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THE SEMICLASSICAL LIMIT OF THE TIME DEPENDENT HARTREE–FOCK EQUATION: THE WEYL SYMBOL OF THE SOLUTION

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For a family of solutions to the time dependent Hartree–Fock equation, depending on the semiclassical parameter h, we prove that if at the initial time the Weyl symbol of the solution is in $L^1(\mathbb{R}^{2n})$ as well as all its derivatives, then this property is true for all time, and we give an asymptotic expansion in powers of h of this Weyl symbol. The main term of the asymptotic expansion is a solution to the Vlasov equation, and the error term is estimated in the norm of $L^1(\mathbb{R}^{2n})$.

1. Introduction

The essential goal of this work is a semiclassical analysis of the solutions of the time dependent Hartree–Fock equation (TDHF) in the framework of trace class h-pseudodifferential operators. This equation describes the time evolution of the density operator of a quantum system in the mean field approximation, in other words, when the number N of particles tends to infinity, the interaction between two particles being of order $1/N$. (See, for instance, [Ammari and Nier 2008; 2009; Bardos et al. 2003; Erdős and Schlein 2009; Fröhlich et al. 2009; Rodnianski and Schlein 2009; Spohn 1980].)

A solution to the TDHF equation is a nonnegative self-adjoint trace class operator $\rho_h(t)$ in $\mathcal{H} = L^2(\mathbb{R}^n)$ (for particles moving in $\mathbb{R}^n$), of trace equal to 1, evolving as a function of t. This operator is usually called the density operator. Its evolution depends on a parameter $h > 0$, and on two potentials V and W, which are here C^∞ real valued functions on $\mathbb{R}^n$, bounded as well as all their derivatives: the first one is the external potential, interacting with all the particles, and the second one describes the interaction between two particles. Then the density operator obeys the equation

$$ih\frac{\partial}{\partial t}\rho_h(t) = -h^2[\Delta, \rho_h(t)] + [V_q(\rho_h(t)), \rho_h(t)], \tag{1-1}$$

where Δ is the Laplacian and $V_q(\rho_h(t))$ is the multiplication operator by the mean quantum potential, defined at each point $x \in \mathbb{R}^n$, and for each time t, according to the principles of quantum mechanics, by

$$V_q(x, \rho_h(t)) = V(x) + \mathrm{Tr}(W_x \rho_h(t)), \tag{1-2}$$

where W_x is the multiplication operator by the function $y \to W(x-y)$. We shall see later the meaning of the commutators in the equation, and the other hypotheses which are needed.

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Using semiclassical analysis, we want to make precise the relationship with the Vlasov equation, which plays the role of TDHF in classical mechanics. A solution of this equation is a nonnegative real-valued function $v(\,\cdot\,,t)$ in $L^1(\mathbb{R}^n)$, depending on $t \in \mathbb{R}$. This function defines the particle density at the point x and at the time t in classical mechanics. Then the mean classical potential at (x,t) is

$$V_{\mathrm{cl}}(x, v(\,\cdot\,,t)) = V(x) + \int_{\mathbb{R}^{2n}} W(x-y)v(y,\eta,t)\,dy\,d\eta. \tag{1-3}$$

Then the density function $v(\,\cdot\,,t)$ satisfies the Vlasov equation, which is the Liouville equation with the mean potential

$$\frac{\partial v}{\partial t} + 2\sum_{j=1}^{n} \xi_j \frac{\partial v}{\partial x_j} - \sum_{j=1}^{n} \frac{\partial V_{\mathrm{cl}}(x, v(\,\cdot\,,t))}{\partial x_j}\frac{\partial v}{\partial \xi_j} = 0. \tag{1-4}$$

The asymptotic relationship, when h tends to 0, between a density operator $\rho_h(t)$ (that is, a nonnegative self-adjoint trace class operator, with trace 1) satisfying the TDHF equation and a density function $v(x,t)$ (a nonnegative real-valued function in $L^1(\mathbb{R}^n)$, with integral 1) satisfying the Vlasov equation will be provided by the semiclassical quantization. We can use either the semiclassical Weyl calculus or the semiclassical Wick symbol. This paper is devoted to the approach by the Weyl calculus. The Wick symbol, which needs weaker hypotheses, will be studied elsewhere (see [Amour et al. 2011]). In this work we also use the semiclassical anti-Wick calculus in Section 2, only to give examples.

The semiclassical Weyl calculus associates to a suitable function F on $\mathbb{R}^{2n}$ an operator, in our case in $L^2(\mathbb{R}^n)$, depending on the parameter $h > 0$, formally defined for $f \in L^2(\mathbb{R}^n)$ by

$$\big(\mathrm{Op}_h^{\mathrm{weyl}}(F)f\big)(x) = (2\pi h)^{-n}\int_{\mathbb{R}^{2n}} e^{(i/h)(x-y)\cdot\xi}\, F\left(\frac{x+y}{2},\xi\right) f(y)\,dy\,d\xi. \tag{1-5}$$

This operator can also be written $F^w(x, hD)$. Let us denote by $W^{m,p}(\mathbb{R}^{2n})$ the Sobolev space of functions which are in $L^p(\mathbb{R}^{2n})$ together with all their derivatives up to the order m ($1 \le p \le +\infty$, $m \ge 0$). In the oldest results on the Weyl calculus, the function F is in $W^{\infty,\infty}(\mathbb{R}^{2n})$ and the operator $\mathrm{Op}_h^{\mathrm{weyl}}(F)$ is a bounded operator in $L^2(\mathbb{R}^n)$. See [Calderón and Vaillancourt 1972; Hörmander 1985a, Chapter 18; Lerner 2010; Taylor 1981] and, in the semiclassical context, [Robert 1987; 1998; Zworski 2012; Dimassi and Sjöstrand 1999; Helffer 1997; Martinez 2002], for example. These results cannot be directly applied to our problem, since our function $v(\,\cdot\,,t)$ is in $L^1(\mathbb{R}^{2n})$, and the operator $\rho_h(t)$ has to be not only bounded, but also trace class. Rather, we shall use, in definition (1-5), symbols F in $W^{\infty,1}(\mathbb{R}^{2n})$. It was proved by C. Rondeaux [1984] that for each function F in $W^{m,1}(\mathbb{R}^{2n})$ (m large enough), the operator $\mathrm{Op}_h^{\mathrm{weyl}}(F)$ formally defined by (1-5) is trace class. This result is very useful for the study of solutions of the TDHF equation. However, in [Rondeaux 1984], there was no parameter h, and the Weyl calculus was not semiclassical, but we need only standard modifications for that.

We want to prove that if at the initial time $t = 0$ the density operator $\rho_h(0)$ is associated by the semiclassical Weyl calculus to a function in $W^{\infty,1}(\mathbb{R}^{2n})$, then for each $t \in \mathbb{R}$, the operator $\rho_h(t)$ is also associated in the same way to another function in $W^{\infty,1}(\mathbb{R}^n)$, and we shall make precise the time evolution of this function. Before giving the precise statement, we recall the standard formula

$$\mathrm{Tr}\big(\mathrm{Op}_h^{\mathrm{weyl}}(F)\big) = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} F(x,\xi)\,dx\,d\xi, \qquad F \in W^{\infty,1}(\mathbb{R}^{2n}). \tag{1-6}$$

Let us recall also that if F is real-valued, then $\mathrm{Op}_h^{\mathrm{weyl}}(F)$ is self-adjoint. By [Rondeaux 1984], we can associate to each nonnegative function F in $W^{\infty,1}(\mathbb{R}^{2n})$ with integral equal to 1 a self-adjoint trace class operator $\rho_h(0)$ with trace 1, in the following way:

$$\rho_h(0) = (2\pi h)^n\, \mathrm{Op}_h^{\mathrm{weyl}}(F). \tag{1-7}$$

However, the positivity of F does not imply the positivity of the operator, which will be another hypothesis. We shall prove that, for a solution $\rho_h(t)$ of the TDHF equation, if a relation like (1-7) exists for $t = 0$, it will exist at each time.

Before the statements of the results, we have to explain the meaning of the TDHF equation and recall the notion of a *classical solution* of TDHF introduced by Bove, Da Prato and Fano [Bove et al. 1974; 1976] (see also [Chadam and Glassey 1975]). Let us denote by $\mathcal{L}^1(\mathcal{H})$ the space of trace class operators $\mathcal{H} = L^2(\mathbb{R}^n)$. Denote by $\mathcal{D}$ the space of operators A in $\mathcal{L}^1(\mathcal{H})$ such that the limit

$$\lim_{t\to 0} \frac{e^{it\Delta} A e^{-it\Delta} - A}{t}$$

exists in $\mathcal{L}^1(\mathcal{H})$. This limit is denoted by $i[\Delta, A]$. It can be easily proved that a trace class operator A is in $\mathcal{D}$ if and only if its commutator with the Laplacian Δ (a priori defined as an operator from $\mathcal{S}(\mathbb{R}^n)$ into $\mathcal{S}'(\mathbb{R}^n)$) can be extended as a trace class operator in $\mathcal{H} = L^2(\mathbb{R}^n)$. A *classical solution* of TDHF (for a fixed $h > 0$) is a map $t \to \rho_h(t)$ in $C^1(\mathbb{R}, \mathcal{L}^1(\mathcal{H})) \bigcap C(\mathbb{R}, \mathcal{D})$ satisfying (1-1). The Cauchy for the TDHF equation was also studied in [Bove et al. 1974; 1976], where it is proved that for each nonnegative self-adjoint operator A in $\mathcal{D}$, and for each $h > 0$, there is a unique classical solution $\rho_h(t)$ of the TDHF equation such that $\rho_h(0) = A$. Moreover, $\rho_h(t)$ is also self-adjoint and nonnegative, and its trace is constant. We have similar properties for the Vlasov equation. If v is a solution of (1-4), and if at an initial time the data $v(\,\cdot\,, 0)$ is in $L^1(\mathbb{R}^{2n})$, and if it is nonnegative, these two properties remain true for all $t \in \mathbb{R}$, and the integral over $\mathbb{R}^{2n}$ of $v(\,\cdot\,, t)$ is constant (see, for instance, [Braun and Hepp 1977]).

Theorem 1.1. *Let $(\rho_h(t))_{(h>0)}$ be a family of classical solutions of the TDHF equation* (1-1), *with V and W real-valued functions in $W^{\infty,\infty}(\mathbb{R}^n)$. We assume that, for every $h > 0$, the operator $\rho_h(0)$ can be written*

$$\rho_h(0) = (2\pi h)^n\, \mathrm{Op}_h^{\mathrm{weyl}}(F_h), \tag{1-8}$$

where F_h is in $W^{\infty,1}(\mathbb{R}^{2n})$, real-valued, and bounded in $W^{\infty,1}(\mathbb{R}^{2n})$ independently of h in $(0, 1]$. *We also assume that the operator $\rho_h(0)$ is nonnegative, and that*

$$\int_{\mathbb{R}^{2n}} F_h(x,\xi)\,dx\,d\xi = 1. \tag{1-9}$$

Then for every $t \in \mathbb{R}$, the operator $\rho_h(t)$ can be written in the form

$$\rho_h(t) = (2\pi h)^n\, \mathrm{Op}_h^{\mathrm{weyl}}(u_h(\,\cdot\,, t)), \tag{1-10}$$

where $u_h(\,\cdot\,, t)$ is in $W^{\infty,1}(\mathbb{R}^{2n})$, bounded in $W^{\infty,1}(\mathbb{R}^{2n})$ independently of h in $(0, 1]$ and of t in a compact set of $\mathbb{R}$. We have, for all $t \in \mathbb{R}$,

$$\int_{\mathbb{R}^{2n}} u_h(x, \xi, t)\, dx\, d\xi = 1. \tag{1-11}$$

The positivity of the operator $\rho_h(t)$ is needed. Then by [Bove et al. 1976], we have $\rho_h(t) \geq 0$ and $\mathrm{Tr}(\rho_h(t)) = 1$ for all t. The condition $\rho_h(0) \geq 0$ is verified if $\rho_h(0) = (2\pi h)^n \operatorname{Op}_h^{\mathrm{AW}}(G)$, with $G \geq 0$ in $L^1(\mathbb{R}^{2n})$, where $\operatorname{Op}_h^{\mathrm{AW}}(G)$ is the anti-Wick operator associated to G (see Section 2).

If there was no interaction between the particles ($W = 0$), the evolution equation (1-1) would be linear, and then we would have

$$\rho_h(t) = e^{-(it/h)H(h)} \rho_h(0) e^{(it/h)H(h)}, \qquad H(h) = -h^2\Delta + V(x). \tag{1-12}$$

In this particular case, the Egorov theorem could be applied. The earliest version of the Egorov theorem says that if A is a pseudodifferential operator and U an invertible Fourier integral operator, then $U^{-1}AU$ is a pseudodifferential operator (see [Hörmander 1985b, Chapter 25]). In the case of an evolution equation like (1-12), it can be proved, without the Fourier integral operators, that if $\rho_h(0)$ is a pseudodifferential operator with a symbol F in $W^{\infty,\infty}(\mathbb{R}^{2n})$, then it is the same for the right-hand side of (1-12). The proof was given (in the semiclassical context) by D. Robert [1987] and M. Zworski [2012], who proved that the error term in the asymptotic expansion is itself a pseudodifferential operator. For this last point, the characterization theorem of R. Beals [1977] is needed.

For our problem, we need an extension of the above Egorov theorem for two reasons: this theorem will be applied for symbols in $W^{\infty,1}(\mathbb{R}^{2n})$ (the Rondeaux class), and for time dependent Hamiltonians. In the proof, we shall use the Beals type characterization of operators with symbols in $W^{\infty,1}(\mathbb{R}^{2n})$, also given by Rondeaux, but with some modifications.

Now we shall give an asymptotic expansion of the function u_h of Theorem 1.1. The first term will be a solution of the Vlasov equation, and the rest will be majorized in the $L^1(\mathbb{R}^{2n})$ norm. One can see in [Domps et al. 1997] a formulation of the physics of this problem.

Theorem 1.2. *Let $(\rho_h(t))_{(h>0)}$ be a family of classical solutions of the TDHF equation* (1-1) *satisfying the hypotheses of Theorem 1.1. Then there exists a sequence of functions $(X, t) \to u_j(X, t, h)$ on $\mathbb{R}^{2n} \times \mathbb{R}$ $(j \geq 0)$ such that*:

- *The function $t \to u_j(\,\cdot\,, t, h)$ is C^∞ from $\mathbb{R}$ into $W^{\infty,1}(\mathbb{R}^{2n})$. For every multi-index (α, β), there exists a function $C_{\alpha\beta}(t)$, bounded on every compact set of $\mathbb{R}$, such that*

$$\left\| \partial_x^\alpha \partial_\xi^\beta u_j(\,\cdot\,, t, h) \right\|_{L^1(\mathbb{R}^{2n})} \leq C_{\alpha\beta}(t) \tag{1-13}$$

  for all $t \in \mathbb{R}$ and $h \in (0, 1]$.

- *If F_h is the function of* (1-8),

$$u_0(X, 0, h) = F_h(X) \quad \text{and} \quad u_j(X, 0, h) = 0, \quad j \geq 1. \tag{1-14}$$

- *The function $u_0(X,t,h)$ verifies the Vlasov equation*

$$\frac{\partial u_0}{\partial t}+2\sum_{j=1}^{n}\xi_j\frac{\partial u_0}{\partial x_j}=\sum_{j=1}^{n}\frac{\partial}{\partial x_j}V_{\mathrm{cl}}\big(u_0(\cdot\,,t)\big)\frac{\partial u_0(\cdot\,,t)}{\partial \xi_j}. \tag{1-15}$$

- *For every $N\ge 1$, the function $u_h(\cdot\,,t)$ defined by* (1-10) *and the function $F^{(N)}(\cdot\,,t,h)$ defined by*

$$F^{(N)}(X,t,h)=\sum_{k=0}^{N-1}h^j u_j(X,t,h) \tag{1-16}$$

satisfy, for all $h\in(0,1]$,

$$\big\|u_h(\cdot\,,t)-F^{(N)}(\cdot\,,t,h)\big\|_{L^1(\mathbb{R}^{2n})}\le C_N(t)h^N, \tag{1-17}$$

where C_N is a function on $\mathbb{R}$ which is bounded on the compact sets of $\mathbb{R}$.

- *For every $N\ge 1$, the operator $\rho_h^{(N)}(t)$ defined by*

$$\rho_h^{(N)}(t)=(2\pi h)^n\,\mathrm{Op}_h^{\mathrm{weyl}}\big(F^{(N)}(\cdot\,,t,h)\big) \tag{1-18}$$

(*where $F^{(N)}(\cdot\,,t,h)$ is the function of* (1-16)) *verifies*

$$\big\|\rho_h(t)-\rho_h^{(N)}(t)\big\|_{\mathscr{L}^1(\mathscr{H})}\le C(t)h^{N+1}. \tag{1-19}$$

In Section 5, we will make precise the construction of the $u_j(X,t,h)$ ($j\ge 1$), and we will prove the theorem. The successive terms $u_j(X,t,h)$ depend on the initial data F_h. If F_h depends on h, without admitting an asymptotic expansion in powers of h, the $u_j(X,t,h)$ will depend on h.

In [Amour et al. 2011], we study the case where $\rho_h(0)$ is trace class but not necessarily a pseudodifferential operator. In this case, the Weyl symbol is not available. It is defined as a function in $L^2(\mathbb{R}^{2n})$ but not necessarily in $L^1(\mathbb{R}^{2n})$, which is the natural space here. Therefore, in this other paper, we shall use the Wick symbol instead of the Weyl symbol, and a relation with the Vlasov equation will appear also.

Since the TDHF appears as a limiting process when the number N of particles tends to infinity, a natural question is the one of the interchange of the two limits, where N tends to infinity and the semiclassical parameter h tends to 0. It is the subject of [Pezzotti and Pulvirenti 2009], where it is shown that the Weyl symbol of the marginal density operator associated to a particle in a system of N particles admits an asymptotic expansion in powers of h; that when N tends to infinity, the Weyl symbol of the marginal density operator tends towards the symbol of a solution of TDHF; that the coefficient of h^j in the asymptotic expansion of the symbol has a limit; and that, for $j=0$, this limit is a solution of the Vlasov equation. See also [Pezzotti 2009; Graffi et al. 2003; Gasser et al. 1998]. We observe that in [Pezzotti and Pulvirenti 2009], the limits are in the sense of $\mathscr{S}'(\mathbb{R}^{2n})$, while in this work and in [Amour et al. 2011], they are in the sense of $L^1(\mathbb{R}^{2n})$.

In Section 2, we will recall some standard results on h-pseudodifferential operators, particularly the semiclassical analogue of the results of [Rondeaux 1984], which need only standard modifications in order to be applied in the semiclassical context. However, we give a different proof of the Beals type characterization theorem for this class, in order to give precisely the number of derivatives which are needed. The results on the composition of operators and the Moyal bracket for the class of Rondeaux operators are stated in Section 3, since, surprisingly, these results are not in [Rondeaux 1984]. Section 4 is devoted to the proofs of Theorem 1.1 and, first, of the analogue of the Egorov theorem for the Rondeaux class and for time dependent Hamiltonians. In Section 5, we prove Theorem 1.2. The results stated in Sections 2 and 3 are proved in Appendices A and B. For Section 2 and Appendix A, we use a technique of A. Unterberger [1980].

2. Weyl calculus and trace class operators

We define $\mathcal{H} = L^2(\mathbb{R}^n)$ and denote by $\mathcal{L}^1(\mathcal{H})$ the set of trace class operators in $\mathcal{H}$. This space is a normed space with the norm defined by

$$\|A\|_{\mathcal{L}^1(\mathcal{H})} = \mathrm{Tr}\big((A^\star A)^{1/2}\big). \tag{2-1}$$

We will denote by $W^{m,p}(\mathbb{R}^{2n})$ (where $1 \leq p \leq +\infty$, and m is an integer ≥ 0 or $+\infty$) the space of functions F which are in $L^p(\mathbb{R}^{2n})$, as well as all their derivatives up to order m.

Since $W^{m,p}(\mathbb{R}^{2n})$ may be considered as an exotic class of symbols, let us explain why definition (1-5) makes sense for such symbols. The semiclassical Weyl calculus sets a bijection between operators from $\mathcal{S}(\mathbb{R}^n)$ into $\mathcal{S}'(\mathbb{R}^n)$, thus admitting a distribution kernel in $\mathcal{S}'(\mathbb{R}^{2n})$ and tempered distributions on $\mathbb{R}^{2n}$ (symbols). This bijection depends on a parameter $h > 0$. For every F in $\mathcal{S}'(\mathbb{R}^{2n})$, we set $\mathrm{Op}_h^{\mathrm{weyl}}(F)$ the operator A defined by (1-5), or equivalently the operator $A : \mathcal{S}(\mathbb{R}^n) \to \mathcal{S}'(\mathbb{R}^n)$ whose distribution kernel is

$$K_A(x, y) = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} F\left(\frac{x+y}{2}, \xi\right) e^{(i/h)(x-y).\xi}\, d\xi. \tag{2-2}$$

This relationship is understood in the sense of distributions and may be inverted. We will denote by $\sigma_h^{\mathrm{weyl}}(A)$ the distribution F (Weyl symbol of A) such that $A = \mathrm{Op}_h^{\mathrm{weyl}}(F)$:

$$F = \sigma_h^{\mathrm{weyl}}(A) \iff A = \mathrm{Op}_h^{\mathrm{weyl}}(F).$$

In view of applications to trace class operators, we can rewrite (1-5) equivalently when F is in $L^1(\mathbb{R}^{2n})$ as

$$\mathrm{Op}_h^{\mathrm{weyl}}(F) = (\pi h)^{-n} \int_{\mathbb{R}^{2n}} F(X) \Sigma_{Xh}\, dX, \tag{2-3}$$

where for $X = (x, \xi)$ in $\mathbb{R}^{2n}$, Σ_{Xh} is the "symmetry" operator defined by

$$(\Sigma_{Xh} f)(u) = e^{(2i/h)(u-x)\xi} f(2x - u), \quad X = (x, \xi) \in \mathbb{R}^{2n}. \tag{2-4}$$

If A is trace class, one has

$$\sigma_h^{\mathrm{weyl}}(A)(X) = 2^n\, \mathrm{Tr}(A \circ \Sigma_{Xh}), \quad X \in \mathbb{R}^{2n}. \tag{2-5}$$

It is shown in [Rondeaux 1984] that if F is in $W^{m,p}(\mathbb{R}^{2n})$ ($1 \leq p < \infty$, m large enough), the operator $\mathrm{Op}_h^{\mathrm{weyl}}(F)$ is in the Schatten class $\mathcal{L}^p(\mathcal{H})$. For $p = +\infty$, this is the classical result of Calderón and Vaillancourt [1972] (see also [Hörmander 1985a]). If F is in $W^{\infty,1}(\mathbb{R}^{2n})$, one has

$$\operatorname{Tr}\bigl(\mathrm{Op}_h^{\mathrm{weyl}}(F)\bigr) = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} F(X)\, dX. \tag{2-6}$$

If F is in $W^{\infty,p}(\mathbb{R}^{2n})$ and G in $W^{\infty,q}(\mathbb{R}^{2n})$ ($p \geq 1$, $q \geq 1$, $\frac{1}{p} + \frac{1}{q} = 1$), one has

$$\operatorname{Tr}\bigl(\mathrm{Op}_h^{\mathrm{weyl}}(F) \circ \mathrm{Op}_h^{\mathrm{weyl}}(G)\bigr) = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} F(X) G(X)\, dX. \tag{2-7}$$

The left-hand side makes sense, since from [Rondeaux 1984], the two operators under composition are respectively $\mathcal{L}^p(\mathcal{H})$ and $\mathcal{L}^q(\mathcal{H})$, and therefore their composition is trace class.

A characterization of the set of operators whose Weyl symbol is in $W^{\infty,1}(\mathbb{R}^{2n})$ is given in [Rondeaux 1984]. This is the analogue of the Beals characterization [1977], which concerns the symbols in $W^{\infty,\infty}(\mathbb{R}^{2n})$. In the next proposition, we recall the results of [Rondeaux 1984], taking into account of the semiclassical parameter h. We denote by $P_j(h) = (h/i)(\partial/\partial x_j)$ the momentum operators and by $Q_j(h)$ the multiplication by x_j. For each operator P, we denote by $(\mathrm{ad}\, P)$ the mapping $Q \to (\mathrm{ad}\, P)(Q) = [P, Q] = PQ - QP$. For every operator A of $\mathcal{S}(\mathbb{R}^n)$ in $\mathcal{S}'(\mathbb{R}^n)$, and for every multi-index (α, β), we set

$$(\mathrm{ad}\, P(h))^{\alpha} (\mathrm{ad}\, Q(h))^{\beta} A = (\mathrm{ad}\, P_1(h))^{\alpha_1} \dots (\mathrm{ad}\, Q_n(h))^{\beta_n} A. \tag{2-8}$$

Proposition 2.1. (a) *If F is in $W^{2n+2,1}(\mathbb{R}^{2n})$, then for all $h > 0$, the operator $\mathrm{Op}_h^{\mathrm{weyl}}(F)$ is trace class and*

$$\bigl\| \mathrm{Op}_h^{\mathrm{weyl}}(F) \bigr\|_{\mathcal{L}^1(\mathcal{H})} \leq C h^{-n} \sum_{|\alpha|+|\beta| \leq 2n+2} h^{(|\alpha|+|\beta|)/2} \| \partial_x^{\alpha} \partial_{\xi}^{\beta} F \|_{L^1(\mathbb{R}^{2n})}. \tag{2-9}$$

(b) *If A is a trace class operator and if for every multi-index (α, β) such that $|\alpha| + |\beta| \leq 2n + 2$ the operator $(\mathrm{ad}\, P(h))^{\alpha} (\mathrm{ad}\, Q(h))^{\beta} A$ is trace class, then the Weyl symbol of A is in $L^1(\mathbb{R}^{2n})$ and*

$$(2\pi h)^{-n} \| \sigma_h^{\mathrm{weyl}}(A) \|_{L^1(\mathbb{R}^{2n})} \leq C \sum_{|\alpha|+|\beta| \leq 2n+2} h^{-(|\alpha|+|\beta|)/2} \bigl\| (\mathrm{ad}\, P(h))^{\alpha} (\mathrm{ad}\, Q(h))^{\beta} A \bigr\|_{\mathcal{L}^1(\mathcal{H})}, \tag{2-10}$$

where the constant C depends only on n.

(c) *The following are equivalent*:

(i) *A family of operators $(A_h)_{0<h\leq 1}$ is of the form $A_h = \mathrm{Op}_h^{\mathrm{weyl}}(F_h)$, where (F_h) is a bounded family of functions in $W^{\infty,1}(\mathbb{R}^{2n})$.*

(ii) *For every $h > 0$, the operator A_h is trace class as well as all iterated commutators of A_h with the operators $P_j(h)$ and $Q_j(h)$, and for every (α, β), the family of norms*

$$h^{n-|\alpha|-|\beta|} \bigl\| (\mathrm{ad}\, P(h))^{\alpha} (\mathrm{ad}\, Q(h))^{\beta} A \bigr\|_{\mathcal{L}^1(\mathcal{H})} \tag{2-11}$$

stays bounded when h varies in $(0, 1]$.

Part (a) is proved in [Rondeaux 1984], without the parameter h, and needs only standard modifications to introduce this parameter. In the same paper, part (c) is proved without the precise estimation (b), which is needed for applications to our nonlinear problem and proved in Appendix A.

For the sake of clarity, it might be useful to recall the well known analogue of Proposition 2.1 for bounded operators and symbols in $W^{\infty,\infty}(\mathbb{R}^{2n})$, that is to say, the Calderón–Vaillancourt and the Beals characterization.

Proposition 2.2. (a) *If F is in $L^\infty(\mathbb{R}^{2n})$ as well as all derivatives up to order $2n+2$, then for all $h>0$, the operator $\mathrm{Op}_h^{\mathrm{weyl}}(F)$ is bounded in $\mathcal{H}=L^2(\mathbb{R}^n)$ and*

$$\big\|\mathrm{Op}_h^{\mathrm{weyl}}(F)\big\|_{\mathcal{L}(\mathcal{H})} \le C \sum_{|\alpha|+|\beta|\le 2n+2} h^{(|\alpha|+|\beta|)/2} \|\partial_x^\alpha \partial_\xi^\beta F\|_{L^\infty(\mathbb{R}^{2n})}. \tag{2-12}$$

(b) *If A is a bounded operator and if, for all multi-indices (α,β) such that $|\alpha|+|\beta|\le 2n+2$, the operator $(\mathrm{ad}\,P(h))^\alpha(\mathrm{ad}\,Q(h))^\beta A$ is bounded, then the Weyl symbol of A is in $L^\infty(\mathbb{R}^{2n})$, and one has*

$$\|\sigma_h^{\mathrm{weyl}}(A)\|_{L^\infty(\mathbb{R}^{2n})} \le C \sum_{|\alpha|+|\beta|\le 2n+2} h^{-(|\alpha|+|\beta|)/2} \big\|(\mathrm{ad}\,P(h))^\alpha(\mathrm{ad}\,Q(h))^\beta A\big\|_{\mathcal{L}(\mathcal{H})}. \tag{2-13}$$

Anti-Wick calculus. The definition of this calculus uses coherent states, in other words the family of functions Ψ_{Xh} in $L^2(\mathbb{R}^n)$, indexed by the parameter $X=(x,\xi)$ in $\mathbb{R}^{2n}$ and depending on $h>0$, defined by

$$\Psi_{X,h}(u) = (\pi h)^{-n/4} e^{-|u-x|^2/2h} e^{(i/h)u.\xi-(i/2h)x.\xi}, \quad X=(x,\xi)\in\mathbb{R}^{2n}. \tag{2-14}$$

These functions will be used, with the anti-Wick calculus recalled below, to give examples of operators satisfying the hypotheses of Theorem 1.1. They will be also helpful in proving Proposition 2.1 in Appendix A. Their two fundamental properties are that

$$|\langle\Psi_{Xh},\Psi_{Yh}\rangle| = e^{-(1/4h)|X-Y|^2}, \quad \|\Psi_{Xh}\|=1, \tag{2-15}$$

and that for all f and g in $\mathcal{H}$,

$$\langle f,g\rangle = (2\pi h)^{-n}\int_{\mathbb{R}^{2n}} \langle f,\Psi_{Xh}\rangle\langle\Psi_{Xh},g\rangle\,dX. \tag{2-16}$$

For every function F in $L^1(\mathbb{R}^{2n})$ and for every $h>0$, the operator $\mathrm{Op}_h^{\mathrm{AW}}(F)$ associated to F by the anti-Wick calculus is the bounded operator in $L^2(\mathbb{R}^n)$ such that for all f and g in $\mathcal{H}$,

$$\langle\mathrm{Op}_h^{\mathrm{AW}}(F)f,g\rangle = (2\pi h)^{-n}\int_{\mathbb{R}^{2n}} a(X)\langle f,\Psi_{Xh}\rangle\langle\Psi_{Xh},g\rangle\,dX. \tag{2-17}$$

If F is in $L^1(\mathbb{R}^{2n})$, we see that $\mathrm{Op}_h^{\mathrm{AW}}(F)$ is indeed trace class in $\mathcal{H}$, and that

$$\big\|\mathrm{Op}_h^{\mathrm{AW}}(F)\big\|_{\mathcal{L}^1(\mathcal{H})} \le (2\pi h)^{-n}\int_{\mathbb{R}^{2n}} |F(X)|\,dX. \tag{2-18}$$

Moreover, one has

$$\mathrm{Tr}\big(\mathrm{Op}_h^{\mathrm{AW}}(F)\big) = (2\pi h)^{-n}\int_{\mathbb{R}^{2n}} F(X)\,dX. \tag{2-19}$$

If $F\ge 0$, the operator $\mathrm{Op}_h^{\mathrm{AW}}(F)$ is self-adjoint and nonnegative. The Weyl symbol of the operator $\mathrm{Op}_h^{\mathrm{AW}}(F)$ is given by

$$\sigma_h^{\mathrm{weyl}}\big(\mathrm{Op}_h^{\mathrm{AW}}(F)\big) = e^{(h/4)\Delta}F, \tag{2-20}$$

where Δ is the Laplacian on $\mathbb{R}^{2n}$. In fact, the operator Σ_{Yh} defined in (2-4) and the operator P_{Xh} of orthogonal projection on $\mathrm{Vect}(\Psi_{Xh})$ satisfy

$$\mathrm{Tr}(P_{Xh}\Sigma_{Yh}) = e^{-|X-Y|^2/h}. \tag{2-21}$$

3. Basic facts on the Moyal bracket

The composition of symbols in the Weyl calculus is a very classical field (see [Hörmander 1985a] or [Robert 1987] for the dependence on the semiclassical parameter h). We need to adapt that to the classes of Rondeaux symbols, and to make precise the dependence on the parameter h.

We define a differential operator $\sigma(\nabla_1, \nabla_2)$ on $\mathbb{R}^{2n} \times \mathbb{R}^{2n}$ by

$$\sigma(\nabla_1, \nabla_2) = \sum_{j=1}^{n} \frac{\partial^2}{\partial y_j \partial \xi_j} - \frac{\partial^2}{\partial x_j \partial \eta_j}, \tag{3-1}$$

where (x, ξ, y, η) denotes the variable of $\mathbb{R}^{2n} \times \mathbb{R}^{2n}$.

Theorem 3.1. *For all functions F in $W^{\infty,p}(\mathbb{R}^{2n})$ and G in $W^{\infty,q}(\mathbb{R}^{2n})$ ($p \geq 1$, $q \geq 1$, $1/p + 1/q = 1$), for all $h > 0$, there exists a function $M_h(F, G, \cdot)$ in $W^{\infty,1}(\mathbb{R}^{2n})$ (Moyal bracket) such that*

$$\Big[\mathrm{Op}_h^{\mathrm{weyl}}(F), \mathrm{Op}_h^{\mathrm{weyl}}(G)\Big] = \mathrm{Op}_h^{\mathrm{weyl}}\big(M_h(F, G, \cdot)\big). \tag{3-2}$$

For all integers $N \geq 2$, one has

$$M_h(F, G, X) = \sum_{k=1}^{N-1} h^k C_k(F, G, X) + R_h^{(N)}(F, G, X), \tag{3-3}$$

where the function $C_k(F, G, X)$ is defined by

$$C_k(F, G, X) = \frac{1}{(2i)^k k!}\big[\sigma(\nabla_1, \nabla_2)^k (F \otimes G)(X, X) - \sigma(\nabla_1, \nabla_2)^k (G \otimes F)(X, X)\big], \tag{3-4}$$

and where the function $R_h^{(N)}(F, G, \cdot)$ is in $W^{\infty,1}(\mathbb{R}^{2n})$. For every integer ℓ, there exists a constant C such that

$$h^{\ell/2}\big\|\nabla^\ell R_h^{(N)}(F, G, \cdot)\big\|_{L^1(\mathbb{R}^{2n})} \leq C \sum_{\substack{|\alpha|+|\beta|\leq \ell+4n+2+2N \\ |\alpha|\geq N,\, |\beta|\geq N}} h^{(\alpha+\beta)/2}\|\nabla^\alpha F\|_{L^p(\mathbb{R}^{2n})}\, \|\nabla^\beta G\|_{L^q(\mathbb{R}^{2n})}. \tag{3-5}$$

The operator $\widehat{R}_h^{(N)}(F, G) = \mathrm{Op}_h^{\mathrm{weyl}}\big(R_h^{(N)}(F, G, \cdot)\big)$ verifies

$$\|\widehat{R}_h^{(N)}(F, G)\|_{\mathscr{L}^1(\mathscr{H})} \leq C h^{-n} \sum_{\substack{|\alpha|+|\beta|\leq 6n+4+2N \\ |\alpha|\geq N,\, |\beta|\geq N}} h^{(\alpha+\beta)/2}\|\nabla^\alpha F\|_{L^p(\mathbb{R}^{2n})}\|\nabla^\beta G\|_{L^q(\mathbb{R}^{2n})}. \tag{3-6}$$

This theorem will be proved in Appendix B. It is also used in [Amour et al. 2011]. We shall also use the well-known analogue of Theorem 3.1, which we recall here in order to be used when needed.

Theorem 3.2. *With the notations of Theorem 3.1, if the functions F and G are in $W^{\infty,\infty}(\mathbb{R}^{2n})$, the function $R_h^{(N)}(F, G, \cdot)$ defined by the equality* (3-3) *verifies, for any $\ell \geq 0$,*

$$h^{\ell/2} \big\| \nabla^\ell R_h^{(N)}(F, G, \cdot) \big\|_{L^\infty(\mathbb{R}^{2n})} \leq C \sum_{\substack{j \geq N, k \geq N \\ \ell+2N \leq j+k \leq \ell+2N+4n+2}} h^{(j+k)/2} \| \nabla^j F \|_{L^\infty(\mathbb{R}^{2n})} \| \nabla^k G \|_{L^\infty(\mathbb{R}^{2n})}. \tag{3-7}$$

The operator $\widehat{R}_h^{(N)}(F, G)$ verifies

$$\| \widehat{R}_h^{(N)}(F, G) \|_{\mathcal{L}(\mathcal{H})} \leq C \sum_{\substack{j \geq N, k \geq N \\ 2N \leq j+k \leq 2N+6n+4}} h^{(j+k)/2} \| \nabla^j F \|_{L^\infty(\mathbb{R}^{2n})} \| \nabla^k G \|_{L^\infty(\mathbb{R}^{2n})}. \tag{3-8}$$

4. The Egorov theorem for trace class operators and proof of Theorem 1.1

We are going to adapt to the case of symbols in $L^1(\mathbb{R}^{2n})$ and trace class operators the idea of the proof of the Egorov theorem contained in [Robert 1987]. The difference with [Robert 1987] comes from the fact that the classes of operators considered here are the classes introduced by Rondeaux and that Hamiltonians are time dependent.

We consider a function $(x, t) \to V(x, t)$ on $\mathbb{R}^n \times \mathbb{R}$, which is real valued, depending in a C^∞ way on x, and continuously on t. We suppose that, for every α, there exists $C_\alpha > 0$ such that

$$|\partial_x^\alpha V(x, t)| \leq C_\alpha, \quad (x, t) \in \mathbb{R}^n \times \mathbb{R}. \tag{4-1}$$

We set

$$H(x, \xi, t) = |\xi|^2 + V(x, t). \tag{4-2}$$

We denote by $V(t)$ the multiplication by $V(\cdot, t)$. We set

$$\widehat{H}_h(t) = -h^2 \Delta + V(t). \tag{4-3}$$

Therefore, $\widehat{H}_h(t) = \mathrm{Op}_h^{\mathrm{weyl}}(H(\cdot, t))$. Let us now recall some facts on unitary propagators (see [Reed and Simon 1975, Section X.12]).

Proposition 4.1. *For all $t \in \mathbb{R}$, let $V(\cdot, t)$ be a C^∞ function on $\mathbb{R}^n$ satisfying* (4-1) *and depending in a C^1 way on $t \in \mathbb{R}$. Let $\widehat{H}_h(t)$ be the operator defined in* (4-3). *For every f in $\mathcal{S}(\mathbb{R}^n)$ and every s in $\mathbb{R}$, there exists a function denoted by $t \to U_h(t, s) f$ that verifies*

$$ih \frac{\partial}{\partial t} U_h(t, s) f = (\widehat{H}_h(t)) U_h(t, s) f, \quad U_h(s, s) f = f. \tag{4-4}$$

The operator $U_h(t, s)$ maps $\mathcal{S}(\mathbb{R}^n)$ into itself and, by duality, $\mathcal{S}'(\mathbb{R}^n)$ into itself. One has $U_h(s, t) = U_h(t, s)^{-1}$. One also has

$$ih \frac{\partial}{\partial s} U_h(t, s) = -U_h(t, s)(\widehat{H}_h(s)). \tag{4-5}$$

For every operator A from $\mathcal{S}(\mathbb{R}^n)$ into $\mathcal{S}'(\mathbb{R}^n)$, let us set

$$G_h(t, s)(A) = U_h(t, s) \circ A \circ U_h(s, t). \tag{4-6}$$

One has

$$ih\frac{\partial}{\partial t}G_h(t,s)(A) = \big[\widehat{H}_h(t), G_h(t,s)(A)\big], \quad G_h(s,s)(A) = A. \tag{4-7}$$

Let us state the analogue of the Egorov theorem for the class of Rondeaux operators [1984].

Theorem 4.2. *Let F be a function defined on $W^{\infty,1}(\mathbb{R}^{2n})$. Let $A_h = \mathrm{Op}_h^{\mathrm{weyl}}(A)$. Then for every $t \in \mathbb{R}$, there exists a function F_{ht} in $W^{\infty,1}(\mathbb{R}^{2n})$ such that*

$$G_h(t,0)(A_h) = \mathrm{Op}_h^{\mathrm{weyl}}(F_{ht}). \tag{4-8}$$

If the function F and the potential $V(\,\cdot\,,t)$ depend on a parameter λ, while staying bounded respectively in $W^{\infty,1}(\mathbb{R}^{2n})$ and in $W^{\infty,\infty}(\mathbb{R}^{2n})$ independently of λ, then the function F_{ht} remains bounded in $W^{\infty,1}(\mathbb{R}^{2n})$ independently of λ, of h in $(0,1]$, and of t in a compact set of $\mathbb{R}$.

Following the idea of Robert [1987], which is related in some sense to Dyson series, we will express our solution $G_h(t,0)(A_h)$ in the form

$$G_h(t,0)(A_h) = \sum_{k=0}^{N-1}\mathrm{Op}_h^{\mathrm{weyl}}\big(D_k(\,\cdot\,,t)\big) + h^N E_N(t,h), \tag{4-9}$$

where the functions $D_k(\,\cdot\,,t)$ will be in $W^{\infty,1}(\mathbb{R}^{2n})$ and $E_N(t,h)$ will be a trace class operator with bounded trace norm. In a second step, we will show that the commutators of $E_N(t,h)$ with the position and momentum operators are also trace class operators, and we will estimate their traces. Finally, we will rely on the characterization recalled in Proposition 2.1 to show that $G_h(t,0)(A_h)$ is itself a pseudodifferential operator, with a symbol in $W^{\infty,1}(\mathbb{R}^{2n})$.

The construction of the terms $D_k(\,\cdot\,,t)$ will use the Hamiltonian flow of $H(\,\cdot\,,t)$. For every function G in $W^{\infty,1}(\mathbb{R}^{2n})$, we call $\Phi_{ts}(G)$ the function on $\mathbb{R}^{2n}$ defined by

$$\frac{\partial\Phi_{t,s}(G)}{\partial t} = \{H(\,\cdot\,,t), \Phi_{ts}(G)\}, \quad \Phi_{s,s}(G) = G. \tag{4-10}$$

Under hypothesis (4-1), one knows that if $(G_\lambda)_{\lambda\in E}$ is a family of bounded functions in $W^{\infty,1}(\mathbb{R}^{2n})$, then $\Phi_{ts}(G_\lambda)$ stays bounded in $W^{\infty,1}(\mathbb{R}^{2n})$ when (t,s) varies in a compact set of $\mathbb{R}^2$ and λ in E.

Lemma 4.3. *For every function G in $W^{\infty,1}(\mathbb{R}^{2n})$ and for (t,s) in $\mathbb{R}^2$, one has*

$$G_h(t,s)\big(\mathrm{OP}_h^{\mathrm{weyl}}(G)\big) = \mathrm{Op}_h^{\mathrm{weyl}}(\Phi_{ts}(G)) + h\int_s^t G_h(t,t_1)\big(\mathrm{Op}_h^{\mathrm{weyl}}(R(\,\cdot\,,t_1,s,h))\big)\,dt_1, \tag{4-11}$$

where the function $R(\,\cdot\,,t_1,s,h)$ is in $W^{\infty,1}(\mathbb{R}^{2n})$. If G depends on some parameter and is bounded in $W^{\infty,1}(\mathbb{R}^{2n})$ independently of this parameter, then the function $R(\,\cdot\,,t_1,s,h)$ associated to G is also bounded in $W^{\infty,1}(\mathbb{R}^{2n})$ independently of this parameter and of (t_1,s) in a compact set of $\mathbb{R}^2$ and of h in $(0,1]$.

Proof of the lemma. From definition (4-10),

$$\frac{\partial}{\partial t}\operatorname{Op}_h^{\text{weyl}}(\Phi_{ts}(G)) = \operatorname{Op}_h^{\text{weyl}}\big(\{H(\cdot\,,t),\,\Phi_{ts}(G)\}\big).$$

With the notations of Theorem 3.1 and with $N=2$, one may write

$$\big[\widehat{H}_h(t),\operatorname{Op}_h^{\text{weyl}}(\Phi_{tsh}(G))\big] = \frac{h}{i}\operatorname{Op}_h^{\text{weyl}}\big(\{H(\cdot\,,t),\,\Phi_{ts}(G)\}\big) + \operatorname{OP}_h^{\text{weyl}}\big(R_h^{(2)}(H(\cdot\,,t),\,\Phi_{ts}(G))\big).$$

Consequently,

$$\frac{\partial}{\partial t}\operatorname{Op}_h^{\text{weyl}}(\Phi_{ts}(G)) - \frac{i}{h}\big[\widehat{H}_h(t),\operatorname{Op}_h^{\text{weyl}}(\Phi_{ts}(G))\big] = -\frac{i}{h}\operatorname{OP}_h^{\text{weyl}}\big(R_h^{(2)}(H(\cdot\,,t),\,\Phi_{ts}(G))\big).$$

On the other hand,

$$\frac{\partial}{\partial t}G_h(t,s)(\operatorname{OP}_h^{\text{weyl}}(G)) - \frac{i}{h}\big[\widehat{H}_h(t),\,G_h(t,s)(\operatorname{OP}_h^{\text{weyl}}(G))\big] = 0.$$

By combining these two equalities, noting that for $t=s$ the two operators $G_h(s,s)(\operatorname{Op}_h^{\text{weyl}}(G))$ and $\operatorname{Op}_h^{\text{weyl}}(\Phi_{ss}(G))$ are equal, and using Duhamel's principle, we obtain (4-11), with

$$R(\cdot\,,t_1,s,h) = -\frac{i}{h}R_h^{(2)}\big(H(\cdot\,,t_1),\,\Phi_{t_1 s}(G)\big).$$

It is well known that when $F(x,\xi)=|\xi|^2$, one has $R_h^{(2)}(F,G)=0$ for every function G. Hence

$$R(\cdot\,,t_1,s,h) = -\frac{i}{h^2}R_h^{(2)}\big(V(\cdot\,,t_1),\,\Phi_{t_1 s}(G)\big).$$

By hypothesis, $V(\cdot\,,t_1)$ is in $W^{\infty,\infty}(\mathbb{R}^n)$ and is bounded independently of t_1. We have seen that $\Phi_{t_1 s}(G)$ is in $W^{\infty,1}(\mathbb{R}^{2n})$, bounded independently of t_1 and of s when (t_1,s) varies in a compact set of $\mathbb{R}^2$. According to Theorem 3.1 applied to the case $N=2$, it follows that $R(\cdot\,,t_1,s,h)$ is in $W^{\infty,1}(\mathbb{R}^{2n})$, bounded independently of t_1 and of s when (t_1,s) varies in a compact set of $\mathbb{R}^2$ and h in $(0,1]$. □

Proof of Theorem 4.2, first step. Let F be a function in $W^{\infty,1}(\mathbb{R}^{2n})$. Let $A_h=\operatorname{Op}_h^{\text{weyl}}(F)$. Let $\Phi_{ts}(G)$ be the function satisfying (4-10). For every $t\in\mathbb{R}$, we define a function $D_0(\cdot\,,t)$ in $W^{\infty,1}(\mathbb{R}^{2n})$ by

$$D_0(\cdot\,,t) = \Phi_{t,0}(F). \tag{4-12}$$

We have seen that this function is in $W^{\infty,1}(\mathbb{R}^{2n})$, bounded independently of t on every compact set of $\mathbb{R}$. By Lemma 4.3 applied to $G=F$ and $s=0$, and from (4-12), one has

$$G_h(t,0)(A_h) = \operatorname{Op}_h^{\text{weyl}}(D_0(t)) + h\int_0^t G_h(t,t_1)\big(\operatorname{Op}_h^{\text{weyl}}(R_1(\cdot\,,t_1,h))\big)\,dt_1,$$

where $R_1(\cdot\,,t_1,h)$ stays bounded in $W^{\infty,1(\mathbb{R}^{2n})}$ when t_1 belongs to a compact set of $\mathbb{R}$ and h is in $(0,1]$. We iterate by applying Lemma 4.3 with $s=t_1$ and $G=R_1(\cdot\,,t_1,h)$. We obtain

$$G_h(t,t_1)\big(\operatorname{Op}_h^{\text{weyl}}(R_1(\cdot\,,t_1,h))\big) = \operatorname{Op}_h^{\text{weyl}}\big(\Phi(t,t_1)(R_1(\cdot\,,t_1,h))\big) + h\int_{t_1}^t G_h(t,t_2)\big(\operatorname{Op}_h^{\text{weyl}}(R_2(\cdot\,,t_2,t_1,h))\big)\,dt_2,$$

where $R_2(\,\cdot\,, t_2, t_1, h)$ stays bounded in $W^{\infty,1}(\mathbb{R}^{2n})$ when (t_1, t_2) belongs to a compact set of $\mathbb{R}^2$ and h is in $(0, 1]$. We define a function $D_1(\,\cdot\,, t)$ in $W^{\infty,1}(\mathbb{R}^{2n})$ by

$$D_1(\,\cdot\,, t) = \int_0^t \Phi(t, t_1)\big(R_1(\,\cdot\,, t_1, h)\big)\, dt_1.$$

This function is in $W^{\infty,1}(\mathbb{R}^{2n})$, bounded independently of t on every compact set of $\mathbb{R}$. We have, if $t > 0$,

$$G_h(t, 0)(A_h) = \mathrm{Op}_h^{\mathrm{weyl}}\big(D_0(t) + hD_1(t)\big) + h^2 \int_{0<t_1<t_2<t} G_h(t, t_2)\big(\mathrm{Op}_h^{\mathrm{weyl}}(R_2(\,\cdot\,, t_2, t_1, h))\big)\, dt_1\, dt_2.$$

Iterating this process, we obtain, for every N, the equality (4-9), with

$$E_N(t, h) = \int_{\Delta_N(t,0)} G_h(t, t_N)\big(\mathrm{Op}_h^{\mathrm{weyl}}(R_N(\,\cdot\,, t_N, \dots, t_1, h))\big)\, dt_1 \dots dt_N, \tag{4-13}$$

where $\Delta_N(t, s)$ is the set defined, if $s < t$, by

$$\Delta_N(t, s) = \big\{(t_1, \dots, t_N) \in \mathbb{R}^N,\ s < t_1 < \cdots < t_N < t\big\}, \tag{4-14}$$

and in a symmetric way if $s > t$. In (4-9), the $D_j(\,\cdot\,, t, h)$ $(j \geq 0)$ and $R_N(\,\cdot\,, t_N, \dots, t_1, h)$ are in $W^{\infty,1}(\mathbb{R}^{2n})$, bounded independently of h in $(0, 1]$, of $(t_1, \dots, t_N)$ in $\Delta_N(t, 0)$, and of t in a compact set of $\mathbb{R}$.

It remains to prove that $E_N(t, h)$ is also a pseudodifferential operator. For that, we shall give in the second step upper bounds for trace norms of iterated commutators of $E_N(t, h)$ with the position and momentum operators. In order to do that, we will use the following lemma, also used in Section 5 and in [Amour et al. 2011]. If an operator A is bounded in $L^2(\mathbb{R}^n)$, as well as all its iterated commutators up to order m, we set

$$I_h^{m\infty}(A) = \sum_{|\alpha|+|\beta|\leq m} \big\|(\mathrm{ad}\, Q(h))^{\beta} (\mathrm{ad}\, P(h))^{\alpha} A\big\|_{\mathscr{L}(\mathscr{H})}. \tag{4-15}$$

If an operator A in $L^2(\mathbb{R}^n)$ is trace class, as well as all its iterated commutators up to order m, we set

$$I_h^{m,\mathrm{tr}}(A) = \sum_{|\alpha|+|\beta|\leq m} \big\|(\mathrm{ad}\, Q(h))^{\beta} (\mathrm{ad}\, P(h))^{\alpha} A\big\|_{\mathscr{L}^1(\mathscr{H})}. \tag{4-16}$$

The aim of the next lemma is to show that these properties are preserved by the mapping $G_h(t, s)$.

Lemma 4.4. *Let $\widehat{H}_h(t)$ be the operator defined in* (4-3), *where $V(\,\cdot\,, t)$ verifies* (4-1). *Let $U_h(t, s)$ denote the unitary propagator and $G_h(t, s)$ the map of Proposition 4.1. Let A be a trace class operator in $\mathscr{H} = L^2(\mathbb{R}^n)$, as well as all iterated commutators* $(\mathrm{ad}\, Q(h))^{\beta}(\mathrm{ad}\, P(h))^{\alpha} A$ *for $|\alpha| + |\beta| \leq m$. Then, for all s and t in $\mathbb{R}$, the operator $G_h(t, s)(A)$ is also trace class, as well as all iterated commutators with the $P_j(h)$ and $Q_j(h)$ up to order m. Moreover, for every compact set K of $\mathbb{R}$, there exists $C_K > 0$ such that*

$$I_h^{m,\mathrm{tr}}(G_h(t, s)(A)) \leq C_K I_h^{m,\mathrm{tr}}(A), \quad (s, t) \in K^2,\ h \in (0, 1]. \tag{4-17}$$

An identical result holds for bounded operators and for the norms $I_h^{m,\infty}$.

Proof of the lemma. By (4-7), one checks that, for every operator A satisfying the hypothesis of the lemma, and for each of the momentum operators $P_j(h)$, the following equality is valid:

$$\frac{\partial}{\partial t}[P_j(h), G_h(t,s)(A)] - \frac{1}{ih}\big[\widehat{H}_h(t), [P_j(h), G_h(t,s)(A)]\big] = \frac{1}{ih}\big[[P_j(h), \widehat{H}_h(t)], G_h(t,s)(A)\big].$$

Then the following equality results by the Duhamel principle:

$$\big[P_j(h), G_h(t,s)(A)\big] = G_h(t,s)\big([P_j(h), A]\big) + \frac{1}{ih}\int_s^t G_h(t,t_1)\big(\big[[P_j(h), \widehat{H}_h(t_1)], G_h(t_1,s)(A)\big]\big)\,dt_1.$$

We have an analogous equality for the position operators $Q_j(h)$. One has

$$[P_j(h), \widehat{H}_h(t)] = \frac{h}{i}\frac{\partial V(\,\cdot\,,t)}{\partial x_j}, \qquad [Q_j(h), \widehat{H}_h(t)] = 2ihP_j(h).$$

We therefore deduce

$$\big[P_j(h), G_h(t,s)(A)\big] = G_h(t,s)\big([P_j(h), A]\big) - \int_s^t G_h(t,t_1)\bigg(\bigg[\frac{\partial V(\,\cdot\,,t_1)}{\partial x_j}, G_h(t_1,s)(A)\bigg]\bigg)\,dt_1,$$

$$\big[Q_j(h), G_h(t,s)(A)\big] = G_h(t,s)\big([Q_j(h), A]\big) + 2\int_s^t G_h(t,t_1)\big(\big[P_j(h), G_h(t_1,s)(A)\big]\big)\,dt_1.$$

If A and its commutators with $P_j(h)$ and $Q_j(h)$ are trace class, we first observe that $[P_j(h), G_h(t,s)(A)]$ is a trace class operator since $G_h(t,s)$ maps $\mathcal{L}^1(\mathcal{H})$ into itself. Using the second equality, we see that $[Q_j(h), G_h(t,s)(A)]$ is also a trace class operator, and that the upper bound (4-17) is proved for $m=1$. We pursue the same reasoning to prove (4-17), by induction, for every m. The analogue of (4-17) for the bounded operators is proved similarly. □

Proof of Theorem 4.2, second step. Following Proposition 2.1, it suffices to show that, for every multi-index (α,β) and for every compact set K of $\mathbb{R}$, there exists $C_{\alpha\beta K} > 0$ such that

$$h^{n-(|\alpha|+|\beta|)}\big\|(\operatorname{ad} P(h))^{\alpha}(\operatorname{ad} Q(h))^{\beta} G_h(t,0)(A_h)\big\|_{\mathcal{L}^1(\mathcal{H})} \le C_{\alpha\beta K} \tag{4-18}$$

for all $t \in K$ and $h \in (0,1]$. In order to achieve this, one will use the asymptotic expansion (4-9) up to an order N that will depend on α and β. Since from the first step, the $D_j(\,\cdot\,,t,h)$ $(j \ge 0)$ of the equality (4-9) belong to $W^{\infty,1}(\mathbb{R}^{2n})$ and are bounded independently of h in $(0,1]$ and of t in a compact set of $\mathbb{R}$, Proposition 2.1 shows that

$$h^{n-(|\alpha|+|\beta|)}\big\|(\operatorname{ad} P(h))^{\alpha}(\operatorname{ad} Q(h))^{\beta}\operatorname{Op}_h^{\mathrm{weyl}}(D_j(\,\cdot\,,t,h))\big\|_{\mathcal{L}^1(\mathcal{H})} \le C_{\alpha\beta K}$$

for all $t \in K$ and $h \in (0,1]$. Let us now derive an analogous upper bound for the term $E_N(t,s,h)$. For that, we use the expression (4-13) of $E_N(t,s,h)$, and we apply Lemma 4.4 with (t,s) replaced by (t,t_N) and A by $\operatorname{Op}_h^{\mathrm{weyl}}(R_N(\,\cdot\,,t_N,\dots,t_1,h))$. Since $R_N(\,\cdot\,,t_N,\dots,t_1,h)$ is in $W^{\infty,1}(\mathbb{R}^{2n})$ and is bounded independently of h in $(0,1]$, of $(t_1,\dots t_N)$ in $\Delta_N(0,t)$, and of t in a compact set of $\mathbb{R}$, Proposition 2.1 shows that, for every integer $m \ge 0$ and every compact set K of $\mathbb{R}$, there exists $C > 0$ such that

$$h^n I_h^{m,\mathrm{tr}}\big(\operatorname{Op}_h^{\mathrm{weyl}}(R_N(\,\cdot\,,t_N,\dots,t_1,h))\big) \le C_{mK}$$

for all $h \in (0, 1]$, $(t_1, \dots, t_N) \in \Delta_N(0, t)$, and $t \in K$. Hence by Lemma 4.4, we deduce that the iterated commutators of $G_h(t, t_N)(\mathrm{Op}_h^{\mathrm{weyl}}(R_N(\,\cdot\,, t_N, \dots, t_1, h)))$ with the position and momentum operators are themselves trace class, and that there exists another constant C_{mK} such that

$$h^n I_h^{m,\mathrm{tr}}\big(G_h(t, t_N)(\mathrm{Op}_h^{\mathrm{weyl}}(R_N(\,\cdot\,, t_N, \dots, t_1, h)))\big) \le C_{mK}.$$

We can therefore write, if $A_h = \mathrm{Op}_h^{\mathrm{weyl}}(F)$, for every multi-index (α, β) and every integer N,

$$h^n \left\| (\mathrm{ad}\, Q(h))^\beta (\mathrm{ad}\, P(h))^\alpha E_N(t, h) \right\|_{\mathscr{L}^1(\mathscr{H})} \le C_{\alpha\beta N}.$$

By reporting this in (4-9), and by choosing $N = |\alpha| + |\beta|$, one deduces (4-18). Using the characterization of Proposition 2.1, Theorem 4.2 follows.

Proof of Theorem 1.1. Let $\rho_h(t)$ be a classical solution of TDHF satisfying the hypotheses of Theorem 1.1. Let us denote by $V_h(t)$ the operator of multiplication by the function

$$x \to V_q(x, \rho_h(t)) = V(x) + \mathrm{Tr}(W_x \circ \rho_h(t)), \quad W_x(y) = W(x - y). \tag{4-19}$$

Under the hypotheses of Theorem 1.1, we have $\rho_h(t) \ge 0$ and $\mathrm{Tr}(\rho_h(t)) = 1$ for all t, and therefore the trace norm of $\rho_h(t)$ is constant. Since all the derivatives of V and W are bounded, it follows that

$$|\partial_x^\alpha V_q(\rho_h(t))(x)| \le C_\alpha, \quad (x, t) \in \mathbb{R}^n \times \mathbb{R}. \tag{4-20}$$

Let $\widehat{H}_h(t)$ denote the operator defined in (4-3), where $V(t)$ is the multiplication by $V_q(x, \rho_h(t))$. With these notations, the TDHF equation can be written

$$ih \frac{d\rho_h(t)}{dt} = [\widehat{H}_h(t), \rho_h(t)]. \tag{4-21}$$

We note that $V_h(t)$ depends on h, but in Theorem 4.2, the potential $V(t)$ may depend on a parameter that could be h. The only requirement is that $V_q(\,\cdot\,, \rho_h(t))$ should be bounded in $W^{\infty,\infty}(\mathbb{R}^n)$ independently of h, which is the case. Denoting by $G_h(t, s)$ the unitary propagator associated to the Hamiltonian $H_h(t)$ as in Proposition 4.1, one therefore has

$$\rho_h(t) = G_h(t, 0)(\rho_h(0)) = G_h(t, 0)(\mathrm{Op}_h^{\mathrm{weyl}}(F_h)).$$

Theorem 1.1 is therefore a particular case of Theorem 4.2. □

5. Proof of Theorem 1.2

We are going to state precisely the explicit construction of an approximate solution of order N, denoted by $\rho_h^{(N)}(t)$, of the TDHF equation. The exact solution $\rho_h(t)$ is determined by the interaction potentials V and W, which belong to $W^{\infty,\infty}(\mathbb{R}^n)$, and the initial data $\rho_h(0)$. We look for an approximate solution with the ansatz (1-18), where $F^{(N)}(t, h)$ is a function $\mathbb{R}^{2n}$ of the form (1-16). The functions $u_j(\,\cdot\,, t)$ in the sum (1-16) will be determined in Proposition 5.1. They will be in $W^{\infty,1}(\mathbb{R}^{2n})$, and they can depend also on h. We will associate to this solution the average quantum potential, like in (1-2):

$$V_q(x, \rho_h^{(N)}(t)) = V(x) + \mathrm{Tr}\big(W_x \rho_h^{(N)}(t)\big). \tag{5-1}$$

By (2-7), if F is in $W^{\infty,1}(\mathbb{R}^{2n})$ and G in $W^{\infty,\infty}(\mathbb{R}^{2n})$, one has

$$\mathrm{Tr}\big(\mathrm{Op}_h^{\mathrm{weyl}}(F)\circ \mathrm{Op}_h^{\mathrm{weyl}}(G)\big) = (2\pi h)^{-n}\int_{\mathbb{R}^{2n}} F(X)G(X)\,dX.$$

Therefore, if $\rho_h^{(N)}(t)$ is defined by (1-18) and $F^{(N)}(t,h)$ by (1-16), we have

$$V_q(x,\rho_h^{(N)}(t)) = V_{\mathrm{cl}}\big(x, F^{(N)}(\,\cdot\,,t,h)\big), \tag{5-2}$$

where, for every function v in $L^1(\mathbb{R}^{2n})$, the function $V_{\mathrm{cl}}(\,\cdot\,,v)$ is defined as in (1-3). One similarly shows that

$$V_q(x,\rho_h^{(N)}(t)) = V_{\mathrm{cl}}\big(x, F^{(N)}(\,\cdot\,,t,h)\big). \tag{5-3}$$

With these notations, the function $u_h(\,\cdot\,,t)$ defined in (1-10) should satisfy

$$\frac{\partial u_h(\,\cdot\,,t)}{\partial t} + 2\sum_{j=1}^{n}\xi_j\frac{\partial u_h(\,\cdot\,,t)}{\partial \xi_j} = \frac{1}{ih}M_h\big(V_{\mathrm{cl}}(u_h(\,\cdot\,,t)),u_h(\,\cdot\,,t)\big), \tag{5-4}$$

where for all suitable functions A and B, $M_h(A,B)$ denotes the Moyal bracket of A and B, defined in (3-2). For all functions A and B in $C^{\infty}(\mathbb{R}^{2n})$, and for every integer $k\geq 0$, let $C_k(A,B,\cdot)$ be the function defined in (3-4). We set $C_0(A,B)=0$. One has $C_1(A,B)=(1/i)\{A,B\}$. Now we will choose the u_j in a such a way that Equation (5-4) is approximatively verified. The construction of the functions u_j of Theorem 1.2 is detailed in the following proposition.

Proposition 5.1. *There exists a sequence of functions $(X,t)\to u_j(X,t)$ on $\mathbb{R}^{2n}\times\mathbb{R}$ $(j\geq 0)$ such that*:

(a) *The function $t\to u_j(\,\cdot\,,t,h)$ is C^{∞} from $\mathbb{R}$ into $W^{\infty,1}(\mathbb{R}^{2n})$. The function $u_j(\,\cdot\,,t,h)$ is bounded in $W^{\infty,1}(\mathbb{R}^{2n})$ independently of h in $(0,1]$ and of t in every compact set of $\mathbb{R}$.*

(b) *One has*

$$u_0(X,0)=F_h(X) \quad \textit{and} \quad u_j(X,0,h)=0, \quad j\geq 1.$$

(c) *For every N, the function $u_N(X,t,h)$ verifies*

$$\frac{\partial u_N}{\partial t} + 2\sum_{j=1}^{n}\xi_j\frac{\partial u_N}{\partial x_j} = \frac{1}{i}\sum_{j+k+\ell=N+1} C_k\big(V_{\mathrm{cl}}(\,\cdot\,,u_j(\,\cdot\,,t,h)),u_\ell(\,\cdot\,,t,h)\big). \tag{5-5}$$

In the sum (5-5), *the indices j and ℓ are ≥ 0 and k is ≥ 1.*

Determination of u_0. For $N=0$, Equation (5-5) reduces to the Vlasov equation,

$$\frac{\partial u_0}{\partial t} + 2\sum_{j=1}^{n}\xi_j\frac{\partial u_0}{\partial x_j} = \sum_{j=1}^{n}\frac{\partial}{\partial x_j}V_{\mathrm{cl}}\big(u_0(\,\cdot\,,t)\big)\frac{\partial u_0(\,\cdot\,,t)}{\partial \xi_j},$$

and we want that $u_0(\,\cdot\,,0)=F_h$, where F_h is the function of (1-6), which is in $W^{\infty,1}(\mathbb{R}^{2n})$. It is well known (see [Braun and Hepp 1977]) that there exists a unique solution u_0 of this Cauchy problem, and that the function u_0 is continuous from $\mathbb{R}$ into $W^{\infty,1}(\mathbb{R}^{2n})$. If F_h stays bounded in $W^{\infty,1}(\mathbb{R}^{2n})$ independently of h, it is also the case for $u_0(\,\cdot\,,t,h)$.

Determination of u_N ($N \geq 1$). For every $N \geq 1$, Equation (5-5) can be written as

$$\begin{aligned}\frac{\partial u_N}{\partial t} + 2\sum_{j=1}^{n} \xi_j \frac{\partial u_N}{\partial x_j} &= \sum_{j=1}^{n} \frac{\partial}{\partial x_j} V_{\mathrm{cl}}\big(u_0(\,\cdot\,, t, h)\big) \frac{\partial u_N(\,\cdot\,, t)}{\partial \xi_j} \\ &\quad + \sum_{j=1}^{n} \frac{\partial}{\partial x_j} V_{\mathrm{cl}}\big(u_N(\,\cdot\,, t, h)\big) \frac{\partial u_0(\,\cdot\,, t, h)}{\partial \xi_j} + G_N(X, t, h), \\ G_N &= \frac{1}{i} \sum_{\substack{j+k+\ell=N+1 \\ j<N,\, \ell<N}} C_k\big(V_{\mathrm{cl}}(u_j(\,\cdot\,, t, h)), u_\ell(\,\cdot\,, t, h)\big).\end{aligned}$$

One also requires that $u_N(X, 0, h) = 0$. To solve this equation, dropping the parameter h for the sake of simplifying notations, let us denote by $X \to \varphi_t(X) = (q(t, X), p(t, X))$ the Hamiltonian flow that is the solution of

$$q'(t, X) = 2p(t, X), \qquad p'(t, X) = -\nabla V(q(t, X)) - \int_{\mathbb{R}^{2n}} \nabla W(q(t, X) - y) u_0(y, \eta, t)\, dy\, d\eta$$

satisfying

$$q(0, X) = x, \quad p(0, X) = \xi, \quad X = (x, \xi).$$

The function v_N defined by $v_N(X, t) = u_N(\varphi_t(X), t)$ should satisfy

$$\frac{\partial v_N}{\partial t} = \sum_{j=1}^{n} \frac{\partial u_0}{\partial \xi_j}\big(\varphi_t(X), t\big) \int_{\mathbb{R}^{2n}} \frac{\partial W}{\partial x_j}\big(q_t(X) - y\big)\, u_N(y, \eta, t)\, dy\, d\eta + \widetilde{G}_N(X, t),$$

where $\widetilde{G}_N(X, t) = G_N(\varphi_t(X), t)$. By using in the integral the change of variables $(y, \eta) = \varphi_t(z, \zeta)$, whose jacobian equals 1, we see that v_N should satisfy

$$\begin{aligned}\frac{\partial v_N}{\partial t}(X, t) &= \widetilde{G}_N(X, t) + \int_{\mathbb{R}^{2n}} A(X, Y, t) v_N(Y, t)\, dY, \\ A(X, Y, t) &= \sum_{j=1}^{n} \frac{\partial u_0}{\partial \xi_j}\big(\varphi_t(X), t\big) \frac{\partial W}{\partial x_j}\big(q_t(X) - q_t(Y)\big).\end{aligned}$$

Moreover, one must have $v_N(\,\cdot\,, 0) = 0$. According to standard results on the Vlasov equation, one knows that $\nabla u_0(\,\cdot\,, t)$ is in $W^{\infty,1}(\mathbb{R}^{2n})$, bounded when t varies in a compact set. The same is true for $\nabla \varphi_t$. If the u_j ($0 \leq j < N$) have been built with the properties of Proposition 5.1, one sees that $G_N(\,\cdot\,, t)$ is in $W^{\infty,1}(\mathbb{R}^{2n})$, bounded when t varies in a compact set. It is also the case for $\widetilde{G}_N(\,\cdot\,, t)$. Then the Cauchy problem verified by v_N and the one verified by u_N can be solved in a standard way.

To prove Theorem 1.2, we will show that the functions $F^{(N)}(t, h)(X)$ defined in (1-16) starting from the $u_j(\,\cdot\,, t, h)$ of Proposition 5.1 and the operators $\rho_h^{(N)}(t)$ defined in (1-18) satisfy (1-17) and (1-19). The next proposition is an intermediate step.

Proposition 5.2. *Let $\rho_h(t)$ be an exact solution of TDHF satisfying the hypotheses of Theorems 1.1 and 1.2. Let $\widehat{H}_h(t)$ be the operator defined in* (4-3), *where $V(t)$ is the multiplication by $V_q(x, \rho_h(t))$. Let u_j*

($j \geq 0$) be the functions of Proposition 5.1, and, for each integer N, let $F^{(N)}$ be the function defined by (1-16) *and $\rho_h^{(N)}(t)$ defined in* (1-18). *Then we can write*

$$i h \frac{d\rho_h^{(N)}(t)}{dt} = [\widehat{H}_h(t), \rho_h^{(N)}(t)] + \mathrm{Op}_h^{\mathrm{weyl}}\big(S_h^{(N)}(\,\cdot\,, t)\big), \tag{5-6}$$

where $S_h^{(N)}(\,\cdot\,, t)$ is in $W^{\infty,1}(\mathbb{R}^{2n})$ and verifies, for every multi-index α,

$$\big\| \nabla^\alpha S_h^{(N)}(\,\cdot\,, t)\big\|_{L^1(\mathbb{R}^{2n})} \leq C_{\alpha N}(t)\big[h^{N+2} + h\big\|\rho_h(t) - \rho_h^{(N)}(t)\big\|_{\mathcal{L}^1(\mathcal{H})}\big], \tag{5-7}$$

where $C_{\alpha N}(t)$ is a function on $\mathbb{R}$ which is bounded on every compact set.

Proof. By (5-5), we have

$$\frac{\partial F^{(N)}}{\partial t} + 2\sum_{j=1}^{n} \xi_j \frac{\partial F^{(N)}}{\partial x_j} = \frac{1}{h}\sum_{k=1}^{N+1} h^k C_k\big(V_{\mathrm{cl}}(\,\cdot\,, F^{(N)}(\,\cdot\,, t, h)), F^{(N)}(\,\cdot\,, t, h)\big) + \Phi^{(N)}(\,\cdot\,, t, h), \tag{5-8}$$

where $\Phi^{(N)}(\,\cdot\,, t, h)$ is a function in $W^{\infty,1}(\mathbb{R}^{2n})$, such that

$$\big\|\nabla^\alpha \Phi^{(N)}(\,\cdot\,, t, h)\big\|_{L^1(\mathbb{R}^{2n})} \leq h^{N+1} C_{\alpha N}(t). \tag{5-9}$$

We define an approximation of the operator $\widehat{H}_h(t)$ by setting

$$\widehat{H}_h^{\mathrm{APP}}(t) = -h^2\Delta + V_{\mathrm{cl}}\big(F^{(N)}(\,\cdot\,, t, h)\big). \tag{5-10}$$

Since $F^{(N)}$ verifies (5-8), we may write

$$i h \frac{d\rho_h^{(N)}(t)}{dt} = \big[\widehat{H}_h^{\mathrm{APP}}(t), \rho_h^{(N)}(t)\big] + \mathrm{Op}_h^{\mathrm{weyl}}\big(T_h^{(N)}(\,\cdot\,, t)\big), \tag{5-11}$$

where the function $T_h^{(N)}(\,\cdot\,, t)$ is defined by

$$T_h^{(N)}(\,\cdot\,, t) = h\Phi^{(N)}(\,\cdot\,, t, h) + R_h^{(N+2)}\big(V_{\mathrm{cl}}(\,\cdot\,, F^{(N)}(\,\cdot\,, t, h)), F^{(N)}(\,\cdot\,, t, h)\big).$$

(For all functions A and B satisfying the hypotheses of Theorem 3.1, we denote by $R_h^{(N)}(A, B, \cdot)$ the function associated by Theorem 3.1 to such functions.) Then by the definition (5-3) of the map V_{cl}, and Proposition 5.1(a), we can write

$$\big\|\nabla_x^\alpha V_{\mathrm{cl}}\big(\,\cdot\,, F^{(N)}(\,\cdot\,, t, h)\big)\big\|_{L^\infty(\mathbb{R}^{2n})} \leq C_{\alpha N}(t), \quad \big\|\nabla^\beta F^{(N)}(\,\cdot\,, t, h))\big\|_{L^1(\mathbb{R}^{2n})} \leq C_{\beta N}(t). \tag{5-12}$$

Using these upper bounds and following Theorem 3.1 on the Moyal bracket, we may write

$$\big\|\nabla^\ell R_h^{(N+2)}\big(V_{\mathrm{cl}}(\,\cdot\,, F^{(N)}(\,\cdot\,, t, h)), F^{(N)}(\,\cdot\,, t, h)\big)\big\|_{L^1(\mathbb{R}^{2n})} \leq C_{\ell N}(t) h^{N+2}.$$

According to these upper bound estimates, and the estimates (5-9) of the derivatives of $\Phi^{(N)}(\,\cdot\,, t, h)$, one has

$$\big\|\nabla^\alpha T_h^{(N)}(\,\cdot\,, t)\big\|_{L^1(\mathbb{R}^{2n})} \leq C_{\alpha N}(t) h^{N+2}. \tag{5-13}$$

According to (5-11), and since

$$\widehat{H}_h^{\mathrm{APP}}(t) - \widehat{H}_h(t) = V_q(\,\cdot\,, \rho_h(t)) - V_q(\,\cdot\,, \rho_h^{(N)}(t)),$$

we can write the equality (5-6) with

$$S_h^{(N)}(\,\cdot\,, t) = T_h^{(N)}(\,\cdot\,, t) + M_h\big(V_q(\,\cdot\,, \rho_h(t)) - V_q(\,\cdot\,, \rho_h^{(N)}(t)),\, F^{(N)}(\,\cdot\,, t, h)\big). \tag{5-14}$$

One has

$$\big\| \nabla_x^\alpha \big(V_q(\,\cdot\,, \rho_h(t)) - V_q(\,\cdot\,, \rho_h^{(N)}(t))\big)\big\|_{L^\infty(\mathbb{R}^{2n})} \le C_\alpha \big\| \rho_h(t) - \rho_h^{(N)}(t)\big\|_{\mathcal{L}^1(\mathcal{H})}.$$

Using all of these estimates and the L^1 norm estimates (5-12) of $F^{(N)}(\,\cdot\,, t, h)$, and using Theorem 3.1 on the Moyal bracket, it results that

$$\big\| \nabla^\alpha M_h\big(V_q(\rho_h(t)) - V_q(\rho_h^{(N)}(t)),\, F^{(N)}(\,\cdot\,, t, h)\big)\big\|_{L^1(\mathbb{R}^{2n})} \le C(t) h \big\| \rho_h(t) - \rho_h^{(N)}(t)\big\|_{\mathcal{L}^1(\mathcal{H})}. \tag{5-15}$$

The norm upper bound estimate (5-7) of $S_h^{(N)}(\,\cdot\,, t)$ results from (5-14), (5-13) and (5-15).

End of the proof of Theorem 1.2. Let $U_h(t, s)$ and $G_h(t, s)$ be the unitary propagator and the mapping defined in Proposition 4.1, associated to the operator $\widehat{H}_h(t)$ of Proposition 5.2. The comparison of equalities (4-21) (verified by the exact solution) and (5-6) (verified by the approximate solution) and the Duhamel principle allow us to write

$$\rho_h(t) - \rho_h^{(N)}(t) = \frac{i}{h} \int_0^t G_h(t, s)\big(\mathrm{Op}_h^{\mathrm{weyl}}(S_h^{(N)}(\,\cdot\,, s))\big)\, ds. \tag{5-16}$$

Since $U_h(t, s)$ is unitary, the map $G_h(t, s)$ preserves the trace norm, and from that we may deduce that

$$\big\| \rho_h(t) - \rho_h^{(N)}(t)\big\|_{\mathcal{L}^1(\mathcal{H})} \le \frac{1}{h} \int_0^t \big\| \mathrm{Op}_h^{\mathrm{weyl}}(S_h^{(N)}(\,\cdot\,, s))\big\|_{\mathcal{L}^1(\mathcal{H})}\, ds.$$

Using Proposition 2.1 and the upper bounds (5-7) of Proposition 5.2, we obtain

$$\big\| \rho_h(t) - \rho_h^{(N)}(t)\big\|_{\mathcal{L}^1(\mathcal{H})} \le \frac{1}{h} \int_0^t C(s)\big[h^{N+2} + h \big\| \rho_h(s) - \rho_h^{(N)}(s)\big\|_{\mathcal{L}^1(\mathcal{H})}\big]\, ds.$$

By the Gronwall lemma, we deduce that, with another constant,

$$\big\| \rho_h(t) - \rho_h^{(N)}(t)\big\|_{\mathcal{L}^1(\mathcal{H})} \le C(t) h^{N+1}.$$

Therefore the Theorem 1.2(1-19) is proved. We deduce from this inequality and from (5-7) that

$$\big\| \nabla^\alpha S_h^{(N)}(\,\cdot\,, t)\big\|_{L^1(\mathbb{R}^{2n})} \le C_{\alpha N}(t) h^{N+2},$$

where $C_{\alpha N}(t)$ is a function on $\mathbb{R}$, bounded on every compact set. From Proposition 2.1 and Lemma 4.4, for every multi-index (α, β), the operators

$$h^{-N-2} (\mathrm{ad}\, Q(h))^\beta (\mathrm{ad}\, P(h))^\alpha G_h(t, s)\big(\mathrm{Op}_h^{\mathrm{weyl}}(S_h^{(N)}(\,\cdot\,, s)\big)$$

are trace class, and their trace norm is bounded, independently of (t, s) in a compact set of $\mathbb{R}$, and of h in $(0, 1]$. By (5-16), for every multi-index (α, β), and for every $N > 0$, there exists a function $C_{\alpha N}(t) > 0$, bounded on every compact set of $\mathbb{R}$, such that

$$\big\| (\mathrm{ad}\, Q(h))^{\beta} (\mathrm{ad}\, P(h))^{\alpha} \big(\rho_h(t) - \rho_h^{(N)}(t) \big) \big\|_{\mathcal{L}^1(\mathcal{H})} \le C_{\alpha N}(t) h^{N+1}.$$

Using Proposition 2.1(b), we deduce

$$(2\pi h)^{-n} \big\| \sigma_h^{\mathrm{weyl}} \big(\rho_h(t) - \rho_h^{(N)}(t) \big) \big\|_{L^1(\mathbb{R}^{2n})} \le C(t) h^{(N+1)-(2n+2)/2}.$$

In other words, with the notations of Theorem 1.2,

$$\big\| u_h(\cdot, t) - F^{(N)}(\cdot, t, h) \big\|_{L^1(\mathbb{R}^{2n})} \le C(t) h^N.$$

This is the Theorem 1.2(1-17), which is proved now. □

Appendix A: Proof of Proposition 2.1

The proof of Proposition 2.1 calls upon a different notion of symbol. One can associate to every bounded operator A in $\mathcal{H}$ a function $S_h(A)$ on $\mathbb{R}^{2n} \times \mathbb{R}^{2n}$ defined by

$$S_h(A)(X, Y) = \frac{\langle A \Psi_{Xh}, \Psi_{Yh} \rangle}{\langle \Psi_{Xh}, \Psi_{Yh} \rangle}, \tag{A-1}$$

where the Ψ_{Xh} are defined in (2-14). An explicit computation of integrals shows that

$$|\langle \Psi_{Xh}, \Psi_{Yh} \rangle| = e^{-(1/4h)|X-Y|^2}, \qquad \|\Psi_{Xh}\| = 1. \tag{A-2}$$

Consequently,

$$|S_h(A)(X, Y)| = e^{(1/4h)|X-Y|^2} |\langle A \Psi_{Xh}, \Psi_{Yh} \rangle|. \tag{A-3}$$

The function $S_h(A)$ is, up to a slight modification, what G. B. Folland [1989] calls the Wick symbol. The following proposition shows that $S_h(A)$ and the Weyl symbol $\sigma_h^{\mathrm{weyl}}(A)$ are related to each other by an integral operator. (By contrast, the Weyl symbol cannot be calculated from what is commonly called the Wick symbol, namely the restriction of $S_h(A)$ to the diagonal.) The function $S_h(A)$ can be majorized (in some norm) and minorized (in another norm) by the trace norm of A (Proposition A.2).

Proposition A.1. *The Weyl symbol of an operator A is related to the function $S_h(A)$ by*

$$S_h(A)(X, Y) = (\pi h)^{-n} \int_{\mathbb{R}^{2n}} e^{-(1/h)(Z-X).(\overline{Z}-\overline{Y})} \sigma_h^{\mathrm{weyl}}(A)(Z)\, dZ, \tag{A-4}$$

$$\sigma_h^{\mathrm{weyl}}(A)(Z) = 2^n (2\pi h)^{-2n} \int_{\mathbb{R}^{4n}} S_h(A)(X, Y) K_h(X, Y, Z)\, dX\, dY, \tag{A-5}$$

$$K_h(X, Y, Z) = e^{-(1/h)(\overline{Z}-\overline{X})(Z-Y)-(1/2h)|X-Y|^2}. \tag{A-6}$$

Proof. By the definition (2-3) of the Weyl calculus, one has

$$A = (\pi h)^{-n} \int_{\mathbb{R}^{2n}} \Sigma_{Zh} \sigma_h^{\mathrm{weyl}}(A)(Z)\, dZ,$$

where Σ_{Zh} is the operator defined in (2-4). An explicit computation shows that

$$\frac{\langle \Sigma_{Zh}\Psi_{Xh}, \Psi_{Yh}\rangle}{\langle \Psi_{Xh}, \Psi_{Yh}\rangle} = e^{-(1/h)(Z-X).(\overline{Z}-\overline{Y})}. \tag{A-7}$$

The equality (A-4) follows. By the fundamental formula (2-16) of coherent states, one has

$$A = (2\pi h)^{-2n} \int_{\mathbb{R}^{4n}} \langle A\Psi_{Xh}, \Psi_{Yh}\rangle P_{XYh}\, dX\, dY, \tag{A-8}$$

where P_{XYh} is the operator defined by

$$P_{XYh} f = \langle f, \Psi_{Xh}\rangle \Psi_{Yh}. \tag{A-9}$$

One knows from (2-5) that

$$\sigma_h^{\mathrm{weyl}}(P_{XYh})(Z) = 2^n \mathrm{Tr}(P_{XYh} \circ \Sigma_Z) = 2^n \langle \Sigma_{Zh}\Psi_{Yh}, \Psi_{Xh}\rangle.$$

By the computation leading to (A-7) (where X and Y are permuted), we may deduce

$$\sigma_h^{\mathrm{weyl}}(A)(Z) = 2^n (2\pi h)^{-2n} \int_{\mathbb{R}^{4n}} S_h(A)(X, Y) \big|\langle \Psi_{Xh}, \Psi_{Yh}\rangle\big|^2 e^{-(1/h)(\overline{Z}-\overline{X})(Z-Y)}\, dX\, dY.$$

Using the equality (2-15) on the scalar product of coherent states, we obtain (A-5). □

Proposition A.2. *Let A be a trace class operator and G a function in $L^1(\mathbb{R}^{2n})$. Then one has*

$$(2\pi h)^{-2n} \int_{\mathbb{R}^{4n}} \left| \langle A\Psi_{Xh}, \Psi_{Yh}\rangle G\left(\frac{X-Y}{\sqrt{h}}\right)\right| dX\, dY \le (2\pi)^{-n} \|G\|_{L^1(\mathbb{R}^{2n})} \|A\|_{\mathscr{L}^1(\mathscr{H})}, \tag{A-10}$$

$$\|A\|_{\mathscr{L}^1(\mathscr{H})} \le (2\pi h)^{-2n} \int_{\mathbb{R}^{4n}} \big|\langle A\Psi_{Xh}, \Psi_{Yh}\rangle\big|\, dX\, dY. \tag{A-11}$$

Proof. We may write $A = B_1 B_2$, where B_1 and B_2 are Hilbert–Schmidt. By using the fundamental property (2-16) of coherent states, one sees that for all X and Y in R^{2n},

$$\langle A\Psi_{Xh}, \Psi_{Yh}\rangle = \langle B_2\Psi_{Xh}, B_1^\star \Psi_{Yh}\rangle = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} u_{Zh}(X) v_{Zh}(Y)\, dZ,$$

where $u_{Zh}(X) = \langle B_2\Psi_{Xh}, \Psi_{Zh}\rangle$ and $v_{Zh}(X) = \langle \Psi_{Zh}, B_1^\star \Psi_{Xh}\rangle$. Let I_h be the left-hand side of (A-10). By Schur's lemma,

$$I_h \le (2\pi h)^{-3n} h^n \|G\|_{L^1(\mathbb{R}^{2n})} \int_{\mathbb{R}^{2n}} \|u_{Zh}\|_{L^2(\mathbb{R}^{2n})} \|v_{Zh}\|_{L^2(\mathbb{R}^{2n})}\, dZ.$$

By (2-16), we have $\|u_{Zh}\|_{L^2(\mathbb{R}^{2n})} = (2\pi h)^{n/2} \|B_2^\star \Psi_{Zh}\|$ and $\|v_{Zh}\|_{L^2(\mathbb{R}^{2n})} = (2\pi h)^{n/2} \|B_1 \Psi_{Zh}\|$. Hence,

$$I_h \le (2\pi h)^{-2n} h^n \|G\|_{L^1(\mathbb{R}^{2n})} \int_{\mathbb{R}^{2n}} \|B_1\Psi_{Zh}\| \|B_2^\star \Psi_{Zh}\|\, dZ.$$

By the fundamental property (2-16) of coherent states,

$$(2\pi h)^{-n} \int_{\mathbb{R}^{2n}} \|B_j \Psi_{Zh}\|^2\, dZ = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} \langle B_j^\star B_j \Psi_{Zh}, \Psi_{Zh}\rangle\, dZ = \mathrm{Tr}(B_j^\star B_j) = \|B_j\|^2_{\mathscr{L}^2(\mathscr{H})},$$

where $\|B_j\|_{\mathscr{L}^2(\mathscr{H})}$ is the Hilbert norm of B_j. Therefore,

$$I_h \leq (2\pi)^{-n} \|G\|_{L^1(\mathbb{R}^{2n})} \ \|B_1\|_{\mathscr{L}^2(\mathscr{H})} \ \|B_2\|_{\mathscr{L}^2(\mathscr{H})}.$$

By taking the infimum over all the decompositions $A = B_1 B_2$, one gets (A-10). The inequality (A-11) is deduced from the equality (A-8) since the operators P_{XYh} have a trace norm equal to 1. □

Proof of Proposition 2.1. For (a), we use the equality (A-4) and integrate by parts, as is done in [Rondeaux 1984]. Thus we see that

$$(2\pi h)^{-2n} \int_{\mathbb{R}^{4n}} e^{-(1/4h)|X-Y|^2} |S_h(A)(X,Y)|\, dX\, dY \leq C h^{-n} \sum_{|\alpha|+|\beta|\leq 2n+2} h^{(|\alpha|+|\beta|)/2} \|\partial_x^\alpha \partial_\xi^\beta F\|_{L^1(\mathbb{R}^{2n})}.$$

One then deduces item (a) (the upper bound estimate of the trace norm of A), using Equation (A-11).

For parts (b) and (c), we are going to integrate by parts in the second equality (A-5) of Proposition A.1. One verifies that the function K_h defined in (A-6) is invariant by the differential operator

$$L(h)K_h = K_h, \quad L(h) = \left(1 + \frac{|X-Y|^2}{h}\right)^{-1} \big(1 + (\overline{Y} - \overline{X})\partial_X\big).$$

Thus equality (A-5) implies, for every integer N,

$$\left|\sigma_h^{\text{weyl}}(A)(Z)\right| \leq 2^n (2\pi h)^{-2n} \int_{\mathbb{R}^{4n}} \left|K_h(X,Y,Z)\right| \left|({}^t L(h))^N S_h(A)(X,Y)\right| dX\, dY.$$

One verifies that

$$|K_h(X,Y,Z)| = e^{-(1/h)|Z-(X+Y/2)|^2 - (1/4h)|X-Y|^2}.$$

One chooses $N = 2n+2$. There exists $C > 0$ such that

$$\left|\sigma_h^{\text{weyl}}(A)(Z)\right| \leq C \sum_{|\alpha|\leq 2n+2} h^{|\alpha|/2} (2\pi h)^{-2n} \int_{\mathbb{R}^{4n}} \left|K_h(X,Y,Z)\right| G\left(\frac{X-Y}{\sqrt{h}}\right) \left|\partial_X^\alpha S_h(A)(X,Y)\right| dX\, dY,$$

where

$$G(X) = (1+|X|)^{-2n-2}.$$

By the classical formulas giving $S_h([P_j(h), A])$ and $S_h([Q_j(h), A])$ as an expression with the derivatives of $S_h(A)$, it follows that

$$\begin{aligned} &\left|\sigma_h^{\text{weyl}}(A)(Z)\right| \\ &\leq C \sum_{|\alpha|+|\beta|\leq 2n+2} h^{-2n-(|\alpha|+|\beta|)/2} \int_{\mathbb{R}^{4n}} e^{-(1/h)|Z-(X+Y/2)|^2 - (1/4h)|X-Y|^2} G\left(\frac{X-Y}{\sqrt{h}}\right) \left|S_h(A_{\alpha\beta h})(X,Y)\right| dX\, dY, \end{aligned}$$

where

$$A_{\alpha\beta h} = (\operatorname{ad} P(h))^\alpha (\operatorname{ad} Q(h))^\beta A.$$

The preceding equality can be also written as

$$\left|\sigma_h^{\text{weyl}}(A)(Z)\right| \leq C \sum_{|\alpha|+|\beta|\leq 2n+2} h^{-2n-(|\alpha|+|\beta|)/2} \int_{\mathbb{R}^{4n}} e^{-\frac{1}{h}\left|Z - \frac{X+Y}{2}\right|^2} G\left(\frac{X-Y}{\sqrt{h}}\right) \left|\langle (A_{\alpha\beta h}\Psi_{Xh}, \Psi_{Yh}\rangle\right| dX\, dY.$$

Item (b) is a consequence of (A-11). Item (c) (an analogue of the Beals characterization) is then easily deduced. □

Appendix B: Proof of Theorems 3.1 and 3.2

First step, common to both theorems. We know that, for all suitable functions F and G, we can write $\mathrm{Op}_h^{\mathrm{weyl}}(F)\circ\mathrm{Op}_h^{\mathrm{weyl}}(G)=\mathrm{Op}_h^{\mathrm{weyl}}(C_h(F,G,\cdot))$, with

$$C_h(F,G,X)=(\pi h)^{-2n}\int_{\mathbb{R}^{4n}}e^{-(2i/h)\sigma(Y-X,Z-X)}F(Y)G(Z)\,dY\,dZ,$$

where σ is the symplectic form $\sigma((x,\xi),(y,\eta))=y\xi-x\eta$. Consequently the Moyal bracket $M_h(F,G,\cdot)$ is defined by $M_h(F,G,X)=C_h(F,G,X)-C_h(G,F,X)$. Thus it suffices to write an asymptotic expansion $C_h(F,G,\cdot)$. We may write $C_h(F,G,X)=\Phi_h(X,1)$ by setting, for every $\theta\in[0,1]$,

$$\Phi_h(X,\theta)=(\pi h)^{-2n}\int_{\mathbb{R}^{4n}}e^{-(2i/h)\sigma(Y-X,Z-X)}F(Y)G\big(X+\theta(Z-X)\big)\,dY\,dZ.$$

Consequently, for every integer N,

$$C_h(F,G,X)=\sum_{k=0}^{N-1}\frac{1}{k!}\partial_t^k\Phi_h(X,0)+\widetilde{R}_h^{(N)}(F,G,X),$$

with

$$\widetilde{R}_h^{(N)}(F,G,X)=\int_0^1\frac{(1-\theta)^{N-1}}{(N-1)!}\partial_\theta^N\Phi_h(X,\theta)\,d\theta.$$

One sees, using integration by parts, that

$$\partial_\theta^k\Phi(X,\theta,h)=\left(\frac{h}{2i}\right)^k(\pi h)^{-2n}\int_{\mathbb{R}^{4n}}e^{-(2i/h)\sigma(Y-X,Z-X)}\big(\sigma(\nabla_1,\nabla_2)^k(F\otimes G)\big)\big(Y,X+\theta(Z-X)\big)\,dY\,dZ.$$

If a function Φ depends only on the Y variable, one has (in the sense of distributions)

$$(\pi h)^{-2n}\int_{\mathbb{R}^{4n}}e^{-(2i/h)\sigma(Y-X,Z-X)}\Phi(Y)\,dY\,dZ=\Phi(X),$$

and similarly if Φ depends only on the Z variable. For $\theta=0$, one has, by the above two equalities,

$$\partial_\theta^k\Phi(X,0,h)=\left(\frac{h}{2i}\right)^k\sigma(\nabla_1,\nabla_2)^k(F\otimes G)(X,X),$$

and therefore we do have indeed the equality (3-3) of Theorem 3.1, by setting

$$R_h^{(N)}(F,G,X)=\widetilde{R}_h^{(N)}(F,G,X)-\widetilde{R}_h^{(N)}(G,F,X). \tag{B-1}$$

It remains to obtain an upper bound for the norm of the two above terms. One also has

$$\widetilde{R}_h^{(N)}(F,G,X)=\left(\frac{h}{2i}\right)^N(\pi h)^{-2n}\int_{\mathbb{R}^{4n}\times[0,1]}\frac{(1-\theta)^{N-1}}{(N-1)!}K_h(X,Y,Z)\Psi(X,Y,Z,\theta)\,dY\,dZ\,d\theta,$$

where

$$K_h(X,Y,Z)=e^{-(2i/h)\sigma(Y-X,Z-X)},$$
$$\Psi(X,Y,Z,\theta)=\big(\sigma(\nabla_1,\nabla_2)^N(F\otimes G)\big)\big(Y,X+\theta(Z-X)\big).$$

The function K_h is invariant by the operator

$$L_h=\left(1+4\frac{|X-Y|^2}{h}+4\frac{|X-Z|^2}{h}\right)^{-1}(1-h\Delta_Y-h\Delta_Z).$$

Therefore, for all integers K and ℓ,

$$\big|\nabla^\ell\widetilde{R}_h^{(N)}(F,G,X)\big|\le\left(\frac{h}{2}\right)^N(\pi h)^{-2n}\int_{\mathbb{R}^{4n}\times[0,1]}\frac{(1-\theta)^{N-1}}{(N-1)!}\big|\nabla^\ell({}^tL)^K\Psi(X,Y,Z,\theta)\big|\,dY\,dZ\,d\theta.$$

Consequently,

$$h^{\ell/2}|\nabla^\ell\widetilde{R}_h^{(N)}(F,G,X)|\le C\sum_{\substack{\alpha+\beta\le\ell+2K+2N\\ \alpha\ge N,\,\beta\ge N}}h^{(\alpha+\beta)/2}I_{\alpha\beta}(X,h),\tag{B-2}$$

$$I_{\alpha\beta}(X,h)$$
$$=h^{-2n}\int_{\mathbb{R}^{4n}\times[0,1]}(1-\theta)^{N-1}\left(1+\frac{|X-Y|+|X-Z|}{\sqrt{h}}\right)^{-2K}|\nabla^\alpha F(Y)|\big|\nabla^\beta G\big(X+\theta(Z-X)\big)\big|\,dY\,dZ\,d\theta.\tag{B-3}$$

End of the proof of Theorem 3.1. We integrate the equality (B-3) with respect to X by making the change of variables

$$X=(1-\theta)^{-1}(\widetilde{X}-\theta\widetilde{Z}),\quad Y=\widetilde{Y},\quad Z=\widetilde{Z}.$$

We obtain

$$\big\|I_{\alpha\beta}(\,\cdot\,,h)\big\|_{L^1(\mathbb{R}^{2n})}$$
$$\le Ch^{-2n}\int_{\mathbb{R}^{6n}\times[0,1]}(1-\theta)^{N-2n-1}\left(1+\frac{|X-Y|+|X-Z|}{\sqrt{h}}\right)^{-2K}|\nabla^\alpha F(Y)||\nabla^\beta G(X)|\,dX\,dY\,dY\,dZ\,d\theta.$$

If one has $N\ge 2n+1$ and chooses $K=2n+1$, we deduce, by using Schur's lemma, that

$$\big\|I_{\alpha\beta}(\,\cdot\,,h)\big\|_{L^1(\mathbb{R}^{2n})}\le C\|\nabla^\alpha F\|_{L^p(\mathbb{R}^{2n})}\,\|\nabla^\beta G\|_{L^q(\mathbb{R}^{2n})}.$$

Adding these inequalities, we obtain

$$h^{\ell/2}\big|\nabla^\ell R_h^{(N,1)}(F,G,X)\big|\le C\sum_{\substack{\alpha+\beta\le\ell+2K+2N\\ \alpha\ge N,\,\beta\ge N}}h^{(\alpha+\beta)/2}\|\nabla^\alpha F\|_{L^p(\mathbb{R}^{2n})}\|\nabla^\beta G\|_{L^q(\mathbb{R}^{2n})}.$$

By proceeding similarly for $\widetilde{R}_h^{(N)}(G,F,\cdot)$, we arrive at the upper bound (3-5) of Theorem 3.1. Part (3-6) is then deduced by Proposition 2.1.

End of the proof of Theorem 3.2. If one chooses $K = 2n + 1$, it follows from (B-3) that

$$\left\| I_{\alpha\beta}(\,\cdot\,, h) \right\|_{L^\infty(\mathbb{R}^{2n})} \leq C \| \nabla^\alpha F \|_{L^\infty(\mathbb{R}^{2n})} \| \nabla^\beta G \|_{L^\infty(\mathbb{R}^{2n})}.$$

By substituting in (B-2), then in (B-1), we obtain the majorization (3-7) of Theorem 3.2.

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