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

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Abstract

This article continues the asymptotic analysis of a nonlinear Schrödinger-Poisson system which models in a far from equilibrium regime the quantum transport in electronic devices like resonant tunneling diodes. Within the reduction to an h-dependent linear problem with uniform regularity estimates for the potential already established in the first part, explicit computations of the asymptotic finite dimensional nonlinear system are derived. They rely on an accurate (phase-space) analysis of the tunnel effect which relies on some kind of Breit-Wigner formula and Fermi golden rule.

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Contents

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1 Introduction

We complete the asymptotic analysis started in [BNP1] of some out-of-equilibrium 1D Schrödinger-Poisson system arising from the modelling of resonant tunelling diodes. This problem is a nonlinear problem whose functional framework was considered in [BDM], [Ni3] within a Landauer-Büttiker approach [BuLa], [ChVi], [Lan] (see also [NiPa], [Pat], [JLPS], [PrSj], [BNP], [BNP1]). We recall that the analysis has been reduced, in [BNP1], to an h-dependent linear problem after providing uniform estimates for the initial semilinear problem. Hence we consider for $h > 0$ going to zero and for some fixed interval $I = [a, b]$ the Schrödinger operator on the real line,

$$P^h := -\frac{d^2}{dx^2} + \tilde{\mathcal{V}}^h - W^h, \quad \tilde{\mathcal{V}}^h := -\mathcal{B} + V^h, \quad V^h \in W^{1,\infty}(a, b)\,, \tag{1.1}$$

where

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

and B is a non-negative constant. The potential $\mathcal{B}$ simply models the applied bias. The family of potentials $(V^h)_{h\in(0,h_0)}$ has uniformly bounded second derivatives $\partial_x^2 V^h = \partial_x^2\tilde{\mathcal{V}}^h$ in $\mathcal{M}_b([a, b])$ which converge weakly to some measure $\mu^0 \in \mathcal{M}_b([a, b])$, with the additional boundary conditions

$$V^h(a) = V^h(b) = 0\,.$$

Recall that this makes a bounded family of functions $\tilde{\mathcal{V}}^h$ in $W^{1,\infty}(a, b)$ and which converges in $\mathcal{C}^{0,\alpha}(I)$, $\alpha < 1$, to a function $\tilde{\mathcal{V}}^0$, $\partial_x^2\tilde{\mathcal{V}}^{(0)}\big|_{(a,b)} = \mu^0\big|_{(a,b)}$. We assume that

$$\inf_{h\in(0,h_0),x\in I} \tilde{\mathcal{V}}^h(x) =: \Lambda_0 > 0. \tag{1.3}$$

Finally, the potential $-W^h$ describes quantum wells according to

$$W^h(x) = \sum_{i=1}^{N} w_i\left(\frac{x-c_i}{h}\right)\,, \tag{1.4}$$

where $c_1 < \ldots < c_N$ are N given points in (a, b) and the functions w_i are continuous[1] positive functions supported in $[-\kappa, \kappa]$ for some fixed $\kappa > 0$. We shall use the convention $c_0 = a$ and $c_{N+1} = b$. The Hamiltonian H^h is the self-adjoint realization of P^h on the real line with domain $H^2(\mathbb{R})$

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

Recall that the notation P is used for the differential operator while H is reserved for some closed non necessary self-adjoint realization as an unbounded operator on L^2.

The potentials w_i, $i = 1, \ldots, N$, is chosen so that the spectrum $\sigma(H_i)$ of the Hamiltonians $H_i = -\Delta - w_i$ satisfies

$$\tilde{\mathcal{V}}^h(c_i) + \inf\sigma(H_i) \geq \kappa_i > 0\,,$$

with κ_i independent of h. With such an assumption the operator H^h has a purely continuous spectrum equal to $[-B, \infty)$.

Due to the applied bias $B \geq 0$, the dispersion relation associated with the Hamiltonian H^h reads

$$\lambda_k := \left|\begin{array}{ll} k^2 & \text{if } k > 0, \\ k^2 - B & \text{if } k < 0. \end{array}\right. \tag{1.6}$$

[1] In [BNP1], the nonlinear analysis was carried out with only $w_i \in L^\infty(I)$.

For $k \in \mathbb{R}$ such that $\lambda_k \in (-B, +\infty) \setminus \{0\}$, the incoming scattering state $\psi_-(k,x)$ is the solution of

$$P^h \psi_-^h(k,\cdot) = \lambda_k \psi_-^h(k,\cdot)\,, \tag{1.7}$$

with the normalization

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

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

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 $\lambda_k \in (-B, 0)$.
This can be reduced to k-dependent transparent boundary conditions

$$\text{for } k>0 \qquad \begin{cases} \left[h\partial_x + i\lambda_k^{1/2}\right] u(a) = 2ike^{i\frac{ka}{h}}, \\ \left[h\partial_x - i(\lambda_k+B)^{1/2}\right] u(b) = 0, \end{cases} \tag{1.8}$$

$$\text{for } k<0 \qquad \begin{cases} \left[h\partial_x + i\lambda_k^{1/2}\right] u(a) = 0, \\ \left[h\partial_x - i(\lambda_k+B)^{1/2}\right] u(b) = 2ike^{i\frac{kb}{h}}\,. \end{cases} \tag{1.9}$$

The coefficients t_k and r_k are the transmission and reflexion coefficients and satisfy for $\lambda_k > 0$

$$|r_k|^2 + \sqrt{\frac{\lambda_k}{\lambda_k+B}}|t_k|^2 = 1. \tag{1.10}$$

Denote, for $i = 1,\dots,N$ by σ_i the set of negative eigenvalues of the Hamiltonian $H_i = -\Delta - w_i$ with $D(H_i) = H^2(\mathbb{R})$

$$\sigma_i := \{e_k^i\}_{k\in K_i} \subset (-\infty;0), \quad K_i \subset \mathbb{N}, \quad i = 1,\dots,N\,. \tag{1.11}$$

The set of asymptotic resonant energies is defined as

$$\mathcal{E}_0 := \bigcup_{i=1}^N \mathcal{E}_i, \quad \mathcal{E}_i := \sigma_i + \tilde{\mathcal{V}}^0(c_i). \tag{1.12}$$

Let us recall as well the notion of asymptotic resonant wells associated with $\lambda \in \mathcal{E}_0$:

$$J_\lambda := \{i \in \{1,\dots,N\} \text{ s. t. } \lambda \in \mathcal{E}_i\}\,.$$

The multiplicity m_λ of the asymptotic resonant energy λ is given by

$$m_\lambda := \# J_\lambda.$$

Like in [BNP1], we focus on positive energies: We fix an energy domain $(\Lambda_*, \Lambda^*) \subset (0, \Lambda_0)$, and we consider the functions

$$\theta \in \mathcal{C}_c^0\left((\Lambda_*, \Lambda^*)\right), \quad \theta \geq 0\,, \tag{1.13}$$

$$\text{and} \qquad g(k) = \theta(\lambda_k)\mathbf{1}_{\mathbb{R}_+}(k)\,. \tag{1.14}$$

The function of the asymptotic momenum is the operator with (continuous in 1D) kernel

$$g(K_-^h)[x,y] = \int_k g(k)\psi_-^h(k,x)\overline{\psi_-^h(k,y)}\ \frac{dk}{2\pi h}\,, \tag{1.15}$$

and we are interested in the asymptotic of the particle density $n^h(x)$ defined by

$$\int_a^b \varphi(x)\ dn^h(x) = \mathrm{Tr}\ \left[g(K_-^h)\varphi(x)\right]\,, \quad \forall\varphi\in\mathcal{C}_c^0((a,b))\,,$$

or equivalently

$$n^h(x) = \int_k g(k)|\psi_-^h(k,x)|^2\ \frac{dk}{2\pi h}\,.$$

The result of [BNP1, Theorem 1.6] states that, possibly after extracting a subsequence, the measure dn^h converges weakly to dn^0 in $\mathcal{M}_b((a,b))$ with

$$dn^0 = \sum_{\lambda\in\mathcal{E}_0}\sum_{i\in J_\lambda} t_i^\lambda\,\theta(\lambda)\,\delta_{x=c_i}\,,\quad t_i^\lambda\in[0,1]\,. \tag{1.16}$$

Our aim here is the accurate determination of the coefficients t_i^λ according to the geometry of the potential.

Recall that this result, [BNP1, Theorem 1.6], is essentially obtained by checking that the t_i^λ's are equal to 1 when the function $g(k)$ is replaced by $\theta(\lambda_k)$ and $g(K_-^h)$ by $\theta(H^h)$. In this article, we focus on the anisotropic case when $g(k)=\theta(\lambda_k)\mathbf{1}_{\mathbb{R}_+}(k)$ cannot be written as a function of the energy. Note that due to the decomposition

$$\theta(H^h) = g_-(K_-^h)+g_+(K_-^h),\qquad g_-(k)=\mathbf{1}_{k<0}\cdot\theta(\lambda_k),\quad g_+(k)=\mathbf{1}_{k>0}\cdot\theta(\lambda_k), \tag{1.17}$$

the result can be tranformed into a result for functions g_- supported on negative momentum and even carries over to more general combination.

2 Assumptions and results

Since (1.16) is a local result on the energy axis while the set of asymptotic resonant energies $\mathcal{E}_0$ is finite, the analysis can be partly simplified after the next assumption.

Assumption 1 *Suppose that the support of function θ and therefore $g(k)=\mathbf{1}_{k>0}\cdot\theta(\lambda_k)$, contains only one asymptotic resonant energy*

$$supp\ \theta\cap\mathcal{E}_0 = \{\lambda_0\}\ .$$

The next assumptions are technically more serious. Some specific configurations allow to handle accurately and quite simply the discussion with respect to the geometry in terms of the Agmon distance.

Definition 2.1 *With an energy $\lambda\in\mathbb{R}$ and a potential $V\in L^\infty(I)$, is associated the Agmon (possibly degenerate) distance $d(.,.;V,\lambda)$ defined by :*

$$\forall x,y\in I,\quad d(x,y;V,\lambda) = \left|\int_x^y \sqrt{(V(t)-\lambda)_+}\,dt\right|. \tag{2.1}$$

Notation 1 *The Agmon distance associated with the asymptotic potential* $\tilde{\mathcal{V}}^0$ *and the asymptotic resonant energy* λ_0 *is denoted by* d_0*. It is defined by*

$$d_0(x,y) := \left| \int_x^y \sqrt{\tilde{\mathcal{V}}^0(\tau) - \lambda_0}\, d\tau \right| ,$$

With this distance, let

$$S_0 := d_0(\cup_{i\in J_{\lambda_0}}\{c_i\}, \partial I), \quad S_U := \max_{i,j\in J_{\lambda_0}} d_0(c_i, c_j), \quad S_I := d_0(a,b) \tag{2.2}$$

be respectively the distance between the λ_0*-resonant wells and the boundary* $\partial I = \{a, b\}$*, the diameter of the union of the resonant wells, and the diameter of the island.*
It is sometimes convenient to introduce the set

$$U = \{c_1, \ldots, c_N\} .$$

Finally, introduce for $\eta_0 > 0$ *the quantity*

$$\tilde{S}_U := \max_{\tau\in[c_1,c_N]} \sqrt{\tilde{\mathcal{V}}^0(\tau) + \eta_0 - \lambda_0}\, |c_N - c_1|,$$

which measures the diameter of the area which contains all the wells.

Notice that $\tilde{S}_U$ is written in terms of some L^∞-norm of the potential instead of an integral. The parameter η_0 is introduced in order to ensure $\tilde{S}_U > S_U$. It can be chosen arbitrarily small.

Definition 2.2 *We say that the* λ_0*-resonant wells are gathered (resp. strongly gathered) if and only if*

$$S_0 + S_U < S_I/2 \quad (\textit{resp.} \quad S_0 + m_{\lambda_0} S_U < S_I/2). \tag{2.3}$$

As $S_0 + S_U$ is the greatest distance from the boundary of the island to the resonant wells, the condition $S_0 + S_U < S_I/2$ expresses that the resonant wells are gathered in one the halves of the island. This explains the terminology.

Definition 2.3 *We say that the wells are isolated if and only if*

$$S_0 > 8\tilde{S}_U \quad \textit{and} \quad m_{\lambda_0} = N. \tag{2.4}$$

Inequality (2.4) means that the wells are confined in the central part of the island.

Theorem 2.4 *Make Assumption 1. Suppose that the* λ_0*-resonant wells are strongly gathered, or suppose that the wells are isolated* ($m_{\lambda_0} = N$) *and gathered with* $N = m_{\lambda_0}$*. Then the two next statements hold:*
i) The coefficients $t_i^{\lambda_0}$, $i \in J_{\lambda_0}$*, are all equal to* 1 *if* $d_0(a, c_i) < d_0(c_i, b)$ *for all* $i \in J_{\lambda_0}$*.*
ii) The coefficients $t_i^{\lambda_0}$, $i \in J_{\lambda_0}$*, are all equal to* 0 *if* $d_0(a, c_i) > d_0(c_i, b)$ *for all* $i \in J_{\lambda_0}$*.*

In the first case the wells are confined in the left-hand half of the island, whereas in the second case the wells are confined in the right-hand side of the island, this partition being done in terms of the Agmon distance d_0. This result can be interpreted in terms of tunneling effect: in case *i)* the tunneling effect is easier from a to the wells than from the wells to b, the particles coming from $-\infty$ (remember $g_+(-|k|) = 0$) are trapped by the wells; in case *ii)*, the particle escape more easily from the wells to b than they get into the wells from a.

Theorem 2.5 *Assume that the wells are isolated according to Definition 2.3 ($m_{\lambda_0} = N$). Let $\lambda_1^h < \ldots < \lambda_{m_{\lambda_0}}^h$ be the eigenvalues of the Dirichlet Hamiltonian H_I^h on $I = [a, b]$ converging to λ_0 as $h \to 0$ with the normalized eigenvectors $\phi_1^h, \ldots, \phi_{m_{\lambda_0}}^h$. Fix $\varepsilon \in (0, 1/2 \min_{0 \le i \ne i' \le N+1} |c_i - c_{i'}|)$ and let $\tilde{\psi}_-^h(k, \cdot)$ be the generalized eigenfunctions of $\tilde{H}^h = H^h + W^h$. Then the coefficient $t_i^{\lambda_0}$, $i = 1, \ldots, m_{\lambda_0}$, is obtained as the limit of the quantity*

$$\sum_{j=1}^{m_{\lambda_0}} \frac{\displaystyle\int_{c_i-\varepsilon}^{c_i+\varepsilon} |\phi_j^h(x)|^2 \, dx}{1 + \dfrac{\sqrt{\lambda_j^h} \left| \left\langle \phi_j^h \, , \, W^h \tilde{\psi}_-^h(-\sqrt{\lambda_j^h + B}, \cdot) \right\rangle \right|^2}{\sqrt{\lambda_j^h + B} \left| \left\langle \phi_j^h \, , \, W^h \tilde{\psi}_-^h(+\sqrt{\lambda_j^h}, \cdot) \right\rangle \right|^2}} \,, \tag{2.5}$$

as $h \to 0$ (after possibly extracting a subsequence).

From this result non trivial cases for which not all the t_i^λ belong to $\{0, 1\}$ will be exhibited in Section 8, in particular in Proposition 8.5 and Proposition 8.6.
When $N = 1$, we will establish that, the coefficient $t_1^{\lambda_0}$ belongs to $(0, 1)$ only if $d_0(a, c_1) = d_0(c_1, b)$. In the case of two wells $N = 2$, the values of $t_1^{\lambda_0}$ and $t_2^{\lambda_0}$ have to fulfill the next rules

1. $t_1^{\lambda_0} = 1$ and $t_2^{\lambda_0} \in [0, 1]$ if $d_0(a, c_1) < d_0(c_2, b)$;
2. $t_1^{\lambda_0} \in [0, 1]$ and $t_2^{\lambda_0} = 0$ if $d_0(a, c_1) > d_0(c_2, b)$;
3. $1 \ge t_1^{\lambda_0} \ge t_2^{\lambda_0} \ge 0$ if $d_0(a, c_1) = d_0(c_2, b)$.

All these rules which were proved only for isolated wells and especially the general condition $t_1^{\lambda_0} \ge t_2^{\lambda_0}$ have a very natural interpretation within the probabilistic presentation of quantum mechanics. They are probably valid in all cases although our proof requires some specific assumptions. They were taken as granted in the numerical applications treated in [BNP]. Note that our results provide essentially a complete understanding of what is going on when there is no interaction of resonances, or when the interaction of resonant states involves only two wells. In the final nonlinear problem presented in [BNP], [BNP1], the coefficients t_i^λ play the role of Lagrange multipliers which have an arbitrary value in $[0, 1]$ when the associated constraint for the asymptotic resonant energy or the Agmon distances is saturated.
Finally note that the assumption $m_{\lambda_0} = N$ in the second case of Theorem 2.4 (isolated and gathered wells) is not crucial. It is assumed here in order to avoid some unessential technicalities which have already been considered in [BNP1] and are treated in the sligthly simpler first case.

3 Reduction of the relevant energy interval

In [BNP1], a small h-dependent energy domain around λ_0 has been introduced. Let H_I^h denote the Dirichlet realization of P^h on the interval $I = [a, b]$ and let $\{\lambda_1^h, \ldots, \lambda_{m_{\lambda_0}}^h\}$ be the ordered eigenvalues converging to λ^0 as $h \to 0$. Set

$$\Omega_h := \{z \in \mathbb{C} \quad \text{s.t.} \quad \mathrm{Re}\,(z) \in K_h, \quad \mathrm{Im}\,(z) \in [-4h, 4h]\} \tag{3.1}$$

$$\text{with} \qquad K_h := [\lambda_0 - \alpha^h, \lambda_0 + \alpha^h] \tag{3.2}$$

$$\text{and} \qquad \alpha^h := 4 \max \left\{h, |\lambda_0 - \lambda_j^h|, \, j = 1, \ldots, m_{\lambda_0}\right\} \,. \tag{3.3}$$

The Proposition 6.4 of [BNP1] yields the next energy interval reduction.

Proposition 3.1 *Under Assumption 1, the convergence*

$$\lim_{h\to 0} Tr\left[g(K_-^h)\varphi(x)\right] - g(\sqrt{\lambda_0})\,Tr\left[\mathbf{1}_{K_h}(H^h)\mathbf{1}_{(0,+\infty)}(K_-^h)\varphi(x)\right] = 0$$

holds for any $\varphi \in \mathcal{C}_c^0((a,b))$ *.*

Hence we will mainly focus on the energies lying in K_h and on the spectral parameters lying in Ω_h in the sequel.

4 Lower bound for the imaginary parts of the resonances

In this simple one-dimensional problem where the potential is piecewise constant outside a compact interval, the resonances are easily introduced after an explicit complex deformation of the transparent boundary conditions (1.8)-(1.9). The operator H_ζ^h is defined for a complex ζ lying in a neighborhood of $\lambda \in (-B, 0)$ by

$$D(H_\zeta^h) = \left\{ u \in H^2(I), \quad \begin{array}{l} \left[h\partial_x + i\zeta^{1/2}\right] u(a) = 0, \\ \left[h\partial_x - i(\zeta + B)^{1/2}\right] u(b) = 0 \end{array} \right\}, \tag{4.1}$$

$$H_\zeta^h u = P^h u = [-h^2\Delta + \mathcal{V}^h(x)]u\,, \quad \forall u \in D(H_\zeta^h)\,. \tag{4.2}$$

The resonances are then exactly the complex values z for which the operator $(H_z^h - z)$ is not injective (see [BNP1] for this specific case and [BaCo], [HeSj1], [HiSi] for more general versions of the complex deformation).
It was proved in [BNP1] that the resonances converging to λ_0 lie in a $\tilde{\mathcal{O}}(e^{-2S_0/h})$-neighborhood of the Dirichlet eigenvalues (see [BNP1, Proposition 5.2]). Hence we get the usual result that the imaginary part of resonances converging to λ_0 are exponentially small

$$\mathrm{Im}\,(z^h) = \tilde{\mathcal{O}}(e^{-\frac{2S_0}{h}})\,.$$

Providing a lower bound for the imaginary part of resonances is a standard result within the semiclassical analysis of resonances (see [HeSj1]). We check it with a more pedestrian approach for our 1D problem where the potential does not fit exactly with the semiclassical setting and has a limited regularity. Note that the lower bound can be much smaller than the upper bound in the multiple well case.

Proposition 4.1 *For any* $\eta > 0$*, there exists a positive constant* $C_\eta > 0$ *such that for any resonance* z^h *converging to* λ_0*, one has*

$$C_\eta e^{-\frac{2S_0 - \eta}{h}} \geq -Im\,(z^h) \geq C_\eta^{-1} e^{-\frac{2(S_0 + S_U) + \eta}{h}}\,. \tag{4.3}$$

Proof: Let z^h such a resonance and u^h a normalized resonant state associated, that is an element in the kernel of $H_{z^h}^h - z^h$ with $L^2(I)$-norm equal to 1. It satisfies

$$-h^2\Delta u^h + \mathcal{V}^h(x)u^h = z^h u^h, \quad \left\|u^h\right\|_{L^2(I)} = 1\,,$$

with the boundary conditions provided by $u^h \in D(H_{z^h}^h)$. By taking the imaginary part of the identity (A.1) applied with $V = \mathcal{V}^h$, $u_2 = u_1 = u^h$, $z = z^h$ and $\varphi \equiv 0$ one gets

$$-\,\mathrm{Im}\,(z^h) = h\mathrm{Re}\,(\sqrt{z^h + B})|u^h(b)|^2 + h\mathrm{Re}\,(\sqrt{z^h})|u^h(a)|^2. \tag{4.4}$$

If the imaginary part of z^h is too small, u^h satisfies a Cauchy problem in $x = a$ with small datas because of the resonant boundary conditions and $\lim_{h\to 0} z^h = \lambda_0 \in (\Lambda_*, \Lambda^*)$. We next check that such a smallness is limited by the normalization assumption $\left\|u^h\right\|_{L^2} = 1$. In order to get this, set

$$F(x) := \begin{pmatrix} u^h(x) \\ ih\dfrac{du^h}{dx}(x) \end{pmatrix}. \tag{4.5}$$

F satisfies the ODE on I

$$ih\frac{dF}{dx} = A^h(x)F(x), \quad A^h(x) := \begin{pmatrix} 0 & 1 \\ z^h - \mathcal{V}^h & 0 \end{pmatrix}, \quad \mathcal{V}^h = \tilde{\mathcal{V}}^h - W^h. \tag{4.6}$$

Endow $\mathbb{C}^2$ with the standard hermitian norm. If $\rho^h(x)$ denotes the spectral radius of $A^h(x)\overline{A^h(x)^T}$, one gets the estimate

$$\left|h\frac{dF}{dx}\right|^2 \leq \rho^h(x)|F(x)|^2. \tag{4.7}$$

By Gronwall's lemma this yields

$$|F(x)| \leq \min\left(|F(a)|e^{\frac{1}{h}\int_a^x |z^h - \mathcal{V}^h(\tau)|^{1/2}\,d\tau}; |F(b)|e^{\frac{1}{h}\int_x^b |z^h - \mathcal{V}^h|^{1/2}\,d\tau}\right), \tag{4.8}$$

for all $x \in I$. The transparent conditions given by $u^h \in D(H^h_{z^h})$ imply

$$|F(a)|^2 = |u^h(a)|^2(1 + |z^h|), \quad |F(b)|^2 = |u^h(b)|^2(1 + |z^h + B|)\,. \tag{4.9}$$

Apply now the Agmon estimate technique like in [DiSj] in order to check that the resonant wave function concentrates in the wells: Taking the real part of the identity (A.1) with $V = \mathcal{V}^h$, $z = z^h$, $u_1 = u_2 = u^h$ and $\varphi(x) = d(x, \operatorname{supp} W^h; \tilde{\mathcal{V}}^h - \varepsilon_0, \operatorname{Re} z^h)$ with $\varepsilon_0 > 0$ leads to

$$\begin{aligned} 0 = \int_a^b \left|h\partial_x(e^{\frac{\varphi}{h}}u^h)\right|^2\,dx + \varepsilon_0\int_{I\setminus\operatorname{supp} W^h}\left|e^{\frac{\varphi}{h}}u^h\right|^2\,dx \\ + \int_{\operatorname{supp} W^h}(\tilde{\mathcal{V}}^h(x) - W^h(x) - \operatorname{Re} z^h)\left|u^h\right|^2\,dx \\ + h\operatorname{Im}[(z^h)^{1/2}]\,e^{2\frac{\varphi(a)}{h}}\left|u^h(a)\right|^2 + h\operatorname{Im}[(z^h + B)^{1/2}]\,e^{2\frac{\varphi(b)}{h}}\left|u^h(b)\right|^2\,. \end{aligned}$$

Since $\lim_{h\to 0} z^h = \lambda_0 > 0$ and $\operatorname{Im}(z^h) = \tilde{\mathcal{O}}(e^{-2S_0/h})$ and from (4.4) we deduce the estimate

$$\begin{aligned} \int_{I\setminus\operatorname{supp} W^h}\left|h\partial_x(e^{\frac{\varphi}{h}}u^h)\right|^2 + \varepsilon_0\left|e^{\frac{\varphi}{h}}u^h\right|^2\,dx \leq \tilde{\mathcal{O}}\left(e^{-4\frac{S_0}{h}}\right)\max\left\{e^{\frac{2\varphi(a)}{h}}, e^{\frac{2\varphi(b)}{h}}\right\} \\ - \int_{\operatorname{supp} W^h}(\tilde{\mathcal{V}}^h(x) - W^h(x) - \operatorname{Re} z^h)\left|u^h\right|^2\,dx\,. \end{aligned}$$

Owing to $\varphi(a) \leq d_0(a, U)$ and $\varphi(b) \leq d_0(b, U)$ for $h > 0$ small enough and to $\left\|u^h\right\|_{L^2} = 1$ we get

$$\int_{I\setminus\operatorname{supp} W^h}\left|h\partial_x(e^{\frac{\varphi}{h}}u^h)\right|^2 + \varepsilon_0\left|e^{\frac{\varphi}{h}}u^h\right|^2\,dx \leq C$$

for some constant independent of $h > 0$ (small enough). Let χ a cut-off function which cancels around the boundary of I. Then, χu^h is close to an eigenfunction for the Dirichlet operator

H_I^h. Using [Hel, p. 30–31] (or [HeSj2]), we can prove that u^h has asymptotically no mass in the non-resonant wells.

From this we conclude that the constant $\kappa_1 > 0$ can be chosen so that there exists $i \in J_{\lambda_0}$ such that the L^2-norm of u^h on $[c_i - \kappa_1 h, c_i + \kappa_1 h]$ is greater than $\frac{1}{2}\frac{1}{m_{\lambda_0}}$, for $h > 0$ small enough. Using (4.8) and integrating on $[c_i - \kappa_1 h, c_i + \kappa_1 h]$, one obtains from (4.8) and (4.9)

$$\frac{1}{4m_{\lambda_0}^2} \le \min\Big(|u^h(a)|^2(1+|z^h|)\int_{c_i-\kappa_1 h}^{c_i+\kappa_1 h} e^{\frac{2}{h}\int_a^x |z^h-\mathcal{V}^h(\tau)|^{1/2}\,d\tau}\,dx\,;$$
$$|u^h(b)|^2(1+|z^h+B|)\int_{c_i-\kappa_1 h}^{c_i+\kappa_1 h} e^{\frac{2}{h}\int_x^b |z^h-\mathcal{V}^h(\tau)|^{1/2}\,d\tau}\,dx\Big)\,. \quad (4.10)$$

In the integral with respect to τ, one can replace $\mathcal{V}^h$ by $\tilde{\mathcal{V}}^h$ *modulo* $\mathcal{O}(h)$, since each well is of diameter κh. Fix now $\varepsilon_1 > 0$. For $h > 0$ small enough we can assume

$$|\tilde{\mathcal{V}}^h(x) - \tilde{\mathcal{V}}^0(x)| \le \varepsilon_1$$
$$\text{and} \quad \left|z^h - \lambda_0\right| \le \varepsilon_1\,.$$

This leads finally to

$$\begin{aligned} 1/(4\,m_{\lambda_0}^2) &\le e^{C\kappa_1}\min\Big(2h|u^h(a)|^2(1+|z^h|)e^{\frac{2(d_0(a,c_i)+C\varepsilon_1}{h}}; 2h|u^h(b)|^2(1+|z^h+B|)e^{\frac{2d_0(c_i,b)+C\varepsilon_1}{h}}\Big) \\ &\le C'\left|\mathrm{Im}\,z^h\right| e^{\frac{2d_0(c_i,\partial I)+C'\varepsilon_1}{h}}\,. \end{aligned}$$

The lower bound of (4.3) appears as a necessary condition owing to $d_0(c_i, \partial I) \le S_0 + S_U$ by taking $C'\varepsilon_1 \le \varepsilon$. □

Remark 4.2 • *Note that in the single well case $N = 1$, $S_U = 0$, one recovers a logarithmic equivalent to $|Im\, z^h|$.*

- *Note that the lower bound of* (4.3) *can be improved slightly by noticing* $d_0(c_i, \partial I)$ *is less than* $\min\{S_0 + S_U, S_I/2\}$.

5 Resolvent estimates around an asymptotic resonant energy

In this section, we play with the explicit expression of the determinant and the inverse of finite dimensional matrices after the Grushin reduction of the resonance problem, in the spirit [TaZw]. The next expression of the resolvent was derived in [BNP1] after introducing a Grushin problem :

$$\mathbf{1}_I(H^h - z)^{-1}\mathbf{1}_I = (H_z^h - z)^{-1} = F(z) - E^+(z)(E^{-+}(z))^{-1}E^-(z)\,, \quad (5.1)$$

for all $z \in \Omega_h$ and where F is a holomorphic trace class operator-valued function. For any compact set $K \subset (a, b)$, there exists c_K such that the estimate

$$\forall \varphi \in \mathcal{C}^0(K), \quad |\mathrm{Tr}\,(F(z)\varphi)| = \mathcal{O}_\varphi(e^{-c_K/h}), \quad h \to 0\,, \quad (5.2)$$

holds uniformly for $z \in \Omega_h$ and $h \in (0, h_0)$. The meromorphic part is of finite rank with poles located exactly at the resonances $z_1^h, \ldots, z_{m_{\lambda_0}}^h$ of P^h.

The labelling of the resonances is done according to the labelling of the Dirichlet eigenvalues $\lambda_1^h, \dots, \lambda_{m_{\lambda_0}}^h$ with $\left|z_j^h - \lambda_j^h\right| = \tilde{\mathcal{O}}\left(e^{-2S_0/h}\right)$.
Moreover, the approximated expansion

$$\begin{aligned} E^{-+}(z) &= \operatorname{diag}\left[\left(z-\lambda_1^h\right),\dots,\left(z-\lambda_{m_{\lambda_0}}^h\right)\right] + \tilde{\mathcal{O}}\left(e^{-\frac{2S_0}{h}}\right) &(5.3)\\ &= \operatorname{diag}\left[\left(z-z_1^h\right),\dots,\left(z-z_{m_{\lambda_0}}^h\right)\right] + \tilde{\mathcal{O}}\left(e^{-\frac{2S_0}{h}}\right), &(5.4)\\ E^-(z) &= E_0^-\psi + \tilde{\mathcal{O}}\left(e^{-\frac{S_0}{2h}}\right), &(5.5)\\ E^+(z) &= \chi E_0^+ + \tilde{\mathcal{O}}\left(e^{-\frac{S_0}{2h}}\right). &(5.6)\end{aligned}$$

hold with $\left\|E_0^+\right\|$ and $\left\|E_0^-\right\|$ uniformly bounded and where ψ and χ are cut-off functions (see [BNP1, Section 5 and Section 6.2]).

Proposition 5.1 *The estimate*

$$\left\|(E^{-+}(\lambda))^{-1}\right\| = \tilde{\mathcal{O}}\left(e^{\frac{2(m_{\lambda_0}-1)S_U}{h}}\left[\min_{j=1,\dots,m_{\lambda_0}} |\lambda - z_j^h|\right]^{-1}\right)$$

holds for any <u>*real*</u> $\lambda \in \Omega_h \cap \mathbb{R}$, *when* $\|\ \|$ *denotes any fixed norm on* $\mathcal{M}_{m_{\lambda_0}}(\mathbb{C})$.

Proof. We start to prove that there exists a function f^h such that

$$\forall z \in \overline{\Omega_h}, \quad \det E^{-+}(z) = \prod_{j=1}^{m_{\lambda_0}} (z - z_j^h) f^h(z) \quad \inf_{h>0} \inf_{\Omega_h} |f^h(z)| \geq c > 0. \tag{5.7}$$

Fix any norm on $\mathcal{M}_{m_{\lambda_0}}(\mathbb{C})$. The function $f^h : z \mapsto \det E^{-+}(z) \prod_{j=1}^{m_{\lambda_0}} (z - z_j^h)^{-1}$ is meromorphic on Ω_h, does not cancel, and has removable singularities at $z = z_j^h$. We apply then the maximum modulus principle to the matrix elements. Because of (5.4) and the location of the resonances we have

$$\det E^{-+}(z) = \prod_{j=1}^{m_{\lambda_0}} (z - z_j^h) + \tilde{\mathcal{O}}\left(e^{-\frac{2S_0}{h}}\right), \tag{5.8}$$

and on the boundary of Ω_h, $|z - z_j^h| \geq Ch$, $C > 0$. Consequently, f is bounded by below by $1/2$ for h sufficiently small. This proves (5.7).
In order to evaluate the norm of $(E^{-+}(z))^{-1}$, we use the representation

$$(E^{-+}(z))^{-1} = \frac{1}{\det E^{-+}(z)} \mathrm{com} E^{-+}(z)^T, \tag{5.9}$$

where $\Gamma(z) := \mathrm{com}E^{-+}(z)^T$ denotes the transpose matrix of the cofactors. Let us make more explicit the form of the general element $\Gamma_{ij}(z)$ in order to get the estimate. In general, by denoting $\varepsilon(z)$ the residual matrix in (5.4) the entry $\Gamma_{ij}(z)$ is a sum of $(m_{\lambda_0} - 1)!$ homogeneous monomials of order $m_{\lambda_0} - 1$ in the matrix elements of $E^{-+}(z)$, among which there are r diagonal elements $(0 \leq r \leq m_{\lambda_0} - 1)$. Such a monomial writes

$$\prod_{k=1}^{r} (z - z_{j_k}^h + \varepsilon_{i_k,i_k}) \prod_{l \notin \{1,\dots,r\}}^{m_{\lambda_0}-1} \varepsilon_{\sigma(i_l),i_l}, \quad \sigma \in \mathfrak{S}_{m_{\lambda_0}-1}\,. \tag{5.10}$$

The estimate of $\left\|(E^{-+}(z))^{-1}\right\|$ is then derived from an upper bound of quantities like

$$t_r^h(z)=\frac{\prod_{k=1}^{r}\left(z-z_{j_k}^h+\varepsilon_{i_k,i_k}\right)\prod_{k\notin\{1,\dots,r\}}^{m_{\lambda_0}-1}\varepsilon_{\sigma(i_k),i_k}}{\prod_{j=1}^{m_{\lambda_0}}(z-z_j^h}\,,\quad 0\leq r\leq m_{\lambda_0}-1. \tag{5.11}$$

For any fixed $r\in\{0,\dots,m_{\lambda_0}-1\}$ and $\lambda\in\mathbb{R}$, the inequality

$$|t_r^h(\lambda)|\leq C_r\max_{0\leq r_1\leq r}\frac{\tilde{\mathcal{O}}\left(e^{-\frac{2(m_{\lambda_0}-r_1-1)S_0}{h}}\right)}{\prod_{k=1}^{m_{\lambda_0}-r_1}|z_{j_k}^h-\lambda|}\leq C_r\max_{0\leq r_1\leq r}\frac{\tilde{\mathcal{O}}\left(e^{-\frac{2(m_{\lambda_0}-r_1-1)S_0}{h}}\right)}{|z_{j_1}^h-\lambda|\prod_{k=2}^{m_{\lambda_0}-r_1}|\mathrm{Im}\,z_{j_k}|}$$

combined with the lower bound (4.3) yields

$$\left|t_r^h(\lambda)\right|\leq C_r\max_{0\leq r_1\leq r}\frac{\tilde{\mathcal{O}}\left(e^{\frac{2(m_{\lambda_0}-r_1-1)S_U}{h}}\right)}{\min_j\left|\lambda-z_j^h\right|}\leq C_r\frac{\tilde{\mathcal{O}}\left(e^{\frac{2(m_{\lambda_0}-1)S_U}{h}}\right)}{\min_j\left|\lambda-z_j^h\right|}\,.$$

□

6 Case of strong gatherness

We prove Theorem 2.4 under the strong gatherness assumption (see Definition 2.2) that we recall here:

$$S_0+m_{\lambda_0}S_U<S_I/2\,. \tag{6.1}$$

Actually the result will be proved under the simplifying assumption that all the wells are λ_0-resonant, $m_{\lambda_0}=N$. The Lemma 6.1 given in the end of this Section will make clear that this assumption is not restrictive.

Proof of Theorem 2.4 under the strong gatherness assumption: First note that the two statements *i)* and *ii)* can be deduced one from the other with a complementary argument provided by the relation (1.17) with the functions of the energy for which $t_j^\lambda=1$ was proved in [BNP1]. Hence we want to prove

$$\lim_{h\to 0}\mathrm{Tr}\,\left[g(K_-^h)\varphi\right]=0$$

in the case ii). According to Proposition 3.1, it is equivalent to

$$\lim_{h\to 0}\mathrm{Tr}\,\left[g^h(K_-^h)\varphi\right]=0\,,$$

with $g^h(k)=\mathbf{1}_{(0,+\infty)}(k)\mathbf{1}_{K_h}(\lambda_k)\,.$

Let $\psi_-(k,x)$ ($\lambda_k\in K_h$) be the generalized eigenfunction defined by (1.8)-(1.9) for the potential $\mathcal{V}^h$ and $\tilde{\psi}_-(k,x)$ be the generalized eigenfunction associated with the filled potential $\tilde{\mathcal{V}}^h=\mathcal{V}^h+W^h\,.$ Set

$$u^h(k,\cdot):=\psi_-^h(k,\cdot)-\tilde{\psi}_-^h(k,\cdot)=(H_{k^2}^h-k^2)^{-1}W^h\tilde{\psi}_-^h(k,\cdot). \tag{6.2}$$

so that

$$|\psi_-^h(k,x)|^2 \leq 2|\tilde{\psi}_-^h(k,x)|^2 + 2|u^h(k,x)|^2\,. \tag{6.3}$$

If we denote by $\tilde{K}_-^h$ the asymptotical momentum for $\tilde{H}^h$, we get for any $\varphi \in \mathcal{C}_c^0((a,b);\mathbb{R}_+)$:

$$0 \leq \mathrm{Tr}\,(g^h(K_-^h)\varphi) \leq \mathrm{Tr}\,(g^h(\tilde{K}_-^h)\varphi) + 2\|\varphi\|_\infty^2 \int_{k>0,\lambda_k\in I_h} \|u^h(k,\cdot)\|_{L_x^2}^2 \frac{dk}{2\pi h}\,. \tag{6.4}$$

If we come back to the expression (5.1) of the resolvent $(H_{k^2}^h - k^2)^{-1}$, we get

$$u^h(k,\cdot) = F(k^2)W^h\tilde{\psi}_-^h(k,\cdot) - E^+(k^2)(E^{-+}(k^2))^{-1}E^-(k^2)W^h\tilde{\psi}_-^h(k,\cdot), \tag{6.5}$$

and finally

$$\|u^h(k,\cdot)\|_{L_x^2}^2 \leq 2\|F(k^2)W^h\tilde{\psi}_-^h(k,\cdot)\|^2 + 2\|T(k^2)W^h\tilde{\psi}_-^h(k,\cdot)\|^2\,, \tag{6.6}$$

by setting

$$T(k^2) := E^+(k^2)(E^{-+}(k^2))^{-1}E^-(k^2)\,. \tag{6.7}$$

The first term of (6.6) uniformly goes to 0 when $h \to 0$, because F is bounded in the operator-norm and $W^h\tilde{\psi}_-^h(k,\cdot)$ is $\tilde{\mathcal{O}}(e^{-d_0(a,U^h)})/h)$, according to the Proposition 6.2 in Section 6.1 of [BNP1]. By Proposition 5.1, it follows that the second term is bounded by

$$\|T(k^2)W^h\tilde{\psi}_-^h(k,\cdot)\|^2 = \tilde{\mathcal{O}}\left(\frac{e^{-\frac{2d(a,U)}{h}}e^{\frac{4(N-1)S_U}{h}}}{\min\limits_{j=1,\ldots,N}|k^2 - z_j^h|^2}\right)\,. \tag{6.8}$$

But, for any resonance $z^h \in \{z_1^h,\ldots,z_N^h\}$, writing $z^h = E^h - i\Gamma^h$, $E^h = \mathrm{Re}\,(z^h)$, $\Gamma^h = -\mathrm{Im}\,(z^h)$, gives

$$\frac{1}{|k^2 - z^h|^2} = \frac{1}{\Gamma^h}\frac{\Gamma_h}{(k^2 - E^h)^2 + {\Gamma^h}^2}. \tag{6.9}$$

The latter factor is uniformly bounded in $L^1(\mathbb{R}_k)$, while the first factor is estimated owing to (4.3) by

$$\frac{1}{\Gamma_h} = \tilde{\mathcal{O}}\left(e^{\frac{2(S_0+S_U)}{h}}\right)\,.$$

By putting all the inequalities together, the integral in (6.4) is dominated by

$$\tilde{\mathcal{O}}\left(e^{-\frac{2d(a,U)}{h}}e^{\frac{4(N-1)S_U}{h}}\right) \times \tilde{\mathcal{O}}\left(e^{\frac{2(S_0+S_U)}{h}}\right)\,.$$

We conclude by recalling the assumptions

$$\begin{aligned} d(a,U) &= S_I - (S_0 + S_U)\\ -2S_I + 4(S_0 &+ NS_U) < 0\,. \end{aligned}$$

□

The next arguments show that the assumption $m_{\lambda_0} = N$ is easily removed. Let $\tilde{H}_{k^2,nr}^h$ be the operator with the same domain as $H_{k^2}^h$ and associated with the potential

$$\tilde{\mathcal{V}}_{nr}^h = \mathcal{V}^h + \sum_{j\in J_{\lambda_0}} w_j\left(\frac{x - c_j}{h}\right)\,,$$

where all the resonant wells are filled. In [BNP1] such an Hamiltonian was denoted by $\tilde{H}_{k^2}(\lambda_0)$ and it was proved (see Proposition 4.3) that it satisfies the same resolvent estimate as $\tilde{H}_{k^2}$. Hence the previous proof carries over to the case when $m_{\lambda_0} < N$ as soon as the generalized eigenfunctions $\tilde{\psi}_{-,nr}^h(k,x)$ corresponding to the partially filled wells share the same properties as the $\tilde{\psi}_-^h(k,x)$. This is given by the next Lemma.

Lemma 6.1 *For $k > 0$ such that $\lambda_k \in K_h$, the pointwise estimate*

$$\tilde{\psi}^h_{-,nr}(k,x) = \tilde{\psi}^h_{-}(k,x) + \tilde{\mathcal{O}}\left(e^{-\frac{d_0(a,U^h_{nr})+d_0(U^h_{nr},x)}{h}}\right)$$

holds for any $x \in I = [a,b]$ with a uniform control of the constants with respect to $x \in I$. The set U^h_{nr} is supp W^h_{nr} with $W^h_{nr} = W^h - \sum_{j\in J_{\lambda_0}} w_j\left(\frac{\cdot - c_j}{h}\right)$.

Proof: The function $\varepsilon(k,\cdot) := \tilde{\psi}^h_{-,nr}(k,\cdot) - \tilde{\psi}^h_{-}(k,\cdot)$ is in the domain of $H^h_{k^2,nr}$ and, since $\tilde{P}^h - W^h_{nr} = P^h_{nr}$, it follows that

$$\tilde{\psi}^h_{-,nr}(k,\cdot) = \tilde{\psi}^h_{-}(k,\cdot) - (H^h_{k^2,nr} - k^2)^{-1} W^h_{nr} \tilde{\psi}^h_{-}(k,\cdot). \tag{6.10}$$

It was shown that $\tilde{\psi}^h_{-}(k,x) = \mathcal{O}(h^{-1})e^{-d_0(a,x)}$ uniformly w.r.t k, whereas the kernel of $(H^h_{k^2,nr} - k^2)^{-1}$ is $\tilde{\mathcal{O}}(e^{-d_0(x,y)})$. □

7 Isolated Wells

We assume in this section $m_{\lambda_0} = N$.

7.1 Preliminary results

In the case of isolated wells, the geometric assumption ensures that the resonances are simple. More precisely, the gaps between the Dirichlet eigenvalues converging to λ_0 are much larger than the imaginary parts of all the corresponding resonances. This does not correspond exactly to the case $m_{\lambda_0} = 1$ because the energy domain $K_h = \Omega_h \cap \mathbb{R}$ has to be splitted into exponentially small energy intervals with a refined analysis which was not really carried out in [BNP1]. This will lead in particular in Section 7.2 to a refined version of the Breit-Wigner type formula for the local density of states already considered in [BNP1] after [GeMa].

The first result which is an application of the universal lower bound of gaps given in [KiSi], introduces the quantity $\tilde{S}_U$.

Proposition 7.1 *Let $\lambda^h_1 < \ldots < \lambda^h_{m_{\lambda_0}}$ be the eigenvalues of H^h_I, the Dirichlet realization of P^h on I converging to λ_0. There exists a constant $C_U > 0$ such that for $h > 0$ sufficiently small*

$$\forall j \neq k, \quad |\lambda^h_j - \lambda^h_k| \geq C_U^{-1} e^{-\frac{\tilde{S}_U}{h}}. \tag{7.1}$$

When the wells are isolated, each disc centered on λ^h_j with radius $(3C_U)^{-1}e^{-\tilde{S}_U/h}$ contains therefore only one resonance of P^h for $h > 0$ small enough.

Proof: Consider the Hamiltonian $\hat{H}^h$ on the whole line $\mathbb{R}$ with domain $H^2(\mathbb{R})$ and defined by

$$\forall u \in H^2(\mathbb{R}), \hat{H}^h u := \hat{P}^h u, \quad \hat{P}^h := -h^2 d^2/dx^2 + \hat{\mathcal{V}}^h, \tag{7.2}$$

$$\hat{\mathcal{V}}^h = \mathbf{1}_{(-\infty,b)} \cdot \mathcal{V}^h(a) + \mathbf{1}_I \cdot \mathcal{V}^h + \mathbf{1}_{(b,\infty)} \cdot \mathcal{V}^h(b). \tag{7.3}$$

The potential $\hat{\mathcal{V}}^h$ is a continuous function constant outside I and coinciding with $\mathcal{V}^h$ on I. By construction, one has

$$\inf \sigma_{\text{ess}}\big(\hat{H}^h\big) \geq \Lambda_0 > \Lambda^*. \tag{7.4}$$

Besides, the number of eigenvalues of $\hat{H}^h$ is bounded w.r.t. $h > 0$. Apply then the Theorem 2 from [KiSi] given in Appendix B with $[a_{KS}, b_{KS}] = [c_1 - \kappa h, c_N + \kappa h]$ and $\alpha_{KS}^2 = \Lambda_0$ (the $_{KS}$ index refers to Kirsch and Simon's notations). This provides a lower bound for the splitting of the eigenvalues of $\hat{H}^h$, lying around λ_0, namely

$$|\hat{\lambda}_j^h - \hat{\lambda}_k^h| \geq Ce^{-\frac{\tilde{S}_U}{h}}. \tag{7.5}$$

Now, if λ^h is one of the eigenvalues of H_I^h in this interval with ϕ^h a corresponding L^2-normalized eigenfunction, one has with the exponential decay estimates (see [BNP1, Proposition 3.3])

$$\hat{H}^h \chi \phi^h = \lambda^h \chi \phi^h + [P^h, \chi]\phi^h, \quad \|[P^h, \chi]\phi^h\|_{L^2} \leq C_\eta e^{-\frac{S_0 - c\eta}{h}}, \tag{7.6}$$

for a smooth cut-off function χ supported in (a, b) and equal to 1 outside an η-neighborhood of its boundary $\partial I = \{a, b\}$. Since H_I^h is self-adjoint, an orthonormal basis of m_{λ_0} eigenvectors ϕ^h's associated with eigenvalues λ^h converging to λ_0 can be considered. The exponential decay of these eigenvectors (see [BNP1, Proposition 3.3]) ensures that the Gram matrix of the $\chi\phi^h$'s is exponentially close the unit matrix. According to [Hel], [HeSj2] (see also [BNP1, Appendix C]), $\hat{H}^h$ has at least m_{λ_0} eigenvalues converging to λ_0.

Conversely, if $\hat{\lambda}^h$ is an eigenvalue of $\hat{H}^h$ with eigenfunction $\hat{\phi}^h$, one has in $L^2(I)$

$$\hat{H}^h \chi \hat{\phi}^h = \hat{\lambda}^h \chi \hat{\phi}^h + [P^h, \chi]\hat{\phi}^h, \tag{7.7}$$

with the same estimate of the remainder term $[P^h, \chi]\hat{\phi}^h$ as in (7.6) owing to the exponential decay of $\hat{\phi}^h$ (Use again the Agmon estimate). A first application of the results of [Hel], [HeSj2] (see also [BNP1, Appendix C]) ensures that there is a bijection between the eigenvalues of H_I^h and the eigenvalues of $\hat{H}^h$ converging to λ_0, with variations of order $\tilde{\mathcal{O}}(e^{-S_0/h})$ which are much smaller than the gaps (7.5). □

The previous localization of resonances can be combined with the Grushin formulation (5.1). Unfortunately this does not produce an accurate enough information. We now want to use the lower bound on the gaps in order to consider separately every pair (λ_j^h, z_j^h) made of a Dirichlet eigenvalue with the associated resonance, although this still allows interacting wells. Improved resolvent estimates and a better description of the generalized wave function is needed. In [BNP1] the kernel of the resolvent $(H_\bullet^h - z)^{-1}$ was studied when $\text{dist}(z, \sigma(H_I^h))$ is larger than h^C (or $e^{-S_1/h}$ with the notations of [BNP1]). Here we have to work with only $\text{dist}(z, \lambda_j^h) \geq (C/100)e^{-\tilde{S}_U/h}$, that is much closer to the Dirichlet eigenvalue λ_j^h ($e^{-\tilde{S}_U/h} = o(e^{-S_U/h}) = o(e^{-S_1/h})$). Let us start with a lemma about the Dirichlet realization which completes the results of [BNP1].

Lemma 7.2 *Let H_I^h be the Dirichlet realization on the interval I of the operator P^h. Let z^h belong to Ω_h with $h \in (0, h_0)$, h_0 small enough. Set*

$$r(h) = \mathit{dist}(z^h, \sigma(H_I^h)),$$

and assume $r(h) > 0$. The kernel of the resolvent $(H_I^h - z^h)^{-1}$ satisfies

$$(H_I^h - z^h)^{-1}[x, y] = \frac{\tilde{\mathcal{O}}\left(e^{-\frac{d_0(x,y) - S_U}{h}}\right)}{\min(r(h), 1)}$$

with uniform constants with respect to $x, y \in I$, when d_0 denotes the Agmon distance $d(., .; \tilde{\mathcal{V}}^0, \lambda_0)$.

Proof: We already proved in [BNP1, Proposition 3.7 and Corollary 3.8] the estimate

$$(H_I^h - z^h)^{-1}[x,y] = \tilde{\mathcal{O}}\left(e^{-\frac{d_0(x,y)}{h}}\right), \quad \text{when } r(h) \geq h^C\,; \tag{7.8}$$

and in [BNP1, Proposition 3.9] the estimate

$$\left|\phi_j^h(x)\right| + \left|\partial_x \phi_j^h(x)\right| = \tilde{\mathcal{O}}\left(e^{-\frac{d_0(x,U)}{h}}\right), \tag{7.9}$$

which holds for any normalized eigenfunction ϕ_j^h associated with an eigenvalue λ_j^h, $j \in \{1,\ldots,m_{\lambda_0}\}$, converging to λ_0 as $h \to 0$. Recall that U gathers all the wells

$$U = \{c_1,\ldots,c_N\}\,.$$

Consider the spectral projector

$$\Pi_I^h = \mathrm{Id} - \frac{1}{2i\pi}\int_{\partial\Omega_h} (z - H_I^h)^{-1}\, dz = \mathrm{Id} - \sum_{j=1}^{m_{\lambda_0}} |\phi_j^h\rangle\langle\phi_j^h|\,.$$

Write for $z \in \Omega_h \setminus \sigma(H_I^h)$

$$\begin{aligned}(H_I^h - z)^{-1} &= (H_I^h - z)^{-1}\Pi_I^h + (H_I^h - z)^{-1}(\mathrm{Id} - \Pi_I^h)\\ &= (H_I^h - z)^{-1}\Pi_I^h + \sum_{j=1}^{m_{\lambda_0}} \frac{1}{\lambda_j^h - z}|\phi_j^h\rangle\langle\phi_j^h|\,,\end{aligned}$$

where the first term is holomorphic with respect to $z \in \Omega_h$. In terms of Schwartz kernels one gets

$$(H_I^h - z)^{-1}\Pi_I^h[x,y] = (H_I^h - z)^{-1}[x,y] - \sum_{j=1}^{m_{\lambda_0}} \frac{1}{\lambda_j^h - z}\phi_j^h(x)\overline{\phi_j^h(y)}\,.$$

The maximum principle combined with the estimate (7.8) for $z \in \partial\Omega_h$ and the decay estimate (7.9) imply

$$\forall z \in \Omega_h, \left|(H_I^h - z)^{-1}\Pi_I^h[x,y]\right| \leq \tilde{\mathcal{O}}\left(e^{-\frac{d_0(x,y)-S_U}{h}}\right).$$

An obvious estimate of the polar term derived again from (7.9) yields the result.

□

Below are two results for the filled wells potential $\tilde{\mathcal{V}}^h$. The first Lemma is a specific case of Proposition 4.3 in [BNP1]. The second one is a consequence of Proposition 6.2 in [BNP1].

Lemma 7.3 *For $z \in \Omega_h$ the resolvent estimate*

$$\left|(\tilde{H}_z^h - z)^{-1}[x,y]\right| = \tilde{\mathcal{O}}\left(e^{-\frac{d_0(x,y)}{h}}\right)$$

holds with uniform constant with respect to $x, y \in I$.

Lemma 7.4 *For $\lambda \in K_h = \Omega_h \cap \mathbb{R}$, the generalized wave functions $\tilde{\psi}_-^h(\sqrt{\lambda},.)$ and $\tilde{\psi}_-^h(-\sqrt{\lambda+B},.)$, which solve* (1.7)-(1.8) *with $W^h \equiv 0$, satisfy*

$$\tilde{\psi}_-^h(\sqrt{\lambda},.) = \tilde{\mathcal{O}}\left(e^{-\frac{d_0(a,x)}{h}}\right) \quad \text{and} \quad \tilde{\psi}_-^h(-\sqrt{\lambda+B},x) = \tilde{\mathcal{O}}\left(e^{-\frac{d_0(x,b)}{h}}\right),$$

with uniform constants with respect to $x \in [a,b]$.

7.2 Breit-Wigner formulas

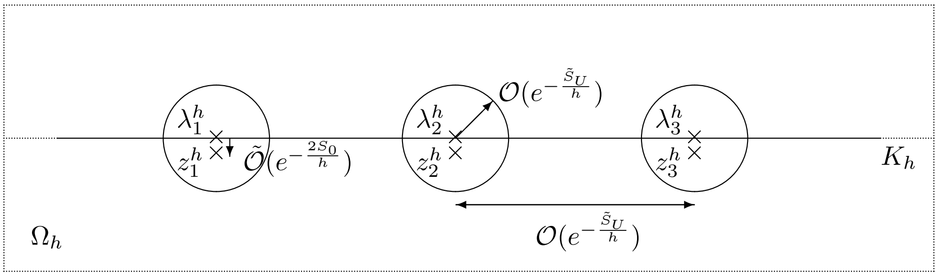
We provide here an accurate information on the resolvent $(H^h_\lambda - \lambda)^{-1} = \mathbf{1}_I (H^h - \lambda)^{-1} \mathbf{1}_I$, for $\lambda \in K_h$, in terms of resonances.
The domain

$$K_h \times \left[-(20C_U)^{-1} e^{-\frac{\tilde{S}_U}{h}}, (20C_U)^{-1} e^{-\frac{\tilde{S}_U}{h}}\right] = \left\{z \in \Omega_h, |\mathrm{Im}\, z| \leq (20C_U)^{-1} e^{-\frac{\tilde{S}_U}{h}}\right\}$$

will be covered by $N_h = \tilde{\mathcal{O}}(e^{\tilde{S}_U/h})$-open discs with radius $(10C_U)^{-1} e^{-\tilde{S}_U/h}$ centered on the real axis. They are labelled so that the m_{λ_0} first ones are centered around the Dirichlet eigenvalues λ^h_j

$$\omega^h_j = \left\{z \in \mathbb{C}, \quad \left|z - \lambda^h_j\right| < (10C_U)^{-1} e^{-\frac{\tilde{S}_U}{h}}\right\},$$

and the notation ω^h_j with $j > m_{\lambda_0}$ is used for all the other ones.



Proposition 7.5 *For $j \in \{1, \ldots, m_{\lambda_0}\}$, let z^h_j be the resonance of H^h associated with the Dirichlet eigenvalue λ^h_j, $\left|z^h_j - \lambda^h_j\right| = \tilde{\mathcal{O}}(e^{-2S_0/h})$. For any $j \in \{1, \ldots, N_h\}$ the resolvent $(H^h_z - z)^{-1}$ is decomposed in ω^h_j as*

$$\left(H^h_z - z\right)^{-1} = g^h_j(z) + \frac{\mathbf{1}_{[1,m_{\lambda_0}]}(j)}{z^h_j - z} A^h_j$$

where $g^h_j(z)$ is an holomorphic operator-valued function of $z \in \omega^h_j$ with the next properties:

1. *For $j \in \{1, \ldots, m_{\lambda_0}\}$, the operator A^h_j is close to the Dirichlet spectral projector $|\phi^h_j\rangle\langle\phi^h_j|$:*

$$\left\|A^h_j - |\phi^h_j\rangle\langle\phi^h_j|\,\right\| = \tilde{\mathcal{O}}\left(e^{-\frac{S_0 - 6\tilde{S}_U}{2h}}\right). \tag{7.10}$$

2. *If χ_1 and $\chi_{1/2}$ are two $\mathcal{C}^\infty_0((a,b))$ cut-off functions such that $\chi_\varrho \equiv 1$ on U and $\partial_x \chi_\varrho$ is supported in $\{x \in (a,b),\ \varrho S_0 - \eta \leq d_0(x,U) \leq \varrho S_0 + \eta\}$ with $\varrho \in \{1/2, 1\}$ and $\eta > 0$, then there is a constant $C_\eta > 0$ and a constant $c > 0$ independent of $\eta > 0$, such that the difference*

$$D^h_j(z) = g^h_j(z) - \left[(\tilde{H}^h_z - z)^{-1}(1 - \chi_{1/2}) + \chi_1 (H^h_I - z)^{-1} \chi_{1/2} - \frac{\mathbf{1}_{[1,m_{\lambda_0}]}(j)}{z^h_j - z} A^h_j\right] \tag{7.11}$$

satisfies

$$\forall z \in \partial\omega^h_j, \quad \left\|D^h_j(z)\right\| \leq C_\eta\, e^{-\frac{S_0 - 6\tilde{S}_U - c\eta}{2h}}. \tag{7.12}$$

Proof: The proof of this result relies on two leading ideas. One is the Laurent expansion (with the exact poles z_j^h) of the meromorphic function $(H_z^h - z)^{-1}$ which is handled like in the proof of Lemma 7.2. The other one is the approximation of the resolvent $(H_z^h - z)^{-1}$ by

$$R^h = (\tilde{H}_z^h - z)^{-1}(1 - \chi_{1/2}) + \chi_1 (H_I^h - z)^{-1} \chi_{1/2}\,, \tag{7.13}$$

already considered in [BNP1, Proposition 4.3].
We focus on the case $j \in \{1, \ldots, m_{\lambda_0}\}$, since the other case $j > m_{\lambda_0}$ will be deduced easily from this one by taking $A_j^h = 0$. The expression (7.13) leads to

$$\begin{aligned} \forall z \in \omega_j^h \setminus \left\{\lambda_j^h\right\}, \qquad & (H_z^h - z)R^h = 1 - \varepsilon = 1 - \varepsilon_0 - \varepsilon_1 \\ \text{with} \qquad & \varepsilon_0 = W^h (\tilde{H}_z^h - z)^{-1}(1 - \chi_{1/2}) \\ \text{and} \qquad & \varepsilon_1 = -\left[P^h, \chi_1\right](H_I^h - z)^{-1}\chi_{1/2}\,. \end{aligned}$$

Lemma 7.3 and Lemma 7.2 provide the estimates

$$\begin{aligned} & \|\varepsilon_0\| \le C_\eta\, e^{-\frac{S_0 - c\eta}{2h}}\,, \\ \text{and} \qquad & \|\varepsilon_1\| \le C_\eta\, \frac{e^{-\frac{S_0 - c\eta - 2S_U}{2h}}}{r(h)} \le C_\eta\,(10C_U)\, e^{-\frac{S_0 - c\eta - 4\tilde{S}_U}{2h}}\,, \end{aligned}$$

for any $z \in \partial\omega_j^h$ with $r(h) = \left|z - \lambda_j^h\right| = (10C_U)^{-1} e^{-\tilde{S}_U/h}$. Hence the assumption $\tilde{S}_U < S_0/4$ and taking $\eta > 0$ small enough ensure the convergence of the series

$$(H_z^h - z)^{-1} = R^h \sum_{k=0}^{\infty} \varepsilon^k = R^h + R^h \sum_{k=1}^{\infty} \varepsilon^k, \quad \text{for } z \in \partial\omega_j^h\,. \tag{7.14}$$

We now consider the Laurent expansion of $(H_z^h - z)^{-1}$ in ω_j^h

$$(H_z^h - z)^{-1} = g_j^h(z) + \frac{1}{z_j^h - z} A_j^h\,, \tag{7.15}$$

where z_j^h is the resonance of H^h lying in ω_j^h according to Proposition 7.1. Computing the residue of $(H_z^h - z)^{-1}$, equal to (7.14) with R_h given by (7.13), along the contour $\partial\omega_j^h$ provide the estimates

$$\left\| A_j^h - |\phi_j^h\rangle\langle\phi_j^h| \,\right\| \le e^{-\frac{S_0 - c\eta}{2h}} + \sup_{z \in \partial\omega_j^h} \left\| R^h \sum_{k=1}^{\infty} \varepsilon^k \right\| \le C'_\eta e^{-\frac{S_0 - c\eta - 4\tilde{S}_U}{2h}} \times e^{\frac{\tilde{S}_U}{h}}\,,$$

after using

$$\|R_h\| \le C\|(\tilde{H}_z - z)^{-1}\| + C\|(H_I - z)^{-1}\| = \mathcal{O}\left(e^{\frac{\tilde{S}_U}{h}}\right)\,.$$

This yields (7.10).
For the second estimate, notice the identity

$$D_j^h(z) = g_j^h(z) - R^h + \frac{1}{z_j^h - z} A_j^h = R^h \sum_{k=1}^{\infty} \varepsilon^k$$

and (7.12) is deduced from

$$\left\| R^h \sum_{k=1}^{\infty} \varepsilon^k \right\| \le C'_\eta e^{-\frac{S_0 - c\eta - 6\tilde{S}_U}{2h}} \quad \text{for } z \in \partial\omega_j^h\,.$$

□

Remark 7.6 *The estimates of the error terms could be improved by studying more carefully the first terms of the series* $\sum_{k=1}^{\infty} \varepsilon^k$ *in the spirit of [HeSj1] or [BNP1, Proposition 4.3]. It is not an essential issue here.*

Below is the Breit-Wigner formula which will be used.

Proposition 7.7 *Assume that the wells are isolated and take the notations* λ_j^h, ϕ_j^h z_j^h *and* ω_j^h *introduced before for* $j \in \{1, \ldots, m_{\lambda_0}\}$. *In* ω_j^h *one has the next equality of meromorphic functions*

$$\langle \phi_j^h \,, (H_z^h - z)^{-1} \phi_j^h \rangle = \frac{1 + \tilde{\mathcal{O}}\left(e^{-\frac{S_0 - 6\tilde{S}_U}{2h}}\right)}{z_j^h - z} + \tilde{\mathcal{O}}\left(e^{-\frac{S_0 - 8\tilde{S}_U}{2h}}\right),$$

and the uniform estimate

$$\left\| g_j^h(z) \right\| = \tilde{\mathcal{O}}\left(e^{-\frac{S_0 - 8\tilde{S}_U}{2h}}\right).$$

Proof: Let us write

$$\langle \phi_j^h \,, (H_z^h - z)^{-1} \phi_j^h \rangle = \langle \phi_j^h \,, g_j^h(z) \phi_j^h \rangle + \frac{1}{z_j^h - z} \langle \phi_j^h \,, A_j^h \phi_j^h \rangle .$$

According to (7.10) the second term has the form

$$\frac{1}{z_j^h - z} \langle \phi_j^h \,, A_j^h \phi_j^h \rangle = \frac{1 + \tilde{\mathcal{O}}\left(e^{-\frac{S_0 - 6\tilde{S}_U}{2h}}\right)}{z_j^h - z} .$$

The first term is holomorphic in ω_j^h and it suffices to find an estimate along $\partial\omega_j^h$. We use the decompostion (7.11)

$$\langle \phi_j^h \,, g_j^h(z) \phi_j^h \rangle = \langle \phi_j^h \,, \left[D_j^h(z) + (\tilde{H}_z^h - z)^{-1}(1 - \chi_{1/2}) \right] \phi_j^h \rangle + \langle \phi_j^h \,, \chi_1 (H_I^h - z)^{-1} (\chi_{1/2}) \phi_j^h \rangle - \frac{1 + \tilde{\mathcal{O}}\left(e^{-\frac{S_0 - 6\tilde{S}_U}{2h}}\right)}{z_j^h - z} .$$

This leads to

$$\langle \phi_j^h \,, g_j^h(z) \phi_j^h \rangle = \tilde{\mathcal{O}}\left(e^{-\frac{S_0 - 6\tilde{S}_U}{2h}}\right) + \frac{z_j^h - \lambda_j^h}{\left(z_j^h - z\right)\left(\lambda_j^h - z\right)} + \frac{\tilde{\mathcal{O}}\left(e^{-\frac{S_0}{2h}}\right)}{\left|\lambda_j^h - z\right|} + \frac{\tilde{\mathcal{O}}\left(e^{-\frac{S_0 - 6\tilde{S}_U}{2h}}\right)}{\left|z_j^h - z\right|},$$

for all $z \in \partial\omega_j^h$ and the maximum principle yields the first result.
The estimate of $\left\| g_j^h(z) \right\|$ follows essentially the same lines. □
We end this section with a reduction of the energy interval which is thiner than the one of Proposition 3.1.

Proposition 7.8 *With the previous notations, set for any* $j \in \{1, \ldots, m_{\lambda_0}\}$

$$K_{j,h} = \omega_j^h \cap \mathbb{R} . \tag{7.16}$$

For any $\varphi \in \mathcal{C}_c^0\left((a,b)\right)$, *the limit*

$$\lim_{h \to 0} Tr\left[g(K_-^h) \varphi(x) \right] - \sum_{j=1}^{m_{\lambda_0}} g(\sqrt{\lambda}_0)\, Tr\left[\mathbf{1}_{K_{j,h}}(H^h) \mathbf{1}_{(0,+\infty)}(K_-^h) \varphi(x) \right] \tag{7.17}$$

is 0.

Proof: We know from (1.16) and [BNP1] that the support of φ can be assumed to be around $U = \{c_1, \dots, c_N\}$, for instance included in $\{x \in (a,b), d_0(x,U) \leq S_0/3\}$. By Proposition 3.1, the first term of (7.17) can be replaced with

$$g(\sqrt{\lambda_0})\mathrm{Tr}\left[\mathbf{1}_{K_h}(H^h)\mathbf{1}_{(0,+\infty)}(K_-^h)\varphi\right] .$$

Moreover we have for $\varphi \geq 0$,

$$\begin{aligned}\mathrm{Tr}\left[\mathbf{1}_{K_h \setminus \cup_{j\leq m_{\lambda_0}} K_{j,h}}(H^h)\mathbf{1}_{(0,+\infty)}(K_-^h)\varphi\right] &\leq \mathrm{Tr}\left[\varphi^{1/2}\mathbf{1}_{K_h\setminus(\cup_{j\leq m_{\lambda_0}}K_{j,h})}(H^h)\varphi^{1/2}\right] \\ &\leq \sum_{j=m_{\lambda_0}+1}^{N_h} \mathrm{Tr}\left[\varphi^{1/2}\mathbf{1}_{K_{j,h}}(H^h)\varphi^{1/2}\right] ,\end{aligned}$$

by introducing $K_{j,h} = \omega_j^h \cap \mathbb{R}$ for $j \in \{m_{\lambda_0}+1, \dots, N_h\}$ and where we recall $N_h = \tilde{\mathcal{O}}\left(e^{\tilde{S}_U/h}\right)$. Proposition 7.5 and especially relation (7.11) give the identity

$$\begin{aligned}\varphi^{1/2}(H^h - \lambda - i0)^{-1}\varphi^{1/2} &= \varphi^{1/2}(H_\lambda^h - \lambda)^{-1}\varphi^{1/2} \\ &= \varphi^{1/2}(\tilde{H}_\lambda^h - \lambda)^{-1}\varphi^{1/2} + \varphi^{1/2}(H_I^h - \lambda)^{-1}\varphi^{1/2} + \varphi^{1/2}D_j^h(\lambda)\varphi^{1/2} ,\end{aligned}$$

valid for all $\lambda \in K_{j,h}$ with $j \in \{m_{\lambda_0+1}, \dots, N_h\}$. Indeed, our choices of supports imply $(1 - \chi_{1/2})\varphi^{1/2} \equiv 0$ and $\varphi^{1/2}\chi_1 \equiv \varphi^{1/2}\chi_{1/2} \equiv \varphi^{1/2}$.
This leads to

$$\frac{1}{2i\pi}\varphi^{1/2}\left[(H^h - \lambda - i0)^{-1} - (H^h - \lambda + i0)\right]\varphi^{1/2} = \frac{1}{2i\pi}\varphi^{1/2}\left[(\tilde{H}_\lambda^h - \lambda)^{-1} + D_j^h(\lambda) - \mathrm{h.c.}\right]\varphi^{1/2} ,$$

where "h.c." stands for "hermitian conjugate". The estimate (7.12) can easily be transformed into a trace-class estimate because of the localization in x and λ. We use Stone's formula for $\mathbf{1}_{K_{j,h}}(H^h)$. After integration w.r.t $\lambda \in K_{j,h}$, $j > m_{\lambda_0}$, and after summing over $j \in \{1, \dots, m_{\lambda_0}\}$, this leads to

$$\sum_{j=m_{\lambda_0}+1}^{N_h} \mathrm{Tr}\left[\varphi^{1/2}\mathbf{1}_{K_{j,h}}(H^h)\varphi^{1/2}\right] = \mathcal{O}\left(e^{-\frac{c}{h}}\right) ,$$

when the wells are assumed isolated. $\square$

7.3 A Fermi-Golden rule

An accurate determination of the coefficients $t_i^{\lambda_0}$ in the case of isolated wells can be done by first elucidating via a Fermi-Golden rule the contribution of positive and negative momenta in the size of the imaginary part of a resonance $z_j^h = E_j^h - i\Gamma_j^h$. We keep the same notations λ_j^h, ϕ_j^h, z_j^h and ω_j^h introduced before for $j \in \{1, \dots, m_{\lambda_0}\}$. The real and imaginary parts of the resonances z_j^h are written according to

$$z_j^h = E_j^h - i\Gamma_j^h , \quad \text{for} \quad j \in \{1, \dots, m_{\lambda_0}\} .$$

Proposition 7.9 *For any $j \in \{1, \dots, m_{\lambda_0}\}$ the idendity*

$$\Gamma_j^h(1 + o(1)) = \frac{|\langle W^h\tilde{\psi}_-^h(\sqrt{\lambda}, \cdot), \phi_j^h\rangle|^2}{4h\sqrt{\lambda}} + \frac{|\langle W^h\tilde{\psi}_-^h(-\sqrt{\lambda+B}, \cdot), \phi_j^h\rangle|^2}{4h\sqrt{\lambda+B}} \tag{7.18}$$

holds for any $\lambda \in \omega_j^h$.

Proof: Let $dE^h(\lambda)$ denote the infinitesimal spectral projection of the whole line Hamiltonian H^h, given by Stone's formula:

$$dE^h(\lambda) = \frac{1}{2i\pi}\left[(H-\lambda-i0)^{-1} - (H-\lambda+i0)^{-1}\right] .$$

We shall compute in two different ways and for a fixed $j \in \{1,\ldots,m_{\lambda_0}\}$ the spectral measure $\left\langle \mathbf{1}_I\phi_j^h\,,\, dE^h(\lambda)\mathbf{1}_I\phi_j^h\right\rangle$ of $\mathbf{1}_I(x)\phi_j$.

First Stone's formula and Proposition 7.7 lead to

$$\begin{aligned}
\left\langle \mathbf{1}_I\phi_j^h\,,\, dE^h(\lambda)\mathbf{1}_I\phi_j^h\right\rangle &= \frac{1}{2i\pi}\left\langle \phi_j^h\,,\, \left[(H_\lambda^h-\lambda)^{-1} - (H_\lambda^{h,\star}-\lambda)^{-1}\right]\phi_j^h\right\rangle \\
&= \frac{1}{2i\pi}\left(1+\tilde{\mathcal{O}}\left(e^{-\frac{S_0-6\tilde{S}_U}{2h}}\right)\right)\left[\frac{1}{z_j^h-\lambda} - \frac{1}{\overline{z_j^h}-\lambda}\right] + \tilde{\mathcal{O}}\left(e^{-\frac{S_0-8\tilde{S}_U}{h}}\right) \\
&= \frac{\Gamma_j^h\left(1+\tilde{\mathcal{O}}\left(e^{-\frac{S_0-6\tilde{S}_U}{2h}}\right)\right)}{\pi\left(\left|\lambda-E_j^h\right|^2+\left|\Gamma_j^h\right|^2\right)} + \tilde{\mathcal{O}}\left(e^{-\frac{S_0-8\tilde{S}_U}{h}}\right) , \qquad (7.19)
\end{aligned}$$

for all $\lambda \in K_{j,h}$.

The second method uses the generalized wave functions :

$$\left\langle \mathbf{1}_I\phi_j^h\,,\, dE^h(\lambda)\mathbf{1}_I\phi_j^h\right\rangle = \frac{|\langle\psi_-^h(\sqrt{\lambda},\cdot),\phi_j^h\rangle|^2}{4\pi h\sqrt{\lambda}} + \frac{|\langle\psi_-^h(-\sqrt{\lambda+B},\cdot),\phi_j^h\rangle|^2}{4\pi h\sqrt{\lambda+B}} .$$

The relation

$$\psi_-^h(k,\cdot) = \tilde{\psi}_-^h(k,\cdot) - \left(H_{\lambda_k}^h-\lambda_k\right)^{-1} W\tilde{\psi}_-^h(k,\cdot) , \qquad (7.20)$$

Proposition 7.5, the exponential decay of ϕ_j^h and $\tilde{\psi}_-^h(k,\cdot)$ in Lemma 7.4 and Proposition 7.7 lead to

$$\begin{aligned}
\left\langle \phi_j^h\,,\, \psi_-^h(k,\cdot)\right\rangle &= \left\langle \phi_j^h\,,\, \tilde{\psi}_-^h(k,\cdot)\right\rangle + \left\langle \phi_j^h\,,\, g_j^h(\lambda_k)W^h\tilde{\psi}_-^h(k,\cdot)\right\rangle \\
&\quad + \frac{1}{z_j^h-\lambda}\left\langle \phi_j^h\,,\, A_j^hW^h\tilde{\psi}_-^h(k,\cdot)\right\rangle \\
&= \tilde{\mathcal{O}}\left(e^{-\frac{S_0}{h}}\right) + \tilde{\mathcal{O}}\left(e^{-\frac{S_0}{h}}\right)\tilde{\mathcal{O}}\left(e^{-\frac{S_0-8\tilde{S}_U}{2h}}\right) \qquad (7.21) \\
&\quad + \frac{1}{z_j^h-\lambda}\left\langle \phi_j^h\,,\, W^h\tilde{\psi}_-^h(k,\cdot)\right\rangle + \frac{\tilde{\mathcal{O}}\left(e^{-\frac{S_0}{h}}\right)\tilde{\mathcal{O}}\left(e^{-\frac{S_0-6\tilde{S}_U}{2h}}\right)}{\left|z_j^h-\lambda\right|} .
\end{aligned}$$

Owing to Proposition 4.1 and the conditions $\tilde{S}_U > S_U$ and $S_0 > 8\tilde{S}_U$, the last term is estimated by

$$\frac{\tilde{\mathcal{O}}\left(e^{-\frac{S_0}{h}}\right)\tilde{\mathcal{O}}\left(e^{-\frac{S_0-6\tilde{S}_U}{2h}}\right)}{\Gamma_j^h} = o\left(\frac{h^{1/2}}{\sqrt{\Gamma_j^h}}\right) .$$

The equality of the two expressions (7.19) and (7.21) for $\lambda = E_j^h$, and again the assumption $S_0 > 8\tilde{S}_U$ imply

$$\begin{aligned}\frac{1}{\Gamma_j^h}(1+o(1)) &= \frac{1}{4h\sqrt{E_j^h}}\left|\frac{\left\langle \phi_j^h\,,\, W^h\tilde{\psi}_-^h(\sqrt{E_j^h},\cdot)\right\rangle}{\Gamma_j^h} + o\left(\frac{h^{1/2}}{\sqrt{\Gamma_j^h}}\right)\right|^2\\ &+\frac{1}{4h\sqrt{E_j^h+B}}\left|\frac{\left\langle \phi_j^h\,,\, W^h\tilde{\psi}_-^h(-\sqrt{E_j^h+B},\cdot)\right\rangle}{\Gamma_j^h} + o\left(\frac{h^{1/2}}{\sqrt{\Gamma_j^h}}\right)\right|^2 .\end{aligned}$$

This yields the result for $\lambda = E_j^h$. For $\lambda \in \omega_j^h$, one writes the equation for $u = \tilde{\psi}_-^h(\sqrt{\lambda},\cdot) - \tilde{\psi}_-^h(\sqrt{E_j^h},\cdot)$ in the form

$$\begin{cases} (\tilde{P}^h - E_j^h)u = \tilde{\mathcal{O}}\left(e^{-\frac{\tilde{S}_U}{h}}\right)\tilde{\psi}_-^h(\sqrt{\lambda},\cdot)\,,\\ h\partial_x u(a) + i\sqrt{E_j^h}u(a) = \tilde{\mathcal{O}}\left(e^{-\frac{\tilde{S}_U}{h}}\right) + \tilde{\mathcal{O}}\left(e^{-\frac{\tilde{S}_U}{h}}\right)\tilde{\psi}_-^h(\sqrt{\lambda},a)\,,\\ h\partial_x u(b) - i\sqrt{E_j^h+B}u(b) = \tilde{\mathcal{O}}\left(e^{-\frac{\tilde{S}_U}{h}}\right)\tilde{\psi}_-^h\left(\sqrt{\lambda},b\right).\end{cases}$$

With the Agmon identity (A.1) with $\varphi = (1-\eta)d_0(a,x)$, $\eta > 0$, one gets

$$\left|\tilde{\psi}_-^h(\sqrt{E_j^h},x) - \tilde{\psi}_-^h(\sqrt{\lambda},x)\right| = \tilde{\mathcal{O}}\left(e^{-\frac{d_0(x,a)+\tilde{S}_U}{h}}\right). \tag{7.22}$$

Note that the right-hand side is $o(\sqrt{h\Gamma_j^h})$ when $x \in \operatorname{supp} W^h$ owing to Proposition 4.1 and the assumption $\tilde{S}_U > S_U$. A similar estimate can be obtained for the momentum $-\sqrt{E_j^h+\lambda}$ with the distance $d_0(x,b)$ instead of $d_0(a,x)$. Hence the result for $\lambda = E_j^h$ implies

$$\begin{aligned}\Gamma_j^h(1+o(1)) &= \frac{1+o(1)}{4h\sqrt{\lambda}}\left|\left\langle \phi_j^h\,,\, W^h\tilde{\psi}_-^h(\sqrt{\lambda},\cdot)\right\rangle + o(\sqrt{h\Gamma_j^h})\right|^2\\ &+\frac{1+o(1)}{4h\sqrt{\lambda+B}}\left|\left\langle \phi_j^h\,,\, W^h\tilde{\psi}_-^h(-\sqrt{\lambda+B},\cdot)\right\rangle + o(\sqrt{h\Gamma_j^h})\right|^2 ,\end{aligned}$$

for all $\lambda \in \omega_j^h$, which yields the result. □

7.4 Values of the coefficients $t_i^{\lambda_0}$

In this paragraph all the previous intermediate results are gathered in order to check that the coeffcients $t_i^{\lambda_0}$ are the limits of the quantities (2.5), when the wells are isolated. We shall prove Theorem 2.5 and the second statement of Theorem 2.4 about isolated wells will come as a corollary.

Proof of Theorem 2.5: The formula (1.16) and the reduction of the energy interval stated in Proposition 7.8 imply that the coefficient t_i^{λ} is the limit of the quantity

$$\sum_{j=1}^{m_{\lambda_0}}\int_{k>0}\int_{c_i-\varepsilon}^{c_i+\varepsilon}\mathbf{1}_{K_{j,h}}(\lambda_k)\left|\psi_-^h(k,x)\right|^2\,dx\frac{dk}{2\pi h} = \sum_{j=1}^{m_{\lambda_0}}\frac{1}{2\pi h}\left\|\mathbf{1}_{K_{j,h}}(\lambda_k)\psi_-^h(k,x)\right\|^2_{L^2(\mathbb{R}_+\times[c_i-\varepsilon,c_i+\varepsilon])},$$

for any fixed $\varepsilon > 0$.
We use again the relation (7.20) between ψ_-^h and $\tilde{\psi}_-^h$ and the decomposition of $(H_{\lambda_k} - \lambda_k)^{-1}$ stated in Proposition 7.5 in order to write when $\lambda_k \in K_{j,h}$

$$\psi_-^h(k,\cdot) = \tilde{\psi}_-^h(k,\cdot) - g_j^h(\lambda_k) W^h \tilde{\psi}_-^h(k,\cdot) - \frac{1}{z_j^h - \lambda_k} \langle \phi_j^h \,,\, W^h \tilde{\psi}_-^h(k,\cdot)\rangle \phi_j^h - \frac{A_j^h - |\phi_j^h\rangle\langle\phi_j^h|}{z_j^h - \lambda_k} W^h \tilde{\psi}_-^h(k,\cdot)\,.$$

By referring to the decay of $\tilde{\psi}_-^h$ stated in Lemma 7.4 and the estimates for $g_j^h(\lambda)$ and $A_j^h - |\phi_j^h\rangle\langle\phi_j^h|$ derived from Propositions 7.5 and 7.7, this leads to

$$\left\| \mathbf{1}_{K_{j,h}}(\lambda_k) \left[\psi_-^h + \frac{1}{z_j^h - \lambda_k} \langle \phi_j^h \,,\, W^h \tilde{\psi}_-^h(k,\cdot)\rangle \phi_j^h \right] \right\|_{L^2(\mathbb{R}_+ \times [c_i - \varepsilon, c_i + \varepsilon])} = \tilde{\mathcal{O}}\left(e^{-\frac{d_0(a, c_i - \varepsilon)}{h}}\right) + \tilde{\mathcal{O}}\left(e^{-\frac{S_0}{h}}\right) \tilde{\mathcal{O}}\left(e^{-\frac{S_0 - 8\tilde{S}_U}{2h}}\right) + \frac{\tilde{\mathcal{O}}\left(e^{-\frac{S_0}{h}}\right) \tilde{\mathcal{O}}\left(e^{-\frac{S_0 - 6\tilde{S}_U}{2h}}\right)}{\sqrt{\Gamma_j^h}}\,.$$

The assumptions $\tilde{S}_U > S_U$ and $S_0 - 8\tilde{S}_U > 0$ combined with the lower bound (4.3) for Γ_j^h leads to

$$h^{-1/2} \left\| \mathbf{1}_{K_{j,h}}(\lambda_k) \left[\psi_-^h + \frac{1}{z_j^h - \lambda_k} \langle \phi_j^h \,,\, W^h \tilde{\psi}_-^h(k,\cdot)\rangle \phi_j^h \right] \right\|_{L^2(\mathbb{R}_+ \times [c_i - \varepsilon, c_i + \varepsilon])} = o(1)\,.$$

The inequality (7.22) provides a comparison between $\tilde{\psi}_-^h(k,\cdot)$ and $\tilde{\psi}_-^h(\sqrt{\lambda_j^h},\cdot)$ which leads to

$$h^{-1/2} \left\| \mathbf{1}_{K_{j,h}}(\lambda_k) \left[\psi_-^h + \frac{1}{z_j^h - \lambda_k} \langle \phi_j^h \,,\, W^h \tilde{\psi}_-^h(\sqrt{\lambda_j^h},\cdot)\rangle \phi_j^h \right] \right\|_{L^2(\mathbb{R}_+ \times [c_i - \varepsilon, c_i + \varepsilon])} = o(1) + \frac{\tilde{\mathcal{O}}\left(e^{-\frac{S_0}{h}}\right) \tilde{\mathcal{O}}\left(e^{-\frac{\tilde{S}_U}{h}}\right)}{\sqrt{h\Gamma_j^h}} = o(1)\,.$$

Computing the integral

$$\int_{\mathbb{R}_+} \int_{c_i - \varepsilon}^{c_i + \varepsilon} \mathbf{1}_{K_{j,h}}(\lambda_k) \frac{\left|\langle \phi_j^h \,,\, W^h \tilde{\psi}_-^h(\sqrt{\lambda_j^h},\cdot)\rangle\right|^2}{\left|\lambda_k - E_j^h\right|^2 + \left|\Gamma_j^h\right|^2} \left|\phi_j^h(x)\right|^2 \, dx \frac{dk}{2\pi h} = \frac{\left|\langle \phi_j^h \,,\, W^h \tilde{\psi}_-^h(\sqrt{\lambda_j^h},\cdot)\rangle\right|^2}{4h\sqrt{\lambda_j^h}\Gamma_j^h} (1 + o(1))\,,$$

and the Fermi golden rule (7.18) with $\lambda = \lambda_j^h$ yields the result. □

Proof of Theorem 2.4 for isolated wells: Assume $d_0(a, c_k) > d_0(c_k, b)$ for all $k \in \{1, \ldots, m_{\lambda_0} = N\}$. The coefficients $t_i^{\lambda_0}$ are obtained as the limits as $h \to 0$ of

$$\sum_{j=1}^{m_{\lambda_0}} \frac{\left|\langle \phi_j^h \,,\, W^h \tilde{\psi}_-^h(\sqrt{\lambda_j^h},\cdot)\rangle\right|^2}{4h\sqrt{\lambda_j^h}\Gamma_j^h} \int_{c_i - \varepsilon}^{c_i + \varepsilon} \left|\phi_j^h x\right|^2 \, dx\,.$$

But the assumption $d_0(a,c_k) > d_0(c_k,b)$ for all k, implies

$$\left|\langle \phi_j^h\,,\,W^h\tilde{\psi}_-^h(\sqrt{\lambda_j^h},\cdot)\rangle\right|^2 = \tilde{\mathcal{O}}\left(e^{-\frac{S_I}{h}}\right)\,,$$

while the lower bound (4.3) implies

$$\frac{1}{h\Gamma_j^h} = \tilde{\mathcal{O}}\left(e^{\frac{2S_0+2S_U}{h}}\right).$$

The condition $S_0 + S_U < S_I/2$ yields $t_i^{\lambda_0} = 0$, for all $i \in \{1,\ldots,m_{\lambda_0}\}$. □

8 Explicit asymptotic values

In this section we derive from an accurate asymptotic analysis of the quantities (2.5) some explicit rules for the coefficients t_i^λ when the wells are not gathered like in Theorem 2.4. In the two cases $N=1$ or $N=2$ with isolated wells, this provides a complete description of all the possible limits $dn^0\big|_{(a,b)}$, which was summarized in the end of Section 2.

We first need a simple description of the Dirichlet eigenfunctions ϕ_j^h.

Lemma 8.1 *Assume $N = m_{\lambda_0} = 1$ or $N = m_{\lambda_0} = 2$. For $i \in \{1,2\}$, let u_i denote a normalized eigenvector ($u_2 = 0$ when $N=1$) of $-\Delta - w_i$ associated with the eigenvalue $\lambda_0 + \tilde{\mathcal{V}}^0(c_i)$. Then there exists $\alpha^h \in \mathbb{R}$ ($\alpha^h = 0$ if $N=1$) such that the Dirichlet eigenvectors ϕ_j^h satisfy*

$$\begin{pmatrix} \phi_1^h \\ \phi_2^h \end{pmatrix} = \begin{pmatrix} \cos\alpha^h & -\sin\alpha^h \\ \sin\alpha^h & \cos\alpha^h \end{pmatrix} \begin{pmatrix} u_1\left(\frac{\cdot - c_1}{h}\right) \\ u_2\left(\frac{\cdot - c_2}{h}\right) \end{pmatrix} + o_{L^2(I)}(1)\,.$$

Proof: We now from Theorem 3.6 in [BNP1] that the eigenvector ϕ_j^h can be written

$$\phi_j^h = \sum_i p_{ji}^h \psi_i^h + o(1)\,,$$

where $(p_{ij})_{1\le ij\le m_{\lambda_0}}$ is a unitary matrix and where the ψ_i^h is a normalized eigenvectors for the one well problem around c_i. By making use of the uniform $W^{1,\infty}$ estimate of $\tilde{\mathcal{V}}^h$ in a small interval $[c_i - \varepsilon, c_i + \varepsilon]$ with $\varepsilon > 0$ independent of $h > 0$ but arbitrarily small like in Theorem 3.4 of [BNP1], the exponential decay of Dirichlet eigenvectors in the classically forbidden region allows to replace ψ_i^h with u_i with an arbitrarily small error. □

Another ingredient of this asymptotic analysis is an accurate description of the generalized eigenfunctions of $\tilde{H}^h$ in the interval $I = [a,b]$. Introduce the Agmon distance associated with the potential $\tilde{\mathcal{V}}^h$ at the energy λ_k:

$$\tilde{d}_h(x,y) = d(x,y;\tilde{\mathcal{V}}^h,\lambda_k) = \left|\int_x^y \sqrt{\tilde{\mathcal{V}}^h(t) - \lambda_k}\;dt\right|\,. \tag{8.1}$$

The comparison with the first order WKB approximation has to be considered. When $\tilde{\mathcal{V}}^h$ is regular it is a classical result which has to be adapted in our case. The first order approximation $\psi_{app}^h(k,x)$ is defined according to

case $k>0$ **:** $\psi^h_{app}(k,x) = (\tilde{\mathcal{V}}^h(x)-\lambda_k)^{-1/4}\left[C_-(k)e^{-\tilde{d}_h(a,x)/h} + C_+(k)e^{\tilde{d}_h(a,x)/h}\right]$ where $(C_-(k),C_+(k))$ solves the system

$$\left\{\begin{array}{l}\left[-(\tilde{\mathcal{V}}^h(a)-\lambda_k)^{1/2}+i\sqrt{\lambda_k}\right]C_-(k) = 2ike^{i\frac{ka}{h}}\left(\tilde{\mathcal{V}}^h(a)-\lambda_k\right)^{1/4}\,,\\ \left[-(\tilde{\mathcal{V}}^h(b)-\lambda_k)^{1/2}-i\sqrt{\lambda_k+B}\right]C_-(k)\\ \quad+\left[\left(\tilde{\mathcal{V}}^h(b)-\lambda_k\right)^{1/2}-i\sqrt{\lambda_k+B}\right]\left(C_+(k)e^{2\frac{\tilde{d}_h(a,b)}{h}}\right)=0\,,\end{array}\right. \tag{8.2}$$

case $k<0$: $\psi^h_{app}(k,x) = (\tilde{\mathcal{V}}^h(x)-\lambda_k)^{-1/4}\left[C_-(k)e^{\tilde{d}_h(x,b)/h} + C_+(k)e^{-\tilde{d}_h(x,b)/h}\right]$ where $(C_-(k),C_+(k))$ solves the system

$$\left\{\begin{array}{l}\left[-(\tilde{\mathcal{V}}^h(a)-i\lambda_k)^{1/2}+i\sqrt{\lambda_k}\right]\left(C_-(k)e^{2\frac{\tilde{d}_h(a,b)}{h}}\right)\\ \qquad\qquad+\left[(\tilde{\mathcal{V}}^h(a)-\lambda_k)^{1/2}+i\sqrt{\lambda_k}\right]C_+(k)=0\,,\\ \left[\left(\tilde{\mathcal{V}}^h(b)-\lambda_k\right)^{1/2}-i\sqrt{\lambda_k+B}\right]C_+(k) = 2ike^{i\frac{kb}{h}}(\tilde{\mathcal{V}}^h(b)-\lambda_k)^{1/4}.\end{array}\right. \tag{8.3}$$

In our case, its rather technical proof which requires all the regularity and convergence assumptions on $\tilde{\mathcal{V}}^h$, namely $\partial_x^2\tilde{\mathcal{V}}^h = \mu^0$ in $\mathcal{M}_b(I)$, is deferred to a forthcoming article (see [Ni4])

Proposition 8.2 *For any $k\in\mathbb{R}$ such that $\lambda_k\in[\Lambda_*,\Lambda^*]$, consider the generalized wave function $\tilde{\psi}(k,x)$ restricted to the interval I and given by (1.7)-(1.8) with $W^h\equiv 0$. By introducing the Agmon distance $\tilde{d}_h$ associated with the potential $\tilde{\mathcal{V}}^h$ and the energy λ_k according to (8.1), take the function ψ^h_{app} defined above. Then the difference converges to 0 with the weighted estimates*

$$\max_{x\in[a,b]}\left|e^{\frac{\tilde{d}_h(a,x)}{h}}\left(\tilde{\psi}^h(k,x)-\psi^h_{app}(k,x)\right)\right|\overset{h\to 0}{\to} 0 \qquad \text{for } k>0\,,$$
$$\max_{x\in[a,b]}\left|e^{\frac{\tilde{d}_h(x,b)}{h}}\left(\tilde{\psi}^h(k,x)-\psi^h_{app}(k,x)\right)\right|\overset{h\to 0}{\to} 0 \qquad \text{for } k<0\,.$$

We shall make the next simplifying assumption, which ensures that some factors do not vanish asymptotically.

Assumption 2 *Assume that the well potentials w_i, $i=1$ or 2, are even and that the eigenvector u_i corresponds to the first or second eigenvalue.*

Proposition 8.3 *Take the same notations and conventions when $N=1$ as before. Let $\tilde{d}_h$ denotes the Agmon distance for the h-dependent potential $\tilde{\mathcal{V}}^h$ at the energy $\lambda_k\in\Omega_h$ and set for $i=1$ or $i=2$*

$$\gamma_{i,\pm} = \frac{C_\pm(\lambda_0^{1/2})}{(\tilde{\mathcal{V}}^0(c_i)-\lambda_0)^{1/4}}\int_{\mathbb{R}} w_i(y)u_i(y)\,dy \pm C_\pm(\lambda_0^{1/2})(\tilde{\mathcal{V}}^0(c_i)-\lambda_0)^{1/4}\int_{\mathbb{R}} y\,w_i(y)\,u_i(y)\,dy\,. \tag{8.4}$$

Then the equality

$$\begin{pmatrix}\langle\phi_1^h\,,\,W^h\tilde{\psi}^h_-(k,\cdot)\rangle\\ \langle\phi_2^h\,,\,W^h\tilde{\psi}^h_-(k,\cdot)\rangle\end{pmatrix} = \begin{pmatrix}\cos\alpha^h & -\sin\alpha^h\\ \sin\alpha^h & \cos\alpha^h\end{pmatrix}\begin{pmatrix}\gamma_{1,-}e^{-\frac{\tilde{d}_h(a,c_1)}{h}}\\ \gamma_{2,-}e^{-\frac{\tilde{d}_h(a,c_2)}{h}}\end{pmatrix}+o\left(e^{\frac{-\tilde{d}_h(a,c_1)}{h}}\right)$$

holds for $k>0$, while the symmetric relation for $k<0$ writes

$$\begin{pmatrix} \langle \phi_1^h\,,\, W^h\tilde{\psi}_-^h(k,\cdot)\rangle \\ \langle \phi_2^h\,,\, W^h\tilde{\psi}_-^h(k,\cdot)\rangle \end{pmatrix} = \begin{pmatrix} \cos\alpha^h & -\sin\alpha^h \\ \sin\alpha^h & \cos\alpha^h \end{pmatrix} \begin{pmatrix} \gamma_{1,+}e^{-\frac{\tilde{d}_h(c_1,b)}{h}} \\ \gamma_{2,+}e^{-\frac{\tilde{d}_h(c_2,b)}{h}} \end{pmatrix} + o\left(e^{-\frac{\tilde{d}_h(c_2,b)}{h}}\right).$$

Proof: Let us focus on the case $k>0$. First the localisation of the potential W^h and Proposition 8.2 implies

$$\left\| W^h\tilde{\psi_-}(k,\cdot)\right\|_{L^2} = \mathcal{O}\left(e^{-\frac{\tilde{d}_h(a,c_1)}{h}}\right).$$

Hence Lemma 8.1 reduces the problem to an accurate calculation of

$$\begin{aligned}
&\left\langle u_i\left(\frac{\cdot - c_i}{h}\right)\,,\, W^h\tilde{\psi}_-^h(k,\cdot)\right\rangle \\
&= \int_{\mathbb{R}} w_i(y)u_i(y)\tilde{\psi}_-^h\,(k, c_i+hy)\;dy + o\left(e^{-\frac{\tilde{d}_h(a,c_1)}{h}}\right) \\
&= \int_{\mathbb{R}} w_i(y)u_i(y)\frac{C_-(k)}{\left(\tilde{\mathcal{V}}^h(c_i+hy)-\lambda_k\right)^{1/4}} e^{-\frac{\tilde{d}_h(a,c_1+hy)}{h}}\;dy + o\left(e^{-\frac{\tilde{d}_h(a,c_1)}{h}}\right) \\
&= e^{-\frac{\tilde{d}_h(a,c_1)}{h}}\int_{\mathbb{R}} w_i(y)u_i(y)\frac{C_-(k)\left(1-\left(\tilde{\mathcal{V}}^h(c_i)-\lambda_k\right)^{1/2}y\right)}{\left(\tilde{\mathcal{V}}^h(c_i+hy)-\lambda_k\right)^{1/4}}\;dy + o\left(e^{-\frac{\tilde{d}_h(a,c_1)}{h}}\right) \\
&= e^{-\frac{\tilde{d}_h(a,c_1)}{h}}\gamma_{i,-} + o\left(e^{-\frac{\tilde{d}_h(a,c_1)}{h}}\right).
\end{aligned}$$

We used the Taylor expansion of $\tilde{d}_h$ with the known uniform regularity of $\tilde{\mathcal{V}}^h$ in $W^{1,\infty}(I)$. □

Remark 8.4 *The Assumption 2 is not necessary in the previous proof but it ensures that the coefficients $\gamma_{i,\pm}$ do not vanish.*

Proposition 8.5 *Make the technical additional Assumption 2 with $N=m_{\lambda_0}=1$. The asymptotic of (2.5) can lead to values $t_1^{\lambda_0}\in(0,1)$ when and only when $d_0(a,c_1)=d_0(c_1,b)$.*

Proof: When $N=m_{\lambda_0}=1$, the single well is isolated and Theorem 2.5 and Proposition 8.3 can be used. This leads to the value $t_1^{\lambda_0}$ as the limit of

$$\begin{aligned}
&\frac{1}{1+\frac{\sqrt{\lambda_0}}{\sqrt{\lambda_0+B}}\left|\frac{\gamma_{1,-}e^{-\frac{\tilde{d}_h(a,c_1)}{h}}+o\left(e^{-\frac{\tilde{d}_h(a,c_1)}{h}}\right)}{\gamma_{1,+}e^{-\frac{\tilde{d}_h(c_1,b)}{h}}+o\left(e^{-\frac{\tilde{d}_h(c_1,b)}{h}}\right)}\right|^2} \\
&\qquad = \left(1+\frac{\sqrt{\lambda_0}}{\sqrt{\lambda_0+B}}\left|\frac{\gamma_{1,-}}{\gamma_{1,+}}e^{-\frac{\tilde{d}_h(a,c_1)-\tilde{d}_h(c_1,b)}{h}}(1+o(1))\right|^2\right)^{-1},
\end{aligned}$$

where $\tilde{d}_h$ is the Agmon distance at the energy λ_j^h. Any value in $[0,1]$ can be achieved depending on the convergence of $\tilde{d}_h(a,c_1)$ and $\tilde{d}_h(c_1,b)$ to their asymptotic values $d_0(a,c_1)$ and $d_0(c_1,b)$. The discussion of the comparison of the asymptotic distances yields the result. □

Proposition 8.6 *Take $N = m_{\lambda_0} = 2$ and assume that the two wells are isolated with the technical additional condition 2. Assume also $|\lambda_2^h - \lambda_1^h| = o(h)$. Then the coefficients $t_i^{\lambda_0}$, $i = 1, 2$ have to fulfill the rules*

- $t_1^{\lambda_0} = 1$ *and* $t_2^{\lambda_0} \in [0,1]$ $d_0(a, c_1) < d_0(c_2, b)$.
- $t_1^{\lambda_0} \in [0,1]$ *and* $t_2^{\lambda_0} = 0$ *if* $d_0(a, c_1) > d_0(c_2, b)$.
- $1 \geq t_1^{\lambda_0} \geq t_2^{\lambda_0} \geq 0$ *if* $d_0(a, c_1) = d_0(c_2, b)$.

Remark 8.7 *When $|\lambda_2^h - \lambda_1^h| \geq h^2$, it is no interaction between the wells and we can apply results for the gathered wells with $m_{\lambda_0} = 1$.*

Proof: According to Theorem 2.5 and Proposition 8.3 we have to study the limits of the two quantities

$$\tau_1^h = \frac{\cos^2 \alpha^h}{1 + \frac{\sqrt{\lambda_0}(1+o(1))}{\sqrt{\lambda_0 + B}} \left| \frac{\cos \alpha^h \gamma_{1,+} e^{-\frac{\tilde{d}_h(c_1,b)}{h}} - \sin \alpha^h \gamma_{2,+} e^{-\frac{\tilde{d}_h(c_2,b)}{h}} + o\left(e^{-\frac{\tilde{d}_h(c_2,b)}{h}}\right)}{\cos \alpha^h \gamma_{1,-} e^{-\frac{\tilde{d}_h(a,c_1)}{h}} - \sin \alpha^h \gamma_{2,-} e^{-\frac{\tilde{d}_h(a,c_2)}{h}} + o\left(e^{-\frac{\tilde{d}_h(a,c_1)}{h}}\right)} \right|^2}$$
$$+ \frac{\sin^2 \alpha^h}{1 + \frac{\sqrt{\lambda_0}(1+o(1))}{\sqrt{\lambda_0 + B}} \left| \frac{\sin \alpha^h \gamma_{1,+} e^{-\frac{\tilde{d}_h(c_1,b)}{h}} + \cos \alpha^h \gamma_{2,+} e^{-\frac{\tilde{d}_h(c_2,b)}{h}} + o\left(e^{-\frac{\tilde{d}_h(c_2,b)}{h}}\right)}{\sin \alpha^h \gamma_{1,-} e^{-\frac{\tilde{d}_h(a,c_1)}{h}} + \cos \alpha^h \gamma_{2,-} e^{-\frac{\tilde{d}_h(a,c_2)}{h}} + o\left(e^{-\frac{\tilde{d}_h(a,c_1)}{h}}\right)} \right|^2}$$

and

$$\tau_2^h = \frac{\sin^2 \alpha^h}{1 + \frac{\sqrt{\lambda_0}(1+o(1))}{\sqrt{\lambda_0 + B}} \left| \frac{\cos \alpha^h \gamma_{1,+} e^{-\frac{\tilde{d}_h(c_1,b)}{h}} - \sin \alpha^h \gamma_{2,+} e^{-\frac{\tilde{d}_h(c_2,b)}{h}} + o\left(e^{-\frac{\tilde{d}_h(c_2,b)}{h}}\right)}{\cos \alpha^h \gamma_{1,-} e^{-\frac{\tilde{d}_h(a,c_1)}{h}} - \sin \alpha^h \gamma_{2,-} e^{-\frac{\tilde{d}_h(a,c_2)}{h}} + o\left(e^{-\frac{\tilde{d}_h(a,c_1)}{h}}\right)} \right|^2}$$
$$+ \frac{\cos^2 \alpha^h}{1 + \frac{\sqrt{\lambda_0}(1+o(1))}{\sqrt{\lambda_0 + B}} \left| \frac{\sin \alpha^h \gamma_{1,+} e^{-\frac{\tilde{d}_h(c_1,b)}{h}} + \cos \alpha^h \gamma_{2,+} e^{-\frac{\tilde{d}_h(c_2,b)}{h}} + o(e^{-\frac{\tilde{d}_h(c_2,b)}{h}})}{\sin \alpha^h \gamma_{1,-} e^{-\frac{\tilde{d}_h(a,c_1)}{h}} + \cos \alpha^h \gamma_{2,-} e^{-\frac{\tilde{d}_h(a,c_2)}{h}} + o\left(e^{-\frac{\tilde{d}_h(a,c_1)}{h}}\right)} \right|^2}$$

The difference between this two numbers equals

$$\tau_1^h - \tau_2^h = (\cos^2 \alpha^h - \sin^2 \alpha^h) \left[\frac{1}{1 + \frac{\sqrt{\lambda_0}(1+o(1))}{\sqrt{\lambda_0 + B}} \varrho(\cos \alpha^h, -\sin \alpha^h)^2} \right.$$
$$\left. - \frac{1}{1 + \frac{\sqrt{\lambda_0}(1+o(1))}{\sqrt{\lambda_0 + B}} \varrho(\sin \alpha^h, \cos \alpha^h)^2} \right],$$

where the coefficient ϱ is given by

$$\varrho(\beta_1,\beta_2)=\left|\frac{\beta_1\gamma_{1,+}e^{-\frac{\tilde d_h(c_1,b)}{h}}+\beta_2\gamma_{2,+}e^{-\frac{\tilde d_h(c_2,b)}{h}}+o\left(e^{-\frac{\tilde d_h(c_2,b)}{h}}\right)}{\beta_1\gamma_{1,-}e^{-\frac{\tilde d_h(a,c_1)}{h}}+\beta_2\gamma_{2,-}e^{-\frac{\tilde d_h(a,c_2)}{h}}+o\left(e^{-\frac{\tilde d_h(a,c_1)}{h}}\right)}\right|.$$

An easy computation of the main term of the numerator shows that the difference

$$\varrho(\sin\alpha^h,\cos\alpha^h)^2-\varrho(\cos\alpha^h,-\sin\alpha^h)^2$$

is a non negative number times

$$\left[|\gamma_{1,+}|^2|\gamma_{2,-}|^2\cos^4\alpha^h-|\gamma_{2,+}|^2|\gamma_{1,-}|^2\sin^4\alpha^h\right]e^{-\frac{\tilde d_h(a,c_1)+\tilde d_h(c_2,b)}{h}}\quad+\quad o\left(e^{-\frac{\tilde d_h(a,c_1)+\tilde d_h(c_2,b)}{h}}\right).$$

The expression (8.4) shows that the two products $\gamma_{2,-}\gamma_{1,+}$ and $\gamma_{1,-}\gamma_{2,+}$ are equal. Hence the difference $\tau_1^h-\tau_2^h$ is always non negative, which leads to

$$t_1^{\lambda_0}\geq t_2^{\lambda_0}\,. \tag{8.5}$$

in all cases.

It remains to check $t_1^{\lambda_0}=1$ when $d_0(a,c_1)<d_0(c_2,b)$ because the second case is obtained via a complement argument and the third one says nothing but (8.5). Three possibilities have to be considered: $\cos\alpha^h\to 0$ as $h\to 0$, $\sin\alpha^h\to 0$ as $h\to 0$ or $|\sin\alpha^h||\cos\alpha^h|\geq\delta>0$.

Assume $\lim_{h\to 0}\cos\alpha^h=0$. Then one has

$$\tau_1^h=o(1)+\frac{1+o(1)}{1+\mathcal{O}\left(e^{-2\frac{\tilde d_h(c_2,b)-\tilde d_h(a,c_1)}{h}}\right)}\overset{h\to 0}{\to}1\,.$$

The case $\lim_{h\to 0}\sin\alpha^h=0$ is the same as the previous one after replacing α^h with $\frac{\pi}{2}-\alpha^h$.

Assume $\cos\alpha^h\geq\delta>0$. This leads to

$$\tau_1^h=\frac{\cos^2\alpha^h}{1+\mathcal{O}\left(e^{-2\frac{\tilde d_h(c_2,b)-\tilde d_h(a,c_1)}{h}}\right)}+\frac{\sin^2\alpha^h}{1+\mathcal{O}\left(e^{-2\frac{\tilde d_h(c_2,b)-\tilde d_h(a,c_1)}{h}}\right)}\overset{h\to 0}{\to}1\,.$$

□

A Agmon energy 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 $P:=-h^2d^2/dx^2+V$. Then for any u_1,u_2 in $H^2(\Omega)$, and setting $v_j:=e^{\varphi/h}u_j$ one has:*

$$\begin{aligned}\int_\alpha^\beta e^{2\frac{\varphi}{h}}(P-z)u_1\bar u_2dx &= \int_\alpha^\beta hv_1'\overline{hv_2'}dx+\int_\alpha^\beta(V-z-\varphi'^2)v_1\bar v_2dx\\ &\quad+\int_\alpha^\beta h\varphi'(v_1'\bar v_2-v_1\bar v_2')dx\\ &\quad+h^2\left(e^{2\frac{\varphi(\alpha)}{h}}u_1'\bar u_2(\alpha)-e^{2\frac{\varphi(\beta)}{h}}u_1'\bar u_2(\beta)\right).\end{aligned} \tag{A.1}$$

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

B Universal lower bound for gaps

Lemma B.1 *Let (a_{KS}, b_{KS}) be an interval and let V be a real valued continuous on $\mathbb{R}$. Let E_n and E_{n-1} be the $(n+1)^{th}$ and n^{th} eigenvalues of $-d^2/dx^2 + V$ and let*

$$\lambda = \max_{E \in [E_{n-1}, E_n],\, x \in (a_{KS}, b_{KS})} |E - V(x)|^{1/2}.$$

If $V(x) \geq E_n + \alpha^2$ on $\mathbb{R} \setminus [a_{KS}, b_{KS}]$ for some $\alpha > 0$, then

$$E_n - E_{n-1} \geq \frac{\pi}{2} \left[\frac{1}{2\lambda^2} + \frac{\lambda}{2\sqrt{|E_n|}(\lambda^2 + |E_n|)} \right]^{-1} e^{-\lambda(b_{KS} - a_{KS})}.$$

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