

# On a General Feshbach Method<sup>1</sup>

Slimane Benaïcha <sup>2</sup>, Mustapha Djaï <sup>3</sup>, Bekkai Messirdi <sup>2</sup>

and Abdelkader Rahmani <sup>2</sup>

<sup>2</sup> Université d'Oran, Es-sénia, Oran, Algeria  
bmessirdi@yahoo.fr

<sup>3</sup> Centre Universitaire de Saida, Algeria

## Abstract

We present a general reduction Feshbach method that can be applied in particular to the spectral study of operators including the hamiltonian of the Born-Oppenheimer approximation and also to Fredholm operators.

This method reduces the study on the first case to the one of a pseudodifferential matrix, and in the second case to a matrix acting between two finite dimensional euclidian spaces. The stability theorem of the Fredholm character and the index is originally obtained as a consequence of this reduction.

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## 1. Introduction

The M. Born and R. Oppenheimer approximation's technique [3] has been of interest to many authors (see [8], [9], [13], [14]), see also [1] and [5] for physics motivations.

Broadly speaking, one studies the behaviour of a N-body system when we send the mass  $M$  of some particles (the nuclear mass for the molecule case), to  $+\infty$ . Thus we are lead to the study of a cut out Hamiltonian of the type:

$$P(h) = -h^2 \Delta_x + h^2 p(\partial_y) + Q(x) , Q(x) = -\Delta_y + V(x, y)$$

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on  $L^2(\mathbb{R}_x^n \times \mathbb{R}_y^p)$ , when  $h$  tends to 0. Here  $p(\partial_y)$  which stands for the isotropic term, is a second order operator that will not be of importance for us in the sequel and then it will be ignored.  $h$  is proportionnal to  $\frac{1}{\sqrt{M}}$ ,  $V$  is the sum of all the interactions between the particles, and  $Q(x)$  is the electronic Hamiltonian defined on  $L^2(\mathbb{R}_y^p)$ .

M. Born and R. Oppenheimer realized that the study of  $P(h)$  can be approximately reduced, modulo  $\mathcal{O}(h^3)$  when  $h$  is small enough, to the one of the family of operators  $-h^2\Delta_x + \lambda_j(x)$ ,  $j = 1, \dots, N$ , on  $\bigoplus_1^N L^2(\mathbb{R}_x^n)$  where  $\lambda_1(x) < \lambda_2(x) \leq \dots \leq \lambda_N(x)$  are the (so called electronic levels) first  $N$  discrete eigenvalues of  $Q(x)$ .

In fact, we are interested in the spectral properties of  $P(h)$  near a fixed energy level  $E_0$ . The method allow us to deal only with  $\lambda_j(x)$  verifying  $\inf_{x \in \mathbb{R}^n} \lambda_j(x) \leq E_0$ . The minimums of  $\lambda_j(x)$  can be physically interpreted as the equilibrium positions of the nuclei around which those will gravitate in a molecular system.

The spectral study of  $P(h)$  can be reduced to that of semiclassical analytic pseudodifferential matrix operator  $F(z)$  on  $\bigoplus_1^N L^2(\mathbb{R}_x^n)$ . The principal part of  $F(z)$  is equal modulo  $\mathcal{O}(h^4)$  to the diagonal matrix  $diag(-h^2\Delta_x + \lambda_j(x))_{1 \leq j \leq N}$  corresponding to the original intuition of M. Born and R. Oppenheimer. If  $\sigma$  stands for the spectrum, we have the following equivalence:

$$z \in \sigma(P(h)) \iff z \in \sigma(F(z))$$

The way in which the spectral reduction of  $P(h)$  and this equivalence are obtained relies on the construction of a matrix operator, the so-called Grushin operator, acting on a greater space by means of the eigenfunctions of  $Q(x)$  associated with the eigenvalues  $\lambda_1(x), \lambda_2(x), \dots, \lambda_N(x)$ .

This is the Feshbach method introduced by Feshbach in [6] which is also used in several situations to study the eigenvalues and resonances of  $P(h)$  in the semiclassical limit where the potential function  $V(x, y)$  is smooth (see. [4], [7], [9], [11]) and recently in [13] and [14] where  $V(x, y)$  has singular Coulombic interactions. WKB type expansions for the eigenvalues and resonances of  $P(h)$  are obtained by virtue of the Feshbach method and the pseudodifferential operators calculus (see. [2], [12]).

In the same spirit, another result of reduction has been established by B. Messirdi and G. Djellouli in [10] for Fredholm type operators. They give the Feshbach method in a slightly different way that can be applied to the Fredholm class operators. The idea was to construct a Grushin operator by means only of the nullity and the deficiency (index). The eigenvalues or the eigenfunctions are not used in this case. They show then in a simple and original manner the stability theorem for Fredholm operators also a result of spectral reduction of these operators.

Here we plan to present this reduction scheme that can be applied in the first case to a general class of operators of the type  $P(x, y, hD_x, D_y)$  which in particular contain the Hamiltonians of the Born-Oppenheimer approximation and in the second case to Fredholm operators.

We describe in this framework some results of Messirdi [9], Messirdi-Senoussaoui [13] and Messirdi-Senoussaoui-Djellouli [14] concerning the study of the discrete spectrum and the resonances of molecular systems and the results of Messirdi-Djellouli [10] about the stability of the Fredholm character and the index under a small perturbation by virtue of the Feshbach reduction method.

## 2. Feshbach method for a general Hamiltonians

We study the discrete spectrum of a general class of Born-Oppenheimer hamiltonians of the type;

$$P(h) = -h^2\Delta_x + P(x, y, D_y) \quad \text{on } L^2(\mathbb{R}^n \times \mathbb{R}^p), \quad n, p \in \mathbb{N}^*$$

when  $h$  tends to  $0^+$ , and  $P(x, y, D_y) = Q(x)$  is a pseudodifferential operator on  $L^2(\mathbb{R}_y^p)$  satisfying the following assumptions:

**(H1)** For all  $x \in \mathbb{R}^n$ ,  $Q(x)$  is selfadjoint on  $L^2(\mathbb{R}_y^p)$  with  $x$ -independent domain  $D$  and  $Q(x) \in C_b^\infty(\mathbb{R}^n, \mathcal{L}(D, L^2(\mathbb{R}_y^p)))$ . ( $C_b^\infty$  stands for the space of functions that are uniformly bounded together with all their derivatives and  $\mathcal{L}(H_1, H_2)$  denotes the space of bounded linear operators from a Hilbert space  $H_1$  to another Hilbert space  $H_2$ ).

**(H2)** For any  $x \in \mathbb{R}^n$ , the spectrum  $\sigma(Q(x))$  of  $Q(x)$  has two disjoint components :

$$\sigma(Q(x)) = \{\lambda_1(x), \lambda_2(x), \dots, \lambda_N(x)\} \cup \sigma_0(x)$$

where  $\lambda_1(x) < \lambda_2(x) \leq \dots \leq \lambda_N(x)$  depends continuously on  $x$  and are separated by a gap from  $\sigma_0(x)$  :

$$\inf_{x \in \mathbb{R}^n} \sigma_0(x) > \sup_{x \in \mathbb{R}^n} \{\lambda_1(x), \lambda_2(x), \dots, \lambda_N(x)\} + \delta \quad , \quad \delta > 0$$

In order to avoid regularity problems at infinity of the values  $(\lambda_j(x))_{1 \leq j \leq N}$ , we shall in addition assume that

$$\inf_{j \neq k, |x| \geq C} |\lambda_j(x) - \lambda_k(x)| \geq \frac{1}{C} \quad , \quad C > 0$$

**Examples:**

1)  $Q(x) = -\Delta_y + (1 + x^2)^{2l} \sum_{j=1}^p \mu_j y_j^2$ ,  $y = (y_1, \dots, y_p)$ ,  $x^2 = \sum_{i=1}^n x_i^2$  if  $x = (x_1, \dots, x_n)$  and  $\mu_j > 0$  for all  $j \in \{1, \dots, p\}$ .  $Q(x)$  satisfies the assumptions (H1) and (H2) with  $D = H^2(\mathbb{R}_y^p) \cap \{\varphi \in L^2(\mathbb{R}_y^p) ; y_j^2 \varphi \in L^2(\mathbb{R}_y^p), j = 1, \dots, p\}$ ,  $\lambda_\alpha(x) = \sum_{j=1}^p \sqrt{\mu_j} (2\alpha_j + 1)(1 + x^2)^l$ ,  $\alpha = (\alpha_1, \dots, \alpha_p) \in \mathbb{N}^p$  and  $\sigma_0(x) = \{\lambda_\alpha(x) ; \alpha \in \mathbb{N}^p \setminus I_N\}$  where  $I_N \subset \mathbb{N}^p$ ,  $\text{cardinal}(I_N) = N$ .

2)  $Q(x) = -\Delta_y + V(x, y)$  when the interaction  $V(x, y)$  is real and regular in the sense that  $V \in C_b^\infty(\mathbb{R}^n, \mathcal{L}(H^2(\mathbb{R}_y^p), L^2(\mathbb{R}_y^p)))$  and satisfying the conditions (H2). ◀

Furthermore, under the assumptions (H1) and (H2), one can use the constructions made in [Me] and obtain an orthonormalized family  $\{v_1(x), \dots, v_N(x)\}$  in  $L^2(\mathbb{R}_y^p)$  such that:

- $\forall j \in \{1, \dots, N\}$ ,  $v_j(x) \in C_b^\infty(\mathbb{R}_x^n, D)$
- $\{v_1(x), \dots, v_N(x)\}$  is a basis of  $\bigoplus_1^N \ker(Q(x) - \lambda_j(x))$ ,  $\forall x \in \mathbb{R}^n$

If  $\pi(x) = \sum_{j=1}^N \langle \cdot, v_j(x) \rangle_{L^2(\mathbb{R}_y^p)} v_j(x)$  and  $\widehat{\pi}(x) = 1 - \pi(x)$  then (H2) ensures in particular that

$$\widehat{\pi}(x)Q(x)\widehat{\pi}(x) - z > 0 \quad , \quad \forall z \in \mathbb{C} \text{ such that } \text{Re } z < \inf_{x \in \mathbb{R}^n} \sigma_0(x) \quad (2.1)$$

Define the following operators:

$$R^- : \bigoplus_1^N L^2(\mathbb{R}_x^n) \longrightarrow L^2(\mathbb{R}_x^n \times \mathbb{R}_y^p) \quad (2.2)$$

$$u^- = (u_1^-, \dots, u_N^-) \longmapsto R^- u^- = \sum_{j=1}^N u_j^- v_j(x)$$

and

$$R^+ = (R^-)^* : L^2(\mathbb{R}_x^n \times \mathbb{R}_y^p) \longrightarrow \bigoplus_1^N L^2(\mathbb{R}_x^n)$$

$$u \longmapsto R^+ u = \bigoplus_{j=1}^N \langle u, v_j(x) \rangle_{L^2(\mathbb{R}_y^p)} \quad (2.3)$$

We then consider a Grushin problem that will lead to the Feshbach reduction. For  $z \in \mathbb{C}$  define

$$\mathcal{P}(z) = \begin{pmatrix} (P(h) - z) & R^- \\ R^+ & 0 \end{pmatrix} \quad (2.4)$$

from  $H^2(\mathbb{R}_x^n, D) \oplus (\oplus_1^N L^2(\mathbb{R}_x^n))$  into  $L^2(\mathbb{R}_x^n \times \mathbb{R}_y^p) \oplus (\oplus_1^N H^2(\mathbb{R}_x^n))$ .

The matrix  $\mathcal{P}(z)$  can be considered as a  $h$ -pseudodifferential operator in  $x$  associated with the operator-valued symbol

$$p(x \ \xi; z) = \begin{pmatrix} (\xi^2 + Q(x) - z) & R^- \\ R^+ & 0 \end{pmatrix} \tag{2.5}$$

with  $p(x \ \xi; z) \in C^\infty(T^*\mathbb{R}_x^n, \mathcal{L}(D \oplus (\oplus_1^N L^2(\mathbb{R}_x^n), L^2(\mathbb{R}_x^n \times \mathbb{R}_y^p) \oplus (\oplus_1^N L^2(\mathbb{R}_x^n)))$ .

Thanks to (2.1) the symbol  $p(x \ \xi; z)$  is invertible for any  $(x, \xi) \in T^*\mathbb{R}_x^n$  and its inverse is given by

$$q(x \ \xi; z) = \begin{pmatrix} \widehat{\pi}(x)(\xi^2 + \widehat{\pi}(x)Q(x)\widehat{\pi}(x) - z)^{-1}\widehat{\pi}(x) & R^- \\ R^+ & (z - \xi^2 - \lambda_j(x))_{1 \leq j \leq N} \end{pmatrix} \tag{2.6}$$

By virtue of (H1) one can consider the weyl quantification  $\mathcal{Q}(z)$  of  $q(x, \xi; z)$  defined on  $L^2(\mathbb{R}_x^n, D)$  by the oscillatory integral

$$\mathcal{Q}(z) = Op_h^w(q(x \ \xi; z))u(x) = (2\pi h)^{-n/2} \int e^{i(x-y)\xi/h} q\left(\frac{x+y}{2} \ \xi; z\right)u(y)dyd\xi$$

and use the composition formula of  $h$ -pseudodifferential operators. It then follows that

$$\begin{cases} \mathcal{P}(z)\mathcal{Q}(z) = 1 + \mathcal{O}(h) \\ \mathcal{Q}(z)\mathcal{P}(z) = 1 + \mathcal{O}(h) \end{cases}$$

uniformly with respect to  $h$ .

Consequently, if  $h$  is small enough  $\mathcal{P}(z)$  is invertible and its inverse is given by the Neumann series.

Writing

$$\mathcal{P}^{-1}(z) = \begin{pmatrix} a(z) & a^+(z) \\ a^-(z) & a^{-+}(z) \end{pmatrix}$$

We see that  $a(z)$ ,  $a^\pm(z)$  and  $a^{-+}(z)$  are  $h$ -pseudodifferential operators analytic on  $z$ . The principal symbol of  $a^{-+}(z)$  is  $(z - \xi^2 - \lambda_j(x))_{1 \leq j \leq N}$ .

The principal interest in having considered the operator  $\mathcal{P}(z)$  is that it reduces the spectral study of  $P(h)$  of that of a matrix operator much simpler and only acting on the variable  $x$  as it is shown in the following proposition.

**Proposition 2.1:** We have the following equivalence:

$$z \in \sigma(P(h)) \iff z \in \sigma(F(z))$$

where  $F(z) = z - a^{-+}(z)$ , called the Feshbach operator, is a  $N \times N$  matrix of bounded  $h$ -pseudodifferential operators on  $\bigoplus_1^N L^2(\mathbb{R}_x^n)$  with principal symbol  $\text{diag}(\xi^2 + \lambda_j(x))_{1 \leq j \leq N}$ .

**Proof:** We have

$$(P(h) - z)u = v \iff \mathcal{P}(z)(u \bigoplus 0) = (v \bigoplus R^+u) \tag{2.7}$$

$$\iff (u \bigoplus 0) = \mathcal{P}^{-1}(z)(v \bigoplus R^+u)$$

$$\iff \begin{cases} a(z)v + a^+(z)R^+u = u \\ a^-(z)v + a^{-+}(z)R^+u = 0 \end{cases}$$

and

$$a^{-+}(z)\alpha = \beta \iff \mathcal{P}^{-1}(z)(0 \bigoplus \alpha) = (a^+(z)\alpha \bigoplus \beta) \tag{2.8}$$

$$\iff (0 \bigoplus \alpha) = \mathcal{P}(z)(a^+(z)\alpha \bigoplus \beta)$$

$$\iff \begin{cases} (P(h) - z)a^+(z)\alpha + R^-\beta = 0 \\ R^+a^+(z)\alpha = \alpha \end{cases}$$

If  $z \notin \sigma(P)$ , we obtain from (2.8)

$$a^+(z)\alpha = -(P(h) - z)^{-1}R^-\beta \quad \text{and} \quad \alpha = -R^+(P(h) - z)^{-1}R^-\beta$$

thus  $z \notin \sigma(F(z))$  and

$$(z - F(z))^{-1} = R^+(z - P(h))^{-1}R^- \tag{2.9}$$

Conversly, if  $z \notin \sigma(F(z))$  then (2.7) gives

$$R^+u = -(z - F(z))^{-1}a^-(z)v \quad \text{and} \quad u = [a(z) - a^+(z)(z - F(z))^{-1}a^-(z)]v$$

Therefore,  $z \notin \sigma(P(h))$  and

$$(z - P(h))^{-1} = a^+(z)(z - F(z))^{-1}a^-(z) - a(z) \tag{2.10}$$



these formulae show that since  $a(z)$ ,  $a^\pm(z)$  and  $a^{-+}(z)$  depend analytically on  $z$ , then a singularity of  $(z - P(h))^{-1}$  is necessarily a singularity of  $(z - F(z))^{-1}$  and conversely.

### 3. Eigenvalues of polyatomic molecules

A potential  $\frac{1}{|x \pm y|}$  is not within the framework in a natural way in the pseudodifferential calculus since the derivatives of order  $k$  of such potential will have a singularity stronger than  $k$  (of order  $\frac{1}{|x \pm y|^{k+1}}$ ). We will show that, modulo a change of variables, the use of such a computation and the Feshbach reduction in the Coulombian case are still possible.

Now if  $P(h) = -h^2 \Delta_x + Q(x)$  on  $L^2(\mathbb{R}^{3n} \times \mathbb{R}^{3p})$  where the real potential function  $V(x, y)$  may have Coulomb-type singularities  $\pm \frac{1}{|y_l - x_j|}$ ,  $+\frac{1}{|x_j - x_k|}$ ,  $x_j, y_l \in \mathbb{R}^3$ ,  $x = (x_1, \dots, x_n) \in \mathbb{R}^{3n}$ ,  $y = (y_1, \dots, y_p) \in \mathbb{R}^{3p}$ , the eigenvalues and eigenfunctions of  $Q(x) = -\Delta_y + V(x, y)$  are only  $C^2$  with respect to the  $x$ -variables.

Nevertheless, by introducing some  $x$ -dependent changes in the  $y$ -variables that will regularize  $Q(x)$  and permit an adaptable semiclassical pseudodifferential calculus (see [13], [14]).

Indeed, if  $x_0, x \in \mathbb{R}^{3n} \setminus \mathcal{C}$  where  $\mathcal{C}$  denotes the collision set :

$$\mathcal{C} = \{x = (x_1, \dots, x_n) \in \mathbb{R}^{3n} \ ; \ \exists j \neq k, x_j = x_k\}$$

and  $x$  is close enough to  $x_0$ , we consider the change  $y \longrightarrow y'$  defined by:

$$y = F_0(x, y') = (F_{x_0}(x, y'_1), \dots, F_{x_0}(x, y'_p))$$

where

$$y_l = F_{x_0}(x, y'_l) = y'_l + \sum_{j=1}^n (x_j - x_j^0) f_j(y'_l) \ , \ l \in \{1, \dots, p\} \tag{3.1}$$

$x_0 = (x_1^0, \dots, x_n^0)$  and  $f_j \in C_0^\infty(\mathbb{R}^3, \mathbb{R})$  such that  $f_j(x_0^k) = \delta_{jk}$  (kroenecker symbol). In particular, we have  $F_{x_0}(x, x_j^0) = x_j$ ,  $j \in \{1, \dots, n\}$ .

We associate with (3.1) the unitary operator on  $L^2(\mathbb{R}^3)$  defined by

$$\mathcal{U}_{x_0} \varphi(x, y'_l) = \varphi(x, F_{x_0}(x, y'_l)) \left| \det(\partial_{y'_l} F_{x_0}(x, y'_l)) \right|^{1/2} \ , \ l \in \{1, \dots, p\} \tag{3.2}$$

It is then easy to observe that for any  $j \in \{1, \dots, n\}$  and  $l \in \{1, \dots, p\}$

$$\mathcal{U}_{x_0} \frac{1}{|y_l \pm x_j|} \in C^\infty(\Omega_{x_0}, \mathcal{L}(H^2(\mathbb{R}^3), L^2(\mathbb{R}^3))) \tag{3.3}$$

where  $\Omega_{x_0}$  is a small neighborhood of  $x_0$ . It also follows that

$$V(x, F_0(x, y'))(-\Delta_y + 1)^{-1} \in C^\infty(\Omega_{x_0}, \mathcal{L}(L^2(\mathbb{R}_y^{3p}))) \tag{3.4}$$

We only consider the first electronic level  $\lambda_1(x)$  ( $N = 1$ ) which is assumed to be separated by a gap from the rest of the spectrum of  $Q(x)$  and that  $\lambda_1^{-1}(]-\infty, E_0])$  is compact where  $E_0$  is a fixed energy such that  $E_0 < \inf\{\sigma(Q(x)) \setminus \{\lambda_1(x)\}\}$ .

By compacity, we cover  $\lambda_1^{-1}(]-\infty, E_0])$  by a finite number of neighborhoods  $(\Omega_l)_{1 \leq l \leq M}$  associated with unitary transformations  $\mathcal{U}_l$  of the type (3.2) satisfying (3.3) and (3.4).

Setting  $W = \mathbb{R}_x^{3n} \setminus \bigcup_{l=1}^M \Omega_l$ , one can modify  $P(h)$  near  $W$  such that the modified operator  $\widehat{P}(h)$  becomes smooth with respect to  $x$  in  $W$  and  $\sigma(\widehat{P}(h)) = \sigma(P(h)) + \mathcal{O}(e^{-\varepsilon/h})$ ,  $\varepsilon > 0$  (see [13], [14]).

Setting also  $\Omega_0 = \mathbb{R}_x^{3n} \setminus \lambda_1^{-1}(]-\infty, E_0])$  and considering the localized matrix operator  $\widehat{\mathcal{P}}(z)$  associated with  $\widehat{P}(h)$  as in (2.4)

$$\widehat{\mathcal{P}}(z) = \sum_{l=0}^M \chi_l(x) \mathcal{U}_l \chi_l(x) \widetilde{P}_l(z) \chi_l(x) \mathcal{U}_l^{-1} \chi_l(x) \tag{3.5}$$

where  $(\chi_l^4)_{0 \leq l \leq M}$  is an adapted partition of unity of  $(\Omega_l)_{0 \leq l \leq M}$  and  $\widetilde{P}_l(z)$ 's are smooth pseudodifferential operators with operator-valued symbol while  $\mathcal{U}_0$  is the identity.

By the techniques developed in the second section we get that  $\widehat{\mathcal{P}}(z)$  is a smooth invertible  $h$ -pseudodifferential operator. Writing

$$\widehat{\mathcal{P}}^{-1}(z) = \begin{pmatrix} \widehat{a}(z) & \widehat{a}^+(z) \\ \widehat{a}^-(z) & \widehat{a}^{-+}(z) \end{pmatrix}$$

and using the fact that the transformations  $\mathcal{U}_l$  only act on the  $y$ -variables, we obtain

**Theorem 3.1:**  $\widehat{F}(z) = z - \widehat{a}^{-+}(z)$  is a smooth  $h$ -pseudodifferential operator, with principal symbol  $\xi^2 + \lambda_1(x)$ . Moreover,

$$z \in \sigma(\widehat{P}(h)) \iff z \in \sigma(\widehat{F}(z))$$

For more detail about these results, the interested reader may consult [8], [13] and [14].

## 4. Resonances of polyatomic molecules

In this Section we describe the results of [14] concerning the resonances of the hamiltonian  $P(h) = -h^2 \Delta_x - \Delta_y + V(x, y)$  on  $L^2(\mathbb{R}_x^{3n} \times \mathbb{R}_y^{3p})$  where

$$V(x, y) = \sum_{j,k=1}^n \frac{\alpha_{jk}}{|x_j - x_k|} + \sum_{\substack{1 \leq l \leq p \\ 1 \leq k \leq n}} \frac{\alpha_{lk}^\pm}{|y_l \pm x_k|} + \sum_{\substack{l,q=1 \\ l \neq q}}^p \frac{\beta_{lq}}{|y_l - y_q|} \tag{4.1}$$

$x = (x_1, \dots, x_n) \in \mathbb{R}_x^{3n}$ ,  $y = (y_1, \dots, y_p) \in \mathbb{R}_y^{3p}$ ,  $\alpha_{jk}, \alpha_{lk}^\pm$  and  $\beta_{lq}$  are real constants and  $\alpha_{jk} > 0, \forall j, k \in \{1, \dots, n\}$ .  $W(x) = \sum_{j,k=1}^n \frac{\alpha_{jk}}{|x_j - x_k|}$  denotes the interactions between the nuclei of the molecule and  $(V(x, y) - W(x))$  the nuclei-electrons and electrons-electrons interactions,  $\alpha_{lk}^\pm$  indicates the charges of the molecule in particular if  $\alpha_{lk}^+ = \alpha_{lk}^-$  the molecule is symmetric.

$P(h)$  with domain  $H^2(\mathbb{R}_x^{3n} \times \mathbb{R}_y^{3p})$  is self adjoint in  $L^2(\mathbb{R}_x^{3n} \times \mathbb{R}_y^{3p})$  and one can define the resonances of  $P(h)$  as the discrete eigenvalues of the distorted Hamiltonian  $P_\mu(h)$  ( $\mu \in \mathbb{C}$  small enough,  $\text{Im } \mu > 0$ ) obtained by the analytic distorsion (see [14]):

$$x_j \longrightarrow x_j + \mu\omega(x_j) \quad , \quad 1 \leq j \leq n \tag{4.2}$$

$$y_l \longrightarrow y_l + \mu\omega(y_l) \quad , \quad 1 \leq l \leq p$$

where  $\omega$  is a smooth vector field of  $\mathbb{R}^3$ ,  $\omega = 0$  near the collision set  $\mathcal{C}$  of all nuclei of the molecule and  $\omega$  is the identity far from  $\mathcal{C}$ .  $P_\mu(h)$  is defined by  $U_\mu P(h) U_\mu^{-1}$  such that

$$U_\mu \varphi(x, y) = \varphi((x_1 + \mu\omega(x_1), \dots, x_n + \mu\omega(x_n) , y_1 + \mu\omega(y_1), \dots, y_p + \mu\omega(y_p)) |J|^{1/2} \tag{4.3}$$

where  $J = J(x, y, \mu) = \prod_{j=1}^n \det(1 + \mu D\omega(x_j)) \prod_{l=1}^p \det(1 + \mu D\omega(y_l))$  is the Jacobian of the transformation (4.2).

Under this distorsion the domains and the singularities of  $V(x, y)$  are not changed and  $P(h)$  can be analytically extended to small complex values of  $\mu$ .

However, the technique of the thirt Section is not sufficient in this case since the classically allowed region with respect to  $x$ ,  $\lambda_1^{-1}(] - \infty, E_0])$  is now unbounded if the scattering energy level  $E_0 \in \sigma_{ess}(P(h)) \setminus \{\text{thresholds of } P(h)\}$ .

We assume (H2) to  $\sigma(Q(x)) \cap ] - \infty, E_0]$  for all  $x$  outside  $\mathcal{C}$  and also the existence of a constant  $C > 0$  such that

$$\sup_{x \in \mathbb{R}_x^{3n} \setminus \mathcal{C}} \tilde{\lambda}_N(x) \leq C$$

where  $\tilde{\lambda}_N(x) = \lambda_N(x) - W(x)$  (this last assumption is automatically satisfied if e.g.  $\alpha_{lk}^\pm \leq 0$ ).

Thus, one must first make a change of variables whose purpose is to localize in a compact region the  $x$ -dependent singularities with respect to  $y$ . After that the previous idea can be adapted to  $P_\mu(h)$  and the study of  $P_\mu(h)$  can be reduced to the one of a matrix of  $h$ -pseudodifferential operators on  $L^2(\mathbb{R}_x^{3n})$ .

More precisely, we costruct a change of type

$$y = (y_1, \dots, y_p) \longrightarrow y' = (\tau_x(y_1), \dots, \tau_x(y_p))$$

for  $x \in \mathbb{R}_x^{3n} \setminus \mathcal{C}$  such that

$$\tau_x(y_l) = \frac{y_l}{|x|} \quad \text{if } |y_l| \leq |x|$$

$$\tau_x(y_l) = Ay_l \quad \text{if } |y_l| \geq 2A|x| \tag{4.4}$$

$l \in \{1, \dots, p\}$ , and  $A > 0$  is fixed large enough.

The singularities become localized in the ball  $|y'| \leq 1$  and  $\widehat{P}_\mu(h)$  the regularization of  $P_\mu(h)$  in the elliptic region is now smooth. One can then use the techniques of Section 3 and by the Feshbach method we get:

**Theorem 4.1:** *For any complex number  $z$  close enough to  $E_0$  there exists a family of  $N \times N$  matrices  $\widehat{F}_\mu(z)$  of  $h$ -pseudodifferential operators on  $\mathbb{R}_x^{3n}$  depending analitically on  $\mu$  (complex small enough),  $\text{Im } \mu > 0$ , such that*

$$z \in \sigma(\widehat{P}_\mu(h)) \iff z \in \sigma(\widehat{F}_\mu(z))$$

## 5. Feshbach reduction of Fredholm operators

We present here the Feshbach method that can be applied to the class of Fredholm operators (see [10]). Our trick is to reduce the problem to the inversion of a Grushin problem using no spectral tools.

Let  $(P_z)_{z \in \omega}$  be a continuous family on an open complex set  $\omega$  of linear operators between two complex Hilbert spaces  $H_1$  and  $H_2$ .

We assume that for a certain point  $z_0$  of  $\omega$ ,  $P_{z_0}$  is a Fredholm operator with index  $(n_0 - d_0)$ ,  $n_0$  is the nullity and  $d_0$  the deficiency of  $P_{z_0}$ .

By analogy with the Grushin operator introduced precedently we set

$$\mathcal{P}(z) = \begin{pmatrix} P_z & R_0^- \\ R_0^+ & 0 \end{pmatrix}$$

which is acting on  $H_1 \oplus \mathbb{C}^{d_0}$  into  $H_2 \oplus \mathbb{C}^{n_0}$  where  $R_0^+$  and  $R_0^-$  are bounded linear operators respectively from  $H_1$  to  $\mathbb{C}^{n_0}$  and from  $\mathbb{C}^{d_0}$  to  $H_2$ , with maximum ranks such that

$$\begin{cases} \text{Ran } P_{z_0} \oplus \text{Ran } R_0^- = H_2 \\ R_0^+ |_{\ker P} \text{ is invertible} \end{cases}$$

Accordingly,  $\mathcal{P}(z)$  becomes invertible for  $z$  in an enough small complex neighborhood  $\Omega$  of  $z_0$  contained in  $\omega$ . Its inverse is given by

$$\mathcal{P}^{-1}(z) = \begin{pmatrix} a(z) & a^+(z) \\ a^-(z) & a^{-+}(z) \end{pmatrix}$$

where  $a(z)$ ,  $a^\pm(z)$  and  $a^{-+}(z)$  are bounded and depends continuously on  $z$  in  $\Omega$ ,  $a(z) \in \mathcal{L}(H_1, H_2)$ ,  $a^+(z) \in \mathcal{L}(\mathbb{C}^{n_0}, H_1)$ ,  $a^-(z) \in \mathcal{L}(H_2, \mathbb{C}^{d_0})$  and  $a^{-+}(z) \in \mathcal{L}(\mathbb{C}^{n_0}, \mathbb{C}^{d_0})$ .

Furthermore,  $a^{-+}(z_0) = 0$  and  $a^\pm(z)$  remains with maximal ranks in  $\Omega$ .

Now, for a given  $g$  in  $H_2$ , we have in view of (2.7)

$$P_z f = g \iff \begin{cases} a(z)g + a^+(z)R_0^+ f = f \\ a^-(z)g + a^{-+}(z)R_0^+ f = 0 \end{cases} \tag{5.1}$$

and thus the equation  $P_z f = g$  admits a solution  $f$  in  $H_1$  if and only if  $a^-(z)g \in \text{Ran}(a^{-+}(z))$ . This ensures that the map  $\rho(\dot{g}) = \widehat{a^-(z)g}$  is an isomorphism from the quotient space  $H_2/\text{Ran}P_z$  into  $\mathbb{C}^{d_0}/\text{Ran}(a^{-+}(z))$  where  $\bullet$  and  $\wedge$  are respectively the equivalence classes in  $H_2/\text{Ran}P_z$  and  $\mathbb{C}^{d_0}/\text{Ran}(a^{-+}(z))$ .

Consequently,

$$\dim(H_2/\text{Ran}P_z) = \dim(\mathbb{C}^{d_0}/\text{Ran}(a^{-+}(z))) < +\infty, \quad \forall z \in \Omega \tag{5.2}$$

Conversly, if  $\alpha \in \mathbb{C}^{n_0}$  and  $\beta \in \mathbb{C}^{d_0}$ , then using (2.8) we have

$$a^{-+}(z)\alpha = \beta \iff \begin{cases} P_z a^+(z)\alpha + R_0^-\beta = 0 \\ R_0^+ a^+(z)\alpha = \alpha \end{cases} \tag{5.3}$$

We deduce that  $\dim(\text{Ran}a^+(z)) = n_0$  and  $a^+(z)$  is an isomorphism from  $\ker a^{-+}(z)$  into  $\ker P_z$ .

Finally,

$$\dim(\ker P_z) = \dim(\ker a^{-+}(z)) < +\infty, \quad \forall z \in \Omega \tag{5.4}$$

We then have established the following stability result:

**Theorem 5.1:** *For any  $z$  in  $\Omega$ ,  $P_z$  is a Fredholm operator with index independent of  $z$ .*

$$\text{index}(P_z) = \text{index}(a^{-+}(z)) = n_0 - d_0, \quad \forall z \in \Omega \tag{5.5}$$

**Remark 5.2:** *Now If  $\Omega$  is an open complex connected neighborhood of 0 verifying the foregoing conditions,  $H_1 \subset H_2$  with a dense inclusion and  $P_z = P - z$  where  $P$  is a Fredholm operator such that  $n_0 = \dim(\ker P) < +\infty$  and  $d_0 = \dim(H_2/\text{Ran}P) < +\infty$ . We also suppose that  $P_z$  is invertible for at least a point of  $\Omega$  different from 0. Then  $a^{-+}(z)$  is also invertible at the same point by virtue of (5.2) and (5.5) and  $n_0 = d_0$ . We get a reduction result as follows*

$$z \in \sigma(P) \iff \det(a^{-+}(z)) = 0$$

The identities (2.9) and (2.10) are also obtained here.

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