On the Time-Dependent Born-Oppenheimer Approximation with Smooth Potential

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Abstract

We give a general reduction scheme for the study of the quantum propagator of molecular Schrödinger operators with smooth potentials. This reduction is made up to infinitely (resp. exponentially) small error terms with respect to the inverse square root of the mass of the nuclei, depending on the C^∞ (resp. analytic) smoothness of the interactions. Then we apply this result to the case when an electronic level is isolated from the rest of the spectrum of the electronic Hamiltonian.

1 Introduction

In this note we investigate the solutions of the molecular Schrödinger equation:

$$ih\frac{\partial\varphi}{\partial t} = (-h^2\Delta_x - \Delta_y + V(x,y))\varphi \tag{1.1}$$

as $h \to 0_+$. Here $x \in I\!R^n$ represents the position of the nuclei, $y \in I\!R^p$ the position of the electrons, and h^{-2} is the quotient of their respective masses. We assume that the real-valued potential V is $C^\infty(I\!R^{n+p})$-smooth and bounded, and the electronic Hamiltonian

$$Q(x) := -\Delta_y + V(x,y)$$

admits a gap in its spectrum $\sigma(Q(x))$, so that we can write:

$$\sigma(Q(x)) = \sigma_1(x) \cup \sigma_2(x) \text{ with } \inf_{x\in I\!R^n} \text{dist } (\sigma_1(x), \sigma_2(x)) \geq \delta_0 > 0. \tag{1.2}$$

With these notations, we also assume

$$\sigma_1(x) \text{ is uniformly bounded with respect to } x \in I\!R^n, \tag{1.3}$$

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and we denote $\Pi_j(x)$ $(j=1,2)$ the spectral projections of $Q(x)$ corresponding to $\sigma_j(x)$ (extending their definition on $L^2(I\!R^{n+p})$ in an obvious way and denoting Π_j these extensions).

Then, denoting $(E_P(\lambda))_{\lambda\in I\!R}$ the family of spectral projections of $P := -h^2\Delta_x + Q(x)$, we prove:

Theorem 1.1 *For any $\lambda_0 \in I\!R$ there exists an orthogonal projection Π on $L^2(I\!R^{n+p})$ such that*

$$\Pi = \Pi_1 + \mathcal{O}(h) \sim \Pi_1 + \sum_{j\geq 1} h^j \Pi^{(j)}$$

and such that any solution φ of (1.1) with initial data $\varphi_0 \in \mathrm{Ran}\, E_P((-\infty, \lambda_0])$ satisfies:

$$\varphi = e^{-itP_1/h}\Pi\varphi_0 + e^{-itP_2/h}(1-\Pi)\varphi_0 + \mathcal{O}(|t|h^\infty\|\varphi_0\|)$$

uniformly with respect to h small enough, $t\in I\!R$ and $\varphi_0 \in \mathrm{Ran}\, E_P((-\infty,\lambda_0])$, with:

$$P_1 = \Pi P \Pi \quad ; \quad P_2 = (1-\Pi)P(1-\Pi).$$

Moreover, for any $j\geq 1$, $\Pi^{(j)}$ is a semiclassical pseudodifferential operator with bounded operator-valued symbol $\pi_j(x,\xi) \in C_b^\infty\left(I\!R^{2n}; \mathcal{L}(L^2(I\!R^p_y))\right)$.

Theorem 1.2 *In the particular case where $\mathrm{Rank}\,\Pi_1(x) = k < \infty$ for all $x \in I\!R^n$, then there exists a semiclassical pseudodifferential operator*

$$W \;:\; L^2(I\!R^{n+p}) \to \left(L^2(I\!R^n)\right)^{\oplus k}$$

with operator-valued symbol and a $k\times k$ selfadjoint matrix A of semiclassical pseudodifferential operators on $L^2(I\!R^n)$ such that the restriction U of W to $\mathrm{Ran}\,\Pi$:

$$U \;:\; \mathrm{Ran}\,\Pi \to \left(L^2(I\!R^n)\right)^{\oplus k}$$

is a unitary operator which satisfies:

$$UP_1\Pi = AU\Pi$$

(in particular, $e^{-itP_1/h}\Pi = U^*e^{-itA/h}U\Pi$ for all $t\in I\!R$).

Moreover, the symbol $a(x,\xi)$ of A has the following form:

$$a(x,\xi) = \xi^2\mathbf{I}_k + \mu(x) + hr(x,\xi) \sim \xi^2\mathbf{I}_k + \mu(x) + \sum_{j\geq 0} h^{j+1} r_j$$

where $\mathbf{I}_k$ is the identity matrix of $\mathbb{C}^k$, $\mu(x)$ is the matrix of $\Pi_1(x)Q(x)$ in a smooth orthonormal basis of $(u_1(x), ..., u_k(x))$ of $\mathrm{Ran}\,\Pi_1$, and the r_j's satisfy $\partial^\alpha r_j(x,\xi) = \mathcal{O}(\langle\xi\rangle^2)$ for any multi-index α and uniformly with respect to $(x,\xi)\in I\!R^{n+p}$ and $h>0$ small enough.

Using the standard construction of the quantum evolution for scalar semiclassical pseudodifferential operators (see e.g. [Ro, MeSj, Bu] and references therein), we immediately deduce from this theorem:

Corollary 1.3 *Assume in addition $k = 1$. Then, for any $t \in \mathbb{R}$ there exists a semiclassical Fourier-Integral operator F_t on $L^2(\mathbb{R}^n)$ of the form:*

$$F_t\psi(x) = (2\pi h)^{-n} \int e^{i\phi(t,x,y,\eta)/h} b(t,x,y,\eta;h)\psi(y)dyd\eta \tag{1.4}$$

(where $b \sim \sum_j h^j b_j$ is a semiclassical symbol of order 0 and ϕ is a smooth phase function with non negative imaginary part), such that any solution φ of (1.1) with initial data φ_0 satisfying

$$\|(1-\Pi)\varphi_0\| + \|E_P([\lambda_0,+\infty))\varphi_0\| = \mathcal{O}(h^\infty)$$

can be written as:

$$\varphi = W^* F_t W \varphi_0 + \mathcal{O}\left(h^\infty\right). \tag{1.5}$$

In the analytic case, these results can be improved as follows:

Theorem 1.4 (Analytic Case) *If in addition V is analytic with respect to x and bounded in a complex strip $\{|\mathrm{Im}\, x| \leq \delta\}$ for some $\delta > 0$, then the statements of Theorem 1.1 and Corollary 1.3 remain valid if one replaces every "$\mathcal{O}(h^\infty)$" by "$\mathcal{O}(e^{-\varepsilon/h})$ for some $\varepsilon > 0$".*

Remark 1.5 *In the particular case $\varphi_0 = \Pi\psi$ where ψ is a wave packet as in [HaJo], then the formula (1.5) permits by a stationary phase argument to get a full asymptotic expansion of φ as $h \to 0_+$. In particular, the results of [HaJo] can be recovered in that way.*

Remark 1.6 *In a forthcoming paper, we plan to generalize our results to the case where $Q(x)$ does not necessarily admits a gap in its spectrum, but a gap exists in $\sigma(Q(x)) \cap (-\infty, \lambda_0]$. We also plan to investigate the case of Coulomb-interactions by using the tools developed in [KMSW].*

Proof of Theorem 1.1 - It is an almost direct consequence of the constructions made in [So] (see also [NeSo]): taking $f \in C_0^\infty(\mathbb{R})$ such that $f = 1$ on $[\inf \sigma(P), \lambda_0]$ and following these constructions, one obtains a semiclassical pseudodifferential operator (with operator-valued symbol)

$$\Pi = \Pi(x, hD_x; h) \sim \sum_{j \geq 0} h^j \Pi^{(j)}(x, hD_x)$$

such that Π is an orthogonal projection, $\Pi = \Pi_1 + \mathcal{O}(h)$ and

$$\|f(P)[\Pi, P]\| = \mathcal{O}(h^\infty).$$

For the sake of completeness, let us recall briefly this construction: Choose a loop $\gamma(x)$ incircling $\sigma_1(Q(x))$ and depending smoothly on x, and define for ξ small enough:

$$\widetilde{\pi}(x,\xi) = \frac{1}{2\pi h}\int_{\gamma(x)} (z-\xi^2+Q(x))^{\#(-1)}dz$$

where $\#(-1)$ means that we take the inverse with respect to the symbolic calculus of semiclassical pseudodifferential operators (with operator-valued symbols). Then, since the previous integral does not change if we slightly move $\gamma(x)$, one can eliminate ξ^2 in the denominators of the expansion and obtain $\widetilde{\pi}(x,\xi) = \sum_{j\geq 0} h^j\widetilde{\pi}_j(x,\xi)$ where $\widetilde{\pi}_j$ is polynomial of order j with respect to ξ (and can therefore be extended to all ξ in $\mathbb{R}^n$). Then denoting $\widetilde{\Pi}_j$ the Weyl quantization of $\widetilde{\pi}_j$ and taking $g\in C_0^\infty(\mathbb{R})$ such

that $gf=f$, one can resum in a standard way the formal series of operators: $\sum h^j g(P)\widetilde{\Pi}_j$ and $\sum h^j\widetilde{\Pi}_j g(P)$. Denoting $g(P)\Pi_0$ and $\Pi_0 g(P)$ the resulting operators, one can see that the operator $\Pi_g := g(P)\Pi_0 + (1-g(P))\Pi_0 g(P) + (1-g(P))\Pi_1(1-g(P))$ has a spectrum concentrated modulo $\mathcal{O}(h)$ near 0 and 1. Then, Π is defined as the spectral projection of Π_g associated to the part of its spectrum close to 1.

Now, observing that $\varphi = f(P)\varphi$ for all time, we can re-write (1.1) as:

$$ih\partial_t\Pi\varphi = P_1\Pi\varphi + R_1\varphi \tag{1.6}$$

$$ih\partial_t(1-\Pi)\varphi = P_2(1-\Pi)\varphi + R_2\varphi \tag{1.7}$$

with $R_1 = \Pi[\Pi,P]f(P) = \mathcal{O}(h^\infty)$ and $R_2 = (1-\Pi)[P,\Pi]f(P) = \mathcal{O}(h^\infty)$, and we deduce from (1.6) and (1.7):

$$\Pi\varphi(t) = e^{-itP_1/h}\Pi\varphi_0 + \int_0^t e^{i(s-t)P_1/h}R_1\varphi(s)ds \tag{1.8}$$

$$(1-\Pi)\varphi(t) = e^{-itP_2/h}(1-\Pi)\varphi_0 + \int_0^t e^{i(s-t)P_2/h}R_2\varphi(s)ds \tag{1.9}$$

from which the result follows immediately. $\diamond$

Proof of Theorem 1.2 - Since $\Pi - \Pi_1 = \mathcal{O}(h)$, for h small enough we can consider the operator $\mathcal{U}$ defined by:

$$\mathcal{U} = (\Pi_1\Pi + (1-\Pi_1)(1-\Pi))\left(1-(\Pi-\Pi_1)^2\right)^{-1/2}$$

and straighforward computations show that:

$$\mathcal{U}^*\mathcal{U} = \mathcal{U}\mathcal{U}^* = 1 \quad \text{and} \quad \Pi_1\mathcal{U} = \mathcal{U}\Pi.$$

Moreover, $\mathcal{U}$ is a semiclassical pseudodifferential operator with operator-valued symbol and it differs from the identity by $\mathcal{O}(h)$. Then, given a smooth orthonormal basis of $(u_1(x),...,u_k(x))$ of $\operatorname{Ran}\Pi_1$, we define W by:

$$W\psi = \langle\mathcal{U}\psi, u_1(x,y)\rangle_{L^2(\mathbb{R}^p_y)} \oplus\cdots\oplus \langle\mathcal{U}\psi, u_k(x,y)\rangle_{L^2(\mathbb{R}^p_y)}.$$

By the properties of $\mathcal{U}$ we see that $W\Pi = W$, and since $W^*(\alpha_1 \oplus \cdots \oplus \alpha_k) = \mathcal{U}^*(\alpha_1 u_1 + \cdots + \alpha_k u_k)$ we also obtain:

$$W^*W = \mathcal{U}^*\Pi_1\mathcal{U} = \Pi \ ; \ WW^* = 1$$

which implies the unitarity of the restriction U of W to $\operatorname{Ran}\Pi$. Moreover, defining $A := UP_1U^*$, we see that A satisfies all the assertions of Theorem 1.2. $\diamond$

Proof of Corollary 1.3 - By the assumptions we have

$$\varphi = e^{-itP/h}\varphi_0 = e^{-itP/h}E_P((-\infty, \lambda_0])\varphi_0 + \mathcal{O}(h^\infty)$$

and thus using theorem 1.1:

$$\varphi = e^{-itP_1/h}\Pi E_P((-\infty, \lambda_0])\varphi_0 + \mathcal{O}(h^\infty) = e^{-itP_1/h}\Pi\varphi_0 + \mathcal{O}(h^\infty).$$

Now by Theorem 1.2:

$$e^{-itP_1/h}\Pi = U^*e^{-itA/h}U\Pi$$

which finally gives

$$\varphi = U^*e^{-itA/h}U\Pi\varphi_0 + \mathcal{O}(h^\infty) = W^*e^{-itA/h}W\varphi_0 + \mathcal{O}(h^\infty).$$

Then the result follows from standard results on the quantum evolution of scalar semiclassical pseudodifferential operators (see [Ro, MeSj, Bu] and references therein). $\diamond$

Proof of Theorem 1.4 - When V is analytic, the construction of Π made in [So] satisfies analytic estimates of the type:

$$\|\Pi^{(j)}\| \leq C^{j+1}j!$$

where $C > 0$ is a constant (which depends on λ_0), and j runs over all the integers. By resummation (and following ideas of [Sj]), this permits to obtain:

$$\|f(P)[\Pi, P]\| = \mathcal{O}(e^{-\varepsilon/h})$$

for some $\varepsilon > 0$. Then the previous proof of Theorem 1.1 can be followed again, allowing error terms exponentially small as $h \to 0_+$.

The improvement of Corollary 1.3 is less direct: first remaining at the level of formal power series in h, one constructs as in [So] a family $(\widetilde{\Pi}^{(j)})_{j\geq 0}$ of semiclassical pseudodifferential operators with analytic coefficients, which are actually *differential* with respect to x and satisfy:

$$[P, \sum_{j\geq 0} h^j\widetilde{\Pi}^{(j)}] = 0 \quad \text{formally.}$$

Moreover, every $\widetilde{\Pi}^{(j)}$ is of degree j and its operator-valued symbol $\widetilde{\pi}_j(x,\xi)$ (polynomial in ξ) satisfies:

$$\|\widetilde{\pi}_j(x,\xi)\|_{\mathcal{L}(L^2(I\!\!R^p))} \leq C^{j+1}\langle\xi\rangle^j j!$$

for some constant $C>0$ and uniformly on $\{|\mathrm{Im}\, x|\leq\delta'\}\times\mathbb{C}^n$ with $0<\delta'<\delta$. Then denoting $\widetilde{\Pi}:=\sum_{j\geq 0} h^j\widetilde{\Pi}^{(j)}$ (formal series) and using the analytic expansion at $s=0$ of $(1-s^2)^{-1/2}=\sum_{j\geq 0}\nu_j s^{2j}$, we can define the following formal version of $\mathcal{U}$:

$$\widetilde{\mathcal{U}} := (\Pi_1\widetilde{\Pi}+(1-\Pi_1)(1-\widetilde{\Pi}))\sum_{j\geq 0}\nu_j(\widetilde{\Pi}-\Pi_1)^{2j} = 1+\sum_{j\geq 1}h^jT_j$$

where the T_j's are again semiclassical differential operators with analytic operator-valued symbols t_j satisfying:

$$\|t_j(x,\xi)\|_{\mathcal{L}(L^2(I\!\!R^p))} \leq C^{j+1}\langle\xi\rangle^j j!$$

with some possibly new positive constant C. Denote $\mu_1(x)$ the (unique) eigenvalue of $Q(x)$ on $\mathrm{Ran}\,\Pi_1(x)$ and $u_1(x)$ a corresponding normalized eigenfunction. Since $\mu_1(x)$ is isolated in $\sigma(Q(x))$ we know that it depends analytically on x in a complex strip, and the same can be assumed for u_1. Then for $\psi\in C^\infty(I\!\!R^n_x;L^2(I\!\!R^p_y))$ we set:

$$\widetilde{W}\psi(x;h) := \langle\widetilde{\mathcal{U}}\psi, u_1(x)\rangle_{L^2(I\!\!R^p_y)}$$

which is a formal series in h with coefficients in $C^\infty(I\!\!R^n)$, and we denote by $\widetilde{W}^*$ the formal adjoint of $\widetilde{W}$ defined by:

$$\widetilde{W}^*\alpha = \widetilde{\mathcal{U}}^*(\alpha(x)u_1(x,y))$$

for any $\alpha\in C^\infty(I\!\!R^n)$, where $\widetilde{\mathcal{U}}^* := 1+\sum_{j\geq 1}h^jT_j^*$. Then it is easy to check that $\widetilde{W}\widetilde{W}^*=1$ and $\widetilde{W}^*\widetilde{W}=\widetilde{\Pi}$ formally. Finally we set

$$\widetilde{A} := \widetilde{W}\widetilde{\Pi}P\widetilde{\Pi}\widetilde{W}^* = \sum_{j\geq 0}h^jA_j$$

where the A_j's are scalar semiclassical differential operators with analytic symbols a_j satisfying:

$$|a_j(x,\xi)|\leq C^{j+1}\langle\xi\rangle^{2+j}j!$$

for x in some complex strip around $I\!\!R^n$. Moreover, $a_0(x,\xi)=\xi^2+\mu_1(x)$.

Then, the standard analytic construction of $e^{-it\widetilde{A}/h}$ (see e.g. [Sj] Section 9, [HeSj] Appendix a.3) can be performed formally, and gives rise to a phase function $\phi=\phi(t,x,y,\eta)$ and a formal analytic symbol $b=\sum_{j\geq 0}h^jb_j(t,x,y,\eta)$

with $|b_j| \leq C^{j+1}\langle\eta\rangle^j j!$, such that the formal Fourier integral operator defined by (1.4) satisfies formally:

$$F_t^* F_t = F_t F_t^* = 1 \quad ; \quad F_t^*(ih\partial_t F_t) = (ih\partial_t F_t)F_t^* = \widetilde{A} \quad ; \quad F_0 = 1.$$

As a consequence, given any φ_0 in the Schwartz space $\mathcal{S}(I\!R_x^n; L^2(I\!R_y^p))$, the series

$$\widetilde{\varphi} := \widetilde{W}^* F_t \widetilde{W}\varphi_0 = \sum_{j\geq 0} h^j \varphi^{(j)}$$

(where $\varphi^{(j)} = \varphi^{(j)}(x;h) := (2\pi h)^{-n}\int e^{i\phi(t,x,y,\eta)/h} b_j(t,x,y,\eta)dyd\eta$) satisfies formally:

$$ih\partial_t\widetilde{\varphi} = \widetilde{\Pi}P\widetilde{\Pi}\widetilde{\varphi} \quad ; \quad \widetilde{\varphi}\,|_{t=0} = \widetilde{\Pi}\varphi_0$$

and

$$\|\varphi^{(j)}\|_{L^2(I\!R^{n+p})} \leq C^{j+1} j! \|\langle hD_x\rangle^j\varphi_0\|_{L^2(I\!R^{n+p})}. \tag{1.10}$$

Moreover, by construction $\widetilde{\Pi}\widetilde{W}^* = \widetilde{W}^*$ (so that $\widetilde{\Pi}\varphi = \widetilde{\varphi}$), and $\widetilde{\Pi}P = P\widetilde{\Pi}$. Therefore, $\widetilde{\varphi}$ actually solves formally the problem:

$$ih\partial_t\widetilde{\varphi} = P\widetilde{\varphi} \quad ; \quad \widetilde{\varphi}\,|_{t=0} = \widetilde{\Pi}\varphi_0.$$

Now, if in addition $f(P)\varphi_0 = \varphi_0$ for some $f \in C_0^\infty(I\!R)$, we can write:

$$\|\langle hD_x\rangle^j\varphi_0\| = \|\left(\langle hD_x\rangle^j\langle P\rangle^{-j}\right)\left(\langle P\rangle^j f(P)\rangle\right)\varphi_0\| \leq C_1^{j+1}\|\langle hD_x\rangle^j\langle P\rangle^{-j}\|\cdot\|\varphi_0\|$$

for some positive constant C_1, and using that

$$\|\langle hD_x\rangle^j\langle P\rangle^{-j}\| \leq C_2^{j+1} \text{ uniformly for } 0 \leq j \leq \frac{1}{C_2 h}$$

for any $C_2 > 0$ large enough (see e.g. [So]), we deduce from (1.10) in this case:

$$\|\varphi^{(j)}\|_{L^2(I\!R^{n+p})} \leq C_3^{j+1} j! \|\varphi_0\|_{L^2(I\!R^{n+p})} \quad (0 \leq j \leq \frac{1}{C_2 h})$$

with $C_3 = CC_1C_2$. As a consequence, we can take an analytic resummation $\widehat{\varphi}$ of $\sum_{j\geq 0} h^j\varphi^{(j)}$ in the sense of [Sj] and it satisfies:

$$ih\partial_t\widehat{\varphi} = P\widehat{\varphi} + \mathcal{O}(e^{-\varepsilon/h})$$

for some $\varepsilon > 0$. Moreover, by [So] the construction of Π can be made in such a way that $\Pi f(P) = \widehat{\Pi}f(P) + \mathcal{O}(e^{-\varepsilon'/h})$ for some $\varepsilon' > 0$, where $\widehat{\Pi}f(P)$ is an analytic resummation of $\widetilde{\Pi}f(P)$.

Therefore $\widehat{\varphi}$ also satisfies in that case:

$$\widehat{\varphi}\,|_{t=0} = \Pi\varphi_0 + \mathcal{O}(e^{-\varepsilon/h})$$

with some possibly new $\varepsilon > 0$ constant.

Now, take φ_0 such that:

$$\|(1-\Pi)\varphi_0\| + \|E_P([\lambda_0, +\infty))\varphi_0\| = \mathcal{O}(e^{-\varepsilon_0/h})$$

for some $\varepsilon_0 > 0$. Then $\|(1-f(P))\varphi_0\|$ is exponentially small for any $f \in C_0^\infty(I\!R)$ such that $f = 1$ near $[\inf \sigma(P), \lambda_0]$, and the previous construction can be applied to $f(P)\varphi_0$ and gives rise to a Fourier integral operator F_t such that the function $\widehat{\varphi} = F_t f(P)\varphi_0$ satisfies:

$$ih\partial_t\widehat{\varphi} = P\widehat{\varphi} + \mathcal{O}(e^{-\varepsilon/h}) \quad ; \quad \widehat{\varphi}\,|_{t=0} = \Pi f(P)\varphi_0 + \mathcal{O}(e^{-\varepsilon/h})$$

for some $\varepsilon > 0$. As a consequence, the unitarity of $e^{-itP/h}$ gives:

$$\|\widehat{\varphi} - e^{-itP/h}\Pi f(P)\varphi_0\| = \mathcal{O}(e^{-\varepsilon/h})$$

and also:

$$\|e^{-itP/h}(1-\Pi)\varphi_0\| + \|e^{-itP/h}\Pi(1-f(P))\varphi_0\| = \mathcal{O}(e^{-\varepsilon/h}).$$

Summing-up we obtain:

$$\|\widehat{\varphi} - e^{-itP/h}\varphi_0\| = \mathcal{O}(e^{-\varepsilon/h})$$

from which the result follows. ◇

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