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On the stability of the Schwartz class under the magnetic Schrödinger flow

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We prove that the Schwartz class is stable under the magnetic Schrödinger flow when the magnetic 2-form is non-degenerate and does not oscillate too much at infinity.

1. Introduction

1.1. Motivation and context

This paper is devoted to describing the solutions to the magnetic Schrödinger equation. Let $\mathbf{B}$ be a smooth and closed 2-form on $\mathbb{R}^d$. Let $\mathbf{A} : \mathbb{R}^d \to \mathbb{R}^d$ be a 1-form (identified with a vector field) such that $\mathrm{d}\mathbf{A} = \mathbf{B}$. The magnetic Schrödinger operator is the essentially self-adjoint (see [4, Theorem 1.2.2]) differential operator

$$\mathscr{L}_h = (-ih\nabla - \mathbf{A})^2 = \sum_{j=1}^{d} L_j^2,$$

where $h > 0$ and, for all $j \in \{1, \dots, j\}$, $L_j = -ih\partial_j - A_j$. Its domain is given by

$$\begin{aligned}\mathrm{Dom}(\mathscr{L}_h) &= \{\psi \in L^2(\mathbb{R}^d) : (-ih\nabla - \mathbf{A})\psi \in L^2(\mathbb{R}^d), \\ &\qquad (-ih\nabla - \mathbf{A})^2\psi \in L^2(\mathbb{R}^d)\} \\ &= \{\psi \in L^2(\mathbb{R}^d) : (-ih\nabla - \mathbf{A})^2\psi \in L^2(\mathbb{R}^d)\}.\end{aligned}$$

The time dependent magnetic Schrödinger equation is given by

$$-ih\partial_t\psi = \mathscr{L}_h\psi, \qquad \psi(0) = \psi_0 \in \mathrm{Dom}(\mathscr{L}_h). \tag{1.1}$$

By Stone's theorem, this Cauchy problem admits a unique solution, evolving in the domain of $\mathscr{L}_h$, and it is given by

$$\forall t \in \mathbb{R}, \quad \psi(t) = e^{\frac{it\mathscr{L}_h}{h}}\psi_0.$$

By unitarity of the flow, we have

$$\forall t \in \mathbb{R}, \quad \|\psi(t)\| = \|\psi_0\|, \quad \|\mathscr{L}_h \psi(t)\| = \|\mathscr{L}_h \psi_0\|,$$

where $\|\cdot\|$ denotes the usual norm on $L^2(\mathbb{R}^d)$. This norm controls the rough phase space localization of the quantum state $\psi(t)$; a natural question is to know to which extent a strong phase space localization of ψ_0 is preserved by the flow. More precisely, this paper was inspired by the following rather naive question. Is it true that

$$\psi_0 \in \mathscr{S}(\mathbb{R}^d) \quad \Longrightarrow \quad \forall t \in \mathbb{R}, \quad \psi(t) \in \mathscr{S}(\mathbb{R}^d) \quad ? \tag{1.2}$$

If so, what kind of explicit control do we have in terms of the Schwartz semi-norms?

These questions are motivated by the recent investigation of the propagation of coherent states by the magnetic Hamiltonian flow in two dimensions (see the Ph. D. thesis of the first author [2]). The present paper gives a positive answer to (1.2). Our explicit estimates of the Schwartz semi-norms (in terms of the semiclassical parameter h), combined with the use of the Birkhoff normal form from [14], turn out to be the key ingredients in the study by [3] of the propagation of coherent states up to times of order h^{-N}, for all $N \in \mathbb{N}$. This gives a quantum analog to the low energy (say of order ε) classical propagation for times of order $\varepsilon^{-\infty}$ (see [14, Theorem 1.2]). Taking into account the analysis of [6], one can even hope to extend these results to three dimensions where the classical dynamics has a more complex behavior.

Independently of this motivation, the answer to (1.2) has an interest of its own, especially because it lives at the confluence of two closely related domains: hypoellipticity and semiclassical analysis with magnetic fields. On these vast subjects, the literature is enormous, and we only refer to [4, 7, 9–11, 13, 16, 17]. In this paper, we will use many classical ideas from these two contexts, and provide an elementary and self-contained presentation.

1.2. Main results

Let us now describe our assumptions and results.

Let $\mathscr{P}$ be the class defined by

$$\mathscr{P} = \{\psi \in \mathscr{C}^\infty(\mathbb{R}^d) : \forall \alpha \in \mathbb{N}^d, \exists (C, m) \in \mathbb{R}_+ \times \mathbb{R}_+, \\ \forall x \in \mathbb{R}^d, |\partial^\alpha \psi| \leqslant C\langle x \rangle^m\}.$$

The following assumption will hold throughout the paper, where we identify $\mathbf{B}$ with its antisymmetric matrix obtained in the usual basis $(\mathrm{d}x_j \wedge \mathrm{d}x_k; j < k)$.

Assumption 1.1. We assume that

(i) $\mathbf{A}$ belongs to $\mathscr{P}$ (in particular $\mathbf{B} \in \mathscr{P}$),

(ii) there exists $b_0 > 0$ such that, for all $x \in \mathbb{R}^d$,

$$\mathrm{Tr}^+\mathbf{B}(x) \geqslant b_0,$$

where $\mathrm{Tr}^+\mathbf{B}(x)$ denotes the sum of the moduli of the eigenvalues with positive imaginary part of the matrix $\mathbf{B}(x)$,

(iii) for all $\alpha \in \mathbb{N}^d$, there exists $C > 0$ such that, for all $x \in \mathbb{R}^d$, $\|\partial^\alpha \mathbf{B}(x)\| \leqslant C\|\mathbf{B}(x)\|$, where $\|\cdot\|$ denotes a norm on the space of matrices.

Assumption 1.1 is stronger than really necessary as we can see in our proofs.

A basic example of magnetic field satisfying Assumption 1.1 when $d = 2$ is given by

$$A_1 = 0, \quad A_2(x_1, x_2) = x_1 + \frac{x_1^3}{3} + x_2^2 x_1.$$

In this case, the magnetic field is a function

$$B(x_1, x_2) = \mathrm{Tr}^+\mathbf{B}(x) = 1 + x_1^2 + x_2^2 \geqslant 1.$$

More generally, in two dimensions, a magnetic field is identified with a scalar function, and it satisfies (ii) if and only if its absolute value if bounded from below by a positive constant. In three dimensions, $\mathbf{B}$ can be seen as a vector field through Euclidean duality and $\mathrm{Tr}^+\mathbf{B} = \|\mathbf{B}\|$. Thus, the assumption (ii) just means that $\|\mathbf{B}\|$ is bounded from below by a positive constant. The positivity of item (ii) has an important consequence on the semiclassical behavior of the ground-energy (the infimum of the spectrum), as shown by the following lemma (see [8, Theorem 2.2]).

Lemma 1.2. *We have*

$$\inf \mathrm{sp}(\mathscr{L}_h) = h \inf_{x \in \mathbb{R}^d} \mathrm{Tr}^+\mathbf{B}(x) + o(h).$$

In particular, there exist $C>0$ and $h_0>0$, such that, for all $h\in(0,h_0)$, $\mathscr{L}_h$ is bijective and

$$\|\mathscr{L}_h^{-1}\|\leqslant Ch^{-1}.$$

In the following, we will always assume that h is small enough and such that $\mathscr{L}_h$ is invertible.

Definition 1.3. For all $n\in\mathbb{N}$, we let

$$\mathrm{Dom}(\mathscr{L}_h^n)=\{\psi\in L^2(\mathbb{R}^d):\forall\ell\in\{1,\dots,n\}:\mathscr{L}_h^{\ell-1}\psi\in\mathrm{Dom}(\mathscr{L}_h)\}.$$

The operator $\mathscr{L}_h^n$ is defined by induction by

$$\forall\psi\in\mathrm{Dom}(\mathscr{L}_h^n),\quad \mathscr{L}_h^n\psi=\mathscr{L}_h(\mathscr{L}_h^{n-1}\psi).$$

The operator $(\mathrm{Dom}(\mathscr{L}_h^n),\mathscr{L}_h^n)$ is self-adjoint and invertible. The following theorem proves some magnetic elliptic estimates, showing that iterations of the magnetic laplacian $\mathscr{L}_h$ control iterations of the magnetic derivatives $(L_j)_{1\leqslant j\leqslant d}$. This will be an important tool on the proof of the main result of the paper.

Theorem 1.4. *Let Assumption 1.1 hold. Let $n\in\mathbb{N}$. There exist $h_0>0$ and $C>0$ such that, for all $h\in(0,h_0)$, and all $\psi\in\mathrm{Dom}(\mathscr{L}_h^n)$,*

$$\sum_{\sigma\in\mathfrak{A}(2n)}\|L_\sigma\psi\|\leqslant Ch^{-3n/2}\|\mathscr{L}_h^n\psi\|, \tag{1.3}$$

where, for $k\in\mathbb{N}$, $\mathfrak{A}(k)=\cup_{p=0}^k\{1,\dots,d\}^{\{1,\dots,p\}}$, and for $p\in\mathbb{N}$, for $\sigma\in\{1,\dots,d\}^{\{1,\dots,p\}}$, $L_\sigma:=L_{\sigma(1)}\dots L_{\sigma(p)}$, with the convention $L_\emptyset=\mathrm{Id}$.

In the case where $\mathbf{A}$ is bounded, Theorem 1.3 is closely related to [16, Theorem 3], which deals with the context of general Gårding inequalities.

Definition 1.5. For all $k\in\mathbb{N}$ and all $\psi\in\mathscr{S}(\mathbb{R}^d)$, we let

$$p_k(\psi)=\max_{\substack{(\alpha,\beta)\in\mathbb{N}^{2d}\\|\alpha|+|\beta|\leqslant k}}\|x^\alpha\partial^\beta\psi\|_\infty.$$

We can now state the main result of this paper.

Theorem 1.6. *Let Assumption 1.1 hold. For all $t \in \mathbb{R}$, we have*

$$e^{\frac{it\mathscr{L}_h}{h}} \mathscr{S}(\mathbb{R}^d) \subset \mathscr{S}(\mathbb{R}^d).$$

More precisely, for all $M \in \mathbb{N}^*$, for all $k \in \mathbb{N}$, there exist $h_0 > 0$, $C > 0$, $N \in \mathbb{N}^*$ and $K \in \mathbb{N}$, such that, for all $h \in (0, h_0)$, and for all $\psi_0 \in \mathscr{S}(\mathbb{R}^d)$, and all $t \in [0, h^{-M}]$,

$$p_k(e^{\frac{it\mathscr{L}_h}{h}} \psi_0) \leqslant Ch^{-N} p_K(\psi_0).$$

Theorem 1.6 is related to the (pseudo-differential) analysis in [17, Section 7]. In this work, under the assumption that the derivatives of order two or higher of the symbol of the propagator should be bounded, a parametrix of the evolution operator was constructed. Closely related is also the paper [15, Corollary 2.11], based on the analysis of coherent states, where the derivatives of order three or higher of the symbol have to be bounded. Our approach here is more directly related to the structure of the magnetic Laplacian, and is reminiscent of the analysis in [11] of the ellipticity of certain algebras of non-commuting vector fields.

Finally, it would be quite interesting to explore time-dependent magnetic fields. In order to tackle this problem, we should first analyse what happens in finite time by means of the results of [12]. However, our method, which is based on estimates of the iterates of $\mathscr{L}_h$ and their commutation with the evolution $e^{i\frac{t}{h}\mathscr{L}_h}$, would need to be refined in order to apply to the the time dependent case.

1.3. Organisation of the proofs

In Section 2, we prove Theorem 1.4 by using a regularization argument involving exponentially weighted estimates and commutator estimates. In Section 3, we apply our magnetic elliptic estimates to prove Theorem 1.6.

2. Magnetic elliptic estimates

This section is devoted to the proof of Theorem 1.4.

2.1. Density argument

Let us explain here why it is sufficient to prove Theorem 1.4 for $\psi \in \mathscr{S}(\mathbb{R}^d)$.

Let us consider $f \in L^2(\mathbb{R}^d)$. There is a unique $\psi \in \mathrm{Dom}(\mathscr{L}_h^n)$ such that $\mathscr{L}_h^n \psi = f$. Consider $f_k \in \mathscr{C}_0^\infty(\mathbb{R}^d)$ converging to f in $L^2(\mathbb{R}^d)$ and consider the unique $\psi_k \in \mathrm{Dom}(\mathscr{L}_h^n)$ such that $\mathscr{L}_h^n \psi_k = f_k$. Note that, by continuity of $(\mathscr{L}_h^n)^{-1}$, ψ_k converges to ψ in $L^2(\mathbb{R}^d)$.

Lemma 2.1. *We let*

$$H^\infty_{\exp}(\mathbb{R}^d) = \{\psi \in L^2(\mathbb{R}^d) : \forall \alpha \in \mathbb{N}^d, \exists \beta > 0 : e^{\beta\langle x\rangle}\partial^\alpha \psi \in L^2(\mathbb{R}^d)\}.$$

Consider $f \in H^\infty_{\exp}(\mathbb{R}^d)$. Then, the unique solution $u \in \mathrm{Dom}(\mathscr{L}_h)$ to $\mathscr{L}_h u = f$ satisfies $u \in H^\infty_{\exp}(\mathbb{R}^d)$.

Proof. The proof follows from the classical Agmon estimates (see [1, 5]). Consider $\beta > 0$ such that $e^{\beta\langle x\rangle} f \in L^2(\mathbb{R}^d)$. Let $\varepsilon > 0$ and $\Phi_\varepsilon = \beta \min(\langle x\rangle, \varepsilon^{-1})$. We have the Agmon formula (see [13, Section 4.2]):

$$\mathrm{Re}\,\langle \mathscr{L}_h u, e^{2\Phi_\varepsilon} u\rangle = \int_{\mathbb{R}^d} |(-ih\nabla - \mathbf{A})e^{\Phi_\varepsilon} u|^2 \mathrm{d}x - h^2 \|\nabla \Phi_\varepsilon e^{\Phi_\varepsilon} u\|^2.$$

In particular,

$$\int_{\mathbb{R}^d} |(-ih\nabla - \mathbf{A})e^{\Phi_\varepsilon} u|^2 \mathrm{d}x - \beta^2 h^2 \|e^{\Phi_\varepsilon} u\|^2 \leqslant \|e^{\Phi_\varepsilon} f\| \|e^{\Phi_\varepsilon} u\|. \tag{2.1}$$

On the other hand, by Lemma 1.2, we get, for some $c > 0$,

$$(hc - \beta^2 h^2)\|e^{\Phi_\varepsilon} u\|^2 \leqslant \int_{\mathbb{R}^d} |(-ih\nabla - \mathbf{A})e^{\Phi_\varepsilon} u|^2 \mathrm{d}x - \beta^2 h^2 \|e^{\Phi_\varepsilon} u\|^2.$$

Choosing β small enough, we get, for some $C(h) > 0$ independent of ε,

$$\|e^{\Phi_\varepsilon} u\| \leqslant C(h) \|e^{\Phi_\varepsilon} f\|.$$

Then, we take the limit $\varepsilon \to 0$ and apply Fatou's Lemma to find

$$\|e^{\beta\langle x\rangle} u\| \leqslant C(h) \|e^{\beta\langle x\rangle} f\|. \tag{2.2}$$

Coming back to (2.1), and replacing β by $\tilde\beta < \beta$, we get

$$\int_{\mathbb{R}^d} |e^{\Phi_\varepsilon}(-ih\nabla - \mathbf{A} - ih\nabla\Phi_\varepsilon) u|^2 \mathrm{d}x - \tilde\beta^2 h^2 \|e^{\Phi_\varepsilon} u\|^2 \leqslant \|e^{\Phi_\varepsilon} f\| \|e^{\Phi_\varepsilon} u\|.$$

Thus,

$$\frac{h^2}{2}\int_{\mathbb{R}^d} |e^{\Phi_\varepsilon}\nabla u|^2 \mathrm{d}x \leqslant \|e^{\Phi_\varepsilon} f\|\|e^{\Phi_\varepsilon} u\| + \tilde{\beta}^2 h^2 \|e^{\Phi_\varepsilon} u\|^2 + 2\|(ih\nabla\Phi_\varepsilon + \mathbf{A})e^{\Phi_\varepsilon} u\|^2$$
$$\leqslant \|e^{\Phi_\varepsilon} f\|\|e^{\Phi_\varepsilon} u\| + \tilde{\beta}^2 h^2 \|e^{\Phi_\varepsilon} u\|^2 + 4\|\nabla\Phi_\varepsilon e^{\Phi_\varepsilon} u\|^2 + 4\|\mathbf{A} e^{\Phi_\varepsilon} u\|^2.$$

Using that $\mathbf{A} \in \mathscr{P}$, (2.2), and Fatou's Lemma, we get $e^{\tilde{\beta}\langle x\rangle}\nabla u \in L^2(\mathbb{R}^d)$.

Considering the equation $\mathscr{L}_h u = f$, we get, in the sense of tempered distributions,

$$-h^2\Delta u = f - |\mathbf{A}|^2 u - ih(\nabla\cdot\mathbf{A})u - 2ih(\mathbf{A}\cdot\nabla)u. \tag{2.3}$$

Noticing that we have just controlled the terms of order at most one, we deduce that, for some $\beta > 0$,

$$e^{\beta\langle x\rangle}\Delta u \in L^2(\mathbb{R}^d),$$

and also

$$\Delta\left(e^{\beta\langle x\rangle}u\right) \in L^2(\mathbb{R}^d).$$

By Fourier transform, we get

$$e^{\beta\langle x\rangle}u \in H^2(\mathbb{R}^d),$$

which implies that, for all $\alpha \in \mathbb{N}^d$ with $|\alpha| \leqslant 2$,

$$e^{\beta\langle x\rangle}\partial^\alpha u \in L^2(\mathbb{R}^d).$$

The higher order derivatives can be controlled by induction (taking successive derivatives of (2.3)). □

Remark 2.2. By the Sobolev embeddings, we have $H^\infty_{\exp}(\mathbb{R}^d) \subset \mathscr{S}(\mathbb{R}^d)$.

By Lemma 2.1, we see that $\psi_k \in \mathscr{S}(\mathbb{R}^d)$. Assume that (1.3) holds for any $\psi \in \mathscr{S}(\mathbb{R}^d)$, with $\psi = \psi_k - \psi_\ell$, for all $(k,\ell) \in \mathbb{N}^2$, this shows that, for all $\sigma \in \mathfrak{A}(2n)$, $(L_\sigma\psi_n)_{n\in\mathbb{N}}$ is a Cauchy sequence in $L^2(\mathbb{R}^d)$. Thus, in the sense of distributions, $L_\sigma\psi \in L^2(\mathbb{R}^d)$. It remains to use again (1.3) with $\psi = \psi_k$ and to take the limit $k \to +\infty$.

2.2. Preliminary lemmas

Lemma 2.3. *For all* $\psi \in \mathrm{Dom}(\mathscr{L}_h)$*, we have*

$$\|(-ih\nabla - \mathbf{A})\psi\|^2 \leqslant \frac{1}{2}\|\psi\|^2_{\mathscr{L}_h}$$

where $\|\psi\|^2_{\mathscr{L}_h} = \|\psi\|^2 + \|\mathscr{L}_h\psi\|^2$.

Proof. We recall that, by definition of the domain, for all $\psi \in \mathrm{Dom}(\mathscr{L}_h)$,

$$\langle \mathscr{L}_h\psi, \psi\rangle = \|(-ih\nabla - \mathbf{A})\psi\|^2 = \sum_{j=1}^{d} \|L_j\psi\|^2,$$

so that

$$\sum_{j=1}^{d} \|L_j\psi\|^2 \leqslant \|\psi\|\|\mathscr{L}_h\psi\|.$$

□

Lemma 2.4. *There exist* $C > 0$ *and* $h_0 > 0$ *such that, for all* $\psi \in \mathscr{S}(\mathbb{R}^d)$ *and all* $h \in (0, h_0)$*,*

$$\|\langle\mathbf{B}\rangle\psi\| + \|\langle\mathbf{B}\rangle^{\frac{1}{2}}(-ih\nabla - \mathbf{A})\psi\| \leqslant Ch^{-1}\|\psi\|_{\mathscr{L}_h}. \tag{2.4}$$

Moreover, for all $\psi \in \mathrm{Dom}(\mathscr{L}_h)$*, we have*

$$\mathbf{B}\psi \in L^2(\mathbb{R}^d) \quad \text{and} \quad |\mathbf{B}|^{\frac{1}{2}}(-ih\nabla - \mathbf{A})\psi \in L^2(\mathbb{R}^d),$$

and (2.4) *holds for* $\psi \in \mathrm{Dom}(\mathscr{L}_h)$.

Proof. By integration by parts and using Assumption 1.1 (iii),

$$\begin{aligned}\int_{\mathbb{R}^d} \langle\mathbf{B}\rangle|(-ih\nabla - \mathbf{A})\psi|^2 \mathrm{d}x &= \langle\langle\mathbf{B}\rangle(-ih\nabla - \mathbf{A})\psi, (-ih\nabla - \mathbf{A})\psi\rangle \\ &\leqslant \langle\mathscr{L}_h\psi, \langle\mathbf{B}\rangle\psi\rangle + C\|\langle\mathbf{B}\rangle\psi\|\|(-ih\nabla - \mathbf{A})\psi\| \\ &\leqslant C\|\langle\mathbf{B}\rangle\psi\|\|\psi\|_{\mathscr{L}_h}.\end{aligned} \tag{2.5}$$

Then, we have

$$\int_{\mathbb{R}^d} |h\mathbf{B}|^2|\psi|^2 \mathrm{d}x = \sum_{(k,\ell)\in\{1,\ldots,d\}^2} \int_{\mathbb{R}^d} |hB_{k,\ell}|^2|\psi|^2 \mathrm{d}x$$

and we write

$$\sum_{(k,\ell)\in\{1,\dots,d\}^2} \int_{\mathbb{R}^d} |hB_{k,\ell}|^2|\psi|^2 \mathrm{d}x = \sum_{(k,\ell)\in\{1,\dots,d\}^2} |\langle [L_k, L_\ell]\psi, hB_{k,\ell}\psi\rangle| \\ \leqslant Ch\|\langle \mathbf{B}\rangle\psi\|\|(-ih\nabla - \mathbf{A})\psi\| \\ + Ch\int_{\mathbb{R}^d} \langle \mathbf{B}\rangle|(-ih\nabla - \mathbf{A})\psi|^2\mathrm{d}x,$$

where we used an integration by parts and Assumption 1.1.

By (2.5), it follows

$$\int_{\mathbb{R}^d} |\mathbf{B}|^2|\psi|^2\mathrm{d}x \leqslant Ch^{-1}\|\langle\mathbf{B}\rangle\psi\|\|\psi\|_{\mathscr{L}_h}$$

and then

$$\|\langle\mathbf{B}\rangle\psi\| \leqslant Ch^{-1}\|\psi\|_{\mathscr{L}_h}.$$

Using again (2.5), the conclusion follows. □

2.3. Case $n = 1$

The estimate of Theorem 1.4 is obvious when $n = 0$. Let us consider the case when $n = 1$ to explain the principle producing these estimates.

Lemma 2.5. *There exist $C > 0$, $h_0 > 0$ such that, for all $\psi \in \mathscr{S}(\mathbb{R}^d)$ and all $h \in (0, h_0)$,*

$$\|L_1^2\psi\| + \|L_2^2\psi\| + \|L_1L_2\psi\| + \|L_2L_1\psi\| \leqslant Ch^{-1}\|\mathscr{L}_h\psi\|.$$

Proof. Let us consider $\psi \in \mathscr{S}(\mathbb{R}^d)$ and let

$$\mathscr{L}_h\psi = f.$$

Consider $j \in \{1,\dots,d\}$. We have

$$\mathscr{L}_h(L_j\psi) = L_jf + [\mathscr{L}_h, L_j]\psi,$$

and

$$\|(-ih\nabla - \mathbf{A})(L_j\psi)\|^2 = \langle L_jf, L_j\psi\rangle + \langle[\mathscr{L}_h, L_j]\psi, L_j\psi\rangle,$$

We have

$$[\mathscr{L}_h, L_j] = \sum_{k=1}^{d}[L_k^2, L_j] = \sum_{k=1}^{d}\left([L_k, L_j]L_k + L_k[L_k, L_j]\right).$$

Thus,

$$\begin{aligned}|\langle[\mathscr{L}_h, L_j]\psi, L_j\psi\rangle| \leqslant C\|\mathbf{B}\psi\|\|(-ih\nabla-\mathbf{A})\psi\|\\ + C\int_{\mathbb{R}^d}|\mathbf{B}||(-ih\nabla-\mathbf{A})\psi|^2\mathrm{d}x.\end{aligned}$$

We have, for all $\varepsilon\in(0,1)$,

$$|\langle L_j f, L_j\psi\rangle| \leqslant \varepsilon\|L_j^2\psi\|^2 + C_\varepsilon\|f\|^2,$$

and then, for ε small enough,

$$\begin{aligned}\|(-ih\nabla-\mathbf{A})(L_j\psi)\|^2 \leqslant C\|f\|^2 + C\|\mathbf{B}\psi\|\|(-ih\nabla-\mathbf{A})\psi\|\\ + C\int_{\mathbb{R}^d}|\mathbf{B}||(-ih\nabla-\mathbf{A})\psi|^2\mathrm{d}x.\end{aligned}$$

With Lemma 2.3, noting that $\|\psi\|^2_{\mathscr{L}_h} \leqslant C(1+h^{-2})\|f\|^2$, we find

$$\|(-ih\nabla-\mathbf{A})(L_j\psi)\|^2 \leqslant Ch^{-3}\|f\|^2.$$

□

2.4. Induction

Let $n\in\mathbb{N}^*$. Let us assume that, for all $k\in\{1,\ldots,n\}$, the ellipticity property (1.3) is true. Let us consider $f,\psi\in\mathscr{S}(\mathbb{R}^d)$ such that

$$\mathscr{L}_h\psi = f.$$

Consider $\sigma\in\mathfrak{A}(2n)$. Since the functions are in the Schwartz class, all the following computations are justified.

We have

$$\mathscr{L}_h L_\sigma\psi = L_\sigma f + [\mathscr{L}_h, L_\sigma]\psi,$$

and then

$$\langle\mathscr{L}_h L_\sigma\psi, L_\sigma\psi\rangle = \langle L_\sigma f, L_\sigma\psi\rangle + \langle[\mathscr{L}_h, L_\sigma]\psi, L_\sigma\psi\rangle. \tag{2.6}$$

By using the Cauchy-Schwarz inequality and the induction assumption, we have for all $\varepsilon\in(0,1)$,

$$|\langle L_\sigma f, L_\sigma\psi\rangle| \leqslant Ch^{-3n}\|\mathscr{L}_h^n f\|\|\mathscr{L}_h^n\psi\| \leqslant Ch^{-3n}\|\mathscr{L}_h^{n+1}\psi\|^2 + Ch^{-3n}\|\mathscr{L}_h^n\psi\|^2,$$

so that, by Lemma 1.2,

$$|\langle L_\sigma f, L_\sigma \psi\rangle| \leqslant Ch^{-(3n+2)}\|\mathscr{L}_h^{n+1}\psi\|^2.$$

Let us now deal with $\langle [\mathscr{L}_h, L_\sigma]\psi, L_\sigma\psi\rangle$. The commutator $[\mathscr{L}_h, L_\sigma]$ is the sum of various terms. Each of them is the composition of at most $2n-2$ of the L_j and with exactly one of the $B_{k,\ell}$. By commuting the $B_{k,\ell}$ to put it on the left, and using Assumption 1.1, we get

$$\|[\mathscr{L}_h, L_\sigma]\psi\| \leqslant C \sum_{\tau\in\mathfrak{A}(2n-2)} \|\langle \mathbf{B}\rangle L_\tau \psi\|.$$

By applying Lemma 2.4, and then the induction assumption, we get

$$\|[\mathscr{L}_h, L_\sigma]\psi\| \leqslant Ch^{-1} \sum_{\tau\in\mathfrak{A}(2n-2)} \|L_\tau\psi\|_{\mathscr{L}_h} \leqslant Ch^{-(3n-1)/2}\|\mathscr{L}_h^n\psi\|.$$

Thus, we deduce

$$|\langle \mathscr{L}_h L_\sigma\psi, L_\sigma\psi\rangle| \leqslant Ch^{-3n-1/2}\|\mathscr{L}_h^{n+1}\psi\|^2.$$

This shows that, for all $\gamma\in\mathfrak{A}(2n+1)$,

$$\|L_\gamma\psi\| \leqslant Ch^{-(3n/2+1)}\|\mathscr{L}_h^{n+1}\psi\|. \tag{2.7}$$

Now, we want to get the control for $\gamma\in\mathfrak{A}(2n+2)$. Let $\sigma\in\mathfrak{A}(2n+1)$. We consider again (2.6). By integration by parts, we can write

$$\langle L_\sigma f, L_\sigma\psi\rangle = \langle L_{\check\sigma} f, L_{\hat\sigma}\psi\rangle,$$

with $\check\sigma\in\mathfrak{A}(2n)$ and $\hat\sigma\in\mathfrak{A}(2n+2)$. Thus, by Cauchy-Schwarz, and the induction assumption, for all $\varepsilon>0$, there exists $C>0$ such that

$$|\langle L_\sigma f, L_\sigma\psi\rangle| \leqslant \varepsilon\|L_{\hat\sigma}\psi\|^2 + Ch^{-3n/2}\|\mathscr{L}_h^{n+1}\psi\|^2. \tag{2.8}$$

As previously, we have

$$\|[\mathscr{L}_h, L_\sigma]\psi\| \leqslant C \sum_{\tau\in\mathfrak{A}(2n-1)} \|\langle \mathbf{B}\rangle L_\tau \psi\|.$$

We use Lemma 2.4 and (2.7) to find

$$\|[\mathscr{L}_h, L_\sigma]\psi\| \leqslant Ch^{-1} \sum_{\tau\in\mathfrak{A}(2n-1)} \|L_\tau\psi\|_{\mathscr{L}_h} \leqslant Ch^{-(3n/2+2)}\|\mathscr{L}_h^{n+1}\psi\|.$$

Then, with Cauchy-Schwarz and (2.7), we get

$$|\langle [\mathscr{L}_h, L_\sigma]\psi, L_\sigma\psi\rangle| \leqslant Ch^{-(3n+3)}\|\mathscr{L}_h^{n+1}\psi\|^2. \tag{2.9}$$

From (2.6), (2.8), and (2.9), summing over $\sigma \in \mathfrak{A}(2n+1)$, and choosing ε small enough, we get (1.3) with n replaced by $n+1$.

This achieves the proof of Theorem 1.4 when $\psi \in \mathscr{S}(\mathbb{R}^d)$ and it remains to use the discussion of Section 2.1 when $\psi \in \mathrm{Dom}(\mathscr{L}_h^n)$.

3. Application to the evolution problem

We can now prove Theorem 1.6. Let $\psi_0 \in \mathscr{S}(\mathbb{R}^d)$. We denote by $\psi(\cdot)$ the solution to the Schrödinger equation (1.1).

Notation. For $\kappa, \lambda \in \mathbb{N}$, we define $\Pi_{\kappa,\lambda}$ the set of the operators P that are composition of operators taken among $(L_j)_{1\leqslant j\leqslant d}$ and and $(x_k)_{1\leqslant k\leqslant d}$ with κ occurences of x and λ occurences of L. We also set $\Pi = \bigcup_{(\kappa,\lambda)\in\mathbb{N}^2} \Pi_{\kappa,\lambda}$.

The aim of this section is to prove the following proposition.

Proposition 3.1. *Let $(\kappa,\lambda) \in \mathbb{N}^2$ and consider $P \in \Pi_{\kappa,\lambda}$. There exist $h_0 > 0$, $C \geqslant 0$ and $N \in \mathbb{N}$ such that, for all $t \geqslant 0$, and all $\psi_0 \in \mathscr{S}(\mathbb{R}^d)$, for $\lambda \leqslant 2n \leqslant \lambda + 1$,*

$$\|P\psi(t)\| \leqslant Ch^{-N}(1+t^\kappa) \sum_{|\alpha|\leqslant\kappa : |\alpha|+\nu\leqslant\kappa+n} \|\mathscr{L}_h^\nu x^\alpha \psi_0\|.$$

This proposition implies the control of the Schwartz semi-norms and achieves the proof of Theorem 1.6. Indeed, from Sobolev embeddings, for all $k \in \mathbb{N}$, there exists $K \in \mathbb{N}$ such that for all $f \in \mathscr{S}(\mathbb{R}^d)$,

$$p_k(f) \leqslant \max_{|\alpha|,|\beta|\leqslant K} \|x^\alpha \partial^\beta f\|.$$

Using now that $\partial_j = (-ih)^{-1}(L_j + A_j)$, and $A \in \mathscr{P}$, there exists $C > 0$ and $N \in \mathbb{N}$ such that, for all $f \in L^2(\mathbb{R}^d)$, if $\|Pf\| < +\infty$ for all $P \in \Pi$, then

$x^\alpha \partial^\beta f \in L^2(\mathbb{R}^d)$ for all $\alpha, \beta \in \mathbb{N}^d$, and

$$\|x^\alpha \partial^\beta f\| \leqslant Ch^{-N} \sum_{P \in R} \|Pf\|,$$

where R is a finite part of Π. Then, Proposition 3.1 implies, for N, κ and n large enough,

$$\|x^\alpha \partial^\beta \psi(t)\| \leqslant Ch^{-N} \sum_{P \in R} \big\|P\psi(t)\big\| \leqslant Ch^{-N}(1+t^\kappa) \sum_{|\gamma| \leqslant \kappa, |\nu| \leqslant n} \|\mathscr{L}_h^\nu x^\gamma \psi_0\|.$$

Finally, we conclude by

$$\|\mathscr{L}_h^\nu x^\alpha \psi_0\| \leqslant C\|(1+x^2)^m \mathscr{L}_h^\nu x^\alpha \psi_0\|_\infty \leqslant Cp_K(\psi_0),$$

for m, K large enough.

3.1. Case when $\kappa = 0$

For all $t \geqslant 0$, we have, by definition,

$$\psi(t) = e^{\frac{it}{h}\mathscr{L}_h} \psi_0.$$

For all $\ell \in \mathbb{N}$, we get

$$\mathscr{L}_h^\ell \psi(t) = e^{\frac{it}{h}\mathscr{L}_h} \mathscr{L}_h^\ell \psi_0.$$

Applying Theorem 1.4, this establishes the estimate of Proposition 3.1 when $\kappa = 0$.

3.2. Case when $\kappa = 1$

Before starting the induction procedure, let us understand first the mechanism with only one occurence of x. Let $j \in \{1, \ldots, d\}$. We have

$$-ih\partial_t(x_j\psi) = \mathscr{L}_h(x_j\psi) + [x_j, \mathscr{L}_h]\psi.$$

Note that $[x_j, \mathscr{L}_h] = 2hL_j$. With the Duhamel formula, we have, for all $t \geqslant 0$,

$$x_j\psi(t) = e^{\frac{it}{h}\mathscr{L}_h}(x_j\psi_0) + \int_0^t e^{\frac{i(t-s)}{h}\mathscr{L}_h} 2L_j\psi(s)\mathrm{d}s. \tag{3.1}$$

With Lemma 2.3, we get

$$\|x_j\psi(t)\| \leqslant \|x_j\psi_0\| + 2\int_0^t \|L_j\psi(s)\|\mathrm{d}s \leqslant \|x_j\psi_0\| + \sqrt{2}\int_0^t \|\psi(s)\|_{\mathscr{L}_h}\mathrm{d}s.$$

Since the evolution is unitary, we get, for all $t \geqslant 0$,

$$\|x_j\psi(t)\| \leqslant \|x_j\psi_0\| + 2\int_0^t \|L_j\psi(s)\|\mathrm{d}s \leqslant \|x_j\psi_0\| + t\sqrt{2}\|\psi_0\|_{\mathscr{L}_h}.$$

More generally, with (3.1), we have, for all $\ell \in \mathbb{N}$,

$$\mathscr{L}_h^\ell x_j\psi(t) = e^{\frac{it}{h}\mathscr{L}_h}\mathscr{L}_h^\ell(x_j\psi_0) + \int_0^t e^{\frac{i(t-s)}{h}\mathscr{L}_h}2\mathscr{L}_h^\ell L_j\psi(s)\mathrm{d}s.$$

so that

$$\begin{aligned}\|\mathscr{L}_h^\ell x_j\psi(t)\| &\leqslant \|\mathscr{L}_h^\ell(x_j\psi_0)\| + 2\int_0^t \|\mathscr{L}_h^\ell L_j\psi(s)\|\mathrm{d}s\\ &\leqslant \|\mathscr{L}_h^\ell(x_j\psi_0)\| + Ch^{-N}\int_0^t \|\mathscr{L}_h^{\ell+1}\psi(s)\|\mathrm{d}s\\ &\leqslant \|\mathscr{L}_h^\ell(x_j\psi_0)\| + Cth^{-N}\|\mathscr{L}_h^{\ell+1}\psi_0\|.\end{aligned}$$

It remains to apply Theorem 1.4 and to commute the x_j with the L_k.

3.3. Induction

Let us now end the proof of Proposition 3.1 by induction. We set the following two induction assumptions. For $\kappa \in \mathbb{N}$, let

$\mathscr{Q}_\kappa : \forall n \in \mathbb{N}$, $\forall \alpha \in \mathbb{N}^d$, $|\alpha| = \kappa$, $\exists N \in \mathbb{N}$ s.t.
$$\|\mathscr{L}_h^n x^\alpha\psi(t)\| \leqslant \|\mathscr{L}_h^n x^\alpha\psi_0\| + C\sum_{|\beta|\leqslant\kappa-1:|\beta|+\nu\leqslant\kappa+n}\|\mathscr{L}_h^\nu x^\beta\psi_0\|h^{-N}(1+t^\kappa)\,;$$

and

$$\mathscr{P}_\kappa : \forall P \in \Pi_{\kappa,\lambda},\ \|P\psi(t)\| \leqslant C\sum_{|\alpha|\leqslant\kappa:|\alpha|+\nu\leqslant\kappa+n}\|\mathscr{L}_h^\nu x^\alpha\psi_0\|h^{-N}(1+t^\kappa),$$

for $\lambda \leqslant 2n \leqslant \lambda + 1$.

We have proved propositions $\mathscr{P}_0$, $\mathscr{Q}_0$ and $\mathscr{Q}_1$. We assume now that for a given $\kappa \in \mathbb{N}^*$, for any $k \leqslant \kappa$, $\mathscr{Q}_k$ and $\mathscr{P}_k$ hold, and we prove $\mathscr{P}_{\kappa+1}$ and

$\mathscr{Q}_{\kappa+1}$. We begin with $\mathscr{Q}_{\kappa+1}$. Let $\alpha \in \mathbb{N}^d$, with $|\alpha| = \kappa + 1$ and $n \in \mathbb{N}$. We have

$$-ih\partial_t\big(\mathscr{L}_h^n x^\alpha \psi(t)\big) = \mathscr{L}_h^{n+1} x^\alpha \psi(t) + \mathscr{L}_h^n [x^\alpha, \mathscr{L}_h]\psi(t).$$

Then, noting that

$$[x^\alpha, \mathscr{L}_h] = hP_1$$

with P_1 a sum of elements in $\Pi_{\kappa,1}$, we get from the Duhamel formula

$$\mathscr{L}_h^n x^\alpha \psi(t) = e^{\frac{it}{h}\mathscr{L}_h} \mathscr{L}_h^n x^\alpha \psi_0 + i\int_0^t e^{i\frac{t-s}{h}\mathscr{L}_h} \mathscr{L}_h^n P_1 \psi(s)\mathrm{d}s.$$

As $\mathscr{L}_h^n P_1$ is a sum of elements in $\Pi_{\kappa,(2n+1)}$, we can apply $\mathscr{P}_\kappa$, and integrating in time and using the unitariness of $e^{i\frac{t}{h}\mathscr{L}_h}$, we find, for some integer $N \in \mathbb{N}$

$$\|\mathscr{L}_h^n x^\alpha \psi(t)\| \leqslant \|\mathscr{L}_h^n x^\alpha \psi_0\| + Ch^{-N} \sum_{|\beta|\leqslant\kappa : |\beta|+\nu\leqslant\kappa+n+1} \|\mathscr{L}_h^\nu x^\beta \psi_0\|(1+t^{\kappa+1})$$

that proves $\mathscr{Q}_{\kappa+1}$. It remains to prove $\mathscr{P}_{\kappa+1}$. We consider so some $P \in \Pi_{\kappa+1,\lambda}$, for a given $\lambda \in \mathbb{N}$. Then, because of the commutation relation of the $(x_k)_{1\leqslant k\leqslant d}$ with the $(L_j)_{1\leqslant j\leqslant d}$, that is $[x_k, L_j] = -ih\delta_{k,j}$, there is $\alpha \in \mathbb{N}^d$, $|\alpha| = \kappa + 1$ such that

$$P = P_2 + P_3 x^\alpha$$

with P_2 a sum of elements in $\Pi_{\kappa,\lambda-1}$ and $P_3 \in \Pi_{0,\lambda}$. So

$$\|P\psi(t)\| \leqslant \|P_2\psi(t)\| + \|P_3\psi(t)\|.$$

Then, applying $\mathscr{P}_\kappa$, we get, for some integer $N \in \mathbb{N}$

$$\|P_2\psi(t)\| \leqslant Ch^{-N}(1+t^\kappa) \sum_{|\beta|\leqslant\kappa : |\beta|+\nu\leqslant\kappa+n} \|\mathscr{L}_h^\nu x^\beta \psi_0\| \tag{3.2}$$

and applying Theorem 1.4 along with $\mathscr{Q}_{\kappa+1}$, for some integer $N \in \mathbb{N}$, and for $\lambda \leqslant 2n \leqslant \lambda + 1$, we have

$$\begin{aligned} \|P_3 x^\alpha \psi(t)\| &\leqslant Ch^{-n}\|\mathscr{L}^n x^\alpha \psi(t)\| \\ &\leqslant Ch^{-N}(1+t^{\kappa+1})\left(\|\mathscr{L}^n x^\alpha \psi_0\| + \sum_{|\beta|\leqslant\kappa : |\beta|+\nu\leqslant\kappa+n+1} \|\mathscr{L}_h^\nu x^\beta \psi_0\|\right). \end{aligned} \tag{3.3}$$

Now, gathering (3.2) and (3.3), we find, for some integer N,

$$\|P\psi(t)\| \leqslant Ch^{-N}(1+t^{\kappa+1}) \sum_{|\beta|\leqslant\kappa+1:|\beta|+\nu\leqslant\kappa+n+1} \|\mathscr{L}_h^{\nu} x^{\beta}\psi_0\|$$

that proves $\mathscr{P}_{\kappa+1}$ and achieves the proof of Proposition 3.1.

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