FESHBACH REDUCTION SCHEME FOR GENERAL HAMILTONIANS IN THE BORN-OPPENHEIMER APPROXIMATION

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Abstract. We study the spectral properties of resonances of general Hamiltonians in the Born-Oppenheimer approximation. We prove that this study can be reduced to the one of a family of finite matrices of semiclassical h-pseudodifferential operators. More precisely, we show that any resonance which is close enough to the real axis can be obtained from the discrete spectrum of one of these matrixes.

1. **Introduction**

The Born-Oppenheimer approximation [2] consists in studying the spectrum of the Schrödinger operator:

$$H = -h^2\Delta_x - \Delta_y + V(x,y)$$

where $x \in \mathbb{R}^n$ represents the position of the nuclei, $y \in \mathbb{R}^p$ is the position of the electrons, h is proportional to the inverse of the square-root of the nuclear mass and $V(x,y)$ is the interaction potential.

Many efforts have been made in order to study in the semiclassical limit the spectrum and resonances of H (see e.g. [4], [8], [10], [13], [15],...). These authors have shown that in many situations it is still possible to perform, by Grushin's method, semiclassical constructions related to the existence of some hidden effective semiclassical operator.

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When one wants to study the eigenvalues and resonances of H, it is shown in [8] that one can reduce the problem to a finite matrix of regular h-pseudodifferential operators, even when V admits singularities of Coulomb-type.

It has been proved, both for diatomic molecules [13] and for polyatomic molecules [8], that the study of resonances of H can be reduced to a matrix of h-pseudodifferential operators.

Here we plan to give a unified version of the two results in [13] and [8], which can be applied to the general class of operators of the type

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

where $P(x, y, D_y)$ is a pseudodifferential operator on $L^2\left(\mathbb{R}^p_y\right)$ (the so-called electronic Hamiltonian and its eigenvalues are the so-called electronic levels).

By using the h-pseudodifferential operators with operator-valued symbol (see [1, 19]) and the general Feshbach reduction scheme, the study of resonances of $P(h)$ on $L^2\left(\mathbb{R}^n_x \times \mathbb{R}^p_y\right)$ is reduced to the discrete spectrum of a matrix of h-pseudodifferential operators $F_\theta(z)$ on $\left(L^2(\mathbb{R}^n_x)\right)^{\oplus M}$ (the so-called effective Hamiltonian) with principal symbol the diagonal matrix $diag\left(\xi^2 + \lambda_j\left(xe^\theta\right)\right)_{1\leq j\leq M}$ where $M > 0$ depends on the energy level and $(\lambda_j(x))_{1\leq j\leq M}$ are the electronic levels. In particular, we obtain the following equivalence:

$$z \text{ is a resonance of } P(h) \Leftrightarrow \exists\theta \in \mathbb{C},\ \operatorname{Im}\theta > 0,\ z \in \sigma_{disc}(F_\theta(z)).$$

2. Assumptions

We study the resonances of a general class of Born-Oppenheimer Hamiltonian of the type:

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

when h tends to 0^+, $P(x, y, D_y)$ is a pseudodifferential operator on $L^2\left(\mathbb{R}^p_y\right)$ with x-independent domain.

We assume that:

$(H1)$ For every $x \in \mathbb{R}^n$, $P(x, y, D_y)$ is selfadjoint and bounded from below on $L^2\left(\mathbb{R}_y^p\right)$. $P(x, y, D_y)$ can be analytically extended on the complex strip

$$D_\delta = \{x \in \mathbb{C}^n, \ \ |\mathrm{Im}\, x| \leq \delta < \mathrm{Re}\, x >\}, \ \delta > 0.$$

$(H2)$ The spectrum of the pseudodifferential operator $P(x, y, D_y)$ has two disjoint components for every $x \in \mathbb{R}^n$:

$$Sp\left(P(x, y, D_y)\right) = \{\lambda_1(x), \lambda_2(x), ..., \lambda_M(x)\} \cup \sigma(x)$$

where $\lambda_1(x), \lambda_2(x), ..., \lambda_M(x)$ are eigenvalues of $P(x, y, D_y)$ depend continuously on $x \in \mathbb{R}^n$ and can be analytically extended on D_δ. There is a gap between the two components:

$$\inf_{\lambda \in \sigma(x), j \in \{1, \dots, M\}} |\lambda_j(x) - \lambda| \geq \delta.$$

In particular, this implies that the spectral projector $\pi(x)$ of $P(x, y, D_y)$ associated to $\{\lambda_1(x), \lambda_2(x), ..., \lambda_M(x)\}$ is C^2-regular with respect to x (see [3]).

$(H3)$ We also assume that $\lambda_1(x), \lambda_2(x), ..., \lambda_M(x)$ are separated at the infinity:

$$\exists \widetilde{C} > 0, \ \ \inf_{\substack{j \neq k \\ |x| \geq C}} |\lambda_j(x) - \lambda_k(x)| \geq \widetilde{C}, \ C > 0.$$

This last assumption is essential in our work to obtain a good behavior of the spectral projectors of $P(x, y, D_y)$ where $|x| \to +\infty$. This is because our technique stand strongly on pseudodifferential calculus, which requires a lot of regularity with respect to x.

$(H4)$ $P(x, y, D_y) \in C_b^\infty\left(\mathbb{R}^n, \mathcal{L}\left(\mathcal{D}\left(P(x, y, D_y)\right), L^2\left(\mathbb{R}_y^p\right)\right)\right)$, here C_b^∞ denotes the space of C^∞-functions that have their derivatives of any order uniformly bounded.

Examples:

- The operator $P(x,y,D_y) = -\frac{d^2}{dy^2} + \left(1+x^2\right)^{2l} y^2$, $x \in \mathbb{R}, l \in \mathbb{R}$ satisfies the assumptions (H1) to (H3) with domain

$$\mathcal{D}\left(P\left(x,y,D_y\right)\right) = H^2\left(\mathbb{R}_y\right) \cap \left\{\varphi \in L^2\left(\mathbb{R}_y\right);\ y^2\varphi \in L^2\left(\mathbb{R}_y\right)\ \right\},$$

$$\lambda_j(x) = (2j+1)\left(1+x^2\right)^l;\ j = 1, ..., M \text{ and}$$

$$\sigma(x) = \left\{(2j+1)\left(1+x^2\right)^l;\ j \geq M+1\right\}.$$

- A second example is the Born-Oppenheimer Hamiltonian (see e.g [15, 8]) for the differential operator

$$P\left(x,y,D_y\right) = -\Delta_y + V\left(x,y\right),$$

where $V(x,y)$ is the Coulomb interaction potential. For the study of resonances of $P(h)$ in this example see the work of Martinez-Messirdi [13].

3. Preliminaries and main result

In this paper we characterize the resonances of $P(h)$ by using the analytic dilation introduced by Hunziker [6]. More precisely, for θ real small enough we consider the transformation $x \longmapsto xe^{\theta}$ and the associated dilation operator U_θ defined by:

$$U_\theta \varphi(x,y) = e^{n\theta/2}\varphi\left(xe^{\theta}, y\right), \quad \varphi \in C_0^\infty\left(\mathbb{R}_x^n \times \mathbb{R}_y^p\right)$$

U_θ is an unitary operator on $L^2\left(\mathbb{R}_x^n \times \mathbb{R}_y^p\right)$. Now let the dilation $P_\theta(h) = U_\theta P(h) U_\theta^{-1}$ of the operator $P(h)$:

$$P_\theta(h) = -h^2 e^{-2\theta}\Delta_x + P\left(xe^{\theta}, y, D_y\right).$$

Then using the assumption (H_1) the family $P_\theta(h)$ can be extended to small enough complex values of θ as an analytic family of type A (see e.g [7, 17]).

Definition 3.1. *We say that a complex number ρ is a resonance of $P(h)$ if $\operatorname{Re}\rho > \inf \sigma_{ess}(P(h))$ and if there exists θ small enough, $\operatorname{Im}\theta > 0$, such that $\rho \in \sigma_{disc}(P_\theta(h))$ (see* [12]*). σ_{ess} and σ_{disc} are respectively the essential and the discrete spectrum.*

Notation 3.2. *We denote by* $\Gamma(h)$ *the set of resonances of the operator* $P(h)$ *.*

We need to recall some basic facts about h-pseudodifferential operators (see e.g. [11, 18, 19]).

A family of unbounded operators $A(h)$ on $L^2(\mathbb{R}^n)$, with fixed domain $H^{k_0}(\mathbb{R}^n)$ $k_0 \geq 0$, is said to be h-pseudodifferential if there exists a sequence $(a_j(x,\xi))_{j\in\mathbb{N}}$ of C^∞-functions on $\mathbb{R}^{2n}$ satisfying:

$$\forall j \in \mathbb{N}, \forall \alpha, \beta \in \mathbb{N}^n, \;\; \left|\partial_x^\alpha \partial_\xi^\beta a_j(x,\xi)\right| = \mathcal{O}\left(<\xi>^{k_0-|\beta|}\right)$$

uniformly on $\mathbb{R}^n$, with $<\xi>=\left(1+|\xi|^2\right)^{1/2}$ and for any $N \in \mathbb{N}$ large enough, $A(h)$ can be written

$$A(h) = \sum_{j=0}^{N} h^j Op_h^w(a_j) + h^N R_N(h)$$

where $R_N(h)$ is uniformly bounded on $L^2(\mathbb{R}^n)$ as $h \to 0^+$, and Op_h^w denotes the Weyl h-quantization of symbols:

$$Op_h^w(a_j)\varphi(x) = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} e^{\frac{i}{h}<x-y,\xi>} a_j\left(\frac{x+y}{2},\xi\right)\varphi(y)\,dyd\xi.$$

The function a_0 is called the principal symbol of $A(h)$.

Denote now $\lambda_0 = \inf\left\{Sp\left(P\left(x,y,D_y\right)\right) \setminus \left\{\lambda_1(x), \lambda_2(x), ..., \lambda_M(x)\right\}\right\}$.

Our main result is:

Theorem 3.3. *Under assumptions* $(H1)$ *to* $(H4)$*, and for any* z *complex close enough to* λ_0*, there exists a family of* $M \times M$*-matrixes* $A_\theta^{-+}(z)$*,* θ *complex small enough, of* h*-pseudodifferential operators on* $\mathbb{R}^n$ *depending analytically on* θ *such that:*

$$z \in \Gamma(h) \Leftrightarrow \exists \theta \in \mathbb{C}, \;\; \operatorname{Im}\theta > 0, 0 \in \sigma_{disc}(A_\theta^{-+}(z)).$$

In particular, $F(z) = z - A_\theta^{-+}(z)$ *has the diagonal matrix* $diag\left(\xi^2 + \lambda_j\left(xe^\theta\right)\right)_{1\leq j\leq M}$ *as principal symbol.*

4. The dilation Feshbach method

The Feshbach reduction is a way to construct an effective Hamiltonian of the spectral problem of $P_\theta(h)$. To get this construction in the context of h-pseudodifferential calculus we make use of a so-called Grushin problem involving a convenient choice of sections of $Ran\pi(x)$, where $\pi(x)$ denotes the orthogonal projector onto the eigenspace of $P(x,y,D_y)$ associated to $\{\lambda_1(x),\lambda_2(x),...,\lambda_M(x)\}$.

In fact, since we are interested in the resonances of $P(h)$, we make all these constructions for the analytic dilation $P_\theta(h)$ of $P(h)$.

Using the constructions made in [14], we have the following lemma:

Lemma 4.1. *Under (H1) to (H4), there exists an orthonormal family* $\left\{v_1^\theta(x), v_2^\theta(x),...,v_M^\theta(x)\right\}$ *in* $\mathcal{D}(P(x,y,D_y))$ *depending analytically with respect to* θ *complex small enough such that:*

1.: $v_j^\theta(x)\in C_b^\infty(\mathbb{R}^n,\mathcal{D}(P(x,y,D_y)))$ *for all* $j\in\{1,...,M\}$,

2.: $\left\{v_1^\theta(x),...,v_M^\theta(x)\right\}$ *generate the space* $\bigoplus_{j=1}^{M}\ker\left(P\left(xe^\theta,y,D_y\right)-\lambda_j\left(xe^\theta\right)\right)$.

If $\overset{M}{\underset{j=1}{\oplus}}\psi_j=(\psi_1,...,\psi_M)\in\left(L^2(\mathbb{R}^n)\right)^{\oplus M}$ and $\varphi\in L^2(\mathbb{R}^n,\mathcal{D}(P(x,y,D_y)))$ then we define the two following operators $R_\theta^\pm$ by:

$$\begin{array}{rcl} R_\theta^-:\bigoplus_{j=1}^{M}L^2(\mathbb{R}^n) & \longmapsto & L^2(\mathbb{R}^n,\mathcal{D}(P(x,y,D_y))) \\ \psi=\overset{M}{\underset{j=1}{\oplus}}\psi_j & \longrightarrow & R_\theta^-\psi=\sum_{j=1}^{M}\psi_j v_j^\theta(x) \end{array}$$

and

$$\begin{array}{rcl} R_\theta^+=\left(R_\theta^-\right)^*:L^2(\mathbb{R}^n,\mathcal{D}(P(x,y,D_y))) & \longrightarrow & \bigoplus_{j=1}^{M}L^2(\mathbb{R}^n) \\ \varphi & \longmapsto & R_\theta^+\varphi=\overset{M}{\underset{j=1}{\oplus}}<\varphi,v_j^\theta(x)>_{L^2(\mathbb{R}^n)}. \end{array}$$

We then consider a Grushin problem that will lead to the Feshbach reduction. For $z\in\mathbb{C}$, we consider the following matrix operator:

$$\mathcal{P}_\theta(z)=\begin{pmatrix} P_\theta(h)-z & R_\theta^- \\ R_\theta^+ & 0 \end{pmatrix} \text{ on } L^2(\mathbb{R}^n,\mathcal{D}(P(x,y,D_y)))\oplus\left(L^2(\mathbb{R}^n)\right)^{\oplus M}.$$

Then we have:

Theorem 4.2. *Assume (H1) to (H4). Then for any z complex such that* $\operatorname{Re} z < \lambda_0$, *the Grushin operator* $\mathcal{P}_\theta(\lambda)$ *maps* $H^2(\mathbb{R}^n, \mathcal{D}(P(x,y,D_y))) \oplus \left(L^2(\mathbb{R}^n)\right)^{\oplus M}$ *into* $L^2\left(\mathbb{R}^n, L^2(\mathbb{R}^p)\right) \oplus \left(L^2(\mathbb{R}^n)\right)^{\oplus M}$, *is invertible and its inverse is of the form:*

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

then $A_\theta(z)$, $A_\theta^\pm(z)$ *and* $A_\theta^{-+}(z)$ *are h-pseudodifferential operators. Moreover, we have the following spectral reduction:*

$$z \in Sp(P_\theta(h)) \Longleftrightarrow \exists \theta \in \mathbb{C},\ \operatorname{Im}\theta > 0,\ z \in Sp(F_\theta(z)) \tag{4.1}$$

where $F_\theta(z) = z - A_\theta^{-+}(z)$ *is a $M \times M$ matrix of h-pseudodifferential operators on* $\left(L^2(\mathbb{R}^n)\right)^{\oplus M}$ *with the diagonal matrix diag* $\left(\xi^2 + \lambda_j\left(xe^\theta\right)\right)_{1\le j\le M}$ *as principal symbol.*

Proof. We can consider the Grushin operator $\mathcal{P}_\theta(z)$ as an h-pseudodifferential operator with operator-valued symbol $p_\theta(x,\xi;z)$ given by:

$$p_\theta(x,\xi;z) = \begin{pmatrix} \xi^2 + P\left(xe^\theta, y, D_y\right) - z & R_\theta^- \\ R_\theta^+ & 0 \end{pmatrix}. \tag{4.2}$$

Using the fact that for any $z \in \mathbb{C}$ such that $\operatorname{Re} z < \lambda_0$ and $x \in \mathbb{R}^n$,

$$\operatorname{Re}\left(\widehat{\pi}_\theta(x)\, P\left(xe^\theta, y, D_y\right) \widehat{\pi}_\theta(x) - z\right) > 0 \tag{4.3}$$

the symbol $p_\theta(x,\xi;z)$ is invertible and its inverse $q_\theta(x,\xi;z)$ is given by:

$$q_\theta(x,\xi;z) = \begin{pmatrix} r_\theta(x,\xi;z) & R_\theta^- \\ R_\theta^+ & \left(z - \xi^2 - \lambda_j\left(xe^\theta\right)\right)_{1\le j\le M} \end{pmatrix} \tag{4.4}$$

where

$$r_\theta(x,\xi;z) = \widehat{\pi}_\theta(x)\left(\xi^2 + \widehat{\pi}_\theta(x)\, P\left(xe^\theta, y, D_y\right) \widehat{\pi}_\theta(x) - z\right)^{-1} \widehat{\pi}_\theta(x),$$

$\widehat{\pi}_\theta(x) = 1 - \pi_\theta(x)$, $\pi_\theta(x)$ denotes the orthogonal projection on the space $\bigoplus_{j=1}^{M} \ker\left(P\left(xe^\theta, y, D_y\right) - \lambda_j\left(xe^\theta\right)\right)$.

Due to $(H4)$ and (4.3), we can consider the Weyl quantification $Q_\theta(z) = Op_h^w(q_\theta(x,\xi;z)) : L^2\left(\mathbb{R}^n, L^2(\mathbb{R}^p)\right) \oplus \left(L^2(\mathbb{R}^n)\right)^{\oplus M} \longrightarrow H^2\left(\mathbb{R}^n, \mathcal{D}\left(P(x,y,D_y)\right)\right) \oplus \left(L^2(\mathbb{R}^n)\right)^{\oplus M}$.

The symbolic calculus and especially the composition theorem of h-pseudodifferential operators allows us to obtain,

$$\begin{cases} \mathcal{P}_\theta(z)\, Q_\theta(z) = I + hR_1; & \|R_1\|_{\mathcal{L}\left(L^2(\mathbb{R}^n, L^2(\mathbb{R}^p)) \oplus (L^2(\mathbb{R}^n))^{\oplus M}\right)} = \mathcal{O}(1) \\ Q_\theta(z)\, \mathcal{P}_\theta(z) = I + hR_2; & \|R_2\|_{\mathcal{L}\left(H^2(\mathbb{R}^n, \mathcal{D}(P(x,y,D_y))) \oplus (L^2(\mathbb{R}^n))^{\oplus M}\right)} = \mathcal{O}(1) \end{cases}.$$

Here, the estimates of $\|R_1\|$ and $\|R_2\|$ are uniform with respect to h. As a consequence, for h small enough, $\mathcal{P}_\theta(z)$ is invertible and its inverse is given by the Neumann series:

$$(\mathcal{P}_\theta(z))^{-1} = Q_\theta(z)\left(I + \sum_{k=1}^{+\infty} h^k R_1^k\right) = \left(I + \sum_{k=1}^{+\infty} h^k R_2^k\right) Q_\theta(z). \tag{4.5}$$

In view of (4.5) and the expression of the symbol $q_\theta(x,\xi;z)$ it remains to prove the equivalence (4.1). This comes from the two following algebraic identities:

$$\begin{aligned} ((P_\theta(h) - z)\, u = v) \quad &\Leftrightarrow \quad \mathcal{P}_\theta(z)\,(u \oplus 0) = v \oplus (< u, \underset{j=1}{\overset{M}{\oplus}} v_j^\theta(x) >_{L^2(\mathbb{R}^p)}) \\ &\Leftrightarrow \quad (u \oplus 0) = (\mathcal{P}_\theta(z))^{-1}\,(v \oplus (< u, \underset{j=1}{\overset{M}{\oplus}} v_j^\theta(x) >_{L^2(\mathbb{R}^p)})) \end{aligned}$$

$$((P_\theta(h) - z)\, u = v) \Leftrightarrow \begin{cases} u = A_\theta(z)\ v + A_\theta^+(z)\,(< u, \underset{j=1}{\overset{M}{\oplus}} v_j^\theta(x) >_{L^2(\mathbb{R}^p)}) \\ 0 = A_\theta^-(z)\, v + A_\theta^{-+}(z)\,(< u, \underset{j=1}{\overset{M}{\oplus}} v_j^\theta(x) >_{L^2(\mathbb{R}^p)}) \end{cases} \tag{4.6}$$

and

$$\begin{aligned} \left(A_\theta^{-+}(z)\,\alpha = \beta\right) \quad &\Leftrightarrow \quad (\mathcal{P}_\theta(z))^{-1}\,(0 \oplus \alpha) = \left(A_\theta^+(z)\,\alpha\right) \oplus \beta \\ &\Leftrightarrow \quad 0 \oplus \alpha = \mathcal{P}_\theta(z)\,(\left(A_\theta^+(z)\,\alpha\right) \oplus \beta) \end{aligned}$$

$$\left(A_\theta^{-+}(z)\,\alpha = \beta\right) \Leftrightarrow \begin{cases} 0 = (P_\theta(h) - z)\left(A_\theta^+(z)\,\alpha\right) + \underset{j=1}{\overset{M}{\oplus}} v_j^\theta(x)\,\beta \\ \alpha = < A_\theta^+(z)\,\alpha, \underset{j=1}{\overset{M}{\oplus}} v_j^\theta(x) >_{L^2(\mathbb{R}^p)} \end{cases}. \tag{4.7}$$

If $z \notin Sp\left(P_\theta\left(h\right)\right)$, then from (4.7) we deduce:

$$A_\theta^{-+}\left(z\right)\alpha = \beta \Leftrightarrow \begin{cases} A_\theta^{+}\left(z\right)\alpha = -\left(P_\theta\left(h\right)-z\right)^{-1}\left(\underset{j=1}{\overset{M}{\oplus}} v_j^\theta\left(x\right)\beta\right) \\ \alpha =< -\left(P_\theta\left(h\right)-z\right)^{-1}\left(\underset{j=1}{\overset{M}{\oplus}} v_j^\theta\left(x\right).\right), \underset{j=1}{\overset{M}{\oplus}} v_j^\theta\left(x\right) >_{L^2(\mathbb{R}^p)} \beta \end{cases}.$$

In particular,

$$0 \notin Sp\left(A_\theta^{-+}\left(z\right)\right) \text{ and } \left(A_\theta^{-+}\left(z\right)\right)^{-1} = -<\left(P_\theta\left(h\right)-z\right)^{-1}\left(\underset{j=1}{\overset{M}{\oplus}} v_j^\theta\left(x\right).\right), \underset{j=1}{\overset{M}{\oplus}} v_j^\theta\left(x\right) >_{L^2(\mathbb{R}^p)}.$$

Conversely, if $0 \notin Sp\left(A_\theta^{-+}\left(z\right)\right)$, then (4.6) gives:

$$\left(P_\theta\left(h\right)-z\right)u = v \Leftrightarrow \begin{cases} < u, \underset{j=1}{\overset{M}{\oplus}} v_j^\theta\left(x\right) >_{L^2(\mathbb{R}^p)} = -\left(A_\theta^{-+}\left(z\right)\right)^{-1}\left(A_\theta^{-}\left(z\right)v\right) \\ u = A_\theta\left(z\right)v - A_\theta^{+}\left(z\right)\left(A_\theta^{-+}\left(z\right)\right)^{-1}A_\theta^{-}\left(z\right)v \end{cases}.$$

As a consequence,

$$z \notin Sp\left(P_\theta\left(h\right)\right) \text{ and } \left(P_\theta\left(h\right)-z\right)^{-1} = A_\theta\left(z\right) - A_\theta^{+}\left(z\right)\left(A_\theta^{-+}\left(z\right)\right)^{-1}A_\theta^{-}\left(z\right).$$

□

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