ON THE BORN-OPPENHEIMER APPROXIMATION OF DIATOMIC MOLECULAR RESONANCES

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Abstract. We give a new reduction of a general diatomic molecular Hamiltonian, without modifying it near the collision set of nuclei. The resulting effective Hamiltonian is the sum of a smooth semiclassical pseudodifferential operator (the semiclassical parameter being the inverse of the square-root of the nuclear mass), and a semibounded operator localised in the elliptic region corresponding to the nuclear collision set. We also study its behaviour on exponential weights, and give several applications where molecular resonances appear and can be well located.

Keywords: Resonances; Born-Oppenheimer approximation; Effective Hamiltonian

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1. Introduction

This paper is devoted to the Born-Oppenheimer reduction of a diatomic molecular Hamiltonian, near energy levels where resonances may appear.

The principle of the Born-Oppenheimer reduction goes back to 1927 with the work [BoOp], where the fact that the nuclei are much heavier than the electrons is exploited in order to approximate the complete molecular Schrödinger operator by a reduced Hamiltonian, acting on the positions of the nuclei only, and in which the electrons are involved through the effective electric potential they create only. This principle has been widely used by chemists since that period, but the mathematically rigorous justifications of this reduction are much more recent. They started with [CDS], where it has been justified up to error-terms of order $h^2 := M^{-1}_{\text{nucl}}$ ($M_{\text{nucl}}$ being the average mass of the nuclei), and continued with [Ha1, Ma1] (up to $O(h^\infty)$, but concerning smooth interactions only), [Ha2] (up to $O(h^\infty)$ for bounded states of diatomic molecules), [KMSW] (exact reduction for bounded states of polyatomic molecules), [Ha3, Ha4, MaSo1, MaSo2] (up to $O(h^\infty)$ for the quantum evolution problem). Let us also mention results on the Born-Oppenheimer reduction for the scattering process [Ra, KMW1, KMW2].

Concerning the reduction for resonant (or metastable) states with singular (Coulomb-type) interactions, to our knowledge it is treated in [MaMe] only. In that paper, following ideas from [KMSW], a regularisation of the Hamiltonian is constructed far from the collision set of the nuclei, and this gives rise to an effective Hamiltonian of pseudodifferential type. However, this effective Hamiltonian is not constructed for the exact molecular Hamiltonian, but for a modified one where the singularity coming from the collision set of the nuclei has been artificially removed. Because of this, additional assumptions have to be done in order to be able to compare the resonances obtained from the effective Hamiltonian to those of the original Hamiltonian.

Indeed, the main inconvenient of [MaMe] lies in some precise assumption (see condition (ii) of Proposition 6.1 in [MaMe]) that involves the unmodified operator directly, and appears to be difficult to verify in general.

Here, we construct an effective Hamiltonian for the unmodified molecular Schrödinger operator, in such a way that the contribution of the collision set of the nuclei is clearly individuated and separated from its complementary. The resulting effective Hamiltonian appears to be the sum of a semiclassical pseudodifferential operator (where, as usual, the semiclassical parameter is the inverse of the square-root of the nuclear mass), and a semibounded operator localised near the collision set of the nuclei. Thanks to this localisation it is possible to apply a general technique (originated in [HeSj2]) in order to compare the resonances of the full effective Hamiltonian to those of its pseudodifferential part.

In the next section, we prove an abstract result of reduction, similar to the Feshbach standard result, but with the difference that the nuclei position-space is split in two parts, each of them giving rise to separated contributions in the final effective Hamiltonian (see Theorem 2.1). In Section 3, we apply
this result to the particular case of a diatomic molecular Hamiltonian, with Coulomb singularities. Then, in Section 3 we give a representation of the effective Hamiltonian in terms of a matrix operator, that can be split into a smooth pseudodifferential part and an operator localised into the elliptic region (see Theorem 4.1). In addition, the conjugation of these operators by an exponential weight-function is studied, too. This is used in Section 5 to investigate their action on WKB solutions. In Section 6, a general method (taken from [HeS]) is described, in order to compare the resonances of the full effective Hamiltonian to those of its pseudodifferential part. Finally, in Section 7, we give a list of applications where our result, together with other techniques, permits to locate molecular resonances and give estimates on their widths.

2. AN ABSTRACT SPLITTING RESULT

Let $\mathcal{H}_Q$ be a Hilbert space. We consider a general (unbounded) closed operator $P$ with domain $\mathcal{D}_P$ on $\mathcal{H} := L^2(\mathbb{R}^n) \otimes \mathcal{H}_Q$, that can be written on the form,

$$P = K_0 \otimes I + \int_{\mathbb{R}^n} Q(x) dx =: K_0 \otimes I + Q,$$

where $K_0$ is a closed operator on $L^2(\mathbb{R}^n)$ with dense domain $\mathcal{D}_0$, such that,

$$\text{Re} K_0 \geq 0,$$

(2.1)

and, for almost all $x \in \mathbb{R}^n$, $Q(x)$ is a lower semi-bounded closed operator on $\mathcal{H}_Q$, with lower semi-bound $-C_0$ and dense domain $\mathcal{D}_Q$, both independent of $x$. In particular, one has,

$$\mathcal{D}_P = \mathcal{D}_0 \otimes \mathcal{D}_Q.$$

We are interested in the spectrum of $P$ near some real interval $I_0 := (-\infty, \lambda_0]$, and we assume the existence of two open subsets $W_0$ and $W_1$ of $\mathbb{R}^n$, together with a continuous family of projections $(\Pi(x))_{x \in \mathbb{R}^n}$ on $\mathcal{H}_Q$ and some $\delta_0 \geq \delta_1 > 0$, such that,

$$W_0 \cup W_1 = \mathbb{R}^n;$$

$$\text{Re} Q(x) \geq \lambda_0 + \delta_0 \quad \text{a.e. on } W_0;$$

$$\Pi(x) : \mathcal{D}_Q \to \mathcal{D}_Q;$$

(2.2)

$$[Q(x), \Pi(x)] = 0 \quad \text{a.e. on } W_1;$$

$$\text{Re}(Q(x) - \lambda_0 - \delta_1)(1 - \Pi(x)) \geq 0 \quad \text{a.e. on } W_1.$$

We set

$$\Pi := \int_{\mathbb{R}^n} \Pi(x) dx ; \quad \mathcal{H}_{\text{red}} := \Pi(\mathcal{H}) \subset \mathcal{H},$$

Our aim is to reduce the spectral study of $P$ near $I_0$, to that of an operator acting on the ‘reduced’ space $\mathcal{H}_{\text{red}}$ (as in the standard Feshbach method), but in such a way that the contributions of $Q_0 := \int_{W_0} Q(x) dx$ and $Q_1 := \int_{W_1} Q(x) dx$ are clearly individuated and separated (the idea is that, in the applications, $Q_1$ is a “smooth” operator, while $Q_0$ is “singular” but elliptic).
Let \( \varphi_0, \varphi_1, \psi_0, \psi_1 \in C^\infty(\mathbb{R}^n, [0, 1]) \) be cut-off functions such that,

\[
\text{Supp} \varphi_j \cup \text{Supp} \psi_j \subset W_j \quad (j = 0, 1);
\]

(2.3) \[
\varphi_0^2 + \varphi_1^2 = 1 \quad \text{on} \quad \mathbb{R}^n;
\]

\[
\psi_j = 1 \quad \text{on} \quad \text{Supp} \varphi_j \quad (j = 0, 1).
\]

We set,

\[
P_0 = K_0 + Q_0 := K_0 + Q + (\lambda_0 + \delta_0 + C_0)(1 - \psi_0);
\]

(2.4) \[
P_1 = K_0 + Q_1 := K_0 + Q\psi_1 + (\lambda_0 + \delta_0)(1 - \psi_1);
\]

\[
\hat{\Pi} := I - \Pi.
\]

In particular, one has \( \varphi_j P_j = \varphi_j P \) and \( P_j \varphi_j = P \varphi_j \) for \( j = 0, 1 \). Moreover, by construction, one also has,

(2.5) \[
\text{Re} P_0 \geq \lambda_0 + \delta_0;
\]

\[
\text{Re} \hat{\Pi}(P_1 - \lambda_0 - \delta_1)\hat{\Pi} \geq 0,
\]

and thus, for \( z \) in a small enough complex neighborhood of \( I_0 \), both \( P_0 - z \) and the restriction of \( \hat{\Pi}P_1\hat{\Pi} - z \) to the range of \( \hat{\Pi} \) are invertible, with bounded inverse. We set,

\[
X_0 = X_0(z) := \hat{\Pi}(P_0 - z)^{-1}\hat{\Pi};
\]

\[
X_1 = X_1(z) := \hat{\Pi}\left(\hat{\Pi}(P_1 - z)\hat{\Pi}\right)^{-1}\hat{\Pi};
\]

\[
M_j := [P_j, \Pi] \quad (j = 0, 1);
\]

\[
T_j := [K_0, \varphi_j] \quad (j = 0, 1);
\]

(2.6) \[
Y = Y(z) := \varphi_0 X_0 T_0 + \varphi_1 X_1 T_1;
\]

\[
Y' = Y'(z) := T_0 X_0 \varphi_0 + T_1 X_1 \varphi_1;
\]

\[
Y_1 := \varphi_0 X_0 M_0 \varphi_0 + \varphi_1 X_1 M_1 \varphi_1;
\]

\[
Y_2 := \varphi_0 X_0 M_0 \varphi_0 + \varphi_1 X_1 M_1 \varphi_1;
\]

\[
Y_3 := \varphi_0 X_0 T_0 + \varphi_1 M_1 X_1 T_1;
\]

\[
Y_4 := \varphi_0 X_0 \varphi_0 + \varphi_1 M_1 \varphi_1.
\]

Observe that \( Y \) and \( Y' \) are bounded operators on \( \mathcal{H} \) and, in the applications, they will actually be very small. Our result is,

**Theorem 2.1.** Assume \( ||Y(z)|| < 1 \) and \( ||Y'(z)|| < 1 \). Then, for \( z \) in a small enough complex neighborhood of \( I_0 \), one has the equivalence,

\[
z \in \sigma(P) \iff 0 \in \sigma(A(z)),
\]

where,

\[
A(z) = \Pi (z - P) \Pi + B : \mathcal{H}_{\text{red}} \cap \mathcal{D}_P \rightarrow \mathcal{H}_{\text{red}},
\]

with,

\[
B(z) := \Pi (-Y_2 + (M_0 + Y_3 - Y_4)(1 + Y)^{-1}(1 - Y_1))\Pi.
\]

**Proof.** For \( z \in \mathbb{C} \) near \( I_0 \), we consider the Grushin problem,

(2.7) \[
\mathcal{G}(z) := \begin{pmatrix} P - z & I \\ \Pi & 0 \end{pmatrix} : \mathcal{D}_P \oplus \mathcal{H}_{\text{red}} \rightarrow \mathcal{H} \oplus \mathcal{H}_{\text{red}}.
\]
We also consider,

\[ G_j(z) := \begin{pmatrix} P_j - z I \\ \Pi \\ 0 \end{pmatrix} \quad (j = 0, 1). \]

It is straightforward to check that \( G_j(z) \) \((j = 0, 1)\) invertible, with inverse given by,

\[ G_j(z)^{-1} := \begin{pmatrix} X_j \\ \Pi(1 + M_j X_j) \\ \Pi(z - P_j - M_j X_j M_j) \end{pmatrix}. \]

Setting \( F(z) := \varphi_0 G_0^{-1} \varphi_0 + \varphi_1 G_1^{-1} \varphi_1 \) and \( U := \varphi_0 X_0 \varphi_0 + \varphi_1 X_1 \varphi_1 \), we find,

\[ F(z) := \begin{pmatrix} U \\ \Pi(1 + Y'_1) \\ \Pi(z - P - Y_2) \end{pmatrix}, \]

with,

\[ Y'_1 := \varphi_0 M_0 X_0 \varphi_0 + \varphi_1 M_1 X_1 \varphi_1, \]

and then, using that \( \varphi_0 [P, \Pi] = \varphi_0 M_0 \), \( \varphi_1 [P, \Pi] = \varphi_1 M_1 \), \( U \Pi = 0 \), \( Y'_1 \Pi = 0 \), and \( Y_4 \Pi = \Pi Y_4 \),

\[ F(z) G(z) := \begin{pmatrix} I + Y \\ G_1 \\ 0 \end{pmatrix}, \]

with,

\[ G_1 := -\Pi M_0 - Y_3 + \Pi Y_4. \]

Therefore, the operator,

\[ \left(1 + \begin{pmatrix} I & 0 \\ G_1 \\ 0 \end{pmatrix}\right)^{-1} F(z) = \begin{pmatrix} (I + Y)^{-1} & 0 \\ -G_1 (I + Y)^{-1} & I \end{pmatrix} F(z) \]

is a left-inverse for \( G(z) \).

In the same way, using that \( \Pi Y_2 \Pi = Y_2 \), we also find,

\[ G(z) F(z) := \begin{pmatrix} 1 + Y' \\ 0 \\ G_2 \end{pmatrix}, \]

with,

\[ G_2 := M_0 - T_0 X_0 M_0 \varphi_0 - T_1 X_1 M_1 \varphi_1 - Y_2 \Pi. \]

This proves that \( G(z) \) is surjective, too, and thus invertible with inverse given by \( G(z) \). Moreover, if \( A(z) \) stands for the coefficient \((2, 2)\) of \( G(z)^{-1} \), one has the standard algebraic property,

\[ z \in \sigma(P) \iff 0 \in \sigma(A(z)). \]

By definition, we also have \( A(z) = \Pi(z - P - Y_2) - G_1 (1 + Y)^{-1} (1 - Y_1) \), and the result follows. \( \square \)

**Remark 2.2.** If we neglect all the terms involving \( Y \), \( M_1 = [K_0, \Pi], T_1 \) or \( T_2 \) (that will all be small in the applications we have in mind), we see that the operator \( A(z) \) reduces to its principal part \( A_0(z) \), given by,

\[ A_0(z) := \Pi(z - P - RX_0 R) \Pi, \]

with \( R := [Q, \Pi] = \varphi_0 [Q, \Pi] \varphi_0 \).
3. Diatomic molecular resonances

3.1. The model. We consider the selfadjoint operator \( H \) on \( L^2(\mathbb{R}^3_x \times \mathbb{R}^3_y) \), with domain \( \mathcal{H}^2(\mathbb{R}^3_x \times \mathbb{R}^3_y) \) defined as

\[
H = -\hbar^2 \Delta + H_{el}(x)
\]

\[
H_{el}(x) = \tilde{H}_{el}(x) + \frac{\alpha}{|x|}
\]

\[
\tilde{H}_{el}(x) = -\Delta_y + V(x,y)
\]

(3.1)

with

\[
V(x,y) = \sum_{j=1}^{n} \left( \frac{\alpha^+}{|y_j + x|} + \frac{\alpha^-}{|y_j - x|} \right) + \sum_{j,k=1}^{n} \frac{\alpha_{jk}}{|y_j - y_k|}
\]

where \( \alpha, \alpha^\pm, \text{ and } \alpha_{jk} \) are real constant and \( \alpha > 0, \alpha^\pm < 0. \)

In this model, \( x \) stands for the relative position of the nuclei, \( y \) for the position of the electrons, and \( \hbar^2 \) for the ratio between the electronic and nuclear masses. In particular, \( H_{el} \) is the electronic Hamiltonian with electronic mass normalized at \( m = \frac{1}{2} \).

Let us define the resonances of \( P \) by using the analytic distortion introduced in [Hu].

Let \( \omega : \mathbb{R}^3 \to \mathbb{R}^3 \) be a smooth odd vector field such that

- \( \omega(x) = 0 \) for \( |x| \leq R \) (\( R > 0 \) large enough);
- \( \omega(x) = x \) for \( |x| >> 1 \),
- For any rotation \( R \) on \( \mathbb{R}^3 \), one has \( \omega(Rx) = R\omega(x) \).

(In other words, we take \( \omega(x) \) on the form \( \omega(x) = \chi(|x|)x \) with \( \chi(t) = 0 \) when \( t \leq R \), and \( \chi(t) = 1 \) for \( t >> 1 \).) For \( \mu \in \mathbb{R} \) small enough, we consider the transformation

\[
F_{\mu}(x,y) = (x + \mu \omega(x), y_1 + \mu \omega(y_1), \ldots, y_p + \mu \omega(y_p))
\]

and the analytic distortion \( U_\mu \) associated to \( F_\mu \) defined as

\[
U_\mu \phi(x,y) = \phi(F_\mu(x,y)).
\]

Then the family,

\[
H_\mu = U_\mu H U_\mu^{-1}
\]

can be extended to small complex values of \( \mu \), and we can give the following definition:

**Definition 3.1.** A complex number \( \rho \) is a resonance of \( H \) if \( \text{Re} \rho > \inf \sigma_{ess}(H) \) and there exists \( \mu \) small enough, with \( \text{Im} \mu > 0 \), such that \( \rho \in \sigma_{disc}(H_\mu) \).

**Remark 3.2.** Using the self-adjointness of \( H \), one can prove that this is also equivalent to \( \overline{\rho} \in \sigma_{disc}(H_{\overline{\mu}}) \).

In the following we denote by \( \Gamma(H) \) the set of such resonances.
3.2. General assumptions and reduction. We assume that, for some fixed \( \lambda_0 \in \mathbb{R} \), and for all \( x \in \mathbb{R}^3 \), one has,

\[
\sigma(H_{el}(x)) \cap (-\infty, \lambda_0] \text{ is discrete.}
\]

Moreover, we also assume the existence of some finite \( m \geq 1 \), such that

\[
\# \sigma(\tilde{H}_{el}(x)) \cap [-\infty, \lambda_0) \leq N.
\]

Let us denote by

\[
\tilde{\lambda}_1(x) < \tilde{\lambda}_2(x) \leq \cdots \leq \tilde{\lambda}_N(x)
\]

the first \( N \) eigenvalues of \( H_{el}(x) \) and assume there exists a gap between them and the rest of the spectrum of \( H_{el}(x) \), that is, there exists some \( \delta > 0 \), such that,

\[
\inf_{x \in \mathbb{R}^3} \text{dist}\left( \sigma(\tilde{H}_{el}(x)) \setminus \{ \tilde{\lambda}_1(x), \ldots, \tilde{\lambda}_N(x) \}, \{ \tilde{\lambda}_1(x), \ldots, \tilde{\lambda}_N(x) \} \right) \geq \delta.
\]

This fact implies that the spectral projection \( \Pi_{el}(x) \) of \( \tilde{H}_{el}(x) \) associated to \( \{ \tilde{\lambda}_1(x), \ldots, \tilde{\lambda}_N(x) \} \) is \( C^2 \) with respect to \( x \in \mathbb{R}^3 \) (see [CoSe, CDS]).

In the following, we set

\[
\lambda_j(x) := \tilde{\lambda}_j(x) + \frac{\alpha}{|x|}, \quad j = 1, \ldots, N.
\]

Since \( \alpha_0 < 0 \) then there exists \( C > 0 \) such that

\[
\lambda_N(x) \leq C + \frac{\alpha}{|x|}.
\]

For \( x \neq 0 \), we set

\[
\tilde{H}_{el}^\mu(x) = U_\mu \tilde{H}_{el}(x + \mu \omega(x)) U_\mu^{-1}
\]

and

\[
H_{el}^\mu(x) = \tilde{H}_{el}^\mu(x) + \frac{\alpha}{|x + \mu \omega(x)|}.
\]

By Lemma 2.1 in [MaMe], we also know that there exists \( C_1 > 0 \) such that, for all \( x \neq 0 \)

\[
\lambda_1(x) \geq \frac{\alpha}{|x|} - C_1.
\]

For \( x \in \mathbb{R}^n \), let \( \gamma(x) \) be a continuous family of simple loops of \( \mathbb{C} \), enclosing \( \{ \tilde{\lambda}_j(x) : j = 1, \ldots, N \} \) and having the rests of \( \sigma(H_{el}(x)) \) in its exterior.

By the gap condition, we may assume that

\[
\min_{x \in \mathbb{R}^3} \text{dist}(\gamma(x), \sigma(\tilde{H}_{el}(x))) \geq \frac{\delta}{2} > 0
\]

Moreover, \( \gamma(x) \) can be taken in some fix compact set of \( \mathbb{C} \).

Thanks to Lemma 2.3 of [MaMe], if \( \mu \in \mathbb{C} \) is small enough, then for any \( x \in \mathbb{R}^3 \) and \( z \in \gamma(x) \), the operator \((z - \tilde{H}_{el}^\mu(x))^{-1}\) exists and satisfies

\[
(z - \tilde{H}_{el}^\mu(x))^{-1} - (z - \tilde{H}_{el}(x))^{-1} = O(|\mu|)
\]

uniformly. Then, for \( \mu \in \mathbb{C} \) sufficiently small, we can define,

\[
\Pi_{el}^\mu(x) = \int_{\gamma(x)} (z - \tilde{H}_{el}^\mu(x))^{-1} \, dx.
\]
At that point, we fix $\mu = i\mu'$ with $\mu' > 0$ small enough, and we apply Theorem 2.1 with,

- $\mathcal{H}_Q := L^2(\mathbb{R}^p)$;
- $K_0 := -\hbar^2U_\mu \Delta U_\mu^{-1} = [(1 + \mu' d\omega(x))^{-1} hD_x]^2$;
- $Q(x) := H^i_\mu(x)$;
- $\mathcal{D}_Q := H^2(\mathbb{R}^p)$;
- $P := H_\mu$;
- $\mathcal{D}_P := H^2(\mathbb{R}^3)$;
- $\mathcal{W}_0 := \{|x| < 2\delta_1\}$ with $\delta_1 > 0$ arbitrarily small;
- $\mathcal{W}_1 := \{|x| > \delta_1\}$;
- $\Pi(x) = \Pi_\mu(x)$.

We observe that all the properties are satisfied (with, indeed, $\delta_0$ arbitrarily large), and in addition, endowing $H^s(\mathbb{R}^3)$ with the semiclassical norm $||u||_{H^s} := ||h^{-s/2}(\xi)^s \hat{u}(\xi/h)||_{L^2}$ (where $\hat{u}$ stands for the usual Fourier transform), we see that,

$$X_0, X_1 = \mathcal{O}(1) : H^{-1}(\mathbb{R}^3; L^2(\mathbb{R}^p)) \to H^1(\mathbb{R}^3; L^2(\mathbb{R}^p)),$$

and thus, we have,

$$\tag{3.5} Y, Y' = \mathcal{O}(h) : H^{-1}(\mathbb{R}^3; L^2(\mathbb{R}^p)) \to L^2(\mathbb{R}^3; L^2(\mathbb{R}^p)).$$

Moreover, using the fact that, for any function $f$, one has,

$$((I + \mu' d\omega(x))^{-1} \nabla_x - (I + \mu' d\omega(y))^{-1} \nabla_y) f(x + \mu \omega(x) - y - \mu \omega(y)) = 0,$$

we see that we can use the same argument as in CoSe, CD, and conclude that $\Pi_\mu(x)$ is $C^2$ with respect to $x \in \mathbb{R}^3$. As a consequence, and since $K_0$ is a 0-th order semiclassical differential operator of degree 2 with respect to $x$, and $[Q, \Pi] = 0$ everywhere, we also have,

$\tag{3.6} M_0 = M_1 = \mathcal{O}(h) : L^2(\mathbb{R}^3; L^2(\mathbb{R}^p)) \to H^{-1}(\mathbb{R}^3; L^2(\mathbb{R}^p));$

$$M_0 = M_1 = \mathcal{O}(h) : H^1(\mathbb{R}^3; L^2(\mathbb{R}^p)) \to L^2(\mathbb{R}^3; L^2(\mathbb{R}^p)).$$

We also deduce that $||Y_2|| + ||Y_3|| = \mathcal{O}(h^2)$, and since $\Pi M_0 \Pi = 0$ and $\Pi Y_4 \Pi = 0$, in that case Theorem 2.1 becomes,

**Theorem 3.3.** For $h > 0$ small enough and $z$ in a small enough complex neighborhood of $(-\infty, \lambda_0)$, one has the equivalence,

$$z \in \Gamma(H) \iff 0 \in \sigma(A_\mu(z)),$$

where,

$$A_\mu(z) = \Pi_\mu(z - H_\mu) \Pi_\mu + B_\mu(z) : \mathcal{H}_{\text{red}} \cap \mathcal{D}_P \to \mathcal{H}_{\text{red}},$$

with,

$$B_\mu(z) = \Pi_\mu(-Y_2 + (M_0 + Y_3 - Y_4)(1 + Y)^{-1}(1 - Y_1)) \Pi_\mu = \mathcal{O}(h^2).$$

**Remark 3.4.** Using Remark 2.2 we see that this is also equivalent to:

$0 \in \sigma(A_\mu(\mathcal{T})).$

**Remark 3.5.** In particular, the principal part of $A_\mu(z)$ is given by,

$$A_\mu^0(z) := \Pi_\mu(z - H_\mu) \Pi_\mu = U_\mu \Pi_\mu(z - H) \Pi_\mu U_\mu^{-1}.$$
4. Smooth representation of the effective Hamiltonian

Now, we are interested in the structure of the effective Hamiltonian $A_\mu(z)$, and in particular in its possible representation as a semiclassical pseudodifferential operator, at least away from $x = 0$. In view of the study of its action on WKB-type functions, we also study the conjugated operators $e^{s/h}A_\mu(z)e^{-s/h}$ for convenient functions $s = s(x)$.

Since $\Pi(x)$ depend continuously on $x \in \mathbb{R}^3$ and one can find $m$ continuous section $v_1(x), \ldots, v_N(x)$ generating $\text{Ran}\Pi(x)$ and we can also assume that they form an orthonormal family. Moreover, one can easily check that $\tilde{\lambda}_1(x), \tilde{\lambda}_2(x), \ldots, \tilde{\lambda}_N(x)$ depend on $|x|$ only, and can be reindexed in such a way that each of the them depends analytically on $x \neq 0$.

The arguments of [MaMe] show that one can construct finite family of bounded open sets $(\Omega_j)_{0 \leq j \leq J}$ in $\mathbb{R}^n$, with $\Omega_0 \subset \{\psi_1 = 0\}$, and a corresponding family of unitary operators $U_j(x)$ ($j = 0, \ldots, J; x \in \Omega_j$), with $U_0 = 1$ such that (denoting by $U_j$ the unitary operator on $L^2(\Omega_j; L^2(\mathbb{R}^{3p}) \simeq L^2(\Omega_j) \otimes L^2(\mathbb{R}^{3p})$ induced by the action of $U_j(x)$ on $L^2(\mathbb{R}^{3p})$)

\begin{itemize}
  \item $\mathbb{R}^{3p} = \bigcup_{j=0}^{J} \Omega_j$;
  \item For all $j = 0, \ldots, J$ and $x \in \Omega_j$, $U_j(x)$ leaves $H^2(\mathbb{R}^{3p})$ invariant;
  \item For all $j$, the operator $U_j(-h^2\Delta_x)U_j^{-1}$ is a semiclassical differential operator with operator-valued symbol, of the form,
  \[ U_j(-h^2\Delta_x)U_j^{-1} = (-h^2\Delta_x) + h \sum_{|\beta| \leq 1} \omega_{\beta,j}(x; h)(hD_x)^\beta, \]
\end{itemize}

where $\omega_{\beta,j}(-\Delta_y + 1) \omega_{\beta,j}^{-1} \in C^\infty(\Omega_j; \mathcal{L}(L^2(\mathbb{R}^{3p})))$ for any $\gamma \in \mathbb{N}^n$ (here, $\mathcal{L}(L^2(\mathbb{R}^{3p}))$ stands for the Banach space of bounded operators on $L^2(\mathbb{R}^{3p})$, and the quantity $||\partial_\gamma^\beta \omega_{\beta,j}(x; h)(-\Delta_y + 1) \omega_{\beta,j}^{-1} ||_{\mathcal{L}(L^2(\mathbb{R}^{3p}))}$ is bounded uniformly with respect to $h$ small enough and locally uniformly with respect to $x \in \Omega_j$;

\begin{itemize}
  \item For all $j$, the operators $U_j(x)Q(x)\psi_1U_j(x)^{-1}$ and $U_j(x)(-\Delta_y + 1)U_j(x)^{-1}$ are in $C^\infty(\Omega_j; \mathcal{L}(H^2(\mathbb{R}^{3p}), L^2(\mathbb{R}^{3p}))$ ;
\end{itemize}

In particular, following the terminology of [MaSo2], one can check that the corresponding operator $P_j$ (defined as in (2.4)) is a twisted pseudodifferential operator on $\mathbb{R}^3$ associated with $(\Omega_j, U_j)_{j=0, \ldots, J}$.

Moreover, if we also assume that the $\tilde{\lambda}_j$’s are non degenerate and separated at infinity, in the sense that there exists $C > 0$ such that,

\begin{equation}
\inf_{j \neq k} |\tilde{\lambda}_j(x) - \tilde{\lambda}_k(x)| \geq \frac{1}{C}, \quad \text{for } |x| \geq C, \tag{4.1} \end{equation}

then, by Proposition 5.1 of [MaMe], for $\mu \in \mathbb{C}$ small enough, there exist $m$ functions $w_{k,\mu}(x, y) \in C^0(\mathbb{R}^2; H^2(\mathbb{R}^{3p}))$, $k = 1, \ldots N$, depending analytically
on $\mu$ near 0, such that
\[
\langle w_{k,\mu}, w_{\ell,\bar{\mu}} \rangle_{L^2(\mathbb{R}^{3p})} = \delta_{k,\ell};
\]
For $x \in W_1$, $(w_{k,\mu})_{1 \leq k \leq N}$ form a basis of $\text{Ran} \Pi^\mu_{el}(x)$;
\[
w_{k,\mu} \in C^\infty(W_0, H^2(\mathbb{R}^{3p}));
\]
(4.2) For $|x|$ large enough, $w_{k,\mu}$ is an eigenfunction of $Q_\mu(x)$
associated with $\lambda_k(x + \mu \omega(x))$;
For $j = 1, \ldots, J$, $U_j(x)w_{k,\mu} \in C^\infty(\Omega_j, H^2(\mathbb{R}^{3p}))$.

For $u \in L^2(\mathbb{R}^{n+p})$ and $x \in \mathbb{R}^n$, we set,
\[
\tilde{\Pi}^\mu_{el}(x)u := \sum_{k=1}^N \langle u, w_{k,\bar{\mu}} \rangle_{L^2(\mathbb{R}^{3p})} w_{k,\mu}.
\]
In particular, for $x \in W_1$, one has $\tilde{\Pi}^\mu_{el}(x) = \Pi^\mu_{el}(x)$, and we also observe that, if $\delta_0$ has been chosen small enough (in the definition of $W_0$), then, for $x \in W_0 \setminus \{0\}$, one has $\text{Re} Q(x) \geq \lambda_0 + \delta_0$. As a consequence, all the properties (2.2) are satisfied with $\Pi(x) := \tilde{\Pi}^\mu_{el}(x)$, too.

In the following we set
\[
R^-_\mu : \bigoplus_i L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^{3+3p}),
R^-_\mu(u_1^-, \ldots, u_N^-) = \sum_{k=1}^N u_k^- w_{k,\mu}
\]
and
\[
R^+_\mu = (R^-_\mu)^* : L^2(\mathbb{R}^{3+3p}) \to \bigoplus_i L^2(\mathbb{R}^3),
R^+_\mu g = \bigoplus_i \langle g, w_{k,\bar{\mu}} \rangle_{L^2(\mathbb{R}^{3p})},
\]
so that we have,
\[
R^+_\mu R^-_\mu = I ; \quad R^-_\mu R^+_\mu = \tilde{\Pi}^\mu_{el} = \Pi.
\]
As a consequence, $R^+_\mu$ sends isomorphically $\mathcal{H}_{\text{red}}$ into $L^2(\mathbb{R}^3)^{\oplus N}$, with inverse $R^-_\mu$. Moreover, by construction we also see that $R^-_\mu$ sends $H^2(\mathbb{R}^{3+3p})$ into $H^2(\mathbb{R}^3)$. Thus, in this case the study of the Grushin operator introduced in (2.7) is equivalent to that of,
\[
\tilde{\mathcal{G}}(z) := \begin{pmatrix} I & 0 \\ 0 & R^+_\mu \end{pmatrix} \begin{pmatrix} P - z & I \\ I & 0 \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & R^-_\mu \end{pmatrix}
\]
\[
= \begin{pmatrix} P - z & R^-_\mu \\ R^+_\mu & 0 \end{pmatrix} : \mathcal{D}_P \oplus L^2(\mathbb{R}^3)^{\oplus N} \to \mathcal{H} \oplus H^2(\mathbb{R}^3)^{\oplus N},
\]
and Theorem 2.3 gives us the first assertion of the following result:

**Theorem 4.1.** Let $\mu = i\mu'$ with $\mu' > 0$ fixed small enough. For $h > 0$ small enough and $z$ in a small enough complex neighborhood of $(-\infty, \lambda_0]$, one has the equivalence,
\[
z \in \Gamma(H) \iff 0 \in \sigma(\tilde{\mathcal{A}}_\mu(z)),
\]
where,
\[
\tilde{\mathcal{A}}_\mu(z) = R^+_\mu \left(z - H_\mu + \tilde{B}_\mu(z)\right) R^-_\mu : H^2(\mathbb{R}^3)^{\oplus N} \to L^2(\mathbb{R}^3)^{\oplus N},
\]
with,
\[ \tilde{B}_\mu(z) = -Y_2 + (M_0 + Y_3 - Y_4)(1 + Y)^{-1}(1 - Y_1) \]
\[ = -RX_0 R + \mathcal{O}(h). \]
Here, \( R := [Q, \Pi] = \varphi_0 [Q, \Pi] \varphi_0 \).
Moreover, if \( s = s(x) \in C_0^\infty(\mathbb{R}^3; \mathbb{R}) \) satisfies \( |\nabla s(x)|^2 \leq \theta(x, z) \), with,
\[ \theta(x, z) := \min\{\lambda_0 + \delta_0 - \text{Re} \, z, \inf \sigma(\text{Re} \, \Pi(Q(x) - z) \Pi)\} - \frac{1}{2} \delta_1, \]
then, \( e^{s(x)/h} \tilde{A}_\mu(z) e^{-s(x)/h} \) can be written as,
\[ e^{s(x)/h} \tilde{A}_\mu(z) e^{-s(x)/h} = \Lambda_{\mu,s}(z) + L_{\mu,s}(z) \psi_0 + \Theta_{\mu,s}(z) \]
where \( \Lambda_{\mu,s}(z) \) is a matrix of pseudodifferential operators on \( \mathbb{R}^3 \), \( X_{1,s} := e^{s(x)/h} X_1 e^{-s(x)/h} \), \( M_{1,s} := e^{s(x)/h} M_1 e^{-s(x)/h} \), and
\[ L_{\mu,s}(z) = -R_\mu^+(H_{\mu}^\omega - \lambda_0 - \delta_0)(1 - \psi_1) + RX_0 s(z) R \] \[ \Rightarrow L_{\mu,s}(z) = \mathcal{O}(h) \]
\[ \Theta_{\mu,s}(z) = 0 \]
\[ = L^2(\mathbb{R}^3 + p) \to L^2(\mathbb{R}^3) \otimes \mathbb{N}, \]
with \( X_{0,s} := e^{s(x)/h} X_0 e^{-s(x)/h} \). The principal symbol of \( \Lambda_{\mu,s}(z) \) is of the form,
\[ \sigma_{\mu,s}(x, \xi; z) := \left( z - ((I + \mu^t d\omega(x))^{-1} (\xi + i \nabla s(x)))^2 \right) \]
where \( I_N \) stands for the \( N \times N \) identity matrix, and \( \mathcal{M}_\mu(x) \) is a \( N \times N \) matrix of smooth functions on \( \mathbb{R}^3 \) with eigenvalues \( \lambda_1(x + \mu \omega(x)), \ldots, \lambda_N(x + \mu \omega(x)) \)
for \( x \in \mathbb{R}^3 \setminus W_0 \), and satisfying \( \text{Re} \, \mathcal{M}_\mu(z) \geq \lambda_0 + \delta_0 \) for \( x \in W_0 \). Finally, there exists a constant \( C > 0 \) such that,
\[ \text{Re} \, e^{s(x)/h} L_{\mu,s}(z) e^{-s(x)/h} \leq C. \]
Here, \( \psi_0 \) and \( \psi_1 \) are the two functions defined as in \( \text{[23]} \).}

**Remark 4.2.** Again, using Remark \( \text{[32]} \) we see that this is also equivalent to: \( 0 \in \sigma(\tilde{A}_\mu(\tau)) \).

**Proof.** We have to prove \( \text{(4.4)} \). Using the same notations as in \( \text{[23]} \), we have,
\[ H_\mu = P = P_1 + (Q - \lambda_0 - \delta_0)(1 - \psi_1) = P_1 + (Q - \lambda_0 - \delta_0)(1 - \psi_1) \psi_0, \]
and thus,
\[ \tilde{A}_\mu(z) = R_\mu^+(z - P_1) R_\mu^- \left( \tilde{B}_\mu(z) - (Q - \lambda_0 - \delta_0)(1 - \psi_1) \psi_0 \right) R_\mu^- \]
The fact that \( R_\mu^+(z - P_1) R_\mu^- \) is a matrix of smooth semiclassical pseudodifferential operators on \( \mathbb{R}^3 \) is a direct consequence of the fact that \( P_1 \) is a twisted pseudodifferential operator associated with the family \( (\Omega_j, U_j)_{j=0, \ldots, J} \), and that the same is true for \( R_\mu^\pm \) (see \( \text{MaSo2} \) for the terminology and details). Moreover, its symbol is a second-order polynomial with respect to \( \xi \), and its principal symbol is of the form \( z - ((I + \mu^t d\omega(x))^{-1} \xi)^2 - \mathcal{M}_\mu(x) \), where \( \mathcal{M}_\mu(x) \) is the matrix,
\[ \mathcal{M}_\mu(x) := R_\mu^+(Q(x) \psi_1(x) + (\lambda_0 + \delta_0)(1 - \psi_1(x))) R_\mu^- \].
In particular, when \( x \in \mathbb{R}^3 \setminus W_0 \), then \( \psi_1(x) = 1 \), and the eigenvalues of \( \mathcal{M}_\mu(x) \) are those of \( Q(x)\Pi_\mu^0(x) \), that is, \( \lambda_1(x + \mu \omega(x)), \ldots, \lambda_N(x + \mu \omega(x)) \). Moreover, when \( x \in W_0 \), then \( \text{Re} \, Q(x) \geq \lambda_0 + \delta_0 \), and thus \( \text{Re} \, \mathcal{M}_\mu(x) \geq \lambda_0 + \delta_0 \), too. As a consequence, \( e^{s/h} R_\mu^+ (z - P_1) R_\mu^+ e^{-s/h} \) is a pseudodifferential operator, too, with principal symbol \( z - ((I + \mu^l \delta \omega(x))^{-1}(\xi + i\nabla s))^2 - \mathcal{M}_\mu(x) \).

In view of (4.7), and since \( R_\mu^+ (Q - \lambda_0 - \delta_0)(1 - \psi_1)\psi_0 R_\mu^- \) commutes with \( e^{s/h} \), now we are reduced to study \( R_\mu^+ e^{s/h} \tilde{B}_\mu(z) e^{-s/h} R_\mu^- \). We first prove

**Lemma 4.3.** If \( s(x) \in C^\infty_0(\mathbb{R}^3; \mathbb{R}) \) satisfies \( |\nabla s(x)|^2 \leq \theta(x, z) \), then, for \( j = 0, 1 \), one has
\[
\text{Re} \, e^{s(x)/h} X_j(z) e^{-s(x)/h} \geq 0,
\]
and
\[
e^{s(x)/h} X_j(z) e^{-s(x)/h} = O(1) : L^2(\mathbb{R}^3; L^2(\mathbb{R}^P)) \to H^2(\mathbb{R}^3; L^2(\mathbb{R}^P)),
\]
uniformly as \( h \to 0_+ \). Moreover, \( e^{s(x)/h} X_1(z) e^{-s(x)/h} \) is a twisted pseudodifferential operator associated with the family \( (\Omega_j, U_j)_{j=0,\ldots,J} \).

**Proof.** We have
\[
e^{s(x)/h} \tilde{\Pi}(P_j - z) \tilde{\Pi} e^{-s(x)/h} = \tilde{\Pi}(e^{s(x)/h} K_0 e^{-s(x)/h} + Q_j - z) \tilde{\Pi},
\]
and the principal symbol \( k_s \) of the semiclassical differential operator \( e^{s(x)/h} K_0 e^{-s(x)/h} \) is given by
\[
k_s(x, \xi) = ((I + \mu^l \delta \omega(x))^{-1}(\xi + i\nabla s(x)))^2,
\]
and thus, for \( \mu \) small enough,
\[
\text{Re} \, k_s(x, \xi) = (1 + O(|\mu|)) \xi^2 - (1 + O(|\mu|)) |\nabla s|^2 \geq \frac{1}{2} \xi^2 - \theta(x, z) - \frac{1}{8} \delta_1.
\]
As a consequence, for \( h > 0 \) small enough, we obtain
\[
(4.8) \quad \text{Re} \, e^{s(x)/h} \tilde{\Pi}(P_j - z) \tilde{\Pi} e^{-s(x)/h} \geq \text{Re} \, \tilde{\Pi} \left( \frac{1}{2} h^2 \Delta_x + Q_j - \theta(x, z) - \frac{1}{4} \delta_1 \right) \tilde{\Pi}
\]
\[
\geq \text{Re} \, \tilde{\Pi} \left( \frac{1}{2} h^2 \Delta_x + \frac{1}{4} \delta_1 \right) \tilde{\Pi}.
\]
Since \( e^{s(x)/h} X_j(z) e^{-s(x)/h} = \left( e^{s(x)/h} \tilde{\Pi}(P_j - z) \tilde{\Pi} e^{-s(x)/h} \right)_{|\text{Ran} \tilde{\Pi}}^{-1} \tilde{\Pi} \), the first two results follow. Moreover, for \( j = 1 \), we know that \( e^{s(x)/h} \tilde{\Pi}(P_1 - z) \tilde{\Pi} e^{-s(x)/h} \) is a twisted pseudodifferential operator associated with the family \( (\Omega_j, U_j)_{j=0,\ldots,J} \). Thus, so is \( e^{s/h} G_1(z) e^{-s/h} \), and (4.8) shows that it is elliptic. Then, the last result follows from the general theory of [MaSo2]. □

This lemma allows us to extend the result of Theorem 2.1 by taking into account the weight \( e^{s/h} \). Indeed, working with \( e^{s/h} G_j(z) e^{-s/h} \) instead of \( G_j(z) \), we see that all the arguments can be repeated, the main point being that, in this case, \( Q(x) \) will be substituted with \( Q(x) - ((I + \mu^l \delta \omega(x))^{-1}(\xi + i\nabla s))^2 \), and \( K_0 \) will be \( ((I + \mu^l \delta \omega(x))^{-1}(D_x + i\nabla s))^2 + ((I + \mu^l \delta \omega(x))^{-1}(\xi + i\nabla s))^2 \), leaving satisfied the conditions (2.1)–(2.2).
In particular, according to the expression of $\tilde{B}_\mu(z)$ and the definition of $Y$ given in [2.6], and adding an index $s$ to the operators, meaning that they are conjugated with $e^{s/h}$ (when they don’t commute with it), we have,

$$\tilde{B}_{\mu,s}(z) = e^{s/h} \tilde{B}_\mu(z)e^{-s/h} = -Y_{2,s} + (M_{0,s} - Y_{4,s} + B_0T_{0,s} + B_1T_{1,s})(1 - Y_{1,s})$$

with,

$$B_0, B_1 = O(h) : H^{-1}(\mathbb{R}^3; L^2(\mathbb{R}^p)) \to L^2(\mathbb{R}^3; L^2(\mathbb{R}^p)).$$

Thus, using the expressions of $Y_2$ and $Y_1$ given in [2.6] and the definition of $R$,

$$\tilde{B}_{\mu,s}(z) = -\varphi_1 M_{1,s} X_{1,s} M_{1,s} \varphi_1$$

$$+ (M_{0,s} - Y_{4,s} + B_0T_{0,s} + B_1T_{1,s})(1 - \varphi_1 X_{1,s} M_{1,s} X_{1,s}) + B_2 \psi_0,$$

with $B_2 = -RX_{0,s}R + O(h)$.

Now, since $T_0$ and $T_1$ are differential operators with coefficients supported in $\{\psi_0 = 1\}$, and since $\Pi(M_0 - Y_4)\Pi = 0$, we deduce,

$$R_\mu^+ \tilde{B}_{\mu,s}(z) R_\mu^- = \Lambda_{\mu,1} - R_\mu^+(M_{0,s} - Y_{4,s} + B_0^b T_{0,s} + B_1^b T_{1,s}) \varphi_1 X_{1,s} M_{1,s} R_\mu^- \varphi_1$$

$$+ R_\mu^+ B_2^\prime R_\mu^- \psi_0,$$

with

$$\Lambda_{\mu,1} := -\varphi_1 R_\mu^+ M_{1,s} X_{1,s} M_{1,s} R_\mu^- \varphi_1;$$

$$B_2^\prime = -RX_{0,s}R + O(h).$$

By the arguments of [MaSo2], we see that $\Lambda_{\mu,1}$ is a semiclassical pseudodifferential operator of order $-2$ (and thus $O(h^2)$ on $L^2(\mathbb{R}^3)$). Moreover, since $[Q, \Pi] \varphi_1 = 0$, we have $M_0 \varphi_1 = [K_0, \Pi] \varphi_1 = M_1 \varphi_1$, and $Y_4 \varphi_1 = \varphi_0 M_1 \varphi_0 \varphi_1 + \varphi_1 M_1 \varphi_1^2$, as a consequence (still with the arguments of [MaSo2]), we see that $R_\mu^+(M_{0,s} - Y_{4,s}) \varphi_1 X_{1,s} M_{1,s} R_\mu^- \varphi_1$ is a semiclassical pseudodifferential operator of order $-2$, too. Hence, we are led to,

$$R_\mu^+ \tilde{B}_{\mu,s}(z) R_\mu^- = \Lambda_{\mu,1}^\prime - R_\mu^+(B_0^b T_{0,s} + B_1^b T_{1,s}) \varphi_1 X_{1,s} M_{1,s} R_\mu^- \varphi_1 + R_\mu^+ B_2^\prime R_\mu^- \psi_0,$$

where $\Lambda_{\mu,1}^\prime$ is a semiclassical pseudodifferential operator of order $-2$. We prove,

Lemma 4.4. For $k = 1, 2$, one has,

$$T_{k,s} X_{1,s} M_{1,s} (1 - \psi_0) = O(h^\infty) : L^2(\mathbb{R}^{3+p}) \to L^2(\mathbb{R}^{3+p}).$$

Proof. We write $X_{1,s} M_{1,s}$ by using the general expression of a twisted pseudodifferential operator (see [MaSo2], Definition 4.4), namely,

$$X_{1,s} M_{1,s} = \sum_{j=0}^J U_j^{-1} \chi_j A_j^N U_j \chi_j + O(h^N),$$

where $N \geq 1$ is arbitrary, $\chi_j \in C_0^\infty(\mathbb{R}^3)$ is supported in $\Omega_j$, and $A_j^N$ is a pseudodifferential operator (of degree -1) with respect to the variable $x$, with operator-valued symbol. Then, the result immediately follows from the fact that $T_{k,s}$ is a first-order differential operator with smooth coefficients supported in $\{\psi_0 = 1\}$. □
Then, formula \((4.4)\) follows by setting,

\[ \begin{align*}
\Lambda_{\mu,s} &:= R_0^+ (z - P_1) R_0^- + \Lambda_{\mu,1}; \\
L_{\mu,s} &:= R_0^+ (B_2^0 - (B_0^1 T_{0,s} + B_1^s T_{1,s}) \varphi_1 X_{1,s} M_{1,s} R_0^- \varphi_1 \\
& \quad - (Q - \lambda_0 - \delta_0)(1 - \psi_1)) R_0^-; \\
\Theta_{\mu,s}(z) &:= - R_0^+ (B_0^1 T_{0,s} + B_1^s T_{1,s}) \varphi_1 X_{1,s} M_{1,s} R_0^- \varphi_1 (1 - \psi_0). 
\end{align*} \] (4.9)

5. Action on WKB solutions

In this section, we study the action of \(\tilde{A}_\mu(z)\) on WKB functions of the type \(a(x, h)e^{-s(x)/h}\), where the symbol \(a(x, h)\) admits some semiclassical expansion of the type,

\[
a(x, h) \sim \sum_{k \geq 0} h^{k/2} a_k(x)
\]
as \(h \to 0^+\). We first prove,

**Proposition 5.1.** Let \(u \in L^2(\mathbb{R}^{3+p})\) such that, for all \(j = 0, 1, \ldots, r\), and \(x \in \Omega_j\), \(U_j(x)u(x, y)\) that can be written as \(U_j(x)u(x, y) = a_j(x, y; h)e^{-s(x)/h}\)

with \(s \in C^\infty(\mathbb{R}^3; \mathbb{R})\) independent of \(h\), \(|\nabla s(x)|^2 \leq \theta(x, z)\), \(a_j \in C^\infty(\Omega_j; L^2(\mathbb{R}^p))\), \(a_j\) admits in \(C^\infty(\Omega_j; L^2(\mathbb{R}^p))\) an asymptotic expansion of the type,

\[
a_j(x, y; h) \sim \sum_{k \geq 0} h^{k/2} a_{j,k}(x, y)
\]
as \(h \to 0^+\), with \(a_{j,k}(x, y) \in C^\infty(\Omega_j; L^2(\mathbb{R}^p))\) independent of \(h\). Then, for any \(\chi_j \in C^\infty(\Omega_j)\), the function \(e^{s/h} U_j \chi_j X_1(z) u\) admits in \(C^\infty(\Omega_j; H^2(\mathbb{R}^p))\) an asymptotic expansion of the type,

\[
e^{s/h} U_j \chi_j X_1(z) u(x, y, h) \sim \sum_{k \geq 0} h^{k/2} b_{j,k}(x, y; z),
\]

with,

\[
b_{j,0} := U_j [\hat{\Pi} (Q_1(x) - [(1 + \mu^l d\omega)^{-1} \nabla s]^2 - z) \hat{\Pi}]^{-1}\hat{\Pi} U^{-1}_{j,0}\chi_j a_{j,0}.
\]

Moreover, the support in \(x\) of \(b_{j,k}\) is included in the union of the supports in \(x\) of \(\chi_j a_{j,0}, \chi_j a_{j,1}, \ldots, \chi_j a_{j,k}\).

**Proof.** Let \(\tilde{\chi}_j \in C^\infty(\Omega_j)\) such that \(\tilde{\chi}_j \chi_j = \chi_j\). As we have seen in the previous section, \(e^{s/h} G_1(z)^{-1} e^{-s/h}\) is an elliptic twisted pseudodifferential operator. Thus, by the general theory of [MaSo2] (in particular Propositions 4.6, 4.10 and 4.14), we know that \(U_j \tilde{\chi}_j e^{s/h} G_1(z)^{-1} e^{-s/h} U^{-1}_{j,0} \tilde{\chi}_j\) is a bounded \(h\)-admissible operator on \(L^2(\mathbb{R}^3; L^2(\mathbb{R}^p \oplus \mathbb{C}^m))\) (with operator-valued symbol). In particular, \(U_j \tilde{\chi}_j e^{s/h} X_1(z) e^{-s/h} U^{-1}_{j,0} \tilde{\chi}_j\) is a bounded \(h\)-admissible operator on \(L^2(\mathbb{R}^3; L^2(\mathbb{R}^p))\). This means that, for any \(M \geq 1\), it can be written as,

\[
U_j \tilde{\chi}_j e^{s/h} X_1(z) e^{-s/h} U^{-1}_{j,0} \tilde{\chi}_j v(x, y) = \frac{1}{(2\pi h)^n} \int e^{i(x-x')/\xi} q_M(x, \xi) v(x', y) dx'd\xi + R_M v,
\]
with \( |R_M| = \mathcal{O}(h^M) \) and \( q_M \) is an operator-valued symbol, acting on \( L^2(\mathbb{R}^p) \). The symbolic calculus also gives us,
\[
q_M = q_0 + \mathcal{O}(h),
\]
with,
\[
q_0(x, \xi) := U_j \tilde{\chi}_j \hat{\Pi} \left( |(1 + \mu^\dagger d\omega)^{-1}(\xi + i\nabla s)|^2 + Q_1(x) - z \right)^{-1} \hat{\Pi} U_j^{-1} \tilde{\chi}_j.
\]
In particular, taking \( v = a \), and observing that \( e^{-s/h} \) commutes with \( U_j^{-1} \tilde{\chi}_j \), we obtain,
\[
U_j \tilde{\chi}_j e^{s/h} X_1(z) \tilde{\chi}_j u(x, y) = \frac{1}{(2\pi h)^n} \int e^{i(x-x')\xi/h} q_N(x, \xi) a(x', y) dx' d\xi + \mathcal{O}(h^N).
\]
The stationary-phase theorem applied to this integral (with critical point \( \xi = 0 \) and \( x' = x \)) immediately gives,
\[
U_j \tilde{\chi}_j e^{s/h} X_1(z) \tilde{\chi}_j u(x, y) \sim \sum_{k \geq 0} h^{k/2} \bar{b}_{j,k}(x, y; z),
\]
in \( C^\infty(\Omega_j; H^2(\mathbb{R}^p)) \), with,
\[
\bar{b}_{j,0} := U_j \hat{\Pi} (Q_1(x) - [(1 + \mu^\dagger d\omega)^{-1}\nabla s] - z) \hat{\Pi} U_j^{-1} \tilde{\chi}_j^2 a_{j,0},
\]
and \( \text{Supp} b_{j,k} \subset \bigcup_{0 \leq \ell \leq k} \text{Supp} \tilde{\chi}_j a_{j,\ell} \). On the other hand, using the representation of twisted \( h \)-admissible operators given in \[\text{MaSo2}, \text{Definition 4.4}\] (that we apply to \( e^{s/h} X_1(z) e^{-s/h} \)), and still by the stationary phase theorem, we also have,
\[
U_j \tilde{\chi}_j e^{s/h} X_1(z)(1 - \tilde{\chi}_j) u(x, y) \sim 0
\]
in \( C^\infty(\Omega_j; H^2(\mathbb{R}^p)) \). As a consequence, we have,
\[
U_j \tilde{\chi}_j e^{s/h} X_1(z) u(x, y) \sim U_j \tilde{\chi}_j e^{s/h} X_1(z) \tilde{\chi}_j u(x, y)
\]
\[
\sim \chi_j U_j \tilde{\chi}_j e^{s/h} X_1(z) \tilde{\chi}_j u(x, y),
\]
and the result follows from \[\text{[5.1]}\].

**Corollary 5.2.** Let \( u \in (L^2(\mathbb{R}^3))^{\leq N} \) that can be written as \( u(x; h) = a(x; h) e^{-s(x)/h} \) with \( s \in C^\infty_c(\mathbb{R}^3; \mathbb{R}) \) independent of \( h \), \( |\nabla s(x)|^2 \leq \theta(x, z) \), \( a \in (C^\infty(\mathbb{R}^3))^{\leq N} \) admitting an asymptotic expansion of the type,
\[
a(x; h) \sim \sum_{k \geq 0} h^{k/2} a_k(x)
\]
as \( h \to 0_+ \), with \( a_k(x) \in (C^\infty(\mathbb{R}^3))^{\leq N} \), \( \text{Supp} a_k \subset \mathcal{W}_0^0 \). Then, \( e^{s/h} \tilde{A}_\mu(z) u \) admits a semiclassical asymptotic expansion of the type,
\[
e^{s/h} \tilde{A}_\mu(z) u(x; h) \sim \sum_{k \geq 0} h^{k/2} b_k(x; z),
\]
with,
\[
b_0(x; z) := \sigma_{\mu,s}(x; 0; z) a_0 = \left( z + ((I + \mu^\dagger d\omega(x))^{-1}\nabla s(x))^2 \right) a_0 - \mathcal{M}_\mu(a_0),
\]
and \( \text{Supp} b_k(\cdot; z) \subset \mathcal{W}_0^0 \).
Proof. Indeed, by Proposition 5.1 and (4.2), we see that, for any $j = 0, \ldots, r$ and $\chi_j \in C_0^\infty(\Omega_j)$, we have,

$$U_j \chi_j X_{1,s} M_{1,s} R_{\mu,s} \varphi_1 a(x, y; h) \sim \sum_{k \geq 0} h^{k/2} b_{j,k}(x, y; z),$$

with $\text{Supp} \ b_{j,k} \subset W_0^\Omega \times \mathbb{R}^p$. In particular,

$$(5.2) \quad \psi_0 U_j \chi_j X_{1,s} M_{1,s} R_{\mu,s} \varphi_1 a(x, y; h) = \mathcal{O}(h^{\infty}),$$

together with all its derivatives in $x$. Now, by (4.4), and using that $\psi_0 u = 0$, we have,

$$e^{s(x)/h} \tilde{A}_\mu(z) u = \Lambda_{\mu,s}(z) a + \Theta_{\mu,s}(z) a,$$

where $\Theta$ is given in (4.9), and is of the form

$$\Theta_{\mu,s}(z) = L'_{\mu,s}(z) \varphi_1 X_{1,s} M_{1,s} R_{\mu,s} (1 - \psi_0)$$

Looking more carefully at the expression of $L'_{\mu,s}(z)$, we see that it involves only twisted pseudodifferential operators, except $X_0$ that always appears on the form $X_0 T_0$ (this is due to the expressions of the operators $Y$ and $Y_3$ given in (2.6), and to the fact that $L'_{\mu,s}(z)$ does not involve $Y_1$, $Y_2$ nor $Y_3$). Therefore, since the coefficients of $T_0$ are supported in $\{ x \neq 0 \}$, and the same holds for $\varphi_1$, one can deduce from (5.2) and the general theory of [MaSo2] that one has,

$$\Theta_{\mu,s}(z) a = \mathcal{O}(h^{\infty}),$$

together with all its derivatives. As a consequence, we obtain,

$$e^{s(x)/h} \tilde{A}_\mu(z) u \sim \Lambda_{\mu,s}(z) a,$$

and the result follows from the fact that $\Lambda_{\mu,s}$ is a pseudodifferential operator with principal symbol $\sigma_{\mu,s}(x, \xi; z)$, and from a standard stationary-phase expansion. \hfill \Box

6. Location of resonances

In order to determine the resonances of $H$ near $\lambda_0$, we see on (4.3) that it is necessary to know the spectrum of $\tilde{A}_\mu(z)$ near 0. But we see on (4.4) with $s = 0$ that $\tilde{A}_\mu(z)$ is not really a pseudodifferential operator (not even modulo $\mathcal{O}(h^{\infty})$), because of the term $L_{\mu,0}(z) \psi_0$ in its expression. However, because this term is localised in the region where $\text{Re} \Lambda_{\mu,0} \leq -\delta_0 + Ch$, and has a real part $\leq C'h$ (with $C, C'$ positive constants), there exists a general method, due to Helffer and Sjöstrand [HeSj2], to compare the eigenvalues of $\tilde{A}_\mu(z)$ to those of,

$$\tilde{A}_\mu(z) := \Lambda_{\mu,0}(z) + \Theta_{\mu,0}(z) = \tilde{A}_\mu(z) - L_{\mu,0}(z).$$

Assume for instance that $\tilde{A}_\mu(z)$ admits an isolated eigenvalue $\rho_0 = \rho_0(z)$ close to 0 (with normalised eigenfunction $u_0$), call $\Pi_0$ the spectral projector of $\tilde{A}_\mu(z)$ associated with $\rho_0$, $\tilde{\Pi}_0 := 1 - \Pi_0$, and assume that the reduced resolvent $\tilde{\Pi}_0(\tilde{A}_\mu(z) - \rho)^{-1}\Pi_0$ is not exponentially large for $\rho$ in a small
(\(h\)-dependent) neighbourhood of 0. Then, for \(\rho\) is his neighbourhood, one considers the two Grushin problems,

\[
\mathcal{G}_0(\rho) := \begin{pmatrix}
\hat{A}_\mu - \rho & u_0 \\
\langle \cdot, u_0 \rangle & 0
\end{pmatrix};
\]

\[
\mathcal{G}(\rho) := \begin{pmatrix}
\hat{A}_\mu - \rho & \chi_1 u_0 \\
\langle \cdot, u_0 \rangle & 0
\end{pmatrix},
\]

where we have omitted the variable \(z\), and where \(\chi_1 \in \mathcal{C}^\infty(\mathbb{R}^n)\) is such that \(\chi_1(x) = 1\) for \(|x| \geq 3\delta_1\), \(\chi_1(x) = 0\) for \(|x| \leq 2\delta_1\). Then, by construction \(\mathcal{G}_0(\rho)\) is invertible, and we denote its inverse by,

\[
\mathcal{G}_0(\rho)^{-1} = \begin{pmatrix}
E_0(\rho) & E_0^+(\rho) \\
E_0^-(\rho) & E_0^-(\rho)
\end{pmatrix},
\]

then a candidate for the inverse of \(\mathcal{G}(\rho)\) is given by (see also [HeSj2], Formula (9.22)),

\[
\mathcal{F}(\rho) := \begin{pmatrix}
\chi_1 E_0(\rho) & E_0^+(\rho) \\
E_0^-(\rho) & E_0^-(\rho)
\end{pmatrix},
\]

where \(\chi_2 \in \mathcal{C}^\infty(\mathbb{R}^n)\) is such that \(\chi_1(x) = 1\) for \(|x| \geq 4\delta_1\), \(\chi_1(x) = 0\) for \(|x| \leq 3\delta_1\), and \(B\) is defined as,

\[
B := \tilde{A}_\mu - C\chi_3,
\]

with \(\chi_3 \in \mathcal{C}^\infty(\mathbb{R}^n)\) such that \(\chi_1(x) = 1\) near \(\{\text{Re} M_\mu(x) \leq \lambda_0\}\), \(\chi_1(x) = 0\) for \(|x| \leq \delta_2\) (where \(\delta_2 > 4\delta_1\)), and \(C > 0\) is taken sufficiently large in order that \(\text{Re} B \leq -\delta_0\).

Indeed, taking advantage of the fact that \(u_0\) is exponentially small near 0, and that, thanks to (4.5), the operators satisfy the same type of estimates as in [HeSj2], Proposition 9.3, we see as in [HeSj2], Section 9, that one has,

\[
\mathcal{G}(\rho)\mathcal{F}(\rho) = I + \mathcal{O}(e^{-\alpha_0/h}),
\]

where \(\alpha_0 > 0\) mainly depends on the distance between the support of \(\chi_3\) and 0. By a similar procedure, an approximate left-inverse of \(\mathcal{G}(\rho)\) can also be found, and as in [HeSj2], this permits to show the existence of an eigenvalue \(\rho_1(z)\) of \(\hat{A}_\mu(z)\) exponentially close to \(\rho_0(z)\). Finally, the corresponding resonance of \(H\) is obtained by solving the equation \(\rho_1(z) = 0\), and we see on Theorem 4.1 that this leads to a unique value \(z_1\) close to \(\lambda_0\).

As in [HeSj2], this argument can also be extended to a set of resonances of \(\hat{A}_\mu\) separated from the rest of its spectrum.

### 7. Applications

In this section we discuss some applications to cases where resonances can be located quite well, and estimates on their widths can be obtained. We do not give details on the proofs (that may result rather long) but just give indications on them.
7.1. **Shape resonances.** In this subsection we assume that \( N = 1 \), and that the first electronic level \( \lambda_1(x) \) presents, at some energy \( \lambda_0 \), the geometric situation of a well in an island, as described in [HeSj2], that is,

- There is an open bounded connected set \( \tilde{O} \) (the island) and a compact set \( U \subset \tilde{O} \) (the well) such that \( \lambda_1 \leq \lambda_0 \) on \( U \cup \tilde{O}^c \), \( \lambda_1 > \lambda_0 \) on \( O \setminus U \);
- The set \( \tilde{O}^c \times \mathbb{R}^3 \) is non trapping for the Hamiltonian \( \xi^2 + \lambda_1(x) \) at energy level \( \lambda_0 \);
- \( \lambda_1(x) \) admits a limit \( \lambda_1^\infty < \lambda_0 \) as \( |x| \to \infty \), \( x \) in a complex sector of the form \( \{|\text{Im} x| < \delta |\text{Re} x|\} \) with \( \delta > 0 \).

**Remark 7.1.** Note that the limit \( |x| \to \infty \) in \( H_{el}(x) \) can be deduced, by a change of variable, from the semiclassical limit of \( -\hbar^2 \Delta y + W(y) \), with \( \hbar := |x|^{-\frac{1}{2}} \), and \( W(y) := \alpha + \sum_{j} (\alpha_j^+ |y_j + \theta|^{-1} + \alpha_j^- |y_j - \theta|^{-1}) + \sum_{j,k} \alpha_{jk} |y_j - y_k|^{-1} \), where \( \theta \) is any element of the unit sphere of \( \mathbb{R}^3 \). In particular, the limit \( \lambda_1^\infty \) can be seen to exist for \( p = 1 \), and to be equal to the smallest between the first eigenvalue of \( -\Delta y + \alpha_1^+ |y|^{-1} \), and that of \( -\Delta y + \alpha_1^- |y|^{-1} \). The case \( p \geq 2 \) seems to be more delicate to treat, but it is reasonable to think that the limit should exist, too.

In this situation, we can adapt some of the arguments of [HeSj2] (see also [LaMa] for a more simplified version) to the operator \( \Lambda_{\mu,0}(z) \) given in (4.4) for \( s = 0 \). Moreover, the properties of \( L_{\mu,s} \) and \( L'_{\mu,s} \) (in particular (4.6)) allows us to extend the Agmon estimates appearing in [HeSj2] to the whole operator \( \tilde{A}_\mu(z) \).

In addition, the non degeneracy of \( \lambda_1(x) \) and the rotational symmetry of \( H_{el}(x) \) (namely, that rotating simultaneously \( x \) and \( y_j \) \( (j = 1, \ldots, p) \) with the same rotation of \( \mathbb{R}^3 \), leaves \( H_{el}(x) \) unchanged), one can see as in [KMSW], Theorem 2.1 (see also [GKMISS]) that one can construct the functions \( w_{k,\mu} \) in such a way that \( \tilde{A}_\mu(z) \) commutes with the operator of angular momentum with respect to \( x \). In particular, working in polar coordinates \( (r, \theta) \in \mathbb{R}_+ \times S^2 \), denoting by \( Y_{\ell,m} \) the spherical harmonic of degree \( \ell \) and order \( m \), and \( \mathcal{H}_\ell \) the subspace of \( L^2(S^2) \) spanned by \( \{Y_{\ell,m} : |m| \leq \ell\} \), one can decompose \( \tilde{A}_\mu(z) \) as (see, e.g., [So]),

\[
\tilde{A}_\mu(z) = \bigoplus_{\ell \geq 0} \tilde{A}_\mu^\ell(z) \otimes 1_{\mathcal{H}_\ell},
\]

where the action of \( \tilde{A}_\mu^\ell(z) \) on \( L^2(\mathbb{R}_+, r^2 dr) \) is defined by,

\[
\tilde{A}_\mu^\ell(z) \alpha(r) := \langle \tilde{A}_\mu(z) \alpha(r) Y_{\ell,m}(\theta), Y_{\ell,m}(\theta) \rangle_{L^2(S^2)},
\]

where actually the right-hand side does not depend on \( m \).

Then, taking the cutoff functions \( \varphi_0, \varphi_1, \psi_0, \psi_1 \) radial, we see on (4.4) (with \( s = 0 \)) that \( \tilde{A}_\mu^\ell(z) \) can be written as,

\[
\tilde{A}_\mu^\ell(z) = z - F_\mu^\ell(z) - S_\mu^\ell(z) \psi_0 - T_\mu^\ell(z),
\]
with $T_\mu^\ell(z) = \mathcal{O}(h^\infty)$, $\text{Re} S_\mu^\ell(z) \leq Ch$, and $F_\mu^\ell(z)$ given by,

$$F_\mu^\ell(z)u(r) := (F_\mu(z)u(r)Y_{\ell,m}(\theta), Y_{\ell,m}(\theta))_{L^2(S^2)},$$

where $F_\mu(z)$ is a rotational-invariant semiclassical pseudodifferential operator on $L^2(\mathbb{R}^3)$, with symbol $f_\mu(x, \xi; z)$ satisfying,

$$f_\mu(x, \xi) = [(I + \mu^l d\omega(x))^{-1} \xi]^2 + \lambda_\mu(x) + \mathcal{O}(h^2),$$

where $\lambda_\mu$ is a smooth function of $|x|$ such that,

$$\lambda_\mu(|x|) = \lambda_1(x + \mu \omega(x)) \quad \text{for } |x| \geq 2\delta_1;$$

$$\text{Re} \lambda_\mu(x) \geq \lambda_0 + \delta_0 \quad \text{for } |x| \leq 2\delta_1.$$

Setting $v(r) = ru(r)$, this leads to a problem on $L^2(\mathbb{R}^+, dr)$ with Dirichlet boundary condition at 0, and with principal part,

$$P_\mu = -h^2 \left( \frac{d}{(1 + \bar{\omega}(r))dr} \right)^2 + \lambda_\mu(r).$$

Then, thanks also to [15], one can adapt the arguments of [HeS2], Section 9, to the operator $F_\mu^\ell(z) + T_\mu^\ell(z)$, and, by the method described in Section 6 one can show the existence of resonances of $H$ near $\lambda_0$, with exponentially small widths.

### 7.2. Microlocal tunneling.

Here we assume $N = 2$, and that the second electronic level $\lambda_2(x)$ forms a well at some energy $\lambda_0$, while the first one $\lambda_1(x)$ is non trapping at $\lambda_0$. More precisely, we assume that $\lambda_2(x)$ is simple (so that $\lambda_1$ and $\lambda_2$ are automatically rotationally invariant), and that,

- The set $U := \{\lambda_2 \leq \lambda_0\}$ is compact;
- $\lambda_2(x)$ admits a limit $\lambda_2^\infty > \lambda_0$ as $|x| \to \infty$, $x$ in a complex sector of the form $\Gamma_\delta := \{ |\text{Im} x| < \delta | \text{Re} x| \}$ with $\delta > 0$;
- $\lambda_1(x)$ admits a limit $\lambda_1^\infty < \lambda_0$ as $|x| \to \infty$, $x \in \Gamma_\delta$;
- The set $\{\lambda_1(x) = \lambda_0\}$ is reduced to a single point.

In this case, using again the rotational symmetry and the simplicity of $\lambda_1$ and $\lambda_2$, the operator $A_\mu(z)$ can be written as,

$$\hat{A}_\mu(z) = \bigoplus_{\ell \geq 0} \hat{A}_\mu^\ell(z) \otimes 1_{\mathcal{H}_\ell},$$

where, as before, $\mathcal{H}_\ell$ is the subspace of $L^2(S^2)$ spanned by the spherical harmonics $Y_{\ell,m} (-\ell \leq m \leq \ell)$, and $\hat{A}_\mu^\ell(z)$ is a $2 \times 2$ matrix acting on $L^2(\mathbb{R}^+, r^2dr) \oplus L^2(\mathbb{R}^+, r^2dr)$, of the form,

$$\hat{A}_\mu^\ell(z) = z - F_\mu^\ell(z) - S_\mu^\ell(z)\psi_0 - T_\mu^\ell(z),$$

still with $T_\mu^\ell(z) = \mathcal{O}(h^\infty)$, $\text{Re} S_\mu^\ell(z) \leq Ch$, and $F_\mu^\ell(z)$ is given by,

$$F_\mu^\ell(z)u(r) := (F_\mu(z)u(r)Y_{\ell,m}(\theta), Y_{\ell,m}(\theta))_{L^2(S^2)},$$

where $F_\mu(z)$ is a rotational-invariant $2 \times 2$ matrix of semiclassical pseudodifferential operators, with symbol $f_\mu(x, \xi; z)$ satisfying,

$$f_\mu(x, \xi) = [(I + \mu^l d\omega(x))^{-1} \xi]^2 I_2 + \Lambda_\mu(x) + \mathcal{O}(h^2),$$

$$\Lambda_\mu(x) = \mathcal{O}(h^\infty).$$
where $\Lambda_\mu$ is a $2 \times 2$ matrix-valued smooth function such that,

$$
\Lambda_\mu(x) = \begin{pmatrix}
\lambda_1(x + \mu \omega(x)) & 0 \\
0 & \lambda_2(x + \mu \omega(x))
\end{pmatrix}
$$

for $|x| \geq 2\delta_1$;

$$
\Re \Lambda_\mu(x) \geq \lambda_0 + \delta_0 \quad \text{for } |x| \leq 2\delta_1.
$$

In this situation, one can work in the same spirit as in [Ma3] (but in a simpler way, here, since the operator is already distorted, and thus only compactly supported weights are necessary) and prove the existence of resonances near $\lambda_0$ with exponentially small widths as $h \to 0_+$. Alternatively, one can also adapt the arguments of [FMW], where particular solutions to such a system are constructed.

7.3. Molecular predissociation. In this subsection we take $N = 3$, and we assume that the second and third level cross on some disc $\{|x| = r_0\}$. More precisely, we assume that the first 3 eigenvalues can be re-indexed in such a way that they become smooth functions of $r = |x|$, and that they satisfy,

- The set $U := \{r > 0; \lambda_2(r) \leq \lambda_0\}$ is a bounded interval $[r_1, r_2]$;
- $\lambda_2(r)$ admits a limit $\lambda_2^\infty > \lambda_0$ as $r \to \infty$, $r$ in a complex sector of the form $\Gamma_\delta := \{\Im r < \delta | \Re r|\}$ with $\delta > 0$;
- $\lambda_3(r)$ admits a limit $\lambda_3^\infty < \lambda_0$ as $r \to \infty$, $r$ in $\Gamma_\delta$;
- $\lambda_1(r)$ admits a limit $\lambda_1^\infty < \lambda_3^\infty$ as $r \to \infty$, $r$ in $\Gamma_\delta$;
- The set $\{\lambda_3(r) = \lambda_0\}$ is reduced to a single point belonging to $(0, r_3)$;
- The set $\{\lambda_1(r) = \lambda_0\}$ is reduced to a single point belonging to $(0, r_1)$;
- For all $r > 0$, $\lambda_1(r) < \min\{\lambda_2(r), \lambda_3(r)\}$.

Then, following [Kl], one can prove the existence of resonances near $\lambda_0$ with exponentially small widths as $h \to 0_+$.

7.4. Crossing levels. We take again $N = 3$, and we assume that the second and third level cross on some disc $\{|x| = r_0\}$. More precisely, we assume that the first 3 eigenvalues can be re-indexed in such a way that they become smooth functions of $r = |x|$, and that they satisfy,

- The set $U := \{r > 0; \lambda_2(r) \leq \lambda_0\}$ is a bounded interval $[r_1, r_2]$ with $r_1 < r_2$ and $\lambda'_2(r_j) \neq 0$ for $j = 1, 2$;
- $\lambda_2(r)$ admits a limit $\lambda_2^\infty > \lambda_0$ as $r \to \infty$, $r$ in a complex sector of the form $\Gamma_\delta := \{\Im r < \delta | \Re r|\}$ with $\delta > 0$;
- $\lambda_3(r)$ admits a limit $\lambda_3^\infty < \lambda_0$ as $r \to \infty$, $r$ in $\Gamma_\delta$;
- $\lambda_1(r)$ admits a limit $\lambda_1^\infty < \lambda_3^\infty$ as $r \to \infty$, $r$ in $\Gamma_\delta$;
- The set $\{\lambda_3(r) = \lambda_0\}$ is reduced to the set $\{r_2\}$;
- The set $\{\lambda_1(r) = \lambda_0\}$ is reduced to a single point belonging to $(0, r_1)$;
- For all $r > 0$, $\lambda_1(r) < \min\{\lambda_2(r), \lambda_3(r)\}$.

Then, one can adapt the arguments of [FMW] (see, in particular, Remarks 2.2 and 8.8 in [FMW]) and prove the existence of resonances at a distance $O(h^{2/3})$ of $\lambda_0$, with widths of size $h^{5/3}$. 


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