The Weyl symbol of Schrödinger semigroups

L. AMOUR, L. JAGER AND J. NOURRIGAT

Université de Reims

Abstract

In this paper, we study the Weyl symbol of the Schrödinger semigroup $e^{-tH}$, $H = -\Delta + V$, $t > 0$, on $L^2(\mathbb{R}^n)$, with nonnegative potentials $V$ in $L^1_{\text{loc}}$. Some general estimates like the $L^\infty$ norm concerning the symbol $u$ are derived. In the case of large dimension, typically for nearest neighbor or mean field interaction potentials, we prove estimates with parameters independent of the dimension for the derivatives $\partial_\alpha x \partial_\beta \xi u$. In particular, this implies that the symbol of the Schrödinger semigroups belongs to the class of symbols introduced in [1] in a high-dimensional setting. In addition, a commutator estimate concerning the semigroup is proved.

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1 Introduction.

Let $V$ be a nonnegative function in $L^1_{\text{loc}}(\mathbb{R}^n)$. It is known that $H = -\Delta + V(x)$ is essentially selfadjoint on $C_0^\infty(\mathbb{R}^n)$ and we also denote by $H$ its unique selfadjoint extension. We may also suppose that $V$ is only in $L^1_{\text{loc}}(\mathbb{R}^n)$ and use Theorem X.32 in [7] to define $H$ as a selfadjoint operator with a suitable domain. In this paper, we are interested in the Weyl symbol $u(\cdot, t)$ of $e^{-tH}$, for each $t > 0$. Since this operator is bounded in $L^2(\mathbb{R}^n)$, its Weyl symbol is a priori a tempered distribution $U(t)$ on $\mathbb{R}^{2n}$ which satisfies,

$$< e^{-tH} f, g > = < U(t), H(f, g, \cdot) >,$$

for all $f$ and $g$ in $\mathcal{S}(\mathbb{R}^n)$, where $H(f, g, x, \xi)$ is the Wigner function (c.f. [3] or [6]),

$$H(f, g, x, \xi) = (2\pi)^{-n} \int_{\mathbb{R}^n} e^{iv \cdot \xi} f \left( x - \frac{v}{2} \right) g \left( x + \frac{v}{2} \right) dv.$$ (2)

The aim of this work is to study this Weyl symbol when $V$ is a $C^\infty$ potential describing a large number of particles in interaction, either for a nearest neighbor interaction model in a lattice, or for a mean field approximation model. Our hypotheses on the interaction potentials will in particular imply that $u(\cdot, t)$,
the symbol of \( e^{-tH} \), is a \( C^\infty \) function on \( \mathbb{R}^{2n} \) and we shall give estimates for its derivatives showing that \( u(\cdot, t) \) belongs to a class of symbols allowing a Weyl calculus in large dimension. This calculus is developed in [2] for the composition of symbols and in [1] for norm estimates, where the constants implied in the inequalities are independent of the dimension.

Let us specify this class of symbols. In [2] and [1], we say that a continuous function \( F \) on \( \mathbb{R}^{2n} \) is in \( S_m(M, \rho, \delta) \) (where \( m \) is an integer \( \geq 0 \), \( M \geq 0 \), and \( \rho \) and \( \delta \) are two sequences \( (\rho_j)_{j \leq n} \) and \( (\delta_j)_{j \leq n} \) of real numbers \( \geq 0 \)) if, for all multi-indices \( \alpha \) and \( \beta \) in \( \mathbb{N}^n \) satisfying \( 0 \leq \alpha_j, \beta_j \leq m \), the derivative
\[
\partial_\alpha x \partial_\beta \xi F
\]
is a continuous and bounded function verifying,
\[
\| \partial_\alpha x \partial_\beta \xi F \|_{L^\infty(\mathbb{R}^{2n})} \leq M \prod_{j \leq n} \rho_j^{\alpha_j} \delta_j^{\beta_j}.
\] (3)

Then, for functions belonging to the classes \( S_m(M, \rho, \delta) \), we develop in [2] and [1] a Weyl calculus in large dimension.

In the first section, the symbol \( u(\cdot, t) \) of the semigroup is proved to be in \( L^\infty(\mathbb{R}^{2n}) \) with \( |u(\cdot, t)| \leq 1 \) almost everywhere and additionally, \( \int_{\mathbb{R}^n} u(x, \xi, t) dx \) and \( \partial_\xi^\beta u(\cdot, t) \) are estimated, without further regularity hypothesis on the interaction potential \( V \). In the second section, we consider the semigroup in a large dimension setting with regular potentials and obtain estimates on all the derivatives of the symbol proving in particular that it lies in the class \( S_m(M, \rho, \delta) \) above. Supplementary assumptions on potentials regarding the large dimension are naturally necessary at this step. Then, in the third section, two examples of Schrödinger semigroups in large dimension, satisfying the assumptions of section 2, are considered, namely, the nearest neighbor and the mean field approximation potentials. Moreover, a commutator property is also proved.

2 First properties of the symbol of the semigroup.

The first step consists in writing the Weyl symbol of \( e^{-tH} \) with the Feynman Kac formula, under rather general hypotheses on the potential \( V \). We make the choice to not first express the symbol with the distribution kernel, in order to avoid the use of Brownian bridges. Let \( T > 0 \) and \( n \) be an integer \( \geq 1 \). We denote by \( B \) the Banach space of continuous functions \( \omega \) on \( [0, T] \) taking values into \( \mathbb{R}^n \) and vanishing at \( t = 0 \). This space is endowed with the supremum norm, with the Borel \( \sigma \)-algebra \( \mathcal{B} \) and with the Wiener measure \( \mu \) of variance 1 (c.f. Kuo [5]).

**Proposition 2.1.** Let \( V \geq 0 \) be a function in \( L^1_{\text{loc}}(\mathbb{R}^n) \). Let \( U(t) \) be the Weyl symbol of the operator \( e^{-tH} \), first considered as a tempered distribution on \( \mathbb{R}^{2n} \). Then, \( U(t) \) is identified with a function \( u(\cdot, t) \) in \( L^\infty(\mathbb{R}^{2n}) \). We have, for each \( t \) in \( (0, T] \) and for almost every \( (x, \xi) \) in \( \mathbb{R}^{2n} \),
\[ u(x, \xi, t) = \int_B e^{-\omega(t) \xi} e^{-\int_0^t V(x - \frac{\omega(s)}{2}) + \omega(s)) ds} d\mu(\omega). \]  

Moreover, the following inequality holds,

\[ |u(\cdot, t)| \leq 1, \]

almost everywhere on \( \mathbb{R}^{2n} \), for each \( t \in [0, T] \).

One notices that the above integral involves all of the trajectories of the Brownian motion with a starting and a finishing point that are symmetric with respect to \( x \).

**Proof.** Let \( f \) and \( g \) in \( S(\mathbb{R}^n) \). When \( V \geq 0 \) belongs to \( L^1_{\text{loc}}(\mathbb{R}^n) \), one may apply Feynman Kac formula (c.f. B. Simon \[8\] or \[9\]) written as,

\[ < e^{-tH} f, g > = \int_{\mathbb{R}^n \times B} f(x + \omega(t)) \overline{g(x)} e^{-\int_0^t V(x + \omega(s)) ds} dxd\mu(\omega). \]  

According to the Wigner function definition, we have for all \( x \) and \( y \) in \( \mathbb{R}^n \),

\[ f(x) \overline{g(y)} = \int_{\mathbb{R}^n} H \left(f, g, \frac{x + y}{2}, \xi\right) e^{-i(x-y) \cdot \xi} d\xi. \]

Consequently, for all \( \omega \) in \( B \),

\[ f(x + \omega(t)) \overline{g(y)} = \int_{\mathbb{R}^n} H \left(f, g, x + \frac{\omega(t)}{2}, \xi\right) e^{-i\omega(t) \cdot \xi} d\xi. \]

The Weyl symbol \( U(t) \) of \( e^{-tH} \) being a priori defined as a tempered distribution on \( \mathbb{R}^{2n} \), thus satisfies, for all \( F \) in \( S(\mathbb{R}^{2n}) \),

\[ < U(t), F > = \int_{\mathbb{R}^{2n} \times B} F \left(x + \frac{\omega(t)}{2}, \xi\right) e^{-i\omega(t) \cdot \xi} e^{-\int_0^t V(x + \omega(s)) ds} dxd\xi d\mu(\omega). \]

The above identity shows that, for all \( F \) in \( S(\mathbb{R}^{2n}) \),

\[ |< U(t), F >| \leq \| F \|_{L^1(\mathbb{R}^{2n})}. \]

As a consequence, \( U(t) \) is identified with a function \( u(\cdot, t) \) in \( L^\infty(\mathbb{R}^{2n}) \), with a \( L^\infty(\mathbb{R}^{2n}) \) norm smaller or equal than 1, and satisfying \[4\] and \[5\]. The proposition is then proved. \( \square \)

As a first consequence of Proposition 2.1, we give below two corollaries which do not assume that the potential \( V \) is differentiable.

**Corollary 2.2.** For every multi-index \( \beta \), for each \( t \geq 0 \), the derivative \( \partial_\xi^\beta u(x, \xi, t) \) understood in the sense of distributions, is a function in \( L^\infty(\mathbb{R}^{2n}) \), which satisfies,

\[ \| \partial_\xi^\beta u(\cdot, t) \|_{L^\infty(\mathbb{R}^{2n})} \leq t^{\beta/2} \prod_{j \leq n} A_{\beta_j}, \quad A_k = \frac{2^{k/2}}{\sqrt{\pi}} \Gamma((k + 1)/2). \]  

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Let $m$ be an integer $\geq 0$. If the multi-index $\beta$ verifies $\beta_j \leq m$ for all $j \leq n$, then we have,

$$\|\partial^\beta u(\cdot, t)\|_{L^\infty(\mathbb{R}^{2n})} \leq B_m^{\beta/2} t^{\beta/2}, \quad B_m = \max_{k \leq m} A_k. \quad (8)$$

When $m \geq 4$, we have $B_m = A_m$.

Proof. We use the notation $\omega(t) = (\omega_1(t), ..., \omega_n(t))$. In view of Proposition 2.1,

$$\|\partial^\beta u(\cdot, t)\|_{L^\infty(\mathbb{R}^{2n})} \leq \int_B \prod_{j \leq n} |\omega_j(t)|^{\beta_j} d\mu(\omega).$$

According to Kuo [5], we know that,

$$\int_B \prod_{j \leq n} |\omega_j(t)|^{\beta_j} d\mu(\omega) = t^{\beta/2} \prod_{j \leq n} A_{\beta_j}, \quad (9)$$

where the $A_k$ are given in (7). This proves the corollary. \(\square\)

Corollary 2.3. If $V \geq 0$ and if the right hand side below defines a convergent integral, then, for each $t > 0$ and for almost every $\xi$ in $\mathbb{R}^n$, the function $u(\cdot, \xi, t)$ belongs to $L^1(\mathbb{R}^n)$, and we have,

$$\int_{\mathbb{R}^n} |u(x, \xi, t)| dx \leq \int_{\mathbb{R}^n} e^{-tV(x)} dx. \quad (10)$$

Proof. From (4), we see

$$|u(x, \xi, t)| \leq \int_B e^{-\int_0^t V(x - \frac{\omega(s)}{t} + \omega(s)) ds} d\mu(\omega).$$

Since the function $x \mapsto e^{-tx}$ is convex, using Jensen inequality and integrating over $x \in \mathbb{R}^n$, for almost every $\xi \in \mathbb{R}^n$, lead to inequality (10). The corollary is thus proved. \(\square\)

3 The large dimension setting.

We shall here give Hamiltonians $H_\Lambda$ for systems with a large number of particles indexed on $\Lambda$, for which we shall obtain estimates on the derivatives of the Weyl symbol $u_\Lambda(\cdot, t)$ of $e^{-tH_\Lambda}$. These estimates prove in particular that $u_\Lambda(\cdot, t)$ belongs to the class of symbols studied in [2] and [1], allowing a Weyl calculus where all the constants in the inequalities are independent of $\Lambda$. The assumptions on the interaction potentials $V_\Lambda$ are stated below. In the next section, we shall give two examples of Hamiltonians satisfying these hypotheses.

We suppose that the functions $V_\Lambda$ are given, $\geq 0$, $C^\infty$ on $\mathbb{R}^\Lambda$, for each finite subset $\Lambda$ in $\Gamma$, for a given infinite countable set $\Gamma$. For all integers $m \geq 0$, we denote by $\mathcal{M}_m(\Lambda)$ the set of multi-indices $\alpha$ in $\mathbb{N}^\Lambda$
such that $0 \leq \alpha_j \leq m$, for all $j \in \Lambda$. For each multi-index $\alpha$, $S(\alpha)$ denotes the set of sites $j \in \Lambda$ such that $\alpha_j \neq 0$.

Set $m \geq 1$. We also assume that there exists $C_m > 0$ such that, for all finite subsets $\Lambda$ in $\Gamma$, for all $\alpha$ in $\mathcal{M}_m(\Lambda)$, we have for all $x \in \mathbb{R}^\Lambda$

$$
\sum_{0 \neq \beta \leq \alpha} |\partial^\beta V_\alpha(x)| \leq C_m |S(\alpha)|. \quad \text{(11)}
$$

We set,

$$
H_\Lambda = -\Delta_\Lambda + V_\Lambda(x)
$$

and $U_\Lambda(t)$ denotes the Weyl symbol of $e^{-tH_\Lambda}$ which, according to Proposition 2.1, is a tempered distribution on $\mathbb{R}^\Lambda \times \mathbb{R}^\Lambda$ identified with a function $u_\Lambda(\cdot, t)$ in $L^\infty(\mathbb{R}^\Lambda \times \mathbb{R}^\Lambda)$.

**Theorem 3.1.** With these notations, let the functions $V_\Lambda \geq 0$ in $C^\infty(\mathbb{R}^\Lambda)$ be given for all finite subsets $\Lambda$ of $\Gamma$. Let $m \geq 1$. We suppose that there exists $C_m > 0$ independent of $\Lambda$, such that (11) is satisfied. For each $t > 0$, and for every finite subset $\Lambda$ of $\Gamma$, let $u_\Lambda(\cdot, t)$ be the Weyl symbol of $e^{-tH_\Lambda}$, which is identified with a function in $L^\infty(\mathbb{R}^\Lambda \times \mathbb{R}^\Lambda)$ in view of Proposition 2.1. Then, for each $\alpha$ and $\beta$ in $\mathcal{M}_m(\Lambda)$, the derivative $\partial^\beta \partial^\alpha U_\Lambda(\cdot, t)$, understood in the sense of distributions, is a function in $L^\infty(\mathbb{R}^\Lambda \times \mathbb{R}^\Lambda)$ which satisfies,

$$
\| \partial^\alpha \partial^\beta U_\Lambda(\cdot, t) \|_{L^\infty(\mathbb{R}^\Lambda \times \mathbb{R}^\Lambda)} \leq m^{|S(\alpha)|} e^{tC_m |S(\alpha)|} B_m |\beta|^{\beta}/\beta!, \quad \text{(13)}
$$

where $B_m$ is defined in (7) and (8), and $C_m$ in (11) (these constants are independent of $\Lambda$).

**Proof.** According to Proposition 2.1, we have for all $F$ in $\mathcal{S}(\mathbb{R}^\Lambda \times \mathbb{R}^\Lambda)$,

$$
| \partial^\alpha \partial^\beta U_\Lambda(t), F > | \leq \| F \|_{L^1(\mathbb{R}^\Lambda \times \mathbb{R}^\Lambda)} \sup_{(x, \omega) \in \mathbb{R}^\Lambda \times B} \left| \partial^\alpha x \partial^\beta \omega e^{-t\int_0^\infty V_\Lambda(x+\omega(s))ds} \right| \int_B \prod_{j \in \Lambda} |\omega_j(t)|^{|\beta|/\beta!} \text{d}\mu(\omega). \quad \text{(14)}
$$

We shall use a multi-dimensional variant of Faà di Bruno formula due to Constantine Savits [4]. For each multi-index $\alpha$, denote by $F(\alpha)$ the set of mappings $\varphi$ from the set of multi-indices $0 \neq \beta \leq \alpha$ into the set of integers $\geq 0$, such that

$$
\sum_{\beta \neq 0 \beta \leq \alpha} \varphi(\beta) \beta = \alpha.
$$

Constantine Savits formula is rewritten as,

$$
\partial^\alpha e^{W(x)} \propto \sum_{\varphi \in F(\alpha)} \prod_{\beta \neq 0 \beta \leq \alpha} \frac{1}{\varphi(\beta)!} \left[ \frac{\partial^\beta W(x)}{\beta!} \right]^{\varphi(\beta)}. \quad \text{(15)}
$$

For each $t > 0$ and for almost all $\omega$ in $B$, we apply this formula with

$$
W(x) = -\int_0^t V_\Lambda(x + \omega(s))ds.
$$
Since $V_\Lambda \geq 0$, we obtain
\[
\sup_{(x,\omega)\in\mathbb{R}^\Lambda \times B} \left| \partial_x^\alpha e^{f_0} V_\Lambda (x+\omega(s)) ds \right| \leq \alpha ! \sum_{\varphi \in F(\alpha)} \prod_{0 \neq \beta \leq \alpha} \frac{1}{\varphi(\beta)!} \left[ \frac{t \| \partial^\beta V_\Lambda \|_{L^\infty}}{\beta!} \right] \varphi(\beta).
\]

Besides,
\[
\sum_{\varphi \in F(\alpha)} \prod_{0 \neq \beta \leq \alpha} \frac{1}{\varphi(\beta)!} \left[ \frac{t \| \partial^\beta V_\Lambda \|_{L^\infty}}{\beta!} \right] \varphi(\beta) \leq \exp \left[ \sum_{0 \neq \beta \leq \alpha} \frac{t \| \partial^\beta V_\Lambda \|_{L^\infty}}{\beta!} \right].
\]

The last factor in (14) is bounded using (9)(8) and the above right hand side is bounded using the hypothesis (11). We then deduce that,
\[
| \partial_x^\alpha \partial^\beta U_\Lambda (t), F | \leq \alpha ! \| F \|_{L^1(\mathbb{R}^\Lambda)} e^{tC_m |S(\alpha)|} B_m |S(\beta)| t^{\beta/2}.
\]

Since $\alpha$ is in $M_m(\Lambda)$, we have $\alpha ! \leq m |S(\alpha)|$. The proof of Theorem 3.1 is then completed. \[\square\]

**Remark 3.2.** Theorem 3.1 shows that, if the family of functions $(V_\Lambda)$ verifies (11) with $C_m > 0$, then, for all $t > 0$, and for each $m \geq 0$, the family of functions $u_\Lambda (\cdot, t)$ belongs to the class $S_m(1, \rho, \delta)$ defined in (3), where $\rho_j = me^{tC_m}$ and $\delta_j = B_m \sqrt{t}$ for all $j \in \Gamma$. We remark that $\rho_j$ and $\delta_j$ depend on $m$ but not on $\Lambda$, and thus, not on the dimension.

4 Examples and application.

4.1 Two examples.

We shall in this section give two examples of family of potentials $(V_\Lambda)$ satisfying (11) for all integers $m \geq 1$. The first one corresponds to the nearest neighbor interaction in a lattice and the second one corresponds to the mean field approximation model.

**Example 4.1.** Set $\Gamma = \mathbb{Z}^d$ ($d \geq 1$). Let $F$ and $G$ be two nonnegative functions in $C^\infty(\mathbb{R})$, bounded together with all their derivatives. For each finite subset $\Lambda$ of $\Gamma$, we set,
\[
V_\Lambda (x) = \sum_{j \in \Lambda} F(x_j) + \sum_{(j,k) \in \Lambda^2 \ |j-k|_\infty \leq 1} G(x_j - x_k).
\]

Then, for all integers $m \geq 1$, there exists $C_m > 0$ such that the family of functions $(V_\Lambda)$ satisfies (11).

**Example 4.2.** Let $\Gamma$ be an infinite countable set. Fix a function $G \geq 0$ in $C^\infty(\mathbb{R})$, bounded together with all its derivatives. Let, for each finite subset $\Lambda$ of $\Gamma$,
\[
V_\Lambda (x) = \frac{1}{|\Lambda|} \sum_{(j,k) \in \Lambda^2} G(x_j - x_k).
\]

Then, for any integer $m \geq 1$, there is $C_m > 0$ such that the family of potentials $(V_\Lambda)$ is verifying (11).
4.2 Application.

For all finite subsets $\Lambda$ in $\Gamma$, choose a function $p_\Lambda \geq 0$ in the Schwarz space $\mathcal{S}(\mathbb{R}^\Lambda \times \mathbb{R}^\Lambda)$. It is known that the Weyl operator $\text{Op}^{\text{Weyl}}(p_\Lambda)$ is trace class. We suppose that its trace equals 1.

For all finite subsets $\Lambda$ in $\Gamma$, suppose that the functions $V_\Lambda \geq 0$ in $\mathbb{R}^\Lambda$ are given satisfying the conditions of Example 4.1 or Example 4.2, and denote by $H_\Lambda$ the Hamiltonian defined in (12). Let $A$ be a function on $\mathbb{R}$ and denote by $A_j$ the multiplication operator by the function $A(x_j)$ ($j \in \Lambda$). The function $A$ is chosen to be polynomial to avoid a long development on pseudodifferential operators.

**Proposition 4.3.** With these notations, there exists a constant $C > 0$ such that, for all finite subsets $\Lambda$ of $\Gamma$, for each $t$ in $(0, 1]$, for every $j$ in $\Lambda$, we have,

$$\left| \text{Tr}([A_j, e^{-tH_\Lambda}] \circ \text{Op}^{\text{Weyl}}(p_\Lambda)) \right| \leq C\sqrt{t}.$$ 

**Proof.** Let $F_{\Lambda,t}$ be the Weyl symbol of the commutator $[A_j, e^{-tH_\Lambda}]$. According to Theorem 3.1 and to the Weyl calculus in one dimension, there exists $C > 0$ such that, for all finite $\Lambda$ in $\Gamma$, and for any $t$ in $(0, 1]$,

$$\|F_{\Lambda,t}\|_{L_\infty(\mathbb{R}^\Lambda \times \mathbb{R}^\Lambda)} \leq C\sqrt{t}.$$ 

It is known that,

$$\text{Tr}([A_j, e^{-tH_\Lambda}] \circ \text{Op}^{\text{Weyl}}(p_\Lambda)) = (2\pi)^{-|\Lambda|} \int_{\mathbb{R}^\Lambda \times \mathbb{R}^\Lambda} F_{\Lambda,t}(x, \xi)p_\Lambda(x, \xi)dxd\xi,$$

$$\text{Tr}(\text{Op}^{\text{Weyl}}(p_\Lambda)) = (2\pi)^{-|\Lambda|} \int_{\mathbb{R}^\Lambda \times \mathbb{R}^\Lambda} p_\Lambda(x, \xi)dxd\xi = 1.$$ 

The proposition then follows. \qed

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E-mail address: \{laurent.amour, lisette.jager, jean.nourrigat\}@univ-reims.fr

Address: LMR EA 4535 and FR CNRS 3399, Université de Reims Champagne-Ardenne, Moulin de la Housse, BP 1039, 51687 REIMS Cedex 2, France.