On a General Born–Oppenheimer Reduction Scheme

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Abstract

We perform a general reduction scheme that can be applied in particular to the spectral study of operators of the type $P = P(x, y, hD_x, D_y)$ as h tends to zero. This scheme permits to reduce the study of P to the one of a semiclassical matrix operator of the type $A = A(x, hD_x)$. Here, for any fixed $(x, \xi) \in \mathbb{R}^n$, the eigenvalues of the principal symbol $a(x, \xi)$ of A are eigenvalues of the operator $P(x, y, \xi, D_y)$.

1 Introduction

In the last decade, many efforts have been made by several authors in order to apply semiclassical techniques to problems in which extra nonsemiclassical variables occur (see, e.g., [GMS, Ha, KMSW, Ne, NeSo, So]). Such efforts have shown that, despite the presence of these extra variables, in many situations it is still possible to perform semiclassical constructions related to the existence of some hidden effective semiclassical operator.

In particular, this has been completely clarified in the case of the spectral study of molecules. In this case, the Hamiltonian can be written in the form

$$H = -h^2\Delta_x - \Delta_y + V(x, y) = -h^2\Delta_x + H_{\mathrm{el}}(x),$$

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 sum of all the interactions. The operator $H_{\mathrm{el}}(x)$ is the so-called electronic Hamiltonian and its eigenvalues are the so-called electronic levels. Then, by using the symbolic calculus, it has been proved in [KMSW] that

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the spectral study of H on $L^2(\mathbb{R}^{n+p})$ can be reduced to that of a semiclassical pseudodifferential matrix operator $H_{eff} = H_{eff}(x, hD_x)$ on $L^2(\mathbb{R}^n)^{\oplus N}$, where $N > 0$ depends on the energy level. Moreover, the principal part of H_{eff} can be explicitly related to the electronic levels in agreement with the original intuition of M. Born and R. Oppenheimer. Let us observe that, actually, $H_{eff} = H_{eff}^{\lambda}$ also depends on the spectral parameter λ, but this dependence is analytic and involves only $\mathcal{O}(h^2)$ terms. In compensation, the reduction is exact in the sense that one has the following equivalence (without error-terms):

$$\lambda \in \sigma(H) \;\Leftrightarrow\; \lambda \in \sigma(H_{eff}^{\lambda}). \tag{1.1}$$

(Here σ stands for the spectrum.) If one accepts error-terms of size $\mathcal{O}(h^{\infty})$, then other techniques exist that permit to construct a λ-independent effective Hamiltonian (see, e.g., [NeSo, So]). However, when one wants to study exponentially small quantitities (such as the tunneling effect), it becomes necessary to use (1.1).

The way in which (1.1) has been proved relies on the construction of an operator acting on a greater space (the so-called Grushin operator), by means of the eigenfunctions of $H_{\rm el}(x)$.

In the same spirit, another result of reduction has been proved in [GMS] for differential operators of the type $P(x, y, hD_x + D_y)$, where $P(x, y, \xi)$ is periodic in y. Here again, the idea was to construct a Grushin operator by means of the eigenfunctions of the operator $Q(x) := P(x, y, D_y)$.

Although these two constructions seem to be rather different from one each other, actually there exists some unified way to see them. Indeed, in both cases the construction is based on the eigenfunctions of the operator obtained by substituting a vector (say, ξ) to the operator hD_x (that is, the same procedure that relates quantum mechanics to classical mechanics). In the first case, the operator one obtains is $\xi^2 + H_{\rm el}(x)$ (that has the same eigenfunctions as $H_{\rm el}(x)$), and in the second case, one obtains $P(x, y, \xi + D_y)$, the eigenfunctions of which are deduced from those of $P(x, y, D_y)$ by conjugating with $e^{i\xi\cdot y}$. Because of the explicit dependence of these eigenfunctions with respect to ξ (indeed, trivial in the first case), the constructions performed in [KMSW, GMS] could be done without particular problems.

Here we plan to give a unified version of these reduction schemes, that can be applied to a general class of operators of the type $P(x, y, hD_x, D_y)$. In particular, we have to solve the additional difficulty that the eigenfunctions of $P(x, y, \xi, D_y)$ may depend on ξ in an essentially arbitrary way. However, our assumtions will permit us to quantize this dependence, and to obtain in this way a Grushin problem in the same spirit as in [KMSW, GMS]. Note that we consider only time-independent problems here: For related time-dependent results, one may consult e.g. [HaJo, MaSo, PST, SpTe].

2 Assumptions and Result

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two Hilbert spaces such that $\mathcal{H}_1 \subset \mathcal{H}_2$ and the natural injection $\mathcal{H}_1 \hookrightarrow \mathcal{H}_2$ is continuous. We denote by $\mathcal{H}_{1,2} := \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$ the space of bounded linear operators from $\mathcal{H}_1$ to $\mathcal{H}_2$ and we consider a family of operator-valued functions $(p_h)_{0<h\leq h_0}$ in $C^\infty(\mathbb{R}^{2n}; \mathcal{H}_{1,2})$ (here $h_0 > 0$ is some fixed small number), such that $p_h(x,\xi) = p_0(x,\xi) + hr_h(x,\xi)$ with p_0 independent of h, and for every multi-index $\alpha \in \mathbb{N}^{2n}$,

$$\|\partial^\alpha p_0(x,\xi)\|_{\mathcal{H}_{1,2}} + \|\partial^\alpha r_h(x,\xi)\|_{\mathcal{H}_{1,2}} = \mathcal{O}(1) \tag{2.1}$$

uniformly with respect to $h \in (0, h_0]$ and $(x,\xi) \in \mathbb{R}^{2n}$. For any $h > 0$ small we define the pseudodifferential operator P_h with symbol p_h by

$$\begin{array}{cccc} P_h : & L^2(\mathbb{R}^n, \mathcal{H}_1) & \to & L^2(\mathbb{R}^n, \mathcal{H}_2), \\ & u & \mapsto & P_h u, \end{array}$$

where for almost all $x \in \mathbb{R}^n$, $P_h u(x) \in \mathcal{H}_2$ is defined by the oscillatory integral (the so-called Weyl quantization of p_h, see, e.g., [Ma1])

$$P_h u(x) = \mathrm{Op}_h^W(p_h)u(x) := \frac{1}{(2\pi h)^n} \int e^{i(x-y)\xi/h} p_h\left(\frac{x+y}{2}, \xi\right) u(y)dy\, d\xi. \tag{2.2}$$

Note that P_h maps continuously $L^2(\mathbb{R}^n, \mathcal{H}_1)$ into $L^2(\mathbb{R}^n, \mathcal{H}_2)$, thanks to (a slight generalization of) the Calderón–Vaillancourt theorem (see [Ma1], Theorem 2.8.1).

We assume that for any $(x,\xi) \in \mathbb{R}^{2n}$, the spectrum $\sigma(p_0(x,\xi))$ of $p_0(x,\xi)$ contains a finite subset $\sigma_1(x,\xi)$ such that the following conditions hold for all $(x,\xi) \in \mathbb{R}^{2n}$:

(H1) There exist $\varphi_1, \dots, \varphi_m \in C_b^\infty(\mathbb{R}^{2n}; \mathcal{H}_1)$ such that for all $(x,\xi) \in \mathbb{R}^{2n}$ the family $(\varphi_1(x,\xi), \dots, \varphi_m(x,\xi))$ forms an orthonormal basis of the vector space $\mathcal{E}(x,\xi) := \sum_{\lambda\in\sigma_1(x,\xi)} \sum_{k\geq 1} \mathrm{Ker}(p_0(x,\xi) - \lambda)^k$. (Here C_b^∞ stands for the space of functions that are uniformly bounded together with all their derivatives.)

(H2) The space $\mathcal{H}_2$ can be split into $\mathcal{H}_2 = \mathcal{E}(x,\xi) \oplus \mathcal{F}(x,\xi)$ where $\mathcal{F}(x,\xi)$ is stable under $p_0(x,\xi)$, in the sense that $p_0(x,\xi)$ maps $\mathcal{F}(x,\xi) \cap \mathcal{H}_1$ into $\mathcal{F}(x,\xi)$. Moreover the two (nonorthogonal) projections $\Pi_{\mathcal{E}/\mathcal{F}}$ and $\Pi_{\mathcal{F}/\mathcal{E}}$ associated with the decomposition $\mathcal{H}_2 = \mathcal{E}(x,\xi) \oplus \mathcal{F}(x,\xi)$ are uniformly bounded and depend continuously on (x,ξ) in $\mathbb{R}^{2n}$.

In particular $\sigma_1(x,\xi)$ is included in the discrete spectrum of $p_0(x,\xi)$ and consists in the eigenvalues of the $m \times m$ complex matrix

$$M(x,\xi) = (\langle p_0(x,\xi)\varphi_k(x,\xi), \varphi_j(x,\xi)\rangle)_{1\leq j,k\leq m}\,, \tag{2.3}$$

where $\langle \cdot, \cdot \rangle$ stands for the scalar product in $\mathcal{H}_2$.

Setting

$$\sigma_{\mathcal{F}} := \bigcup_{(x,\xi)\in I\!R^{2n}} \sigma\left(p_0(x,\xi)\left|_{\mathcal{F}(x,\xi)\cap\mathcal{H}_1}\right.\right),$$

our main result is the following:

Theorem 2.1 *Assume (2.1) and (H1)–(H2). Then for any $z \in \mathbb{C}\backslash\sigma_{\mathcal{F}}$ there exists a $m\times m$ matrix of h-pseudodifferential operators $A_z = \left(A_z^{j,k}\right)_{1\leq j,k\leq m}$, bounded on $L^2(I\!R^n)^{\oplus m}$, with principal symbol $M(x,\xi)$, and such that the following equivalence holds:*

$$z\in\sigma(P_h) \iff z\in\sigma(A_z).$$

Moreover, A_z depends analytically on z in the interior of $\mathbb{C}\backslash\sigma_{\mathcal{F}}$.

Example For $x\in I\!R^n$, let $Q(x)$ be a (possibly unbounded) nonnegative self-adjoint operator on some Hilbert space $\mathcal{H}_2$ with domain $\mathcal{H}_1$, such that $\sigma(Q(x)) = \{\lambda_1(x),\dots,\lambda_m(x)\}\cup\Sigma(x)$, where $\lambda_1(x),\dots,\lambda_m(x)$ depend continuously on x, remain uniformly separated outside some compact subset of $I\!R^n$, and $\inf\Sigma(x)\geq \max\{\lambda_1(x),\dots,\lambda_m(x)\}+\delta$ for some $\delta>0$ and for all $x\in I\!R^n$. Assume also that $Q(x)$ depends smoothly on x and is uniformly bounded together with all its derivatives as an operator from $\mathcal{H}_1$ to $\mathcal{H}_2$. Then our result can be applied with

$$P_h = \left(-h^2\Delta_x + Q(x)+1\right)^{-1}$$

and

$$\sigma_1(x,\xi) = \left\{\left(\xi^2+\lambda_j(x)+1\right)^{-1},\ 1\leq j\leq m\right\}.$$

Indeed, using the method of [DiSj], Section 8, we see that both (2.2) and (2.1) are satisfied, and $p_0(x,\xi) = \left(\xi^2+Q(x)+1\right)^{-1}$. Moreover, the constructions made in [KMSW] show the existence of an orthonormal family $(\varphi_1(x),\dots,\varphi_m(x))$ in $\mathcal{H}_2$, which depends smoothly on $x\in I\!R^n$, has all its derivatives uniformly bounded in $\mathcal{H}_2$, and generates $\bigoplus_{j=1}^m \mathrm{Ker}(Q(x)-\lambda_j(x))$. Since, by the spectral mapping theorem, this latter space is also equal to

$$\bigoplus_{j=1}^m \mathrm{Ker}\left(\left(\xi^2+Q(x)+1\right)^{-1} - \left(\xi^2+\lambda_j(x)+1\right)^{-1}\right),$$

we see that (H1) is satisfied, too. Finally, Condition (H2) is automatically satisfied by taking $\mathcal{F}(x,\xi)$ as the orthogonal space of $\mathcal{E}(x,\xi)$, since $p_0(x,\xi)$ is self-adjoint on $\mathcal{H}_2$. In this case $\sigma_{\mathcal{F}} = (0,(1+\lambda_+)^{-1}]$ with

$$\lambda_+ := \inf_{I\!R^n}\left(\sigma(Q(x))\backslash\{\lambda_1(x),\dots,\lambda_m(x)\}\right),$$

and our result permits to recover the reduction method used, e.g., in [Ma2] (see also [KMSW] for the Coulombic case), for studying the spectrum of the molecular Schrödinger operator $H := -h^2\Delta_x + Q(x)$ (typically, $Q(x) = -\Delta_y + V(x,y)$ acts on $L^2(I\!R^p_y)$ where y stands for the electronic position variables).

Remark As one can see from the proof, there is no real problem to generalize this theorem to unbounded symbols that, instead of (2.1), satisfy, e.g., estimates of the type

$$\|\partial^\alpha p_0(x,\xi)\|_{\mathcal{H}_{1,2}} + \|\partial^\alpha r_h(x,\xi)\|_{\mathcal{H}_{1,2}} = \mathcal{O}(\langle\xi\rangle^k)$$

for some $k \geq 0$. However, as we have illustrated in the previous example, it is often possible, in the applications, to transform the problem in order to deal with bounded symbols only.

3 Proof

The idea of the proof is to reduce the problem to the inversion of some Grushin problem, and to use the semiclassical symbolic calculus in order to construct the inverse.

We denote by B the operator $L^2(I\!R^n)^{\oplus m} \to L^2(I\!R^n;\mathcal{H}_2)$ defined by

$$B(u_1 \oplus \ldots \oplus u_m) = \sum_{j=1}^m \frac{1}{(2\pi h)^n}\int e^{i(x-y)\xi/h}\varphi_j\left(\frac{x+y}{2},\xi\right)u_j(y)dy\,d\xi,$$

and we denote by B^* its adjoint $L^2(I\!R^n;\mathcal{H}_2) \to L^2(I\!R^n)^{\oplus m}$, given by

$$Bu(x) = \bigoplus_{j=1}^m \frac{1}{(2\pi h)^n}\int e^{i(x-y)\xi/h}\left\langle u(y),\varphi_j\left(\frac{x+y}{2},\xi\right)\right\rangle_{\mathcal{H}_2} dy\,d\xi.$$

Then for $z \in \mathbb{C}$ we consider the following matrix operator (the so-called Grushin operator):

$$\mathcal{P}(z) := \begin{pmatrix} P_h - z & B \\ B^* & 0 \end{pmatrix}$$

that maps $L^2(I\!R^n;\mathcal{H}_1) \oplus L^2(I\!R^n)^{\oplus m}$ into $L^2(I\!R^n;\mathcal{H}_2) \oplus L^2(I\!R^n)^{\oplus m}$. In particular, we see that $\mathcal{P}(z)$ can be seen as an h-pseudodifferential operator with operator-valued principal symbol $\mathcal{P}_z(x,\xi)$ given by

$$\mathcal{P}_z(x,\xi) = \begin{pmatrix} p_0(x,\xi) - z & b(x,\xi) \\ b^*(x,\xi) & 0 \end{pmatrix} \;:\; \mathcal{H}_1 \oplus \mathbb{C}^n \to \mathcal{H}_2 \oplus \mathbb{C}^n \tag{3.1}$$

where $b(x,\xi)(\alpha_1,\ldots,\alpha_m) = \alpha_1\varphi_1(x,\xi) + \ldots + \alpha_m\varphi_m(x,\xi)$, $(\alpha_1,\ldots,\alpha_m \in \mathbb{C})$, and $b^*(x,\xi)f = \left(\langle f,\varphi_1(x,\xi)\rangle_{\mathcal{H}_2},\ldots\langle v,\varphi_m(x,\xi)\rangle_{\mathcal{H}_2}\right)$, $(f \in \mathcal{H}_1)$. In order to show that $\mathcal{P}(z)$ is invertible, we first prove the following lemma:

Lemma 3.1 *Denote by $\Pi^0_{\mathcal{E}}$ the orthogonal projection onto $\mathcal{E}(x,\xi)$. Then for all $z \in \mathbb{C}\backslash\sigma_{\mathcal{F}}$ and for all $(x,\xi) \in I\!R^{2n}$, the operator $\mathcal{P}_z(x,\xi)$ defined in (3.1) is invertible and its inverse is given by*

$$\mathcal{P}_z(x,\xi)^{-1} =: \mathcal{Q}_z(x,\xi) = \begin{pmatrix} Q_z(x,\xi) & Q_z^+(x,\xi) \\ Q_z^-(x,\xi) & Q_z^\pm(x,\xi) \end{pmatrix}$$

where, for $g \in \mathcal{H}_2$ and $\beta = (\beta_1, \dots, \beta_m) \in \mathbb{C}^n$,

$$\begin{aligned}
Q_z(x,\xi)g &:= \left(1 - \Pi^0_{\mathcal{E}}\right)(p_0'(x,\xi) - z)^{-1}\Pi_{\mathcal{F}/\mathcal{E}}g,\\
Q_z^+(x,\xi)\beta &:= \sum_{j=1}^m \beta_j\varphi_j,\\
Q_z^-(x,\xi)g &:= \left(\left\langle\left(1 + (p_0(x,\xi) - z)\Pi^0_{\mathcal{E}}(p_0'(x,\xi) - z)^{-1}\right)\Pi_{\mathcal{E}/\mathcal{F}}g, \varphi_j\right\rangle\right)_{1\le j\le m}\\
Q_z^\pm(x,\xi)\beta &:= (z - M(x,\xi))\,\beta.
\end{aligned}$$

Here we have denoted by $(p_0'(x,\xi) - z)^{-1}$ the inverse of $(p_0(x,\xi) - z)\big|_{\mathcal{F}(x,\xi)}$.

Proof For $g \in \mathcal{H}_2$ and $\beta = (\beta_1, \dots, \beta_m) \in \mathbb{C}^n$ we have to solve the problem

$$\mathcal{P}_z(x,\xi)(f \oplus \alpha) = g \oplus \beta \tag{3.2}$$

where the unknown $f \oplus \alpha = f \oplus (\alpha_1, \dots, \alpha_m)$ is in $\mathcal{H}_1 \oplus \mathbb{C}^n$. We can rewrite (3.2) as

$$\begin{cases} (p_0(x,\xi) - z)\,f + \sum_{j=1}^m \alpha_j\varphi_j(x,\xi) = g\\ \langle f, \varphi_j(x,\xi)\rangle = \beta_j \quad (j = 1, \dots, m),\end{cases}$$

and, writing $f = f_{\mathcal{E}} + f_{\mathcal{F}}$ with $f_{\mathcal{E}} \in \mathcal{E}(x,\xi)$ and $f_{\mathcal{F}} \in \mathcal{F}(x,\xi)$, we obtain (since $(\varphi_1(x,\xi), \dots, \varphi_m(x,\xi))$ is an orthonormal basis of $\mathcal{E}(x,\xi)$),

$$\begin{cases} f_{\mathcal{E}} = \sum_{j=1}^m \left(\beta_j - \langle f_{\mathcal{F}}, \varphi_j\rangle\right)\varphi_j\\ (p_0 - z)\,f_{\mathcal{F}} + (p_0 - z)f_{\mathcal{E}} + \sum_{j=1}^m \alpha_j\varphi_j = g.\end{cases} \tag{3.3}$$

(Here we have omitted the dependence on (x,ξ) to simplify the notation.) Since both spaces $\mathcal{E}(x,\xi)$ and $\mathcal{F}(x,\xi)$ are stable under $p_0(x,\xi)$ we see that (3.3) is equivalent to

$$\begin{cases} f_{\mathcal{E}} = \sum_{j=1}^m \left(\beta_j - \langle f_{\mathcal{F}}, \varphi_j\rangle\right)\varphi_j\\ (p_0 - z)\,f_{\mathcal{F}} = \Pi_{\mathcal{F}/\mathcal{E}}g\\ (p_0 - z)\,f_{\mathcal{E}} + \sum_{j=1}^m \alpha_j\varphi_j = \Pi_{\mathcal{E}/\mathcal{F}}g,\end{cases} \tag{3.4}$$

and thus, since by assumption $(p_0 - z)\big|_{\mathcal{F}(x,\xi)}$ is invertible for all $(x,\xi) \in \mathbb{R}^n$,

$$\begin{cases} f_{\mathcal{F}} = (p_0' - z)^{-1}\,\Pi_{\mathcal{F}/\mathcal{E}}g\\ f_{\mathcal{E}} = \sum_{j=1}^m \left(\beta_j - \langle f_{\mathcal{F}}, \varphi_j\rangle\right)\varphi_j\\ \alpha_j = \left\langle \Pi_{\mathcal{E}/\mathcal{F}}g - (p_0 - z)\,f_{\mathcal{E}}, \varphi_j\right\rangle \quad (j = 1\dots, m).\end{cases} \tag{3.5}$$

In particular $f_{\mathcal{F}}$, $f_{\mathcal{E}}$, $\alpha_1, \dots, \alpha_m$ can all be determined in function of g and β and, using (2.3) and the fact that $\Pi^0_{\mathcal{E}}v = \sum_{j=1}^m \langle v, \varphi_j\rangle\varphi_j$, we obtain the formulae given in the lemma. $\diamond$

The next step is important, since it will permit us to construct the inverse of $\mathcal{P}(z)$ by means of the symbolic calculus of h-pseudodifferential operators (see [Ma1] and the appendix of [GMS]).

Lemma 3.2 *For any $z \in \mathbb{C} \setminus \sigma_{\mathcal{F}}$, the application*

$$\begin{array}{rccc} \mathcal{Q}_z : & \mathbb{R}^{2n} & \to & \mathcal{L}\left(\mathcal{H}_2 \oplus \mathbb{C}^n ; \mathcal{H}_1 \oplus \mathbb{C}^n\right) \\ & (x,\xi) & \mapsto & Q_z(x,\xi) \end{array}$$

is C^∞ and uniformly bounded together with all its derivatives on $\mathbb{R}^{2n}$. Moreover, it depends analytically on z in the interior of $\mathbb{C} \setminus \sigma_{\mathcal{F}}$.

Proof Thanks to Assumptions (H1) and (H2), it is straighforward to verify that $\mathcal{Q}_z(x,\xi)$ is uniformly bounded on $\mathbb{R}^{2n}$ as an operator $\mathcal{H}_2 \oplus \mathbb{C}^n \to \mathcal{H}_1 \oplus \mathbb{C}^n$. Since, moreover, $\mathcal{P}_z(x,\xi)$ depends smoothly on (x,ξ) and is uniformly bounded together with all its derivatives, the continuity and the differentialbility follows by writing, for all $(x,\xi),(x'\xi') \in \mathbb{R}^{2n}$,

$$\mathcal{Q}_z(x,\xi) - \mathcal{Q}_z(x',\xi') = \mathcal{Q}_z(x,\xi)\left(\mathcal{P}_z(x',\xi') - \mathcal{P}_z(x,\xi)\right)\mathcal{Q}_z(x',\xi').$$

This permits to obtain

$$\left(\nabla_{x,\xi}\mathcal{Q}_z\right)(x,\xi) = -\mathcal{Q}_z(x,\xi)\left(\nabla_{x,\xi}\mathcal{P}_z\right)(x,\xi)\mathcal{Q}_z(x,\xi)$$

and the result follows by differentialting iteratively this equality. The analyticity of $\mathcal{Q}_z(x,\xi)$ with respect to z is also a direct consequence of the analytic dependence of $\mathcal{P}_z(x,\xi)$ on z. $\diamond$

Thanks to Lemma 3.2, we can consider the Weyl quantization $\mathcal{Q}(z) = \mathrm{Op}_h^W(\mathcal{Q}_z)$ of $\mathcal{Q}_z(x,\xi)$, defined on $L^2(\mathbb{R}^n;\mathcal{H}_2 \oplus \mathbb{C}^n) \simeq L^2(\mathbb{R}^n;\mathcal{H}_2) \oplus L^2(\mathbb{R}^n)^{\oplus m}$ by the oscillatory integral

$$\mathcal{Q}(z)\psi(x) = \frac{1}{(2\pi h)^n}\int e^{i(x-y)\xi/h}\mathcal{Q}_z\left(\frac{x+y}{2},\xi\right)\psi(y)dy\,d\xi.$$

Here $\psi = u \oplus u_1 \oplus \ldots \oplus u_m \in L^2(\mathbb{R}^n;\mathcal{H}_2) \oplus L^2(\mathbb{R}^n)^{\oplus m}$. By the Calderón–Vaillancourt theorem, $\mathcal{Q}(z)$ is a bounded operator from $L^2(\mathbb{R}^n;\mathcal{H}_2) \oplus L^2(\mathbb{R}^n)^{\oplus m}$ to $L^2(\mathbb{R}^n;\mathcal{H}_1) \oplus L^2(\mathbb{R}^n)^{\oplus m}$, and as a consequence we can perform the two compositions $\mathcal{Q}(z)\mathcal{P}(z)$ and $\mathcal{P}(z)\mathcal{Q}(z)$. Moreover, the symbolic calculus permits us to estimate it as follows:

$$\mathcal{Q}(z)\mathcal{P}(z) = \mathrm{Op}_h^W(\mathcal{Q}_z\mathcal{P}_z) + hR_1 = I + hR_1$$

with

$$\|R_1\|_{\mathcal{L}(L^2(\mathbb{R}^n;\mathcal{H}_1)\oplus L^2(\mathbb{R}^n)^{\oplus m})} = \mathcal{O}(1)$$

uniformly with respect to h. Similarly, we also have

$$\mathcal{P}(z)\mathcal{Q}(z) = \mathrm{Op}_h^W(\mathcal{P}_z\mathcal{Q}_z) + hR_2 = I + hR_2$$

with

$$\|R_2\|_{\mathcal{L}(L^2(\mathbb{R}^n;\mathcal{H}_2)\oplus L^2(\mathbb{R}^n)^{\oplus m})} = \mathcal{O}(1)$$

uniformly with respect to h. As a consequence, for h small enough $\mathcal{P}(z)$ is invertible and its inverse is given by the convergent Neuman series

$$\mathcal{P}(z)^{-1} = \left(\sum_{k=1}^{+\infty} h^k R_1^k \right) \circ \mathcal{Q}(z) = \mathcal{Q}(z) \circ \left(\sum_{k=1}^{+\infty} h^k R_2^k \right). \tag{3.6}$$

Therefore, we have proved the first part of the following proposition:

Proposition 3.3 *The operator $\mathcal{P}(z)$; $L^2(I\!R^n;\mathcal{H}_1)\oplus L^2(I\!R^n)^{\oplus m} \to L^2(I\!R^n;\mathcal{H}_2)\oplus L^2(I\!R^n)^{\oplus m}$ is invertible and its inverse can be written as*

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

where $Q(z)$, $Q^+(z)$, $Q^-(z)$, and $Q^{\pm}(z)$ are h-pseudodifferential operators with principal symbols $Q_z(x,\xi)$, $Q_z^+(x,\xi)$, $Q_z^-(x,\xi)$, and $Q_z^{\pm}(x,\xi)$ respectively. Moreover, we have the following equivalence:

$$z \in \sigma(P_h) \Longleftrightarrow 0 \in \sigma\left(Q^{\pm}(z)\right). \tag{3.7}$$

Proof In view of (3.6) it remains only to prove that $Q(z)$, $Q^+(z)$, $Q^-(z)$, and $Q^{\pm}(z)$ are h-pseudodifferential operators and that the equivalence (3.7) holds. The first assertion comes from the fact that $\mathcal{P}(z)^{-1}$ is the inverse of an elliptic h-pseudodifferential operator, and it can be proved in a standard way by using the Beals characterization theorem, see [DiSj], Proposition 8.3. The second assertion comes from the two following series of algebraic identities:

$$\begin{aligned}(P_h - z)u = v \quad &\Leftrightarrow \quad \mathcal{P}(z)(u \oplus 0) = v \oplus B^*u \Leftrightarrow \mathcal{Q}(z)(v \oplus B^*u) = u \oplus 0 \\ &\Leftrightarrow \quad \begin{cases} Q(z)v + Q^+(z)B^*u = u, \\ Q^-(z)v + Q^{\pm}(z)B^*u = 0, \end{cases}\end{aligned} \tag{3.8}$$

and

$$\begin{aligned}Q^{\pm}(z)\alpha = \beta \quad &\Leftrightarrow \quad \mathcal{Q}(z)(0 \oplus \alpha) = Q^+(z)\alpha \oplus \beta \Leftrightarrow \mathcal{P}(z)(Q^+(z)\alpha \oplus \beta) = 0 \oplus \alpha \\ &\Leftrightarrow \quad \begin{cases} (P_h - z)Q^+(z)\alpha + B\beta = 0, \\ B^*Q^+(z)\alpha = \alpha. \end{cases}\end{aligned} \tag{3.9}$$

Since we also have $B^*Q^+(z) = 1$ (just write explicitly that $\mathcal{P}(z)\mathcal{Q}(z) = I$), we see that if $z \notin \sigma(P_h)$, then (3.9) permits to obtain the following equivalence:

$$Q^{\pm}(z)\alpha = \beta \;\Leftrightarrow\; \alpha = -B^*(P_h - z)^{-1}B\beta.$$

In particular $0 \notin \sigma(Q^{\pm}(z))$ and

$$Q^{\pm}(z)^{-1} = -B^*(P_h - z)^{-1}B. \tag{3.10}$$

Conversely, if $0 \notin \sigma(Q^{\pm}(z))$, then (3.8) gives the following equivalence:

$$(P_h - z)u = v \;\Leftrightarrow\; \begin{cases} B^*u = -Q^{\pm}(z)^{-1}Q^-(z)v, \\ u = Q(z)v - Q^+(z)Q^{\pm}(z)^{-1}Q^-(z)v. \end{cases}$$

Moreover, the fact that $B^*Q(z) = 0$ and $B^*Q^+(z) = 1$ shows that, actually, the first equation of the latter system is implied by the second one. As a consequence, in this case we have

$$(P_h - z)u = v \iff u = Q(z)v - Q^+(z)Q^\pm(z)^{-1}Q^-(z)v,$$

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

$$(P_h - z)^{-1} = Q(z) - Q^+(z)Q^\pm(z)^{-1}Q^-(z). \tag{3.11}$$

This completes the proof of the proposition. $\diamond$

To complete the proof of the theorem, it just remains to observe that, by construction, $Q^\pm(s)$ is a h-pseudodifferential operator on $L^2(\mathbb{R}^n)^{\oplus m}$, that is, a $m \times m$ matrix of pseudodifferential operators on $L^2(\mathbb{R}^n)$. Therefore the theorem follows from Proposition 3.3 and Lemma 3.1 by setting $A_z = Q^\pm(z) - z$. $\diamond$

References

[DiSj] Dimassi, M., Sjöstrand, J.: Spectral Asymptotics in the Semiclassical Limit, London Math. Soc. Lecture Notes Series 268, Cambridge University Press (1999).

[GMS] Gérard, C., Martinez, A., Sjöstrand, J.: A mathematical approach to the effective hamiltonian in perturbed periodic problems, (joint work with C.Gérard and J.Sjstrand), Comm. Math. Physics Vol.142, n2 (1991).

[Ha] G. Hagedorn, *High Order Corrections to the time-independent Born-Oppenheimer Approximation*, Ann. Inst. H. Poincaré 47 (1987) 1-16

[HaJo] G. Hagedorn, A. Joye, *A Time–Dependent Born–Oppenheimer Approximation with Exponentially Small Error Estimates*, Preprint mp_arc. 00-209 (2000)

[Ho] Hörmander, L.: The Analysis of Linear Partial Differential Operators, Vol. I to IV. Springer Verlag (1985).

[KMSW] Klein, M., Martinez, A., Seiler, R., Wang, X.: On the Born-Oppenheimer Expansion for Polyatomic Molecules, Comm. Math. Phys. 143, p. 607-639 (1992).

[Ma1] Martinez, A.: An Introduction to Semiclassical and Microlocal Analysis, Springer-Verlag New–York, UTX Series, 2002

[Ma2] Martinez, A.: Développements asymptotiques et effet tunnel dans l'approximation de Born-Oppenheimer, Ann.Inst.H.Poincaré, Vol.49, n3, (1989), p. 239-257.

[MaSo] Martinez, A., Sordoni, V.: A general reduction scheme for the time-dependent Born-Oppenheimer approximation, C.R.Acad.Sci. Paris, Ser. I 334 (2002) 185-188

[Ne] G. Nenciu, *Linear Adiabatic theory: I.Exponential Estimates*, Comm. Math. Phys., 152 (1993).

[NeSo] G.Nenciu, V.Sordoni, *Semiclassical Limit for Multistate Klein-Gordon Systems: Almost Invariant Subspaces and Scattering Theory*, Preprint Bologna (2001)

[PST] Panati, G., Spohn, H., Teufel, S.: Space-Adiabatic Perturbation Theory, Preprint Technische Universität München (2002)

[So] V.Sordoni, *Scattering for Multistate Schrödinger Systems in the Semi-classical Limit*, Preprint Bologna (2001) and to appear in Comm. Part. Diff. Eq. (2002)

[SpTe] Spohn, S., Teufel, S.: Adiabatic Decoupling and Time -Dependent Born-Oppenheimer Theory, Comm. Math. Phys. 224 (1) (2001) 113-132