]}\right)\chi_y + \chi_x(\tilde{H}_I^h(\lambda_0) - z)^{-1}\left(\prod_{j=1}^{k} \varepsilon_{[j+1]}\right)\chi_y, \tag{4.17}$$

where $[\ell]$ stands for the class of ℓ *modulo* 2. Each term involves $k+1$ resolvents, which induces a prefactor $(C_\eta e^{\frac{c\eta}{2h}})^{k+1}$ in the estimate

$$\forall k \geq 1, \quad \|\chi_x \cdot R(\lambda)\varepsilon^k \cdot \chi_y\| \leq (C_\eta e^{\frac{c\eta}{2h}})^{k+1} e^{-\frac{\varphi_k(x,y)}{h}},$$

with

$$\varphi_k(x,y) = \min\{L_k(x,y), L_k(y,x)\}, \quad L_k(x,y) = \tilde{d}(x,\partial I) + (k-1)\frac{S_0^z}{2} + \tilde{d}(y,\tilde{U}_\lambda^h).$$

We conclude, since $\varphi_k(x,y) \geq \tilde{d}(x,y) + (k-2)S_0^z$, that the serie is convergent (the convergence is uniform w.r.t $z \in \Omega_h$). Again the pointwise estimate is provided by Appendix E.
i)-c) To finish the proof of *i*), it remains the case $\lambda \neq \lambda_0$, $\mathrm{dist}(z,\lambda_0) \geq \alpha_h/2$ or $|\mathrm{Im}(z)| \geq 2h$. The strategy is essentially the same as in *i*)-b): we replace $H_z^h = \tilde{H}_z^h(\lambda)$ by $\tilde{H}_z^h$ far away from the wells and by $\tilde{H}_I^h(\lambda) = H_I^h$ around non λ-resonant wells, which are all the wells. Consider this time

$$S_0^z := d(U^h, \partial I), \quad \text{with } U^h = \mathrm{supp} W^h$$

and χ, ψ such that $0 \leq \chi, \psi \leq 1$, $\chi \equiv 1$ in the set $\{x \in I, \tilde{d}(x, U^h) \leq S_0^z - \eta\}$, $\psi \equiv 1$ in the set $\{\tilde{d}(x, U^h) \leq (S_0^z - \eta)/2\}$ and $\psi \equiv 0$ in the set $\{\tilde{d}(x, U^h) \geq (S_0^z + \eta)/2\}$. Choose as an approximate right inverse (well defined for $z \in \Omega_h$ such that $|\mathrm{Im}(z)| > h$ or $\mathrm{dist}(z, \Lambda_0) \geq \alpha_h/2$)

$$R = (\tilde{H}_z^h - z)^{-1}(1 - \psi) + \chi(H_I^h - z)^{-1}\psi,$$

and as an approximate left inverse

$$L = (1 - \psi)(\tilde{H}_z^h - z)^{-1} + \psi(\tilde{H}_I^h - z)^{-1}.$$

One obtains again a norm-convergent series thanks to resolvent estimates and the pointwise estimates of the kernel are derived from Appendix E.
ii) We start again like for *i*) by the case where $\lambda = \lambda_0$, $J_{\lambda_0} = \{1, \ldots, N\}$. For H_0^h being the Dirichlet h-Laplacian on I, write, since $(H_0^h + i)\varphi = (\tilde{H}_z^h + i - z - \tilde{\mathcal{V}}^h)\varphi$:

$$\begin{aligned} \varphi(\tilde{H}_z^h - z)^{-1} &= (H_0^h + i)^{-1}\varphi[1 + (z + i - \tilde{\mathcal{V}}^h)](\tilde{H}_z^h - z)^{-1} \\ &\quad + (H_0^h + i)^{-1}[P^h, \varphi](\tilde{H}_z^h - z)^{-1}. \end{aligned} \tag{4.18}$$

One sees that the first term of the r.h.s of (4.18) is trace-class with the announced estimates because $(H_0^h + i)^{-1}$ is trace-class whereas the second factor is uniformly bounded. For the last term, use again that $(H_0^h + i)^{-1}$ is trace-class and the fact that we obtained estimates for $(\tilde{H}_z^h - z)^{-1}$ in the $H^{1,h}$-norm. The result follows by taking the adjoint. In the case $\lambda = \lambda_0$, $z \in \Omega_h$ and $m_{\lambda_0} < N$, use the series $R(\lambda_0)\sum_{k=0}^{\infty} \varepsilon^k$ to see that

$$(\tilde{H}_z^h(\lambda_0) - z)^{-1} = \left[(\tilde{H}_z^h - z)^{-1}(1 - \tilde{\psi}) + \chi(\tilde{H}_I^h(\lambda_0) - z)^{-1}\tilde{\psi}\right]\left[1 + \mathcal{O}(e^{-\frac{c}{h}})\right], \tag{4.19}$$

and notice that the first factor is trace-class. Finally, one has something similar for $\lambda \neq \lambda_0$ and suitable z

$$(H_z^h - z)^{-1} = \left[(\tilde{H}_z^h - z)^{-1}(1 - \tilde{\psi}) + \chi(H_I^h - z)^{-1}\tilde{\psi}\right]\left[1 + \mathcal{O}(e^{-\frac{c}{h}})\right]. \tag{4.20}$$

□

5 Localizing resonances

The formalism of Grushin's Problem provides a convenient way to treat simultaneously the question of the invertibility of the operator$(H_z^h - z)$ raised in the latter section, and (through a perturbative formulation) to localize the resonances of P^h. We refer the reader to the appendix of [HeSj1] or to [SjZw] for a general presentation of this technique. Fix the reference energy to the value $\lambda_0 \in (\Lambda_*, \Lambda^*)$ and work in the set Ω_h defined in (4.3). Denote by $\lambda_1^h, \ldots, \lambda_n^h$ the eigenvalues of H_I^h converging to λ_0 (they lie in K_h), and $\phi_1^h, \ldots, \phi_{m_{\lambda_0}}^h$ a corresponding orthonormal system of eigenvectors. Start by writing the Grushin's problem for the Dirichlet realization H_I^h:

$$\begin{cases} (H_I^h - z)u + R_0^- u^- = v, \\ R_0^+ u = v^+, \end{cases} \tag{5.1}$$

with

$$(u, u^-) \in D(H_I^h) \times \mathbb{C}^{m_{\lambda_0}}, \quad (v, v^+) \in L^2(I) \times \mathbb{C}^{m_{\lambda_0}},$$

$$R_0^- : \mathbb{C}^{m_{\lambda_0}} \longrightarrow L^2(I), \quad u^- := \begin{pmatrix} u_1^- \\ \vdots \\ u_{m_{\lambda_0}}^- \end{pmatrix} \mapsto R_0^- u^- := \sum_{j=1}^{m_{\lambda_0}} u_j^- \phi_j^h, \tag{5.2}$$

and

$$R_0^+ : L^2(I) \longrightarrow \mathbb{C}^{m_{\lambda_0}}, \quad u \mapsto R_0^+ u := \begin{pmatrix} \langle u, \phi_1^h \rangle_{L^2} \\ \vdots \\ \langle u, \phi_{m_{\lambda_0}}^h \rangle_{L^2} \end{pmatrix}. \tag{5.3}$$

Set $F'' := \operatorname{span}\{\phi_j^h\}_{j=1}^n$, $F' := (F'')^\perp$. Then, this problem is invertible and the solution is given, with obvious notations by

$$\begin{cases} u' &= (H_I^{h\prime} - z)^{-1} v', \\ u'' &= \displaystyle\sum_{j=1}^{m_{\lambda_0}} \langle u, \phi_j^h \rangle \phi_j^h = \sum_{j=1}^{m_{\lambda_0}} v_j^+ \phi_j^h, \\ u_j^- &= \langle v, \phi_j^h \rangle + (z - \lambda_j^h) v_j^+, \quad j = 1, \dots, m_{\lambda_0}, \end{cases} \tag{5.4}$$

where $H_I^{h\prime}$ denotes the restriction of H_I^h to F'. In terms of operators

$$\begin{cases} u = E_0(z) v + E_0^+ v^+, \\ u^- = E_0^- v + E_0^{-+}(z) v^+, \end{cases} \tag{5.5}$$

with

$$E_0(z) v = (H'^h_I - z)^{-1} \Pi_I^h v, \qquad E_0^+ v^+ = \sum_{j=1}^{m_{\lambda_0}} v_j^+ \phi_j^h,$$

$$E_0^- v = \begin{pmatrix} \langle v, \phi_1^h \rangle_{L^2} \\ \vdots \\ \langle v, \phi_{m_{\lambda_0}}^h \rangle_{L^2} \end{pmatrix}, \qquad E_0^{-+}(z) v^+ = \operatorname{diag}(z - \lambda_j^h)\, v^+,$$

and Π_I^h is the orthogonal projector onto F' :

$$\Pi_I^h v := \left(1 - \sum_{j=1}^{m_{\lambda_0}} |\phi_j^h\rangle\langle\phi_j^h| \right) v\,. \tag{5.6}$$

Finally, write

$$\mathcal{H}_I^h(z) := \begin{pmatrix} H_I^h - z & R_0^- \\ R_0^+ & 0 \end{pmatrix}, \quad \mathcal{E}_I^h(z) := (\mathcal{H}_I^h(z))^{-1} = \begin{pmatrix} E_0(z) & E_0^+ \\ E_0^- & E_0^{-+}(z) \end{pmatrix}. \tag{5.7}$$

Now we perturb the problem in order to obtain the resonant problem. Like in the proof of Proposition 4.3, set

$$S_0 := \tilde{d}_0(U_{\lambda_0}^h, \partial I), \tag{5.8}$$

where $\tilde{d}_0$ is the Agmon distance for the potential $\mathcal{V}^0$ at the energy λ_0. For $\eta > 0$ small, fix two smooth cut-off functions χ, ψ such that $0 \le \chi, \psi \le 1$, $\chi \equiv 1$ in the set $\{x \in I, d(x, U_{\lambda_0}^h) \le S_0 - \eta\}$, $\psi \equiv 1$ in the set $\{d(x, U_{\lambda_0}^h) \le (S_0 - \eta)/2\}$ and $\psi \equiv 0$ in the set $\{d(x, U_{\lambda_0}^h) \ge (S_0 + \eta)/2\}$. Define

$$\mathcal{H}(z; h) := \begin{pmatrix} H_z^h - z & \chi R_0^- \\ R_0^+ & 0 \end{pmatrix}, \quad z \in \Omega_h. \tag{5.9}$$

Far from the resonant wells, H_z^h looks like $\tilde{H}_z^h(\lambda_0)$ and around the wells the Dirichlet problem (with all the wells) is a good approximation of H_z^h. This leads to set

$$\mathcal{F}(z;h) := \begin{pmatrix} \chi E_0 \psi + (\tilde{H}_z^h(\lambda_0) - z)^{-1}(1-\psi) & \chi E_0^+ \\ E_0^- \psi & E_0^{-+} \end{pmatrix}. \tag{5.10}$$

One shows that

$$\mathcal{H}(z;h)\,\mathcal{F}(z;h) = 1 + \mathcal{K}(z;h)$$

and $\mathcal{K}$ satisfies the estimate

$$\mathcal{K}(z;h) = \begin{pmatrix} \tilde{\mathcal{O}}\left(e^{-\frac{S_0}{2h}}\right) & \tilde{\mathcal{O}}\left(e^{-\frac{S_0}{h}}\right) \\ \tilde{\mathcal{O}}\left(e^{-\frac{S_0}{2h}}\right) & \tilde{\mathcal{O}}\left(e^{-\frac{2S_0}{h}}\right) \end{pmatrix}. \tag{5.11}$$

More precise computations with the second order expansion of the Neumann series and using the resolvent esimates of Proposition 4.3 can be done. When all the wells are resonant, $m_{\lambda_0} = N$, details are given by the direct transcription of [HeSj1, pp. 117-128]. The more general case was treated in [Pat, pp. 178-189].

Proposition 5.1 *With the notations* (4.3) *and* (5.8) *and for $z \in \Omega_h$, the operator is invertible, and the inverse is given by the norm convergent series*

$$\mathcal{H}(z;h)^{-1} = \mathcal{F}(z;h)\sum_{j=0}^{\infty}(-1)^j\mathcal{K}^j(z;h) = \begin{pmatrix} E(z;h) & E^+(z;h) \\ E^-(z;h) & E^{-+}(z;h) \end{pmatrix},$$

with

$$E^{-+}(z) = E_0^{-+} + \tilde{\mathcal{O}}\left(e^{-\frac{2S_0}{h}}\right)$$

Moreover, it is uniformly norm-bounded holomorphic function of $z \in \Omega_h$.

Within the Grushin problem approach, the inversibility of $H_z^h - z$ is reduced to the question of invertibility of the finite-dimensional block $E^{-+}(z)$ (see the Schur complement formula (6.7)). In particular, considering $\det(E^{-+}(z))$ leads to the next standard approximation result of resonances by Dirichlet eigenvalues.

Proposition 5.2 *Take the notation* (4.3) *and* (5.8)*. The operator P^h has exactly m_{λ_0} resonances (counted with multiplicity) $z_1^h, \ldots, z_{m_{\lambda_0}}^h$ in Ω_h. They satisfy*

$$\forall j \in \{1, \ldots, m_{\lambda_0}\}, \quad |z_j^h - \lambda_j^h| = \tilde{\mathcal{O}}\left(e^{-\frac{2S_0}{h}}\right).$$

and have negative imaginary parts.

6 Local density of states

We end the proof of Theorem 1.6 by considering the asymptotic behaviour of the density associated with a function of the energy.

Proposition 6.1 *Let $\theta \in \mathcal{C}_c^0((\Lambda_*, \Lambda^*))$ and keep the notations (4.4) under Assumptions 1, 3 and 4. The particle density $dn_{\theta_\lambda}[V^h]$ defined for $g(k) = \theta(\lambda_k)$ satisfies the next weak* asymptotic in $\mathcal{M}_b((a,b))$: For all $\varphi \in \mathcal{C}_c^0((a,b))$,*

$$\lim_{h\to 0} \int_a^b \varphi(x)\ dn_{\theta_\lambda} = \lim_{h\to 0} Tr\left[\theta(H^h)\varphi\right] = \lim_{h\to 0} Tr\left[(\theta.1_{K_h})(H^h)\varphi\right]$$
$$= \sum_{i\in J_{\lambda_0}} \theta(\lambda_0)\,\varphi(c_i)\,. \quad (6.1)$$

This result which is a Breit-Wigner type formula for the density of states like in [GeMa] will be proved in two steps : 1) eliminating the non resonant energies; 2) specifying the contribution of resonant states.

6.1 Eliminating the non resonant energies

We first check that the density goes to 0 in (a,b) as h goes to 0 when all the wells are filled, that is for $\tilde{H}^h$ and then reduce the more general non resonant energy problem to this case after using an approximate resolvent provided by (4.19)-(4.20). We start with a simple accurate estimate.

Proposition 6.2 *Let $\tilde{\psi}_-^h(k,\cdot)$ the incoming scattering states of $\tilde{H}^h$, such that $\lambda_k \in [\Lambda_*, \Lambda^*]$. The function $\tilde{\psi}_-^h(k,\cdot)$ is uniformly bounded with respect to $x \in [a,b]$ and k. Moreover one has the uniform pointwise estimate*

$$\begin{aligned} \tilde{\psi}_-^h(k,x) &= \mathcal{O}\left(h^{-1/2} e^{-\frac{\tilde{d}_h(a,x)}{h}}\right), \quad k>0, \\ \textit{and}\quad \tilde{\psi}_-^h(k,x) &= \mathcal{O}\left(h^{-1/2} e^{-\frac{\tilde{d}_h(b,x)}{h}}\right), \quad k<0\,, \end{aligned}$$

where $\tilde{d}_h$ stands for the Agmon distance for the potential $\tilde{\mathcal{V}}^h$ at the energy λ_k .

Proof: We focus on the case $k>0$ (if $k<0$, just swap a and b). Start by noticing that for given k, the function $A_k^h : x \mapsto |\tilde{\psi}_-^h(k,x)|^2$ satisfies

$$h^2 \frac{d^2}{dx^2} A_k^h = 2|h\partial_x \tilde{\psi}_-^h(k,\cdot)|^2 + 2(\tilde{\mathcal{V}}^h - \lambda_k)|\tilde{\psi}_-^h(k,\cdot)|^2 \geq 0. \quad (6.2)$$

It follows that the function $h\partial_x A_k^h$ is increasing on I. But the scattering condition (1.17) says that this functions vanishes at $x=b$. So the function A_k^h is convex and decreasing on I. It suffices now to show that the family $(A_k^h(a))_k$ is uniformly bounded. But it equals

$$A_k^h(a) = |\tilde{\psi}_-^h(k,a)|^2 = \left|e^{i\frac{ka}{h}} + r_k e^{-i\frac{ka}{h}}\right|^2, \quad (6.3)$$

which is bounded according to (1.16).
Now use the Agmon estimate of Appendix A with $V = \tilde{\mathcal{V}}^h$, $z = \lambda_k$, $u = v = \tilde{\psi}_-^h(k,\cdot)$ and $\varphi = \tilde{d}_h(a,x)$. Since $\tilde{P}^h u = zu$, and $V - \varphi'^2 - z = 0$, this leads after taking the real part to

$$\begin{aligned} \left\|h\partial_x\left(e^{\frac{\varphi}{h}}\tilde{\psi}_-^h(k,\cdot)\right)\right\|^2_{L^2(I)} &\leq h^2 e^{\frac{2\varphi(a)}{h}} \left|\mathrm{Re}(h\partial_x\tilde{\psi}_-^h(k,a)\overline{\tilde{\psi}_-^h(k,a)})\right| \\ &\quad + h^2 e^{\frac{2\varphi(b)}{h}} \left|\mathrm{Re}(h\partial_x\tilde{\psi}_-^h(k,b)\overline{\tilde{\psi}_-^h(k,b)})\right| \quad (6.4) \\ &\leq 2|k|A_k^h(a)^{1/2} = \mathcal{O}(1)\,. \quad (6.5) \end{aligned}$$

Writing

$$e^{\frac{\varphi(x)}{h}}\tilde{\psi}_-^h(k,x) = \tilde{\psi}_-^h(k,a) + h^{-1}\int_a^x h\partial_x\left(e^{\frac{\varphi(t)}{h}}\tilde{\psi}_-^h(k,t)\right)dt$$

and Schwarz's inequality yield the result. □

Corollary 6.3 *Let $\theta \in \mathcal{C}_c^0((\Lambda_*,\Lambda^*))$ and $\varphi \in \mathcal{C}_c^0((a,b))$. The operator $\theta(\tilde{H}^h)\varphi$ is trace-class with a trace estimated by*

$$Tr[\theta(\tilde{H}^h)\varphi] = \tilde{\mathcal{O}}\left(e^{-\dfrac{c\ dist(supp\,\varphi,\partial I)}{h}}\right),$$

where $dist(x,y) = |x-y|$ and c is a positive constant. The family of measures $(dn_{\theta_\lambda}[\tilde{V}^h])_{h>0}$ weakly converges to 0 in $\mathcal{M}_b((a,b))$.

Proof: The function φ can be assumed non negative. We write

$$\begin{aligned}\int_a^b \varphi(x)\ dn_{\theta_\lambda}[\tilde{V}^h](x) &= \mathrm{Tr}\left[\varphi^{1/2}\theta(\tilde{H}^h)\varphi^{1/2}\right]\\ &= \int_a^b\int_{\mathbb{R}}\theta(\lambda_k)\left|\tilde{\psi}_-^h(k,x)\right|^2\varphi(x)\frac{dk}{2\pi h},\end{aligned}$$

after using the expression of the kernel of $\theta(\tilde{H}^h)$. Proposition 6.2 combined with the fact that the Agmon distance $\tilde{d}_h$ associated with $\tilde{\mathcal{V}}$ and an energy $\lambda \in (\Lambda_*,\Lambda^*)$ is uniformly equivalent to the Euclidean distance, yields the result after integration. □

Thanks to this result one easily gets rid of non resonant energies.

Proposition 6.4 *Consider the energy interval K_h defined in (4.4) and set $\tilde{\theta}^h(\lambda) := (1-1_{K_h}(\lambda))\cdot\theta(\lambda)$. Then in restriction to (a,b), the measure $dn^h_{\tilde{\theta}^h_\lambda}$ weakly converges to 0 as h goes to 0:*

$$\forall\varphi \in \mathcal{C}_c^0((a,b)),\ \lim_{h\to 0} Tr\,(\tilde{\theta}^h(H^h)\varphi) = 0\,.$$

Proof: We again assume again $\varphi \geq 0$ and apply Stone's formula in order to compute the trace of $\varphi^{1/2}\mathbf{1}_I\tilde{\theta}^h(H^h)\mathbf{1}_I\varphi^{1/2}$. By referring to Proposition 4.1 and by using successively (4.19)-(4.20) one obtains

$$\mathrm{Tr}\,(\tilde{\theta}^h(H^h)\varphi) = \mathrm{Tr}\,(\tilde{\theta}^h(\tilde{H}^h)(1-\tilde{\psi})\varphi) + \mathrm{Tr}\,(\chi\tilde{\theta}^h(H_I^h)\tilde{\varphi}) + \mathcal{O}\left(h^{-2}e^{-\frac{c}{h}}\right), \quad h\to 0. \tag{6.6}$$

The first term can be estimated by

$$0 \leq \mathrm{Tr}\,(\tilde{\theta}^h(\tilde{H}^h)(1-\tilde{\psi})\varphi) \leq \mathrm{Tr}\,(\theta(\tilde{H}^h)(1-\tilde{\psi})\varphi)\,,$$

with a right-hand side converging to 0 by Corollary 6.3. Meanwhile the second term cancels since H_I^h has no spectrum on the support of $\tilde{\theta}^h$. This finishes the proof. □

6.2 Contribution of resonant states

Let us first go back to the Grushin problem introduced in Section 5. According to Proposition 5.1, and estimates (5.11) we have

$$\mathcal{H}(z;h)^{-1} := \begin{pmatrix} E(z) & E^+(z) \\ E^-(z) & E^{-+}(z) \end{pmatrix} = \mathcal{F}(z;h) \begin{pmatrix} 1+\varepsilon(z) & \varepsilon^+(z) \\ \varepsilon^-(z) & 1+\varepsilon^{-+}(z) \end{pmatrix},$$

with $\varepsilon^\bullet(z) = \tilde{\mathcal{O}}(e^{-S_0/2h})$ uniformly in $z \in \Omega_h$. This implies

$$[H_z^h - z]^{-1} = E(z) - E^+(z)(E^{-+}(z))^{-1}E^-(z)\,. \tag{6.7}$$

Coming back to the definition (5.10) of $\mathcal{F}^h(z)$, this can be improved into

$$E(z) = (\tilde{H}_z^h(\lambda_0) - z)^{-1}(1-\psi)(1+\varepsilon) + \chi E_0(z)\psi(1+\varepsilon) + \chi E_0^+\varepsilon^- \tag{6.8}$$

$$E^+(z) = \chi E_0^+ + (\tilde{H}_z^h(\lambda_0) - z)^{-1}(1-\psi)\varepsilon^+ + \chi E_0^+\varepsilon^{-+} + \chi E_0(z)\psi\varepsilon^+ \tag{6.9}$$

$$E^-(z) = E_0^-\psi + E_0(z)\psi\varepsilon + E_0^{-+}(z)\varepsilon^- \tag{6.10}$$

$$E^{-+}(z) = E_0^{-+}(z) + \tilde{\mathcal{O}}\left(e^{-\frac{2S_0}{h}}\right). \tag{6.11}$$

We are now ready to apply Stone's formula with a complex deformation of the integration contour. Before this, we write under an adapted form the polar part coming from (6.11).

Lemma 6.5 *Set $\tilde{\Omega}_h := [\lambda_0 - \alpha^h/2, \lambda_0 - \alpha^h/2] \times [-2ih, 2ih]$ For z in $\Omega_h \setminus \tilde{\Omega}_h$, there exists a constant $c > 0$ and a matrix-valued meromorphic function G such that*

$$E^{-+}(z)^{-1} = E_0^{-+}(z)^{-1} + G(z), \quad \|G(z)\| = \mathcal{O}\left(e^{-\frac{c}{h}}\right), \quad h \to 0\,.$$

Proof: Fix any matrix-norm on $\mathbb{C}^{m_{\lambda_0}}$ and use again (6.11) to see that

$$\begin{aligned} E^{-+}(z) &= (1 + F(z)E_0^{-+}(z)^{-1})E_0^{-+}(z), \quad z \neq \lambda_j^h, \\ \|F(z)\| &= \mathcal{O}\left(e^{-\frac{2S}{h}}\right), \quad 0 < S < S_0 \quad \text{for } z \in \Omega_h \setminus \tilde{\Omega}_h\,. \end{aligned} \tag{6.12}$$

Because of the expression of $E_0^{-+}(z)$,

$$\|F(z)E_0^{-+}(z)^{-1}\| = \mathcal{O}\left(e^{-\frac{2S}{h}}\right)\left(\min_{j=1,\dots,m_{\lambda_0}} |z - \lambda_j^h|\right)^{-1}.$$

For $z \neq z_j^h$, $j = 1, \dots, m_{\lambda_0}$

$$E^{-+}(z)^{-1} = E_0^{-+}(z)^{-1}[1 + F(z)E_0^{-+}(z)^{-1}]^{-1} \tag{6.13}$$

and the condition $z \in \Omega_h \setminus \tilde{\Omega}_h$ implies $\min_{j=1,\dots,m_{\lambda_0}} \left|z - \lambda_j^h\right| \geq h$. Therefore, the Neumann expansion of $[1 + F(z)E_0^{-+}(z)^{-1}]^{-1}$ converges, which yields the result. □

We can end the proof of Theorem 1.6 with the
Proof of Proposition 6.1: Owing to Proposition 6.4 it is enough to consider the trace

$$\mathbf{1}_I(\mathbf{1}_{K_h}.\theta)(H^h)\mathbf{1}_I\varphi.$$

According to Stone's formula and Proposition 4.1 one gets for non negative functions $\theta \in \mathcal{C}_c^0((\Lambda_*, \Lambda^*))$, and $\varphi \in \mathcal{C}_c^0(I)$,

$$\mathbf{1}_I(\mathbf{1}_{K_h}.\theta)(H^h)\mathbf{1}_I\varphi = \frac{-1}{2i\pi}\int_{K_h+i0}\theta(\lambda)(\lambda - H_\lambda^h)^{-1}\varphi\ d\lambda + \frac{1}{2i\pi}\int_{K_h-i0}\theta(\lambda)(\lambda - H_\lambda'^h)^{-1}\varphi\ d\lambda\,, \tag{6.14}$$

where $(H_z'^h - z)^{-1}$ denotes the (meromorphic continuation from the lower-half complex plane) of the truncated resolvent $\mathbf{1}_I(H^h - z)^{-1}\mathbf{1}_I$, corresponding to the anti-resonant boundary conditions (see Remark 9).

For fixed $\varepsilon > 0$, consider the contour C_ε made by the segments $(\Lambda_* + i\varepsilon, \Lambda^* + i\varepsilon) \cap \Omega_h$ and $(\Lambda_* - i\varepsilon, \Lambda^* - i\varepsilon) \cap \Omega_h$ scoured in opposite way, the first one by real parts increasing (see Figure 2). This contour in homotopic to the union of the circle γ_h and the contour C'_ε (depicted in the Figure 2) which lies on the square root Riemann surface ramified along $\mathbb{R}_+$. Part of the deformation takes place on the second sheet where resonances appear as poles. Meanwhile in the lower half-plane (first sheet) the resolvent is given by the anti-resonant boundary conditions (see Remark 9). The operator corresponding to these dual transparent boundary conditions is denoted by $H_z'^h$ and its resolvent, $[H_z'^h - z]^{-1}$, has the same properties as $[H_z^h - z]^{-1}$, up to the sign of imaginary parts. Since for any given function $\varphi \in \mathcal{C}_c^0((a,b))$, the functional $\theta \mapsto \mathrm{Tr}\,[\theta(H^h)\varphi]$ defines a non negative

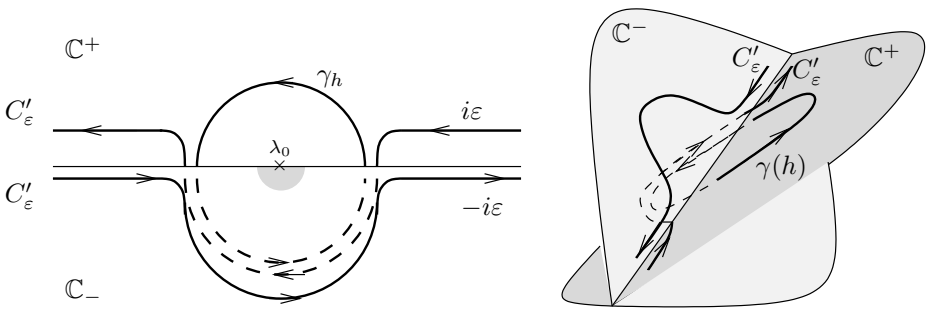


Figure 2: Application of Stone's formula. Resonances lie on the second sheet and close to λ_0 (semi-circle gray).

measure while the right-hand side $\sum_{i\in J_{\lambda_0}}\theta(\lambda_0)\varphi(c_i)$ of (6.1) is also a positive functional of θ, the function θ can be replaced by a polynomial approximation on the interval $[\Lambda_*, \Lambda^*]$. Use polynomial approximations from below (resp. from above) in order to get a lower bound (resp. upper bound) of the limit in (6.1). Hence we can assume that θ is a polynomial function on $[\Lambda_*, \Lambda^*]$, which allows the complex deformation of the contour integral.

We first integrate the polar part. Consider first the integral over γ_h, which involves only $(H_z^h - z)^{-1}$. Use expression (6.7) first. Let us note immediately that $E(z)$ is a holomorphic function in a neighborhood of γ_h, its integral is null. Then, one can rewrite

$$E^-(z) = E_0^-\psi + \tilde{\mathcal{O}}\left(e^{-\frac{S_0}{2h}}\right), \quad E^+(z) = \chi E_0^+ + \tilde{\mathcal{O}}\left(e^{-\frac{S_0}{2h}}\right). \tag{6.15}$$

These estimates hold in the norm of trace-class operators since these operators are of finite-rank. On the contour γ_h, one has

$$E^{-+}(z)^{-1} = E_0^{-+}(z)^{-1} + G(z), \quad G(z) = \mathcal{O}(1), \tag{6.16}$$

so coming back to (6.7)

$$E_0^+(z-H_z^h)^{-1} = -E(z) + \chi E_0^+ E_0^{-+}(z)^{-1} E_0^- \psi + \mathcal{O}\left(e^{-\frac{S_0}{2h}}\right), \quad h \to 0. \tag{6.17}$$

If now we integrate over γ_h, and since $\theta(\lambda_j^h) = \theta(\lambda_0) + o(1)$, it comes

$$\int_{\gamma_h} \theta(z)(H_z^h - z)^{-1}\varphi \frac{dz}{2i\pi} = 0 + \theta(\lambda_0)\chi E_0^+ E_0^- \psi\varphi + o(1)\|\varphi\|_\infty. \tag{6.18}$$

Note that $E_0^+ E_0^-$ is nothing but the orthogonal projector on the Dirichlet states $\sum_{j=1}^{m_{\lambda_0}} |\phi_j^h\rangle\langle\phi_j^h|$. Taking now the trace, and using its cyclicity, one has with the approximation of the Dirichlet states by superpositions of the eigenfunctions of the one-well problem in Theorem 3.6

$$\begin{aligned}
\mathrm{Tr}\left[\chi \sum_{j=1}^{m_{\lambda_0}} |\phi_j^h\rangle\langle\phi_j^h|\psi\varphi\right] &= \mathrm{Tr}\left[\sum_{j=1}^{m_{\lambda_0}} |\phi_j^h\rangle\langle\phi_j^h|\psi\varphi\right] && (6.19)\\
&= \sum_{j=1}^{m_{\lambda_0}} \left\langle \phi_j^h, \phi_j^h \psi\varphi\right\rangle_{L^2} && (6.20)\\
&= \sum_{j\in J(\lambda_0)} \varphi(c_j) + o(1)\|\varphi\|_\infty\,. && (6.21)
\end{aligned}$$

Let us come to the contour C'_ε of which the projection on $\mathbb{C}$ lies in $\Omega_h \setminus \tilde{\Omega}_h$. Note that the polar part coming from $(H_z'^h - z)^{-1}$ is to be treated with the integral of the polar part coming from $(H_z^h - z)^{-1}$. Since (with obvious notations)

$$E'^{-+}(z)^{-1} - E^{-+}(z)^{-1} = E'^{-+}(z)^{-1}(E^{-+}(z) - E'^{-+}(z))E^{-+}(z)^{-1}\,,$$

Lemma 6.5 implies that the difference is then exponentially small because the resonances and anti-resonances are at distance greater than h from C'_ε.

It remains the holomorphic part over C'_ε. Because the polar part is treated, one can compute this integral after the inverse homotopy leading back to C_ε. But coming back to the expansion series (6.8) of $E(z)$ (resp. $E'(z)$) with main term given by $\tilde{H}_z^h$ (resp. $\tilde{H'}_z^h$), the application of Stone's formula gives that the contribution of these terms is zero by Proposition 6.4. □

A Agmon identity

Here we just give the basic energy identity.

Lemma A.1 *Let $\Omega := (\alpha, \beta)$ an open interval, $V \in L^\infty(\omega)$, $z \in \mathbb{C}$ and φ a Lipschitz real function on Ω. Denote by P the Schrödinger operator $P := -h^2 d^2/dx^2 + V$. Then for any u_1, u_2 in $H^2(\Omega)$, and setting $v_j := e^{\varphi/h} u_j$ one has:*

$$\begin{aligned}
\int_\alpha^\beta e^{\frac{2\varphi}{h}}(P-z)u_1\bar{u}_2 dx &= \int_\alpha^\beta h v_1' \overline{h v_2'} dx + \int_\alpha^\beta (V - z - \varphi'^2) v_1 \bar{v}_2 dx\\
&+ \int_\alpha^\beta h\varphi'(v_1'\bar{v}_2 - v_1\bar{v}_2')dx\\
&+ h^2\left(e^{\frac{2\varphi(\alpha)}{h}} u_1'\bar{u}_2(\alpha) - e^{\frac{2\varphi(\beta)}{h}} u_1'\bar{u}_2(\beta)\right)\,.
\end{aligned}$$

This identity is obtained after conjugation of hd/dx by $e^{\varphi/h}$ and integration by parts.

B Monotony Principle

A little variation of [Ni2] provides the next result.

Proposition B.1 *For $i = 1, 2$, let V_i two non negative functions in $L^\infty(I)$ and $H_i := H_B^h + V_i$. Consider a function $F \in \mathcal{S}(\mathbb{R})$ which is decreasing on $[-B, +\infty)$. Write $F_\lambda(k) = F(\lambda_k)$ and define dn_{F_λ} according to* (1.35) *and* (1.20)*. Then the inequality*

$$\int_I (V_2 - V_1) dn_F[V_2] \leq \int_I (V_2 - V_1) dn_F[V_1]$$

holds.

This inequality is a convexity inequality which is a key ingredient in the analysis of thermondynamical equilibria of Schrödinger-Poisson systems (see [Ni1], [Ni2]). Here the assumption $V_i \geq 0$ ensures $\sigma(H_i) \subset [-B, +\infty)$. The convexity inequality with a continuous spectrum has been proved in [Ni2], with the assumption that the potential is 0 at infinity. Here the different values 0 and $-B$ for $x < a$ and $x > b$ do not bring any additional difficulties in this simple one-dimensional problem.

C Spectral approximation

We refer the reader to [Hel], [HeSj2] for the details. Recall that if E and F are two given closed subspaces of a Hilbert space $\mathcal{H}$, with orthogonal projections Π_E and Π_F, the non-symmetric distance from E to F, denoted by $\vec{d}(E, F) \in [0, 1]$ is the norm of operator $(1 - \Pi_F)\Pi_E$, and if $\vec{d}(E, F) < 1$, Π_F induces on E a continuous injection on its range with bounded inverse. Moreover, if at the same time $\vec{d}(F, E) < 1$, the latter distances are equal. In particular E and F have same dimension.

Proposition C.1 *Let A an unbounded self-adjoint operator on $\mathcal{H}$ and $\Lambda := [\lambda_-, \lambda_+] \subset \mathbb{R}$. Suppose that there exists $\varepsilon > 0$, N linearly independent vectors $\psi_1, \ldots, \psi_N$ in the domain of A,$\mu_1, \ldots, \mu_N$, N complex numbers in Λ such that $A\psi_j = \mu_j \psi_j + r_j$, with $\|r_j\| \leq \varepsilon$. If A has no spectrum in $\{x, 0 < dist(x, \Lambda) \leq a\}$ for some $a > 0$, then the subspaces $E := Span(\psi_1, \ldots, \psi_N)$ and F equal to the spectral subspace $\mathbf{1}_\Lambda(A)\mathcal{H}$ verify*

$$\vec{d}(E, F) \leq \left(\frac{N}{\rho_*}\right)^{1/2} \frac{\varepsilon}{a},$$

where ρ_* is the smallest eigenvalue of the Gram matrix with entries $\langle \psi_i, \psi_j \rangle$.

In particular if A is known to have only discrete spectrum and if the directed distance $\vec{d}(E, F)$ can be proved in this way to be smaller than 1, then A has at least N eigenvalues lying in Λ.

D Scattering states for the barrier

Proposition D.1 *Let $V_0(x) := \Lambda^*$ on I and $H_0^h := -h^2\Delta + V_0 - B \cdot \mathbf{1}_{(b,\infty)}$, and $\{\psi_-^h(k, \cdot)\}_k$ its scattering states. Set $S_k := \sqrt{(\Lambda^* - \lambda_k)}$, $\lambda_k < \Lambda^*$. Then one has as $h \to 0$, and uniformly for $x \in I$, for $k > 0$*

$$|\psi_-^h(k, x)|^2 = \frac{4k^2}{\Lambda^*} e^{-\frac{S_k(x-a)}{h}} \left(1 + \mathcal{O}\left(e^{-\frac{2S_k(b-x)}{h}}\right)\right),$$

$$|\psi_-^h(-k, x)|^2 = \frac{4k^2}{\Lambda^* + B} e^{\frac{S_k(x-b)}{h}} \left(1 + \mathcal{O}\left(e^{-\frac{2S_k(x-a)}{h}}\right)\right).$$

It suffices to solve explicitly on I the system characterizing $\psi_-^h(k,\cdot)$ on the explicit basis of solutions to the ODE (since the potential is constant on I). Use the scattering conditions (1.17)-(1.18) . These conditions are still valid when $\lambda < 0$ because of the choice of the square root indeed. Finally the computation reduces to the solving of 2 by 2 affine systems. We just give the final result.

E Pointwise estimate for the resolvent

The next result shows that no Lipschitz regularity is necessary in dimension 1 in order to transform weighted L^2-estimates into pointwise estimates of the Green functions. Once the weighted L^2-estimates are obtained from the Agmon identity of Appendix A, it suffices to use the equation after the regularization of the Agmon distance which is possible because the $\tilde{\mathcal{O}}$ estimates can absorb little exponential errors.

Proposition E.1 *Let $H = -h^2\Delta + \mathcal{V}$ be a closed operator with $\mathcal{V} \in L^\infty(I)$, $I = [a,b]$, $D(H) \subset H^2(I)$, with dual H' and $D(H') \subset H^2(I)$. Fix $z \in \mathbb{C}$ such that $z \notin \sigma(H)$ for all $h \in (0,h_0)$. We assume that there is a distance $d \in \mathcal{C}^0(I \times I)$, such that the resolvent estimate*

$$\|\chi_x(z-H)^{-1}\chi_y\|_{\mathcal{L}(L^2)} \leq C_\eta A(h) e^{\frac{-d(x,y)+\eta}{h}}$$

holds for all $(x,y,h) \in I \times I \times (0,h_0)$ as soon as $\eta \in (0,\eta_0)$, with $\eta_0 > 0$ small enough and χ_p generically denotes a cut-off functions supported in $|x-p| = \mathcal{O}(\eta)$. Then the pointwise estimate

$$|(z-H)^{-1}[x,y]| = \tilde{\mathcal{O}}\left(A(h)e^{\frac{-d(x,y)}{h}}\right),$$

holds with uniform constants with respect to $(x,y,h) \in I \times I \times (0,h_0)$.

Proof: Let $y_0 \in I$ be fixed. Consider a smooth function $\varphi \in \mathcal{C}^\infty(I)$ which is an aproximation of $d(x,y_0)$, such that $\|\varphi - d(.,y_0)\|_{L^\infty} \leq \eta$ and $f \in L^2(I)$.
Let u be the solution to $(H-z)u = \chi_{y_0} f$, then

$$e^{\frac{\varphi}{h}}(-h^2\Delta + \mathcal{V} - z)e^{-\frac{\varphi}{h}}\left(e^{\frac{\varphi}{h}}u\right) = e^{\frac{\varphi}{h}}\chi_{y_0} f.$$

By defining $v = e^{\varphi/h}u$, the assumption leads to the estimate

$$\|v\|_{L^2} \leq C_\eta\, A(h)\, e^{\frac{c\eta}{h}}\, \|\chi_{y_0} f\|. \tag{E.1}$$

Using the relation

$$e^{\frac{\varphi}{h}}(-(h\partial_x)^2 + V - z)e^{-\frac{\varphi}{h}} = -h^2\partial_x^2 + 2h\varphi'\partial_x + h\varphi'' + V - (\varphi')^2 - z,$$

we can write

$$[C - h^2\partial_x^2 + 2h\varphi'\partial_x]v = e^{\frac{\varphi}{h}}\chi_{y_0} f + Cv + h\varphi'' v - (V - (\varphi')^2 - z)v, \tag{E.2}$$

where C is a strictly positive constant large enough. The regularity of φ implies

$$\|v\|_{H^{2,h}} \leq C_\eta\, e^{\frac{c\eta}{h}}\, \|\chi_{y_0}\tilde{f}\|_{L^2}.$$

In dimension one, $H^{2,h}$ is continously embedded in $\mathcal{C}^0([a,b])$. Then the application $f \mapsto e^{\varphi/h}(H-z)^{-1}e^{-\varphi/h}\chi_{y_0} f$ is continuous from $L^2([a,b])$ onto $\mathcal{C}^0([a,b])$ with the above uniform estimate.
By duality, $\chi_{y_0}e^{-\varphi/h}(H'-z)^{-1}e^{-\varphi/h}$ is continuous from $(\mathcal{M}_b(I), \|\cdot\|_b)$ onto L^2.

By changing y_0 into x_0 and H into H', this says that the L^2-norm $v_1 = \chi_{x_0} e^{d(x_0, y_0 - c\eta)/h}(H - z)^{-1}\delta_{y_0}$ has an $L^2(I)$-norm bounded by $C_\eta A(h)$. A bootstrap with (E.2) leads to the uniform estimate of $|v_1(x)|$, which yields the pointwise resolvent estimate. $\square$

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