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Born-Oppenheimer approximation for an atom in constant magnetic fields

By

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Abstract

We announce our recent results about a reduction scheme for the study of the quantum evolution of an atom in constant magnetic fields by the method developed by Martinez, Nenciu and Sordoni based on the construction of almost invariant subspace. Using the center of mass coordinates and constructing the almost invariant subspace different from that of Martinez and Sordoni, we obtain the reduced Hamiltonian which does not include the vector potential terms of the nucleus. Using the reduced evolution we also obtain the asymptotic expansion of the evolution for a specific localized initial data, which verifies the straight motion of an atom in constant magnetic fields.

§ 1. Introduction

The main purpose of this article is to announce the results of [1] on the Born-Oppenheimer approximation for an atom in constant magnetic fields.

The Hamiltonian of an atom with a nucleus and N electrons moving in constant magnetic fields has the form

$$\hat{P} = \frac{1}{2m}(D_{x_1} - e_1 A(x_1))^2 + \sum_{i=2}^{N+1} \frac{1}{2m_e}(D_{x_i} - eA(x_i))^2 + \sum_{i<j} V_{ij}(x_i - x_j) + \sum_{i=1}^{N+1} V_i(x_i). \tag{1.1}$$

Here $x_1 \in \mathbb{R}^3$ (resp., m) denotes the position (resp., the mass) of the nucleus, $x_j, j \geq 2$ (resp., m_e) denote the position (resp., the mass) of electrons and V_{ij} (resp., V_i) are

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interaction (resp., external) potentials. e_1 (resp., e) denotes the charge of the nucleus (resp., electrons) and A denotes the vector potential.

In the Born-Oppenheimer approximation framework without magnetic fields, the Hamiltonian of some nuclei and electrons is written as

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

where we denote the coordinates of the electrons by y and that of the nuclei by x and h^2 is the ratio of electronic and nuclear mass. Our purpose is to study the asymptotics of the solution to the Schrödinger equation $ih\partial_t\varphi = P(h)\varphi$ as $h \to 0$. Since the electrons change their state adiabatically, if the electrons are in bound states for the fixed nuclei, i.e. the bound states for $P_e(x) := -\Delta_y + V(x,y)$ at the initial time, we expect the electrons remain in the bound states even after time passes. This suggests there is an almost invariant subspace close to the electronic bound states under the evolution $e^{-itP(h)/h}$.

The almost invariant subspaces are described by the projections (see Nenciu [17, 18]). If an orthogonal projection Π satisfies $[P(h),\Pi] = \mathcal{O}(h^\infty)$, then $e^{-itP/h}\Pi = \Pi e^{-itP/h} + \mathcal{O}(h^\infty|t|)$ holds which means $\mathrm{Ran}\Pi$ is the almost invariant subspace. We expect there exists such a projection Π such that $\Pi - \Pi_0 = \mathcal{O}(h)$ where $\Pi_0 = \int^\oplus \Pi_0(x)dx$ and $\Pi_0(x)$ is the spectral projection onto an arbitrarily chosen part of the discrete spectrum of $P_e(x)$ separated from the other part of the spectrum. In the case of Born-Oppenheimer approximation the almost invariant subspace does not seem to exist according to the physical intuition saying that the adiabatic decoupling becomes weaker and weaker when the energy increases. However for any cutoff function χ a projection Π which satisfies $[P(h),\Pi]\chi(P) = \mathcal{O}(h^\infty)$ is constructed by Sordoni [21]. Using the projection Π the quantum evolution $e^{-itP/h}$ of the molecule is reduced to the evolution of the nuclei $e^{-itG/h}$ where G is a $k \times k$ matrix of semiclassical pseudodifferential operators $H^2(\mathbb{R}^n_x) \to L^2(\mathbb{R}^n_x)$, of the nuclear variables, k being the rank of Π_0 (see Martinez-Sordoni [15, 16]). The symbol of G is written as $g = \xi^2 I_k + \mu(x) + \sum_{j=1}^\infty g_j h^j$, where I_k is the k-dimensional identity matrix and $\mu(x)$ is a matrix of $\Pi_0 P_e(x)$ in a basis of $\mathrm{Ran}\Pi_0$.

In semiclassical limit the quantum evolution of generalized coherent states admits an asymptotic expansion each term of which is a generalized coherent state centered at the point reached by the classical flow (see Combescure-Robert [3] and Combescure [2]). In [16] Martinez and Sordoni applied this expansion to G in order to obtain the evolution of a specific localized initial data.

When there is a constant magnetic field, the coordinates of the particles perpendicular to the magnetic field stay in a bounded region as in the classical mechanics. When there are N particles, the center of mass of the particles does not move freely, so that we cannot divide the motion of the particles into the internal and external motion. However, if the total charge of the particles is zero, there is a subspace $\mathcal{H}_{bound}$ of $L^2(\mathbb{R}^{3N})$ such that internal coordinates of the particles in the state in $\mathcal{H}_{bound}$ stay in a bounded region and the particles travel to infinity across the magnetic field (see Gérard-Łaba [4]). Thus we expect when there is an atom, the electrons around the nucleus offset the influence of the magnetic fields. Hence it seems to be natural that the vector potential terms do not appear in the reduced Hamiltonian G. The Born-Oppenheimer approximation with magnetic fields is also dealt with by Martinez-Sordoni [16] but in their construction the term $h^2(D_x - eA(x))^2$ remains in G. We obtain in [1] a reduction scheme from $\hat{P}$ in (1.1) to G without vector potential terms.

To obtain such G we change the coordinates to the new coordinates where the independent variables are the center of mass and the relative position of the electrons. The difficulty in our construction of Π is that when we expand the symbol of the resolvent $(P-z)^{-1}$ in formal power series in h as $\sum_{j=0}^{\infty} q_j(x,\xi;z)h^j$ where q_j are operators on $L^2(\mathbb{R}^{3N}_y)$, the power of y contained in $q_j(z)$ becomes of higher order as j increases.

§ 2. Adiabatic theory and Born-Oppenheimer approximation

We recall the Adiabatic theory and Born-Oppenheimer approximation (see Nenciu [17], Nenciu-Sordoni [19] Martinez-Sordoni [15],[16]).

§ 2.1. Adiabatic theory and almost invariant subspace

Consider the evolution, $U_h(t,t_0)$, given by

$$ih\frac{d}{dt}U_h(t,t_0) = H(t)U_h(t,t_0),\ U_h(t_0,t_0) = 1$$

Since this is hard to integrate, we need obtain information without integrating this equation. For this purpose we find out almost invariant subspaces, $\mathcal{K}(t;h)$ under the evolution $U_h(t,t_0)$;

$$U_h(t,t_0)\mathcal{K}(t_0;h) \cong \mathcal{K}(t;h).$$

Assume that $\mathcal{K}(t_0;h)$ is obtained by a projection $\Pi_h(t)$ as $\Pi_h(t)U_h(t,t_0) \cong U_h(t,t_0)\Pi_h(t_0)$. Then that $\mathcal{K}(t_0;h)$ is almost invariant means

$$\Pi_h(t)U_h(t,t_0) \cong U_h(t,t_0)\Pi_h(t_0),$$

or

$$\Pi_h(t) \cong U_h(t,t_0)\Pi_h(t_0)U_h(t,t_0)^{-1}.$$

If we differentiate it we have

$$ih\frac{d}{dt}\Pi_h(t) \cong [H(t),\Pi_h(t)]$$

Nenciu [17] constructed such an almost invariant subspace by recurrent relation.

§ 2.2. Born-Oppenheimer approximation

For simplicity we consider the case without magnetic fields. Hamiltonian of n nuclei and N electrons is written as follows:

$$P = -\sum_{i=1}^{n} \frac{1}{2m}\Delta_{x_i} - \sum_{i=1}^{N} \frac{1}{2m_e}\Delta_{y_i} + \sum_{i<j} V_{ij}(x_i - x_j) + \sum_{i<j} \tilde{V}_{ij}(y_i - y_j) + \sum_{i,j} \hat{V}_{ij}(x_i - y_j)$$

Here $x_i \in \mathbb{R}^3$ (resp., m) denote the position (resp., the mass) of the nuclei, $y_i \in \mathbb{R}^3$ (resp., m_e) denote the position (resp., the mass) of electrons and V_{ij}, $\tilde{V}_{ij}$ and $\hat{V}_{ij}$ are interaction potentials.

Since the electrons are lighter than the nuclei, they move rapidly and adjust their state adiabatically as the nuclei move more slowly. To demonstrate this mathematically we change the scale and rewrite the Hamiltonian as

$$P(h) = -h^2 \sum_{i=1}^{n} \Delta_{x_i} - \sum_{i=1}^{N} \Delta_{y_i} + V(x, y)$$

where $h^2 = \frac{m_e}{m}$. Then our aim is to study the asymptotics of the solution of the Schrödinger equation

$$ih\partial_t \varphi = P(h)\varphi$$

as $h \to 0$. We introduce the electronic Hamiltonian

$$P_e(x) := -\sum_{i=1}^{N} \Delta_{y_i} + V(x, y).$$

We deal with the given part of the discrete spectrum $\sigma_0(x)$ of $P_e(x)$ such that

$$\sigma(P_e(x)) = \sigma_0(x) \cup \sigma_1(x)$$

$$\exists d > 0, \ \inf_{x \in \mathbb{R}^3} \operatorname{dist}(\sigma_0(x), \sigma_1(x)) \geq d$$

This assumption is called the gap condition. We denote the spectral projection corresponding to $\sigma_0(x)$ by $\Pi_0(x)$ and assume $\operatorname{Rank}(\operatorname{Ran}\Pi_0(x)) = k < \infty$. Let $(u_1(x), \ldots, u_k(x))$ be the smooth orthonormal basis of $\operatorname{Ran}\Pi_0(x)$.

Sordoni [21] constructed for any cutoff function $\chi \in C_0^\infty(\mathbb{R})$, a projection Π such that $\Pi - \Pi_0 = \mathcal{O}(h)$, where $\Pi_0 := \int^{\oplus} \Pi_0(x)dx$, and $[P, \Pi]\chi(P) := (P\Pi - \Pi P)\chi(P) =$

$\mathcal{O}(h^\infty)$, and therefore as in the adiabatic theory we have

$$\begin{aligned} e^{-itP/h}\Pi\chi(P) &= \Pi\chi(P)e^{-itP/h} + i\int_0^t e^{-isP/h}[\Pi, P]\chi(P)e^{i(s-t)P/h}ds \\ &= \Pi\chi(P)e^{-itP/h} + \mathcal{O}(h^\infty|t|). \end{aligned}$$

Thus, $\mathrm{Ran}(\Pi\chi(P))$ is almost invariant.

Using Π Martinez and Sordoni proved the following theorem.

Theorem 2.1 (Martinez-Sordoni [15],[16]). *There exist a h-admissible operator with operator valued symbol $W : L^2(\mathbb{R}^{3(n+N)}) \to (L^2(\mathbb{R}^{3n}_x))^{\oplus k}$ and $G : (L^2(\mathbb{R}^{3n}_x))^{\oplus k} \to (L^2(\mathbb{R}^{3n}_x))^{\oplus k}$, $k \times k$ self-adjoint matrix of h-admissible operators on $L^2(\mathbb{R}^{3n}_x)$ such that the following are satisfied.*
The restriction U of W to $\mathrm{Ran}\Pi$*:*

$$U : \mathrm{Ran}\Pi \to (L^2(\mathbb{R}^{3n}_x))^{\oplus k}$$

is unitary. If $\varphi_0 \in \mathrm{Ran}\chi(P)$, then

$$e^{-itP/h}\Pi\varphi_0 = U^* e^{-itG/h} U\Pi\varphi_0 + \mathcal{O}(|t|h^\infty\|\varphi_0\|).$$

The symbol $g(x,\xi)$ of G has the following form

$$g(x,\xi) = \xi^2 I_k + \mu(x) + \sum_{i\geq 1} h^j g_j(x,\xi),$$

where $\mu(x)$ is the matrix of $\Pi_0 P_e(x)$ in $(u_1(x), \dots, u_k(x))$.

This theorem means that the motion of all the particles is reduced to the motion of only the nuclei.

§ 3. Some preliminaries

We suppose the magnetic field is parallel to the third axis, so that the vector potential is written as

$$A(x) = \begin{pmatrix} 0 & -b & 0 \\ b & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} x.$$

where $b > 0$ is a constant. We also suppose that the total charge of the particles is zero i.e. $e_1 + Ne = 0$. Setting the mass of electrons to $1/2$ and denoting m/m_e by m again, we introduce new coordinates $(x, y_2, \dots, y_{N+1}) = (x, y) \in \mathbb{R}^3 \times \mathbb{R}^{3N}$ by setting

$$
\begin{aligned}
x &= \frac{1}{M}\left(mx_1 + \sum_{i=2}^{N+1} x_i\right),\ M = m+N \\
y_i &= x_i - x_1,\ 2 \le i \le N+1.
\end{aligned}
\tag{3.1}
$$

Here M is the total mass, x is the position of center of mass and y_i is the position of the electrons relative to the nucleus. With this choice of coordinates, the Hamiltonian is transformed into another Hamiltonian

$$
\tilde{P} = h^2 D_x^2 - 2h^2 e \sum_{i=2}^{N+1} A(y_i) D_x + \sum_{i=2}^{N+1} \tilde{L}_i(x)^2 + h^2 \tilde{Q} + V(x,y)
$$

where $h^2 = \frac{1}{M}$, $\tilde{L}_i(x) = D_{y_i} - eA(y_i + x)$, and writing $f = \sum_{i=2}^{N+1} y_i$, $V(x,y)$ and $\tilde{Q} = \tilde{Q}_1 + \tilde{Q}_2$ are as follows:

$$
\begin{aligned}
V(x,y;h) &= \sum_{i=2}^{N+1} V_{1i}(-y_i) + \sum_{2\le i<j} V_{ij}(y_i - y_j) \\
&\quad + V_1\left(x - h^2 f\right) + \sum_{i=2}^{N+1} V_i\left(x + y_i - h^2 f\right), \\
\tilde{Q}_1 &= \frac{1}{1-Nh^2}\left(\sum_{i=2}^{N+1} \tilde{L}_i(x)\right)^2, \\
\tilde{Q}_2 &= \frac{1}{1-Nh^2}\left[2\sum_{i=2}^{N+1} \tilde{L}_i(x)\left(\sum_{i=2}^{N+1} eA\left(y_i + h^2 f\right)\right) + \left(\sum_{i=2}^{N+1} eA\left(y_i + h^2 f\right)\right)^2\right] \\
&\quad + 2\sum_{i=2}^{N+1} e\tilde{L}_i(x) A(f) + Nh^2 e^2 A(f)^2.
\end{aligned}
$$

Applying the unitary transformation $\mathcal{V} := \exp\left(-ieA(x)\sum_{i=2}^{N+1} y_i\right)$ and its inverse to $\tilde{P}$ we have

$$
\begin{aligned}
P &= \mathcal{V}\tilde{P}\mathcal{V}^* \\
&= h^2 D_x^2 + P_e - 4h^2 e \sum_{i=2}^{N+1} A(y_i) D_x + h^2 Q
\end{aligned}
$$

Here, $P_e(x) = \sum_{i=2}^{N+1} L_i^2 + V_0(x,y)$ and $Q = Q_1 + Q_2 + h^{-2}(V(x,y;h) - V_0(x,y))$, where

$L_i = D_{y_i} - eA(y_i)$ and

$$Q_1 = \frac{1}{1-Nh^2}\left(\sum_{i=2}^{N+1} L_i\right)^2,$$

$$Q_2 = \frac{1}{1-Nh^2}\left[2\sum_{i=2}^{N+1} L_i\left(\sum_{i=2}^{N+1} eA\left(y_i + h^2 f\right)\right) + \left(\sum_{i=2}^{N+1} eA\left(y_i + h^2 f\right)\right)^2\right]$$
$$+ 2\sum_{i=2}^{N+1} eL_i A(f) + (3+Nh^2)e^2 A(f)^2,$$

$$V_0(x,y) = \sum_{i=2}^{N+1} V_{1i}(-y_i) + \sum_{2\le i<j} V_{ij}(y_i - y_j) + V_1(x) + \sum_{i=2}^{N+1} V_i(x+y_i).$$

Note that $V_0(x,y)$ is the zeroth order terms with respect to h of formal Taylor expansion of $V(x,y;h)$.

We suppose interaction potentials V_{ij} and the external potentials V_i satisfy the following assumptions.

(H1) (i) V_{ij} are real valued function Δ-bounded with relative bound smaller than 1.

(ii) $V_i \in C^\infty$ are real valued function and for any $\alpha \in \mathbb{N}^3$ there exist a constant C_α such that

$$|\partial^\alpha V_i(r)| \le C_\alpha.$$

We also suppose that

(H2) The spectrum $\sigma(P_e(x))$ is the union of two disjoint components $\sigma_j(x),\ j = 0,1$, such that $\sigma_0(x)$ is a part of discrete spectrum of $P_e(x)$ with the corresponding subspace of $L^2(\mathbb{R}^{3N})$ being finite dimensional and there exists a number $d > 0$ such that

$$\inf_{x\in\mathbb{R}^3} \operatorname{dist}(\sigma_0(x), \sigma_1(x)) \ge d.$$

Remark. Since by the assumption (H1) V_i is uniformly continuous, the dimension of the subspace associated with $\sigma_0(x)$ is independent of x by [Kato [12], IV Theorem 3.16].

We denote by $\Pi_0(x)$ the spectral projection of $P_e(x)$ corresponding to $\sigma_0(x)$. We also suppose the following assumption.

(H3) $\mathrm{Ran}\Pi_0(x)$ is spanned by a orthonormal basis $(u_1(x,y), \dots, u_k(x,y)) \in C^\infty(\mathbb{R}^3; L^2_y)$ such that

$$\int_{\mathbb{R}^{3N}} |u_i(x,y)|^2 e^{2\alpha|y|} dy < C,$$

$$\int_{\mathbb{R}^{3N}} |\partial_x^\beta u_i(x,y)|^2 dy < C_\beta, \ \forall \beta \in \mathbb{N}^3 \tag{3.2}$$

where constants $C > 0$, $\alpha > 0$ and C_β do not depend on x.

§ 4. Main results

Our main results are concerned with the almost invariant subspace which is close to electronic eigenspace. In the following theorem, $a = \mathcal{O}(h^\infty)$ means $a = \mathcal{O}(h^K)$ for any $K \in \mathbb{N}$.

Theorem 4.1. *Assume (H1)-(H3) hold true. Then for any $\Phi \in C_0^\infty(\mathbb{R})$ such that $\Phi = 1$ on some interval there exists a orthogonal projection $\Pi(h)$ on $L^2(\mathbb{R}^{3(N+1)})$ such that*

$$\|\Pi - \Pi_0\|_{L^2(\mathbb{R}^{3(N+1)})} = \mathcal{O}(h),$$

and, for any $\chi \in C_0^\infty(\mathbb{R})$ such that $\chi\Phi = \chi$, we have

$$\|\chi(P)[\Pi, P]\|_{L^2(\mathbb{R}^{3(N+1)})} + \|[\Pi, P]\chi(P)\|_{L^2(\mathbb{R}^{3(N+1)})} = \mathcal{O}(h^\infty).$$

Using Π we have the following theorem.

Theorem 4.2. *If φ is the solution of $ih\partial_t\varphi = P\varphi$ with initial data φ_0 satisfying $\chi(P)\varphi_0 = \varphi_0$ for some $\chi \in C_0^\infty(\mathbb{R})$ such that $\chi\Phi = \chi$ where Φ is as in Theorem 4.1, then*

$$\varphi = e^{-itP_1/h}\Pi\varphi_0 + e^{-itP_2/h}(1 - \Pi)\varphi_0 + \mathcal{O}(|t|h^\infty\|\varphi_0\|), \tag{4.1}$$

where $P_1 := \Pi P \Pi$ and $P_2 = (1 - \Pi)P(1 - \Pi)$ are self-adjoint on a domain containing $D(P)$.

We can reduce the evolution $e^{-itP_1/h}$ to an evolution on the L^2 space of only nuclear variables. To state the next result we use h-admissible operators.

Theorem 4.3. *There exist a h-admissible operator*

$$W : L^2(\mathbb{R}^{3(N+1)}) \to (L^2(\mathbb{R}^3_x))^{\oplus k}$$

with operator valued symbol and a $k \times k$ self-adjoint matrix G of h-admissible operators on $L^2(\mathbb{R}^3_x)$ such that the restriction U of W to $\mathrm{Ran}\Pi$*:*

$$U : \mathrm{Ran}\Pi \to (L^2(\mathbb{R}^3_x))^{\oplus k}$$

is a unitary operator which satisfies

$$UP_1\Pi = GU\Pi,$$

so that $e^{-itP_1/h}\Pi = U^* e^{-itG/h} U\Pi$. *The symbol* $g(x,\xi)$ *of* G *has the following form:*

$$g(x,\xi) = \xi^2 I_k + \mu(x) + \sum_{j\geq 1} h^j g_j(x,\xi), \tag{4.2}$$

where I_k *is the* k*-dimensional identity matrix and* $\mu(x)$ *is the matrix of* $\Pi_0(x)P_e(x)$ *in* $(u_1(x),\dots,u_k(x))$. *The component in the* j*th low and* m*th column of* g_1 *is*

$$\begin{aligned}(g_1)_{jm} = &-2i\sum_{n=1}^{3}(u_j(x),\partial_{x_n}u_m(x))_{L^2_y}\,\xi_n\\ &-4e\sum_{n=1}^{3}(u_j(x),(\sum_{\ell=2}^{N+1}A(y_\ell))_n u_m(x))_{L^2_y}\xi_n,\end{aligned}\tag{4.3}$$

where $(\sum_{\ell=2}^{N+1}A(y_\ell))_n$ *is the* n*th component of* $\sum_{\ell=2}^{N+1}A(y_\ell)$, *and* $g_j \in S^0(\mathbb{R}^3\times\mathbb{R}^3)$, $j \geq 2$, *so that* $Op_h^w(g_j) \in \mathcal{L}(L^2(\mathbb{R}^{3(N+1)}))$, $j\geq 2$.

Remark. Terms including the vector potential of the nucleus such as $-2heA(x)\xi$ do not appear in g. In particular if the external potentials do not exist (i.e. $V_i \equiv 0$), P_e and u_i are independent of x, so that the first term of (4.3) vanishes and the second term is independent of x. Actually higher order terms are also independent of x in this case since the Hamiltonian P does not include terms depending on x. Thus, the Hamilton flow of g is a straight line. This is not obvious because the internal and external motions are not separated in magnetic fields.

The next result is concerned with more explicit expression of the solution of the Schrödinger equation for a special initial data. We assume $k = 1$ and set $\tilde{u}_1(x) := \mathcal{V}^* u_1(x)$. Then $\tilde{u}_1(x) \in \mathrm{Ran}\tilde{\Pi}_0(x)$ where

$$\tilde{\Pi}_0(x) := \mathcal{V}^*\Pi_0(x)\mathcal{V},$$

which is the spectral projection of $\tilde{P}_e(x) = \sum_{i=2}^{N+1}\tilde{L}_i(x)^2 + V_0(x,y)$ corresponding to $\sigma_0(x)$. Let $\alpha_t = (x_t,\xi_t)$ be the solution of

$$x_t = \frac{\partial g}{\partial \xi}(x_t,\xi_t),\ \xi_t = -\frac{\partial g}{\partial x}(x_t,\xi_t) \tag{4.4}$$

starting from initial data $\alpha_0 = (x_0,\xi_0)$. Let (η_n,ζ_n), $n = 1,2,3$ be the independent solutions of

$$\begin{pmatrix}\dot{\eta}\\ \dot{\zeta}\end{pmatrix} = JM_t\begin{pmatrix}\eta\\ \zeta\end{pmatrix}, \tag{4.5}$$

with initial data

$$(\eta_n)_j|_{t=0} = \delta_{jn},\ (\zeta_n)_j|_{t=0} = i\delta_{jn},$$

where $(\eta_n)_j$ is the jth component of η_n,

$$J = \begin{pmatrix} 0 & \mathbb{I} \\ -\mathbb{I} & 0 \end{pmatrix},$$

$\mathbb{I}$ being the unit matrix and M_t is the Hessian of g at α_t.

Theorem 4.4. *Let $k = 1$ and $\tilde{\varphi}_0 \in L^2(\mathbb{R}^{3(N+1)})$ be as follows*

$$\tilde{\varphi}_0 = (\pi h)^{-3/4}\tilde{\Pi}\chi(\tilde{P})(e^{ix\xi_0/h-(x-x_0)^2/2h}\tilde{u}_1(x)),$$

where $\tilde{\Pi} = \mathcal{V}^*\Pi\mathcal{V}$, and $\chi = 1$ near $\xi_0^2 + \mu(x_0)$. Then there exists $C > 0$ such that for any integer $J \geq 1$ one has

$$\begin{aligned} e^{-it\tilde{P}/h}\tilde{\varphi}_0 =& (\pi h)^{-3/4}(e^{ix\xi_t/h-(x-x_t)^2/2h}\tilde{u}_1(x)) \\ &+ h^{1/2}e^{i\delta_t/h}\sum_{\mu=0}^{\ell_J} c_\mu(t;h)\phi_{\ell,t}\tilde{v}_\ell(x) + \mathcal{O}(h^{J/4}), \end{aligned} \tag{4.6}$$

where

$$c_\ell(t;h) = \sum_{j=0}^{j_\ell} h^{j/2}c_{\ell,j}(t),$$

$c_{\ell,j}$ are given by the polynomials with respect to $\partial^\gamma g(x_t,\xi_t)$ and $\mathrm{Re}\eta_n$, $\mathrm{Im}\eta_n$, $\mathrm{Re}\zeta_n$, $\mathrm{Im}\zeta_n$, $1 \leq n \leq 3$, $\delta_t := \int_0^t(\dot{x}_s\xi_s - g(x_s,\xi_s))ds + (x_0\xi_0 - x_t\xi_t)/2$, $\tilde{v}_\ell \in C^\infty(\mathbb{R}^3; L^2_y(\mathbb{R}^{3N}))$ and $\phi_{\ell,t}$ is a generalized coherent state centered at (x_t,ξ_t). The estimate is uniform with respect to (t,h) such that $h > 0$ is small enough and $t < C^{-1}\ln\frac{1}{h}$.

§ 5. Sketch of the proof of Theorem 4.1

We sketch the proof of Theorem 4.1. We denote by $p(x,\xi;h) = \xi^2 + \sum_{i=2}^{N+1} L_i^2 - 4h^2e\sum_{i=2}^{N+1} A(y_i)\xi + h^2Q + V(x,y)$ the symbol of P and by $p_0(x,\xi) := \xi^2 + \sum_{i=2}^{N+1} L_i^2 + V_0(x,y)$ its principal symbol. Then we have

$$(p(x,\xi;h) - z)\#q_0(x,\xi;z) = 1 - r(x,\xi;h,z),$$

where $q_0 := (p_0 - z)^{-1}$ and $r(x,\xi;h,z) = \sum_{j\geq 1} r^j(x,\xi;z)h^j$. Here

$$a(x,\xi)\#b(x,\xi) = \sum_{\alpha,\beta}\frac{h^{|\alpha+\beta|}(-1)^{|\alpha|}}{(2i)^{|\alpha+\beta|}\alpha!\beta!}(\partial_x^\alpha\partial_\xi^\beta a(x,\xi))(\partial_\xi^\alpha\partial_x^\beta b(x,\xi)),$$

at a formal series level. We define

$$q(x,\xi;h,z) = \sum_{j\geq 1} q_j(x,\xi;z)h^j,$$

by

$$q := q_0 + q_0 \# \sum_{j \geq 1} r^{\# j}.$$

Here $r^{\# j} = r \# \cdots \# r$ where the number of r is j.

Let us set

$$\Gamma(x, \xi) := \{z \in \mathbb{C}; z - \xi^2 \in \gamma(x)\},$$

and let us define

$$\hat{\pi}_j(x, \xi) = \frac{i}{2\pi} \oint_{\Gamma(x,\xi)} q_j(x, \xi; z) dz. \tag{5.1}$$

Then we have the following Lemma.

Lemma 5.1. *For any $j \in \mathbb{N}$ and $r, s \in \mathbb{R}$, $\hat{\pi}_j(x, \xi) \in S^j(\mathbb{R}^3 \times \mathbb{R}^3; \mathcal{L}(L_y^{2,r}, L_y^{2,r+s}))$ where $L_y^{2,s} := \{u : (1 + |y|^2)^{s/2} u \in L_y^2\}$ and $\hat{\pi}(x, \xi) \in S^m(\mathbb{R}^3 \times \mathbb{R}^3; \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ means*

$$\sup_{(x,\xi) \in \mathbb{R}^3 \times \mathbb{R}^3} \|\partial_x^\alpha \partial_\xi^\beta \hat{\pi}(x, \xi)\|_{\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)} (1 + |\xi|)^{-m + |\beta|} < \infty, \tag{5.2}$$

for any $\alpha, \beta \in \mathbb{N}^3$.

We define

$$\begin{aligned}
\hat{\Pi}_j u(x) &= Op_h^w(\hat{\pi}_j(x, \xi)) u(x) \\
&= \frac{1}{(2\pi h)^3} \int \left(\int e^{i(x-y)\xi/h} \pi_j(\frac{x+y}{2}, \xi) u(y) dy \right) d\xi.
\end{aligned}$$

The operator $\hat{\Pi}_j$ is not bounded but by a localization in energy we obtain a bounded operator.

Lemma 5.2. *For any $\Phi \in C_0^\infty(\mathbb{R})$ such that $\Phi = 1$ on some interval, $\Phi(P)\hat{\Pi}_j$ is bounded in $L^2(\mathbb{R}^{3(N+1)})$.*

We resum in a standard way

$$\hat{\Pi}\Phi(P) := \Pi_0 \Phi(P) + \sum_{j \geq 1} \hat{\Pi}_j \Phi(P) h^j,$$

$$\Phi(P)\hat{\Pi} := \Phi(P)\Pi_0 + \sum_{j \geq 1} \Phi(P)\hat{\Pi}_j h^j.$$

We define

$$\hat{\Pi}_\Phi := \Phi(P)\hat{\Pi} + (1 - \Phi(P))\hat{\Pi}\Phi(P) + (1 - \Phi(P))\Pi_0(1 - \Phi(P)).$$

Since $\sum_{j \geq 0} q_j h^j$ is formally the symbol of $(P - z)^{-1}$, we have the following lemma as in Sordoni [21].

Lemma 5.3. *Let $\chi \in C_0^\infty(\mathbb{R})$ satisfy $\chi\Phi = \chi$ where Φ is as in Lemma 5.2. Then for all $N \in \mathbb{N}$*

$$\|\chi(P)[\hat{\Pi}_\Phi, P]\| + \|[\hat{\Pi}_\Phi, P]\chi(P)\| = \mathcal{O}(h^N),$$

$$\|\chi(P)(\hat{\Pi}_\Phi^2 - \hat{\Pi}_\Phi)\| + \|(\hat{\Pi}_\Phi^2 - \hat{\Pi}_\Phi)\chi(P)\| = \mathcal{O}(h^N).$$

Since $\hat{\Pi}_\Phi - \Pi_0 = \mathcal{O}(h)$, for sufficiently small h the spectrum of $\hat{\Pi}_\Phi$ is concentrated near 0 and 1, so that the set $\{z \in \mathbb{C}; |z-1| = 1/2\}$ is in the resolvent set of $\hat{\Pi}_\Phi$ for sufficiently small h. We define

$$\Pi := \frac{i}{2\pi}\oint_{|z-1|=1/2} (\hat{\Pi}_\Phi - z)^{-1} dz.$$

Then as in Sordoni [21] we have

$$\Pi - \hat{\Pi}_\Phi = \frac{i}{2\pi}(\hat{\Pi}_\Phi^2 - \hat{\Pi}_\Phi)\oint_{|z-1|=1/2} (\hat{\Pi}_\Phi - z)^{-1}(2\hat{\Pi}_\Phi - 1)(1 - \hat{\Pi}_\Phi - z)^{-1}(1-z)^{-1} dz.$$

Theorem 4.1 follows from this formula and Lemma 5.3.

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