Resonances for a General Hamiltonian in the Born-Oppenheimer Approximation

by

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Abstract: We study the discrete spectrum of a general class of Born-Oppenheimer Hamiltonians of the type:

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

when h tends to 0^+, here $P(x,y,D_y)$ is a pseudodifferential operator on $L^2(\mathbb{R}^p_y)$. In the case where the first eigenvalue $\lambda_1(x)$ of $P(x,y,D_y)$ on $L^2(\mathbb{R}^p_y)$ admits one non degenerate point-well, we obtain WKB-type expansions for all order in $h^{1/2}$ of eigenvalues (in the interval $[0, C_0h]$, $C_0 > 0$) and associated normalized eigenfunctions of H, and this for all orders in $h^{1/2}$.

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0 Introduction

The Born-Oppenheimer approximation is a method introduced in [2] to analyse the spectrum of molecules. It consists in studying the behavior of the associate Hamiltonian when the nuclear mass tends to infinity. This Hamiltonian can be written in the form:

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

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.

In the last decade, many efforts have been made in order to study in the semiclassical limit the spectrum of P (see e.g. [24], [12], [14], [17], [20], [**?**],...). 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.

It has been proved, both for smooth potentials [14] and for the physically interesting case of Coulomb interaction potentials (see , [12, 20]), the existence for the operator P of asymptotic expansions for eigenvalues and associated eigenfunctions of the types:

$$\sum_{j\geq 0} \alpha_j h^{j/2} \text{ and } e^{-\psi(x)/h}\left(\sum_{j\geq 0} a_j(x,y)\, h^{j/2}\right),$$

where $\psi(x)$ is the Agmon distance between x and the potential well.

Here we plan to give a unified version of the two results in [14] and [12], which can be applied to the general class of operators of the type $H = -h^2\Delta_x + P(x, y, D_y)$, where $P(x, y, D_y)$ is a pseudodifferential operator on $\mathcal{H}_2 = L^2(\mathbb{R}_y^p)$ (the so-called electronic Hamiltonian and its eigenvalues are the so-called electronic levels).

By using the h-pseudodifferential operators with operator-valued symbol and the general Feshbach reduction scheme (see [1, 22]), the spectral study of H on $L^2(\mathbb{R}_x^n \times \mathbb{R}_y^p)$ is reduced to that of a matrix of h-pseudodifferential operators $F(\lambda)$ on $\left(L^2(\mathbb{R}_x^n)\right)^{\oplus m}$ (the so-called effective Hamiltonian) with principal symbol the diagonal matrix $diag\left(\xi^2 + \lambda_j(x)\right)_{1\le j\le m}$ where $m > 0$ depends on the energy level and $(\lambda_j(x))_{1\le j\le m}$ are the electronic levels. In particular, we obtain the following equivalence:

$$\lambda \in Sp(H) \Longleftrightarrow \lambda \in Sp(F(\lambda))$$

(here Sp stands for the spectrum).

The general theory of Helffer and Sjöstrand in [8] can be applied to the operator $F(\lambda)$ and shows the existence of formal WKB-type expansions for eigenfunctions of this operator. This finally gives the formal WKB-type expansions for the operator H itself.

The argument of Martinez in [14] gives a justification to the formal WKB-constructions by showing that, modulo an error of size $\mathcal{O}(h^\infty)$, the formal eigenfunctions approximate correctly the true eigenfunctions of H.

The plan of this paper is the following. In the first section we introduce our assumptions and give preliminaries. The spectral reduction of the problem is given in the second section. The third section is devoted to state our main result and apply the reduction theorem obtained in the section 2 to establish the proof.

1 Assumptions and preliminaries

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

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

when h tends to 0^+, $P(x, y, D_y)$ is a pseudodifferential operator on $L^2(\mathbb{R}_y^p)$ 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 $L^2(\mathbb{R}_y^p)$. $P(x, y, D_y)$ can be analytically extended on the complex strip

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

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

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

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:

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

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:

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

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.

$(H4)$ $P(x, y, D_y) \in C_b^\infty\left(\mathbb{R}^n, \mathcal{L}\left(\mathcal{D}(P(x, y, D_y)), L^2(\mathbb{R}_y^p)\right)\right)$, 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

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

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

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

- A second example is the Born-Oppenheimer Hamiltonian (see e.g [20, **?**, 12]) for the differential operator

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

where $V(x, y)$ is the Coulomb interaction potential. For the study of resonances of $P(h)$ in this example see the works of Martinez-Messirdi [17] and those of Messirdi-Senoussaoui-Djellouli [**?**].

2 Preliminaries and main result

In this paper we characterize the resonances of $P(h)$ by using the analytic dilation introduced by Hunziker [10]. More precisely, for θ real small enough we consider the transformation xe^θ 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 $L^2\left(\mathbb{R}^n_x \times \mathbb{R}^p_y\right)$. 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 familly $P_\theta(h)$ can be extended to small enough complex values of θ as analytic family of type A (see e.g [11, **?**]).

Definition 1 *We say that a complex number ρ is a resonance of $P(h)$ if $\operatorname{Re}\rho > \inf \sigma_{ess}(P(h))$ and there exists θ small enough, $\operatorname{Im}\theta > 0$, such that $\rho \in \sigma_{disc}(P(h))$. σ_{ess} and σ_{disc} are respectively the essential and the discrete spectrum.*

Notation 2 *We denote by $\Gamma(h)$ the set of resonances of the operator $P(h)$.*

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 symboles:

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

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

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

Our main result is:

Theorem 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 $\left(\xi^2 + \lambda_j(x)\right)_{1\leq j\leq M}$ as principal symbol.

3 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 [18], we have the following lemma:

Lemma 4 *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:

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

and

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

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 5 *Assume (H1) to (H4). Then for any z complex such that* $\operatorname{Re} z < \lambda_0$*, the Grushin operator* $\mathcal{P}_\theta(\lambda) : H^2(\mathbb{R}^n, \mathcal{D}(P(x,y,D_y))) \oplus \left(L^2(\mathbb{R}^n)\right)^{\oplus M} \longrightarrow L^2\left(\mathbb{R}^n, L^2(\mathbb{R}^p)\right) \oplus \left(L^2(\mathbb{R}^n)\right)^{\oplus M}$ *, if we write it's inverse as:*

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

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

$$z \in Sp(P_\theta(h)) \Longleftrightarrow z \in Sp(F_\theta(z)), \ \operatorname{Im}\theta > 0 \tag{2.1}$$

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:

$$p_\theta(x,\xi;z) = \begin{pmatrix} \xi^2 + P\left(xe^\theta, y, D_y\right) - z & R_\theta^- \\ R_\theta^+ & 0 \end{pmatrix}. \tag{2.2}$$

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

$$\operatorname{Re}\left(\widehat{\pi}_\theta(x) P\left(xe^\theta, y, D_y\right) \widehat{\pi}_\theta(x) - z\right) > 0 \tag{2.3}$$

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

$$q_\theta(x,\xi;z) = \begin{pmatrix} \widehat{\pi}_\theta(x)\left(\xi^2 + \widehat{\pi}_\theta(x) P\left(xe^\theta, y, D_y\right)\widehat{\pi}_\theta(x) - z\right)^{-1}\widehat{\pi}_\theta(x) & R_\theta^- \\ R_\theta^+ & \left(z - \xi^2 - \lambda_j\left(xe^\theta\right)\right)_{1\le j\le M} \end{pmatrix} \tag{2.4}$$

where $\widehat{\pi}_\theta(x) = 1 - \pi_\theta(x)$, $\pi_\theta(x)$ 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 (2.3), we can consider the Weyl quantification $Q_\theta(z) = Op_h^w(q_\theta(x,\xi;z)) : L^2\left(\mathbb{R}^n, L^2(\mathbb{R}^p)\right) \oplus \left(L^2(\mathbb{R}^n)\right)^{\oplus M} \longrightarrow H^2(\mathbb{R}^n, \mathcal{D}(P(x,y,D_y))) \oplus \left(L^2(\mathbb{R}^n)\right)^{\oplus M}$.
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:

$$(\mathcal{P}_\theta(z))^{-1} = Q_\theta(z)\left(I + \sum_{k=1}^{+\infty} h^k R_1^k\right) = \left(I + \sum_{k=1}^{+\infty} h^k R_2^k\right) Q_\theta(z). \tag{2.5}$$

In view of (2.5) and the expression of the symbol $q_\theta(x,\xi;z)$ it remains to prove the equivalence (2.1). This comes from the two following algebraic identities:

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

$$
((P_\theta(h)-z)\,u=v) \Leftrightarrow \begin{cases} u=A_\theta(z)\;v+A_\theta^+(z)(<u,\overset{M}{\underset{j=1}{\oplus}} v_j^\theta(x)>_{L^2(\mathbb{R}^p)})\\ 0=A_\theta^-(z)\,v+A_\theta^{-+}(z)(<u,\overset{M}{\underset{j=1}{\oplus}} v_j^\theta(x)>_{L^2(\mathbb{R}^p)}) \end{cases} \tag{2.6}
$$

and

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

$$
\left(A_\theta^{-+}(z)\,\alpha=\beta\right) \Leftrightarrow \begin{cases} 0=(P_\theta(h)-z)\left(A_\theta^+(z)\,\alpha\right)+\overset{M}{\underset{j=1}{\oplus}} v_j^\theta(x)\,\beta\\ \alpha=<A_\theta^+(z)\,\alpha,\overset{M}{\underset{j=1}{\oplus}} v_j^\theta(x)>_{L^2(\mathbb{R}^p)} \end{cases}. \tag{2.7}
$$

If $z\notin Sp(P_\theta(h))$, then from (2.7) we deduce:

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

In particular,

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

Conversely, if $0\notin Sp\left(A_\theta^{-+}(z)\right)$, then (2.6) gives:

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

As a consequence,

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

$\blacksquare$

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