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Asymptotic Expansions for a General Hamiltonians in the Born-Oppenheimer Approximation

Abderrahmane Senoussaoui*

Université Libre de Bruxelles,
Département de Mathématiques,
Campus Plaine ULB, CP214 Bld du Triomphe, B-1050,
Bruxelles-BELGIUM.

Abstract

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

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

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

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I. 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 $x \in \mathbf{R^n}$ represents the position of the nuclei, $y \in \mathbf{R^p}$ 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.[4],[6],[7],[8],[9],[10],...). 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[7] and for the physically interesting case of Coulomb interaction potentials (see ,[6,9]), the existence for the operator P of asymptotic expansions for eigenvalues and associated eigenfunctions of the types:

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*Permanent address: Université d'Oran Es-sénia, Département de Mathématiques, Faculté des Sciences, B.P. 1524 El-Mnaouer, Oran 31000, ALGERIA.

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

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

Here we plan to give a unified version of the two results in[7] and[6], which can be applied to the general class of operators of the type $H = -h^2\Delta_x + P\left(x,y,D_y\right)$, where $P\left(x,y,D_y\right)$ is a pseudodifferential operator on $\mathcal{H}_2 = L^2\left(\mathbf{R}^{\mathbf{p}}_{\mathbf{y}}\right)$ (the so-called electronic Hamiltonian and its eigenvalues are the so-called electronic levels).

By using the h-pseudodifferential operators with operator-valued symbol and the general Feshbach reduction scheme (see[1,11]), the spectral study of H on $L^2\left(\mathbf{R}^{\mathbf{n}}_{\mathbf{x}}\times\mathbf{R}^{\mathbf{p}}_{\mathbf{y}}\right)$ is reduced to that of a matrix of h-pseudodifferential operators $F\left(\lambda\right)$ on $\left(L^2\left(\mathbf{R}^{\mathbf{n}}_{\mathbf{x}}\right)\right)^{\oplus m}$ (the so-called effective Hamiltonian) with principal symbol the diagonal matrix $diag\left(\xi^2+\lambda_j\left(x\right)\right)_{1\leq j\leq m}$ where $m>0$ depends on the energy level and $\left(\lambda_j\left(x\right)\right)_{1\leq j\leq m}$ are the electronic levels. In particular, we obtain the following equivalence:

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

(here Sp stands for the spectrum).

The general theory of Helffer and Sjöstrand in[5] can be applied to the operator $F\left(\lambda\right)$ 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[7] gives a justification to the formal WKB-constructions by showing that, modulo an error of size $\mathcal{O}\left(h^\infty\right)$, 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.

II. ASSUMPTIONS AND PRELIMINARIES

On the pseudodifferential operator $Q\left(x\right)=P\left(x,y,D_y\right)$, we assume (H1), (H2) and (H3) below.

(H1) For every $x\in\mathbf{R}^{\mathbf{n}}$, $Q\left(x\right)$ is selfadjoint and bounded from below on $\mathcal{H}_2$ with x-independent domain $\mathcal{H}_1$.

(H2) The spectrum of the pseudodifferential operator $Q\left(x\right)$ has two disjoint components for every $x\in\mathbf{R}^{\mathbf{n}}$:

$$Sp\left(Q\left(x\right)\right)=\left\{\lambda_1\left(x\right),\lambda_2\left(x\right),...,\lambda_m\left(x\right)\right\}\cup\Gamma\left(x\right)$$

where $\lambda_1\left(x\right),\lambda_2\left(x\right),...,\lambda_m\left(x\right)$ depend continuously on x, there is a gap between them and the rest of $Sp\left(Q\left(x\right)\right)$ more precisely:

$$\exists\delta>0,\quad\inf\Gamma\left(x\right)>\max\left\{\lambda_1\left(x\right),\lambda_2\left(x\right),...,\lambda_m\left(x\right)\right\}+\delta,\ \forall x\in\mathbf{R}^{\mathbf{n}}$$

and remain uniformly separated outside some compact subset of $\mathbf{R}^{\mathbf{n}}$:

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

(H3) $Q\left(x\right)\in C_b^\infty\left(\mathbf{R}^{\mathbf{n}},\mathcal{L}\left(\mathcal{H}_1,\mathcal{H}_2\right)\right)$, $Q\left(x\right)$ depends smoothly on x and is uniformly bounded together with all its derivatives as an operator from $\mathcal{H}_1$ to $\mathcal{H}_2$.

Examples:

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

$$\mathcal{H}_1 = H^2(\mathbf{R_y}) \cap \{\varphi \in L^2(\mathbf{R_y});\ y^2\varphi \in L^2(\mathbf{R_y})\ \},$$

$$\lambda_j(x) = (2j+1)\left(1+x^2\right)^l;\ j = 1, ..., m$$

$$\text{and } \Gamma(x) = \left\{(2j+1)\left(1+x^2\right)^l;\ j \geq m+1\right\}$$

- A second example is given in[9,10] for the differential operator $\widehat{Q}(x) = U(x)\left(-\Delta_y + V(x,y)\right)U^{-1}(x)$ where $U(x)$ is a diffeomorphism regularizing the physical case of the Coulomb interaction potential $V(x,y)$.

We denote by $S^m\left(\mathbf{R^{2n}}, \mathcal{L}(\mathbf{A},\mathbf{B})\right)$ the space of operator-valued symbols of order $m \in \mathbf{R}$:

$$\left\{a : \mathbf{R^{2n}} \mapsto \mathcal{L}(\mathbf{A},\mathbf{B}) \in \mathbf{C}^\infty;\ \forall(\alpha,\beta) \in \mathbf{R^{2n}},\ \left\|\partial_\mathbf{x}^\alpha \partial_\xi^\beta \mathbf{a}(\mathbf{x},\xi)\right\|_{\mathcal{L}(\mathbf{A},\mathbf{B})} = \mathcal{O}(<\xi>^\mathbf{m})\right\}$$

with $<\xi> = \left(1+|\xi|^2\right)^{1/2}$ and $\mathcal{L}(A,B)$ the space of bounded linear operators from the Hilbert space A to the Hilbert space B.

For $\varphi \in \mathcal{S}(\mathbf{R^n}, \mathbf{A})$ (the Schwartz space), $x \in \mathbf{R^n}$ and $a \in S^m\left(\mathbf{R^{2n}}, \mathcal{L}(\mathbf{A},\mathbf{B})\right)$, the h-pseudodifferential operator (the Weyl quantification of the symbol a) is defined by:

$$Op_h^w(a)\varphi(x) = (2\pi h)^{-1} \int_{\mathbf{R^{2n}}} e^{\frac{i}{h}<x-y,\xi>} a\left(\frac{x+y}{2}, \xi\right)\varphi(y)\, dyd\xi.$$

Note that $Op_h^w(a)$ maps continuously $\mathcal{S}(\mathbf{R^n},\mathbf{A})$ into $\mathcal{S}(\mathbf{R^n},\mathbf{B})$. In particular, due to a slight generalization of the Caldéron-Vaillancourt theorem (see[3,11]), if $m \leq 0$ then $Op_h^w(a) \in \mathcal{L}\left(L^2(\mathbf{R^n},\mathbf{A}), L^2(\mathbf{R^n},\mathbf{B})\right)$.

Using the constructions made in[6] lemma 1.1, we have the following lemma:

Lemma 1.1: *Under (H1) to (H3), there exist an orthonormal family* $\{u_1(x), u_2(x), ..., u_m(x)\}$ *in* $\mathcal{H}_2$ *such that:*

1. $\forall j \in \{1,...,m\},\ u_j(x) \in C_b^\infty(\mathbf{R^n}, \mathcal{H}_2)$,
2. $\{u_1(x), u_2(x), ..., u_m(x)\}$ *generates the space* $\bigoplus_{j=1}^m \ker(Q(x) - \lambda_j(x))$.

III. FESHBACH REDUCTION

If $\overset{m}{\underset{j=1}{\oplus}} \psi_j = (\psi_1, ..., \psi_m) \in \left(L^2(\mathbf{R^n})\right)^{\oplus m}$ and $\varphi \in L^2(\mathbf{R^n}, \mathcal{H}_1)$ then we define:

$$\overset{m}{\underset{j=1}{\oplus}} u_j(x)\left(\overset{m}{\underset{j=1}{\oplus}} \psi_j\right) = \sum_{j=1}^m u_j(x)\psi_j,\ \ <\varphi, \overset{m}{\underset{j=1}{\oplus}} u_j(x)>_{\mathcal{H}_2} = \overset{m}{\underset{j=1}{\oplus}} (<\varphi, u_j(x)>_{\mathcal{H}_2}).$$

For $\lambda \in \mathbf{R}$, we consider the following matrix operator (the so-called Grushin operator):

$$\mathcal{P}(\lambda) = \begin{pmatrix} & \overset{m}{\underset{j=1}{\oplus}} u_j(x) \\ <\cdot, \overset{m}{\underset{j=1}{\oplus}} u_j(x)>_{\mathcal{H}_2} & 0 \end{pmatrix} \text{ on } L^2(\mathbf{R^n}, \mathcal{H}_1) \oplus \left(L^2(\mathbf{R^n})\right)^{\oplus m}.$$

Denote by $\lambda_+ = \inf_{x\in\mathbf{R^n}} \{Sp(Q(x)) \setminus \{\lambda_1(x), \lambda_2(x), ..., \lambda_m(x)\}\}$. Then we have:

Theorem 2.1: *Assume (H1)-(H3). Then for any* $\lambda < \lambda_+$, *the Grushin operator* $\mathcal{P}(\lambda) : H^2(\mathbf{R^n}, \mathcal{H}_1) \oplus \left(L^2(\mathbf{R^n})\right)^{\oplus m} \longrightarrow L^2(\mathbf{R^n}, \mathcal{H}_2) \oplus \left(L^2(\mathbf{R^n})\right)^{\oplus m}$ *is invertible and its inverse can be written as:*

$$\mathcal{P}(\lambda)^{-1} = \begin{pmatrix} E(\lambda) & E_+(\lambda) \\ E_-(\lambda) & E_{-+}(\lambda) \end{pmatrix}$$

where $E(\lambda), E_\pm(\lambda)$ *and* $E_{-+}(\lambda)$ *are h-pseudodifferential operators.*

Moreover, we have the following equivalence:

$$\lambda \in Sp(H) \Longleftrightarrow \lambda \in Sp(F(\lambda)) \tag{2.1}$$

where $F(\lambda) = \lambda - E_{-+}(\lambda)$ *is a* $m \times m$ *matrix of h-pseudodifferential operators on* $(L^2(\mathbf{R}^\mathbf{n}))^{\oplus m}$ *with the diagonal matrix diag* $(\xi^2 + \lambda_j(x))_{1\le j\le m}$ *as principal symbol.*

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

$$p_\lambda(x,\xi) = \begin{pmatrix} \xi^2 + Q(x) - \lambda & \overset{m}{\underset{j=1}{\oplus}} u_j(x) \\ <., \overset{m}{\underset{j=1}{\oplus}} u_j(x) >_{\mathcal{H}_2} & 0 \end{pmatrix} \tag{2.2}$$

Using the fact that for any $\lambda < \lambda_+$ and $x \in \mathbf{R}^\mathbf{n}$,

$$\widehat{\pi}(x) Q(x) \widehat{\pi}(x) - \lambda > 0 \tag{2.3}$$

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

$$q_\lambda(x,\xi) = \begin{pmatrix} \widehat{\pi}(x)\left(\xi^2 + \widehat{\pi}(x) Q(x) \widehat{\pi}(x) - \lambda\right)^{-1} \widehat{\pi}(x) & \overset{m}{\underset{j=1}{\oplus}} u_j(x) \\ <., \overset{m}{\underset{j=1}{\oplus}} u_j(x) >_{\mathcal{H}_2} & \left(\lambda - \xi^2 - \lambda_j(x)\right)_{1\le j\le m} \end{pmatrix} \tag{2.4}$$

where $\widehat{\pi}(x) = 1 - \pi(x)$, $\pi(x)$ denotes the orthogonal projection on the space $\bigoplus_{j=1}^{m} \ker(Q(x) - \lambda_j(x))$.

Due to (H3) and (2.3), we can consider the Weyl quantification $Q(\lambda) = Op_h^w(q_\lambda) : L^2(\mathbf{R}^\mathbf{n}, \mathcal{H}_2) \oplus (L^2(\mathbf{R}^\mathbf{n}))^{\oplus m} \longrightarrow H^2(\mathbf{R}^\mathbf{n}, \mathcal{H}_1) \oplus (L^2(\mathbf{R}^\mathbf{n}))^{\oplus m}$ .ially the composition theorem of h-pseudodiff-erential operators allows us to obtain,

$$\begin{cases} \mathcal{P}(\lambda) Q(\lambda) = I + hR_1; \ \|R_1\|_{\mathcal{L}\left(L^2(\mathbf{R}^\mathbf{n}, \mathcal{H}_2) \oplus (L^2(\mathbf{R}^\mathbf{n}))^{\oplus m}\right)} = \mathcal{O}(1) \\ Q(\lambda) \mathcal{P}(\lambda) = I + hR_2; \ \|R_2\|_{\mathcal{L}\left(H^2(\mathbf{R}^\mathbf{n}, \mathcal{H}_1) \oplus (L^2(\mathbf{R}^\mathbf{n}))^{\oplus m}\right)} = \mathcal{O}(1) \end{cases}.$$

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

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

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

$$\begin{aligned} ((H-\lambda)u = v) &\Leftrightarrow \mathcal{P}(\lambda)(u \oplus 0) = v \oplus (<u, \overset{m}{\underset{j=1}{\oplus}} u_j(x) >_{\mathcal{H}_2}) \\ &\Leftrightarrow (u \oplus 0) = \mathcal{P}(\lambda)^{-1}(v \oplus (<u, \overset{m}{\underset{j=1}{\oplus}} u_j(x) >_{\mathcal{H}_2})) \end{aligned}$$

$$((H-\lambda)u = v) \Leftrightarrow \begin{cases} u = E(\lambda)v + E_+(\lambda)(<u, \overset{m}{\underset{j=1}{\oplus}} u_j(x) >_{\mathcal{H}_2}) \\ 0 = E_-(\lambda)v + E_{-+}(\lambda)(<u, \overset{m}{\underset{j=1}{\oplus}} u_j(x) >_{\mathcal{H}_2}) \end{cases} \tag{2.6}$$

and

$$\begin{aligned}(E_{-+}(\lambda)\alpha=\beta) &\Leftrightarrow \mathcal{P}(\lambda)^{-1}(0\oplus\alpha)=(E_{+}(\lambda)\alpha)\oplus\beta\\ &\Leftrightarrow 0\oplus\alpha=\mathcal{P}(\lambda)((E_{+}(\lambda)\alpha)\oplus\beta)\end{aligned}$$

$$(E_{-+}(\lambda)\alpha=\beta)\Leftrightarrow\begin{cases}0=(H-\lambda)(E_{+}(\lambda)\alpha)+\overset{m}{\underset{j=1}{\oplus}}u_j(x)\beta\\ \alpha=<E_{+}(\lambda)\alpha,\overset{m}{\underset{j=1}{\oplus}}u_j(x)>_{\mathcal{H}_2}\end{cases}. \tag{2.7}$$

If $\lambda\notin Sp(H)$, then from (2.7) we deduce:

$$E_{-+}(\lambda)\alpha=\beta\Leftrightarrow\begin{cases}E_{+}(\lambda)\alpha=-(H-\lambda)^{-1}(\overset{m}{\underset{j=1}{\oplus}}u_j(x)\beta)\\ \alpha=<-(H-\lambda)^{-1}(\overset{m}{\underset{j=1}{\oplus}}u_j(x).),\overset{m}{\underset{j=1}{\oplus}}u_j(x)>_{\mathcal{H}_2}\beta\end{cases}.$$

In particular,

$$0\notin Sp(E_{-+}(\lambda))\text{ and }E_{-+}(\lambda)^{-1}=-<(H-\lambda)^{-1}(\overset{m}{\underset{j=1}{\oplus}}u_j(x).),\overset{m}{\underset{j=1}{\oplus}}u_j(x)>_{\mathcal{H}_2}.$$

Conversely, if $0\notin Sp(E_{-+}(\lambda))$, then (2.6) gives:

$$(H-\lambda)u=v\Leftrightarrow\begin{cases}<u,\overset{m}{\underset{j=1}{\oplus}}u_j(x)>_{\mathcal{H}_2}=-E_{-+}(\lambda)^{-1}(E_{-}(\lambda)v)\\ u=E(\lambda)v-E_{+}(\lambda)E_{-+}(\lambda)^{-1}E_{-}(\lambda)v\end{cases}.$$

As a consequence,

$$\lambda\notin Sp(H)\text{ and }(H-\lambda)^{-1}=E(\lambda)-E_{+}(\lambda)E_{-+}(\lambda)^{-1}E_{-}(\lambda)$$

IV. WKB-CONSTRUCTIONS

In this section we will give asymptotic expansions in powers of $h^{1/2}$ for eigenvalues and eigenfunctions of H near the potential well formed by the first electronic level $\lambda_1(x)$ of $Q(x)$. Assume (H2) with $m=1$. By adding a constant to $Q(x)$ and a translation in the variable x, we assume that $\lambda_1(x)$ has a minimum strict at zero (a one point well not degenerate):

$$0=\inf_{x\in\mathbf{R^n}}\lambda_1(x),\quad \underline{\lim}_{|x|\mapsto\infty}\lambda_1(x)>0,\ \lambda_1^{-1}(0)=\{0\},\ \lambda_1''(0)>0.$$

Denoting by $\psi(x)$ the distance between $x\in\mathbf{R^n}$ and 0 in the Agmon metric $\lambda_1(x)dx^2$, it is known (see[5]) that there is a neighborhood Ω of 0 such that:

$$\psi\in C^\infty(\Omega,\mathbf{R}),\ (\nabla\psi)^2(x)=\lambda_1(x),\ \forall x\in\Omega.$$

We fix some (arbitrarily large) constant $C_0>0$ outside the spectrum of the harmonic oscillator $H_0=-\Delta_x+\frac{1}{2}<\lambda_1''(0)x,x>_{\mathbf{R^n}}$. Denote by $e_1,...,e_{N_0}$ the eigenvalues of H_0 in $[0,C_0]$,

$$Sp(H_0)=\left\{\sum_{i=1}^{n}(2\alpha_i+1)\sqrt{\mu_i};\ \alpha=(\alpha_1,...,\alpha_n)\in\mathbf{N^n}\right\}$$

where $\mu_1,...,\mu_n$ are the eigenvalues of the matrix $\lambda_1''(0)$. The main result is as follows:

Theorem 3.1. *Assume (H1)-(H3). H has N_0 eigenvalues $E_1(h)$, $E_2(h)$, ..., $E_{N_0}(h)$ in $[0,C_0h]$ such that, for every $j\in\{1,...,N_0\}$ and for h sufficiently small, $E_j(h)$ admit the following asymptotic expansion:*

$$E_j(h) = e_j h + \sum_{k\geq 1} \alpha_{j,k} h^{1+k/2} \quad \textit{modulo } \mathcal{O}(h^\infty) \tag{3.1}$$

$\alpha_{j,k} \in \mathbf{R}$. *If* $E_j(h)$ *is asymptotically simple (in the sense that the expansion* (3.1) *determines* $E_j(h)$ *in a unique way), then the associated normalized eigenfunction* $\varphi_j(x, y; h)$ *satisfies:*

$$e^{\psi(x)/h} \varphi_j(x, y; h) = h^{-m_j} \sum_{k\geq 0} a_{j,k}(x, y)\, h^{k/2} \quad \textit{modulo } \mathcal{O}(h^\infty)$$

in $C^\infty(\Omega, \mathcal{H}_1)$, *where* $a_{0,0} = \widetilde{a}_0(x)\, u_1(x, y)$, $\widetilde{a}_0(x) \neq 0$, $\forall x \in \Omega$, $m_j \in \mathbf{R}$, $m_1 = n/4$.

Before turning to the proof of the theorem 3.1, let us recall some basic facts on formal h-pseudodifferential operators with operator valued symbol. If Ω is an open set in $\mathbf{R^n}$, H is a Hilbert space and $m \in \mathbf{R}$, we introduce the space of formal power series:

$$S^m(\Omega, H) = \left\{ \sum_{k\geq 0} h^{-m+k/2} s_k(x)\,;\; s_k \in C^\infty(\Omega, H) \right\}. \tag{3.2}$$

For $\psi \in C^\infty(\Omega, \mathbf{R})$ and $\mathcal{V}$ a neighborhood of 0 in $\mathbf{R^n}$ we set

$$\Omega^* = \{(x, \xi) \in \Omega \times \mathbf{C}^n;\; \xi - i\nabla\psi(x) \in \mathcal{V}\} \tag{3.3}$$

and the space of formal symbol

$$S^0(\Omega^*, \mathcal{L}(H, K)) = \left\{ \sum_{k\geq 0} h^k p_k(x, \xi)\,;\; p_k \in C^\infty(\Omega^*, \mathcal{L}(H, K)) \right\} \tag{3.4}$$

where H, K denote Hilbert spaces. For any symbol $b(x, \xi, h) = b = \sum_{k\geq 0} h^k b_k \in S^0(\Omega^*, \mathcal{L}(H, K))$, one can define the action of the operator of symbol b on $e^{-\psi(x)/h} S^m(\Omega, H)$ by setting for $s \in S^m(\Omega, H)$:

$$e^{\psi(x)/h} Op_h^w(b) \left(e^{-\psi(x)/h} s\right)$$

$$= \sum_{\alpha\in\mathbf{N^n}} \frac{h^{|\alpha|}}{i^{|\alpha|}\alpha!} \partial_z^\alpha \left[\partial_\xi^\alpha b\left(\frac{x+z}{2}, i\nabla\psi(x), h\right) s(z, h)\, e^{-\mathcal{K}(x,z)/h} \right]_{z=x} \tag{3.5}$$

where

$$\mathcal{K}(x, z) = \psi(z) - \psi(x) - (z - x)\nabla\psi(x) = \mathcal{O}\left(|z - x|^2\right).$$

$Op_h^w(b)$ is called a formal h-pseudodifferential operator, this definition coincides with a formal stationary phase expansion.

One can verify as in[11] that

$$e^{\psi(x)/h} Op_h^w(b) \left(e^{-\psi(x)/h} s\right) \in S^m(\Omega, K).$$

Furthermore, if G is an Hilbert space and $c = \sum_{j\geq 0} h^j c_j \in S^0(\Omega^*, \mathcal{L}(K, G))$, then $Op_h^w(c) \circ Op_h^w(b) = Op_h^w(d)$ is a formal h-pseudodifferential operator with symbol $d(x, \xi, h) = \sum_{j\geq 0} h^j d_j(x, \xi) \in S^0(\Omega^*, \mathcal{L}(H, G))$ given by:

$$d_j(x, \xi) = \sum_{|\alpha|+|\beta|+k+l=j} \frac{(-1)^{|\beta|}}{\alpha!\beta!\,(2i)^{|\alpha|+|\beta|}} \left(\partial_\xi^\alpha \partial_x^\beta b_k\right) \left(\partial_\xi^\alpha \partial_x^\alpha c_l\right). \tag{3.6}$$

Proof of theorem 3.1: The main idea of the proof is to use a simplified formal version of the theorem 2.1. For $\lambda < \lambda_+$ we set

$$\widetilde{\mathcal{P}}(\lambda) = \begin{pmatrix} H-\lambda & u_1(x) \\ <.,u_1(x)>_{\mathcal{H}_2} & 0 \end{pmatrix} \text{ on } e^{-\psi(x)/h}S^m(\Omega, \mathcal{H}_1 \oplus \mathbf{C}),$$

$\widetilde{\mathcal{P}}(\lambda)$ is a formal h-pseudodifferential operator with symbol

$$\widetilde{p}(x,\xi;\lambda) = \begin{pmatrix} \xi^2 + Q(x) - \lambda & u_1(x) \\ <.,u_1(x)>_{\mathcal{H}_2} & 0 \end{pmatrix} \in S^0(\Omega^*, \mathcal{L}(\mathcal{H}_1 \oplus \mathbf{C}, \mathcal{H}_2 \oplus \mathbf{C}))$$

where Ω^* is defined as in (3.3) with $\psi(x)$ being the Agmon distance. As in the proof of the theorem 2.1, the inverse of the symbol $\widetilde{p}(x,\xi;\lambda)$ is given by:

$$q_0(x,\xi;\lambda) = \begin{pmatrix} \widehat{\pi}(x)\left(\xi^2 + \widehat{\pi}(x)Q(x)\widehat{\pi}(x) - \lambda\right)^{-1}\widehat{\pi}(x) & u_1(x) \\ <.,u_1(x)>_{\mathcal{H}_2} & \lambda - \xi^2 - \lambda_1(x) \end{pmatrix}. \tag{3.7}$$

This permit us, using the composition formula (3.6), to construct a formal h-pseudodifferential operator $\widetilde{\mathcal{Q}}(\lambda)$ of symbol (see[7],[11])

$$q_\lambda(x,\xi,h) = q_0(x,\xi;\lambda) + \sum_{k\geq 1} h^k q_k(x,\xi;\lambda) \in S^0(\Omega^*, \mathcal{L}(\mathcal{H}_2 \oplus \mathbf{C}, \mathcal{H}_1 \oplus \mathbf{C}))$$

such that

$$\widetilde{\mathcal{P}}(\lambda)\widetilde{\mathcal{Q}}(\lambda) = Id \quad \text{on } e^{-\psi(x)/h}S^m(\Omega, \mathcal{H}_2 \oplus \mathbf{C}). \tag{3.8}$$

Writing

$$\widetilde{\mathcal{Q}}(\lambda) = \begin{pmatrix} \widetilde{E}(\lambda) & \widetilde{E}_+(\lambda) \\ \widetilde{E}_-(\lambda) & \widetilde{E}_{-+}(\lambda) \end{pmatrix}$$

and setting $\widetilde{F}(\lambda) = \lambda - \widetilde{E}_{-+}(\lambda)$, by construction, the operator $\widetilde{F}(\lambda)$ is a nice formal h-pseudodifferential operator with scalar symbol

$$e_\lambda(x,\xi,h) = \xi^2 + \lambda_1(x) + \sum_{k\geq 1} h^k e_k(x,\xi;\lambda) \in S^0(\Omega^*, \mathbf{C}).$$

Since $\widetilde{F}(\lambda)$ is formally selfadjoint and $\lambda_1(x)$ admits a nondegenerate minimum at 0, the construction of Helffer and Sjöstrand in[5] Sect.3 gives N_0 formal series $\widetilde{E}_j(h;\lambda)$ for $j \in \{1,..,N_0\}$ of the form:

$$\widetilde{E}_j(h;\lambda) = e_j h + \sum_{k\geq 1} h^{1+k/2} e_{j,k}(\lambda) \quad \text{and} \quad a_j(x,h;\lambda) \in S^{m_j}(\Omega;\mathbf{C}) \tag{3.9}$$

such that

$$\left(\widetilde{F}(\lambda) - \widetilde{E}_j(h;\lambda)\right)\left(e^{-\psi(x)/h}a_j(x,h;\lambda)\right) = 0 \text{ in } e^{-\psi(x)/h}S^{m_j}(\Omega;\mathbf{C}). \tag{3.10}$$

Fix $j \in \{1,..,N_0\}$. Using the analytical dependence in λ of the symbol $e_\lambda(x,\xi,h)$ of $\widetilde{F}(\lambda)$ and applying again the construction of Helffer and Sjöstrand for $\widetilde{F}\left(e_j h + \lambda' h^{3/2}\right)$ (λ' indicates a new parameter), this gives formal series of the form:

$$\widetilde{E}'_j(h;\lambda') = e_j h + e_{j,1}h^{3/2} + \sum_{k\geq 2} h^{1+k/2}\widetilde{e}_{j,k}(\lambda').$$

Setting $\lambda' = e_{j,1} + \lambda'' h^{1/2}$ (where λ'' indicates a new parameter) and reiterating this process, we obtain finally formal series (independent of λ):

$$\widetilde{E}_j(h) = e_j h + \sum_{k\geq 1} h^{1+k/2} e_{j,k} \text{ and } a_j(x,h) \in S^{m_j}(\Omega; \mathbf{C}).$$

Furthermore, we have:

$$\left(\widetilde{F}\left(\widetilde{E}_j(h)\right) - \widetilde{E}_j(h)\right)\left(e^{-\psi(x)/h} a_j(x,h)\right) = 0 \text{ in } e^{-\psi(x)/h} S^{m_j}(\Omega; \mathbf{C}) \tag{3.11}$$

$$< a_j(.,h), a_{j'}(.,h) >_\psi = \delta_{jj'} + \mathcal{O}(h) \tag{3.12}$$

where (3.12) holds in the sense of formal power series in h with complex coefficients. The inner product $< .,. >_\psi$ is defined by a formal stationary phase expansion at 0:

$$< u(x,h), v(x,h) >_\psi = \int_\Omega e^{-2\psi(x)/h} u(x,h) \overline{v(x,h)} dx.$$

Using (3.8) and the definitions of $\widetilde{\mathcal{P}}(\lambda)$ and $\widetilde{\mathcal{Q}}(\lambda)$, the equation (3.11) yields that the formal symbol:

$$b_j(x,y;h) = e^{\psi(x)/h} \widetilde{E}_+\left(\widetilde{E}_j(h)\right)\left(e^{-\psi(x)/h} a_j(x,h)\right) \in S^{m_j}(\Omega; \mathcal{H}_1) \tag{3.13}$$

solves

$$\left(H - \widetilde{E}_j(h)\right)\left(e^{-\psi(x)/h} b_j(x,y;h)\right) = 0 \text{ in } e^{-\psi(x)/h} S^{m_j}(\Omega; \mathcal{H}_2). \tag{3.14}$$

Since

$$\widetilde{E}_+(\lambda) = u_1(x,.) + \mathcal{O}(h) \text{ and } < u_1(x,.), u_1(x,.) >_{\mathcal{H}_2} = 1, \tag{3.15}$$

we get

$$< e^{-\psi(x)/h} b_j(.,.;h), e^{-\psi(x)/h} b_{j'}(.,.;h) >_{L^2(\Omega\times\mathbf{R^p})} = \delta_{jj'} + \mathcal{O}(h). \tag{3.16}$$

By a standard argument in[7] and[5] Sec.5, one can show that the eigenvalues $E_j(h)$ of H in $[0, C_0 h]$ ($C_0 > 0$ arbitrarily large) admit for asymptotic expansions $\widetilde{E}_j(h)$ found above. Moreover, if $E_j(h)$ is asymptotically simple, the formal series $e^{-\psi(x)/h} b_j(x,y;h)$ are the asymptotic expansions for the associated normalized eigenfunctions $\varphi_j(x,y;h)$ $(j = 1, ..., N_0)$. This is the case for the first eigenfunction $\varphi_1(x,y;h)$ (since $E_1(h)$ is simple) and $m_1 = n/4$ is chosen for the normalization.TCIMACRO

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