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ESTIMATES ON THE MOLECULAR DYNAMICS FOR THE PREDISSOCIATION PROCESS

PHILIPPE BRIET[1] & ANDRÉ MARTINEZ[2]

Abstract. We study the survival probability associated with a semiclassical matrix Schrödinger operator that models the predissociation of a general molecule in the Born-Oppenheimer approximation. We show that it is given by its usual time-dependent exponential contribution, up to a reminder term that is small in the semiclassical parameter and for which we find the main contribution. The result applies in any dimension, and in presence of a number of resonances that may tend to infinity as the semiclassical parameter tends to 0.

Keywords: Resonances; Born-Oppenheimer approximation; eigenvalue crossing; quantum evolution; survival probability.

Subject classifications: 35P15; 35C20; 35S99; 47A75.

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1. Introduction

The molecular predissociation is one of most well known quantum phenomena giving rise to metastable states and resonances. This corresponds when a bound state molecule dissociates to the continuum through tunneling see e.g. [Kr, La, St, Ze]. The rigorous description of this phenomena goes back to [Kl] with further developments in [DuMe] and, more recently, in [GrMa].

In the context of the Born-Oppenheimer approximation, the transition can occur when a confining electronic curve near a given energy E (e.g. E is a local minimum) crosses a dissociative electronic level (that is, a curve having a limit smaller than E at infinity). Such a situation occurs for instance in the SH molecule : see [LeSu].

After reduction to an effective Hamiltonian, this phenomena can be described by a 2×2 matrix H of semiclassical pseudodifferential operators (see, e.g., [KMSW, MaSo]), with small parameter h corresponding to the square root of the inverse of the mass of the nuclei, and with principal part that is diagonal and consists of two Schrödinger operators.

In this paper we consider predissociation resonances from a dynamical point of view, i.e. in terms of exponential behavior in time of the quantum evolution e^{-itH} associated with that system.

Our main motivation is the recent series of works around the case where $H = H_0 + \kappa V$ is the perturbation of an operator with an embedded eigenvalue: See, e.g., [CGH, CoSo, JeNe, Her, Hu2] and references therein. In all of these papers, denoting by φ the corresponding eigenfunction of H_0, the survival probability $\langle e^{-itH}\varphi, \varphi\rangle$ is studied. Roughly speaking, they show that the embedded eigenvalue gives rise to a resonance ρ, and the previous quantity behaves like $e^{-it\rho}\|\varphi\|^2$ with an error-term typically $\mathcal{O}(\kappa^2)$. Moreover, inserting a cutoff in energy, the error-term has a polynomial decay in time at infinity.

The starting point of our work is the following observation: in the case of the molecular predissociation, H can be seen as a perturbation of a matrix Schrödinger operator admitting embedded eigenvalues. Therefore, a similar procedure can be done in order to study the quantum evolution. However, in contrast with the case $H = H_0 + \kappa V$, the small parameter is involved

in the unperturbed operator, too, making very delicate the extension of the methods used for it. In order to overcome this difficulty, we use the definition of resonances based of complex distortion (see, e.g., [Hu1]), and we replace the arguments of regular perturbation theory (used, e.g., in [CGH]) by those of semiclassical microlocal analysis.

In this way, we can essentially generalize the previous results, and in the case of an isolated resonance ρ with a gap $a(h) >> h^2$, our result takes the form,

$$\langle e^{-itH} g(H)\varphi, \varphi\rangle = e^{-it\rho} b(\varphi, h) + \mathcal{O}\left(\frac{h^2}{a(h)} \min_{0\leq k\leq \nu} \{\frac{1}{[(1+t)a(h)]^k}\} \|\varphi\|^2\right),$$

where $b(\varphi, h)$ is the residue at ρ of $z \mapsto \langle (z-H)^{-1}\varphi, \varphi\rangle$, and $\nu \geq 0$ depends on the regularity of the energy cutoff g (see Theorem 4.1 for a more complete result with several resonances). In addition, we also have an expression for the main contribution of the remainder term (see Remark 4.3). In the case where ν can be taken positive, this also leads to the fact that the error term remains negligible up to times of order $Ch^{-1}|\text{Im } \rho|^{-1}$ with $C > 0$, $C \sim \nu$ as $\nu \to \infty$, that is much beyond the life-time of the resonant state (see Remark 4.4).

Our results must also be compared with that of [NSZ], where a polynomial bound is obtained for the rest in the quantum evolution, in the case of a scalar semiclassical Schrödinger operator.

Let us briefly describe the content of the paper. In the next section, we give a precise description of the model and assumptions. Section 3 is devoted to the definition of resonances by means of complex distortion theory. Our main result is given in Section 4, whose proof is spread over Sections 5 to 9. Section 10 contains the proof of a corollary where the energy cutoff has been removed and we discuss in Section 11 the non-trapping case. Finally, some examples of application are given in Section 12, and the Appendix contains the proof of some technical results.

2. Assumptions

We consider the semiclassical 2×2 matrix Schrödinger operator,

$$H = H_0 + h\mathcal{W}(x, hD_x) = \begin{pmatrix} P_1 & 0 \\ 0 & P_2 \end{pmatrix} + h\mathcal{W}(x, hD_x) \tag{2.1}$$

on the Hilbert space $\mathcal{H} := L^2(\mathbb{R}^n) \oplus L^2(\mathbb{R}^n)$, with,

$$P_j := -h^2\Delta + V_j(x) \quad (j = 1, 2),$$

where $x = (x_1, \dots, x_n)$ is the current variable in $\mathbb{R}^n$ ($n \geq 1$), $h > 0$ denotes the semiclassical parameter, and

$$\mathcal{W}(x, hD_x) = \begin{pmatrix} 0 & W \\ W^* & 0 \end{pmatrix}$$

with $W = w(x, hD_x)$ is a first-order semiclassical pseudodifferential operators, in the sense that, for all $\alpha \in \mathbb{N}^{2n}$, $\partial^\alpha w(x, \xi) = \mathcal{O}(1 + |\xi|)$ uniformly on $\mathbb{R}^{2n}$.

This is typically the kind of operator one obtains in the Born-Oppenheimer approximation, after reduction to an effective Hamiltonian (see [KMSW, MaSo]).

We assume,

Assumption 1. *The potentials V_1 and V_2 are smooth and bounded on $\mathbb{R}^n$, and satisfy,*

(2.2) *The set $U := \{V_1 \leq 0\}$ is bounded ;*

(2.3) $\liminf_{|x|\to\infty} V_1 > 0;$

(2.4) *V_2 has a strictly negative limit $-\Gamma$ as $|x| \to \infty$;*

(2.5) *$V_2 > 0$ on U.*

In particular, H with domain $\mathcal{D}_H := H^2(\mathbb{R}^n) \oplus H^2(\mathbb{R}^n)$ is selfadjoint.

Since we have to consider the resonances of H near the energy level $E = 0$, we also assume,

Assumption 2. *The potentials V_1 and V_2 extend to bounded holomorphic functions near a complex sector of the form, $\mathcal{S}_{R_0,\delta} := \{x \in \mathbb{C}^n\,;\, |\mathrm{Re}\, x| \geq R_0\,,\, |\mathrm{Im}\, x| \leq \delta|\mathrm{Re}\, x|\}$, with $R_0, \delta > 0$. Moreover V_2 tends to its limit at ∞ in this sector and $\mathrm{Re}\, V_1$ stays away from 0 in this sector.*

Assumption 3. *The symbol $w(x, \xi)$ of W extends to a holomorphic functions in (x, ξ) near,*

$$\widetilde{\mathcal{S}}_{R_0,\delta} := \mathcal{S}_{R_0,\delta} \times \{\xi \in \mathbb{C}^n\,; |\mathrm{Im}\, \xi| \leq \delta\langle \mathrm{Re}\, x\rangle\},$$

and, for real x, w is a smooth function of x with values in the set of holomorphic functions of ξ near $\{|\mathrm{Im}\,\xi| \leq \delta\}$. Moreover, we assume that, for any $\alpha \in \mathbb{N}^{2n}$, it satisfies

$$\partial^\alpha w(x,\xi) = \mathcal{O}(\langle \mathrm{Re}\,\xi\rangle) \quad \textit{uniformly on } \widetilde{\mathcal{S}}_{R_0,\delta} \cup (\mathbb{R}^n \times \{|\mathrm{Im}\,\xi| \leq \delta\})\,. \tag{2.6}$$

Under the previous assumption we plan to study the quantum evolution of the operator P given in (2.1), where $\mathcal{W}$ is defined as

$$\mathcal{W} := \begin{pmatrix} 0 & \mathrm{Op}_h^L(w) \\ \mathrm{Op}_h^R(\overline{w}) & 0 \end{pmatrix}$$

where for any symbol $a(x,\xi)$ we use the following quantizations,

$$\mathrm{Op}_h^L(a)u(x) = \frac{1}{(2\pi h)^n}\int e^{i(x-y)\xi/h} a(x,\xi)u(y)dyd\xi;$$
$$\mathrm{Op}_h^R(a)u(x) = \frac{1}{(2\pi h)^n}\int e^{i(x-y)\xi/h} a(y,\xi)u(y)dyd\xi.$$

Finally, we assume,

Assumption [V] (Virial condition)

$$2V_2(x) + x\nabla V_2(x) < 0 \ \text{ on } \{V_2 \leq 0\},$$

or, more generally,

Assumption [NT]

$$E = 0 \text{ is a non-trapping energy for } V_2.$$

The fact that 0 is a non-trapping energy for V_2 means that, for any $(x,\xi) \in p_2^{-1}(0)$, one has $|\exp tH_{p_2}(x,\xi)| \to +\infty$ as $t \to \infty$, where $p_2(x,\xi) := \xi^2 + V_2(x)$ is the symbol of P_2, and $H_{p_2} := (\nabla_\xi p_2, -\nabla_x p_2)$ is the Hamilton field of p_2. It is equivalent to the existence of a function $G \in C^\infty(\mathbb{R}^{2n};\mathbb{R})$ supported near $\{p_2 = 0\}$ (where $p_2(x,\xi) := \xi^2 + V_2(x)$), and satisfying,

$$H_{p_2}G(x,\xi) > 0 \ \text{ on } \{p_2 = 0\}. \tag{2.7}$$

Note that Assumption [V] is nothing but (2.7) with $G(x,\xi) = x\cdot\xi$. Moreover, thanks to Assumption 2, we see that this condition is automatically satisfied for $|x|$ large enough.

3. Resonances

In the previous situation, the essential spectrum of H_0 is $[-\Gamma, +\infty)$. The resonances of H can be defined by using a complex distortion in the following way: Let $f(x) \in C^\infty(\mathbb{R}^n, \mathbb{R}^n)$ such that $f(x) = 0$ for $|x| \leq R_0$, $f(x) = x$ for $|x|$ large enough. For $\theta \neq 0$ small enough, we define the distorted operator H_θ as the value at $\nu = i\theta$ of the extension to the complex of the operator $U_\nu H U_\nu^{-1}$ which is defined for ν real, and analytic in ν for ν small enough, where we have set,

$$U_\nu \phi(x) := \det(1 + \nu df(x))^{1/2} \phi(x + \nu f(x)). \tag{3.1}$$

Since we have a pseudodifferential operator $w(x, hD_x)$, the fact that $U_\nu H U_\nu^{-1}$ is analytic in ν is not completely standard but can be done without problem (thanks to Assumption 3). By using the Weyl Perturbation Theorem, one can also see that there exists $\varepsilon_0 > 0$ such that for any $\pm\theta > 0$ small enough, the spectrum of H_θ is discrete in $\{z \in \mathbb{C}\,;\, \mathrm{Re}\, z \in [-\varepsilon_0, \varepsilon_0],\ \pm \mathrm{Im}\, z \geq \mp \varepsilon_0 \theta\}$, and contained in $\{\pm \mathrm{Im}\, z \leq 0\}$. When θ is positive, the eigenvalues of H_θ are called the resonances of H [Hu1, HeSj2, HeMa], they form a set denoted by $\mathrm{Res}(H)$ (on the contrary, when $\theta < 0$, the eigenvalues of H_θ are just the complex conjugates of the resonances of H, and are called anti-resonances).

Let us observe that the resonances of H can also be viewed as the poles of the meromorphic extension, from $\{\mathrm{Im}\, z > 0\}$, of some matrix elements of the resolvent $R(z) := (H - z)^{-1}$ (see, e.g., [ReSi, HeMa]).

By adapting techniques of [HeSj1, HeSj2] (see also [Kl, GrMa]), one can prove that, in our situation, the resonances of H near 0 are close to the eigenvalues of the operator

$$\widetilde{H} := \begin{pmatrix} -h^2\Delta + V_1 & 0 \\ 0 & -h^2\Delta + \widetilde{V}_2 \end{pmatrix} + h\mathcal{W}(x, hD_x), \tag{3.2}$$

where $\widetilde{V}_2 \in C^\infty(\mathbb{R}^n; \mathbb{R})$ coincides with V_2 in $\{V_2 \geq \delta\}$ ($\delta > 0$ is fixed arbitrarily small), and is such that $\inf \widetilde{V}_2 > 0$. The precise statement is the following one : Let $I(h)$ be a closed interval included in $(-\varepsilon_0, \varepsilon_0)$, and $a(h) > 0$ such that $a(h) \to 0$ as $h \to 0_+$, and, for all $\varepsilon > 0$ there exists $C_\varepsilon > 0$ satisfying,

$$a(h) \geq \frac{1}{C_\varepsilon} e^{-\varepsilon/h}; \tag{3.3}$$

$$\sigma(\widetilde{H}) \cap ((I(h) + [-3a(h), 3a(h)]) \backslash I(h)) = \emptyset, \tag{3.4}$$

for all $h > 0$ small enough. Then, there exist two constants $\varepsilon_1, C_0 > 0$ and a bijection,

$$\widetilde{\beta} \,:\, \sigma(\widetilde{H}) \cap I(h) \,\to\, \mathrm{Res}(H) \cap \Omega(h),$$

where we have set,

$$\Omega(h) := (I(h) + [-a(h), a(h)) + i[-\varepsilon_1, 0],$$

such that,

$$\widetilde{\beta}(\lambda) - \lambda = \mathcal{O}(e^{-C_0/h}),$$

uniformly as $h \to 0_+$.

In particular, since the eigenvalues of $\widetilde{P}$ are real, one obtains that, for any $\varepsilon > 0$, the resonances ρ in $\Omega(h)$ satisfy,

$$\mathrm{Im}\, \rho = \mathcal{O}(e^{-C_0/h}).$$

In what follows, we will show that, under an additional assumption, these resonances are also closed to the eigenvalues of P_1.

Remark 3.1. *Actually, under an assumption of analyticity on W slightly stronger that Assumption 3 (see* [GrMa]*), or if W has a simpler form (see* [Kl]*), C_0 can be taken arbitrarily close to $2d(U, \{V_2 \leq 0\})$, where d stands for the Agmon distance associated with the potential $\min(V_2, V_1)$, that is, the pseudo-distance associated with the pseudo-metric $\max(0, \min(V_2, V_1))dx^2$.*

4. Main Result

For our purpose, we need to have a stronger gap between $I(h)$ and the rest of the spectrum of P_1. Namely, we assume the existence of $a(h) > 0$, such that,

$$\begin{aligned} &\frac{h^2}{a(h)} \to 0 \;\text{ as }\; h \to 0_+; \\ &\sigma(P_1) \cap ((I(h) + [-3a(h), 3a(h)])\backslash I(h)) = \emptyset, \end{aligned} \tag{4.1}$$

Then, we denote by $u_1, \ldots, u_m$ an orthonormal basis of eigenfunctions of P_1 corresponding to its eigenvalues $\lambda_1, \ldots, \lambda_m$ in $I(h)$ (we recall that $m = m(h) = \mathcal{O}(h^{-n})$). For $j = 1, \ldots, m$, we also set,

$$\phi_j := \begin{pmatrix} u_j \\ 0 \end{pmatrix} \in L^2(\mathbb{R}^n) \oplus L^2(\mathbb{R}^n),$$

so that ϕ_j is an eigenvector of,

$$H_0 := \begin{pmatrix} -h^2\Delta + V_1 & 0 \\ 0 & -h^2\Delta + V_2 \end{pmatrix},$$

with eigenvalue λ_j imbedded in its continuous spectrum $[\Gamma, +\infty)$.

Theorem 4.1. *Suppose Assumptions 1-3, (4.1), and Assumption [V] or [NT]. Let $g \in L^\infty(\mathbb{R})$ supported in $(I(h) + (-2a(h), 2a(h)))$ with $g = 1$ on $I(h) + [-a(h), a(h)]$, and such that, for some $\nu \geq 0$, one has,*

$$\begin{aligned} &g, g', \dots, g^{(\nu)} \in L^\infty(R); \\ &g^{(k)} = \mathcal{O}(a(h)^{-k}) \quad (k = 1, \dots, \nu). \end{aligned} \tag{4.2}$$

Then, for all $t \in \mathbb{R}$ and $\varphi \in \mathrm{Span}\{\phi_1, \dots, \phi_m\}$, one has,

$$\langle e^{-itH} g(H)\varphi, \varphi\rangle = \sum_{j=1}^{m} e^{-it\rho_j} b_j(\varphi, h) + r(t, \varphi, h), \tag{4.3}$$

where $\rho_1, \dots, \rho_m$ are the resonances of H lying in $\Omega(h) := I(h) + [-a(h), a(h)] - i[0, \varepsilon_1]$, and satisfy,

$$\rho_j = \lambda_j + \mathcal{O}(h^2), \tag{4.4}$$

$r(t, \varphi, h)$ is such that,

$$r(t, \varphi, h) = \mathcal{O}\left(\frac{h^2}{a(h)} \min_{0 \leq k \leq \nu} \{\frac{1}{[(1+t)a(h)]^k}\} \|\varphi\|^2\right), \tag{4.5}$$

uniformly with respect to $h > 0$ small enough, $t \geq 0$, and $\varphi \in \mathrm{Span}(\phi_1, \dots \phi_m)$. Here $b_j(\varphi, h)$ is the residue at ρ_j of the meromorphic extension from $\{\mathrm{Im}\, z > 0\}$ of the function,

$$z \mapsto \langle (z - H)^{-1}\varphi, \varphi\rangle.$$

and satisfies: There exists a $m \times m$ matrix $M(z)$ depending analytically on $z \in \Omega(h)$, with

$$\|M(z)\| = \mathcal{O}(h^2), \tag{4.6}$$

such that,

$$\begin{aligned} &b_j(\varphi, h) \text{ is the residue at } \rho_j \text{ of the meromorphic function} \\ &z \mapsto \langle (z - \Lambda + M(z))^{-1}\alpha_\varphi, \alpha_\varphi\rangle_{\mathbb{C}^m}, \end{aligned} \tag{4.7}$$

where $\alpha_\varphi := (\langle\varphi, \phi_1\rangle, \dots, \langle\varphi, \phi_m\rangle)$ and $\Lambda := \mathrm{diag}(\lambda_1, \dots, \lambda_m)$.

If in addition one assumes that $\lambda_1, \dots, \lambda_m$ are all simple, and the gap $\widetilde{a}(h) := \min_{j \neq k} |\lambda_j - \lambda_k|$ is such that,

$$h^2/\widetilde{a}(h) \to 0 \text{ as } h \to 0_+, \tag{4.8}$$

then, $b_j(\varphi, h)$ satisfies,

$$b_j(\varphi, h) = |\langle \varphi, \phi_j \rangle|^2 + \mathcal{O}\left((h^2 + h^4(a\widetilde{a})^{-1})\|\varphi\|^2\right), \tag{4.9}$$

uniformly with respect to $h > 0$ small enough and $\varphi \in \mathrm{Span}(\phi_1, \dots \phi_m)$.

Remark 4.2. *Actually, our proof also gives a generalization of a result given in* [CGH] *for the case $m = 1$: see Propositions 7.1 and 7.3.*

Remark 4.3. *Concerning the remainder term, we will see in the proof that it is of the form*

$$r(t, \varphi, h) = r_0(t, \varphi, h) + \mathcal{O}\left(\frac{h^4}{(a(h))^2} \min_{0 \le k \le \nu} \{\frac{1}{[(1+t)a(h)]^k}\}\|\varphi\|^2\right)$$

with

$$\begin{aligned} r_0(t, \varphi, h) = &- h^2 \lim_{\varepsilon, \varepsilon' \to 0_+} \sum_{j,k} \langle \varphi, \phi_j \rangle \overline{\langle \varphi, \phi_k \rangle} \\ &\times \langle e^{-itP_2} g(P_2)(P_2 - \lambda_j - i\varepsilon)^{-1} W^* u_j, (P_2 - \lambda_k + i\varepsilon')^{-1} W^* u_k \rangle. \end{aligned} \tag{4.10}$$

Remark 4.4. *In particular, one has $|r(t, \varphi, h)| << |e^{-it\rho_j}|$ as long as $0 \le t << \frac{1}{|\mathrm{Im}\ \rho_j|} \ln(a(h)/h^2)$ that is much beyond the life time. In the case $\nu \ge 1$, since $|\mathrm{Im}\ \rho_j|$ is exponentially small w.r.t. h , this can indeed be improved by allowing times up to $\frac{C_0 \nu}{h|\mathrm{Im}\ \rho_j|}$ for some constant $C_0 > 0$ independent of ν.*

Remark 4.5. *Let us observe that, in the particular case where $m = 1$, one obtains $b_1(\varphi, h) = |\langle \varphi, \phi_1 \rangle|^2 + \mathcal{O}\left((h^2 + h^4/a^2)\|\varphi\|^2\right)$. Therefore, in the situation of the Theorem with (4.8), a mere application of the previous result for each λ_j would give $b_j(\varphi, h) = |\langle \varphi, \phi_j \rangle|^2 + \mathcal{O}\left((h^2 + h^4/\widetilde{a}^2)\|\varphi\|^2\right)$, and compared with (4.9) this is a weaker result if $\widetilde{a}(h) << a(h)$.*

As a corollary, for the case without energy cutoff, we also obtain,

Corollary 4.6. *In the general situation of Theorem 4.1 (without the assumption on the simplicity of the λ_j's), one has,*

$$\langle e^{-itH}\varphi, \varphi \rangle = \sum_{j=1}^{m} e^{-it\rho_j} b_j(\varphi, h) + \mathcal{O}\left((h^2 + h^4 a(h)^{-2})\|\varphi\|^2\right).$$

In the sequels, we will concentrate on the detailed proof of Theorem 4.1 in the case of Assumption [V]. The more general case of Assumption [NT] can be proved in a similar way by using the Helffer-Sjöstrand framework of resonances theory [HeSj2], and will be outlined in Section 11.

5. Preliminaries

In order to prove Theorem 4.1, we start from the Stone formula,

(5.1)
$$\langle e^{-itH} g(H)\varphi,\varphi\rangle = \lim_{\varepsilon\to 0_+} \frac{1}{2i\pi}\int_{\mathbb{R}} e^{-it\lambda} g(\lambda)\langle (R(\lambda+i\varepsilon)-R(\lambda-i\varepsilon))\varphi,\varphi\rangle d\lambda,$$

where $R(z) := (H-z)^{-1}$. In the sequels, we also denote by $R_\theta(z) := (H_\theta - z)^{-1}$ the distorted resolvent, and by $\varphi_\theta := U_{i\theta}\varphi$ the distortion of φ (observe that, thanks to the analyticity of V_1 and the ellipticity of P_1, each function u_j can be distorted without problem). In particular, by standard arguments (see, e.g., [ReSi, HeMa]), one has $\langle R(z)\varphi,\varphi\rangle = \langle R_\theta(z)\varphi_\theta,\varphi_{-\theta}\rangle$. From now on, we fix $\theta>0$ small enough and, thanks to the fact that $g=1$ on $I(h)+[-a(h),a(h)]$, we can slightly deform the contour of integration in this region, and rewrite (5.1) as,

(5.2)
$$\langle e^{-itH} g(H)\varphi,\varphi\rangle = \frac{1}{2i\pi}\int_{\gamma_+} e^{-itz} g(\mathrm{Re}\ z)\langle R_\theta(z)\varphi_\theta,\varphi_{-\theta}\rangle dz - \frac{1}{2i\pi}\int_{\gamma_-} e^{-itz} g(\mathrm{Re}\ z)\langle R_{-\theta}(z)\varphi_{-\theta},\varphi_\theta\rangle dz,$$

where the complex contour $\gamma_\pm$ can be parametrized by Re z, coincides with $\mathbb{R}$ away from $I(h)+(-a(h),a(h))$, and is included in $\{\pm\mathrm{Im}\ z>0\}$ on $I(h)+(-a(h),a(h))$.

Here we anticipate by using (4.4) and, proceeding as in [CGH], we see that (5.2) can be transformed into,

$$\langle e^{-itH} g(H)\varphi,\varphi\rangle = \sum_{j=1}^{m} e^{-it\rho_j} b_j(\varphi,h) + r(t,\varphi,h), \tag{5.3}$$

where $b_j(\varphi,h)$ is the residue at ρ_j of the meromorphic function

$$z\mapsto -\langle R_\theta(z)\varphi_\theta,\varphi_{-\theta}\rangle,$$

and $r(t,\varphi,h)$ is given by,

(5.4)
$$r(t,\varphi,h) := \frac{1}{2i\pi}\int_{\gamma_-} e^{-itz} g(\mathrm{Re}\ z)\left(\langle R_\theta(z)\varphi_\theta,\varphi_{-\theta}\rangle - \langle R_{-\theta}(z)\varphi_{-\theta},\varphi_\theta\rangle\right) dz,$$

where γ_- is chosen in such a way that it stays below the ρ_j's. Thus, the proof will consist in estimating both $b_j(\varphi,h)$ and $r(t,\varphi,h)$.

6. The Grushin problems

From now on (up to Section 11), we suppose Assumption [V].

In order to have good enough estimates on the resolvent, and in particular to compare it with that of P_1, for z in $\Omega(h) := (I(h)+[-a(h), a(h)])+i[-\varepsilon_1, \varepsilon_1]$, we specify our choice of distorsion. In (3.1), we take F such that,

$$\left\{ \begin{array}{l} f(x) = x \text{ in a neighborhood of the sea } \{V_2 \leq 0\}; \\ F = 0 \text{ in a neighborhood of the well } U = \{V_1 \leq 0\}. \end{array} \right. \tag{6.1}$$

With such a distorsion, it is well known (see, e.g., [BCD]) that, under Assumption [V], the distorted operator P_2^θ satifies,

$$\|(P_2^\theta - z)^{-1}\|_{\mathcal{L}(L^2(\mathbb{R}^n))} = \mathcal{O}(1), \tag{6.2}$$

uniformly with respect to $h > 0$ small enough and $z \in \Omega(h)$.

We introduce the two following Grushin problems,

$$\mathcal{G}(z) := \begin{pmatrix} H_\theta - z & L_- \\ L_+ & 0 \end{pmatrix} : \mathcal{D}_H \times \mathbb{C}^m \to \mathcal{H} \times \mathbb{C}^m,$$

$$\mathcal{G}_0(z) := \begin{pmatrix} H_0^\theta - z & L_- \\ L_+ & 0 \end{pmatrix} : \mathcal{D}_H \times \mathbb{C}^m \to \mathcal{H} \times \mathbb{C}^m,$$

where H_0^θ stands for the distorted Hamiltonian obtained from H_0, and $L_\pm$ are defined as,

$$L_-(\alpha_1, \ldots, \alpha_m) := \sum_{j=1}^m \alpha_j \phi_j^\theta; \tag{6.3}$$

$$L_+ u := L_-^* u = (\langle u, \phi_1^{-\theta}\rangle, \ldots, \langle u, \phi_m^{-\theta}\rangle). \tag{6.4}$$

with $\phi_j^{\pm\theta} := U_{\pm i\theta}\phi_j$.

It is elementary to check that $\mathcal{G}_0(z)$ is invertible, with inverse given by,

$$\mathcal{G}_0(z)^{-1} = \begin{pmatrix} \widehat{\Pi}_\theta \widehat{R}_0^\theta(z) \widehat{\Pi}_\theta & L_- \\ L_+ & z - \Lambda \end{pmatrix},$$

where $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_m)$, $\widehat{\Pi}_\theta := 1 - \Pi_\theta$ with Π_θ the spectral projection of H_0^θ associated with the eigenvalues $(\lambda_1, \ldots, \lambda_m)$, that is,

$$\Pi_\theta u := \sum_{j=1}^m \langle u, \phi_j^{-\theta}\rangle \phi_j^\theta,$$

and $\widehat{R}_0^\theta(z)$ is the reduced resolvent of H_0^θ i.e. the inverse of the restriction of $H_0^\theta - z$ to the range of $\widehat{\Pi}_\theta$.

In addition to (6.2), we have,

Lemma 6.1.

$$\|(\widehat{P}_1^{\pm\theta} - z)^{-1}\|_{\mathcal{L}(L^2(\mathbb{R}^n))} = \mathcal{O}(a(h)^{-1}),$$

uniformly with respect to $h > 0$ small enough and $z \in \Omega(h)$.

Proof. See Appendix 1. □

In order to prove that $\mathcal{G}(z)$ is invertible, too, and to compare its inverse with $\mathcal{G}_0(z)^{-1}$, we compute the product,

$$\mathcal{G}(z)\mathcal{G}_0(z)^{-1} =: \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}.$$

Using that $H_\theta = H_0^\theta + h\mathcal{W}_\theta$ (where $\mathcal{W}_\theta$ stands for the distorted operator obtained from $\mathcal{W}$), we find,

$$\begin{aligned} A_{11} &= 1 + h\mathcal{W}_\theta \widehat{R}_0^\theta(z); \\ A_{12} &= h\mathcal{W}_\theta L_-; \\ A_{21} &= 0; \\ A_{22} &= I_{\mathbb{C}^m}. \end{aligned}$$

Then, we observe,

$$\widehat{\Pi}_\theta = \begin{pmatrix} \widehat{\Pi}_1^\theta & 0 \\ 0 & 1 \end{pmatrix},$$

and,

$$\widehat{R}_0^\theta(z) = \begin{pmatrix} \widehat{\Pi}_1^\theta \widehat{R}_1^\theta(z) \widehat{\Pi}_1^\theta & 0 \\ 0 & R_2^\theta(z) \end{pmatrix},$$

where $R_2^\theta(z)$ is the resolvent of P_2^θ (the distorted operator obtained from P_2), and $\widehat{R}_1^\theta(z)$ is the reduced resolvent of P_1^θ. Thus, denoting by W_θ the distorted operator obtained from $W = w(x, hD_x)$, and W_θ^* that obtained from W^*, we find,

$$h\mathcal{W}_\theta \widehat{R}_0^\theta(z) = \begin{pmatrix} 0 & hW_\theta R_2^\theta(z) \\ hW_\theta^* \widehat{\Pi}_1^\theta \widehat{R}_1^\theta(z) \widehat{\Pi}_1^\theta & 0 \end{pmatrix}.$$

Here we must be aware that this operator is not $\mathcal{O}(h)$, since $\widehat{\Pi}_1^\theta \widehat{R}_1^\theta(z) \widehat{\Pi}_1^\theta$ is $\mathcal{O}(a(h)^{-1})$ only. However, the other off-diagonal operator $hW_\theta R_2^\theta(z)$ is $\mathcal{O}(h)$, and this is enough, for instance, to invert $1 + h\mathcal{W}_\theta \widehat{R}_0^\theta(z)$ without problem. From now on, we set,

$$Q_1(z) := W_\theta^* \widehat{\Pi}_1^\theta \widehat{R}_1^\theta(z) \widehat{\Pi}_1^\theta = \mathcal{O}(a(h)^{-1}) \ ; \ Q_2(z) := W_\theta R_2^\theta(z) = \mathcal{O}(1). \tag{6.5}$$

In particular,

$$K(z) := h^2 Q_1(z) Q_2(z) = \mathcal{O}(h^2/a(h)), \tag{6.6}$$

and thus, by assumption (4.1), the operator $1-K$ is invertible for $h>0$ small enough. Then, a straightforward computation shows that $\mathcal{G}(z)\mathcal{G}_0(z)^{-1}$ is invertible, with inverse given by,

$$\mathcal{F}(z) := \begin{pmatrix} B_1(z) & B_2(z) \\ 0 & I_{\mathbb{C}^m} \end{pmatrix},$$

where,

$$B_1(z) := \begin{pmatrix} 1+h^2Q_2(1-K)^{-1}Q_1 & -hQ_2(1-K)^{-1} \\ -h(1-K)^{-1}Q_1 & (1-K)^{-1} \end{pmatrix},$$

and

$$B_2(z) := h^2 \begin{pmatrix} 0 & Q_2(1-K)^{-1} \\ 0 & (1-K)^{-1} \end{pmatrix} \mathcal{W}_\theta L_-. \tag{6.7}$$

(Here, we have also used the fact that the first component of $\mathcal{W}_\theta\phi_j$ is identically 0.)

A similar computation shows that $\mathcal{G}_0(z)^{-1}\mathcal{G}(z)$ is invertible, too, and, as a consequence, so is $\mathcal{G}(z)$, with inverse,

$$\mathcal{G}(z)^{-1} = \mathcal{G}_0(z)^{-1}\mathcal{F}(z) = \begin{pmatrix} E(z) & E_+(z) \\ E_-(z) & E_{-+}(z) \end{pmatrix}, \tag{6.8}$$

where,

$$\begin{aligned} E(z) &:= \widehat{\Pi}_\theta \widehat{R}_0^\theta(z)\widehat{\Pi}_\theta B_1(z) \\ E_+(z) &:= L_- + \widehat{\Pi}_\theta \widehat{R}_0^\theta(z) B_2(z) \\ E_-(z) &:= L_+B_1 \\ E_{-+}(z) &:= z-\Lambda + L_+B_2(z). \end{aligned} \tag{6.9}$$

We set,

$$M(z) := L_+B_2(z) = M_0(z) + M_1(z),$$

with

$$M_0(z) := h^2 L_+ \begin{pmatrix} 0 & Q_2(z) \\ 0 & 1 \end{pmatrix} \mathcal{W}_\theta L_-,$$

and

$$M_1(z) := L_+B_2(z) - M_0(z). \tag{6.10}$$

One can prove,

Lemma 6.2. *One has,*

$$\|M_0(z)\|_{\mathcal{L}(\mathbb{C}^m)} = \mathcal{O}(h^2);$$
$$\|M_1(z)\|_{\mathcal{L}(\mathbb{C}^m)} = \mathcal{O}(h^4/a(h)) = o(h^2),$$

uniformly with respect to $h>0$ small enough and $z\in\Omega(h)$.

Proof. See Appendix 2. □

In particular,

$$\|M(z)\|_{\mathcal{L}(\mathbb{C}^m)} = \mathcal{O}(h^2), \tag{6.11}$$

uniformly with respect to $z \in \Omega(h)$ and $h > 0$ small enough. Since $h^2/a(h) \to 0$, by standard perturbation theory we deduce,

$$\mathrm{Sp}(\Lambda + M(z)) = \{\lambda_1(z), \dots, \lambda_m(z)\},$$

with,

$$\lambda_j(z) = \lambda_j + \mathcal{O}(h^2).$$

As a consequence the solutions $z \in \Omega(h)$ of the problem,

$$0 \in \sigma(E_{-+}(z)),$$

are all of the form,

$$z = \lambda_j + \mathcal{O}(h^2),$$

for some j. Deforming continuously $(E_{-+}(z))$ into $z - \Lambda$ (e.g., by setting $\Lambda_t(z) := z - \Lambda + tM(z)$, $0 \le t \le 1$), and following continuously the roots of the determinant of $\Lambda_t(z)$ as t varies from 0 to 1, we also see that all the values of j are reached by such solutions. Since we also know that these solutions are precisely the resonances of H in $\Omega(h)$ (see (7.4)), we have proved (4.4).

7. The reduced resolvent

In this section, we still consider the Grushin problem given by $\mathcal{G}(z)$, but we will solve it in a different way, in order to obtain the inverse in terms of the reduced resolvent $\widehat{R}_\theta(z)$ of H_θ (instead of that of H_0^θ), as in the usual Feshbach method.

Indeed, denoting by $\widehat{H}_\theta$ the restriction of $\widehat{\Pi}_\theta H_\theta$ to the range of $\widehat{\Pi}_\theta$, for all z such that $\mathrm{Im}\, z > 0$ we can define the reduced resolvent $\widehat{R}_\theta(z)$ as the inverse of $\widehat{H}_\theta - z$, and it is straightforward to verify that, for such z, the inverse of $\mathcal{G}(z)$ is given by,

$$\mathcal{G}(z)^{-1} = \begin{pmatrix} E(z) & E_+(z) \\ E_-(z) & E_{-+}(z) \end{pmatrix},$$

with,

$$\begin{aligned} E(z) &:= \widehat{\Pi}_\theta \widehat{R}_\theta(z) \widehat{\Pi}_\theta \\ E_+(z) &:= (1 - h\widehat{\Pi}_\theta \widehat{R}_\theta(z) \widehat{\Pi}_\theta \mathcal{W}_\theta) L_- \\ E_-(z) &:= L_+(1 - h\mathcal{W}_\theta \widehat{\Pi}_\theta \widehat{R}_\theta(z) \widehat{\Pi}_\theta) \\ E_{-+}(z) &:= z - \Lambda + h^2(\langle \mathcal{W}_\theta \widehat{\Pi}_\theta \widehat{R}_\theta(z) \widehat{\Pi}_\theta \mathcal{W}_\theta \phi_k^\theta, \phi_j^{-\theta} \rangle)_{1 \le j,k \le m}. \end{aligned} \tag{7.1}$$

Comparing with (6.9), we obtain in particular (still for $\mathrm{Im}\, z > 0$, for which the computations of the previous section remain valid),

$$\widehat{\Pi}_\theta \widehat{R}_\theta(z) \widehat{\Pi}_\theta = \widehat{\Pi}_\theta \widehat{R}_0^\theta(z) \widehat{\Pi}_\theta B_1(z). \tag{7.2}$$

Now, since both expressions are holomorphic in $\{\mathrm{Im}\, z > 0\}$, and the right-hand side extends analytically in $\Omega(h)$, we conclude that so does $\widehat{\Pi}_\theta \widehat{R}_\theta(z) \widehat{\Pi}_\theta$, and the identity remains valid in $\Omega(h)$.

In addition, the expression $\langle W_\theta \widehat{\Pi}_\theta \widehat{R}_\theta(z) \widehat{\Pi}_\theta W_\theta \phi_k^\theta, \phi_j^{-\theta} \rangle$ is actually independent of θ, and is nothing but the meromorphic extension to $\Omega(h)$ of the function (holomorphic in $\{\mathrm{Im}\, z > 0\}$),

$$F_{j,k}(z) := \langle \mathcal{W} \widehat{\Pi} \widehat{R}(z) \widehat{\Pi} \mathcal{W} \phi_k, \phi_j \rangle \tag{7.3}$$

Finally, in order to estimates the residues appearing in (5.3), let us recall the well known formula for the whole resolvent of H_θ. For $z \in \Omega(h) \backslash \{\rho_1, \dots, \rho_m\}$, one has,

$$R_\theta(z) = E(z) - E_+(z) \left(E_{-+}(z)\right)^{-1} E_-(z). \tag{7.4}$$

In view of (7.1)-(7.2), we know that the operators $E(z)$, $E_\pm(z)$ and $E_{-+}(z)$ depend analytically on z in $\Omega(h)$. Therefore, in formula (7.4), the only possible poles come from $\left(E_{-+}(z)\right)^{-1}$.

Therefore, we have proved,

Proposition 7.1. *The distorted resolvent $R_\theta(z)$ of H is given by (7.4), where the operators $E(z)$, $E_\pm(z)$ and $E_{-+}(z)$ are given in (7.1). Moreover, the resonances of H in $\Omega(h)$ are exactly the roots of the equation,*

$$\det(z - \Lambda + h^2 F(z)) = 0,$$

where $F(z)$ is the $m \times m$ matrix with coefficients $F_{j,k}(z)$ $(1 \leq j, k \leq m)$ given by (7.3).

In the particular case where $m = 1$, let us observe that, at first glance, $F_{1,1}(z)$ can be estimated by $\mathcal{O}(a(h)^{-1})$, and its holomorphic derivative $F'_{1,1}(z)$ by $\mathcal{O}(a(h)^{-2})$ (this is because of the presence of the reduced resolvent in $F_{1,1}(z)$). For the resonance, this leads to,

$$\rho_1 = \lambda_1 - h^2 F_{1,1}(\rho_1) = \lambda_1 + \mathcal{O}(h^2/a(h)) = \lambda_1 - h^2 F_{1,1}(\lambda_1) + \mathcal{O}(h^4/a(h)^3),$$

which, compared to the result given in [CGH] seems much less interesting. But actually, looking more precisely to the expression of $F(z)$, one can prove,

Lemma 7.2. *In the case $m = 1$, one has,*

$$|F_{1,1}(z)| + |F'_{1,1}(z)| = \mathcal{O}(1),$$

uniformly with respect to $h > 0$ small enough and $z \in \Omega(h)$.

Proof. Using (7.2), we have,

$$\begin{aligned} F_{1,1}(z) &= \langle \mathcal{W}_\theta \widehat{\Pi}_\theta \widehat{R}_0^\theta(z) \widehat{\Pi}_\theta B_1(z) \mathcal{W}_\theta \phi_1^\theta, \phi_1^{-\theta} \rangle \\ &= \langle B_1(z) \mathcal{W}_\theta \phi_1^\theta, \widehat{\Pi}_{-\theta} \widehat{R}_0^{-\theta}(\overline{z}) \widehat{\Pi}_{-\theta} (\mathcal{W}_\theta)^* \phi_1^{-\theta} \rangle, \end{aligned}$$

and since,

$$(\mathcal{W}_\theta)^* \phi_1^{-\theta} = \begin{pmatrix} 0 \\ W_{-\theta} u_j^{-\theta}, \end{pmatrix}$$

we have,

$$\widehat{\Pi}_{-\theta} \widehat{R}_0^{-\theta}(\overline{z}) \widehat{\Pi}_{-\theta} (\mathcal{W}_\theta)^* \phi_1^{-\theta} = \begin{pmatrix} 0 \\ R_2^{-\theta}(\overline{z}) W_{-\theta} u_j^{-\theta}, \end{pmatrix} \tag{7.5}$$

Hence, $\|\widehat{\Pi}_{-\theta} \widehat{R}_0^{-\theta}(\overline{z}) \widehat{\Pi}_{-\theta} (\mathcal{W}_\theta)^* \phi_1^{-\theta}\|_{L^2} = \mathcal{O}(1)$, and since also $\|B_1(z)\|_{\mathcal{L}(L^2)} = \mathcal{O}(1)$, we deduce,

$$F_{1,1}(z) = \mathcal{O}(1).$$

(Here, we have used the fact that $\|u_j^{\pm\theta}\|_{L^2} = \mathcal{O}(1)$.)

On the other hand, taking the derivate with respect to z, we obtain,

$$F'_{1,1}(z) = \langle \mathcal{W}_\theta \widehat{\Pi}_\theta \widehat{R}_\theta(z)^2 \widehat{\Pi}_\theta \mathcal{W}_\theta \phi_1^\theta, \phi_1^{-\theta} \rangle$$

Then, applying (7.2) with θ replaced by $-\theta$, and z replaced by $\overline{z}$, and then taking the adjoint, we obtain,

$$\widehat{\Pi}_\theta \widehat{R}_\theta(z) \widehat{\Pi}_\theta = B_1^*(z) \widehat{\Pi}_\theta \widehat{R}_0^\theta(z) \widehat{\Pi}_\theta, \tag{7.6}$$

with $B^*(z) = I + \mathcal{O}(h^2/a)$ in $\mathcal{L}(L^2)$. Using both (7.2) and (7.6), we are led to,

$$F'_{1,1}(z) = \langle B_1^*(z) \widehat{\Pi}_\theta \widehat{R}_0^\theta(z) \widehat{\Pi}_\theta \mathcal{W}_\theta \phi_1^\theta, B_1(z)^* \widehat{\Pi}_{-\theta} \widehat{R}_0^{-\theta}(\overline{z}) \widehat{\Pi}_{-\theta} (\mathcal{W}_\theta)^* \phi_1^{-\theta} \rangle.$$

Thus, we can conclude as before (see (7.5)) that $F'_{1,1}(z) = \mathcal{O}(1)$. □

As a consequence, we obtained the following generalization of the result of [CGH]:

Theorem 7.3. *Suppose Assumptions 1-3, (4.1), and $m = 1$. Then, the resonance $\rho_1(h)$ of H that is the closest one to $\lambda_1(h)$ satisfies,*

$$\rho_1(h) = \lambda_1(h) - h^2 F_{1,1}(\lambda_1(h)) + \mathcal{O}(h^4),$$

uniformly for $h > 0$ small enough. Here, $F_{1,1}(z)$ is defined in (7.3).

8. Estimates on the residues

Going back to (5.3), and using (7.4), we deduce,

$$b_j(\varphi, h) = \text{Residue}_{z=\rho_j} \langle E_+(z) \left(E_{-+}(z)\right)^{-1} E_-(z)\varphi_\theta, \varphi_{-\theta}\rangle. \tag{8.1}$$

Since $\varphi \in \text{Span}(\phi_1, \dots, \phi_m)$, it can be written as,

$$\varphi = \sum_{j=1}^{m} \alpha_j \phi_j, \tag{8.2}$$

($\alpha_j \in \mathbb{C}$), and thus we see on (7.1) that we actually have,

$$E_-(z)\varphi_\theta = L_+\varphi_\theta = (\alpha_1, \dots, \alpha_m).$$

In a similar way, since $\widehat{\Pi}_\theta^* = \widehat{\Pi}_{-\theta}$, we also find,

$$E_+(z)^*\varphi_{-\theta} = (\alpha_1, \dots, \alpha_m).$$

Inserting into (8.1), and setting,

$$\alpha_\varphi := (\alpha_1, \dots, \alpha_m) \in \mathbb{C}^m,$$

we obtain,

$$b_j(\varphi, h) = \text{Residue}_{z=\rho_j} \langle E_{-+}(z)^{-1}\alpha_\varphi, \alpha_\varphi\rangle_{\mathbb{C}^m}. \tag{8.3}$$

Therefore, using (6.9)-(6.11), we deduce (4.6)-(4.7).

Now, assuming that the λ_j's are simple and that (4.8) is satisfied, we write,

$$E_{-+}(z) = (z - \Lambda + M_0(z)) \left(1 + (z - \Lambda + M_0(z))^{-1} M_1(z)\right). \tag{8.4}$$

Moreover, using (8.3) and denoting by γ_j the oriented boundary of the disc centered in λ_j of radius $\widetilde{a}(h)/2$, we have,

$$b_j(\varphi, h) = \frac{1}{2i\pi} \int_{\gamma_j} \langle E_{-+}(z)^{-1}\alpha_\varphi, \alpha_\varphi\rangle dz. \tag{8.5}$$

When $z \in \gamma_j$, we have $\|(z - \Lambda)^{-1}\| = \mathcal{O}(\widetilde{a}^{-1})$ and thus, using (4.8),

$$\|(z - \Lambda + M_0(z))^{-1}\| = \|(1 + (z - \Lambda)^{-1} M_0(z))^{-1}(z - \Lambda)^{-1}\| = \mathcal{O}(\widetilde{a}^{-1}).$$

Moreover, using (6.11), we have,

$$\|(z - \Lambda + M_0(z))^{-1} M_1(z)\| = \mathcal{O}(h^4/(a\widetilde{a})) = o(1),$$

and thus, by (8.4), for $z \in \gamma_j$,

$$\begin{aligned} E_{-+}(z)^{-1} &= \left(1 + \mathcal{O}(h^4/(a\widetilde{a})\right) (z - \Lambda - M_0(z))^{-1} \\ &= (z - \Lambda + M_0(z))^{-1} + \mathcal{O}(h^4/(a\widetilde{a}^2)), \end{aligned}$$

and thus, since the length of γ_j is $\mathcal{O}(\widetilde{a})$,

(8.6)
$$\int_{\gamma_j} \langle E_{-+}(z)^{-1}\alpha_\varphi, \alpha_\varphi\rangle dz = \int_{\gamma_j} \langle (z-\Lambda+M_0(z))^{-1}\alpha_\varphi, \alpha_\varphi\rangle dz + \mathcal{O}\left(\frac{h^4}{a\widetilde{a}}\right)\|\varphi\|^2.$$

On the other hand, we see on its definition that we have,

$$M_0(z) = h^2\left(\langle W_\theta R_2^\theta(z) W_\theta^* u_k^\theta, u_j^{-\theta}\rangle\right)_{1\le j,k\le m},$$

and, introducing the operator $\widetilde{P}_2 := -h^2\Delta + \widetilde{V}_2$ where $\widetilde{V}_2$ is as in (3.2), the exponential decay of $u_j^{\pm\theta}$ away from U and Agmon estimates (see [HeSj2]) show that,

$$\langle W_\theta R_2^\theta W_\theta^* u_k^\theta, u_j^{-\theta}\rangle = \langle W\widetilde{R}_2(z)W^* u_k, u_j\rangle + \mathcal{O}(e^{-\delta/h}),$$

for some constant $\delta > 0$, and with $\widetilde{R}_2(z) := (\widetilde{P}_2 - z)^{-1}$. Setting

$$\widetilde{M}_0(z) := \left(\langle W_\theta R_2^\theta W_\theta^* u_k^\theta, u_j^{-\theta}\rangle = \langle W\widetilde{R}_2(z)W^* u_k, u_j\rangle\right)_{1\le j,k\le m},$$

we deduce as before,

(8.7)
$$\int_{\gamma_j} \langle E_{-+}(z)^{-1}\alpha_\varphi, \alpha_\varphi\rangle dz = \int_{\gamma_j} \langle (z-\Lambda+\widetilde{M}_0(z))^{-1}\alpha_\varphi, \alpha_\varphi\rangle dz + \mathcal{O}\left(\frac{h^4}{a\widetilde{a}}\right)\|\varphi\|^2,$$

where the matrix $\widetilde{M}_0(z)$ is $\mathcal{O}(h^2)$, depends analytically on $z \in \Omega(h)$, and is selfadjoint when z is real. As a consequence, thanks to the gap condition on the λ_j's, we see that the matrix $\Lambda - \widetilde{M}_0(z)$ can be diagonalized in a basis $(e_1(z), \dots, e_m(z))$ of $\mathbb{C}^m$, that depends analytically on $z \in \Omega(h)$, is orthonormal when z is real, and the corresponding change of basis is given by a matrix $A(z)$ satisfying,

$$^tA(z)A(z) = I_{\mathbb{C}^m};$$

$$A(z) = I_{\mathbb{C}^m} + \mathcal{O}(h^2);$$

$$^tA(z)(z-\Lambda+\widetilde{M}_0(z))^{-1}A(z) = \mathrm{diag}\left(\frac{1}{z-\mu_1(z)}, \dots, \frac{1}{z-\mu_m(z)}\right),$$

where the eigenvalues $\mu_1(z), \dots, \mu_m(z)$ of $\Lambda - \widetilde{M}_0(z)$ satisfy,

$$\mu_j(z) = \lambda_j + f_j(z)$$

with $f_j(z) = \mathcal{O}(h^2)$. Note that f_j are real on the real. Since

$$\frac{d}{dz}\widetilde{M}_0(z) = \mathcal{O}(h^2),$$

we see by a standard Hellmann-Feynman argument that, in this situation, we also have,

$$\mu_j'(z) = f_j'(z) = \mathcal{O}(h^2).$$

Moreover, the poles $\widetilde{\lambda}_1, \dots, \widetilde{\lambda}_m$ of $\langle (z-\Lambda-\widetilde{M}_0(z))^{-1}\alpha_\varphi, \alpha_\varphi\rangle$ are the solutions of an equation,

$$z = \mu_j(z)$$

for some $j = 1, \dots, m$. Thus, they are necessarily simple, and since $\mu_j(\overline{z}) = \overline{\mu_j(z)}$, they must be real. Finally, we obtain,

(8.8)
$$\frac{1}{2i\pi}\int_{\gamma_j} \langle (z-\Lambda-\widetilde{M}_0(z))^{-1}\alpha_\varphi, \alpha_\varphi\rangle dz = (1-f_j'(\widetilde{\lambda}_j))^{-1}|\alpha_j|^2 + \mathcal{O}(h^2\|\varphi\|^2)$$
$$= |\alpha_j|^2 + \mathcal{O}(h^2\|\varphi\|^2),$$

and (4.9) follows from (8.5), (8.7) and (8.8).

9. Estimates on the rest

We have to estimate the quantity,

$$S_\theta(z) := \langle R_\theta(z)\varphi_\theta, \varphi_{-\theta}\rangle - \langle R_{-\theta}(z)\varphi_{-\theta}, \varphi_\theta\rangle, \tag{9.1}$$

for $z \in \gamma_-$ where, setting $\widetilde{I} = [\alpha, \beta] := I(h) + [-a, a]$, we choose the contour γ_- as,

$$\gamma_- := (\mathbb{R}\backslash\widetilde{I}) \cup (\alpha - i[0,a]) \cup ([\alpha,\beta] - ia) \cup (\beta - i[0,a]).$$

We first compute $v = (v_1, v_2) := R_\theta(z)\varphi_\theta$. Denoting by $u := \sum_j \alpha_j u_j$ the first component of φ, we find,

$$v_1 = (P_1^\theta - z)^{-1}(1-T_\theta)^{-1}u_\theta$$
$$v_2 = -h(P_2^\theta - z)^{-1}W_\theta^* v_1,$$

with

$$T_\theta := h^2 W_\theta (P_2^\theta - z)^{-1} W_\theta^* (P_1^\theta - z)^{-1} = \mathcal{O}(h^2/a(h)).$$

Then, using that $(P_1 - z)^{-1}u = \sum_k \alpha_k(\lambda_k - z)^{-1}u_k$, that the u_j's are orthogonal to each other, and that z stays at a distance greater than $a/2$ from the λ_j's, we deduce,

$$\langle R_\theta(z)\varphi_\theta, \varphi_{-\theta}\rangle = \langle v_1, u_{-\theta}\rangle = \sum_j \frac{|\alpha_j|^2}{\lambda_j - z} + \sum_{j,k}\frac{\alpha_j\overline{\alpha_k}}{\lambda_k - z}\langle T_\theta u_j^\theta, u_k^{-\theta}\rangle + \mathcal{O}(h^4a^{-3}).$$

Using again that the u_j's are eigenfunction of P_1, this lead us to,

$$\langle R_\theta(z)\varphi_\theta, \varphi_{-\theta}\rangle = \sum_j \frac{|\alpha_j|^2}{\lambda_j - z} + h^2\sum_{j,k}\frac{\alpha_j\overline{\alpha_k}}{(\lambda_k - z)(\lambda_j - z)}\langle W_\theta R_2^\theta(z) W_\theta^* u_j^\theta, u_k^{-\theta}\rangle$$
$$+ \mathcal{O}(h^4a^{-3}\|\varphi\|^2).$$

Here we observe that the quantity $\langle W_\theta R_2^\theta(z) W_\theta^* u_j^\theta, u_k^{-\theta}\rangle$ is nothing but the holomorphic continuation from $\{\mathrm{Im}\ z > 0\}$ through the real axis of the function $z \mapsto \langle R_2(z) W^* u_j, W^* u_k\rangle$. From now on, we denote this continuation by $\langle \widetilde{R}_2(z) W^* u_j, W^* u_k\rangle$.

Changing θ into $-\theta$, we also find an analog expression for $\langle R_{-\theta}(z)\varphi_{-\theta}, \varphi_\theta\rangle$, and making their difference, we obtain,

(9.2)
$$S_\theta(z) = h^2 \sum_{j,k} \frac{\alpha_j \overline{\alpha_k}}{(\lambda_k - z)(\lambda_j - z)} \langle (\widetilde{R}_2(z) - R_2(z)) W^* u_j, W^* u_k\rangle + \mathcal{O}(h^4 a^{-3} \|\varphi\|^2).$$

Multiplying by $e^{-itz} g(\mathrm{Re}\ z)$ and integrating over γ_-, we obtain the required estimate of $r(t, \varphi, h)$ in the case $\nu = 0$

For the case $\nu > 0$, as in [CGH] we use the formula,

$$e^{-izt} = (1+t)^{-\nu} \left(1 + i\frac{d}{dz}\right)^\nu e^{-izt},$$

and we make k integrations by parts with respect to z $(0 \le k \le \nu)$. This makes appear the composition of a finite number of resolvents and additional negative powers of $\lambda_j - z$, and the estimate follows in the same way.

Moreover, setting

(9.3)
$$r_0(t, \varphi, h) := \frac{h^2}{2i\pi} \sum_{j,k} \int_{\gamma_-} \frac{e^{-itz} g(\mathrm{Re}\ z)}{(\lambda_k - z)(\lambda_j - z)} \langle (\widetilde{R}_2(z) - R_2(z)) W^* u_j, W^* u_k\rangle$$

we see on (9.2) that we have $r(t, \varphi, h) = r_0(t, \varphi, h) + \mathcal{O}(h^4 a^{-2} \|\varphi\|^2)$. In addition, in (9.3), we can change (λ_j, λ_k) into $(\lambda_j + i\varepsilon, \lambda_k + i\varepsilon')$ and take the limit as $\varepsilon, \varepsilon' \to 0_+$. Before taking this limit, we can also deform γ_- into $\mathbb{R}$, and this transforms $\widetilde{R}_2(z) - R_2(z)$ into $\widetilde{R}_2(\lambda + i0) - R_2(\lambda - i0)$. By the spectral theorem, this leads to the expression (4.10) of Remark 4.3. □

10. Proof of Corollary 4.6

We first prove,

Lemma 10.1.

$$\sum_{j=1}^m b_j(\varphi, h) = \left(1 + \mathcal{O}(h^2 + h^4/a^2)\right) \|\varphi\|^2.$$

Proof. We write,

$$E_{-+}(z) = (z - \Lambda + M_0(z)) \left(1 + (z - \Lambda + M_0(z))^{-1} M_1(z)\right), \tag{10.1}$$

and, using (8.3) and denoting by γ the oriented boundary of the rectangle $\{z \in \mathbb{C}\,;\, \mathrm{Re}\, z \in I(h) + [-a(h), a(h)],\ |\mathrm{Im}\, z| \leq \varepsilon_1\}$, we have,

$$\sum_{j=1}^{m} b_j(\varphi, h) = \frac{1}{2i\pi} \int_\gamma \langle E_{-+}(z)^{-1} \alpha_\varphi, \alpha_\varphi \rangle dz. \tag{10.2}$$

We divide γ into its vertical part $\gamma^{\mathbf{v}}$ and its horizontal one $\gamma^{\mathbf{h}}$.

When $z \in \gamma^{\mathbf{h}}$, since z remains at a distance ε_1 of $\mathbb{R}$, we have $\|(z - \Lambda)^{-1}\| = \mathcal{O}(1)$ and thus,

$$\|(z - \Lambda + M_0(z))^{-1}\| = \|(1 + (z - \Lambda)^{-1} M_0(z))^{-1} (z - \Lambda)^{-1}\| = \mathcal{O}(1).$$

Moreover, still for $z \in \gamma^{\mathbf{h}}$, we see on (6.6) that $K(z) = \mathcal{O}(h^2)$, and thus, by (6.7) and (6.10), $\|M_1(z)\| = \mathcal{O}(h^4)$. As a consequence

$$\|(z - \Lambda + M_0(z))^{-1} M_1(z)\| = \mathcal{O}(h^4), \quad (z \in \gamma^{\mathbf{h}}).$$

Therefore, by (10.1), for such z we can write,

$$\begin{aligned} E_{-+}(z)^{-1} &= \left(1 + \mathcal{O}(h^4)\right) (z - \Lambda - M_0(z))^{-1} \\ &= (z - \Lambda - M_0(z))^{-1} + \mathcal{O}(h^4), \end{aligned}$$

and thus,

$$\int_{\gamma^{\mathbf{h}}} \langle E_{-+}(z)^{-1} \alpha_\varphi, \alpha_\varphi \rangle dz = \int_{\gamma^{\mathbf{h}}} \langle (z - \Lambda - M_0(z))^{-1} \alpha_\varphi, \alpha_\varphi \rangle dz + \mathcal{O}(h^4) \|\varphi\|^2. \tag{10.3}$$

On the other hand, when $z \in \gamma^{\mathbf{v}}$, we can write $z = z_1 + i z_2$ with $z_1, z_2 \in \mathbb{R}$, $\mathrm{dist}(z_1, I(h)) = a(h)$, $|z_2| \leq \varepsilon_1$. Therefore, for such z we have, $\|(z - \Lambda + M_0(z)))^{-1}\| = \mathcal{O}((a + |z_2|)^{-1})$, $\|K(z)\| = \mathcal{O}(h^2 (a + |z_2|)^{-1})$, and $\|M_1(z)\| = \mathcal{O}(h^4 (a + |z_2|)^{-1})$. Proceeding as before, we deduce,

$$E_{-+}(z)^{-1} = (z - \Lambda - M_0(z))^{-1} + \mathcal{O}(h^4/(a + |z_2|)^3) \|\varphi\|^2,$$

and thus, integrating in z_2 on $[-\varepsilon_1, \varepsilon_1]$,

$$\int_{\gamma^{\mathbf{v}}} \langle E_{-+}(z)^{-1} \alpha_\varphi, \alpha_\varphi \rangle dz = \int_{\gamma^{\mathbf{v}}} \langle (z - \Lambda - M_0(z))^{-1} \alpha_\varphi, \alpha_\varphi \rangle dz + \mathcal{O}(h^4/a(h)^2) \|\varphi\|^2. \tag{10.4}$$

We deduce from (10.3)-(10.4),

$$\int_{\gamma} \langle E_{-+}(z)^{-1} \alpha_\varphi, \alpha_\varphi \rangle dz = \int_{\gamma} \langle (z - \Lambda - M_0(z))^{-1} \alpha_\varphi, \alpha_\varphi \rangle dz + \mathcal{O}(h^4/a(h)^2) \|\varphi\|^2. \tag{10.5}$$

At this point, we make the key observation that, by definition, $M_0(z)$ extends analytically in some h-independent complex neighborhood of $I(h)$, where it is $\mathcal{O}(h^2)$ in norm. As a consequence, modifying the complex contour γ into another one that stays at some fix positive distance from $I(h)$, we deduce from (10.5),

(10.6)
$$\int_\gamma \langle E_{-+}(z)^{-1}\alpha_\varphi, \alpha_\varphi\rangle dz = \int_\gamma \langle (z-\Lambda)^{-1}\alpha_\varphi, \alpha_\varphi\rangle dz + \mathcal{O}(h^2 + h^4/a(h)^2)\|\varphi\|^2.$$

Going back to (10.2), this gives,

$$\sum_{j=1}^m b_j(\varphi, h) = \sum_{j=1}^m |\alpha_j|^2 + \mathcal{O}(h^2 + h^4/a(h)^2)\|\varphi\|^2 = \left(1 + \mathcal{O}(h^2 + h^4/a^2)\right)\|\varphi\|^2,$$

and (4.9) is proved. □

Now, applying Theorem 4.1 with $t = 0$, we obtain,

$$\langle g(H)\varphi, \varphi\rangle = \sum_{j=1}^m b_j(\varphi, h) + \mathcal{O}(e^{-M/h})$$

and thus, by the previous lemma,

$$\langle g(H)\varphi, \varphi\rangle = \|\varphi\|^2 + \mathcal{O}(h^2 + h^4/a^2)\|\varphi\|^2.$$

Hence,

$$\langle (1 - g(H))\varphi, \varphi\rangle = \mathcal{O}(h^2 + h^4/a^2)\|\varphi\|^2, \tag{10.7}$$

and we can chose g in such a way that $0 \le g \le 1$. In that case, (10.7) can be re-written as,

$$\|(1 - g(H))^{\frac{1}{2}}\varphi\|^2 = \mathcal{O}(h^2 + h^4/a^2)\|\varphi\|^2,$$

and Corollary 4.6 follows by writing,

$$\begin{aligned}\langle e^{-itH}\varphi, \varphi\rangle &= \langle e^{-itH} g(H)\varphi, \varphi\rangle + \langle e^{-itH}(1 - g(H))\varphi, \varphi\rangle \\ &= \langle e^{-itH} g(H)\varphi, \varphi\rangle + \langle e^{-itH}(1 - g(H))^{\frac{1}{2}}\varphi, (1 - g(H))^{\frac{1}{2}}\varphi\rangle \\ &= \langle e^{-itH} g(H)\varphi, \varphi\rangle + \mathcal{O}(\|(1 - g(H))^{\frac{1}{2}}\varphi\|^2).\end{aligned}$$

11. The non-trapping case

In the case when only Assumption [NT] is assumed (instead of Assumption [V]), the strategy of the proof is the same. However, an important ingredient for the estimates on the residues was the uniform boundedness of the resolvent of P_2^θ. Therefore, in order to generalize this proof one needs a framework where $(P_2 - z)^{-1}$ becomes bounded uniformly with respect to

h. This is provided by the theory of resonances developed by Helffer and Sjöstrand in [HeSj2]. Without entering too much into details, let us just recall that this theory consists in changing $L^2(\mathbb{R}^n)$ into a space $\mathcal{H}_{\theta G}$, that contains $C_0^\infty(\mathbb{R}^n)$, and that depends on a positive small enough parameter θ and a function $G \in C^\infty(\mathbb{R}^{2n};\mathbb{R})$ supported near $\{p_2 = 0\}$ (where $p_2(x,\xi) := \xi^2 + V_2(x)$), and satisfying,

$$|p_2(x,\xi) - i\theta H_{p_2} G(x,\xi)| \geq \frac{\theta}{C}\langle\xi\rangle^2,$$

for some constant $C > 0$. Then, one has,

$$\|(P_2 - z)^{-1}\|_{\mathcal{L}(\mathcal{H}_{\theta G})} = \mathcal{O}(1/\theta), \tag{11.1}$$

uniformly with respect to $h > 0$ small enough and z close to 0. Let us also recall that pseudodifferential operators with analytic symbols on complex sectors can act on $\mathcal{H}_{\theta G}$, and their representation involves the restriction of their symbol to the complex Lagrangian manifold,

$$\Lambda_{\theta G} := \{(x + i\theta\partial_\xi G(x,\xi), \xi - i\theta\partial_x G(x,\xi))\,;\,(x,\xi) \in \mathbb{R}^{2n}\}.$$

Moreover, a whole symbolic calculus can be performed for such operators, where only the restrictions to $\Lambda_{\theta G}$ of the symbols are involved. Finally, as in the L^2-case, an analog of Sobolev spaces can be introduced by inserting a weight, and we denote by $\mathcal{H}^2_{\theta G}$ the analog of $H^2(\mathbb{R}^n)$ in this context. In particular, we have,

$$P_1\,,\,P_2\,:\mathcal{H}^2_{\theta G} \to \mathcal{H}_{\theta G}.$$

Then, setting $D_{\theta G} := \mathcal{H}^2_{\theta G} \times \mathcal{H}^2_{\theta G}$ and $\widetilde{\mathcal{H}}_{\theta G} := \mathcal{H}_{\theta G} \times \mathcal{H}_{\theta G}$, we consider the two Grushin problems $\mathcal{G}(z)$ and $\mathcal{G}_0(z)$ as in Section 6, but this time without distortion, as operators : $D_{\theta G} \times \mathbb{C}^m \to \widetilde{\mathcal{H}}_{\theta G} \times \mathbb{C}^m$, and with the scalar product replaced (in the definition of L_+) by the duality-bracket between $\widetilde{\mathcal{H}}_{\theta G}$ and $\widetilde{\mathcal{H}}_{-\theta G}$.

Then the proof of the estimates on the residues proceeds in the same way, in particular the fact that G is supported near $\{p_2 = 0\}$ (thus, away from the well U) makes valid an analog of Lemma 6.1 in this context. Indeed, the norm in $\mathcal{H}_{\theta G}$ is equivalent to a weighted norm of the same type as in (**??**), but this time with a weight G that is no more compactly supported (but still supported in a neighborhood of $\{p_2 = 0\}$): see [HeSj2], Formula (9.48). For the same reason, the estimates of Lemma 6.2 on $M_0(z)$ and $M_1(z)$ can be generalized, too, and all of Sections 8 and 10 remain valid.

The same procedure applies to estimate the remainder term $r(t,\varphi,h)$.

12. Examples

12.1. **The one dimensional case.** When $n=1$, if we assume,

$$V_1' \neq 0 \text{ on } \{V_1=0\},$$

then it is well known (see, e.g., HeRo) that the eigenvalues of P_1 are all simple and separated by a gap of order h. Then, we can take $|I(h)|=\mathcal{O}(h)$, $a=\widetilde{a}\sim h$, and we also have $m=\mathcal{O}(1)$. Moreover, in this case Assumption [NT] on V_2 is equivalent to,

$$V_2' \neq 0 \text{ on } \{V_2=0\}, \text{ and } \{V_2\leq 0\} \text{ has no bounded connected component.}$$

For instance $V_2(x)=-\Gamma+\alpha(1+x^2)^{-1}$, (with $\alpha>0$ sufficiently large, so that $V_2>0$ on $\{V_1\leq 0\}$) satisfies all the assumptions (including Assumption [V]).

In such a situation, (4.9) becomes,

$$b_j(\varphi,h)=|\langle\varphi,\phi_j\rangle|^2+\mathcal{O}(h^2)\|\varphi\|^2, \tag{12.1}$$

and, with Corollary 4.6, this gives,

$$\langle e^{-itH}\varphi,\varphi\rangle=\sum_{j=1}^{m}e^{-it\rho_j}|\langle\varphi,\phi_j\rangle|^2+\mathcal{O}(h^2)\|\varphi\|^2. \tag{12.2}$$

12.2. **The non-degenerate point-well.** In addition to Assumption 1, let us suppose,

$$U=\{0\},\ \mathrm{Hess}\,V_1(0)>0.$$

Then, it is well known (see [HeSj1, Si]) that the spectrum of P_1 near 0 consists of eigenvalues admitting asymptotic expansions as $h\to 0_+$, of the form,

$$\lambda_j(h)\sim\sum_{k\geq 0}\lambda_{j,k}h^{1+\frac{k}{2}},$$

where $\lambda_{j,0}$ is the j-th eigenvalue of the harmonic oscillator $-\Delta+\frac{1}{2}\langle\mathrm{Hess}\,V_1(0)x,x\rangle$.

As for V_2, one can take $V_2(x)=-\Gamma+\alpha(1+x^2)^{-1}$ with $\alpha,\Gamma>0$ arbitrary. Then Assumption [V] is satisfied, and choosing $I(h)=[0,Ch]$ with $C\notin\{\lambda_{j,0}\,;\,j\geq 1\}$, we see that the general assumptions of Theorem 4.1 are satisfied with $a(h)\sim h$. Thus, (12.1) remains valid in this case.

Moreover, in the case $n = 1$, all the $\lambda_{j,0}$'s are simple, and thus so are the λ_j's, with a gap $\widetilde{a} \sim h$, and (12.2) is valid, too.

When $n \geq 2$, some $\lambda_{j,0}$ may have some multiplicity. This is for instance the case if we take $n = 2$ and $V_1(x_1, x_2) = x_1^2 + 4x_2^2 + x_1^2 x_2 + \mathcal{O}(|x|^4)$ uniformly near 0. Then (see [HeSj1], end of Section 3), the asymptotic of the first eigenvalues of P_1 can be computed, and one finds,

$$\begin{aligned}
\lambda_1(h) &= 3h + \mathcal{O}(h^2);\\
\lambda_2(h) &= 5h + \mathcal{O}(h^{\frac{3}{2}});\\
\lambda_3(h) &= 7h - \alpha h^{\frac{3}{2}} + \mathcal{O}(h^2);\\
\lambda_4(h) &= 7h + \alpha h^{\frac{3}{2}} + \mathcal{O}(h^2);\\
\lambda_5(h) &= 9h + \mathcal{O}(h^{\frac{3}{2}}),
\end{aligned}$$

with $\alpha := \int y_1^2 y_2 v_1(y_1) w_2(y_2) v_3(y_1) w_1(y_2) dy_1 dy_2 > 0$, where v_j stands for the normalized j-th eigenfunction of $-d_{y_1}^2 + y_1^2$, and w_j for the normalized j-th eigenfunction of $-d_{y_2}^2 + 4y_2^2$.

Thus, we can apply Theorem 4.1 with $I(h) = [0, 8h]$, $a(h) = h/2$, and $\widetilde{a}(h) = 2\alpha h^{\frac{3}{2}}$.

13. Appendix

13.1. **Appendix 1: Proof of Lemma 6.1.** We do it for P_1^θ only, since the sign of θ is not involved in the proof. Let $\eta, \psi, \chi \in C_0^\infty(\mathbb{R}^n)$ be such that,

$$\begin{aligned}
&\inf_{\mathbb{R}^n}(V_1 + \eta) > 0;\\
&\psi = 1 \text{ in a neighborhood of } \operatorname{Supp}\eta;\\
&\chi = 1 \text{ in a neighborhood of } \operatorname{Supp}\psi;\\
&\operatorname{Supp}\chi \subset \mathbb{R}^n \backslash \operatorname{Supp} F.
\end{aligned}$$

We denote by,

$$\widetilde{P}_1^\theta := P_1^\theta + \eta$$

the perturbation of P_1^θ where the well U has been filled with η (the so-called "filled-well" operator). By analogy with a technique used in [HeSj2], Section 9 (in particular Formula (9.22)), we consider the operator,

$$X(z) := \chi(\widehat{P}_1^\theta - z)^{-1}\psi + (\widetilde{P}_1^\theta - z)^{-1}(1 - \psi).$$

By a straightforward computation, we have,

$$(P_1^\theta - z)\widehat{\Pi}_1^\theta X(z)\widehat{\Pi}_1^\theta = \widehat{\Pi}_1^\theta + Y(z), \tag{13.1}$$

with,

$$Y(z) := \widehat{\Pi}_1^\theta \left(-\chi \Pi_1^\theta \psi + [P_1^\theta, \chi](\widehat{P}_1^\theta - z)^{-1}\psi - \eta(\widetilde{P}_1^\theta - z)^{-1}(1-\psi)\right) \widehat{\Pi}_1^\theta.$$

Then, denoting by d_1 the Agmon distance associated with V_1, one observes that both $d_1(\mathrm{Supp}\,\nabla\chi, \mathrm{Supp}\,\psi)$ and $d_1(\mathrm{Supp}\,\eta, \mathrm{Supp}\,(1-\psi)$ are positive numbers. Therefore, one can apply e.g. the Propositions 9.3 and 9.4 in [HeSj2] (or, more directly, Agmon estimates on P_1^θ, uniformly with respect to θ) to deduce the existence of some $\delta_1 > 0$, independent of θ, such that,

$$\|[P_1^\theta, \chi](\widehat{P}_1^\theta - z)^{-1}\psi - \eta(\widetilde{P}_1^\theta - z)^{-1}(1-\psi)\|_{\mathcal{L}(L^2)} = \mathcal{O}(e^{-2\delta_1/h}). \tag{13.2}$$

Moreover, since $\widehat{\Pi}_1^\theta \Pi_1^\theta = \Pi_1^\theta \widehat{\Pi}_1^\theta = 0$, we have,

$$\widehat{\Pi}_1^\theta \left(\chi \Pi_1^\theta \psi)\right) \widehat{\Pi}_1^\theta = \widehat{\Pi}_1^\theta \left((\chi - 1)\Pi_1^\theta(\psi - 1))\right) \widehat{\Pi}_1^\theta,$$

and Agmon estimates on P_1^θ show the existence of $\delta_2 > 0$, still independent of θ, such that, for all $j = 1, \dots, m$, one has,

$$\|(1-\psi)u_j^\theta\|_{L^2} = \mathcal{O}(e^{-2\delta_2/h}),$$

and therefore, since $m(h) = \mathcal{O}(h^{-n})$,

$$\|\widehat{\Pi}_1^\theta \left(\chi \Pi_1^\theta \psi)\right) \widehat{\Pi}_1^\theta\|_{\mathcal{L}(L^2)} = \mathcal{O}(e^{-\delta_2/h}). \tag{13.3}$$

From (13.2)-(13.3), we obtain,

$$\|Y(z)\|_{\mathcal{L}(L^2)} = \mathcal{O}(e^{-\delta_3/h}),$$

for some constant $\delta_3 > 0$. Going back to (13.1), we deduce,

$$(\widehat{P}_1^\theta - z)^{-1} = \widehat{\Pi}_1^\theta X(z) \widehat{\Pi}_1^\theta (1 + \mathcal{O}(e^{-\delta_3/h})). \tag{13.4}$$

On the other hand, since the distortion coincides with the identity on the supports of χ and of ψ, we have,

$$X(z) := \chi(\widehat{P}_1 - z)^{-1}\psi + (\widetilde{P}_1^\theta - z)^{-1}(1-\psi),$$

and by construction $\|(\widetilde{P}_1^\theta - z)^{-1}\| = \mathcal{O}(1)$ and $\|(\widehat{P}_1 - z)^{-1}\| = \mathcal{O}(1/a)$. Hence, by (13.4), Lemma 6.1 follows.

13.2. **Appendix 2: Proof of Lemma 6.2.** In view of (6.5), (6.6), it is enough to prove that, if A is a bounded operator on $L^2(\mathbb{R}^n)$, then the matrix $M_A := (\langle A u_k^\theta, u_j^{-\theta}\rangle_{L^2(\mathbb{R}^n)})_{1\le j,k\le m}$ satisfies,

$$\|M_A\|_{\mathcal{L}(\mathbb{C}^m)} = \mathcal{O}(\|A\|_{\mathcal{L}(L^2)}), \tag{13.5}$$

uniformly with respect to $h > 0$ small enough. In order to prove (13.5), we take $\alpha = (\alpha_1, \dots, \alpha_m) \in \mathbb{C}^m$, and we write,

$$\|M_A\alpha\|^2 = \sum_{j=1}^m |\sum_{k=1}^m \alpha_k \langle Au_k^\theta, u_j^{-\theta}\rangle_{L^2(\mathbb{R}^n)}|^2 = \sum_{j=1}^m |\langle A\widetilde{\alpha}, u_j^{-\theta}\rangle_{L^2(\mathbb{R}^n)}|^2,$$

where $\widetilde{\alpha} := \sum_{k=1}^m \alpha_k u_k^\theta$. Then, we denote by $D \subset \mathbb{R}^n$ and open set such that

$$U \subset D \subset \mathbb{R}^n \backslash \mathrm{Supp}\, F,$$

In particular, on D we have $u_k^{\pm\theta} = u_k$, and, by Agmon estimates, we know that the norms $\|u_k^{\pm\theta}\|_{L^2(\mathbb{R}^n\backslash D)}$ are exponentially small, uniformly with respect to θ. Therefore, since $m = \mathcal{O}(h^{-n})$, we can write,

$$\|M_A\alpha\|^2 = \sum_{j=1}^m |\langle A\widetilde{\alpha}, u_j\rangle_{L^2(D)}|^2 + \mathcal{O}(e^{-c/h})\|A\widetilde{\alpha}\|_{L^2}^2, \tag{13.6}$$

where $c > 0$ is independent of α, θ, and h. Then, we use the fact that, for the same reason (and since $\langle u_k^\theta, u_j^{-\theta}\rangle_{L^2} = \delta_{j,k}$), we have,

$$\langle u_k, u_j\rangle_{L^2(D)} = \delta_{j,k} + \mathcal{O}(e^{-c/h}), \tag{13.7}$$

where the positive constant c may be different from the previous one. This permits us to show (e.g., by diagonalizing the family $(u_k)_{1\le k\le m}$ in $L^2(D)$ by means of a matrix $B = I + \mathcal{O}(e^{-\delta/h})$) that one has,

$$\sum_{j=1}^m |\langle A\widetilde{\alpha}, Tu_j\rangle_{L^2(D)}|^2 = \mathcal{O}(\|A\widetilde{\alpha}\|_{L^2(D)}^2),$$

uniformly with respect to h and α. Hence, inserting in (13.6), we find,

$$\|M_A\alpha\|^2 = \mathcal{O}(\|A\widetilde{\alpha}\|_{L^2(D)}^2 + e^{-c/h}\|A\widetilde{\alpha}\|_{L^2}^2),$$

and thus,

$$\|M_A\alpha\|^2 = \mathcal{O}(\|A\widetilde{\alpha}\|_{L^2}^2) = \mathcal{O}(\|A\|^2 \cdot \|\widetilde{\alpha}\|_{L^2}^2),$$

and the result follows by observing that (using the decay properties of the $u_k^{\pm\theta}$'s and (13.7) again),

$$\|\widetilde{\alpha}\|_{L^2} = \mathcal{O}(\|\widetilde{\alpha}\|_{L^2(D)} + e^{-c/h}\|\alpha\|_{\mathbb{C}^m}) = \mathcal{O}(\|\alpha\|_{\mathbb{C}^m}).$$

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