

A Priori Estimation of the Resolvent on Approximation of Born-Oppenheimer

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Abstract: In this study, we estimate the resolvent of the two bodies Shrodinger operator perturbed by a potential of Coulombian type on Hilbert space when h tends to zero. Using the Feshbach method, we first distorted it and then reduced it to a diagonal matrix. We considered a case where two energy levels cross in the classical forbidden region. Under the assumption that the second energy level admits a non degenerate point well and virial conditions on the others levels, a good estimate of the resolvent were observed.

Key words: Distorsion, eigenvalues, estimation, resolvent, resonances

INTRODUCTION

The Born-Oppenheimer approximation technical^[1] has instigated many works one can find in bibliography the recent papers like^[2-5].

It consists to study the behaviour of a many body systems, in the limit of small parameter h as the particles masses (masses of nuclei) tends to infinity; (see the references therein for more information), we can describe it with a Hamiltonian of type $P = -h^2\Delta_x - \Delta_y + V(x, y)$ on $L^2(\mathbb{R}_x^3 \times \mathbb{R}_y^{3p})$, when $h \rightarrow 0$ and V denote the interaction potentials between the nuclei of the molecule and the nuclei electrons.

The idea is to replace the operator

$Q(x) = -\Delta_y + V(x, y)$ (in $L^2(\mathbb{R}_y^{3p})$ \mathcal{X} fixed) by the so-called electronic levels which be a family of its discrete eigenvalues: $\lambda_1(x), \lambda_2(x), \lambda_3(x), \dots$ and to study the operators P which can be approximatively given by $-h^2\Delta_x + \lambda_j(x)$, on $L^2(\mathbb{R}_x^3)$.

Martinez and Messirdi's works, are about spectral proprieties of P near the energy level E_0 such that $\inf_{\mathbb{R}^n} \lambda_j \leq E_0$. Martinez in^[6], studies the case where $\lambda_1(x)$ admits a nondegenerate strict minimum at some energy level λ_0 , the eigenvalues of P near λ_0 admits a complete asymptotic expansion in half-powers of h ^[2].

Messerdi and Martinez^[7] considers the case where λ_2 admits a minimum, such appears resonances for P . He gives an estimation of the resolvent of $O(h^{-1})$ at the neighbourhood of 0.

In this study we try to generalize this work to approximate the resolvent of P where V is a potential of Coulombian type at the neighbourhood of a point $x_0 \neq 0$.

In fact, we estimate the resolvent of the operator F_μ^ζ , given by a reduction of the distorted operator P_μ^ζ , of P modified by a truncature ζ ^[8], and we try to have a good evaluation of the order of $O(h^{-1/2})$.

We apply the Feshbach method to study the distorted operator P_μ^ζ which allows us to goback to the initial problem and we put the virial conditions on λ_1 and λ_3 .

Hypothesis and results

Hypothesis: Let the operator

$$P = -h^2\Delta_x - \Delta_y + V(x, y) \tag{1}$$

on $L^2(\mathbb{R}_x^3 \times \mathbb{R}_y^{3p})$, when h tends to 0. $V(x, y) = V(x, y_1, y_2, y_3, \dots, y_p)$ is an interaction potential of Coulombian type

$$V(x, y) = \frac{\alpha}{|x|} + \sum_{j=1}^p \left[\frac{\alpha_j^+}{|y_j + x|} + \frac{\alpha_j^-}{|y_j - x|} \right] + \sum_{\substack{j,k=1 \\ j \neq k}}^p \frac{\alpha_{jk}}{|y_j - y_k|} \tag{2}$$

where $\alpha, \alpha_j^\pm, \alpha_{jk}$ are real constants, $\alpha > 0$ (α_j^\pm is the charges of the nuclei).

It is well known that P with domain $H^2(\mathbb{R}_x^3 \times \mathbb{R}_y^{3p})$ is essentially self-adjoint on $L^2(\mathbb{R}_x^3 \times \mathbb{R}_y^{3p})$.

For $x \neq 0$, $Q(x) = -\Delta_y + V(x, y)$ with domain $H^2(\mathbb{R}_y^{3p})$ is essentially self-adjoint on $L^2(\mathbb{R}_y^{3p})$

Remark 1.1: The domain of $Q(x)$ is independent of x . To describe our main results we introduce the following assumptions:

(H1) $\forall x \in \mathbb{R}^{3n} \setminus \{0\}$, $\# \sigma_{\text{disc}}(Q(x)) \geq 3$

Let λ_0 an energy level such that: $\lambda_j \cap [-\infty, \lambda_0] \leq 3$, denoting $\lambda_1(x), \lambda_2(x), \lambda_3(x)$ the first three eigenvalues of $Q(x)$.

(H2) we assume that the first three eigenvalues λ_j , $\forall j \in \{1, 2, 3\}$ are simple at infinity:

$$|x| \geq C \Rightarrow \inf_{j,k \in \{1,2,3\}} |\lambda_j(x) - \lambda_k(x)| \geq \frac{1}{C} \tag{3}$$

and

$$\lim_{j,k \in \{1,2,3\}} \text{dist}(\lambda_j(x) - \lambda_k(x)) \setminus \{\lambda_1(x), \lambda_2(x), \lambda_3(x)\} > 0$$

this means

$\exists \delta_1 > 0, \forall x \neq 0$, and $\lambda \in \sigma(Q(x)) \setminus \{\lambda_1(x), \lambda_2(x), \lambda_3(x)\}$, we have

$$\inf_{1 \leq j \leq 3} |\lambda - \lambda_j(x)| \geq \delta_1 \tag{4}$$

Remark 1.2: By Reed-Simon' results^[9], the first eigenvalue is automatically simple.

(H3) we suppose that $\exists c > 0$ such that

$$\forall x \in \mathbb{R}^3 \setminus \{0\}, \lambda_j \leq c + \frac{\alpha}{x}, \quad j \in \{1, 2, 3\} \tag{5}$$

Remark 1.3: This hypothesis is still true for $\alpha_{\pm} < 0$; λ_1 also verifies (H3) and we can see with a simple computation that there exists c_1 such that for all $x \neq 0$

$$\lambda_1(x) \geq -c_1 + \frac{\alpha}{|x|} \tag{6}$$

(H4) We are in the situation where $\lambda_2(x)$ admits a nondegenerate strict minimum; creating a potential well

of the shape $\Gamma : \begin{cases} v_0 = \inf_{x \in \mathbb{R} \setminus \{0\}} \lambda_2(x), \quad v_0 < \lambda_0(x) \\ \lambda_2^{-1}(v_0) = r_0, \quad \lambda_2(x) > 0, \quad \lambda_2''(r_0) > 0 \end{cases}$

$\exists \delta_2 > 0$ such that

$$\forall x \in \mathbb{R}^3 \setminus \{0\}, \lambda_1(x) + \delta_2 < \min \{\lambda_2(x), \lambda_3(x)\}$$

we note by

$$K = \{x \in \mathbb{R}, \lambda_2(x) = \lambda_3(x)\}$$

and for $\delta > 0$, we also note by:

$$K_\delta = \{x \in \mathbb{R}, \text{dist}(x, K) \leq \delta\}$$

Let $\delta_0 > \delta_1 > 0$ such that

* $K_{\delta_0} \setminus K_{\delta_1}$ is simply connex

* $K_{2\delta_0} \cap U = \emptyset$

* The connex composites of $\mathbb{R}^3 \setminus K_{\delta_1}$ are simply connex

(H5) Virial Conditions

It exists $d > 0$ such that for $j \in \{2, 3\}$,

The resonances of P are obtained by an analytic distorsion introduced by Hunziker^[8] and so they are defined as complex numbers ρ_j ($j = 1, \dots, N_0$) such that for all $\varepsilon > 0$ and μ sufficiently small, $\text{Im} \mu > 0$

$\rho_j \in \sigma_{\text{disc}}(P_\mu)$ ^[3]. We denote de set of the resonances of P by: $\sigma(P) = \bigcup_{\text{Im} \mu > 0, |\mu| < \varepsilon} \sigma_{\text{disc}}(P_\mu)$

Where P_μ is obtained by the analytic distorsion satisfying: $P_\mu = U_\mu P_\mu U_\mu^{-1}$. So, P_μ can be extended to small enough complex values of μ as an analytic family of type^[9].

The analytic distorsion U_μ , for μ small enough associated to v is defined on $C_0^\infty(\mathbb{R}_x^3 \times \mathbb{R}_y^{3p})$ by

$$U_\mu \varphi(x, y) = \varphi(x + \mu v(x), y_1 + \mu v(y_1), \dots, y_p + \mu v(y_p)) |J|^{1/2}$$

where $J = J(x, y) = \det(1 + \mu Dv(x)) \prod_{j=1}^p \det(1 + \mu D(y_j))$ is the

Jacobien of the transformation

$$\Psi_\mu : (x, y) \rightarrow (x + \mu v(x), y_1 + \mu v(y_1), \dots, y_p + \mu v(y_p))$$

and $v \in C^\infty(\mathbb{R}^3)$ is a vector field satisfying :

$$\exists N > 0, \text{ large enough such that: } \begin{cases} v(x) = 0, \text{ si } |x| \leq \frac{2}{N} \\ v(x) = x, \text{ si } |x| \geq r_0 - \varepsilon' \end{cases}$$

($\varepsilon' > 0$, small enough, $|r_0| > \frac{3}{N} + \varepsilon'$).

Remark 1.4: The distorsion is close to the potential well.

We localise our operator near the well v_0 by introducing a truncate function $\zeta \in C^\infty(\mathbb{R}^3)$ satisfying:

$$\begin{cases} \zeta = 1, \text{ si } |x| \geq \frac{2}{N} \\ \zeta = 0, \text{ si } |x| \leq \frac{3}{2N} \end{cases}$$

fixing $\alpha_0 > v_0$, we set

$$Q_\mu^\zeta(x) = -U_\mu \Delta_y U_\mu^{-1} + \zeta(x) V_\mu(x, y) + (1 - \zeta(x)) \alpha_0$$

$$V_\mu(x, y) = (x + \mu v(x), y_1 + \mu v(x), \dots, y_p + \mu v(x))$$

We also denote:

$$P_\mu^\zeta = -h^2 U_\mu \Delta_x U_\mu^{-1} + Q_\mu^\zeta(x) \tag{7}$$

With domain $H^2(\mathbb{R}_x^3)$.

Remark 1.5: Like in ^[10], near v_0 , $\sigma(P_\mu)$ and $\sigma(P_\mu^\zeta)$ coincide up to exponentially small error terms. For this we will study P_μ^ζ instead of P_μ .

RESULTS

Here we write the results of our works as following:

Theorem 1.6: Under assumptions (H1) to (H5) and for $\mu \in \mathbb{C}, |\mu|$ and h small enough, we have

$$\left\| (F_\mu^\zeta - z)^{-1} \right\| = O(h^{-1/2})$$

where F_μ^ζ is the Feshbach reduced operator of P_μ^ζ verifying

$$F_\mu^\zeta = -\frac{h^2}{(1 + \mu)^2} \Delta_x I + M_\mu^\zeta + \tilde{R}_\mu^\zeta \text{ and the error } \tilde{R}_\mu^\zeta \text{ is}$$

satisfying: $\left\| \tilde{R}_\mu^\zeta \right\|_{L(H^m \oplus H^m, H^{m-1} \oplus H^{m-1})} = O(h^2)$

We need for our proof the main important theorem for the operator $P_{2,\mu}^\zeta$ which is the distortion of the operator

$$P_{2,\mu}^\zeta : P_{2,\mu}^\zeta = -h^2 U_\mu \Delta_x U_\mu^{-1} + \lambda_2(x + \mu v(x)) \tag{8}$$

at the neighbourhood of point x_0 of the well such that $(\forall \varepsilon) > 0$, small enough, $\left| |x_0| \right|_{r_0 + \varepsilon}$, the distortion $P_{2,\mu}^\zeta$

is in fact a dilatation of angle θ such that $e^\theta = (1 + \mu)$.

We denote it by $P_{2,0}^{\zeta [11]}$ and is defined by

$$P_{2,0}^\zeta = -h^2 \Delta_x + \lambda_2(x e^\theta) \tag{9}$$

Let $e_j, j=1, \dots, N_0$ be the eigenvalues of the operator

$$P_0 = -\frac{d^2}{dr^2} + \frac{1}{2} \lambda_2^+(r_0)(r - r_0)^2 \text{ and } \gamma_j \text{ complex circles}$$

centred at $e_j h$.

Theorem 1.7: Under assumptions (H1)- (H5), for $\theta \in \mathbb{C}, |\theta|$ and h small enough and for $(\forall \varepsilon) > 0$, small enough, $\left| |x_0| \right|_{r_0 + \varepsilon}$, the resolvent of the distorted operator defined by (9) satisfies the estimate

$$\left\| (P_{2,0}^\zeta - z)^{-1} \right\| = O(h^{-1/2}), \text{ uniformly for } z \in [-\varepsilon' - x_0, C_0 h - x_0] \text{ outside of the } \gamma_j.$$

Before we prove this theorem, we introduce the so-called Grushin problem associated to the distorted operator P_μ^ζ .

The reduced Feshbach operator: Now, we try to reduce the operator P_μ^ζ by the Feshbach method into a

$$\text{matricial operator of type: } -\frac{h^2}{(1 + \mu)^2} \Delta_x I + M_\mu^\zeta + \tilde{R}_\mu^\zeta$$

where M_μ^ζ is the matrix of eigenvalues of Q_μ^ζ and \tilde{R}_μ^ζ is the remainder of order $O(h^2)$

The study of the distorted operator P_μ^ζ : We begin our study by the operator Q_μ^ζ which is defined by:

$$Q_\mu^\zeta = U_\mu Q(x + \mu v(x)) U_\mu^{-1} \tag{10}$$

For $x \neq 0$, we denote also

$$\tilde{Q}_\mu(x) = Q_\mu(x) - \frac{\alpha}{|x + \mu v(x)|} \text{ and } \tilde{\lambda}_j(x) = \lambda_j - \frac{\alpha}{|x|}, j \in \{1, 2, 3\}$$

Let $C(x)$ be a family of continuous closed simple loop of C enclosing $\tilde{\lambda}_j(x), j \in \{1, 2, 3\}$ and having the rest of $\sigma(\tilde{Q}_0(x))$ in its exterior. The gap condition (4) permits us to assume that:

$$\min_{x \in \mathbb{R}^3} \text{dist}(\gamma(x), \sigma(\tilde{Q}_0(x))) \geq \frac{\delta}{2} \tag{11}$$

Using the relation (6) and (H3), we can take $C(x)$ compact in a set of C . So, we deduce from (11) the following result^[3].

Lemma 2.1

1. $\forall j, k \in \{1, \dots, p\}, j \neq k, \beta \in \mathbb{N}^{3p}$, the

$$\text{operators } \frac{1}{|y_j \pm x|} (\tilde{Q}_0(x) - z)^{-1}, \frac{1}{|y_j - y_k|} (\tilde{Q}_0(x) - z)^{-1}$$

and $\partial^\beta (\tilde{Q}_0(x) - z)^{-1}$ are uniformly bounded on $L^2(\mathbb{R}_y^{3p}), x \in \mathbb{R}^3, z \in C(x)$

2. If $\mu \in \mathbb{C}$ small enough, then for $x \in \mathbb{R}^3, z \in C(x)$, the

operator $(\tilde{Q}_\mu(x) - z)^{-1}$ exists and satisfies uniformly

$$(\tilde{Q}_\mu(x) - z)^{-1} - (\tilde{Q}_0(x) - z)^{-1} = O(|\mu|).$$

Now we define for $\mu \in \mathbb{C}$ small enough, the spectral projector associated to \tilde{Q}_μ and the interior of $C(x)$.

$$\pi_\mu(x) = \frac{1}{2\pi} \int_{\gamma(x)} (z - \tilde{Q}_\mu(x))^{-1} dz \text{ and } \text{rg} \pi_\mu = 1$$

This projector permits us to construct the Grushin problem associated to the operator P_μ^ζ .

Problem of Grushin associated with the operator P_μ^ζ : We begin this section by the result which is (lemma 1-1 of [12] and proposition 5-1 of [7]).

Proposition 2.2: Assume (H1), (1.7), (1.9), (1.10) hold, then for $\mu \in \mathbb{C}$, $z \in C$ small enough, there exist N functions $\omega_{k,\mu}(x, y) \in C^0(\mathbb{R}^3, H^2(\mathbb{R}^{3p}))$, ($k = 1, 2, 3$), depending analytically on $\mu \in \mathbb{C}$, such that

- i. $\langle \omega_{j,\mu} | \omega_{k,\mu} \rangle_{L^2(\mathbb{R}^{3p})} = \delta_{j,k}$
- ii. For $|x| \geq \frac{3}{N}$, $(\omega_{k,\mu})_{1 \leq k \leq 3}$ form a basis of $\text{Ran } \pi_\mu(x)$
- iii. $\in C^\infty \left(\left\{ |x| < \frac{2}{N} \right\}, H^2(\mathbb{R}^{3p}) \right)$
- iv. For $|x|$ large enough, $\omega_{k,\mu}(x)$ is an eigen function of $Q_\mu(x)$ associated with $\lambda_k(x + \mu\omega(x))$

We first introduce the family $\{\omega_{1,\mu}, \omega_{2,\mu}, \omega_{3,\mu}\}$ of $\text{Ran } \pi_\mu(x)$ depending analytically on μ for μ small enough and normalized in $L^2(\mathbb{R}^{3p})$ by $\langle \omega_{i,\mu}(x), \omega_{j,\mu}(x) \rangle_{L^2(\mathbb{R}^{3p})} = \delta_{ij}$ and then we associate the two following operators

$$R_\mu^- : \bigoplus_1^3 L^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^{3p})$$

$$u^- = (u_1^-, u_2^-, u_3^-) \rightarrow R_\mu^- u^- = \sum_{k=1}^3 u_k^- \omega_{k,\mu}(x)$$

$$R_\mu^+ = (R_\mu^-)^* : L^2(\mathbb{R}^{3p}) \rightarrow \bigoplus_1^3 L^2(\mathbb{R}^3)$$

$$u = {}^t \langle \langle u, \omega_{\bar{1},1} \rangle_Y, \langle u, \omega_{\bar{2},2} \rangle_Y, \langle u, \omega_{\bar{3},3} \rangle_Y \rangle$$

where ${}^t A$ denote the transposed of the operator A , $\langle \cdot, \cdot \rangle_Y$ the inner product on $L^2(\mathbb{R}^{3p})$ and $\langle \cdot, \omega_{\bar{i},i} \rangle_Y$ is the adjoint of the operator $L^2(\mathbb{R}^n) \ni v \mapsto v u_{\mu,i} \in L^2(\mathbb{R}^{n+p})$,

$u_{\mu,k} = u(x + \mu v(x))$ and we put $\hat{\pi}_\mu = 1 - \pi_\mu$, where

$$\pi_\mu = \langle u, \omega_{\bar{1},1} \rangle_Y \omega_{\mu,1} + \langle u, \omega_{\bar{2},2} \rangle_Y \omega_{\mu,2} + \langle u, \omega_{\bar{3},3} \rangle_Y \omega_{\mu,3}.$$

As P_μ^ζ and $\omega_{\mu,k}$, $k=1,2,3$ have analytic extensions with μ , the Grushin problem is then defined, for $z \in C$, by:

$$P_\mu^\zeta(z) = \begin{pmatrix} P_\mu^\zeta - z & R_\mu^+ \\ R_\mu^- & 0 \end{pmatrix} = \begin{pmatrix} P_\mu^\zeta - z & \omega_{1,\mu} & \omega_{2,\mu} & \omega_{3,\mu} \\ \langle \cdot, \omega_{1,\mu} \rangle_Y & 0 & 0 & 0 \\ \langle \cdot, \omega_{2,\mu} \rangle_Y & 0 & 0 & 0 \\ \langle \cdot, \omega_{3,\mu} \rangle_Y & 0 & 0 & 0 \end{pmatrix} \quad (12)$$

which sets on $H^2(\mathbb{R}^{3p}) \oplus (\bigoplus_1^3 L^2(\mathbb{R}^3))$ to $L^2(\mathbb{R}^{3p}) \oplus (\bigoplus_1^3 H^2(\mathbb{R}^3))$

The following proposition, gives the inverse of the operator (12) by using a result of Grushin problem. This is proved in [3,6].

Proposition 2.3: $\forall z \in C$ close enough to λ_0 , P_μ^ζ is invertible and we can write its inverse:

$$P_\mu^{\zeta-1} = \begin{pmatrix} X_{\mu,+}^\zeta & X_{\mu,+}^\zeta \\ X_{\mu,-}^\zeta & X_{\mu,-}^\zeta \end{pmatrix},$$

With $X_\mu^\zeta(z) = (P_\mu^\zeta - z)^{-1} \hat{\pi}_\mu(x)$ where $(P_\mu^\zeta - z)^{-1}$ is the bounded inverse of the restriction of $\hat{\pi}_\mu(P_\mu^\zeta - z)$ to $\{u \in H^2(\mathbb{R}^{3(n+p)}), \hat{\pi}u = u\}$.

$$X_{\mu,+}^\zeta(z) = (\omega_{k,\mu} - X_\mu^\zeta(z) P_\mu^\zeta(\omega_{k,\mu}))_{1 \leq k \leq 3},$$

$$X_{\mu,-}^\zeta(z) = {}^t \langle \langle (1 - P_\mu^\zeta(z) X_\mu^\zeta(\cdot), \omega_{k,\bar{i}} \rangle_{1 \leq k \leq 3} \rangle \text{ and}$$

$$X_{\mu,-}^{\zeta+}(z) = \left(z \delta_{jk} - \langle (P_\mu^\zeta - P_\mu^\zeta X_\mu^\zeta(x) P_\mu^\zeta)(\omega_{j,\mu}), \omega_{j,\bar{i}} \rangle_{L^2(\mathbb{R}^{3p})} \right)_{1 \leq j,k \leq 3}$$

Remark 2.4

1. For $z \in C$, close enough to λ_0 , we have $z \in \sigma(P_\mu^\zeta)$ if and only if $\exists \mu, |\mu|$ small enough and $\text{Im} \mu > 0$, such that $z \in \sigma_{\text{disc}}(X_{\mu,+}^\zeta(z))$ where $X_{\mu,+}^\zeta(z) : \bigoplus_1^3 H^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^3)$, is a pseudo-differential operator of principal symbol defined by the matrix:

$$B(x, \xi, z) = zI - \langle \langle \omega_{j,\mu}(x) | (t_\mu(\xi) + Q_\mu^\zeta(x)) \omega_{k,\mu}(x) \rangle_{L^2(\mathbb{R}^3)} \rangle_{1 \leq j,k \leq 3}$$

and $t_\mu(\xi)$ is the principal symbol of $-h^2 U_\mu \Delta_x U_\mu^{-1}$

2. z is a resonance of the operator P_μ^ζ only and only if, $\exists \mu \in C$, $|\mu|$ small enough $\text{Im} \mu > 0$, such that: $0 \in \sigma_{\text{disc}}(X_{\mu,+}^\zeta)$ or $0 \in \sigma_{\text{disc}}(F_{\mu,+}^\zeta)$ where F_μ^ζ is the Feshbach operator ($F_\mu^\zeta = z - X_{\mu,+}^\zeta$) our goal is to takeback the initial problem to a problem on $L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$.

Reduced Feshbach operator: To reduce the Feshbach operator in a matricial operator, we input:

$$\Phi_\mu^\zeta = P_\mu^\zeta - P_\mu^\zeta X_\mu^\zeta(x) P_\mu^\zeta \quad (13)$$

$$F_\mu^\zeta = \left\langle \left\langle \Phi_\mu^\zeta(\omega_{j,\mu}(x)) \middle| \omega_{k,\bar{\mu}}(x) \right\rangle_Y \right\rangle_{1 \leq j,k \leq 3} \quad (14)$$

and

$$\Phi_{1,\mu}^\zeta(z) = \left\langle \left\langle \Phi_\mu^\zeta(\omega_{1,\mu}(x)) \middle| \omega_{1,\bar{\mu}}(x) \right\rangle \right\rangle_{1 \leq j,k \leq 3} \quad (15)$$

The following proposition give us the estimation of the resolvent of the operator (15).

Proposition 2.5: For $z \in C, |z|$ small enough, $\mu \in C, |\mu|$ small enough, the operate or $(\Phi_\mu^{1\zeta}(z) - z)$ is bijective for $H^2(\mathbb{R}^3)$ to $L^2(\mathbb{R}^3)$. Its inverse is extended for H^m in H^{m+j}
 $H^m = H^m(L^2(\mathbb{R}_x^n), L^2(\mathbb{R}^p)), \forall m \in Z$ and verify for $j = \{1, 2, 3\}$, $h > 0$ small enough:

$$\left\| (\Phi_{1,\mu}^\zeta(z) - z)^{-1} \right\|_{L(H^m, H^{m+j})} \leq \frac{C(m)}{h^j (\text{Im } \mu)}$$

To prove this proposition, we first use a lemma in^[3], to prove the following lemma:

Lemma 2.6: $\forall m \in Z$, the operator $X_\mu^\zeta(z)$ is uniformly is extensible in a bounded operator on $H^m(L^2(\mathbb{R}_x^n), L^2(\mathbb{R}^p)), \forall m \in Z$, for $h > 0, z \in Z$ and $\mu \in Z$ small enough and

$$\left\| X_\mu^\zeta \right\|_{L(H^m, H^{m+2})} = O(h^{-2})$$

See^[3] for the proof.

Lemma 2.7: We assume that

$$\left\| (P_{1,\mu}^\zeta - z)^{-1} \right\|_{L^2(H^m, H^{m+j})} = O\left(\frac{1}{h^j \text{Im } \mu}\right)$$

for $h > 0, z \in C$ and $\mu \in C$ small enough, where

$$P_{1,\mu}^\zeta = -h^2 \frac{1}{(1+\mu)^2} \Delta_x + \lambda_1(x + \mu v(x)) -$$

$$h^2 \frac{1}{(1+\mu)^2} \left\langle \Delta_x(\omega_{1,\mu}(x)) \middle| \omega_{1,\bar{\mu}}(x) \right\rangle_Y -$$

$$-h^2 \left\langle R_\mu(x, D_x)(\omega_{1,\mu}(x)) \middle| \omega_{1,\bar{\mu}}(x) \right\rangle_Y$$

$R_\mu(x, D_x)$, is an differential operator of coefficients C^∞ .

Proof of lemma 2.7: Using (H5) we have:

$$\text{Im} \frac{1}{(1+\mu)^2} \lambda_1(x + \mu v(x)) \leq -\frac{\text{Im } \mu}{C_1}, \text{ so}$$

$$\left\| \left(-h^2 \frac{1}{(1+\mu)^2} \Delta_x + \lambda_1(x + \mu v(x)) - z \right)^{-1} \right\|_{L(L^2(\mathbb{R}^3))} \leq \frac{C_2}{\text{Im } \mu}$$

and we easily deduce with a simple computation that

$$\left\| (P_{1,\mu}^\zeta - z)^{-1} \right\|_{L^2(H^m, H^{m+j})} = O\left(\frac{1}{h^j \text{Im } \mu}\right)$$

Proof of the proposition 2.5: From (13) and (15), we have $\Phi_{1,\mu}^\zeta = \left\langle \left\langle (P_\mu^\zeta - P_\mu^\zeta X_\mu^\zeta(z)) P_\mu^\zeta(\omega_{1,\mu}(x)) \middle| \omega_{1,\bar{\mu}}(x) \right\rangle \right\rangle$, then we substitute P_μ^ζ from (7) with

$$U_\mu \Delta_x U_\mu^{-1} = \frac{1}{(1+\mu)^2} \Delta_x + R_\mu(x, D_x), \text{ where } R_\mu(x, D_x)$$

is a second order differential operator with C^∞ coefficients in x with compact support, analytic in μ and whose derivative of any kind compared to x are $O(|\mu|)$: and we put

$$\Lambda_\mu^\zeta = \frac{1}{(1+\mu)^4} \left\langle \Delta_x X_\mu^\zeta \Delta_x(\omega_{1,\mu}(x)), \omega_{1,\bar{\mu}}(x) \right\rangle_Y + \frac{1}{(1+\mu)^2} \left\langle (R_\mu(x, D_x) X_\mu^\zeta \Delta_x + \Delta_x X_\mu^\zeta R_\mu(x, D_x)) \right\rangle_{(\omega_{1,\mu}(x), \omega_{1,\bar{\mu}}(x))}.$$

Using the fact that

$$\hat{\pi}_\mu \omega_{1,\mu} = 0, X_\mu^\zeta = \hat{\pi}_\mu X_\mu^\zeta \hat{\pi}_\mu, \left\langle \omega_{1,\mu}, \omega_{1,\bar{\mu}} \right\rangle = 1, \text{ we have:}$$

$$\Phi_{1,\mu}^\zeta(z) = \check{P}_{1,\mu}^\zeta - h^4 \Lambda_\mu^\zeta, \text{ where}$$

$$\check{P}_{1,\mu}^\zeta = -h^2 \frac{1}{(1+\mu)^2} \Delta_x + \lambda_1(x + \mu v(x))$$

$$- \frac{1}{(1+\mu)^2} \left\langle \Delta_x(\omega_{1,\mu}(x)) \middle| \omega_{1,\bar{\mu}}(x) \right\rangle_Y$$

$$- h^2 \left\langle R_\mu(x, D_x)(\omega_{1,\mu}(x)) \middle| \omega_{1,\bar{\mu}}(x) \right\rangle_Y$$

We have $R_\mu(x, D_x)$ bounded, so Λ_μ^ζ is $O(h^2)$ from H^m to H^m and we also see from (H5) and lemma2.6 that: for h small enough, $\left\| (P_{1,\mu}^\zeta - z)^{-1} \right\|_{L(L^2)} = O\left(\frac{1}{\text{Im } \mu}\right)$, then, we deduce

$$\left\| (\check{P}_{1,\mu}^\zeta - z)^{-1} \right\|_{L^2(H^m, H^{m+j})} = O\left(\frac{1}{h^j \text{Im } \mu}\right). \text{ Finally we have:}$$

$$\left\| (\Phi_{1,\mu}^\zeta(z) - z)^{-1} \right\|_{L(H^m, H^{m+j})} = O\left(\frac{1}{h^j \text{Im } \mu}\right)$$

Proof of theorems

Proof of theorem 2.1: Proposition3.5 permits us to reduce the Feshbach operator F_μ^ζ in a matricial operator

2x2, A_μ^ζ , where

$$A_\mu^\zeta = \left\{ \left\langle \Phi_\mu^\zeta(\omega_{i,\mu}) + T_\mu^{j\zeta}(\omega_{1,\mu}, \omega_{1,\bar{\mu}}) \right\rangle_{i,j=2,3} \right\}$$

Now, we consider a solution $\alpha = \alpha_1 \oplus \alpha_2 \oplus \alpha_3 \in L^2(\mathbb{R}^n) \oplus L^2(\mathbb{R}^n) \oplus L^2(\mathbb{R}^n)$ of the equation: $F_\mu^\zeta(z)\alpha = z\alpha$

The operators $T_\mu^{j\zeta}$ are defined by:

$$T_\mu^{j\zeta}(z)\alpha_j = -(\Phi_\mu^{1\zeta}(z) - z)^{-1} \left\{ \left\langle \Phi_\mu^\zeta(\alpha_j \omega_{j,\mu}, \omega_{j,\bar{\mu}}) \right\rangle_{j=2,3} \right\},$$

hence, the spectral study of the Feshbach F_μ^ζ becomes the study of the operator A_μ^ζ on $L^2(\mathbb{R}^n) \oplus L^2(\mathbb{R}^n)$ by:

$$\alpha_1 = -(\Phi_\mu^{1\zeta}(z) - z)^{-1} \left\{ \left\langle \Phi_\mu^\zeta(\alpha_2 \omega_{2,\mu}, \omega_{2,\bar{\mu}}) \right\rangle_Y + \left\langle \Phi_\mu^\zeta(\alpha_3 \omega_{3,\mu}, \omega_{3,\bar{\mu}}) \right\rangle_Y \right\}$$

Then the eigenvalues equation of $F_\mu^\zeta(z)$ becomes:

$$\begin{cases} \alpha_1 = (T_\mu^{2\zeta}(z) \oplus T_\mu^{3\zeta}(z))(\alpha_2 \oplus \alpha_3) \\ A_\mu^\zeta(z)(\alpha_2 \oplus \alpha_3) = z(\alpha_2 \oplus \alpha_3) \end{cases}$$

So we establish easily

$$A_\mu^\zeta = -h^2 \frac{1}{(1+\mu)^2} \Delta_x + M_\mu^\zeta + \tilde{R}_\mu^\zeta, \text{ where } M_\mu^\zeta \text{ is a}$$

diagonal matrix outside of $K_{2\delta_0}$ and it equal to:

$$M_\mu^\zeta = \left\{ \left\langle Q_\mu^\zeta(x)(\omega_{i,\mu}) \middle| \omega_{j,\bar{\mu}} \right\rangle_Y \right\}_{i,j=2,3} = \begin{pmatrix} \lambda_2(x + \mu v(x)) & 0 \\ 0 & \lambda_3(x + \mu v(x)) \end{pmatrix}$$

where $\lambda_2(x + \mu v(x))$, $\lambda_3(x + \mu v(x))$ are the eigenvalues of Q_μ^ζ , $\forall x \in \mathbb{R} - \{0\}$

The remainder

$$\|\tilde{R}_\mu^\zeta(z, h)\|_{L(H^m \oplus H^m, H^{m-1} \oplus H^{m-1})} = O(h^2), \forall m \in Z \text{ uniformly}$$

for $h > 0$ and $z \in C$ closed to λ_0

At the end we prove the second result. To describe it, we apply a technical of Briet Combs Duclos^[13].

Let $J_i \in C_0^\infty(|x - x_0| \leq \delta)$, $(\delta) > 0$ fixed small enough and x_0 a point of maximum) and $J_e \in C^\infty(\mathbb{R}^n)$ such that: $J_i = 1$ near x_0 and $J_i^2 + J_e^2 = 1$

J is an identification mapping such that:

$$J: L^2(\mathbb{R}^n) \oplus L^2(\text{supp}J_e) \rightarrow L^2(\mathbb{R}^n) \\ J(u \oplus w) = J_i u + J_e w$$

It is easily proved that: $JJ^* = 1_{L^2(\mathbb{R}^n)}$

Now, if we note P_μ^Ω the Dirichlet realisation of P_μ^ζ on Ω , on Ω , $x = v(x)$ and the distorsion $x + \mu v(x) = xe^0$,

is an analytic dilatation (whose Dirichlet realisation is the operator H_μ^ζ obtained for $\zeta = 1$)). We set

$$H_\theta^i = -h^2 e^{-2\theta} \Delta + \langle \lambda_2''(x_0)(x - x_0), (x - x_0) \rangle e^{2\theta}$$

$$H_\theta = P_\theta^2 = -h^2 e^{-2\theta} \Delta + \lambda_2(xe^0)$$

$H_\theta^c = H_\theta \Big|_{L^2(\text{supp}J_e)}$, with Dirichlet conditions on $\partial \text{supp}J_e$

Remark 3.1: Since $\inf_{x \in \text{supp}J_e} \text{Re} e^{2\theta} \lambda_2(xe^0) > 0$, $(H_\theta^c - z)^{-1}$ is uniformly bounded for $|z|$ and h small enough.

Before we prove the second result, we introduce the following lemma

Lemma 3.2: For all $p \in [0, 1]$, $\| |x|^p (H_\theta^i - z)^{-1} \|_{L(L^2)} = O(h^{\frac{p-1}{2}})$, uniformly for z outside of $\gamma(x)$ $z \in [-\varepsilon - x_0, C_0 h - x_0] + i[-\varepsilon - x_0, C_0 h - x_0]$, $\text{Im} \theta \geq 0$, and h small enough.

Proof of lemma 3.2: If we put $y = \frac{x - x_0}{\sqrt{h}}$, we can

write H_θ^i :

$$H_\theta^i = h H_\theta^0 \tag{16}$$

where $H_\theta^0 = -e^{-2\theta} \Delta_y + \frac{1}{2} \langle \lambda_2''(x_0)y, y \rangle + h^{-1} \Im(\varepsilon)$,

with $\Im(\varepsilon) = \varepsilon(1 + (x - x_0)e^0) + \frac{1}{2}(x - x_0)^2 e^{2\theta}$

It is enough to show that, for $\theta = i\alpha$, $\alpha \geq 0$, small enough. We have from (16)

$$|x|^p (H_\theta^i - z)^{-1} = h^{\frac{p-1}{2}} |y|^2 (H_\theta^0 - zh^{-1})^{-1} \tag{17}$$

and the eigenvalues of the operator H_θ^0 in

$]-\infty, C_0 - x_0] + i \mathbb{R}$ are e_1, \dots, e_N .

We distinguish three cases for $p = 0$.

1/ If $z \in [-Ch - x_0, C_0 h - x_0] + i[-Ch - x_0, C_0 h - x_0]$: we deduce for all $C > 0$, $(H_\theta^0 - zh^{-1})^{-1}$ is bounded on L^2 uniformly for z outside the γ_j , so (17) is verified.

2/ If $z \in [-\varepsilon - x_0, C_0 h - x_0] + i[-\varepsilon - x_0, C_0 h - x_0]$: then for $u \in C_0^\infty(\mathbb{R}^n)$:

$$e^{20}H_0^0 = -\Delta y + \frac{1}{2} \langle \lambda''(x_0)y, y \rangle e^{40} +$$

$$h^{-1}(z + \varepsilon(1 + (x - x_0)e^{30} + \frac{1}{2}(x - x_0)^2 e^{40}))$$

and

$$\text{Im} \langle e^{20}(H_0^0 - zh^{-1})u, u \rangle = \frac{1}{2} \sin 4\alpha \langle \langle \lambda''(x_0)y, y \rangle u, u \rangle - \left[h^{-1}(z \sin 2\alpha + \text{Im } z \cos 2\alpha + h^{-\frac{1}{2}}(y \sin 3\alpha + z \cos 4\alpha)) \right] \|u\|^2$$

We take particularly α small enough and C large enough such that: $C \cos 2\alpha > C_0 \sin 2\alpha$

At least we obtained

$$\left| \langle e^{20}(H_0^0 - zh^{-1})u, u \rangle \right| \geq h^{-\frac{1}{2}}(x_0 \sin 2\alpha + y \sin 3\alpha) \|u\|^2$$

so the result is also verified. It remain the case:

$$3/ \text{If } z \in [-\varepsilon - x_0, -Ch - x_0] + i[-Ch - x_0, C_0 h - x_0]:$$

$$\text{Re} \langle e^{20}(H_0^0 - zh^{-1})u, u \rangle \geq h^{-\frac{1}{2}}(\text{Re } z \cos 4\alpha - \text{Im } z \sin 2\alpha + y \cos 3\alpha)$$

we deduce the estimation when $C > C_0$, α small enough

and C large enough such that $\cos 4\alpha > \sin 2\alpha$

Now we consider the case when $p \neq 0$,

$$e^{20}(H_0^0 - zh^{-1}) = -\Delta + \frac{1}{2} e^{40} \langle \lambda''(x_0)y, y \rangle \text{ and}$$

$$-zh^{-1}e^{20} + h^{-1}e^{20}\mathfrak{I}(\varepsilon)$$

$$\left\| -\Delta + \frac{1}{2} e^{40} \langle \lambda''(x_0)y, y \rangle - zh^{-1}e^{20} + h^{-1}e^{20}\mathfrak{I}(\varepsilon) \right\|$$

$$\geq \left\| \frac{1}{2} \cos 4\alpha \langle \lambda''(x_0)y, y \rangle u \right\|_{L^2} \geq \frac{1}{C} |y|^2 \|u\|_{L^2}$$

if we put $u = (H_0^0 - zh^{-1})^{-1}v$ the result is deduced from a priori standard estimation.

Proof of theorem 1.2: We put $H_0^d = H_0^i \oplus H_0^c$ and $\Pi = H_0 J - J H_0^d$, for z outside the spectrum of H_0 , with a simple calculation we obtain:

$$(H_0 - z)^{-1} = J(H_0^d - z)^{-1} J^* (1 + \Pi(H_0^d - z)^{-1} J^*)^{-1} \quad (18)$$

Using the lemma3.2 (with $p = 2$) and the lemma3.1 of Briet Combs Duclos^[13], we can easily prove that: $\exists \beta < 1$ such that

$$\left\| \Pi(H_0^d - z)^{-1} J^* \right\| \leq \beta \quad (19)$$

Using the lemma3.2 and (19), we obtain from (18)

$$\left\| (H_0 - z)^{-1} \right\| \leq C \left\| (H_0^d - z)^{-1} \right\|, \text{ finally the result is}$$

obtained from lemma3.2 and remark3.1

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