

AN INTRODUCTION TO SEMICLASSICAL ANALYSIS

STÉPHANE NONNENMACHER

Requirements: elementary functional analysis (Hilbert spaces), Fourier transform, theory of distributions. Linear PDEs and semigroup theory. Spectral theory on Hilbert spaces (at least for bounded operators).

Following Matthieu Léautaud's course on Spectral Theory would help.

Bibliography on semiclassical analysis:

- M. Zworski, Semiclassical Analysis, AMS, 2012
- A. Martinez, An Introduction to Semiclassical and Microlocal Analysis, Springer, 2002
- M. Dimassi and J. Sjöstrand, Spectral Asymptotics in the Semi-Classical Limit, Cambridge U Press, 1999

Older books on microlocal analysis (that is, without the $\hbar$ parameter)

- A. Grigis and J. Sjöstrand, Microlocal Analysis for Differential Operators, An Introduction. Cambridge University Press, 1994
- L. Hörmander, The Analysis of Linear Partial Differential Operators, Volumes I-IV, Springer, 1983-85 (a.k.a. "the Bible").

1. INTRODUCTION TO THE COURSE

1.1. What is this all about? Objective: analyse qualitatively and *quantitatively* certain types of linear differential operators appearing in mathematical physics.

1.1.1. Understand the solutions to Schrödinger equation in quantum mechanics. Originally, semiclassical analysis was applied to the equations of quantum mechanics. The dynamics of a massive, nonrelativistic quantum particle is governed by the time-dependent Schrödinger eq. on Hilbert space $u(t) \in L^2(\mathbb{R}^d)$,

$$(1.1) \quad i\hbar\partial_t u(x, t) = \left(-\frac{\hbar^2\Delta}{2m} + \tilde{V}(x) \right) u(x, t).$$

Here Δ is the standard Laplacian on $\mathbb{R}^d$, $\tilde{V}(x)$ is the potential energy of the quantum particle. In these lectures we will generally assume that the function $\tilde{V}(x)$ is smooth, and make some

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extra assumptions about its behaviour at infinity. The differential operator $\tilde{P}_h = -\frac{\hbar^2 \Delta}{2m} + \tilde{V}(x)$ is called the quantum Hamiltonian of the system. In physics, the parameter $\hbar \approx 10^{-34} J.s$ has the dimension of an action, m is the mass of the particle (ex: $m_{electron} \approx 10^{-31} kg$). As is often done in theoretical physics, we will now get rid of these dimensioned parameters.

We will reduce the dimensions of the Schrödinger equation considering a reference energy scale E_0 of the system. In view of the potential energy $\tilde{V}(x)$, the system at this energy will evolve on a typical length scale L_0 . Setting the dimensionless space variable $y = x/L_0$ and dividing $\tilde{P}_h$ by E_0 , we end up with the operator so there remains only a single dimension (length=time), and we are lead to study the operator

(1.2)

$$P_h = \frac{1}{E_0} \tilde{P}_h = -\frac{\hbar^2 \Delta_y}{2mE_0 L^2} + \frac{\tilde{V}(L_0 y)}{E_0}, \quad \text{which we write}$$

(1.3)

$$P_h = -\frac{\hbar^2 \Delta_y}{2} + V(y), \quad \text{with the rescaled energy } V(y) = \frac{\tilde{V}(L_0 y)}{E_0} \text{ and Planck parameter } h = \frac{\hbar}{L_0 \sqrt{mE_0}}.$$

The rescaled parameter is dimensionless, since it is obtained by dividing $\hbar$ by the typical action $S_0 = L_0 \sqrt{mE_0}$ of the system. Saying that $h \ll 1$ amounts to compare Planck's constant $\hbar = 10^{-34} J.s$ with the value of the action S_0 . Rescaling, the time variable by $t = T_0 \tau$ with the characteristic time $T_0 = L_0 \sqrt{m/E_0}$, the Schrödinger equation takes the dimensionless form

$$ih \frac{\partial}{\partial \tau} u(\tau, y) = P_h u(\tau, y).$$

In the following we will abandon the notations (τ, y, h) and revert to using $(t, x, \hbar)$ for the dimensionless variables and Planck parameter.

The assumptions we will make on the potential V will induce that the operator P_h is self-adjoint on $L^2(\mathbb{R}^d)$, with a dense domain $\mathcal{D}(P_h) \subset L^2$; its spectrum will therefore be real. One major goal of quantum mechanics is to analyze quantitatively the spectra of such operators. In the cases we will study, spectra will often have a discrete component made of isolated eigenvalues of finite multiplicities

$$(1.4) \quad P_h u_{\hbar,i} = E_{\hbar,i} u_{\hbar,i}, \quad i = 0, 1, 2, \dots$$

In this situation we will be interested in the following spectral data:

- (1) the distribution of the eigenvalues $\{E_{i,\hbar}\}$, in some fixed interval (indep. of $\hbar$)
- (2) the spatial (and more generally, phase space, or *microlocal*) localization properties of the eigenfunctions $u_{i,\hbar}$.

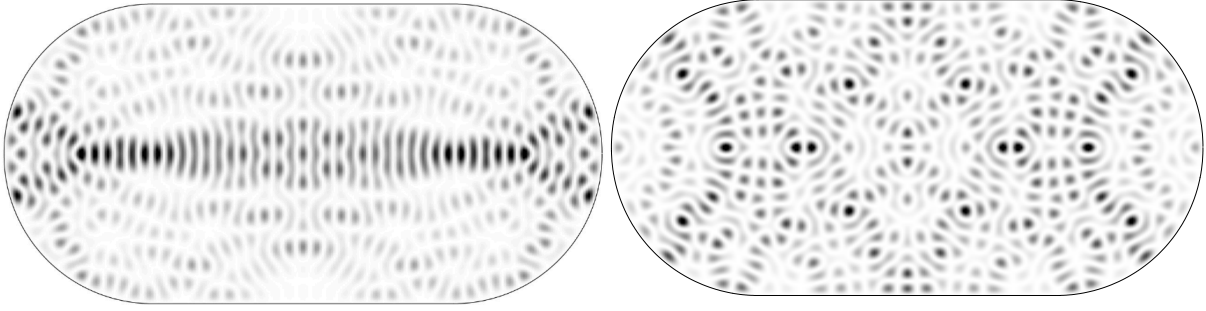


FIGURE 1.1. 2 eigenfunctions of the Laplacian inside a stadium-shaped domain (with Dirichlet boundary conditions). The grey intensity is proportional to $|u_i(x)|^2$.

1.1.2. *Semiclassical limit = fast oscillatory functions.* As often the case in analysis, one can make effective computations only in presence of a small (or large) parameter, meaning in some asymptotic limit. **The semiclassical limit** consists in analyzing the operator P_h in the regime $\hbar \ll 1$. This corresponds to wavefunctions $u(x, t)$ which oscillate fast **in position**, **compared with the macroscopic scales** ($\Delta x \sim 1$).

A local model to keep in mind is that of the Laplacian inside a cavity, say with Dirichlet boundary conditions. It describes the free motion of a quantum particle ($V \equiv 0$, and L_0 is the typical size of the cavity). Then, the equation $-\hbar^2 \Delta u = u$ can be solved locally by linear combinations of **plane waves** with same **wavelength** $2\pi\hbar \ll 1$:

$$u(x) = \int_{\mathbb{S}^{d-1}} \hat{u}(\xi) e^{i\xi \cdot x / \hbar} d\xi.$$

These waves oscillate on scales $\sim \hbar$ much smaller than the global scales of the problem ($L_0 \sim 1$). Here $\hat{u}(\xi)$ is, up to normalization, the (semiclassical) Fourier transform of $u(x)$ (see eq.(1.6) below).

Such oscillatory functions can be very complicated at the microscopic scale (cf. pictures of eigenmodes of billiards). **In general there are no explicit, or even approximate expressions for the eigenmodes.**

Furthermore, because $\hbar$ is in front of the most singular term (in the PDE sense: the highest derivative term), **the limit $\hbar \rightarrow 0$ of the Schrödinger equation is singular.** The spectrum of the operator P_h for $\hbar$ small has nothing in common with the spectrum of the multiplication operator $P_0 = -0\Delta + V(x)$!

What do we gain from studying this semiclassical regime?

Claim. in the semiclassical regime $\hbar \ll 1$, we will be able to connect the Schrödinger equation (a linear PDE) with the **classical mechanics of point particles** (a Hamiltonian Ordinary Differential Equation), and thereby gain nontrivial informations on the eigenmodes $u_{i,\hbar}(x)$.

1.1.3. *Applications of the semiclassical formalism to the wave equation.* Semiclassical analysis is closely connected with the *microlocal analysis* of linear PDEs, which was introduced in the 1960s. The typical example of equation dealt with is the scalar wave equation on $\mathbb{R}^d$. The original equation reads

$$(\partial_t^2 - c^2 \Delta) u(x, t) = 0,$$

where $c > 0$ is the speed of sound, which we assume homogeneous (position-independent) and isotropic. We may then reduce the dimension of this PDE by setting $c = 1$, thereby obtaining a dimensionless wave equation $(\partial_t^2 - \Delta)u = 0$.

What is the connection between the wave equation (with no small parameter involved) and the semiclassical Schrödinger equation?

Firstly, the wave equation is a second order differential equation w.r.t. the time. Since $-\Delta$ is a positive operator, we may factorize the wave equation into

$$(i\partial_t - \sqrt{-\Delta})(i\partial_t + \sqrt{-\Delta})u = 0,$$

that is the product of two first order equations which have the form of the Schrödinger equation

$$(1.5) \quad i\partial_t v = \pm P v, \quad \text{with } P = \sqrt{-\Delta}.$$

Each of these equations (they are mapped to one another by a time reversal) is called the *half-wave equation*. Solving the half-wave equation obviously provides a solution of the wave equation.

Microlocal analysis starts when considering the high frequency components of the solution $v(x, t)$. To do so, we may split the Fourier space $\mathbb{R}^d \ni \eta$ according to the value of $|\eta|$, using a dyadic decomposition (such a decomposition is called a Paley-Littlewood decomposition). Namely, let us consider a *smooth partition of unity* on $\mathbb{R}_+$

$$1 = \chi_0 + \sum_{n \geq 1} \chi_n,$$

with $\text{supp } \chi_n \subset (2^{n-1}, 2^{n+1})$ for all $n \geq 1$, $\text{supp } \chi_0 \subset [0, 2]$. Using this partition of unity, we split the initial data $v(x, 0) = f(x)$ for the equation (1.5) in Fourier space. Namely, using the operator P we define

$$f_n = \chi_n(P)f, \quad \forall n \geq 0.$$

The operators $\chi_n(P)$ are Fourier multipliers. Indeed, if we denote by

$$\mathcal{F}f(\eta) = (2\pi)^{-d/2} \int f(x) e^{-i\eta \cdot x} dx,$$

the Fourier transform of f , each $f_n(x)$ can be obtained by

$$f_n(x) = (2\pi)^{-d/2} \int \mathcal{F}f(\eta) \chi_n(|\eta|) e^{i\eta \cdot x} d\eta.$$

We then have as initial data $f = \sum_{n \geq 0} f_n$, with each component f_n being composed of Fourier modes at scales $|\eta| \sim 2^n$. By the linearity of the equation, we may solve the equation for each component independently. If we take f_n as initial data, the solution $v_n(x, t)$ will also be composed of such Fourier modes for any $t \in \mathbb{R}$. We may rescale this Fourier scale by inserting an artificial parameter $\hbar = \hbar_n \stackrel{\text{def}}{=} 2^{-n}$, and write the half-wave equation as

$$i\hbar \partial_t v_n = P_{\hbar} v_n, \text{ with } P_{\hbar} = \hbar P = \hbar \sqrt{-\Delta}.$$

By doing so, we end up with a *semiclassical* Schrödinger equation (that is, with a small effective parameter $\hbar$), with the solution $v_n(x, t)$ having the property that, at each time t , its semiclassical Fourier transform

$$[\mathcal{F}_{\hbar} v_n](\xi, t) \stackrel{\text{def}}{=} (2\pi\hbar)^{-d/2} \int v_n(x, t) e^{-i\xi \cdot x / \hbar} dx$$

is supported in the annulus $\{|\xi| \in (1/2, 2)\}$. Equivalently if we consider $\Pi_{\hbar} = \mathbb{1}_{(1/2, 2)}(P_{\hbar})$ the spectral projector of $P_{\hbar}$ associated with the interval $(1/2, 2)$, we have at each time $(\Pi_{\hbar} - 1)v_n(t) = 0$.

After this rescaling, the set of equations $\{(i\hbar_n \partial_t - P_{\hbar_n}) v_n = 0, v_n(0) = f_n\}_{n \in \mathbb{N}}$ is viewed as a subset of the family of semiclassical equations $\{(i\hbar \partial_t - P_{\hbar}) v_{\hbar} = 0, v_{\hbar}(0) = f_{\hbar}\}_{\hbar \in [0, 1]}$, with the functions $f_{\hbar}$ assumed to be spectrally concentrated (w.r.t. $P_{\hbar}$) in some fixed interval $I \subset \mathbb{R}_+$. The high-frequency limit $|\eta| \rightarrow \infty$ has been transformed into a semiclassical regime $\hbar \rightarrow 0$ and a fixed momentum scale $|\xi| \sim 1$. The setup is now similar to the preceding one, except that the Schrödinger operator $P_{\hbar} = -\frac{\hbar^2 \Delta}{2} + V(x)$ has been replaced by the *half-wave generator* $P_{\hbar} = \sqrt{-\hbar^2 \Delta}$.

In the case of the wave equation, the corresponding classical dynamics is the *geodesic flow* (or *ray dynamics*). This procedure can be adapted to the case of waves travelling on a smooth Riemannian manifold, with or without boundaries.

1.2. Quantum Mechanics in a nutshell.

1.2.1. *Wavefunctions and probability distributions.* Quantum Mechanics was developed, as a (pretty strong) modification of classical mechanics, more precisely **Hamilton's formulation of conservative (dissipationless) classical mechanics**, which we will review in section 1.4 below.

In classical mechanics, the state of a particle at time t is uniquely and precisely described by the data of its position $x(t)$ and its velocity $\dot{x}(t)$, or equivalently its momentum (in French, “impulsion” or “quantité de mouvement”) $\xi(t)$. Mathematically, a difference between the two points of view is that $\dot{x}(t) \in T\mathbb{R}^d$ is a tangent vector, while $\xi(t) \in T^*\mathbb{R}^d$ is a cotangent vector. This difference is not really relevant when working on $\mathbb{R}^d$, and when the Hamiltonian is of the form $p(x, \xi) = |\xi|^2/2 + V(x)$. The phase space of classical mechanics on $\mathbb{R}^d$ is the cotangent space $T^*\mathbb{R}^d \equiv \mathbb{R}_\xi^d \times \mathbb{R}_x^d$.

In quantum mechanics, the state of a particle (say, an electron) is described by a *wavefunction* $u(x, t)$, which is a time-dependent, complex-valued function $u(t) \in L^2(\mathbb{R}^d)$ with unit norm. The wavefunction $u(t)$ represents the particle as a **wave**, which is hence intrinsically delocalized. Alternatively, it describes a point particle, whose position (or momentum) cannot be known deterministically, but only probabilistically. That is, if one performs a position measurement on the particle at time t , one cannot in advance predict the outcome of the measurement, but **only provide a probability distribution of the outcome**, given by the function $|u(t, x)|^2$ (remind that we require $\|u(t)\|_{L^2} = 1$). The function $u(x, t)$ is called the (*position*) *probability amplitude*.

The wavefunction $u(x, t)$ simultaneously describes the momentum of the particle, which is associated with the Fourier variable, at the scale $\hbar^{-1}$. Namely, the De Broglie correspondence states that a flux of particles of momentum $\xi_0 \in \mathbb{R}^d$ is described by the plane wave

$$u_{\xi_0}(x) = C e^{i \frac{\xi_0 \cdot x}{\hbar}}, \quad x \in \mathbb{R}^d,$$

that is, the momentum ξ_0 corresponds to a wavevector $\eta_0 = \xi_0/\hbar$. Any wavefunction $u(x, t)$ can be decomposed in such Fourier modes, using the semiclassical Fourier transform:

$$(1.6) \quad u(x, t) = \frac{1}{(2\pi\hbar)^{d/2}} \int e^{-i\xi \cdot x/\hbar} \hat{u}(\xi, t) d\xi, \quad \hat{u}(\xi, t) = [\mathcal{F}_\hbar u(t)](\xi) = \frac{1}{(2\pi\hbar)^{d/2}} \int e^{i\xi \cdot x/\hbar} u(x, t) dx$$

Here $\xi \mapsto \hat{u}(\xi, t)$ represents the momentum amplitude of the state $u(t)$. If one proceeds with a momentum measurement (what people actually do in particle accelerators), the outcome is a random variable, following the *momentum probability density* $|\hat{u}(\xi, t)|^2$.

As a result, the same function $u(x, t)$ allows to represent both the position and momentum probability distributions. Clearly, changing the phase of $u(x, t)$ won't change $|u(x, t)|^2$, but it will generally impact the momentum density $|\hat{u}(\xi, t)|^2$.

1.2.2. *Observables in classical and quantum mechanics.* If the wavefunction $u(x)$ is nice enough, say in the Schwartz space $u \in \mathcal{S}(\mathbb{R}^d)$, then the distributions of the position or momentum variables can be described through their *moments*. Namely, for any multi-index¹ $\alpha \in \mathbb{N}^d$, the moment² of this variable, $\mathbb{E}_u x^\alpha$, is finite. This moment can be interpreted as a “diagonal matrix element” of a corresponding *multiplication operator*

$$\text{Op}(x^\alpha) : u(x) \mapsto x^\alpha u(x).$$

For $\alpha \neq 0$ this operator is unbounded on L^2 , but it has a dense domain on which it is selfadjoint. Any function $u \in \mathcal{S}$ belongs to this domain, and we have

$$\mathbb{E}_u x^\alpha = \int_{\mathbb{R}^d} dx |u(x)|^2 x^\alpha = \langle u, \text{Op}(x^\alpha) u \rangle_{L^2(dx)}.$$

Similarly, the moments of the momentum variables can be viewed as matrix elements of corresponding momentum operators. Indeed, for any multi-index $\beta \in \mathbb{N}^d$, the average of the variable ξ^β , for a particle in the state $u(x) \in \mathcal{S}$, is defined as

$$\mathbb{E}_u \xi^\beta = \int_{\mathbb{R}^d} d\xi |\hat{u}(\xi)|^2 \xi^\beta = \langle \hat{u}, \xi^\beta \hat{u} \rangle_{L^2(d\xi)}.$$

Now, we would like to express this matrix element in terms of the original wavefunction $u(x)$. A straightforward computation shows that the multiplication operator by ξ^α is transformed, through the $\hbar$ -Fourier transform, into the differential operator $\left(\frac{\hbar}{i}\partial\right)^\alpha$: for any $u \in \mathcal{S}(\mathbb{R}^d)$,

$$[\mathcal{F}_\hbar^{-1}(\xi^\alpha \hat{u}(\xi))](x) = \left[\left(\frac{\hbar}{i} \partial \right)^\alpha u \right](x).$$

Notation: We will use the notation $\boxed{D = D_x = -i\partial}$ for the symmetric derivative operator.

The above operator will be denoted $\text{Op}_\hbar(\xi^\alpha) \stackrel{\text{def}}{=} (\hbar D_x)^\alpha$, so we may write

$$\mathbb{E}_u \xi^\alpha = \langle u, \text{Op}_\hbar(\xi^\alpha) u \rangle_{L^2(dx)}.$$

Here we have let correspond:

¹ $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_d)$ with $\alpha_i \in \mathbb{N}$, and we note $x^\alpha = x_1^{\alpha_1} x_2^{\alpha_2} \dots x_d^{\alpha_d}$. Similarly, we will note the multi-derivative $\partial^\alpha = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \dots \partial x_d^{\alpha_d}}$, with $|\alpha| = \alpha_1 + \dots + \alpha_d$.

²In physics such expectation values (“averages”) are usually denoted with brackets, $\mathbb{E}_u x^\alpha = \langle x^\alpha \rangle$. We will try not to use this notation, to avoid any confusion with scalar products.

- to the position variable x_j the operator of multiplication by x_j , which we denote $\text{Op}(x_j) = \text{Op}_\hbar(x_j)$ (this operator is independent of $\hbar$).
- to the momentum variable ξ_j the differential operator $\hbar D_{x_j} = \frac{\hbar}{i} \frac{\partial}{\partial x_j} = \text{Op}_\hbar(\xi_j)$ (this “momentum operator” explicitly depends on $\hbar$).

Position and momentum form a first set of variables describing the state of particle. Such variables, which can be experimentally measured, are called *observables* in quantum mechanics.

More generally, one calls *classical observable* a smooth, real valued function on phase space $a \in C^\infty(\mathbb{R}_{x,\xi}^{2d}, \mathbb{R})$, while a *quantum observable* is a *selfadjoint* operator $A : L^2(\mathbb{R}_x^d) \rightarrow L^2(\mathbb{R}_x^d)$ (often unbounded, in which case we’ll assume its domain $\mathcal{D}(A)$ to be dense in L^2). A classical observable can be used to test the localization of a distribution of particles $\rho(x, \xi)$ of particles in phase space through classical averages $\int \rho(x, \xi) a(x, \xi) dx d\xi$. Similarly, quantum observables can be seen as “test operators”, helping to grab the structure of the wavefunction u through *quantum averages* $\langle u, Au \rangle_{L^2}$.

Remark 1.1. What is the interpretation of such a quantum average? As a selfadjoint operator, the operator A can be experimentally measured. For a general state u , the output of the measurement cannot be predicted with certainty, but is described by a real valued random variable, which will take different values if we repeat the measurement many times (reconstructing the same wavefunction u before each measurement). Assuming u is nice enough, that random variable can be described in terms of its moments, which are given by the matrix elements $\langle u, A^n u \rangle$, $n \geq 1$.

In the case when A has pure point spectrum with orthonormal basis $(\phi_i, a_i)_{i \in \mathbb{N}}$, the quantum averages simply depend on the overlaps between u and the eigenmodes ϕ_i :

$$\langle u, A^n u \rangle = \sum_{i \in \mathbb{N}} a_i^n |\langle u, \phi_i \rangle|^2.$$

The measurement of the observable A will give the value a_i with probability $|\langle u, \phi_i \rangle|^2$.

1.2.3. *Quantization: from classical to quantum observables.* Quantum mechanics establishes a correspondence between classical and quantum observables, through a **quantization procedure**

$$(1.7) \quad a \in C^\infty(\mathbb{R}^{2d}) \mapsto A = \text{Op}_\hbar(a)$$

mapping a classical observable (a function on phase space) into a quantum observable (an operator on L^2). This quantization procedure lies at the heart of semiclassical analysis. Our

lectures will be devoted to a precise study of such a quantization procedure, and of its various consequences.

We won't give yet the precise definition of this quantization, but only a few relevant properties:

- (1) the position monomials x^α are quantized into the corresponding multiplication operators
- (2) the momentum monomials ξ^α are quantized into the differential operators $(\hbar D_x)^\alpha$
- (3) quantization is a linear operation: $\text{Op}_\hbar(\alpha a + \beta b) = \alpha \text{Op}_\hbar(a) + \beta \text{Op}_\hbar(b)$ (here we don't pay attention to questions of domains).
- (4) quantization should map real valued functions into (essentially) selfadjoint operators.

The last property is specific to quantum mechanics applications, and will lead to the so-called **Weyl quantization**. In the study of linear PDEs it is often customary to introduce different (yet related) forms of quantization, which do not necessarily satisfy the requirement (4).

By taking linear combination of monomials we get polynomials, which are in some sense “dense” in the set of smooth functions. Hence, it is reasonable to expect the following extension of the above properties:

(1') a smooth function (which does not grow too fast at infinity) $a(x)$ is quantized into the multiplication by $a(x)$.

(2') a smooth function $b(\xi)$ is quantized into the Fourier multiplier $b(\hbar D_x)$, a first example of *pseudodifferential operator*.

We will need to be more precise on the growth conditions we have to impose on the function a, b . We will be lead to introduce various spaces of appropriate functions (which are called *symbols* in this context). Such functions will be smooth, with controlled growth or decay at infinity, and they may depend explicitly on the parameter $\hbar$, still in a controlled way.

Problem 1.2. How to quantize a function (say, a polynomial) depending on both x and ξ ? From the above properties we naturally end up with **ordering questions**. Indeed, the operators $\text{Op}_\hbar(x_j)$ and $\text{Op}_\hbar(\xi_k)$ do not commute, but satisfy the *commutation relations*

$$[\text{Op}_\hbar(x_j), \text{Op}_\hbar(\xi_k)] = i\hbar \delta_{jk} \quad (\text{where } \delta_{jk} \text{ is the Kronecker symbol}).$$

What should then be the quantization of the observable $x_j \xi_j$? We easily check that neither $A_1 \stackrel{\text{def}}{=} \text{Op}_\hbar(x_j) \text{Op}_\hbar(\xi_j)$ nor $A_2 \stackrel{\text{def}}{=} \text{Op}_\hbar(\xi_j) \text{Op}_\hbar(x_j)$ are symmetric operators, so they don't satisfy the requirement 4. A mixture of the two operators, namely $\frac{A_1 + A_2}{2}$, will “do the job”.

Such ordering problems, coming from the noncommutation of operators, are also at the heart of the

Proposition 1.3. [*Heisenberg uncertainty principle*]

For any state $u \in \mathcal{S}(\mathbb{R})$, with $\|u\|_{L^2} = 1$, the variances of the position and momentum variables satisfy the constraint:

$$(\mathbb{E}_u(x^2) - \mathbb{E}_u(x)^2) (\mathbb{E}_u(\xi^2) - \mathbb{E}_u(\xi)^2) \geq \hbar^2/4.$$

This expresses the fact that the uncertainty in position and the uncertainty in momentum (or $\hbar$ -Fourier variable) cannot be simultaneously arbitrarily small.

Exercise 1.4. Prove the uncertainty principle (in 1 dimension). For this aim, consider the state $v_\lambda = xu + i\lambda\hbar D_x u$ for $\lambda \in \mathbb{R}$, and use the fact that $\|v_\lambda\| \geq 0$ for any $\lambda \in \mathbb{R}$.

1.2.4. *Microlocalization of semiclassical states: using observables as “quantum test functions”.* One role of quantized observables $\text{Op}_\hbar(a)$ will be to detect the concentration of a state $u(x)$ (or rather, of a family of $\hbar$ -dependent states $(u_\hbar)_{\hbar \in (0,1]}$) in some phase space region $\Omega \subset \mathbb{R}_x^d \times \mathbb{R}_\xi^d$.

For a spatial region Ω_x (assumed to be a domain of $\mathbb{R}^d$), one measures the weight of $u_\hbar$ in Ω_x by taking the matrix element $\langle u_\hbar, \mathbb{1}_{\Omega_x} u_\hbar \rangle \in [0, 1]$. One can also measure the weight of $u_\hbar$ in a Fourier region Ω_ξ by taking the matrix element $\langle u_\hbar, \mathbb{1}_{\Omega_\xi}(\hbar D_x) u_\hbar \rangle \in [0, 1]$. Notice that this weight corresponds to wavevectors $\eta = \hbar^{-1}\xi$ of moduli $\sim \hbar^{-1}$: we are measuring the weight of large wavevectors, corresponding to oscillations of $u_\hbar(x)$ at the scale $\sim \hbar$.

The idea of microlocal analysis is to measure both types of concentration (space vs. Fourier) simultaneously. For instance, the weight of $u_\hbar$ in the product region $\Omega_x \times \Omega_\xi$ could be defined by $\langle u_\hbar, \mathbb{1}_{\Omega_\xi}(\hbar D_x) \mathbb{1}_{\Omega_x} u_\hbar \rangle$. However, this expression is not so nice: the operator $\mathbb{1}_{\Omega_\xi}(\hbar D_x) \mathbb{1}_{\Omega_x}$ is not selfadjoint, hence is not an observable. Besides, the properties of this operator suffer from the discontinuity of the characteristic functions $\mathbb{1}_{\Omega_x}, \mathbb{1}_{\Omega_\xi}$, namely the fact that the Fourier transform of a discontinuous function exhibits strong fluctuations (Stokes oscillations).

To avoid these problems, it is more reasonable to replace the characteristic functions by smooth functions $\chi_x \in C_c^\infty(\mathbb{R}_x^d, [0, 1])$, $\chi_\xi \in C_c^\infty(\mathbb{R}_\xi^d, [0, 1])$, namely functions satisfying, for some small $\epsilon > 0$,

$$(1.8) \quad \chi_x = 1 \text{ on } \Omega_x, \quad \chi_x \text{ is supported in the } \epsilon - \text{neighbourhood of } \Omega_x$$

This property will be denoted by $\chi_x \succ \mathbb{1}_{\Omega_x}$. Similarly, we may use a smoothened characteristic function in momentum $\chi_\xi \succ \mathbb{1}_{\Omega_\xi}$.

This way, the operators $\text{Op}_\hbar(\chi_x) = \chi_x$ and $\text{Op}_\hbar(\chi_\xi) = \chi_\xi(\hbar D_x)$ are better behaved upon composition, and we could take for the weight in $\Omega_x \times \Omega_\xi$ the scalar product $\langle u_\hbar, \text{Op}_\hbar(\chi_x) \text{Op}_\hbar(\chi_\xi) u_\hbar \rangle$,

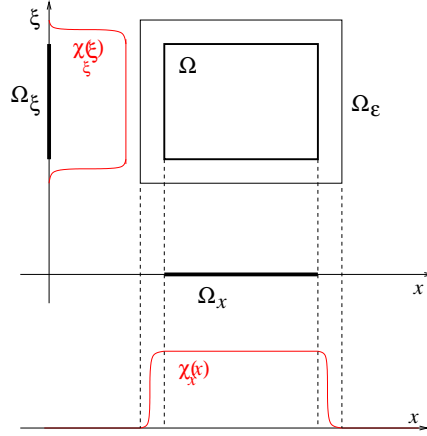


FIGURE 1.2. Microlocalization inside a domain $\Omega = \Omega_x \times \Omega_\xi$ and its ϵ -neighbourhood Ω_ϵ , using smooth cutoff functions.

or its symmetrized version. Another, somewhat more natural possibility would be to take for the weight $\langle u_h, \text{Op}_h(\chi_x \chi_\xi) u_h \rangle$, where the operator $\text{Op}_h(\chi_x \chi_\xi)$ will be selfadjoint if we choose an appropriate (e.g. Weyl) quantization procedure.

From the latter expression, the definition of a phase space weight can be extended to an arbitrary phase space domain $\Omega \subset \mathbb{R}_x^d \times \mathbb{R}_\xi^d$, by smoothing the function $\mathbb{1}_\Omega(x, \xi)$ into some smooth cutoff $\chi_\Omega \in C_c^\infty(\mathbb{R}_{x,\xi}^{2d}, [0, 1])$, $\chi_\Omega \succ \mathbb{1}_\Omega$, and defining the weight by the scalar product $\langle u_h, \text{Op}_h(\chi_\Omega) u_h \rangle$.

Such a phase space weight is called *microlocal*. Here the prefix “micro” does not refer to “microscopic”, but rather to “phase space”, or “simultaneously local in position and Fourier”. There is some freedom in the definition of the weight, since the cutoff χ_Ω , satisfying the analogue of 1.8, is not uniquely defined. Also, the operators $\text{Op}_h(\chi_x) \text{Op}_h(\chi_\xi)$, its symmetric version, and $\text{Op}_h(\chi_x \chi_\xi)$ are not equal, so do they measure the same localization phenomenon? These operators belong to the class of $\hbar$ -pseudodifferential operators; we will see in section 2 that the difference between these operators is of order $\mathcal{O}(\hbar)$, hence becomes negligible in the semiclassical limit.

Another way to interpret a quantized cutoff such as $\text{Op}_h(\chi_\Omega)$ is as an *approximate phase space projector*. Namely, for an arbitrary function u_h , we may view $v_h = \text{Op}_h(\chi_\Omega) u_h$ as the “approximate projection” of u_h in the phase space region Ω . The term “projection” has to be understood with some care. The operator $\text{Op}_h(\chi_\Omega)$ is not a projector, since in general $\text{Op}_h(\chi_\Omega)^2 \neq \text{Op}_h(\chi_\Omega)$. Actually, this operator is not even positive in general. Besides, the cutoff χ_Ω leaks away from Ω (by a margin $\leq \epsilon$), so v_h could also have some components outside Ω .

Nevertheless, this method of “approximate phase space projection” (a more proper term would be “microlocalization”) will be useful to analyze semiclassical families of states $(u_h)_h$. It will lead to the notions of *semiclassical wavefront set* $\text{WF}_h(u_h)$ and of *semiclassical measures* μ_{sc} associated with a sequence of functions $(u_h)_{h \in (0,1]}$, which are two ways to measure the microlocalization of u_h . Roughly speaking, $\text{WF}_h(u_h)$ records the phase space points around which u is NOT microlocally residual, that is, is NOT of size $\mathcal{O}(\hbar^\infty)$ ³, while the semiclassical measure μ_{sc} keeps track of the points where u is not microlocally $o(1)$.

One of the outputs of semiclassical analysis is to give informations on the wavefront sets and semiclassical measures associated with eigenstates $u_{i,h}$ of operators P_h , in the limit $\hbar \searrow 0$. So actually, we will not deal with fixed operators, but with semiclassical families $(P_h)_{h \in (0,1]}$ of operators, indexed by small Planck parameters.

1.3. Time evolution in quantum mechanics. One is naturally interested in the time evolution of the wavefunction, to understand how the particle evolves. In quantum mechanics this evolution is governed by a Schrödinger equation of the type (1.1), where $V(x)$ is the potential energy of the particle at point x . More generally, it will be given by a Schrödinger equation of the form

$$(1.9) \quad i\hbar \partial_t u(t) = P_h u(t), \quad t \in \mathbb{R}, \quad u(0) = u_0,$$

for some self-adjoint operator P_h (usually a differential operator) called the quantum Hamiltonian.

In the next subsection on semigroups, we recall that the Schrödinger equation is *globally well-posed* for any initial data $u_0 \in L^2$, and admits a unique solution $u(t)$ expressed by the action of the Schrödinger group

$$(1.10) \quad u(t) = U_h(t)u_0, \quad t \in \mathbb{R}.$$

which is formally represented by

$$U_h(t) = \exp(-itP_h/\hbar).$$

The group operators $U_h(t) : L^2 \rightarrow L^2$ are all *unitary*, which allows the normalization $\|u(t)\|_{L^2} = 1$ at all times. The operator $U_h(t)$ is usually called the *propagator* associated with the Hamiltonian P_h (it propagates the quantum state u_0 to future times).

³A quantity $Q(\hbar)$ is said to be *microlocally residual* if $Q(\hbar) = \mathcal{O}(\hbar^\infty)$; that is, for any $N \geq 1$, there exists $C_N > 0$ such that $|Q(\hbar)| \leq C_N \hbar^N$ for all $\hbar \in (0, \hbar_0]$.

1.3.1. *Reminder on semigroups.* A strongly continuous group acting on a Hilbert space $\mathcal{H}$ is composed of a function $S : \mathbb{R} \rightarrow \mathcal{L}(\mathcal{H}, \mathcal{H})$ taking values in bounded operators, such that

- (1) $S(0) = Id$
- (2) For any $t, t' \in \mathbb{R}$, $S(t + t') = S(t) \circ S(t')$
- (3) The function $S(t)$ is strongly continuous: for any $u \in L^2$, $\lim_{t \rightarrow 0} \|S(t)u - u\|_{\mathcal{H}} = 0$.

If the operators $S(t)$ are all unitary, one speaks of a unitary group.

One can define the infinitesimal generator of a group $S(t)$. It is a linear operator A on $\mathcal{H}$, which may be unbounded. Its domain $\mathcal{D}(A)$ is defined as the space of vectors $u \in L^2$ such that $\frac{u - S(t)u}{it}$ admits a limit when $t \rightarrow 0$; the limit is then defined to be Au . This shows that $t \mapsto u(t)$ is differentiable at $t = 0$, with

$$\left. \frac{dS(t)u}{dt} \right|_{t=0} = -iAu.$$

By using the 2d property, we see that the function $u(t) = S(t)u_0$ satisfies, for any $t \in \mathbb{R}$, the evolution equation

$$(1.11) \quad i \frac{du(t)}{dt} = Au.$$

The function $u(t) = S(t)u_0$ is solution of this evolution equation in two possible senses:

- if $u_0 \in \mathcal{D}(A)$, then $u(t) \in \mathcal{D}(A)$ for all $t \in \mathbb{R}$, the function $t \mapsto u(t)$ is $C^1(\mathbb{R}, L^2)$, and $u(t)$ satisfies (1.11) in a strong sense.
- if $u_0 \in \mathcal{H} \setminus \mathcal{D}(A)$, then $u(t)$ is a solution of the equation (1.9) in a *weak* sense: for any test function $\psi \in C_c^1(\mathbb{R}_t)$, the state $u_\psi \stackrel{\text{def}}{=} \int_{\mathbb{R}} dt \psi(t)u(t)$ is in the domain of A , and it satisfies $Au_\psi = -iu_{\psi'}$.

For a unitary group, the generator $(A, \mathcal{D}(A))$ is automatically selfadjoint.

1.3.2. *Understanding time evolution: semiclassical propagation of singularities.* A major goal of quantum mechanics is to understand, as quantitatively as possible, the evolved state $u(t)$, depending on the quantum Hamiltonian P_h and the initial state u_0 . In the present semiclassical perspective, this evolution will be linked with another type of evolution, namely a Hamiltonian flow on the phase space $\mathbb{R}_x^d \times \mathbb{R}_\xi^d$ generated by some Hamilton function $p(x, \xi)$, called the *principal symbol* of the family of operators $(P_h)_h$. We have already explained some notion of microlocalization of a state (u_h) . The type of question one would like to address:

Assuming that the initial data (u_h) is microlocalized in some set $\Omega \Subset \mathbb{R}^{2d}$, can we say something about the microlocalization of its evolution $u_h(t) = U_h(t)u_h$?

The formalism we develop below, in particular the Quantum-Classical correspondence (called *Egorov's theorem* in mathematics), allows to answer to this question. The locus of microlocalization (i.e. the wavefront set) of $u_h(t)$ is transported according the Hamiltonian flow $\Phi_p^t : \mathbb{R}^{2d} \rightarrow \mathbb{R}^{2d}$ generated by the function $p(x, \xi)$ (we recall the elementary notions of Hamiltonian mechanics in the next subsection). For example, in the case of the Schrödinger operator $P_h = -\hbar^2 \Delta / 2 + V(x)$, the principal symbol (which is, actually, its full symbol) is $p(x, \xi) = \frac{|\xi|^2}{2} + V(x)$, the sum of the kinetic energy and the potential energy. The Hamiltonian flow just integrates Newton's equations in the case of a conservative dynamics. Proving this connection between classical and quantum transport (through Egorov's theorem) is one of the goals of the present lectures.

Remark. Most actual particles (like the electron, photon, proton..) carry an intrinsic magnetic momentum, called spin, which forces to describe them not as scalar functions $u(x, t)$, but as vector valued functions $\vec{u}(x, t)$, where the vector (actually called a spinor) has dimension 2 or more, depending on the type of the particle. The state space is thus rather $L^2(\mathbb{R}^d, \mathbb{C}^2)$. We will exclusively deal with *scalar* particles, namely particles without spin degrees of freedom.

1.4. A short reminder of Hamiltonian classical mechanics.

1.4.1. *From Newton to Hamilton.* A classical particle on $\mathbb{R}^d$ is described by a trajectory $x(t) \in \mathbb{R}^d$. At each time t it occupies a single point $x(t) \in \mathbb{R}^d$, and has a velocity $\dot{x}(t) = \frac{dx(t)}{dt} \in \mathbb{R}^d$. The motion is determined by Newton's law (1st principle of mechanics):

$$(1.12) \quad m\ddot{x}(t) = F(x(t)),$$

where $F : x \mapsto F(x) \in \mathbb{R}^d$ is the force field at position x (here we assume this force field to be time independent). Since this equation is of second order in time, ODE theory shows that, provided $F(x)$ is smooth near $x(0)$, the **intial data** $(x(0), \dot{x}(0))$ suffice to specify, at least locally in time, the trajectory $(x(t))_{t \in I}$.

Remark 1.5. The trajectory may explode at finite time, e.g. one may have $x(t) \xrightarrow{t \rightarrow T} \infty$ even if F is smooth everywhere. This cannot be the case under appropriate conditions on the force field F (e.g. if $F(x)$ does not grow too fast at infinity).

In the following we will always assume that the trajectories remain finite for any real time, so that $(x(t))_t$ is well-defined for all $t \in \mathbb{R}$. One then says that the flow generated by the force field F is **complete**.

The force field $F(x)$ is said to be **conservative** if it derives from a potential energy (which we will call “potential” for short) $V : x \mapsto V(x) \in \mathbb{R}$.⁴

$$(1.13) \quad F(x) = -\nabla V(x).$$

In this case, the total mechanical energy

$$E(x, \dot{x}) = E_{kin} + V = \frac{m|\dot{x}|^2}{2} + V(x)$$

is preserved during the evolution: $\frac{d}{dt}E(x(t), \dot{x}(t)) = 0$.

It is useful to slightly change variables, by defining the **momentum** of the particle, which in this Euclidean setting reads⁵

$$\xi(t) = m\dot{x}(t).$$

The dynamical variables specifying the motion of the particle are now $(x(t), \xi(t)) \in \mathbb{R}^d \times \mathbb{R}^d$. The mechanical energy can be interpreted as a function defined on the **phase space** $\mathbb{R}^{2d} = \mathbb{R}_x^d \times \mathbb{R}_\xi^d$, called **Hamilton’s function**

$$(1.14) \quad H(x, \xi) = \frac{|\xi|^2}{2m} + V(x).$$

We will denote by $\rho = (x, \xi)$ the generic phase space point.

After this change of variables, Newton’s law (2d order eq. on d variables) can be cast into **Hamilton’s equations** over the phase space (1st order eqs. on $2d$ variables):

$$(1.15) \quad \begin{cases} \dot{x}(t) &= \frac{\partial H}{\partial \xi}(x(t), \xi(t)) \\ \dot{\xi}(t) &= -\frac{\partial H}{\partial x}(x(t), \xi(t)) \end{cases} \iff \dot{\rho}(t) = X_H(\rho)$$

The RHS defines the **Hamiltonian vector field** $\rho \in \mathbb{R}^{2d} \mapsto X_H(\rho) \in T_\rho \mathbb{R}^{2d} \equiv \mathbb{R}^{2d}$, which generates the **Hamiltonian flow** associated with the hamilton function H :

$$\Phi_H^t : \rho(0) = (x(0), \xi(0)) \in \mathbb{R}^{2d} \mapsto \Phi_H^t(\rho(0)) = \rho(t) = (x(t), \xi(t)) \in \mathbb{R}^{2d}.$$

Being a flow means that (provided everything is well-defined),

$$\Phi^{t+s}(\rho) = \Phi^t(\Phi^s(\rho)),$$

both for positive or negative times.

⁴the negative sign implies that the particle “rolls down” the energy landscape: it is attracted by low values of the potential.

⁵Beware that we will use PDE’s notation $\rho = (x, \xi)$ for the position-momentum coordinates and phase space point. In classical mechanics and quantum mechanics, one rather uses the notations (x, p) , or sometimes $x = (q, p)$!

Remark 1.6. This Hamiltonian formalism is not restricted to functions of the form (1.14), but can be generalized to more general functions $H(x, \xi)$ on phase space. Most of what we will say in this subsection applies in this higher generality, and defines a Hamiltonian flow on $\mathbb{R}^{2d}$.

Here again, the flow may not be defined for all time.

Remark 1.7. We will assume that $H \in C^\infty(\mathbb{R}^{2d})$, and that the flow Φ_H^t is complete.

In this context, the conservation of energy now reads as follows:

Proposition 1.8. *The Hamiltonian flow Φ_H^t leaves invariant the value of the Hamiltonian.*

$$\forall t \in \mathbb{R}, \forall \rho \in \mathbb{R}^{2d}, \quad H(\Phi_H^t(\rho)) = H(\rho)$$

Proof. Explicit computation using Hamilton's equations (1.15) lead to the following derivative for the function $H(\rho(t))$:

$$\frac{d}{dt}H(\rho(t)) = \frac{\partial H}{\partial x}(\rho(t)) \cdot \dot{x}(\rho(t)) + \frac{\partial H}{\partial \xi}(\rho(t)) \cdot \dot{\xi}(\rho(t)) = 0.$$

□

As a consequence, the phase space $\mathbb{R}^{2d}$ is naturally **foliated into energy layers**

$$\Sigma_E \stackrel{\text{def}}{=} H^{-1}(E) = \{\rho \in \mathbb{R}^{2d}, H(\rho) = E\},$$

and each layer Σ_E is invariant through the flow Φ_H^t . Hence, one can study the property of the flow Φ_H^t on each energy layer independently of the other ones.

Definition 1.9. A fixed point for the flow Φ_H^t is a point $\rho_c \in \mathbb{R}^{2d}$ for which $X_H(\rho_c) = 0$. Such a point is called **critical**. The corresponding energy $H(\rho_c)$ is called a critical energy.

The implicit function theorem shows that, if the energy E is noncritical, then $\Sigma_E \subset \mathbb{R}^{2d}$ is a smooth embedded hypersurface.

1.4.2. *Symplectic structure.* This formulation of conservative mechanics is equivalent with Newton's formulation. What we gain is a explicit new invariant structure, namely the **symplectic structure** on $T^*\mathbb{R}^d = \mathbb{R}_\xi^d \times \mathbb{R}_x^d$, which is explicitly given by the nondegenerate 2-form on $\mathbb{R}^{2d}$:

$$(1.16) \quad \omega = \sum_{j=1}^d d\xi_j \wedge dx_j.$$

⁶Most physics or mechanics books choose instead $\omega = \sum_{j=1}^d dx_j \wedge d\xi_j$, this sign change is just a matter of convention. We will use the present convention to conform with PDE convention.

This notation means that for any two vectors $V = \begin{pmatrix} V_x \\ V_\xi \end{pmatrix}$, $W = \begin{pmatrix} W_x \\ W_\xi \end{pmatrix} \in T_\rho \mathbb{R}^{2d} \simeq \mathbb{R}^{2d}$,

$$\omega(V, W) = \sum_j V_{\xi_j} W_{x_j} - V_{x_j} W_{\xi_j} = \langle JV, W \rangle, \quad \text{where } J \stackrel{\text{def}}{=} \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}.$$

This 2-form is obviously *nondegenerate* and *closed*. The Hamiltonian vector field can be defined using the symplectic form, by the more intrinsic, coordinate free equation:

$$(1.17) \quad \iota_{X_H} \omega = -dH \iff \forall V \in T_\rho \mathbb{R}^{2d}, \quad \omega(X_H, V) = -dH(V)$$

Definition 1.10. The symplectic form generates the **Poisson bracket** on $\mathbb{R}^{2d}$, which is the following bilinear operator on observables. For any pair of functions $f, g \in C^1(\mathbb{R}^{2d})$, the bracket is the function on $\mathbb{R}^{2d}$ defined by:

$$\{f, g\} \stackrel{\text{def}}{=} \sum_{j=1}^d \frac{\partial f}{\partial \xi_j} \frac{\partial g}{\partial x_j} - \frac{\partial f}{\partial x_j} \frac{\partial g}{\partial \xi_j} = X_f g = -X_g f = dg(X_f) = -df(X_g) = \omega(X_f, X_g)$$

If $f = H$ is the Hamiltonian, we have

$$\{H, g\} = X_H g = dg(X_H),$$

defines the infinitesimal change of the observable g evolved along the Hamiltonian flow Φ_H^t :

$$(1.18) \quad \{H, g\} = \frac{d}{dt} [g \circ \Phi_H^t] \big|_{t=0}.$$

Proposition 1.11. *The Hamiltonian flow Φ_H^t preserves the symplectic form. In other words, the pull-back of ω through the flow is equal to ω :*

$$(\Phi_H^t)^* \omega = \omega$$

Proof. One can write down the explicit infinitesimal transformation of ω under the Hamiltonian vector field X_H , in a slightly sloppy way:

$$\begin{aligned} \dot{\omega} &= \sum d\dot{\xi}_j \wedge dx_j + d\xi_j \wedge d\dot{x}_j \\ &= \sum -d(\partial_{x_j} H) \wedge dx_j + d\xi_j \wedge d(\partial_{\xi_j} H) \\ &= \sum -\left(\partial_{x_j x_k}^2 H dx_k + \partial_{x_j \xi_k}^2 H d\xi_k\right) \wedge dx_j + d\xi_j \wedge \left(\partial_{\xi_j x_k}^2 H dx_k + \partial_{\xi_j \xi_k}^2 H d\xi_k\right) \end{aligned}$$

The cross-terms $d\xi_k \wedge dx_j$ cancel each other. We may now invoke the fact that $(\partial_{x_j x_k}^2 H)$ and $(\partial_{\xi_j \xi_k}^2 H)$ are symmetric matrices, while $dx_k \wedge dx_j$ and $d\xi_j \wedge d\xi_k$ are antisymmetric, to kill the remaining terms, and get $\dot{\omega} = 0$.

A faster (and more geometric proof) uses the Cartan formula:

$$\dot{\omega} = \mathcal{L}_{X_H} \omega = d(\iota_{X_H} \omega) + \iota_{X_H} d\omega.$$

The closedness of ω kills the second term. On the other hand, $\iota_{X_H}\omega = -dH$, so we get zero. $\square$

2. (SEMICLASSICAL) QUANTIZATIONS ON $\mathbb{R}^{2d}$

We now present and investigate the quantization procedure mentioned in the introduction, which maps a function $a(x, \xi)$ (classical observable) to a linear operator $\text{Op}_h(a)$ acting on $L^2(\mathbb{R}^d)$ (or a smaller functional spaces dense in L^2 , like the Schwartz space $\mathcal{S}(\mathbb{R}^d)$). We will actually present a family of quantization procedures (indexed by a parameter $t \in [0, 1]$), compare them, and show that the differences between these different quantizations become small in the semiclassical limit. One particular choice ($t = 1/2$, or Weyl quantization) will have one distinctive advantage, namely map a real-valued function to a symmetric operator.

Notation: Following the use in quantum mechanics, in our notes the scalar product on $L^2(\mathbb{R}^d)$ will always be *antilinear in the first argument*, and linear in the second one:

$$\forall \alpha, \beta \in \mathbb{C}, \quad \langle \alpha u, \beta v \rangle = \bar{\alpha} \beta \langle u, v \rangle.$$

As a prerequisite, a quantization procedure should satisfy the following constraints (at this stage we do not care about the regularity or growth of the function):

- (1) a function $a(x)$ is quantized into the multiplication operator by $a(x)$.
- (2) a polynomial $p(\xi)$ is quantized into the differential operator $p(\hbar D_x)$, where recall the notation $D_x = \frac{1}{i} \partial_x$. (notice that D_{x_j} enjoys the property to be symmetric: $\langle u, D_{x_j} v \rangle = \langle D_{x_j} u, v \rangle$). More generally, a smooth function $a(\xi)$ is mapped to a Fourier multiplier $a(\hbar D_x)$.
- (3) quantization is a linear operator.

What is the use of such a quantization? What form of operators are produced this way?

- (1) The quantum Hamiltonian (the generator of the Schrödinger flow) $P_h = -\frac{\hbar^2 \Delta}{2} + V(x)$ is obtained a quantization of a classical Hamiltonian $p(x, \xi) = \frac{|\xi|^2}{2} + V(x)$.
- (2) the class of operators we obtain contains differential operators, but also a larger class of (semiclassical) **pseudodifferential operators**, or $\hbar$ -pseudodifferential operators ($\hbar$ - Ψ DO for short). Eventhough the Hamiltonian is usually a differential operator, the following derived operators are genuine pseudodifferential ops: its resolvent $(P_h - z)^{-1}$, or its noninteger powers $(P_h - z)^s$, more generally functions $f(P_h)$ which are useful when analyzing its spectrum.
- (3) the class of pseudodifferential operators also contains phase space cutoff operators $\text{Op}_h(\chi)$, $\chi \in C_c^\infty(\mathbb{R}^{2d})$, which are useful to analyze the **microlocalization properties** of wavefunctions, that is, their localization properties both in position and momentum (Fourier) space.

- (4) Although the quantization can be defined for any value of $\hbar > 0$ (e.g. $\hbar = 1$), the theory becomes quantitatively useful in the semiclassical limit $0 < \hbar \ll 1$, and this is the asymptotic regime we'll be considering. The reason is, the Schwartz kernels of operators develop **fast oscillatory phases** in this limit, which allows to use nonstationary vs. stationary phase estimates of relevant integrals, leading to expansions for these objects in terms of asymptotic series in powers of $\hbar$. These semiclassical expansions are at the heart of pseudodifferential calculus, and globally of semiclassical analysis; as a consequence, many properties of operators $\text{Op}_\hbar(a)$ can be directly read in terms of their symbols $a \in C^\infty(\mathbb{R}^{2d})$

Remark. Following the terminology of quantum mechanics, we have called the phase space function $a(x, \xi)$ a *classical observable*, and its quantization $\text{Op}_\hbar(a)$ a *quantum observable*. In the context of linear PDEs, the phase space function $a(x, \xi)$ is called the **symbol** of the (family of) operator(s) $\text{Op}_\hbar(a)$. The *symbol map* is the inverse of the quantization map⁷. This symbol map depends on the specific quantization procedure. We will sometimes speak of right, left, Weyl symbol, in reference to these different quantizations.

2.1. Quantizations of symbols in the Schwartz class $\mathcal{S}(\mathbb{R}^{2d})$.

2.1.1. *Symbols depending on x or ξ .* In order to give a unifying framework for the quantizations of function $f(x)$ and $g(\xi)$, we will write these operators in a similar form. For a while we will let our operators act on wavefunctions $u \in \mathcal{S}(\mathbb{R}^d)$ only. Let us start with the multiplication operator by $f(x)$:

$$\begin{aligned}
 [\text{Op}_\hbar(f)u](x) &= f(x)u(x) \\
 &= \int e^{i\frac{\xi \cdot x}{\hbar}} f(x) (\mathcal{F}_\hbar u)(\xi) \frac{d\xi}{(2\pi\hbar)^{d/2}} \\
 (2.1) \qquad &= \iint e^{i\frac{\xi \cdot (x-y)}{\hbar}} f(x)u(y) \frac{d\xi dy}{(2\pi\hbar)^d}.
 \end{aligned}$$

In the last line the integral is not absolutely convergent, but uses the representation of the delta distribution as an **oscillatory integral**:

$$\delta_0(x) = \int_{\mathbb{R}^d} e^{i\frac{\xi \cdot x}{\hbar}} \frac{d\xi}{(2\pi\hbar)^d}.$$

This expression is a formal way to express the fact that the Fourier transform of the distribution δ_0 is a constant function: $\mathcal{F}_\hbar \delta_0(\xi) = \frac{1}{(2\pi\hbar)^{d/2}}$.

⁷We will see that the quantization is indeed an invertible procedure, at least formally.

Exercise 2.1. Prove this integral representation by multiplying the integrand by the factor $e^{-\epsilon \xi^2}$, and letting $\epsilon \searrow 0$. Later we will alternatively give a meaning to such oscillatory integrals through formal integrations by parts.

The quantization of the momentum function $g = g(\xi)$ can be represented similarly:

$$\begin{aligned} [\text{Op}_h(g)u](x) &= [\mathcal{F}_h^{-1}(g\mathcal{F}_h u)](x) \\ &= \int e^{i\frac{\xi \cdot x}{h}} g(\xi) (\mathcal{F}_h u)(\xi) \frac{d\xi}{(2\pi\hbar)^{d/2}} \\ &= \iint e^{i\frac{\xi \cdot (x-y)}{h}} g(\xi) u(y) \frac{d\xi dy}{(2\pi\hbar)^d}. \end{aligned}$$

Note that this double integral is absolutely convergent as long as $g(\xi)$ decays fast enough when $|\xi| \rightarrow \infty$, e.g. if $g \in \mathcal{S}(\mathbb{R}^d)$.

2.1.2. *General symbols $a(x, \xi)$: Right and Left quantizations.* The composition of these two operators yields the expression:

$$(2.2) \quad [\text{Op}_h(f) \text{Op}_h(g)u](x) = \iint e^{i\frac{\xi \cdot (x-y)}{h}} f(x) g(\xi) u(y) \frac{d\xi dy}{(2\pi\hbar)^d},$$

Viewing this expression as a possible quantization of the function $f(x)g(\xi)$, leads to the following definition for the quantization of a general observable $a(x, \xi)$. We will start by considering very nice symbols, namely assume that $a \in \mathcal{S}(\mathbb{R}^{2d})$ (fast decay in both x and ξ).

Definition 2.2. (*Standard = Kohn-Nirenberg = Right quantization*) For any symbol $a(x, \xi) \in \mathcal{S}(\mathbb{R}^{2d})$, its standard (semiclassical) quantization is defined by

$$[\text{Op}_h^R(a)u](x) \stackrel{\text{def}}{=} \int e^{i\frac{\xi \cdot x}{h}} a(x, \xi) (\mathcal{F}_h u)(\xi) \frac{d\xi}{(2\pi\hbar)^{d/2}} = \iint e^{i\frac{\xi \cdot (x-y)}{h}} a(x, \xi) u(y) \frac{d\xi dy}{(2\pi\hbar)^d}.$$

The integral is absolutely convergent if the wavefunction $u \in L^1(\mathbb{R}^d)$. This operator $\text{Op}_h^R(a)$ will also be denoted by $a(x, hD)$.

This definition generalizes the product (2.2): for the product observable $a(x, \xi) = f(x)g(\xi)$, the right quantization corresponds to

$$\text{Op}_h^R(f(x)g(\xi)) = \text{Op}_h(f(x)) \text{Op}_h(g(\xi)).$$

This ordering corresponds to applying the Fourier multiplier on the *right* and the multiplication operator on the left. This is the reason why this quantization is called the *right quantization*. This quantization generalizes the standard quantization of polynomial symbols in ξ , $a(x, \xi) = \sum_{|\alpha| \leq m} a_\alpha(x) \xi^\alpha$, into differential operators $\text{Op}_1^R(a) = \sum_{|\alpha| \leq m} a_\alpha(x) D^\alpha$, with $D = (-i\partial)$. It is sometimes called the *standard* quantization.

Alternatively, ordering $\text{Op}_h(f)$ and $\text{Op}_h(g)$ in the opposite way to (2.2), we would obtain

$$[\text{Op}_h(g) \text{Op}_h(f)u](x) = \iint e^{i\frac{\xi \cdot (x-y)}{h}} g(\xi) f(y) u(y) \frac{d\xi dy}{(2\pi\hbar)^d} \stackrel{\text{def}}{=} [\text{Op}_h^L(g(\xi) f(x))] u(x)$$

Viewing this as the quantization of $a(x, \xi) = f(x)g(\xi)$, leads to a different quantization, called the *left quantization*, where multiplication precedes differentiation:

Definition 2.3. (*Left quantization*) The *left* (semiclassical) quantization of a symbol $a(x, \xi) \in \mathcal{S}(\mathbb{R}^{2d})$ is defined by

$$[\text{Op}_h^L(a)u](x) \stackrel{\text{def}}{=} \iint e^{i\frac{\xi \cdot (x-y)}{h}} a(y, \xi) u(y) \frac{d\xi dy}{(2\pi\hbar)^d}.$$

Note that the integral is now absolutely convergent, provided $u \in L^\infty(\mathbb{R}^d)$, or even if $u(y)$ grows polynomially when $|y| \rightarrow \infty$.

The right and left quantizations are related to one another by duality.

Lemma 2.4. *For any symbol $a \in \mathcal{S}(\mathbb{R}^{2d})$, and any pair of wavefunctions $u, v \in \mathcal{S}(\mathbb{R}^d)$, we have the symmetry relation*

$$\langle u, \text{Op}_h^R(a)v \rangle_{L^2} = \langle \text{Op}_h^L(\bar{a})u, v \rangle_{L^2}.$$

As a consequence, the formal adjoint of $\text{Op}_h^R(a)$ (viewed as acting on $L^2(\mathbb{R}^d)$) is $\text{Op}_h^L(\bar{a})$.

We will see below that $\text{Op}_h^R(a)$ is bounded on L^2 , so the formal adjoint is the true adjoint.

Proof. Easy exercise by integration by parts.

$$\begin{aligned} \langle u, \text{Op}_h^R(a)v \rangle_{L^2} &= \iiint dx \bar{u}(x) e^{i\frac{\xi \cdot (x-y)}{h}} a(x, \xi) v(y) \frac{d\xi dy}{(2\pi\hbar)^d} \\ &= \iiint dy v(y) \overline{u(x) e^{i\frac{\xi \cdot (y-x)}{h}} \bar{a}(x, \xi)} \frac{d\xi dx}{(2\pi\hbar)^d} \\ &= \langle \text{Op}_h^L(\bar{a})u, v \rangle_{L^2}. \end{aligned}$$

Here we applied the Fubini theorem, using the fact that the integral converges absolutely. $\square$

Claim 2.5. For a generic, real-valued function $a \in \mathcal{S}(\mathbb{R}^{2d})$, the operators $\text{Op}_h^R(a)$ and $\text{Op}_h^L(a)$ act differently on $\mathcal{S}(\mathbb{R}^d)$.

This is the case in particular for symbols of the form $a(x, \xi) = f(x)g(\xi)$, because the operators $\text{Op}_h(f(x))$ and $\text{Op}_h(g(\xi))$ generally do not commute with each other. This is easy to verify when we take for $g(\xi)$ a polynomial of degree ≥ 1 (such a polynomial is not in the Schwartz space, but its action on $\mathcal{S}(\mathbb{R}^d)$ still makes sense).

Example 2.6. For instance, if $g(\xi) = \xi_1$, we get the commutator

$$[hD_{x_1}, f(x)] = \frac{h}{i} \partial_{x_1} f(x), \quad \text{a multiplication operator.}$$

For $g(\xi) = \xi_1 \xi_2$, it gives

$$\begin{aligned} hD_{x_1} hD_{x_2} f(x) &= hD_{x_1} \left(f(x) hD_{x_2} + \frac{h}{i} \partial_{x_2} f(x) \right) \\ &= [hD_{x_1}, f(x)] hD_{x_2} + f(x) hD_{x_1} hD_{x_2} + \frac{h}{i} [hD_{x_1}, \partial_{x_2} f(x)] + \frac{h}{i} \partial_{x_2} f(x) hD_{x_1} \\ \implies [hD_{x_1} hD_{x_2}, f(x)] &= \frac{h}{i} \partial_{x_1} f(x) hD_{x_2} + \frac{h}{i} \partial_{x_2} f(x) hD_{x_1} - h^2 \partial_{x_1 x_2}^2 f(x), \end{aligned}$$

now a first order differential operator, which can be written as the right quantization of the symbol

$$\frac{h}{i} \partial_{x_1} f(x) \xi_2 + \frac{h}{i} \partial_{x_2} f(x) \xi_1 - h^2 \partial_{x_1 x_2}^2 f(x).$$

These examples are differential operators. If $g(\xi)$ is a polynomial of degree n , then $[g(hD_x), f(x)]$ will be a polynomial operator of degree $n - 1$, with the highest degree terms depending on the first derivatives of f .

Remark 2.7. Any Fourier multiplier $\text{Op}_h(g)$ can be expressed as a convolution:

$$[g(hD)u](x) = \mathcal{F}_h^{-1}(g \mathcal{F}_h u) = (\mathcal{F}_h^{-1} g) * u.$$

Hence, the two operators $\text{Op}_h(f) \text{Op}_h(g) = \text{Op}_h^R(fg)$ and $\text{Op}_h(g) \text{Op}_h(f) = \text{Op}_h^L(fg)$ can be expressed by:

$$\begin{aligned} [f(x)g(hD_x)u](x) &= f(x) ((\mathcal{F}_h^{-1} g) * u)(x) = \int f(x) (\mathcal{F}_h^{-1} g)(x - y) u(y) dy, \\ g(hD_x) f(x) u(x) &= (\mathcal{F}_h^{-1} g) * (fu)(x) = \int (\mathcal{F}_h^{-1} g)(x - y) f(y) u(y) dy, \end{aligned}$$

which shows that the Schwartz kernels of the two operators are different if $\mathcal{F}_h^{-1} g$ is a function (hence, if $g \in L^1$), and f is not a constant function. The Right and Left quantizations have interesting support properties, in situations where $a(x, \xi)$ is compactly supported in the x variable.

- (1) Assume $a(x, \xi)$ is supported inside $\{x \in K\} \Subset \mathbb{R}^d$. Then for any $u \in \mathcal{S}$, $\text{Op}_h^R(a)u$ is supported in K .
- (2) Assume $a(x, \xi)$ is supported inside $\{x \in K\} \Subset \mathbb{R}^d$, and $u(x)$ is supported inside $\mathbb{R}^d \setminus K$. Then $\text{Op}_h^L(a)u = 0$.

2.1.3. t - and Weyl quantizations. Quantum mechanics requires that a real valued observable $a(x, \xi)$ should be quantized into a selfadjoint (or at least, symmetric) operator. For a generic

real valued symbol $a(x, \xi)$ (e.g. when $a \in \mathcal{S}$), we've seen that $\text{Op}_h^R(a) \neq \text{Op}_h^L(a) = \text{Op}_h^R(a)^*$, hence this reality property is not satisfied by the Right and Left quantizations. For this reason, quantum mechanics will rather use a more symmetric quantization, called the *Weyl quantization*.

To introduce the Weyl quantization, we notice that the only difference between the Left and Right quantizations is that in the Schwartz kernel of the operators, the symbol a is evaluated at the initial (y), resp. final (x) position. To symmetrize the problem, one may *evaluate the symbol at some convex combination* of the two, namely at a point $tx + (1-t)y$ for some fixed $t \in [0, 1]$. This convention leads to a continuous family of quantizations $\text{Op}_t = \text{Op}_h^t$, indexed by some parameter $t \in [0, 1]$:

$$(2.3) \quad [\text{Op}_h^t(a)u](x) \stackrel{\text{def}}{=} \iint e^{i\frac{\xi \cdot (x-y)}{h}} a(tx + (1-t)y, \xi) u(y) \frac{d\xi dy}{(2\pi\hbar)^d}.$$

In particular we have the identifications $\text{Op}_h^R(a) = \text{Op}_h^1(a)$ and $\text{Op}_h^L(a) = \text{Op}_h^0(a)$.

Remark 2.8. For $a \in \mathcal{S}(\mathbb{R}^{2d})$, the Schwartz kernel of $A = \text{Op}_t(a)$ is the function

$$k_A(x, y) = \int e^{i\frac{\xi \cdot (x-y)}{h}} a(tx + (1-t)y, \xi) \frac{d\xi}{(2\pi\hbar)^d},$$

that is a sort of partial Fourier transform of a . This function is in $\mathcal{S}(\mathbb{R}_x^d \times \mathbb{R}_y^d)$.

Lemma 2.4 easily generalizes to the

Lemma 2.9. *For any symbol $a \in \mathcal{S}(\mathbb{R}^{2d})$ and any $t \in [0, 1]$, we have the formal adjoint relation*

$$(2.4) \quad \text{Op}_h^t(a)^* = \text{Op}_h^{1-t}(\bar{a}).$$

Proof. Same integration by parts for Lemma 2.4. □

The Weyl quantization consists in taking the midpoint $t = 1/2$, that is $\text{Op}_h^W(a) \stackrel{\text{def}}{=} \text{Op}_h^{1/2}(a)$, so that the same quantization appears in the two sides of (2.4).

Definition 2.10. (*Weyl quantization*) Take a symbol $a(x, \xi) \in \mathcal{S}(\mathbb{R}^{2d})$. Then its Weyl quantization is defined by

$$(2.5) \quad [\text{Op}_h^W(a)u](x) \stackrel{\text{def}}{=} \iint e^{i\frac{\xi \cdot (x-y)}{h}} a\left(\frac{x+y}{2}, \xi\right) u(y) \frac{d\xi dy}{(2\pi\hbar)^d}.$$

This expression does not seem very natural at first glance, but it leads to several nice properties. From Lemma 2.9 we straightforwardly derive the following crucial property of the Weyl quantization.

Proposition 2.11. *For any real-valued symbol $a(x, \xi) \in \mathcal{S}(\mathbb{R}^{2d})$, the operator $\text{Op}_h^W(a)$ is symmetric w.r.t. the $L^2(\mathbb{R}^d)$ scalar product.*

We will see below that for such symbols the operator $\text{Op}_h^W(a)$ is bounded on $L^2(\mathbb{R}^d)$, so that it is actually selfadjoint on $L^2(\mathbb{R}^d)$.

2.2. An alternative route to the Weyl quantization: using Weyl-Heisenberg operators. We will recover the Weyl quantization from a different strategy, namely by using the *phase space translation operators*, also called Weyl-Heisenberg operators. These operators form a family of unitary operators on $L^2(\mathbb{R}^d)$, indexed by phase space vectors $V_0 = (x_0, \xi_0) \in \mathbb{R}^{2d}$. They depend on Planck's parameter $\hbar$, but this dependence will be omitted in the formulas: we will call $T_{(x_0, \xi_0)} = T_{V_0}$ the operator performing the translation by the vector $V_0 = (x_0, \xi_0)$.

These operators form a unitary representation of the Heisenberg group. We will not dwell too much into these algebraic considerations, but have a more pedestrian approach.

2.2.1. The (Weyl-Heisenberg) phase space translation operators. To define these operators, we start by purely spatial translations, namely the subclass of operators $T_{(x_0, 0)}$. Translating a state $u \in L^2$ by the space vector x_0 is the obvious operation:

$$(2.6) \quad [T_{(x_0, 0)}u](x) \stackrel{\text{def}}{=} u(x - x_0).$$

Similarly, since momentum and position are exchanged by $\mathcal{F}_h$, we define as follows the pure momentum translations:

$$(2.7) \quad \begin{aligned} \mathcal{F}_h(T_{(0, \xi_0)}u)(\xi) &= \mathcal{F}_h u(\xi - \xi_0) \\ \implies [T_{(0, \xi_0)}u](x) &= e^{i\frac{\xi_0 \cdot x}{\hbar}} u(x). \end{aligned}$$

Hence, $T_{(0, \xi_0)}$ is simply the multiplication operator by the linear phase function corresponding to a plane wave of wavevector $\xi_0/\hbar$, or momentum ξ_0 . Notice that this operator explicitly depends on $\hbar$.

On the phase space $\mathbb{R}^d \times \mathbb{R}^d$, translating by the phase space vector $V_0 = (x_0, \xi_0)$ is simply the combination of the translation by x_0 and by ξ_0 , these translations forming the Galilean group. It thus sounds reasonable to take for $T_{(x_0, \xi_0)}$ the product of the two preceding operators. However, the operators $T_{(x_0, 0)}$ and $T_{(0, \xi_0)}$ do not commute, so one should (again) decide of a “best” ordering to define $T_{(x_0, \xi_0)}$.

Let us look at the commutation properties:

$$\begin{aligned} [T_{(x_0,0)} T_{(0,\xi_0)} u](x) &= e^{i \frac{\xi_0 \cdot (x-x_0)}{\hbar}} u(x-x_0), \quad \text{while} \\ [T_{(0,\xi_0)} T_{(x_0,0)}] u(x) &= e^{i \frac{\xi_0 \cdot x}{\hbar}} u(x-x_0), \end{aligned}$$

hence

$$(2.8) \quad \boxed{T_{(0,\xi_0)} T_{(x_0,0)} = e^{i \frac{\xi_0 \cdot x_0}{\hbar}} T_{(x_0,0)} T_{(0,\xi_0)}}$$

Definition 2.12. We will show below that it is “natural” to define the joint translation $T_{(x_0,\xi_0)}$ by selecting the “median” between the two phases, namely take:

$$(2.9) \quad T_{(x_0,\xi_0)} \stackrel{\text{def}}{=} e^{i \frac{\xi_0 \cdot x_0}{2\hbar}} T_{(x_0,0)} T_{(0,\xi_0)} = e^{-i \frac{\xi_0 \cdot x_0}{2\hbar}} T_{(0,\xi_0)} T_{(x_0,0)}.$$

This definition will be justified by the following expressions of the translation operators.

Lemma 2.13. *The multiplication operator $T_{(0,\xi_0)}$ can be obtained by solving the Schrödinger equation with Hamiltonian $\text{Op}_\hbar(-\xi_0 \cdot x)$, at time $t = 1$. Formally, we may write*

$$T_{(0,\xi_0)} = \exp \left(\frac{i}{\hbar} \text{Op}_\hbar(\xi_0 \cdot x) \right) = \exp \left(-\frac{i}{\hbar} \text{Op}_\hbar(-\xi_0 \cdot x) \right).$$

Similarly, the space translation operator $T_{(x_0,0)}$ can be obtained as the time-1 propagator generated by the quantum Hamiltonian $\text{Op}_\hbar(x_0 \cdot \xi) = x_0 \cdot \hbar D$:

$$T_{(x_0,0)} = \exp \left(-\frac{i}{\hbar} \text{Op}_\hbar(x_0 \cdot \xi) \right) = \exp(-x_0 \cdot \partial_x).$$

Proof. These facts are easily proved, since we are dealing with multiplication operators in position or Fourier space. $\square$

Remark 2.14. The classical Hamiltonian $p(x, \xi) = -\xi_0 \cdot x$ generates the flow $(x(t), \xi(t)) = (x(0), \xi(0) + t\xi_0)$, which at time 1 realizes a translation by $(0, \xi_0)$. In turn, the flow generated by $p(x, \xi) = x_0 \cdot \xi$ gives $(x(t), \xi(t)) = (x(0) + tx_0, \xi(0))$, which at time 1 gives the translation by $(x_0, 0)$.

Now, since the classical translation (x_0, ξ_0) is obtained by the time-1 flow generated by the Hamiltonian $p(x, \xi) = x_0 \cdot \xi - \xi_0 \cdot x$, it sounds natural to define the corresponding quantum translation as the propagator generated by the quantum Hamiltonian $P_\hbar = \text{Op}_\hbar(x_0 \cdot \xi - \xi_0 \cdot x)$:

$$T_{(x_0,\xi_0)} \stackrel{\text{def}}{=} \exp \left(-\frac{i}{\hbar} \text{Op}_\hbar(x_0 \cdot \xi - \xi_0 \cdot x) \right) = \exp \left(-\frac{i}{\hbar} (x_0 \cdot \hbar D_x - \xi_0 \cdot x) \right).$$

Lemma 2.15. *This definition of $T_{(x_0,\xi_0)}$ exactly coincides with the “half phase” Ansatz (2.9).*

Proof. Check, by an explicit computation, that the Schrödinger equation

$$i\hbar\partial_t u(t, x) = (x_0 \cdot hD_x - \xi_0 \cdot x)u(t, x), \quad u(0) = u_0,$$

is solved by $u(t, x) = e^{-it^2 \frac{\xi_0 \cdot x_0}{2\hbar}} e^{it \frac{\xi_0 \cdot x}{\hbar}} u_0(x - tx_0) = e^{it \frac{\xi_0 \cdot (x - tx_0/2)}{\hbar}} u_0(x - tx_0)$. In particular, we see that $u(1) = T_{(x_0, \xi_0)} u_0$. $\square$

Proposition 2.16. (*Algebra relations*) *The family of Weyl-Heisenberg operators satisfies the following composition rules:*

$$(2.10) \quad T_{(x_0, \xi_0)} T_{(x_1, \xi_1)} = e^{i \frac{\xi_0 \cdot x_1 - x_0 \cdot \xi_1}{2\hbar}} T_{(x_0 + x_1, \xi_0 + \xi_1)}.$$

It will be useful to express the extra phase in terms of the symplectic form:

$$\xi_0 \cdot x_1 - x_0 \cdot \xi_1 = \omega(V_0, V_1), \quad \text{where } V_i = (x_i, \xi_i) \quad \text{are the phase space vectors.}$$

So the above composition rule reads

$$(2.11) \quad T_{V_0} T_{V_1} = e^{i \frac{\omega(V_0, V_1)}{2\hbar}} T_{V_0 + V_1}.$$

Proof. A simple computation, using the formulas (2.8). $\square$

Remark 2.17. The commutation rule (2.8) can be viewed as the “exponentiated version” of the commutation formula

$$(2.12) \quad [\text{Op}(x_i), \text{Op}_\hbar(\xi_j)] = i\hbar\delta_{ij}.$$

Both types are called the *Heisenberg commutation relations*. They show that the operators $T_{(x_0, \xi_0)}$ form a unitary projective representation of the Galilean group, called the Heisenberg group.

Claim 2.18. The operators $\{e^{is/\hbar} T_{(x_0, \xi_0)}\}$ represent the *Heisenberg group*, a noncommutative extension of the Galilean group, which includes an extra dimension to take into account the phase:

$$(2.13) \quad (x_0, \xi_0, s_0) \cdot (x_1, \xi_1, s_1) = \left(x_0 + x_1, \xi_0 + \xi_1, s_0 + s_1 + \frac{1}{2} (\xi_0 \cdot x_1 - x_0 \cdot \xi_1) \right).$$

or in a more compact form:

$$(V_0, s_0) \cdot (V_1, s_1) = \left(V_0 + V_1, s_0 + s_1 + \frac{1}{2} \omega(V_0, V_1) \right).$$

2.2.2. Microscopic translations = quantized “phase space Fourier modes”. If we rescale the translation vectors V_0 by $\hbar$, we get the operator

$$T_{\hbar V_0} = T_{(\hbar x_0, \hbar \xi_0)} = \exp(-i \text{Op}_\hbar(x_0 \cdot \xi - \xi_0 \cdot x)) = \exp(i(\xi_0 \cdot x - x_0 \cdot \hbar D_x)).$$

The right hand side suggests to consider the linear exponential function (phase space Fourier mode)

$$(2.14) \quad e_{V_0}(x, \xi) \stackrel{\text{def}}{=} \exp(i(\xi_0 \cdot x - x_0 \cdot \xi)), \quad V_0 = (x_0, \xi_0) \in \mathbb{R}^{2d}.$$

Since this function can be written as the product $e_{(0, \xi_0)}(x)e_{(x_0, 0)}(\xi)$, one easily obtains its Right (resp. Left) quantizations:

$$\text{Op}_h^R(e_{V_0}) = T_{h(0, \xi_0)} T_{h(x_0, 0)}, \quad \text{resp.} \quad \text{Op}_h^L(e_{V_0}) = T_{h(x_0, 0)} T_{h(0, \xi_0)}.$$

Lemma 2.19. *The Weyl quantization of $e_{V_0}(x, \xi)$ is given by the translation operator T_{hV_0} . More generally, for any $t \in [0, 1]$ one has*

$$(2.15) \quad \text{Op}_h^t(e_{V_0}) = e^{ih(t-1/2)\xi_0 \cdot x_0} T_{hV_0}.$$

Proof. We compute the Weyl quantization of e_{V_0} , using the formula (2.3):

$$\begin{aligned} \text{Op}_t(e_{V_0})u(x) &= \iint e^{i\frac{\xi \cdot (x-y)}{h}} e^{i(\xi_0 \cdot (tx + (1-t)y) - x_0 \cdot \xi)} u(y) \frac{d\xi dy}{(2\pi\hbar)^d} \\ &= e^{it\xi_0 \cdot x} \iint e^{i\frac{\xi \cdot (x - \hbar x_0)}{h}} e^{-i\frac{y \cdot (\xi - \hbar(1-t)\xi_0)}{h}} u(y) \frac{d\xi dy}{(2\pi\hbar)^d} \\ &= e^{it\xi_0 \cdot x} \int e^{i\frac{\xi \cdot (x - \hbar x_0)}{h}} [\mathcal{F}_h u](\xi - \hbar(1-t)\xi_0) \frac{d\xi}{(2\pi\hbar)^{d/2}} \\ &= e^{it\xi_0 \cdot x} \int e^{i\frac{(\xi' + \hbar(1-t)\xi_0) \cdot (x - \hbar x_0)}{h}} [\mathcal{F}_h u](\xi') \frac{d\xi'}{(2\pi\hbar)^{d/2}} \\ &= e^{-i\hbar(1-t)\xi_0 \cdot x_0} e^{i\xi_0 \cdot x} u(x - \hbar x_0). \end{aligned}$$

□

Remark. The remarkable property $\text{Op}_h^W(e^{i(\xi_0 \cdot x - x_0 \cdot \xi)}) = e^{i\text{Op}_h^W(i(\xi_0 \cdot x - x_0 \cdot \xi))}$, namely the fact that the Weyl quantization commutes with the exponential, is specific to the linear symbol $\xi_0 \cdot x - x_0 \cdot \xi$; it fails for more general functions.

Since the symbol $a \in \mathcal{S}(\mathbb{R}^{2d})$ can be Fourier decomposed into the (nonsemiclassical) Fourier modes $e_{V_0}(x, \xi)$, we can define its Weyl quantization by linearity in terms of the translation operators. Let us denote as follows the Fourier decomposition of $a \in \mathcal{S}(\mathbb{R}^{2d})$:

$$(2.16) \quad \forall \rho = (x, \xi), \quad a(\rho) = \int \exp(i(\xi_0 \cdot x - x_0 \cdot \xi)) \hat{a}(x_0, \xi_0) \frac{dx_0 d\xi_0}{(2\pi)^d} = \int \exp(i\omega(V_0, \rho)) \hat{a}(V_0) \frac{dV_0}{(2\pi)^d}$$

Remark 2.20. Compared with the standard definition of the Fourier transform, there is a sign change: $-x_0$ is the Fourier parameter conjugate to ξ , while ξ_0 is the Fourier parameter conjugate to x .

With this convention, we gather the following property

Proposition 2.21. *The Weyl quantization of $a \in \mathcal{S}(\mathbb{R}^{2d})$ can be expressed in terms of the (microscopic) translation operators as follows:*

$$(2.17) \quad \text{Op}_h^W(a) = \int T_{h(x_0, \xi_0)} \hat{a}(x_0, \xi_0) \frac{dx_0 d\xi_0}{(2\pi)^d} = \int_{\mathbb{R}^{2d}} T_{hV_0} \hat{a}(V_0) \frac{dV_0}{(2\pi)^d}.$$

This formula looks a bit less “arbitrary” than the original formula (2.5), since it originates from the group of phase space translation operators.

Remark 2.22. This more algebraic definition provides the Weyl quantization specific intertwining properties with respect to the Heisenberg group, but also with respect to the *metaplectic group*, obtained by exponentiating the operators of the form in $\text{Op}_h(Q(x, \xi))$, with $Q(x, \xi)$ a real-valued quadratic form.

2.2.3. *Relations between various quantizations.* Starting from the expression

$$A \stackrel{\text{def}}{=} \text{Op}_h^W(a) = \int \text{Op}_h^W(e_{V_0}) \hat{a}(V_0) \frac{dV_0}{(2\pi)^d},$$

and using (2.15), for $t \in [0, 1]$ we may compute the symbol a_t such that the operator $A = \text{Op}_t(a_t)$. Namely, we want to establish the connection between the t -symbol of an operator A and its Weyl ($t = 1/2$)-symbol. Take $a \in \mathcal{S}(\mathbb{R}^{2d})$. Using the expression (2.15) we obtain

$$(2.18) \quad A = \text{Op}_t(a_t) = \int \text{Op}_h^W(e_{V_0}) e^{-ih(1/2-t)\xi_0 \cdot x_0} \hat{a}_t(V_0) \frac{dV_0}{(2\pi)^d}.$$

Since the Fourier decomposition is unique, this expression shows that the Fourier transforms of a and a_t are related as follows:

$$\hat{a}(V_0) = e^{ih(t-1/2)\xi_0 \cdot x_0} \hat{a}_t(V_0).$$

More generally, the symbols a_t and a_s satisfy

$$(2.19) \quad \hat{a}_t(V_0) = e^{ih(s-t)\xi_0 \cdot x_0} \hat{a}_s(V_0).$$

This expression shows that if $a_s \in \mathcal{S}$, then so does a_t . We also notice that, even if $a_{1/2}$ is defined independently of $\hbar$, the symbols a_s will explicitly depend on $\hbar$. We now express this relation directly between a_s and a_t .

Proposition 2.23. *Assume $A = \text{Op}_t(a_t)$ for $t \in [0, 1]$, with $a_{1/2} \in \mathcal{S}(\mathbb{R}^{2d})$. We get the following expression between the symbols a_t and a_s :*

$$(2.20) \quad a_t(x, \xi) = e^{ih(s-t)\partial_x \cdot \partial_\xi} a_s(x, \xi) = e^{ih(t-s)D_x \cdot D_\xi} a_s(x, \xi).$$

Here the operator $e^{ih(t-s)D_x \cdot D_\xi}$ is defined as a Fourier multiplier on $\mathbb{R}^{2d}$, see (2.20).

Proof. In the integral equation (2.16) for $a_t(x, \xi)$, we express the extra factor $e^{i\hbar(s-t)\xi_0 \cdot x_0}$ through a derivative of the integrand:

$$\begin{aligned}
 (2.21) \quad a_t(x, \xi) &\stackrel{\text{def}}{=} \int e^{i(\xi_0 \cdot x - x_0 \cdot \xi)} \hat{a}_t(x_0, \xi_0) \frac{dx_0 d\xi_0}{(2\pi)^d} \\
 &= \int e^{i\hbar(s-t)\xi_0 \cdot x_0} e^{i(\xi_0 \cdot x - x_0 \cdot \xi)} \hat{a}_s(x_0, \xi_0) \frac{dx_0 d\xi_0}{(2\pi)^d} \\
 &= \int e^{i\hbar(s-t)\partial_x \cdot \partial_\xi} e^{i(\xi_0 \cdot x - x_0 \cdot \xi)} \hat{a}_s(x_0, \xi_0) \frac{dx_0 d\xi_0}{(2\pi)^d} \\
 &= [e^{i\hbar(s-t)\partial_x \cdot \partial_\xi} a_s](x, \xi).
 \end{aligned}$$

□

These exponentiated quadratic differentials will pop up regularly in the next sections. These computations should appear as a preparation for the computations on the composition of Ψ DOs.

2.3. Asymptotic expansions of symbols. In this section we study the behaviour of expressions like (2.20, 2.21) in the limit $\hbar \searrow 0$, to obtain asymptotic expansions in powers of $\hbar$.

What meaning should one give to an expression like (2.20), apart from its Fourier transform version? To avoid too cumbersome notations, we will take $t = 1$, $s = 0$. A naive expansion gives:

$$(2.22) \quad a_1(x, \xi) = [e^{i\hbar D_x \cdot D_\xi} a_0](x, \xi) = \sum_{j \geq 0} \frac{(i\hbar D_y \cdot D_\eta)^j}{j!} a_0(y, \eta)|_{y=x, \eta=\xi},$$

which looks nice in the semiclassical regime, since terms are formally $\mathcal{O}(\hbar^k)$. The trouble is that this series is generally divergent for all values of $\hbar$, since we have no a priori control on the growth of higher derivatives. For instance, the higher derivatives could grow much faster than $j!$ ⁸. Still, this formal series contains nontrivial information, **as an asymptotic expansion**.

2.3.1. Definition of asymptotic expansions.

Definition 2.24. (*Asymptotic expansion*) Let $(a(\hbar))_{\hbar \in (0,1]}$ be a family of elements in some Banach space $\mathcal{B}$, and let $(a_j)_{j \in \mathbb{N}}$ be elements of the same Banach space. We say that the

⁸To get such a control on high derivatives one needs some analyticity condition on a , or at least Gevrey type regularity.

family $(a(\hbar))$ satisfies the asymptotic expansion

$$(2.23) \quad a(\hbar) \sim \sum_{j \geq 0} \hbar^j a_j \quad \text{as } \hbar \searrow 0,$$

if for any $N \geq 0$, there exists $C_N > 0$ such that we have

$$\left\| a(\hbar) - \sum_{j=0}^{N-1} \hbar^j a_j \right\|_{\mathcal{B}} \leq C_N \hbar^N, \quad \forall \hbar \in (0, 1].$$

A similar definition holds for $a(\hbar), a_j$ elements of a Fréchet space $\mathcal{F}$ generated by a countable family of seminorms $(\|\bullet\|_\alpha)$. Then for any $N \geq 0$ and for any α , there exists $C_{\alpha, N} > 0$ such that the corresponding inequality holds for the α -seminorm. We will write

$$a(\hbar) = \sum_{j=0}^{N-1} \hbar^j a_j + \mathcal{O}(\hbar^N)_{\mathcal{B}}, \quad \text{respectively} \quad a(\hbar) = \sum_{j=0}^{N-1} \hbar^j a_j + \mathcal{O}(\hbar^N)_{\mathcal{F}}$$

when we wish to emphasize the topology in which the expansion holds.

The proposition below shows that one can always construct a family $a(\hbar)_{\hbar \in (0, 1]}$ from the knowledge of the elements $(a_j)_{j \in \mathbb{N}}$.

Proposition 2.25. (*Borel's summation Lemma*) *Given any sequence $(a_j \in \mathcal{F})_{j \in \mathbb{N}}$, there exists a function $a : \hbar \in (0, 1] \rightarrow a(\hbar) \in \mathcal{F}$ satisfying the asymptotic expansion (2.23).*

The function $a(\hbar)$ is not unique, however two such functions $a(\hbar), \tilde{a}(\hbar)$ satisfy $a(\hbar) = \tilde{a}(\hbar) + \mathcal{O}(\hbar^\infty)_{\mathcal{F}}$.

Here and below, the notation $\mathcal{O}(\hbar^\infty)$ means $\mathcal{O}(\hbar^N)$ for any $N \geq 0$ (with implicit constants depending on N).

Proof. Let us first treat the case of a Banach space $\mathcal{B}$, with norm $\|\bullet\|$. Choose a cutoff function $\chi \in C_c^\infty[0, \infty)$ with $\chi(t) = 1$ on $[0, 1]$ and $\chi(t) = 0$ for $t \geq 2$. We will select below a sequence $\lambda_j \rightarrow \infty$, and consider the function

$$(2.24) \quad a(\hbar) \stackrel{\text{def}}{=} \sum_{j=0}^{\infty} \hbar^j \chi(\lambda_j \hbar) a_j.$$

Since $\lambda_j \rightarrow \infty$, for any $\hbar \in (0, 1]$ the above series contains finitely many nonzero terms, so that $a(\hbar)$ is well-defined. We want some control on the decay of the terms. The idea is to let λ_j grow sufficiently fast, such that the terms $\hbar^j \chi(\lambda_j \hbar) \|a_j\|$ decay uniformly when $\hbar \rightarrow 0$.

We just notice that

$$\begin{aligned}\hbar^j \chi(\lambda_j \hbar) \|a_j\| &= \hbar^j \chi(\lambda_j \hbar) \frac{\lambda_j \hbar}{\lambda_j \hbar} \|a_j\| \\ &\leq \hbar^{j-1} \frac{2}{\lambda_j} \|a_j\|.\end{aligned}$$

If we assume iteratively

$$\lambda_j > \max(2^{j+1} \|a_j\|, \lambda_{j-1} + 1),$$

we obtain the uniform bound

$$\hbar^j \chi(\lambda_j \hbar) \|a_j\| \leq \hbar^{j-1} / 2^j, \quad \forall j \geq 0, \quad \forall \hbar \in (0, 1].$$

For each given $n > 0$ we want to control

$$(2.25) \quad \left\| a(\hbar) - \sum_{j=0}^n \hbar^j a_j \right\| \leq \sum_{j=0}^{\infty} \hbar^j (\chi(\lambda_j \hbar) - 1_{j \leq n}) \|a_j\|,$$

On the one hand, for $\hbar \geq \lambda_n^{-1}$ we may always find a constant C_n such that

$$\forall h \in [\lambda_n^{-1}, 1], \quad \left\| a(h) - \sum_{j=0}^n h^j a_j \right\| \leq C_n \lambda_n^{-1} \leq C_n h^{n+1},$$

since the LHS is bounded uniformly when $h \leq 1$. On the other hand, for $\hbar < \lambda_n^{-1}$ the sequence in the RHS of (2.24) will start at the order $j = n + 1$, and is equal to

$$\sum_{j=n+1}^{\infty} \hbar^j \chi(\lambda_j \hbar) \|a_j\| \leq \hbar^{n+1} \|a_{n+1}\| + \sum_{j=n+2}^{\infty} \hbar^{j-1} / 2^j \leq \hbar^{n+1} (\|a_{n+1}\| + 1).$$

Putting together these two estimate, we find that for any $h \in (0, 1]$, $\left\| a(h) - \sum_{j=0}^n h^j a_j \right\| \leq \tilde{C}_n h^{n+1}$.

Let us now treat the case of a Fréchet space $\mathcal{F}$, the topology of which is defined by the countable set of seminorms $(\|\bullet\|_{\alpha})_{\alpha \in \mathbb{N}}$. To select the λ_j we proceed by a diagonal argument. Namely, we choose λ_j such as to ensure that the property

$$\hbar^j \chi(\lambda_j \hbar) \|a_j\|_{\alpha} \leq \hbar^{j-1} / 2^j \quad \text{holds for all seminorms with } \alpha \leq j.$$

This can be achieved by taking

$$\lambda_j > \max \left(2^{j+1} \max_{\alpha \leq j} \|a_j\|_{\alpha}, \lambda_{j-1} + 1 \right).$$

Now, given a seminorm α and an index n , let us first assume that the norm index $\alpha \leq n$. Then, in the case $\hbar < \lambda_n^{-1}$ we have

$$(2.26) \quad \left\| a(\hbar) - \sum_{j=0}^n \hbar^j a_j \right\|_{\alpha} \leq \sum_{j=0}^{\infty} \hbar^j (\chi(\lambda_j \hbar) - 1_{j \leq n}) \|a_j\|_{\alpha}$$

$$(2.27) \quad \leq \sum_{j=n+1}^{\infty} \hbar^j \chi(\lambda_j \hbar) \|a_j\|_{\alpha}$$

$$(2.28) \quad \leq \hbar^{n+1} (\|a_{n+1}\|_{\alpha} + 1).$$

As before, the case of $\hbar > \lambda_n^{-1}$ is easy, one just needs to take a large enough constant $C_{\alpha,n} \geq (\|a_{n+1}\|_{\alpha} + 1)$.

Let us finally treat the higher norm indices $\alpha > n$. For this we decompose

$$a(\hbar) - \sum_{j=0}^n \hbar^j a_j = a(\hbar) - \sum_{j=0}^{\alpha} \hbar^j a_j + \sum_{j=n+1}^{\alpha} \hbar^j a_j.$$

Using the bound for the case $n = \alpha$, this leads to

$$\left\| a(\hbar) - \sum_{j=0}^n \hbar^j a_j \right\|_{\alpha} \leq C_{\alpha,\alpha} \hbar^{\alpha+1} + \sum_{j=n+1}^{\alpha} \hbar^j \|a_j\|_{\alpha} \leq \max \left(C_{\alpha,\alpha}, \sum_{j=n+1}^{\alpha} \|a_j\|_{\alpha} \right) \hbar^{n+1} \stackrel{\text{def}}{=} C_{\alpha,n} \hbar^{n+1}.$$

□

2.3.2. A first example of asymptotic expansion for a symbol. Let us now come back to the expression (2.20) giving the t -symbol of an operator, in terms of its s -symbol, and let us focus on the case $s = 0, t = 1$. We want to show that this expression satisfies an asymptotic expansion similar to (2.22) in the topology of the Fréchet space $\mathcal{S}(\mathbb{R}^{2d})$, in the limit $h \searrow 0$.

For this aim, we use a **Taylor expansion with integral remainder** valid for any smooth function $f \in C^{\infty}((-1, 1))$:

$$(2.29) \quad \forall h \in (-1, 1), \quad f(h) = \sum_{j=0}^{N-1} h^j \frac{f^{(j)}(0)}{j!} + \frac{h^N}{(N-1)!} \int_0^1 (1-u)^{N-1} f^{(N)}(uh) du.$$

The Fourier transform of the function $a_1 = e^{ihD_y \cdot D_{\eta}} a_0$ is given by

$$\hat{a}_1(x_0, \xi_0) = e^{-ih\xi_0 \cdot x_0} \hat{a}_0(x_0, \xi_0), \quad (x_0, \xi_0) \in \mathbb{R}^{2d}.$$

If we apply the above Taylor expansion to the exponential $\hbar \mapsto e^{-ih\xi_0 \cdot x_0}$, viewing (x_0, ξ_0) as parameters, we obtain

$$(2.30) \quad e^{-ih\xi_0 \cdot x_0} = \sum_{j=0}^{N-1} \frac{1}{j!} (-ih\xi_0 \cdot x_0)^j + \frac{(ih)^N}{(N-1)!} \int_0^1 (1-u)^{N-1} (-\xi_0 \cdot x_0)^N e^{-iuh\xi_0 \cdot x_0} du$$

Multiplying both sides by $\hat{a}_0(x_0, \xi_0)$, and remembering that $\hat{a}_0 \in \mathcal{S}(\mathbb{R}^{2d})$, the integrand on the RHS,

$$I(x_0, \xi_0; u, \hbar) \stackrel{\text{def}}{=} (1-u)^{N-1} (-\xi_0 \cdot x_0)^N e^{-iuh\xi_0 \cdot x_0} \hat{a}_0(x_0, \xi_0).$$

remains in a bounded set of $\mathcal{S}(\mathbb{R}_{x_0, \xi_0}^{2d})$, uniformly in $\hbar \in (0, 1]$ and $u \in [0, 1]$ (this means that any $\mathcal{S}$ seminorm $\|I(\bullet, u, \hbar)\|_\alpha$ is bounded uniformly in $u, \hbar$). Taking the inverse FT of (2.30), we get the expression

(2.31)

$$\begin{aligned} e^{i\hbar D_y \cdot D_\eta} a_0 &= \sum_{j=0}^{N-1} \frac{1}{j!} (i\hbar D_y \cdot D_\eta)^j a_0 + \frac{(i\hbar)^N}{(N-1)!} \int_0^1 (1-u)^{N-1} (D_y \cdot D_\eta)^N e^{iuh D_y \cdot D_\eta} a_0 du \\ (2.32) \quad &= \sum_{j=0}^{N-1} \frac{1}{j!} (i\hbar D_y \cdot D_\eta)^j a_0 + \frac{(i\hbar)^N}{(N-1)!} \int_0^1 \mathcal{F}^{-1} I(\bullet, u, \hbar) du \end{aligned}$$

Since the Fourier transform is continuous $\mathcal{S} \rightarrow \mathcal{S}$, the function $\mathcal{F}^{-1} I(\bullet, u, \hbar)$ is also bounded in $\mathcal{S}(\mathbb{R}^{2d})$, uniformly in $\hbar, u$. So, when integrating over $u \in [0, 1]$ we obtain a function bounded in $\mathcal{S}(\mathbb{R}^{2d})$, uniformly in $\hbar$: this shows that the last term in (2.31) is of order $\mathcal{O}(\hbar^N)_{\mathcal{S}}$.

We have therefore proved that for any $N \geq 1$,

$$a_1(\hbar) = e^{i\hbar D_y \cdot D_\eta} a_0 = \sum_{j=0}^{N-1} \hbar^j \frac{1}{j!} (i D_y \cdot D_\eta)^j a_0 + \mathcal{O}(\hbar^N)_{\mathcal{S}},$$

showing that once we have fixed the symbol $a_0 \in \mathcal{S}$, the corresponding symbol a_1 satisfies the asymptotic expansion

$$a_1(\hbar) \sim \sum_{j=0}^{N-1} \hbar^j \frac{1}{j!} (i D_y \cdot D_\eta)^j a_0 \quad \text{in } \mathcal{S}(\mathbb{R}^{2d}).$$

The proof works exactly the same for an arbitrary pair (t, s) , and leads to the following rigorous version of the formal series (2.22):

Proposition 2.26. *Consider any pair of indices $(t, s) \in [0, 1]^2$. Choose a function $a_s \in \mathcal{S}(\mathbb{R}^{2d})$. Then the corresponding symbol $a_t(\hbar)$ such that $\text{Op}_\hbar^t(a_t) = \text{Op}_\hbar^s(a_s)$ depends explicitly on $\hbar$, and satisfies the asymptotic expansion:*

(2.33)

$$a_t(\hbar) = e^{i\hbar(t-s)D_x \cdot D_\xi} a_s \sim \sum_{j \geq 0} \hbar^j \frac{(i(t-s))^j}{j!} (D_y \cdot D_\eta)^j a_s \quad \text{in } \mathcal{S}(\mathbb{R}^{2d}), \quad \text{when } \hbar \searrow 0.$$

Remark 2.27. The above proof of the asymptotic expansion combines several ingredients: an exponentiated differential operator, the Fourier transform, and the **Taylor expansion with integral remainder**.

2.3.3. Another route towards asymptotic expansions: (quadratic) stationary phase expansions. We now give an alternative representation of a_t as a function of a_s , which will provide an example of stationary phase expansion. Starting from (2.21), by expressing $\hat{a}_s(V_0)$ in terms of $a_s(y, \eta)$, we get the following integral over $\mathbb{R}^{4d}$:

$$(2.34) \quad a_t(x, \xi; \hbar) = \iint e^{i\hbar(s-t)\xi_0 \cdot x_0} e^{i(\xi_0 \cdot (x-y) - x_0 \cdot (\xi - \eta))} a_s(y, \eta) \frac{dx_0 d\xi_0 dy d\eta}{(2\pi)^{2d}}.$$

The vector $V_0 = (x_0, \xi_0)$ appears in a quadratic expression in the phase. Notice that the integral over V_0 does not converge absolutely, but is an oscillatory integral. However, we may integrate over V_0 , using the following

Lemma 2.28. *Let Q be a nonsingular, symmetric $n \times n$ real valued matrix. Then, the function $x \mapsto e^{\frac{i}{2}\langle x, Qx \rangle}$, which can be viewed as a distribution in $\mathcal{S}'(\mathbb{R}^n)$ admits the following Fourier transform:*

$$(2.35) \quad \mathcal{F}_1 \left(e^{\frac{i}{2}\langle x, Qx \rangle} \right) (\xi) = \frac{e^{i\pi \operatorname{sgn}(Q)/4}}{|\det Q|^{1/2}} e^{-\frac{i}{2}\langle \xi, Q^{-1}\xi \rangle}.$$

Here $\operatorname{sgn}(Q)$ denotes the signature of Q , that is the difference between the numbers of positive and negative eigenvalues of this matrix.

Proof. We first recall the case of the Fourier transform of a real Gaussian: for G a definite positive $n \times n$ matrix, we have

$$\int e^{-\frac{1}{2}\langle x, Gx \rangle} e^{-ix \cdot \xi} \frac{dx}{(2\pi)^{n/2}} = \frac{e^{-\frac{1}{2}\langle \xi, G^{-1}\xi \rangle}}{(\det G)^{1/2}}.$$

Notice that the LHS is an oscillatory integral. We can give a meaning to it by deforming G so that it acquires an imaginary part, still keeping a positive definite real part: the integral is now absolutely convergent, and the Gaussian integration produces the same expression as above, where the square root of $\det G$ is obtained by analytic continuation from its original positive value. When $G = -iQ + \epsilon I$ and $\epsilon \searrow 0$, the expansion of this determinant over the eigenvalues of Q gives $(\det(\epsilon - iQ))^{1/2} = \prod_j (\epsilon - i\lambda_j)^{1/2}$. If $\lambda_j > 0$ this converges to $e^{-i\pi/4} |\lambda_j|^{1/2}$, while for $\lambda_j < 0$ this goes to $e^{+i\pi/4} |\lambda_j|^{1/2}$. Putting back the phases in the numerator, we get (2.35). $\square$

Let us now apply this Lemma to compute the integral in (2.34). The quadratic form in (x_0, ξ_0) is given by the matrix $Q = \hbar(s - t) \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}$, which has signature 0, determinant $|\det Q| = |\hbar(s - t)|^{2d}$, and inverse $Q^{-1} = (\hbar(s - t))^{-1} \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}$. The integral over $dV_0/(2\pi)^d$ thus produces the integral

$$(2.36) \quad a_t(x, \xi; \hbar) = \frac{1}{|s - t|^d} \int \frac{dy d\eta}{(2\pi\hbar)^d} e^{i \frac{(\eta - \xi) \cdot (y - x)}{2\hbar(s - t)}} a_s(y, \eta) = \frac{1}{|s - t|^d} \int \frac{dy d\eta}{(2\pi\hbar)^d} e^{i \frac{\eta \cdot y}{2\hbar(s - t)}} a_s(x + y, \xi + \eta),$$

where in the last equality we just shifted the integration variables. Since $a_0 \in \mathcal{S}$, this integral over (y, η) converges absolutely. In the particular case $t = 1, s = 0$, it gives

$$(2.37) \quad a_1(x, \xi; \hbar) = \int \frac{dy d\eta}{(2\pi\hbar)^d} e^{-i \frac{\eta \cdot y}{2\hbar}} a_0(x + y, \xi + \eta).$$

When $\hbar \searrow 0$, the phase in the integral oscillates faster and faster. To estimate the integral, one should identify the *stationary points* of the oscillatory phase, and expand the integral around these points. Indeed, in the limit $\hbar \searrow 0$, the integral is dominated by the contributions of these stationary points. We thus obtain the **stationary phase expansion** of this integral. In the present case the phase is quadratic in its variables (y, η) , and the unique stationary point is the origin $(0, 0)$.

Of course, the expansion we obtain by this method coincides with the asymptotic expansion shown in the previous subsection. Actually, the proof of the quadratic stationary phase expansion we give below exactly parallels the proof of the last subsection.

2.4. Stationary and nonstationary phase expansions. This gives us the opportunity to introduce a crucial analytical tool of semiclassical analysis, namely nonstationary and stationary phase estimates.

Generally speaking, the goal is to estimate integrals of the type

$$(2.38) \quad I(\hbar) = \int_{\mathbb{R}^n} a(x) e^{i \frac{\varphi(x)}{\hbar}} dx \quad \text{in the limit } \hbar \searrow 0,$$

where $a \in C_c^\infty(\Omega)$ for some bounded domain $\Omega \subset \mathbb{R}^n$, and the phase function $\varphi \in C^\infty(\mathbb{R}^n, \mathbb{R})$ (or $C^\infty(\overline{\Omega}, \mathbb{R})$, since the values of φ outside Ω are irrelevant). This integral is strongly oscillatory when $\hbar \rightarrow 0$, so we expect it to be small in this limit. The question is:

What is the asymptotic behaviour of $I(\hbar)$ when $\hbar \searrow 0$?

The answer to this question will depend on the critical (or *stationary*) points of φ , that is the points $x_c \in \Omega$ such that $\nabla\varphi(x_c) = 0$. We will not give the most general result, but focus on situations where the stationary points of φ are *isolated* and *nondegenerate*.

We will start from a situation directly generalizing integrals of the type (2.36), namely when the phase function is a nondegenerate quadratic form.

2.4.1. Quadratic stationary phase expansion. We consider the case where the phase function $\varphi(x)$ is a nondegenerate quadratic form $\varphi(x) = \langle x, Qx \rangle$, so it has a single stationary point at the origin.

Theorem 2.29. (*Quadratic stationary phase*) Take Q a real symmetric nondegenerate $n \times n$ matrix on $\mathbb{R}^n$, and $a \in C_c^\infty(\Omega, \mathbb{C})$, for $\Omega \Subset \mathbb{R}^n$ a bounded domain. Then the integral

$$(2.39) \quad I(\hbar) = \int a(x) e^{\frac{i\langle x, Qx \rangle}{2\hbar}} dx$$

admits the following asymptotic expansion.

For any $N \geq 0$, there exists C_N (depending on the dimension n and on the form Q), such that

$$(2.40) \quad \left| I(\hbar) - \frac{(2\pi\hbar)^{n/2} e^{i\pi \operatorname{sgn} Q/4}}{|\det Q|^{1/2}} \sum_{j=0}^{N-1} \frac{\hbar^j}{j!} \left(\frac{\langle D, Q^{-1}D \rangle}{2i} \right)^j a|_{x=0} \right| \leq C_N \hbar^{N+n/2} \sum_{|\alpha| \leq 2N+n+1} \|\partial^\alpha a\|_{L^1}.$$

Remark 2.30. The L^1 norm on $\mathbb{R}^n$ can be controlled by a certain seminorm in $\mathcal{S}$:

$$(2.41) \quad \|a\|_{L^1(\mathbb{R}^n)} \leq C_n \sup_x |\langle x \rangle^{n+1} a(x)| = C_n \|\langle x \rangle^{n+1} a\|_{L^\infty}$$

Proof. Again, we will make a little detour through the Fourier side. The integral $I(\hbar)$ can be seen as the bracket between the distribution $e^{\frac{i\langle x, Qx \rangle}{2\hbar}} \in \mathcal{S}'$ and the function $a \in \mathcal{S}$. Through Parseval's formula, this bracket is equal to the bracket between their Fourier transforms. Using Lemma 2.28, this leads to

$$I(\hbar) = \hbar^{n/2} \frac{e^{i\pi \operatorname{sgn}(Q)/4}}{|\det Q|^{1/2}} \int e^{-\frac{i\hbar}{2} \langle \xi, Q^{-1}\xi \rangle} \mathcal{F}_1(a)(\xi) d\xi.$$

Now that $\hbar$ is in the numerator in the exponential, it makes sense to expand the latter in powers of $\hbar$. Instead of the exact Taylor formula like (2.30), it will be sufficient for us to bound the remainder in the Taylor formula as:

$$\left| e^{it} - \sum_{j=0}^{N-1} \frac{(it)^j}{j!} \right| \leq \frac{|t|^N}{N!},$$

so as to get

$$\left| e^{-i\pi \operatorname{sgn}(Q)/4} \frac{|\det Q|^{1/2}}{\hbar^{n/2}} I(\hbar) - \sum_{j=0}^{N-1} \frac{(\hbar/2i)^j}{j!} \int (\langle \xi, Q^{-1}\xi \rangle)^j \mathcal{F}_1(a)(\xi) d\xi \right| \leq \frac{(\hbar/2)^N}{N!} \int \left| (\langle \xi, Q^{-1}\xi \rangle)^N \right| |\mathcal{F}_1(a)(\xi)| d\xi.$$

The right hand side can be estimated from above by

$$C_N \hbar^N \sum_{|\alpha|=2N} \int |\xi^\alpha \mathcal{F}_1 a(\xi)| d\xi \leq C'_N \hbar^N \sum_{|\alpha| \leq 2N+n+1} \|\partial^\alpha a\|_{L^1},$$

where we used the standard estimate

$$(2.42) \quad \|\mathcal{F}_1 a\|_{L^1} \leq C_n \sum_{|\alpha| \leq n+1} \|\partial^\alpha a\|_{L^1}.$$

Each term of order $\hbar^j$ reads:

$$\begin{aligned} \int (\langle \xi, Q^{-1}\xi \rangle)^j \mathcal{F}_1(a)(\xi) d\xi &= \int \mathcal{F}_1 \left((\langle D, Q^{-1}D \rangle)^j a \right) (\xi) d\xi \\ &= (2\pi)^{n/2} (\langle D, Q^{-1}D \rangle)^j a(0). \end{aligned}$$

□

Remark 2.31. The terms in the expansion (2.40) can be computed in a “direct” manner. We Taylor expand $a(x)$ around $x = 0$, to get the formal sum

$$a(x) \sim \sum_{\alpha \in \mathbb{N}^n} \frac{\langle x^\alpha, \partial^\alpha a(0) \rangle}{\alpha!},$$

which is an asymptotic expansion in the limit $|x| \rightarrow 0$. One then explicitly computes each integral of the form $\int x^\alpha e^{\frac{i\langle x, Qx \rangle}{2\hbar}} dx$. Odd monomials ($|\alpha|$ odd) lead to zero due to the parity of the quadratic form, while even monomials lead to the appearance of the matrix Q^{-1} , through a change of variables. The explicit result for the derivatives of order $k = 2j$ is the j -term in (2.40).

In subsection 2.4.3 we will generalize this stationary phase expansion to the case of more general phase functions φ .

Before doing that, we may apply Thm 2.29 to the integral (2.37) expressing $a_1(x, \xi; \hbar)$ in terms of a_0 . This integral is indeed an oscillatory phase integral of the form (2.39) on $\mathbb{R}^n := \mathbb{R}_{y, \eta}^{2d}$, with symmetric matrix $Q(y, \eta) = \frac{1}{2|s-t|} \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}$ and symbol $\tilde{a}(y, \xi) = a_0(x + y, \xi + \eta)$. The theorem provides a *pointwise* asymptotic expansion for $a_1(x, \xi; \hbar)$, that is,

with no informations on the behaviour when changing (x, ξ) . The derivatives of $\tilde{a}(y, \xi)$ at the origin are indeed equal to derivatives of a_0 at the point (x, ξ) , so we indeed recover the terms of the expansion (2.33).

Remark 2.32. The expansion of Thm 2.29 indicates that the integral $I(\hbar)$ is dominated by the germ of a at the stationary point $x_0 = 0$: the behaviour of the function a away from this point is, in some sense, negligible. As we will see in the next subsection, this is a general feature: the nonstationary points of the phase lead to negligible contributions of oscillatory integrals.

2.4.2. Nonstationary phase estimates. Let us now switch to a general phase function $\varphi(x)$ in the definition (2.38) of $I(\hbar)$, and first consider the situation where this phase function admits *no* stationary point on $\overline{\Omega}$ (which contains the support of the symbol a). By the compactness of $\overline{\Omega}$, this means that $|\nabla\varphi|$ is bounded below by a positive number on $\overline{\Omega}$.

Theorem 2.33. (*Nonstationary phase*) Assume that the phase function φ has no stationary point on $\overline{\Omega}$. Then, for any $N \geq 0$, there exists $C_{N,\varphi,a} > 0$ such that

$$|I(\hbar)| \leq C_{N,\varphi,a} \hbar^N, \quad \forall \hbar \in (0, 1], \quad \text{or equivalently} \quad I(\hbar) = \mathcal{O}(\hbar^\infty).$$

A more precise estimate is the following: for any $N \geq 0$,

$$(2.43) \quad |I(\hbar)| \leq C_N \hbar^N \sum_{j=0}^N \left\| \frac{|\partial^j a|}{|\nabla\varphi|^{2N-j}} \right\|_{L^1},$$

where the prefactor C_N depends on the dimension n , the volume $|\Omega|$ and on upper bounds on the derivatives⁹ $\varphi'', \varphi^{(3)}, \dots, \varphi^{(N+1)}$.

Proof. We apply integration by parts using the differential operator

$$L = \frac{\hbar}{i} \frac{\varphi'(x) \cdot \nabla}{|\varphi'(x)|^2}, \quad \text{which satisfies } L e^{i\frac{\varphi(x)}{\hbar}} = e^{i\frac{\varphi(x)}{\hbar}}.$$

We can then write

$$I(\hbar) = \int a \left[L^k e^{i\frac{\varphi}{\hbar}} \right] dx = \int [{}^t L^k a] e^{i\frac{\varphi}{\hbar}} dx.$$

by integrating by parts k times. The transposed operator reads

$${}^t L = -\frac{\hbar}{i} \nabla \cdot \frac{\varphi'(x)}{|\varphi'(x)|^2} = -\frac{\hbar}{i} \left[\nabla, \frac{\varphi'(x)}{|\varphi'(x)|^2} \right] - \frac{\hbar}{i} \frac{\varphi'(x)}{|\varphi'(x)|^2} \cdot \nabla,$$

where the commutator is a function

$$\left[\nabla, \frac{\varphi'(x)}{|\varphi'(x)|^2} \right] = \sum_{j=1}^n \partial_j \left(\frac{\partial_j \varphi(x)}{|\varphi'(x)|^2} \right).$$

⁹To alleviate notations we write $\varphi' = \partial_x \varphi$, $\varphi'' = \partial_x^2 \varphi$ etc.

Since $\varphi' = \nabla\varphi$ never vanishes, we get the pointwise estimate

$$|[{}^tL a](x)| \leq C\hbar \left(\frac{|\varphi''(x)|}{|\varphi'(x)|^2} |a(x)| + \frac{1}{|\varphi'(x)|} |\partial a(x)| \right)$$

Applying this transposed operator again, we find

$$|[{}^tL^2 a](x)| \leq C\hbar^2 \left(\left(\frac{|\varphi''(x)|^2}{|\varphi'(x)|^4} + \frac{|\varphi^{(3)}(x)|}{|\varphi'(x)|^3} \right) |a(x)| + \frac{|\varphi''(x)|}{|\varphi'(x)|^3} |\partial a(x)| + \frac{1}{|\varphi'(x)|^2} |\partial^2 a(x)| \right).$$

The higher derivatives $\varphi''(x)$, $\varphi^{(3)}(x)$ are uniformly bounded on $\overline{\Omega}$, we may absorb them in the constant prefactor, keeping only the dependence in φ' explicit. We thus get the pointwise estimate

$$|[{}^tL^2 a](x)| \leq C_{n,2,\varphi''} \hbar^2 \sum_{j=0}^2 \frac{|\partial^j a(x)|}{|\varphi'(x)|^{4-j}}.$$

An straightforward induction argument shows that for any $N \geq 0$,

$$(2.44) \quad |[{}^tL^N a](x)| \leq C_{n,N,\varphi''} \hbar^N \sum_{j=0}^N \frac{|\partial^j a(x)|}{|\varphi'(x)|^{2N-j}}.$$

As a result, integrating over $x \in \Omega$ we get the result (2.43). $\square$

This estimate will be very helpful in the following. For instance, when deriving *stationary* phase estimates, it allows to take advantage of situations when $\varphi'(x)$ vanishes at some critical point, but $a(x)$ also vanishes up to some order at the same point. It will also allow to get fast decay for states of the form $\text{Op}_{\hbar}(a)u$, away from the support of u .

This nonstationary phase estimate confirms our previous Remark 2.32. When considering a general phase function φ , it will be convenient to (smoothly) truncate the integral $I(\hbar)$ in small neighbourhoods of stationary points, the remaining parts lying in nonstationary regions, and therefore being of order $\mathcal{O}(\hbar^\infty)$.

2.4.3. Nonquadratic stationary phase estimates. We now go back the computation of $I(\hbar)$ in (2.38) with a nonquadratic phase function φ .

Definition 2.34. We assume that all the stationary points of φ are *nondegenerate*: at each stationary point x_c , that is such that $\varphi'(x_c) = 0$, the Hessian matrix $\varphi''(x_c) = (\partial_i \partial_j \varphi(x_c))$ is nonsingular. This implies that x_c is isolated from other stationary points, hence that stationary points form a discrete set. On each precompact set Ω there are at most finitely many stationary points.

Using a smooth finite partition and the nonstationary estimates of the previous section, we may treat separately the neighbourhoods of each stationary point separately.

Theorem 2.35. (*Nonquadratic stationary phase*) We want to estimate the integral (2.38). We assume φ admits a single stationary point $x_0 \in \text{supp } a$, and that this stationary point is nondegenerate ($\varphi''(x_0)$ is nonsingular).

Then there exists a sequence of differential operators $(A_{2k}(x, D))_{k \in \mathbb{N}}$ of orders $\leq 2k$, such that for any $N \geq 0$,

$$(2.45) \quad \left| I(\hbar) - e^{i\varphi(x_0)/\hbar} \sum_{k=0}^{N-1} \hbar^{n/2+k} [A_{2k}(x, D)a(x)]_{|x=x_0} \right| \leq C_N \hbar^{N+n/2} \sum_{|\alpha| \leq 2N+n+1} \|\partial^\alpha a\|_{L^1}.$$

The constant C_N depends on $\text{supp } a$ and φ , but not on $\hbar$ nor the seminorms of a .

The most straightforward way to prove this Theorem is through the Morse Lemma, which allows to transform the phase function φ into a quadratic phase through a well-chosen change of coordinates. This transformation will then allow us to use Thm 2.29.

Proposition 2.36. (*Morse Lemma*) Assume $\varphi(x)$ has a nondegenerate critical point at $x_0 \in \mathbb{R}^n$. Then there exists a change of coordinates $\kappa : \text{neigh}(0) \rightarrow \text{neigh}(x_0)$ defined in some neighbourhood of 0, with $\kappa(0) = x_0$, $\partial\kappa(0) = Id$, such that

$$\varphi(x) = \varphi_2 \circ \kappa^{-1}(x), \quad x \in \text{neigh}(x_0),$$

where $\varphi_2(y) = \varphi(x_0) + \frac{1}{2}\langle y, \varphi''(x_0)y \rangle$ in the corresponding neighbourhood of $y = 0$.

In other words, the diffeomorphism κ “straightens out” the coordinates, such as to absorb the nonquadratic part of φ at $x = x_0$.

Proof. Let us assume that the stationary point $x_0 = 0$, so that the diffeomorphism κ fixes the origin. The Taylor expansion of φ at $x = 0$ can be written locally as

$$\varphi(x) = \varphi(0) + \frac{1}{2}\langle x, \varphi''(0)x \rangle + \mathcal{O}(x^3).$$

Due to the nondegeneracy of $\varphi''(0)$, we may write the RHS as

$$\varphi(x) = \varphi(0) + \frac{1}{2}\langle x, Q(x)x \rangle,$$

where $Q(x)$ is a symmetric nondegenerate matrix, smoothly dependent on x , such that $Q(0) = \varphi''(0)$. The trick now is to construct a diffeomorphism κ with the announced properties, such that

$$\langle x, Q(x)x \rangle = \langle \kappa^{-1}(x), Q(0)\kappa^{-1}(x) \rangle.$$

We try to solve this equation by the Ansatz $\kappa^{-1}(x) = A(x)x$, with $A(x)$ an invertible matrix, smoothly dependent on x , with $A(0) = Id$. Hence, we need to solve (in $A(x)$) the problem

$$(2.46) \quad {}^t A(x) Q(0) A(x) = Q(x).$$

This problem is solved by inverting the function $F : A \mapsto {}^tAQ(0)A$ defined on the space of $n \times n$ matrices, with images in the space of $n \times n$ symmetric matrices. To find a (right) inverse to this function near $A = Id$, we linearize the equation at $A = Id$. Namely, we notice that for an infinitesimal perturbation δA ,

$$F(I + \delta A) = Q(0) + \delta Q + \mathcal{O}(\delta A^2), \quad \delta Q = {}^t\delta A Q(0) + Q(0)\delta A.$$

The differential map $DF : \delta A \mapsto \delta Q$ is surjective, and admits as inverse $\delta A = \frac{1}{2}Q(0)^{-1}\delta Q$. The **implicit function theorem** implies the existence of a map $G : Q \mapsto A$ with $G(Q(0) + \delta Q) = I + \frac{1}{2}Q(0)^{-1}\delta Q + \mathcal{O}(\delta Q^2)$, such that $F \circ G = Id$. As a result, the problem (2.46) can be solved by a matrix $A(x) = G(Q(x))$ depending smoothly on x . $\square$

Let us now come back to the proof of the Thm 2.35. We may choose a cutoff $\chi \in C_c^\infty(\mathbb{R}^d, [0, 1])$ supported inside the neighbourhood $\text{neigh}(x_0)$, image of the coordinate change κ in the Morse Lemma 2.36, while $\chi(x) = 1$ in a smaller neighbourhood of x_0 . This way, we may decompose $I(\hbar)$ into

$$I(\hbar) = I_0(\hbar) + I_1(\hbar), \quad I_0(\hbar) = \int \chi(x)a(x) e^{i\frac{\varphi(x)}{\hbar}} dx, \quad I_1(\hbar) = \int (1 - \chi(x))a(x) e^{i\frac{\varphi(x)}{\hbar}} dx.$$

The integral $I_1(\hbar)$ is easy to treat: the phase φ is nonstationary on the support of $(1 - \chi)a$, so from Thm (2.33) we find $I_1(\hbar) = \mathcal{O}(\hbar^\infty)$.

Applying the Morse Lemma, we may write $I_0(\hbar)$ as an integral with a quadratic stationary phase:

$$I_0(\hbar) = \int \chi a(x) e^{i\frac{\varphi(x)}{\hbar}} dx = \int e^{i\frac{\varphi_2(y)}{\hbar}} (\chi a) \circ \kappa(y) |\det d\kappa(y)| dy.$$

We may then apply the quadratic stationary phase expansion of Theorem 2.29, with the data $Q := \varphi''(x_0)$ and $a := \chi a \circ \kappa(y) |\det d\kappa(y)|$. This proves the expansion of Theorem 2.35, using the fact that all derivatives of $\chi a(x)$ at the point x_0 are equal to the same derivatives of $a(x)$. $\square$

Remark 2.37. Our proof of the stationary phase estimate (2.45) does not explicitly compute the differential operators $A_{2k}(x, D)$. One can actually compute these operators by a more “formal” approach, bypassing the use of the Morse Lemma. The idea is to Taylor expand the phase function around x_0 :

$$\varphi(x) = \varphi_2(x) + g(x), \quad g(x) = \mathcal{O}((x - x_0)^3) \quad \text{when } x \rightarrow x_0,$$

then naively expand the exponential

$$e^{ig(x)/\hbar} a(x) = \sum_{k \geq 0} \frac{(ig(x)/\hbar)^k}{k!} a(x),$$

and finally, for each $k \geq 0$, Taylor expand the product $g(x)^k a(x)$ at $x = x_0$. One thereby obtains a sum of polynomials in $(x - x_0)$, which can be explicitly integrated over the quadratic phase $e^{i\varphi_2/\hbar}$. Some power counting shows that the “dangerous” factor $\hbar^{-k}$ do not ruin the asymptotic expansion. Indeed, the k -term polynomial behaves like $\hbar^{-k} \mathcal{O}((x - x_0)^{3k})$ when $x \rightarrow x_0$. If k is even, integrating over the quadratic phase yields a result of order $\hbar^{-k} \hbar^{n/2} \hbar^{3k/2} = \hbar^{n/2+k/2}$. If k is odd, the lowest order term will come from integrating $\hbar^{-k} \mathcal{O}((x - x_0)^{3k+1})$, and is therefore of order $\hbar^{-k} \hbar^{n/2} \hbar^{(3k+1)/2} = \hbar^{n/2+(k+1)/2}$. The polynomials $A_{2j}(x, D)$ will hence depend on the germs at x_0 of the functions $\frac{(ig(x)/\hbar)^k}{k!} a(x)$ with the condition $k \leq j$ (k even), respectively $k + 1 \leq j$ (k odd).

3. COMPOSING $\hbar$ -PSEUDODIFFERENTIAL OPERATORS

Once we have decided how to quantize classical observables, we want to understand how these operators are composed with each other. Namely, for a given choice of parameter $t \in [0, 1]$ and any two symbols a, b on $\mathbb{R}^{2d}$, what can we say about the operator $\text{Op}_h^t(a) \circ \text{Op}_h^t(b)$? Can we bring it into the form $\text{Op}_h^t(c)$ for some symbol $c(x, \xi)$?

3.0.1. Composing semiclassical differential operators. We have already come across this question, when composing operators $\text{Op}_h(f(x))$ and $\text{Op}_h(g(\xi))$: depending on the choice of ordering, we obtained either $\text{Op}_h^R(f(x)g(\xi))$, or $\text{Op}_h^L(f(x)g(\xi))$.

In the case of differential operators

$$A_h = \sum_{|\alpha| \leq m} a_\alpha(x) (hD)^\alpha = \text{Op}_h^R(a), \quad a(x, \xi) = \sum_{|\alpha| \leq m} a_\alpha(x) \xi^\alpha,$$

say with coefficients $a_\alpha \in \mathcal{S}(\mathbb{R}^d)$, the composition of the two operators still gives a differential operator:

$$\begin{aligned} A_h \circ B_h &= \sum_{|\alpha| \leq m} \sum_{|\beta| \leq n} a_\alpha(x) (hD)^\alpha b_\beta(x) (hD)^\beta \\ &= \sum_{\alpha, \beta} a_\alpha(x) b_\beta(x) (hD)^{\alpha+\beta} + \sum_{\alpha, \beta} a_\alpha(x) [(hD)^\alpha, b_\beta(x)] (hD)^\beta. \end{aligned}$$

The first sum on the RHS is exactly $\text{Op}_h^R(ab)$. In the second sum, each commutator can be written as:

$$\begin{aligned} [(hD)^\alpha, b_\beta(x)]u &= \sum_{\substack{\alpha^{(1)} + \alpha^{(2)} = \alpha \\ |\alpha^{(1)}| > 0}} c_{\alpha^{(1)}, \alpha^{(2)}} h^{|\alpha^{(1)}|} \left[D^{\alpha^{(1)}} b_\beta \right] (hD)^{\alpha^{(2)}} u \\ &= \sum_{\substack{\alpha^{(1)} + \alpha^{(2)} = \alpha \\ |\alpha^{(1)}| > 0}} c_{\alpha^{(1)}, \alpha^{(2)}} h^{|\alpha^{(1)}|} \text{Op}_h^R \left(\left(D^{\alpha^{(1)}} b_\beta \right) (x) \xi^{\alpha^{(2)}} \right) u, \end{aligned}$$

where the $c_{\alpha^{(1)}, \alpha^{(2)}}$ are combinatorial coefficients. The above sum is therefore a differential operator, quantization of a polynomial symbol of order $\mathcal{O}(h)$.

Summing over all the terms α, β , we find that $A_h \circ B_h$ is a differential operator of degree $m + n$. Its symbol depends explicitly on h , and is composed of

- (1) the function $a(x, \xi)b(x, \xi)$, independent of h , called the *principal symbol* of $A_h \circ B_h$,
- (2) a remainder, which is a differential operator of degree $\leq m + n - 1$, whose coefficients depend explicitly on h , and are of order $\mathcal{O}(h)$.

3.1. Computing the symbol of $A \circ B$ for Schwartz symbols. In the case of symbols $a, b \in \mathcal{S}(\mathbb{R}^{2d})$, the Remark 2.8 showed that the Schwartz kernels of the operators $A = \text{Op}_h^t(a)$, $B = \text{Op}_h^t(b)$ both belong to $\mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$; as a result, the kernel $k(x, y; \hbar) = k_{A \circ B}(x, y; \hbar)$ of the composed operator $A \circ B$ belongs to $\mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$ as well, as the convolution of two Schwartz kernels.

Using the partial inverse Fourier transform $y \rightarrow \xi$ we may write this kernel as

$$k(x, y; \hbar) = \int e^{-i\xi \cdot y / \hbar} (\mathcal{F}_{h; y \rightarrow \xi}^{-1} k)(x, \xi) \frac{d\xi}{(2\pi\hbar)^{d/2}} \stackrel{\text{def}}{=} \int e^{i\xi \cdot (x-y) / \hbar} c_1(x, \xi; \hbar) \frac{d\xi}{(2\pi\hbar)^d},$$

where we introduced the function

$$c_1(x, \xi; \hbar) \stackrel{\text{def}}{=} (2\pi\hbar)^{d/2} e^{-i\xi \cdot x / \hbar} (\mathcal{F}_{h; y \rightarrow \xi}^{-1} k)(x, \xi) \in \mathcal{S}(\mathbb{R}^{2d}).$$

In other words, $A \circ B = \text{Op}_h^R(c_1(\hbar))$. From Proposition 2.23, we may as well express $A \circ B$ as the t -quantization of a Schwartz symbol $c = c_t(x, \xi; \hbar)$.

Definition 3.1. For any choice of $t \in [0, 1]$, to any linear operator C with Schwartz kernel $k_C \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$ corresponds a unique function $c_t \in \mathcal{S}(\mathbb{R}^{2d})$ such that $C = \text{Op}_h^t(c_t)$. The function c_t is called the (full) t -symbol of the operator C , and we note $c = \sigma_h^t(C)$. The map $C \mapsto c_t = \sigma_h^t(C)$ depends on both $\hbar$ and the choice of quantization (t). In the case of the Weyl quantization ($t = 1/2$), we write $c_{1/2} = \sigma_h^W(C)$.

Our main questions in this section is:

For $C = \text{Op}_h^t(a) \circ \text{Op}_h^t(b)$, how does the symbol $c_t(\hbar)$ depend on $\hbar$? Can we compute it directly from a, b ?

To answer these questions, we will first give an exact expression for c , using the expression of $\text{Op}_h^t(a)$ and $\text{Op}_h^t(b)$ in terms of Weyl translation operators. In a second step, we will show that the expression for $c_t(x, \xi; \hbar)$ admits an asymptotic series in powers of $\hbar$. Our main asymptotic tool will be the *stationary phase expansions* of the previous section.

3.1.1. Exact expression of the composed symbols. Let us take $a, b \in \mathcal{S}(\mathbb{R}^{2d})$. For the moment we will treat an arbitrary t -quantization. Using the expression

$$A = \text{Op}_h^t(a) = \int \text{Op}_h^t(e_{V_0}) \hat{a}(V_0) \frac{dV_0}{(2\pi)^d},$$

we get

$$A \circ B = \text{Op}_h^t(a) \text{Op}_h^t(b) = \int \text{Op}_h^t(e_{V_0}) \hat{a}(V_0) \frac{dV_0}{(2\pi)^d} \int \text{Op}_h^t(e_{V_1}) \hat{b}(V_1) \frac{dV_1}{(2\pi)^d}.$$

A direct computation, using (2.15), generalizes the composition rule for translation operators (2.10):

$$\text{Op}_h^t(e_{V_0}) \text{Op}_h^t(e_{V_1}) = e^{i\hbar((1-t)\xi_0 \cdot x_1 - t\xi_1 \cdot x_0)} \text{Op}_h^t(e_{V_0+V_1}).$$

From there we get

$$\begin{aligned} A \circ B &= \iint \frac{dV_0 dV_1}{(2\pi)^{2d}} e^{i\hbar((1-t)\xi_0 \cdot x_1 - t\xi_1 \cdot x_0)} \hat{a}(V_0) \hat{b}(V_1) \text{Op}_h^t(e_{V_0+V_1}) \\ &= \iint \frac{dV_+ dV_-}{(2\pi)^{2d}} e^{i\hbar((1-t)\xi_0 \cdot x_1 - t\xi_1 \cdot x_0)} \hat{a}(V_+/2 + V_-) \hat{b}(V_+/2 - V_-) \text{Op}_h^t(e_{V_+}), \end{aligned}$$

where we used the change of variables

$$(V_0, V_1) \mapsto (V_+ = V_0 + V_1, V_- = \frac{1}{2}(V_0 - V_1)).$$

In these coordinates the phase reads

$$\begin{aligned} \varphi_t &= (1-t)(\xi_+/2 + \xi_-) \cdot (x_+/2 - x_-) - t(\xi_+/2 - \xi_-) \cdot (x_+/2 + x_-) \\ &= (1-t)(\xi_+ \cdot x_+/4 - \xi_+ \cdot x_-/2 + \xi_- \cdot x_+/2 - \xi_- \cdot x_-) - t(\xi_+ \cdot x_+/4 + \xi_+ \cdot x_-/2 - \xi_- \cdot x_+/2 - \xi_- \cdot x_-) \\ &= (1-2t)(\xi_+ \cdot x_+/2 - 2\xi_- \cdot x_-) + (-\xi_+ \cdot x_- + \xi_- \cdot x_+)/2. \end{aligned}$$

We can hence identify the Fourier transform of the t -symbol of $C = A \circ B$:

$$(3.1) \quad \hat{c}_t(V_+; \hbar) = \int \frac{dV_-}{(2\pi)^d} e^{i\hbar\varphi_t(V_+, V_-)} \hat{a}(V_+/2 + V_-) \hat{b}(V_+/2 - V_-).$$

Let us distinguish two cases:

- (1) in the case of the Weyl quantization ($t = 1/2$), the phase reads $\frac{1}{2}(\xi_- \cdot x_+ - \xi_+ \cdot x_-) = \frac{1}{2}\omega(V_-, V_+) = \frac{1}{2}\omega(V_0, V_1)$.
- (2) in the case of the right quantization ($t = 1$), the phase reads $-(\xi_+/2 - \xi_-) \cdot (x_+/2 + x_-) = -x_0 \cdot \xi_1$.

3.1.2. Computing the composed symbol in the case of the Weyl quantization. We will restrict ourselves to the Weyl quantization, and omit to indicate the subscripts $\bullet_{1/2}$. The expression (3.1) simplifies to

$$(3.2) \quad \hat{c}(V_+; \hbar) = \int \frac{dV_-}{(2\pi)^d} e^{\frac{i\hbar}{2}\omega(V_-, V_+)} \hat{a}(V_+/2 + V_-) \hat{b}(V_+/2 - V_-) = \int \frac{dV_-}{(2\pi)^d} e^{\frac{i\hbar}{2}\omega(V_0, V_1)} \hat{a}(V_0) \hat{b}(V_1).$$

Can we get a decent expression of c as a function of a, b ? As we had already done in Proposition 2.23, the phase $e^{\frac{i\hbar}{2}\omega(V_0, V_1)}$ is a Fourier multiplier on the space $\mathbb{R}_{\rho_0, \rho_1}^{4d}$: the product $\hat{a}(V_0) \hat{b}(V_1)$ is the Fourier transform of $a(\rho_0)b(\rho_1)$, so $e^{\frac{i\hbar}{2}\omega(V_0, V_1)} \hat{a}(V_0) \hat{b}(V_1)$ is the Fourier

transform of

$$\tilde{c}(\rho_0, \rho_1) \stackrel{\text{def}}{=} e^{\frac{i\hbar}{2}\omega(D_{\rho_0}, D_{\rho_1})} a(\rho_0) b(\rho_1).$$

The inverse symbol $c(\rho; \hbar)$ hence reads

$$(3.3) \quad c(\rho; \hbar) = \int e^{i\omega(V_+, \rho)} \hat{c}(V_+) \frac{dV_+}{(2\pi)^d}$$

$$= \iint e^{i\omega(V_+, \rho)} e^{\frac{i\hbar}{2}\omega(V_-, V_+)} \hat{a}(V_+/2 + V_-) \hat{b}(V_+/2 - V_-) \frac{dV_+ dV_-}{(2\pi)^{2d}}$$

$$(3.4) \quad = \iint e^{i\omega(V_0 + V_1, \rho)} e^{\frac{i\hbar}{2}\omega(V_0, V_1)} \hat{a}(V_0) \hat{b}(V_1) \frac{dV_0 dV_1}{(2\pi)^{2d}}$$

$$(3.5) \quad = \tilde{c}(\rho_0, \rho_1) \upharpoonright_{\rho_0=\rho_1=\rho}$$

$$= e^{\frac{i\hbar}{2}\omega(D_{\rho_0}, D_{\rho_1})} a(\rho_0) b(\rho_1) \upharpoonright_{\rho_0=\rho_1=\rho}.$$

This last line directly connects the symbol $c(\hbar)$ with a, b .

Theorem 3.2. (*composition of Ψ DOs*). Assume $a, b \in \mathcal{S}(\mathbb{R}^{2d})$. Then the operator $\text{Op}_\hbar^W(a) \circ \text{Op}_\hbar^W(b) = \text{Op}_\hbar^W(c(\hbar))$, where for any $\hbar \in (0, 1]$ the symbol $c(\hbar)$ is given by the expression

$$(3.6) \quad c(\rho; \hbar) = e^{\frac{i\hbar}{2}\omega(D_{\rho_0}, D_{\rho_1})} a(\rho_0) b(\rho_1) \upharpoonright_{\rho_0=\rho_1=\rho}$$

$$(3.7) \quad = e^{\frac{i\hbar}{2}(D_{\xi_0} \cdot D_{x_1} - D_{\xi_1} \cdot D_{x_0})} a(\rho_0) b(\rho_1) \upharpoonright_{\rho_0=\rho_1=\rho}$$

$$(3.8) \quad = a(\rho) e^{i\frac{\hbar}{2}\omega(\overleftarrow{D}, \overrightarrow{D})} b(\rho).$$

This symbol $c(\hbar)$ belongs to $\mathcal{S}(\mathbb{R}^{2d})$, with uniformly bounded seminorms w.r.t. $\hbar \in (0, 1]$. We write $c = a \#_\hbar b$, where the $\#_\hbar$ is called the **Moyal product** of the symbols a and b . This product can be defined on the Fourier side, namely by (3.2).

The arrows in the last line indicates that the derivative operator $\overleftarrow{D}$ acts on $a(\rho)$ situated on its left, while the operator $\overrightarrow{D}$ acts on $b(\rho)$ on its right. One has to be a bit careful with these notations, and come back to the more precise (3.6) in case of doubt.

Exercise 3.3. Show that in the case of the right quantization, the composition formula for $\text{Op}_\hbar^R(a) \circ \text{Op}_\hbar^R(b)$ reads

$$c_1(\rho; \hbar) = e^{i\hbar D_{\xi_0} \cdot D_{x_1}} a_1(\rho_0) b_1(\rho_1) \upharpoonright_{\rho_0=\rho_1=\rho}$$

$$= a(\rho) e^{i\hbar \overleftarrow{D}_\xi \cdot \overrightarrow{D}_x} b(\rho).$$

3.1.3. *The composed Weyl symbol as an “oscillatory convolution integral”.* Like in §2.3.3, the formal expression (3.6) can be expressed as an oscillatory convolution integral, and leads to an asymptotic expansion in powers of $\hbar$.

By expanding in (3.4) the Fourier transforms $\hat{a}$, $\hat{b}$, we obtain the oscillatory integral:

$$c(\rho; \hbar) = \iiint \frac{dV_0 dV_1 d\rho_0 d\rho_1}{(2\pi)^{4d}} e^{i\omega(V_0+V_1, \rho)} e^{\frac{i\hbar}{2}\omega(V_0, V_1)} e^{i\omega(\rho_0, V_0) + i\omega(\rho_1, V_1)} a(\rho_0) b(\rho_1).$$

Notice that the Fourier variables $\mathcal{V} = \begin{pmatrix} V_0 \\ V_1 \end{pmatrix} \in \mathbb{R}^{4d}$ only appear in the phase, hence the integral over $\mathcal{V}$ does not converge absolutely. The phase is of the form

$$\begin{aligned} \varphi &= \frac{\hbar}{2} \langle JV_0, V_1 \rangle - \langle V_0, J(\rho - \rho_0) \rangle - \langle V_1, J(\rho - \rho_1) \rangle \\ &= \frac{1}{2} \langle \mathcal{V}, \mathcal{Q}\mathcal{V} \rangle - \langle \mathcal{V}, Z \rangle, \end{aligned}$$

with the $4d \times 4d$ symmetric matrix and $4d$ -vector

$$\mathcal{Q} = \frac{\hbar}{2} \begin{pmatrix} 0 & -J \\ J & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} J(\rho - \rho_0) \\ J(\rho - \rho_1) \end{pmatrix}.$$

The integral over $\mathcal{V}$ thus gives the Fourier transform of this quadratic phase, which was computed in Lemma 2.28. The matrix $\mathcal{Q}$ has signature 0, determinant $|\det \mathcal{Q}| = (\hbar/2)^{4d}$ and inverse $\mathcal{Q}^{-1} = \frac{2}{\hbar} \begin{pmatrix} 0 & -J \\ J & 0 \end{pmatrix}$, so we get

$$\begin{aligned} \iint \frac{d\mathcal{V}}{(2\pi)^{2d}} e^{i(\frac{1}{2}\langle \mathcal{V}, \mathcal{Q}\mathcal{V} \rangle - \langle \mathcal{V}, Z \rangle)} &= \mathcal{F}_1 \left(e^{\frac{i}{2}\langle \mathcal{V}, \mathcal{Q}\mathcal{V} \rangle} \right) (Z), \\ &= \frac{1}{|\det \mathcal{Q}|^{1/2}} \exp \left(-\frac{i}{2} \langle Z, \mathcal{Q}^{-1} Z \rangle \right) \\ &= \left(\frac{2}{\hbar} \right)^{2d} \exp \left(-\frac{2i}{\hbar} \langle J(\rho - \rho_0), (\rho - \rho_1) \rangle \right). \end{aligned}$$

Hence we get the “direct integral” over $\mathbb{R}_{\rho_0, \rho_1}^{4d}$:

$$\begin{aligned} c(\rho; \hbar) &= \iint \frac{d\rho_0 d\rho_1}{(\pi\hbar)^{2d}} e^{-\frac{2i}{\hbar} \langle J(\rho - \rho_0), (\rho - \rho_1) \rangle} a(\rho_0) b(\rho_1) \\ &= \iint \frac{d\rho'_0 d\rho'_1}{(\pi\hbar)^{2d}} e^{-\frac{2i}{\hbar} \omega(\rho'_0, \rho'_1)} a(\rho + \rho'_0) b(\rho + \rho'_1) \end{aligned}$$

after the change of variables $\rho'_i = \rho_i - \rho$.

Proposition 3.4. *The Moyal product of two symbols $a, b \in \mathcal{S}(\mathbb{R}^{2d})$ can be expressed as the following “oscillatory convolution” integral:*

$$(3.9) \quad (a \#_{\hbar} b)(\rho) = \iint \frac{d\rho_0 d\rho_1}{(\pi\hbar)^{2d}} e^{-\frac{2i}{\hbar} \omega(\rho_0, \rho_1)} a(\rho + \rho_0) b(\rho + \rho_1).$$

3.2. Asymptotic expansion of the composed Weyl symbol. Expanding the operator $e^{i\frac{\hbar}{2}\omega(D_{\rho_0}, D_{\rho_1})}$ to finite order and using the Taylor expansion with integral remainder, we find

similarly as in (2.31):

$$(3.10) \quad \begin{aligned} a \#_{\hbar} b(\rho) &= a(\rho) e^{i\frac{\hbar}{2}\omega(\overleftarrow{D}, \overrightarrow{D})} b(\rho) = \sum_{j=0}^{N-1} \frac{(i\hbar/2)^j}{j!} a(\rho) \left(\omega(\overleftarrow{D}, \overrightarrow{D}) \right)^j b(\rho) \\ &+ \frac{(i\hbar/2)^N}{(N-1)!} \int_0^1 du (1-u)^{N-1} a(\rho) \left(\omega(\overleftarrow{D}, \overrightarrow{D}) \right)^N e^{iu\frac{\hbar}{2}\omega(\overleftarrow{D}, \overrightarrow{D})} b(\rho). \end{aligned}$$

From this exact expression, we will extract bounds on the integral term in the RHS, and show that it is indeed a “remainder” smaller than the previous terms. On the Fourier side, the integral over $u \in [0, 1]$ is a linear combination of $(\omega(V_0, V_1))^N e^{iu\frac{\hbar}{2}\omega(V_0, V_1)} \hat{a}(V_0) \hat{b}(V_1)$, which are contained in a bounded set in $\mathcal{S}(\mathbb{R}^{4d})$ uniformly in $u, \hbar$; after integrating over u we are still in a bounded set in $\mathcal{S}$, uniformly in $\hbar \in (0, 1]$. To obtain the integral in (3.10) we take the inverse Fourier transform $V_0, V_1 \rightarrow \rho_0, \rho_1$, which still gives a function contained in a bounded set in $\mathcal{S}(\mathbb{R}^{4d})$. Its restriction on the diagonal $\{\rho_0 = \rho_1\}$ is still in a bounded set in $\mathcal{S}(\mathbb{R}^{2d})$.

More explicitly, one can control the seminorms of $a \#_{\hbar} b$ in terms of those of a, b as follows:

Proposition 3.5. *For $a, b \in \mathcal{S}(\mathbb{R}^{2d})$, the seminorms of $c(\hbar) = a \#_{\hbar} b$ are controlled as follows¹⁰:*

$$(3.11) \quad \begin{aligned} \forall \alpha, \gamma \in \mathbb{N}^{2d}, \forall \rho \in \mathbb{R}^{2d}, \quad |\rho^\gamma \partial^\alpha (a \#_{\hbar} b)(\rho)| &\leq \sum_{j=0}^{N-1} \frac{(\hbar/2)^j}{j!} \left| \rho^\gamma \partial^\alpha \left[a(\rho) \left(\omega(\overleftarrow{D}, \overrightarrow{D}) \right)^j b(\rho) \right] \right| \\ &+ C_{N, \gamma, \alpha} \hbar^N \left\| \langle \rho \rangle^{|\gamma|} \langle D \rangle^{N+|\alpha|+2d+1} a \right\|_{L^1} \left\| \langle D \rangle^{N+|\alpha|+|\gamma|+2d+1} b \right\|_{L^1}. \end{aligned}$$

The norms in the last term could be symmetrized between a and b . They can be replaced by norms of the type $\sum_{|\beta| \leq N+|\alpha|+2d+1} \left\| \langle \rho \rangle^\gamma \partial^\beta a \right\|_{L^1}$.

For $N = 0$ this bound reads

$$\forall \alpha, \gamma \in \mathbb{N}^{2d}, \quad |\rho^\gamma \partial^\alpha (a \#_{\hbar} b)(\rho)| \leq C_{\gamma, \alpha} \left\| \langle \rho \rangle^{|\gamma|} \langle D \rangle^{|\alpha|+2d+1} a \right\|_{L^1} \left\| \langle D \rangle^{|\alpha|+|\gamma|+2d+1} b \right\|_{L^1}.$$

As a consequence, the symbol $c(\hbar)$ belongs to a bounded set in $\mathcal{S}(\mathbb{R}^{2d})$, when $\hbar \in (0, 1]$.

Proof. We only need to show that the integral term in (3.10), which we call $\hbar^N R_N(\rho; \hbar)$, satisfies the bound on the second line of (3.11). For this we work on the Fourier side. Let us

¹⁰Here we use the “Japanese brackets” notation: $\langle \rho \rangle = (1 + |\rho|^2)^{1/2}$, which grows like $|\rho|$ when $\rho \rightarrow \infty$, but is regular and nonvanishing with $\rho \rightarrow 0$. This notation also applies to the differential operator D , obtaining a Fourier multiplier.

first take $\gamma = \alpha = 0$:

$$\begin{aligned} \left| (\omega(V_0, V_1))^N e^{iu\frac{\hbar}{2}\omega(V_0, V_1)} \hat{a}(V_0) \hat{b}(V_1) \right| &\leq C \langle V_0 \rangle^N |\hat{a}(V_0)| \langle V_1 \rangle^N |\hat{b}(V_1)| \\ &= C \left| \widehat{\langle D \rangle^N a}(V_0) \right| \left| \widehat{\langle D \rangle^N b}(V_1) \right|. \end{aligned}$$

To pointwise estimate the N -th order component of $(a \#_{\hbar} b)(\rho)$ we remember that a function in $\mathcal{S}(\mathbb{R}^n)$ is pointwise bounded as follows:

$$\begin{aligned} \forall x \in \mathbb{R}^n \quad |f(x)| &\leq C_n \|\hat{f}\|_{L^1(\mathbb{R}^n)} = C_n \int |\hat{f}(\xi)| \frac{\langle \xi \rangle^{n+1}}{\langle \xi \rangle} \\ &\leq C'_n \left\| \langle \xi \rangle^{n+1} \hat{f} \right\|_{L^\infty} = C'_n \left\| \widehat{\langle D \rangle^{n+1} f} \right\|_{L^\infty} \\ &\leq C'_n \left\| \langle D \rangle^{n+1} f \right\|_{L^1(\mathbb{R}^n)}. \end{aligned}$$

In the case of the remainder term in $c(\rho; \hbar)$, the Fourier transform is realized in dimension $4d$, so after factorizing in two integrals in dimension $2d$, we get

$$\begin{aligned} \forall \rho \in \mathbb{R}^{2d}, \quad |R_N(\rho; \hbar)| &\leq C \left\| (\omega(V_0, V_1))^N e^{iu\frac{\hbar}{2}\omega(V_0, V_1)} \hat{a}(V_0) \hat{b}(V_1) \right\|_{L^1(\mathbb{R}^{4d})} \\ &\leq C \left\| \langle V_0 \rangle^N \hat{a}(V_0) \right\|_{L^1(\mathbb{R}^{2d})} \left\| \langle V_1 \rangle^N \hat{b}(V_1) \right\|_{L^1(\mathbb{R}^{2d})} \\ &\leq C' \left\| \langle D \rangle^{N+2d+1} a \right\|_{L^1(\mathbb{R}^{2d})} \left\| \langle D \rangle^{N+2d+1} b \right\|_{L^1(\mathbb{R}^{2d})}. \end{aligned}$$

Now, differentiating $R_N(\rho; \hbar)$ α times amounts to multiply the Fourier transform by $(i(J(V_0 + V_1)))^\alpha$, which can be bounded by an extra factor $C_\alpha \langle V_0 \rangle^{|\alpha|} \langle V_1 \rangle^{|\alpha|}$, and finally extra factors $\langle D \rangle^{|\alpha|}$ inside each L^1 factor in (3.11).

Finally, multiplying $R_N(\rho; \hbar)$ by ρ^γ amounts to hit the phase $e^{i\omega(V_0+V_1, \rho)}$ by the derivative $D^\gamma_{V_0}$ in the Fourier integral (3.4). Integrating by parts $|\gamma|$ times, the derivative will hit

$$(\omega(V_0, V_1))^N e^{iu\frac{\hbar}{2}\omega(V_0, V_1)} \hat{a}(V_0) \hat{b}(V_1),$$

which will result in either decreasing the order of the polynomial $(\omega(V_0, V_1))^N$, or bringing down factors $\hbar V_1$ from the exponential, or differentiating $\hat{a}(V_0)$. The final integrand is therefore bounded above by

$$\langle V_0 \rangle^N \langle V_1 \rangle^{N+|\gamma|} |\langle D \rangle^{|\gamma|} \hat{a}(V_0)| |\hat{a}(V_1)|,$$

which leads to (3.11) by inverse Fourier transform. $\square$

Remark 3.6. As usual, the L^1 norms as in (3.11) can be bounded by seminorms of $\mathcal{S}$: $\|f\|_{L^1(\mathbb{R}^n)} \leq \|\langle x \rangle^{n+1} f\|_{L^\infty(\mathbb{R}^n)}$.

As a consequence, we obtain the following asymptotic expansion for the Moyal product.

Theorem 3.7. *The Moyal product of two symbols $a, b \in \mathcal{S}(\mathbb{R}^d)$ satisfies the following asymptotic expansion:*

(3.12)

$$\begin{aligned} a \#_{\hbar} b &= \sum_{j=0}^{N-1} \frac{(i\hbar/2)^j}{j!} a(\rho) \left(\omega(\overleftarrow{D}, \overrightarrow{D}) \right)^j b(\rho) + \mathcal{O}(\hbar^N)_{\mathcal{S}} \\ &= a(\rho)b(\rho) + \frac{i\hbar}{2} (D_{\xi}a \cdot D_x b - D_x a \cdot D_{\xi}b) - \frac{\hbar^2}{8} a(\rho) \left(\overleftarrow{D}_{\xi} \cdot \overrightarrow{D}_x - \overleftarrow{D}_x \cdot \overrightarrow{D}_{\xi} \right)^2 b(\rho) + \mathcal{O}(\hbar^3)_{\mathcal{S}} \\ &= a(\rho)b(\rho) - \frac{i\hbar}{2} \{a, b\} - \frac{\hbar^2}{8} a(\rho) \left(\left(\overleftarrow{D}_{\xi} \cdot \overrightarrow{D}_x \right)^2 + \left(\overleftarrow{D}_x \cdot \overrightarrow{D}_{\xi} \right)^2 - 2 \overleftarrow{D}_{\xi} \cdot \overrightarrow{D}_x \overleftarrow{D}_x \cdot \overrightarrow{D}_{\xi} \right) b(\rho) + \mathcal{O}(\hbar^3)_{\mathcal{S}}. \end{aligned}$$

Remark 3.8. This expansion exhibits the following features:

- (1) The first term ($\hbar^0$ term) is equal the *classical pointwise product* of the two symbols. For this reason, the Moyal product can be considered as a *noncommutative deformation* of the (commutative) product of classical observables.
- (2) The second term ($\hbar^1$) is proportional to **the Poisson bracket** of the classical observables, which is antisymmetric w.r.t. exchanging a and b .
- (3) This antisymmetry will be the case for all odd-order terms $\hbar^{2k+1}$, while the even-order terms (like the $\hbar^2$ term above) will be symmetric.

From point 1 we draw the following

Definition 3.9. If we consider initial symbols a, b independent of $\hbar$, the function $c(\hbar) = \sigma_{\hbar}^W(\text{Op}_{\hbar}^W(a) \text{Op}_{\hbar}^W(b))$ explicitly depends on $\hbar$, but its main term (order $\hbar^0$) does not. We call this first term in the expansion (3.12) the *principal symbol* of the operator $\text{Op}_{\hbar}^W(a) \text{Op}_{\hbar}^W(b)$, denoted $\sigma_0(\text{Op}_{\hbar}^W(a) \text{Op}_{\hbar}^W(b))$.

The above property (1). can thus be expressed as

$$\sigma_0^W(\text{Op}_{\hbar}^W(a) \text{Op}_{\hbar}^W(b)) = ab.$$

Claim 3.10. All quantizations $\text{Op}_{\hbar}^t$ lead to the same principal symbol:

$$\text{Op}_{\hbar}^t(a) \text{Op}_{\hbar}^t(b) = \text{Op}_{\hbar}^t(ab) + \mathcal{O}(\hbar).$$

The point (2) will have important consequences concerning the dynamics generated by the Schrödinger equation, as we analyze in the next subsection.

The expansion (3.12) of the product of two pseudodifferential operators embodies the *symbol calculus*, or (semiclassical) *pseudodifferential calculus*, which is at the heart of semiclassical/microlocal analysis. This calculus allows to connect properties of the operators, with

properties of their symbols. For the moment our symbols are all in $\mathcal{S}(\mathbb{R}^{2d})$, but in the next section we will extend this calculus to more general symbol classes. Before that, we present two interesting applications of this calculus:

- the quantum-classical correspondence, expressed through the evolution of observables (Egorov theorem)
- the first notions of (semiclassical) microlocalization: essential supports and wavefront sets.

3.3. Commutator vs. Poisson bracket: the quantum-classical correspondence. So far we have described the quantum dynamics in terms of the evolution of wavefunctions $u(t)$ through the Schrödinger equation

$$i\hbar\partial_t u(x, t) = [P_\hbar u](x, t), \quad u(0, x) = u_0(x).$$

If we want to test the wavefunction $u(t, x)$ through the observable $A_\hbar$, it makes sense to analyze the time evolution of the quantum average $\langle u(t), A_\hbar u(t) \rangle$. Calling $U_\hbar(t) = e^{-itP_\hbar/\hbar}$ the propagator of the Schrödinger equation, this average can be expressed in two ways:

$$\begin{aligned} \langle u(t), A_\hbar u(t) \rangle &= \langle U_\hbar(t)u_0, A_\hbar U_\hbar(t)u_0 \rangle \\ (3.13) \quad &= \langle u_0, U_\hbar(t)^* A_\hbar U_\hbar(t)u_0 \rangle \stackrel{\text{def}}{=} \langle u_0, A_\hbar(t)u_0 \rangle. \end{aligned}$$

In the last expression, we have used the evolution of the observable $A_\hbar$, which is dual to that of wavefunctions. This evolution is called the *Heisenberg evolution* in quantum mechanics. Mathematically, it is just the adjoint action of the Schrödinger group on the observable $A_\hbar$. Notice that $A_\hbar(t)$ remains selfadjoint, and keeps the same spectrum throughout the evolution. A simple computation shows (without paying attention to questions of domains) that the infinitesimal evolution of an observable is given by:

$$(3.14) \quad \frac{d}{dt} A_\hbar(t) = (iP_\hbar/\hbar)A_\hbar(t) + A_\hbar(t)(-iP_\hbar/\hbar) = \frac{i}{\hbar}[P_\hbar, A_\hbar(t)],$$

where we used the standard notation for the commutator between the two operators.

From the points 2 and 3 in Remark 3.8, we draw the following expansion of the commutator:

Corollary 3.11. (*Commutator of Ψ DOs*). *For $a, b \in \mathcal{S}$, the commutator of the corresponding Weyl quantizations satisfy*

$$\begin{aligned} [\text{Op}_\hbar^W(a), \text{Op}_\hbar^W(b)] &= \text{Op}_\hbar^W(a \#_\hbar b - b \#_\hbar a) \\ (3.15) \quad &= \frac{\hbar}{i} \text{Op}_\hbar^W(\{a, b\}) + \text{Op}_\hbar^W(\mathcal{O}(\hbar^3)). \end{aligned}$$

This identity is at the heart of the semiclassical correspondence.

Exercise 3.12. For a general parameter $t \in [0, 1]$, the quantization Op_h^t satisfies the less precise expansion

$$[\text{Op}_h^t(a), \text{Op}_h^t(b)] = \frac{\hbar}{i} \text{Op}_h^t(\{a, b\}) + \text{Op}_h^W(\mathcal{O}(\hbar^2)).$$

A specificity of the Weyl quantization resides in the absence of a term $\mathcal{O}(\hbar^2)$ in the expansion of the commutator.

The fact that **the commutator of two operators is approximately represented by the quantization of the Poisson bracket** is an important property of quantization.

Why is this connection so important?

Because, in a Hamiltonian system generated by a Hamiltonian¹¹ $p(x, \xi)$, we had found in (1.18) that the infinitesimal evolution of an observable a is given by a Poisson bracket:

$$\{p, a(t)\} = \frac{d}{dt}a(t), \quad \text{where } a(t) = (a \circ \Phi_H^t).$$

On the other hand, we have seen above that the infinitesimal quantum evolution of an observable $A = \text{Op}_h^W(a)$, through the dynamics generated by the quantum Hamiltonian $P = \text{Op}_h^W(p)$, is described by a commutator

$$\frac{i}{\hbar} [P, A(t)] = \frac{d}{dt}A(t).$$

Hence, the correspondence (3.15) connects the quantum and classical evolutions of observables, up to a small semiclassical remainder:

$$(3.16) \quad \boxed{\frac{i}{\hbar} [P, A] = \frac{i}{\hbar} [\text{Op}_h^W(p), \text{Op}_h^W(a)] = \text{Op}_h^W(\{p, a\}) + \mathcal{O}(\hbar^2)}$$

The following **Egorov Theorem** formulates this **quantum-classical correspondence between the evolution of classical and quantum observables** in an integrated form. We will first express it with a remainder expressed in the $L^2 \rightarrow L^2$ norm, hence we first need to estimate this norm in terms of the symbol, anticipating on the more general Calderon-Vaillancourt Theorem:

Proposition 3.13. *Let $a \in \mathcal{S}(\mathbb{R}^{2d})$. Then there exists $C(a) > 0$ such that, for any $h \in (0, 1]$ and any $t \in [0, 1]$,*

$$\forall u \in \mathcal{S}(\mathbb{R}^d), \quad \|\text{Op}_h^t(a)u\|_{L^2} \leq C(a)\|u\|_{L^2}.$$

As a result, the operator $\text{Op}_h^t(a)$ can be extended to a bounded operator on $L^2(\mathbb{R}^d)$. The constant $C(a)$ can be estimated as follows: there exists $C_d > 0$ depending on the dimension,

¹¹At this stage, let us assume that the Hamiltonian $p \in \mathcal{S}(\mathbb{R}^{2d})$.

such that we can take

$$C(a) = C_d \sum_{|\alpha| \leq 2d+1} \|\partial^\alpha a\|_{L^1}.$$

Proof. The Fourier transform $\hat{a} \in \mathcal{S}$. From the expression (2.17) of $\text{Op}_h^W(a)$ and the unitarity of the translation operators T_{hV_0} on L^2 , we get:

$$\|\text{Op}_h^W(a)\|_{L^2 \rightarrow L^2} \leq \int |\hat{a}(V_0)| \frac{dV_0}{(2\pi)^d} = (2\pi)^{-d} \|\hat{a}\|_{L^1} \leq C_d \sum_{|\alpha| \leq 2d+1} \|\partial^\alpha a\|_{L^1}.$$

From the relation (2.19) between the symbols of different quantizations, we find that the above bound works as well for all t -quantizations. $\square$

Equipped with this $L^2 \rightarrow L^2$ estimate, we can prove a (relatively basic) form of the quantum-classical correspondence.

Theorem 3.14. (*Egorov theorem - main order - Schwartz symbols*). Take $p, a \in \mathcal{S}(\mathbb{R}^{2d})$ for the classical Hamiltonian and observable, and their quantizations $P_h = \text{Op}_h^W(p)$, $A_h = \text{Op}_h(a)$ for the corresponding quantum operators. Let $a(t)$ (resp. $A_h(t)$) be the classical (resp. quantum) evolution of the observable. Then for each fixed time $t \in \mathbb{R}$,

$$(3.17) \quad A_h(t) = \text{Op}_h^W(a(t)) + \mathcal{O}(\hbar^2)_{L^2 \rightarrow L^2}.$$

For given $T > 0$, the remainder is bounded uniformly for $t \in [-T, T]$.

Proof. The proof will result from the integration of the infinitesimal correspondence (3.16). To alleviate notations, we will call

$$A_0(t) \stackrel{\text{def}}{=} \text{Op}_h^W(a(t)), \quad \text{and} \quad \dot{A}_0(t) \stackrel{\text{def}}{=} \frac{d}{dt} A_0(t) = \text{Op}_h^W(\{p, a(t)\}).$$

Our goal will be to compare $A_h(t)$ with $A_0(t)$. We notice that $A_h(0) = A_0(0)$. It is then tempting to compute the time derivative of $A_h(t) - A_0(t)$:

$$\begin{aligned} \frac{d}{dt} (A_h(t) - A_0(t)) &= \frac{i}{\hbar} [P, A_h(t)] - \text{Op}_h^W(\{p, a(t)\}) \\ &= \frac{i}{\hbar} U_h(t)^* [P, A_h] U_h(t) - \text{Op}_h^W(\{p, a\}(t)), \end{aligned}$$

but we cannot a priori compare both terms. We must use more cleverly the unitarity of $U_h(t)$: we will apply *Duhamel's trick*, which consists in interpolating between $A_0(t)$ and $A_h(t)$ through the following family of operators:

$$(3.18) \quad A(t; s) \stackrel{\text{def}}{=} U_h(s)^* A_0(t - s) U_h(s), \quad t, s \in \mathbb{R}.$$

We notice that $A(t; 0) = A_0(t)$, while $A(t; t) = A_h(t)$. For given $t \in [-T, T]$, the derivative of $A(t; s)$ w.r.t. s gives:

$$\begin{aligned} \frac{d}{ds} A(t; s) &= U_h(s)^* \left(\frac{i}{\hbar} [P, A_0(t-s)] - \dot{A}_0(t-s) \right) U_h(s) \\ &\stackrel{\text{def}}{=} \hbar^2 U_h(s)^* R_2(t-s) U_h(s). \end{aligned}$$

What we gain with this trick is the full control on the operator $A_0(t-s)$ and its time derivative appearing on the right hand side. Indeed, the function $a(t) = a \circ \Phi_p^t$ belongs to a bounded set in $\mathcal{S}(\mathbb{R}^{2d})$ for $t \in [-2T, 2T]$. As a result, we may apply the estimate (3.16) to $A_0(t-s)$:

$$\frac{i}{\hbar} [P, A_0(t-s)] - \dot{A}_0(t-s) = \hbar^2 R_2(t-s; \hbar), \text{ where } R_2(t-s; \hbar) = \text{Op}_h^W(r_2(t-s; \hbar)).$$

The remainder symbol $r_2(t-s; \hbar)$ is bounded in $\mathcal{S}$, uniformly in $t, s \in [-T, T]$ and $\hbar \in (0, 1]$. By integrating over $s \in [0, t]$, we thus find:

$$A(t; t) - A(t; 0) = A_h(t) - A_0(t) = \hbar^2 \int_0^t U_h(s)^* R_2(t-s; \hbar) U_h(s) ds.$$

Since $r_2(t-s; \hbar)$ remains in a bounded set in $\mathcal{S}$, applying Proposition 3.13 we obtain for some constant $C_{a,T} > 0$:

$$\boxed{\|A_h(t) - A_0(t)\|_{L^2 \rightarrow L^2} \leq C_{a,T} |t| \hbar^2, \quad \forall |t| \leq T, \quad \hbar \in (0, 1]}$$

□

Remark 3.15. The remainder $\mathcal{O}(\hbar^2)$ is due to our use of the Weyl quantization. A similar Egorov estimate exists for any t -quantization, yet in general the error will be $\mathcal{O}(\hbar)$.

3.4. A second application of the symbol calculus: essential support and wavefront set. Let us describe a second important application of the asymptotic expansion (3.12) for the Moyal product. We will describe the phase space regions where a semiclassical family of operators $(A_h)_{h \in (0,1]}$, resp. a family of wavefunctions $(u(\hbar))_{h \in (0,1]}$, are essentially concentrated in the limit $\hbar \rightarrow 0$.

3.4.1. Essential supports of symbols / Wavefront sets of operators. One simple application of the expansion (3.12) concerns the case of symbols $a, b \in \mathcal{S}(\mathbb{R}^{2d})$ with disjoint supports¹².

Proposition 3.16. *Assume $a, b \in \mathcal{S}(\mathbb{R}^{2d})$ have disjoint supports. Then the symbol $a \#_{\hbar} b = \mathcal{O}(\hbar^\infty)_{\mathcal{S}}$ (one sometimes says that the symbol is semiclassically residual).*

¹²Most of what follows will later be generalized to symbols not belonging to $\mathcal{S}$.

In the case a, b are compactly supported but $\text{supp } a \cap \text{supp } b \neq \emptyset$, we no longer have $a \#_h b = \mathcal{O}(\hbar^\infty)_{\mathcal{S}}$, yet the symbol $a \#_h b$ will be very small away from $\text{supp } a \cap \text{supp } b$. On the other hand, for each given $\hbar \in (0, 1]$, the support of $a \#_h b$ will in general be the full space $\mathbb{R}^{2d}$. This leads us to replace the notion of support by that of *essential support*.

Definition 3.17. Assume that a family of symbols $(a(h) \in \mathcal{S}(\mathbb{R}^{2d}))_{h \in (0, 1]}$ is uniformly bounded in $\mathcal{S}$, and assume there exists a compact set $K \Subset \mathbb{R}^{2d}$ such that, for any $\chi \in C_b^\infty(\mathbb{R}^{2d})$ with $\text{supp } \chi \cap K = \emptyset$, one has $\chi a(h) \in h^\infty \mathcal{S}$.

We then say that the symbol $a(h)$ has a *compact essential support*, and its essential support $\text{ess-supp } a(h)$ is given by the smallest such set K .

Roughly speaking, the essential support describes the points near which $a(\rho; \hbar)$ is NOT $\mathcal{O}(\hbar^\infty)_{C^\infty}$. Although the definition of $\text{ess-supp } a(h)$ is not easy to apprehend, for an $\hbar$ -independent symbol we recover the usual definition:

Example 3.18. If $a \in C_c^\infty(\mathbb{R}^{2d})$ is independent of $\hbar$, one has $\text{ess-supp } a = \text{supp } a$.

In case our $\hbar$ -dependent symbol is obtained through the Moyal product of two symbols, the following result can be seen as a generalization of Proposition 3.16:

Proposition 3.19. Assume two families of symbols $a(h), b(h)$ are uniformly bounded in $\mathcal{S}(\mathbb{R}^{2d})$, and both have compact essential supports. Then $a \#_h b$ also has compact essential support, and

$$\text{ess-supp}(a \#_h b) \subset \text{ess-supp}(a) \cap \text{ess-supp}(b).$$

For instance, if we take $a, b \in C_c^\infty(\mathbb{R}^{2d})$ independent of $\hbar$, the above Proposition describes the essential support of the symbol $a \#_h b$.

The notion of essential support parallels that of wavefront set, which concerns the corresponding operators.

Definition 3.20. If the essential support of a family of symbols $(a(\hbar))_{\hbar \in (0, 1]}$ is compact, then the *semiclassical wavefront set* of the corresponding family of operators $(A_\hbar = \text{Op}_\hbar^W(a(\hbar)))_{\hbar \in (0, 1]}$ is equal to this essential support:

$$\text{WF}_\hbar(\text{Op}_\hbar(a)) \stackrel{\text{def}}{=} \text{ess-supp } a(h).$$

This notion means that the action of the operator $A = (A_\hbar)_{\hbar \in (0, 1]}$ is negligible outside this compact part of phase space.

Proposition 3.19 can be rephrased as:

$$\text{WF}_\hbar(A \circ B) \subset \text{WF}_\hbar(A) \cap \text{WF}_\hbar(B),$$

provided the objects in the RHS are well-defined.

3.4.2. Wavefront set of a semiclassical family of states. Above we have defined the wavefront set of a family of operators, corresponding to the phase space region where the symbol $a(h)$ of the operator is not negligible. We now define a notion of wavefront set (or of microlocalization) associated with a family of wavefunctions $(u(x, h))_{h \in (0, 1]}$. This notion will describe the regions of phase space where the wavefunctions $u(h)$ are *microlocalized* (notice that $u(h)$ only depends on the space variable $x \in \mathbb{R}^d$).

In general our functions $u(x, h)$ will be allowed to oscillate more and more in x when $h \searrow 0$, so we certainly cannot require them to be in a bounded set of $\mathcal{S}(\mathbb{R}^d)$ (see e.g the Example 3.23 below). For a moment we will assume that our states are L^2 -normalized: $\|u(h)\|_{L^2} = 1$, uniformly in $h \in (0, 1]$.

Definition 3.21. (Wavefront set of u) Let $u = (u(h))_{h \in (0, 1]}$ be a family of normalized $L^2(\mathbb{R}^d)$ functions. The semiclassical wavefront set of this family, $\text{WF}_h(u)$, is a subset of $\mathbb{R}^{2d}$, which we define by its complement. Namely, a point $\rho_0 = (x_0, \xi_0)$ belongs to $\mathbb{C} \text{WF}_h(u)$ iff there exists a symbol $a \in \mathcal{S}(\mathbb{R}^{2d})$ with $a(\rho_0) \neq 0$, such that¹³ $\|\text{Op}_h(a)u(h)\|_{L^2} = \mathcal{O}(h^\infty)$.

From the continuity of the symbol a involved in the definition, we see that the property $\rho_0 \notin \text{WF}_h(u)$ is an open property. As a consequence, $\text{WF}_h(u)$ is necessarily a *closed* subset of $\mathbb{R}^{2d}$.

The definition could let believe that the symbol a has to be selected with a lot of care. We actually have a large freedom to choose this symbol, as shown in the following

Proposition 3.22. Assume $\rho_0 \notin \text{WF}_h(u)$. Then for any $b = b(h) \in \mathcal{S}(\mathbb{R}^{2d})$ with $\text{ess-supp } b$ a sufficiently small neighbourhood of ρ_0 , we have

$$\|\text{Op}_h(b)u(h)\|_{L^2} = \mathcal{O}(h^\infty).$$

Proof. By assumption, there exists $a \in \mathcal{S}(\mathbb{R}^{2d})$ such that $a(\rho_0) \neq 0$ and $\|\text{Op}_h(a)u\|_{L^2} = \mathcal{O}(h^\infty)$. There exists a small neighbourhood U_{ρ_0} such that $|a(\rho)| \geq c > 0$ for all $\rho \in U_{\rho_0}$. Let us construct a symbol $c(h) \in \mathcal{S}$ such that the Moyal product

$$(3.19) \quad c(h) \#_h a = 1 + \mathcal{O}(h^\infty)_{C^\infty(U_{\rho_0})}$$

Such a symbol $c(h)$ is then called a *microlocal inverse* of a in the region U_{ρ_0} .

¹³As we will see later, the condition can be strengthened to $\text{Op}_h(a)u(h) = \mathcal{O}(h^\infty)_{\mathcal{S}}$.

The construction of $c(h)$ proceeds by computing its semiclassical expansion, order by order. Namely, we write formally the Ansatz $c \sim \sum \hbar^j c_j$ and using the expansion of the Moyal product, we solve, order by order in powers of $\hbar$, the equation (3.19):

$$\begin{aligned} \text{order } h^0 : \quad & c_0(\rho)a(\rho) = 1 \implies c_0(\rho) = \frac{1}{a(\rho)} \\ \text{order } h^1 : \quad & c_1(\rho)a(\rho) - \frac{i}{2} \{c_0, a\}(\rho) = 0 \implies c_1(\rho) = 0 \\ \text{order } h^2 : \quad & c_2(\rho)a(\rho) - \frac{i}{2} \{c_1, a\}(\rho) - \frac{1}{8} c_0(\rho) \left(\overleftarrow{D}_\xi \cdot \overrightarrow{D}_x - \overleftarrow{D}_x \cdot \overrightarrow{D}_\xi \right)^2 a(\rho) = 0 \\ & \implies c_2(\rho) = \frac{1}{8a(\rho)} \left[c_0 \left(\overleftarrow{D}_\xi \cdot \overrightarrow{D}_x - \overleftarrow{D}_x \cdot \overrightarrow{D}_\xi \right)^2 a \right](\rho), \end{aligned}$$

and so on. At any order j the term $c_j(\rho)$ is obtained by dividing by $a(\rho)$ an explicit expression involving the functions $a, c_0, c_1, \dots, c_{j-1}$. We thus obtain a sequence of functions $(c_j)_{j \geq 0}$ defined on U_{ρ_0} , which we may extend outside the neighbourhood, to obtain functions $c_j \in \mathcal{S}$. Using Borel's Lemma, there exists a function $c(h) \in \mathcal{S}$ such that $c(h) \sim \sum_j \hbar^j c_j$, and hence satisfies (3.19).

Take a symbol $b(h) \in \mathcal{S}(\mathbb{R}^{2d})$ satisfying $b(h) \sim \sum \hbar^j b_j$, where all $b_j \in C_c^\infty(U_{\rho_0})$, and consider the double Moyal product $b(h) \#_h c(h) \#_h a$. The property (3.19) shows that

$$b(h) \#_h c(h) \#_h a = b(h) \#_h 1 + \mathcal{O}(\hbar^\infty)$$

in $C^\infty(U_{\rho_0})$; but since $b(h)$ is essentially supported inside U_{ρ_0} the above equality also holds in $\mathcal{S}(\mathbb{R}^{2d})$. Quantizing these symbols and using Prop. 3.13, we find

$$\| \text{Op}_\hbar(b)u \|_{L^2} = \| \text{Op}_\hbar(b) \text{Op}_\hbar(c) \text{Op}_\hbar(a)u \|_{L^2} + \mathcal{O}(\hbar^\infty) = \mathcal{O}(\hbar^\infty).$$

□

Let us now give some (characteristic) examples of families $(u(h))_h$. Most of the time, the states $u(h)$ we will consider will belong to $\mathcal{S}$, but with unbounded seminorms when $h \searrow 0$. Our first example is provided by *truncated plane waves*.

Example 3.23. Fix $\xi_0 \in \mathbb{R}^d$ and a function $\chi \in C_c^\infty(\mathbb{R}^d)$ such that $\|\chi\|_{L^2(\mathbb{R}^d)} = 1$, and consider the family of states

$$(3.20) \quad e_{\xi_0}(x; \hbar) = \chi(x) e^{i\xi_0 \cdot x / \hbar}.$$

Its wavefront set $\text{WF}_\hbar(e_{\xi_0}) = \{(x, \xi_0), x \in \text{supp } \chi\} = \text{supp } \chi \times \{\xi_0\}$. In particular, for any function $u \in C_c^\infty(\mathbb{R}^d)$ independent of $\hbar$, the wavefront set $\text{WF}_\hbar(u) = \text{supp } \chi \times \{0\}$.

Another standard example is given by Gaussian wavepackets (also called *coherent states*). These represent the strongest form of microlocalization.

Example 3.24. Fix $\rho_0 = (x_0, \xi_0) \in \mathbb{R}^{2d}$, $\alpha > 0$, and consider the family

$$e_{\rho_0, \alpha}(x; h) = (\pi h)^{-d/4} \exp \left(-\frac{|x - x_0|^2}{2h\alpha^2} + i\xi_0 \cdot x \right).$$

Its semiclassical wavefront set $\text{WF}_h(e_{\rho_0}) = \{\rho_0\}$. For this reason, those coherent states are sometimes considered as “quantum phase space points”.

The wavefront sets of states $(u(h))$ and operators $A = \text{Op}_h(a)$ combine in a natural way:

Proposition 3.25. *Consider a family $(u(h))_h$, and a symbol $a = (a(h))_h$ uniformly bounded in $\mathcal{S}'(\mathbb{R}^{2d})$. Then*

$$(i) \text{WF}_h(\text{Op}_h(a)u) \subset \text{WF}_h(u).$$

$$(ii) \text{ If } a \text{ has a compact essential support, then } \text{WF}_h(\text{Op}_h(a)u) \subset \text{ess-supp } a \cap \text{WF}_h(u).$$

Proof. For the first statement, let us assume that $\rho_0 \notin \text{WF}_h(u)$. We want to prove that $\rho_0 \notin \text{WF}_h(\text{Op}_h(a)u)$. Let us consider a function $c \in C_c^\infty(\mathbb{R}^{2d})$ with a small support U_{ρ_0} near ρ_0 . The expansion of the Moyal product shows that the symbol $b(h) \stackrel{\text{def}}{=} c \#_h a$ has essential support inside U_{ρ_0} . From Proposition 3.22, provided we choose U_{ρ_0} small enough, we'll have $\|\text{Op}_h(b(h))u\|_{L^2} = \mathcal{O}(h^\infty)$. This just proves that $\|\text{Op}_h(c)(\text{Op}_h(a)u)\|_{L^2} = \mathcal{O}(h^\infty)$, hence $\rho_0 \notin \text{WF}_h(\text{Op}_h(a)u)$.

Let us now assume that $\text{ess-supp } a$ is compact. For any $\rho_0 \notin \text{ess-supp } a$, we may consider a symbol b supported in a small neighbourhood of ρ_0 , such that $b(\rho_0) \neq 0$ and $\text{ess-supp } b \cap \text{ess-supp } a = \emptyset$. From Propositions 3.16 and 3.13 we obtain $\|\text{Op}_h(b)\text{Op}_h(a)u\|_{L^2} = \mathcal{O}(h^\infty)$, hence $\rho_0 \notin \text{WF}_h(\text{Op}_h(a)u)$, which proves that $\rho_0 \notin \text{WF}_h(\text{Op}_h(a)u)$. $\square$

Example 3.26. (Microlocal partition of unity of $\mathbb{R}^{2d}$) Let us consider a smooth resolution of identity $1 = \sum_n \chi_n$, where each $\chi_n \in C_c^\infty(\mathbb{R}^{2d})$. We then obtain a decomposition of a state $u \in L^2(\mathbb{R}^d)$ into

$$u = \sum_n \text{Op}_h(\chi_n)u.$$

According to the above Proposition, each term $\text{Op}_h(\chi_n)u$ is microlocalized in $\text{supp } \chi_n \Subset \mathbb{R}^{2d}$, that is $\text{WF}_h(\text{Op}_h(\chi_n)u) \subset \text{supp } \chi_n$.

4. EXTENDING THE QUANTIZATION TO NONDECAYING SYMBOLS

So far we have defined the quantization of symbols of the form $f(x)$, $g(\xi)$, with $f, g \in \mathcal{S}(\mathbb{R}^d)$, or $a \in \mathcal{S}(\mathbb{R}^{2d})$. As we have just seen, such fast decaying functions are useful to analyze the microlocalization of quantum states (we will often use cutoff functions $\chi \in C_c^\infty(\mathbb{R}^{2d})$). However, we also want to be able to quantize unbounded symbols, like the standard Hamiltonian $p(x, \xi) = \frac{|\xi|^2}{2} + V(x)$, which is unbounded in ξ , but can also be unbounded in x , depending on the potential V . We will indeed show that our quantization procedures can be naturally extended to certain *classes of symbols* with appropriate growth properties at infinity.

4.1. The class of uniformly bounded symbols $S(\mathbb{R}^{2d})$. One useful class of symbols is the class $S(\mathbb{R}^{2d})$ of smooth functions, with all derivatives uniformly bounded over $\mathbb{R}^{2d}$. In general we will consider $\hbar$ -dependent symbols $a = (a(\hbar))_{\hbar \in (0,1]}$; an important property of this class is that all bounds on derivatives are uniform w.r.t. $\hbar \in (0, 1]$:

$$S(\mathbb{R}^{2d}) \stackrel{\text{def}}{=} \left\{ a = a(\hbar) \in C^\infty(\mathbb{R}^{2d}), \quad \sup_{\rho \in \mathbb{R}^{2d}} \left| \partial_x^\alpha \partial_\xi^\beta a(\rho; \hbar) \right| \leq C_{\alpha, \beta}, \quad \forall \hbar \in (0, 1] \right\}.$$

For a moment, we will not investigate the limit $\hbar \rightarrow 0$, but **freeze** the value of $\hbar > 0$.

For a symbol $a \in S(\mathbb{R}^{2d})$, and for a wavefunction $u \in \mathcal{S}(\mathbb{R}^d)$, the integral

$$I(u)(x) = \text{Op}_\hbar^t(a)u(x) = \iint e^{i\frac{\xi \cdot (x-y)}{\hbar}} a(tx + (1-t)y, \xi) u(y) \frac{dy d\xi}{(2\pi\hbar)^d}$$

is absolutely convergent in the y variable, but *not* in the ξ variable. Still the presence of an oscillatory phase will help us to give a meaning to such an **oscillatory integral**. The strategy will be to apply sufficiently many *formal* integrations by parts in the variable y , in order to recover an absolutely convergent integral in both variables y, ξ . To proceed, for each ξ we insert the differential operator

$$L_\xi \stackrel{\text{def}}{=} \frac{1 + i\hbar\xi \cdot \partial_y}{1 + |\xi|^2}, \quad \text{which satisfies} \quad L_\xi e^{i\frac{\xi \cdot (x-y)}{\hbar}} = e^{i\frac{\xi \cdot (x-y)}{\hbar}}.$$

Since we assume that $u \in \mathcal{S}(\mathbb{R}^d)$, the integrand decays fast when $|y| \rightarrow \infty$. We are then allowed to integrate by parts w.r.t. the variables $y = (y_1, \dots, y_d)$, which amounts to applying the transposed of this operator, ${}^tL_\xi = \frac{1 - i\hbar\xi \cdot \partial_y}{1 + |\xi|^2}$ to the rest of the integrand:

$$\begin{aligned} I(u) &= \iint \left(L_\xi e^{i\frac{\xi \cdot (x-y)}{\hbar}} \right) a(tx + (1-t)y, \xi) u(y) \frac{dy d\xi}{(2\pi\hbar)^d} \\ &= \iint e^{i\frac{\xi \cdot (x-y)}{\hbar}} {}^tL_\xi [a(tx + (1-t)\bullet, \xi) u(\bullet)](y) \frac{dy d\xi}{(2\pi\hbar)^d}. \end{aligned}$$

The action of ${}^tL_\xi$ on au differentiates the symbol a and the state u , but the resulting product is still fast decaying in y . In the ξ variable we have gained a factor $\frac{\mathcal{O}(\xi)}{1+|\xi|^2}$. Here it is handy to use the “Japanese brackets” notation¹⁴ $\langle \xi \rangle \stackrel{\text{def}}{=} (1 + |\xi|^2)^{1/2}$, and say that our integration by parts has produced an extra decaying factor $\mathcal{O}(\langle \xi \rangle^{-1})$.

Definition 4.1. (Kernels defined by oscillatory integrals) Applying this integration by parts $d + 1$ times, we obtain an integrand behaving like $\mathcal{O}(\langle y \rangle^{-\infty} \langle \xi \rangle^{-d-1})$ at infinity, which makes the integral absolutely convergent in all directions. **This converging integral is be taken as the definition for the oscillatory integral $I(u)$** , and therefore as the definition for the action of the operator $\text{Op}_h^t(a)$ on $u \in \mathcal{S}(\mathbb{R}^d)$.

More general operators: symbols in $\mathcal{S}'(\mathbb{R}^{2d})$. Let us for a while set $\hbar = 1$ to alleviate our notations. The above manipulation are natural if we consider the large class of operators with Schwartz kernels $K(x, y)$ given by tempered distributions on $\mathbb{R}^d \times \mathbb{R}^d$. To simplify the notations, we will restrict ourselves to the Weyl quantization. When the symbol $a \in \mathcal{S}'(\mathbb{R}^d)$, the Schwartz kernel

$$(4.1) \quad K_a(x, y) = \int e^{i\xi \cdot (x-y)} a\left(\frac{x+y}{2}, \xi\right) \frac{d\xi}{(2\pi)^d}$$

is a well-defined Schwartz function, and can be easily expressed in terms of the partial Fourier transform of the symbol a w.r.t. its second variable:

$$K_a(x, y) = (2\pi)^{-d/2} [\mathcal{F}_{\xi \rightarrow z} a] \left(\frac{x+y}{2}, z \right) \Big|_{z=x-y}.$$

Proposition 4.2. *The above formula can be extended to symbols $a \in \mathcal{S}'(\mathbb{R}_{x,\xi}^{2d})$, and defines a kernel $K_a \in \mathcal{S}'(\mathbb{R}_{x,y}^{2d})$. The latter defines a continuous operator $\text{Op}_h^W(a) : \mathcal{S}(\mathbb{R}^d) \rightarrow \mathcal{S}'(\mathbb{R}^d)$.*

Proof. For a function $a \in \mathcal{S}(\mathbb{R}^{2d})$, the formula (4.1) for the kernel $K_a(x, y)$ implies that for any $u, v \in \mathcal{S}(\mathbb{R}^d)$, we have:

$$\begin{aligned} \langle \text{Op}_h^W(a)v, u \rangle_{\mathcal{S}'(\mathbb{R}^d), \mathcal{S}(\mathbb{R}^d)} &= \langle K_a, u(x)v(y) \rangle_{\mathcal{S}'(\mathbb{R}^{2d}), \mathcal{S}(\mathbb{R}^{2d})} \\ &= (2\pi)^{-d/2} \langle [\mathcal{F}_{\xi \rightarrow z} a](s, z), u(s + z/2)v(s - z/2) \rangle_{\mathcal{S}'(\mathbb{R}^{2d}), \mathcal{S}(\mathbb{R}^{2d})}. \end{aligned}$$

Since the function $(s, z) \mapsto u(s + z/2)v(s - z/2)$ defines an element of $\mathcal{S}(\mathbb{R}^{2d})$, the latter bracket still makes sense when $a \in \mathcal{S}'(\mathbb{R}^{2d})$, it defines a distribution $K_a \in \mathcal{S}'(\mathbb{R}_{x,y}^{2d})$. The identification on the first line defines a continuous operator $\text{Op}_h^W(a) : \mathcal{S}(\mathbb{R}^d) \rightarrow \mathcal{S}'(\mathbb{R}^d)$. This interpretation of the integral (4.1) as a distribution allows to use standard regularization tools in the theory of distribution. For instance, the distribution K_a can be obtained as the limit

¹⁴The Japanese bracket behaves like $|\xi|$ when $|\xi| \rightarrow \infty$, but it avoids the problem of singularity and the vanishing of $|\xi|$ at $\xi = 0$.

of a family $K_{a,\epsilon}(x, y) \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$ obtained by inserting the factors $e^{-\epsilon(|y|^2 + |\xi|^2)}$ in the integrand, and taking $\epsilon \rightarrow 0$. $\square$

Back to the class $S(\mathbb{R}^{2d})$. This breadth of Proposition 4.2 has a disadvantage that two operators $A, B : \mathcal{S} \rightarrow \mathcal{S}'$ cannot in general be composed with one another. The important fact about taking a symbol $a \in S(\mathbb{R}^{2d})$ lies in the fact that the resulting operator $\text{Op}_h^W(a)$ maps the space $\mathcal{S}(\mathbb{R}^d)$ to itself.

Theorem 4.3. *For any $a \in S(\mathbb{R}^{2d})$ and any $\hbar \in (0, 1]$, the operator $\text{Op}_h(a)$ acts continuously $\mathcal{S}(\mathbb{R}^d) \rightarrow \mathcal{S}(\mathbb{R}^d)$.*

Remark 4.4. We do not try to control the behaviour of the seminorms when $\hbar \rightarrow 0$. However, by inspecting the occurrences of the factors $\hbar$, one finds that if the derivatives ∂^α involved in the seminorms of $\mathcal{S}(\mathbb{R}^d)$ are replaced by $(\hbar \partial)^\alpha$, then the implied constants are uniform when $\hbar \searrow 0$.

Proof. To alleviate notations we will take $\hbar = 1$. We need to control the seminorms of the function defined by the integral $I(u)$, in terms of the seminorms of u . Again, we will restrict ourselves to the case of Weyl quantization. The action of the differential operator $({}^t L_\xi)^n$ on the product au provides an expression of the type

$$\frac{1}{\langle \xi \rangle^{2n}} (au + * \xi \cdot \partial_y(au) + \cdots * (\xi \cdot \partial_y)^n(au)).$$

(here $*$ just indicates a numerical factor). Since $a \in S(\mathbb{R}^{2d})$, the integrand will be, for any $\ell \geq 0$, bounded above by $\frac{C_a}{\langle \xi \rangle^{n \langle y \rangle^\ell}} (\max_{|\alpha| \leq n} \|\langle y \rangle^\ell \partial^\alpha u\|_{L^\infty})$; hence, if we take $\ell = n = d + 1$, the convergence of $\iint dy d\xi \langle y \rangle^{-d-1} \langle \xi \rangle^{-d-1}$ shows that that

$$|I(u)(x)| \leq C_a \max_{|\alpha| \leq d+1} \|\langle y \rangle^{d+1} \partial^\alpha u\|_{L^\infty}.$$

Here the constant C_a depends on a certain number of S -seminorms of a . Below this constant will vary from line to line.

Differentiating β times $I(u)$ w.r.t. x produces extra factors in the integrand:

$$\partial_x^\beta \left(e^{i\xi \cdot (x-y)} a\left(\frac{x+y}{2}, \xi\right) u(y) \right) = \sum_{\alpha \leq \beta} e^{i\xi \cdot (x-y)} (i\xi)^\alpha \partial_x^{\beta-\alpha} a\left(\frac{x+y}{2}, \xi\right) u(y),$$

so that the integrand now may grow like $\langle \xi \rangle^{|\beta|}$. As a result, we need to integrate by parts $n = |\beta| + d + 1$ times with the operator L_ξ , to let the integrand decay like $\langle \xi \rangle^{-d-1}$, which makes it integrable. In view of the above computation, this will give

$$\|\partial^\beta I(u)\|_{L^\infty} \leq C_a \max_{|\alpha| \leq |\beta| + d + 1} \|\langle y \rangle^{d+1} \partial^\alpha u\|_{L^\infty}.$$

Finally, to show that $\partial^\beta I(u)(x)$ decays like $\langle x \rangle^{-m}$ when $|x| \rightarrow \infty$, we need to apply integration by parts in the variable ξ , using a differential operator “dual” to L_ξ , namely

$$L_x \stackrel{\text{def}}{=} \frac{1 + i\hbar(x-y) \cdot \partial_\xi}{1 + |x-y|^2},$$

which also satisfies $L_x e^{i\frac{\xi \cdot (x-y)}{\hbar}} = e^{i\frac{\xi \cdot (x-y)}{\hbar}}$. We apply m integrations by parts with this operator *after* applying the $|\beta| + d + 1$ integrations by parts with L_ξ , so that we already have enough decay as $|\xi| \rightarrow \infty$. The operator $({}^t L_x)^m$ acts on a sum of terms of the form

$$\sum_{k \leq n} \sum_{\alpha \leq \beta} \frac{(\xi \cdot \partial_y)^k \xi^\alpha}{\langle \xi \rangle^{2n}} \partial_x^{\beta-\alpha} a\left(\frac{x+y}{2}, \xi\right) u(y)$$

The derivatives ∂_ξ will either hit the rational prefactor $\frac{(\xi \cdot \partial_y)^k \xi^\alpha}{\langle \xi \rangle^{2n}}$ (which will improve its decay at infinity), or the symbol $\partial^{\beta-\alpha} a(\bullet, \xi)$ (which leads to a bounded factor), hence the worst term corresponds to hitting only the symbol a :

$$\left| ({}^t L_x)^m \frac{(\xi \cdot \partial_y)^k \xi^\alpha}{\langle \xi \rangle^{2n}} \partial_x^{\beta-\alpha} a\left(\frac{x+y}{2}, \xi\right) u(y) \right| \leq \frac{C_a}{\langle \xi \rangle^{2n-k-|\alpha|} \langle x-y \rangle^m} \max_{|\gamma| \leq k} |\partial^\gamma u(y)|.$$

Taking the worst case $k = n$, $\alpha = \beta$, this gives an upper bound

$$\frac{C_a}{\langle \xi \rangle^{n-|\beta|} \langle x-y \rangle^m} \max_{|\gamma| \leq n} |\partial^\gamma u(y)|.$$

To let appear the seminorms of u , we insert upstairs and downstairs a factor $\langle y \rangle^\ell$, take $n = |\beta| + d + 1$ as above, and get an integrand:

$$\leq \frac{C_a}{\langle \xi \rangle^{d+1} \langle x-y \rangle^m \langle y \rangle^\ell} \langle y \rangle^\ell \max_{|\gamma| \leq |\beta|+d+1} |\partial^\gamma u(y)| \leq \frac{C_a}{\langle \xi \rangle^{d+1} \langle x-y \rangle^m \langle y \rangle^\ell} \max_{|\gamma| \leq |\beta|+d+1} \|\langle y \rangle^\ell \partial^\gamma u\|_{L^\infty}.$$

We can now consider the integral over the RHS. The integral over ξ converges. If $\ell + m \geq d + 1$ the integral over y converges as well. Lemma 4.5 shows that if we take $\ell = \max(m, d + 1)$, the integral over y is bounded by $C \langle x \rangle^{-m}$. We have thus proved that:

$$|\partial^\beta I(u)(x)| \leq \frac{C_a}{\langle x \rangle^m} \max_{|\gamma| \leq |\beta|+d+1} \|\langle y \rangle^{\max(m, d+1)} \partial^\gamma u\|_{L^\infty},$$

where C_a depends on a certain number of seminorms of $a \in S(\mathbb{R}^{2d})$. □

Lemma 4.5. *Consider any pair $(m, \ell) \geq 0$ such that $m + \ell > d$. Then, for any $x \in \mathbb{R}^d$, the integral $I_{d,m,\ell}(x) \stackrel{\text{def}}{=} \int_{\mathbb{R}^d} \langle x-y \rangle^{-m} \langle y \rangle^{-\ell} dy$ converges, and is bounded by*

$$I_{d,m,\ell}(x) \leq C_{d,m,\ell} \left(\begin{cases} \langle x \rangle^{-\ell}, & \text{if } m > d, \\ \langle x \rangle^{-\ell} \log(2 + |x|), & \text{if } m = d, \\ \langle x \rangle^{-\ell-m+d}, & \text{if } m < d \end{cases} + \begin{cases} \langle x \rangle^{-m}, & \text{if } \ell > d, \\ \langle x \rangle^{-m} \log(2 + |x|), & \text{if } \ell = d, \\ \langle x \rangle^{-\ell-m+d}, & \text{if } \ell < d \end{cases} \right).$$

Proof. If $|x| \leq 10$ the result is obvious. Let us then assume that $|x| \geq 10$. We consider the balls $B_0 = B(0, |x|/2)$, $B_1 = B(x, |x|/2)$, and split the integral between B_0, B_1 and $\mathbb{R}^d \setminus (B_0 \cup B_1)$. The first integral

$$\begin{aligned} \int_{B(0, |x|/2)} \langle x - y \rangle^{-m} \langle y \rangle^{-\ell} dy &\asymp \langle x \rangle^{-m} \int_{B(0, |x|/2)} \langle y \rangle^{-\ell} dy \\ &\asymp \langle x \rangle^{-m} \times \begin{cases} 1, & \text{if } \ell > d, \\ \log(|x|), & \text{if } \ell = d, \\ \langle x \rangle^{-\ell+d}, & \text{if } \ell < d. \end{cases} \end{aligned}$$

The integral over $B_1 = B(x, |x|/2)$ gives a similar result. On the complement of $B_0 \cup B_1$, simple trigonometry shows that $\langle x - y \rangle \asymp \langle y \rangle$ with constants uniform w.r.t. x and y , so that the remaining integral is of the order of

$$\int_{\mathbb{R}^d \setminus (B_0 \cup B_1)} \langle y \rangle^{-(m+\ell)} dy \leq \int_{\mathbb{R}^d \setminus B_0} \langle y \rangle^{-(m+\ell)} dy \asymp \langle x \rangle^{-(m+\ell-d)}.$$

In all cases, a simple computation shows that this contribution is smaller or equal to the sum of the two previous ones. $\square$

Example 4.6. If we take $a(x, \xi) \equiv 1$, we obtain a representation of the identity, by recovering the fact that the delta function can be written as $\delta(x - y) = \int e^{i \frac{\xi \cdot (x - y)}{h}} \frac{d\xi}{(2\pi h)^d}$; Equivalently we recover the fact that $\mathcal{F}_h \delta = \frac{1}{(2\pi h)^{d/2}}$.

Example 4.7. Any function $f \in C_b^\infty(\mathbb{R}_x^d)$, leading to the multiplication operator $\text{Op}_h(f)$, is also in the class $S(\mathbb{R}^{2d})$. Any $g \in C_b^\infty(\mathbb{R}_\xi^d)$, leading to the Fourier multiplier $\text{Op}_h(g) = g(hD)$, is also in the class $S(\mathbb{R}^{2d})$.

4.2. Symbols with polynomial growth: order functions. Beyond the class $S(\mathbb{R}^{2d})$, we want to extend the quantization map to symbols $a(x, \xi)$ which may grow as $|x|, |\xi| \rightarrow \infty$. We have seen that formal integration by parts allow to gain factors $\langle \xi \rangle^{-n}$ or $\langle x - y \rangle^{-m}$ in the integrals. For this reason, we will need to assume that the symbols $a(x, \xi)$, and their derivatives, *grow at most polynomially*.

A convenient way to describe such a polynomial growth in phase space is through the notion of *order function*. This notion will allow some flexibility.

Definition 4.8. A function $m : \mathbb{R}^{2d} \rightarrow \mathbb{R}_+^*$ is called an order function if there exists $C_0 > 0, N \in \mathbb{R}$ such that

$$\forall \rho, \rho' \in \mathbb{R}^{2d}, \quad \frac{m(\rho)}{m(\rho')} \leq C_0 \langle \rho - \rho' \rangle^N.$$

As a result, $m(\rho)$ can grow at most polynomially, and can decay at most inverse polynomially when $\rho \rightarrow \infty$.

Example 4.9. Typical order functions will be $m(\rho) = \langle \xi \rangle^N$ for some $N \in \mathbb{R}$, when we only want to allow a growth/decay in momentum: this includes symbols of the type $|\xi|^2 + V(x)$ with a bounded potential. More generally we can use $m(\rho) = \langle \xi \rangle^{N_1} \langle x \rangle^{N_2}$, or $m(\rho) = \langle \rho \rangle^N$ if we want to allow growth/decay both in ξ and x .

To an order function we associate a *symbol class*.

Definition 4.10. Let $m(\rho)$ be an order function. Then we define the symbol class $S(\mathbb{R}^{2d}, m) = S(m)$ as follows:

$$S(m) \stackrel{\text{def}}{=} \{a = a(\hbar) \in C^\infty(\mathbb{R}^{2d}), \forall \alpha \in \mathbb{N}^{2d}, \exists C_\alpha > 0, \forall \rho \in \mathbb{R}^{2d}, \forall \hbar \in (0, 1] \quad |\partial_{x,\xi}^\alpha a(\rho; \hbar)| \leq C_\alpha m(\rho)\}.$$

We notice that from the polynomial growth at infinity, for each $\hbar$ the symbol $a(\hbar)$ is a tempered distribution, so it leads to a well-defined operator $\text{Op}_\hbar(a) : \mathcal{S} \rightarrow \mathcal{S}'$. The space of operators $\{\text{Op}_\hbar(a), a \in S(m)\}$ makes up the class $\Psi_\hbar(m)$ of pseudodifferential operators. We have not specified which quantization we are using, but the Corollary 4.16 below will show that this choice is irrelevant.

Under this notation, the space $S(\mathbb{R}^{2d})$ will be denoted $S(1)$ from now on. The following seminorms generate the topology of $S(m)$:

$$\|a\|_n = \max_{|\alpha| \leq n} \sup_{\hbar \in (0,1]} \sup_{\rho} \frac{|\partial^\alpha a(\rho; \hbar)|}{m(\rho)}, \quad n \in \mathbb{N}.$$

We already know that $\text{Op}_\hbar(a)$ maps $\mathcal{S}$ to $\mathcal{S}'$ continuously. The smoothness of $a \in S(m)$ allows to show, like in the case of $S(1)$, that $\text{Op}_\hbar(a)$ preserves the Schwartz space.

Theorem 4.11. *Let $m(\rho)$ be an order function on $\mathbb{R}^{2d}$. Then for any $a \in S(m)$ and any $\hbar \in (0, 1]$, the operator $\text{Op}_\hbar(a)$ acts continuously $\mathcal{S} \rightarrow \mathcal{S}$. Like in Remark 4.4, the estimates are uniform if one uses the $\hbar$ -seminorms on $\mathcal{S}$.*

Proof. Again we take $\hbar = 1$ in our computations. There is an $N \geq 0$ such that our order function $m(\rho) \leq C \langle \rho \rangle^N$. On the other hand, $\langle \rho \rangle \leq \langle x \rangle + \langle \xi \rangle \leq 2 \langle x \rangle \langle \xi \rangle$, hence $\langle \rho \rangle^N \leq C_N \langle x \rangle^N \langle \xi \rangle^N$. Compared with the proof of Thm 4.3, we need to perform extra integration by parts in y and ξ to cancel the growth of the symbol $a(\frac{x+y}{2}, \xi)$ in the integral $I(u)$. Indeed, applying $(d+1+N)$ times the operator ${}^t L_\xi$, we get an extra factor $\langle \xi \rangle^{-N-(d+1)}$, so that the integral over ξ becomes absolutely convergent. If we want to consider $\partial^\beta I(u)$, we need to apply the same operator $|\beta|$ more times to cancel the extra growth in ξ .

To control the decay of $\partial^\beta I(u)(x)$ in $|x| \rightarrow \infty$, we need to integrate n times with the operator L_x , thereby producing a factor $\langle x - y \rangle^{-n}$. Inserting a factor $\langle y \rangle^\ell$ upstairs and downstairs, the function $\partial^\beta I(u)(x)$ is bounded above by

$$\int dy \frac{C_a \langle x + y \rangle^N \langle \xi \rangle^N}{\langle \xi \rangle^{N+d+1} \langle x - y \rangle^n \langle y \rangle^\ell} \max_{|\alpha| \leq N+|\beta|+d+1} \|\langle y \rangle^\ell \partial^\alpha u\|_{L^\infty},$$

where C_a will (as usual) depend on a certain number of seminorms of $a \in S(m)$. Since the numerator $\langle x + y \rangle^N \leq C_N (\langle x \rangle^N + \langle y \rangle^N)$, we see by using Lemma 4.5 that taking any $n \geq N$ and $\ell = N + \max(d + 1, n)$ produces an upper bound

$$|\partial^\beta I(u)(x)| \leq C_{N,n,|\beta|}(a) \langle x \rangle^{N-n} \max_{|\alpha| \leq N+|\beta|+d+1} \|\langle y \rangle^\ell \partial^\alpha u\|_{L^\infty}.$$

□

Example 4.12. Any monomial $a(x, \xi) = \xi^\alpha$, $\alpha \in \mathbb{N}^d$, belongs to the class $S(\langle \xi \rangle^{|\alpha|})$. The corresponding operator is the differential operator $\text{Op}_h(\xi^\alpha) = (hD_x)^\alpha$. Through the integral defining the Schwartz kernel, we recover the representation of derivatives of the δ distribution through its Fourier transform:

$$K_a(x, y) = \int e^{i \frac{\xi \cdot (x-y)}{h}} \xi^\alpha \frac{d\xi}{(2\pi h)^d} = \left(\frac{h}{i} \right)^{|\alpha|} [\partial^\alpha \delta](x - y).$$

Once we know that if $a \in S(m)$, the operator $\text{Op}_h(a)$ preserves $\mathcal{S}(\mathbb{R}^d)$ it makes sense to compose these operators with each other. Like we did with symbols $a \in \mathcal{S}(\mathbb{R}^{2d})$ in section 3, we are interested in the algebra property of these symbol classes. Let us start by the simple product of two symbols.

Lemma 4.13. *For any two order functions m_1, m_2 , and symbols $a_i \in S(m_i)$, the symbol $a_1 \times a_2 \in S(m_1 m_2)$. In particular, the symbol class $S(1)$ is stable by simple product.*

Proof. Obvious application of the Leibniz rule. □

Considering all symbol classes $S(m)$ together allows to relate them with the Schwartz space. Indeed, the latter is dense in the classes $S(m)$, in a slightly weak sense:

Lemma 4.14. *For any $\epsilon > 0$, the space $\mathcal{S}(\mathbb{R}^{2d})$ is dense in $S(m)$ for the weaker topology of $S(\langle \rho \rangle^\epsilon m) \supset S(m)$.*

Remark. This slight weakening is necessary: we know that $\mathcal{S}$ is not dense in the space $S(1)$, since the constant function $a \equiv 1$ cannot be approached by Schwartz functions for the sup norm: $\|1 - a\|_{L^\infty} \geq 1$ for any $a \in \mathcal{S}$. On the other hand, the sequence $a_n(\rho) = \exp(-|\rho|^2/n) \in \mathcal{S}$ satisfies, for any $\alpha \in \mathbb{N}^{2d}$, $\|\langle \rho \rangle^{-\epsilon} \partial^\alpha (1 - a_n)\|_{L^\infty} \xrightarrow{n \rightarrow \infty} 0$.

This density of $\mathcal{S}$ inside $S(m)$ suggests that the algebra governing the composition of operators should look the same as in Thm 3.2. We thus need to extend the action of the operator $e^{i\frac{\hbar}{2}\omega(D_{\rho_0}, D_{\rho_1})}$ on symbols in $S(m)$.

4.3. Action of exponentiated quadratic differentials on $S(m)$. For symbols $a \in S(m)$, we want to manipulate operators $\text{Op}_\hbar(a)$, for instance compose two operators, or compare operators corresponding to different quantizations. As we've seen above (see Prop. 2.23 and eq. (3.6)), these procedures can be represented by acting on symbols with operators of the type $e^{i\frac{\hbar}{2}\langle D, Q^{-1}D \rangle}$ for some symmetric nondegenerate matrix Q (of dimension $2d$ or $4d$). The action of this operator on $\mathcal{S}$, (and hence also on $\mathcal{S}'$ by duality), had been first defined as a Fourier multiplier. We also expressed this operator on the “direct side” by a convolution operator as in Proposition 3.4.

Before going back to symbols a defined on $\mathbb{R}^d$, we will consider $m(x)$ an order function on $\mathbb{R}_x^n$ (the definition is analogous to Def. 4.8), and study the action of such exponential quadratic derivatives on symbols $a \in S(m)$. (Later we will take $x \rightarrow (x, \xi)$ or $x \rightarrow (x_0, \xi_0, x_1, \xi_1)$).

Proposition 4.15. *Let $m(x)$ be an order function on $\mathbb{R}^n$. Take $a \in S(m, \mathbb{R}_x^n)$, and Q a $n \times n$ symmetric nondegenerate matrix. Then the distribution $e^{i\frac{\hbar}{2}\langle D, Q^{-1}D \rangle}a$ also belongs to $S(m)$. More precisely, the operator $e^{i\frac{\hbar}{2}\langle D, Q^{-1}D \rangle}$ acts continuously $S(m) \rightarrow S(m)$. Moreover, if a is independent of $\hbar$, the symbol $e^{i\frac{\hbar}{2}\langle D, Q^{-1}D \rangle}a$ admits the asymptotic expansion*

$$(4.2) \quad e^{i\frac{\hbar}{2}\langle D, Q^{-1}D \rangle}a \sim \sum_{j \geq 0} \frac{1}{j!} \left(i\frac{\hbar}{2} \langle D, Q^{-1}D \rangle \right)^j a \quad \text{in the class } S(m).$$

Proof. Since the symbol classes $S(m)$ do not have nice properties w.r.t. the Fourier transform, we will study the operator $e^{i\frac{\hbar}{2}\langle D, Q^{-1}D \rangle}$ through its convolution representation (generalizing the expression (2.36)):

$$\left[e^{i\frac{\hbar}{2}\langle D, Q^{-1}D \rangle}a \right](x) = C_Q \int_{\mathbb{R}^n} \exp \left(-i \frac{\langle y, Qy \rangle}{2\hbar} \right) a(x+y) dy,$$

with the prefactor $C_Q = \frac{|\det Q|^{1/2} e^{i\pi \operatorname{sgn} Q/4}}{(2\pi\hbar)^{n/2}}.$

Fixing the point x , we will analyze the oscillatory integral

$$I(x, \hbar) = \int_{\mathbb{R}^n} e^{-i \frac{\langle y, Qy \rangle}{2\hbar}} a(x+y) dy.$$

Since a is not decaying, we split the integral between a compactly supported part, containing the stationary point $y = 0$, and a noncompact part where the phase oscillates, and where we will be able to gain decay using integrations by parts. Let $\chi \in C_c^\infty(\mathbb{R}^n)$, $\chi(y) = 1$ for $|y| \leq 1$,

$\chi(y) = 0$ for $|y| \geq 2$. We write

$$I(x, \hbar) = I_1(x, \hbar) + I_2(x, \hbar), \quad \text{with}$$

$$I_1(x, \hbar) = \int_{\mathbb{R}^n} e^{-i\frac{\langle y, Qy \rangle}{2\hbar}} \chi(y) a(x+y) dy, \quad I_2(x, \hbar) = \int_{\mathbb{R}^n} e^{-i\frac{\langle y, Qy \rangle}{2\hbar}} (1 - \chi(y)) a(x+y) dy.$$

The (quadratic) stationary phase estimate applies to $I_1(\hbar)$, and we get an expansion

$$I_1(x, \hbar) \sim C_Q^{-1} \sum_{j \geq 0} \frac{1}{j!} \left(i \frac{\hbar}{2} \langle D_y, Q^{-1} D_y \rangle \right)^j a(x+y)|_{y=0}.$$

(notice that the terms of the expansion do not depend on χ , since $\chi = 1$ near $y = 0$). As a function of x , each term in the expansion is bounded above by $C\hbar^{n/2+j}m(x)$. If we truncate the expansion at the order N , the remainder is bounded by $2N + n + 1$ derivatives of $a(x+y)$ in the region $\{|y| \leq 2\}$, so the remainder is bounded above by $C_N\hbar^{n/2+N}m(x)$. Hence $|I_1(x, \hbar)| \leq C\hbar^{n/2}m(x)$. If we differentiate I_1 w.r.t. x , we get the same expressions, with $a(x)$ replaced by $\partial^\alpha a(x)$. As a result, we also get

$$(4.3) \quad |\partial^\alpha I_1(x, \hbar)| \leq C_\alpha \hbar^{n/2} m(x).$$

We now want to give a sense to the oscillatory integral $I_2(x, \hbar)$, and show that it is very small. Since the integrand $(1 - \chi(y)) a(x+y)$ may grow polynomially when $|y| \rightarrow \infty$, we will proceed as usual by *formal* integration by parts in the variables y , using the operator

$$L = -\frac{\langle Qy, \hbar D_y \rangle}{|Qy|^2},$$

which is well-defined on the support of $(1 - \chi)$. An important remark is the fact that the denominator satisfies $c|y| \leq |Qy| \leq C|y|$, which will allow us to “gain” factors $\langle y \rangle^{-1}$ after each integration by parts. More precisely, the k -th i.b.p. of $I_2(x, \hbar)$ reads

$$I_2(x, \hbar) = \int_{\mathbb{R}^n} e^{-i\frac{\langle y, Qy \rangle}{2\hbar}} ({}^t L)^k [(1 - \chi(\bullet)) a(x + \bullet)](y) dy.$$

The function $({}^t L)^k [(1 - \chi(\bullet)) a(x + \bullet)]$ can be estimated by using the nonstationary phase estimate (2.44):

$$(4.4) \quad ({}^t L)^k [(1 - \chi(y)) a(x+y)] \leq C_k \hbar^k \sum_{j=0}^k \frac{|\partial_y^j [(1 - \chi(y)) a(x+y)]|}{|y|^{2k-j}} \leq C_k \frac{\hbar^k}{|y|^k} m(x+y).$$

Since $m(x+y) \leq C\langle y \rangle^N m(x)$ for some N , we see that for $k \geq N + n + 1$ the integral becomes absolutely convergent, and satisfies $|I_2(x, \hbar)| \leq C\hbar^k m(x)$. Differentiating $I_2(x)$ w.r.t. x amounts to replacing a with $\partial^\alpha a$, which has the same growth properties, so we also get $|\partial^\alpha I_2(x, \hbar)| \leq C\hbar^k m(x)$.

To summarize, we found $|\partial^\alpha I_2(x, \hbar)| = \mathcal{O}(\hbar^\infty)m(x)$, which is smaller than any term in the expansion. Together with (4.3), this shows that $I(\bullet, \hbar) = e^{i\frac{\hbar}{2}\langle D, Q^{-1}D \rangle}a \in \hbar^{n/2}S(m)$, and satisfies the expansion (4.2). $\square$

4.4. Composition of operators with symbols in $S(m)$. As a first application of Proposition 4.15, we obtain the fact that the class of operators $\Psi_\hbar(m)$ is independent of the chosen quantization.

Corollary 4.16. *Take $t, s \in [0, 1]$, and assume $a_s \in S(m)$ for some order function m . Then the symbol a_t such that $\text{Op}_\hbar^t(a_t) = \text{Op}_\hbar^s(a_s)$ also belongs to $S(m)$.*

Proof. The explicit formula (2.20) is exactly of the type $e^{i\frac{\hbar}{2}\langle D, Q^{-1}D \rangle}a_s$. $\square$

A more interesting corollary concerns the composition of operators. For two symbols $a_i \in S(m_i)$, the symbol $a_1(\rho_1)a_2(\rho_2)$ may be seen as an element of $S(m_1 \otimes m_2, \mathbb{R}^{4d})$. We may then use the expression (3.6) and Prop. 4.15 to define the Moyal product between these two symbols, and obtain the following

Theorem 4.17. *Take two order functions m_1, m_2 and $a_i \in S(m_i)$, $i = 1, 2$. Then the symbol $a_1 \#_\hbar a_2 \in S(m_1 m_2)$. If the a_i are independent of $\hbar \in (0, 1]$, then the symbol $a_1 \#_\hbar a_2$ satisfies the asymptotic expansion*

$$a_1 \#_\hbar a_2 = \sum_{j=0}^{N-1} \frac{(i\hbar/2)^j}{j!} a_1 \left(\omega(\overleftarrow{D}, \overrightarrow{D}) \right)^j a_2 + \mathcal{O}(\hbar^N)_{S(m_1 m_2)}$$

The analysis of the integral $I_2(x, \hbar)$ in the proof of Proposition 4.15 allows to generalize and strengthen the quasi-locality property of Prop. 3.19.

Lemma 4.18. *Consider $a \in C_c^\infty(\mathbb{R}^{2d})$ independent of $\hbar$, and $b \in S(m)$. Then the symbol $a \#_\hbar b \in \mathcal{S}(\mathbb{R}^{2d})$ with seminorms uniform w.r.t. $\hbar \in (0, 1]$. More precisely, for any $\alpha \in \mathbb{N}^{2d}$ and any point $\rho \notin \text{supp } a$ one has the estimate*

$$\partial^\alpha (a \#_\hbar b)(\rho) = \mathcal{O} \left(\left(\frac{\hbar}{\text{dist}(\rho, \text{supp } a)} \right)^\infty \right).$$

Remark 4.19. Being in $\mathcal{S}(\mathbb{R}^{2d})$ with uniform seminorms w.r.t. $\hbar$ is equivalent with being in $S(\langle \rho \rangle^{-\infty}) \stackrel{\text{def}}{=} \bigcap_{N \geq 0} S(\langle \rho \rangle^{-N})$.

Proof. We use the integral expression

$$(4.5) \quad a \#_\hbar b(\rho) = \iint \frac{d\rho_0 d\rho_1}{(\pi\hbar)^{2d}} \exp \left(-\frac{2i}{\hbar} \omega(\rho_0, \rho_1) \right) a(\rho + \rho_0) b(\rho + \rho_1).$$

The integrand is supported in the domain $\{(\rho_0, \rho_1) \in (\text{supp } a - \rho) \times (\text{supp } b - \rho)\}$. If $\rho \notin \text{supp } a$ this domain does not contain the stationary point $(0, 0)$ but is situated at a distance $|(\rho_0, \rho_1)| \geq \text{dist}(\rho, \text{supp } a)$ from the stationary point¹⁵. As a result, we can perform k integrations by parts in the above integral, leading to factors $\left(\frac{\hbar}{|(\rho_0, \rho_1)|}\right)^k$.

If both $a, b \in C_c^\infty$, the integral is bounded above by $C\hbar^{-2d} \left(\frac{\hbar}{|(\rho_0, \rho_1)|}\right)^k \|a\|_{C^k} \|b\|_{C^k}$. Besides, it is compactly supported in ρ_0, ρ_1 , and we get the bound

$$(4.6) \quad |(a \#_{\hbar} b)(\rho)| \leq C \hbar^{k-2d} \frac{\|a\|_{C^k} \|b\|_{C^k}}{(\text{dist}(\rho, \text{supp } a) + \text{dist}(\rho, \text{supp } b))^k}, \quad \rho \notin \text{supp } a \cup \text{supp } b.$$

In the case $b \in S(m)$, the integrand is bounded above by

$$C\hbar^{-2d} m(\rho + \rho_1) \left(\frac{\hbar}{|(\rho_0, \rho_1)|}\right)^k \leq C\hbar^{k-2d} m(\rho) \frac{\langle \rho_1 \rangle^N}{|(\rho_0, \rho_1)|^k} \leq C\hbar^{k-2d} m(\rho) \frac{1}{|(\rho_0, \rho_1)|^{k-N}}.$$

The integrand is compactly supported in ρ_0 . For $k \geq N + 2d + 1$ the integral over ρ_1 converges absolutely, and is bounded above by

$$|(a \#_{\hbar} b)(\rho)| \leq C \hbar^{k-2d} \frac{m(\rho)}{\text{dist}(\rho, \text{supp } a)^{k-N-2d}}.$$

The same estimate holds if we differentiate w.r.t. ρ , which produces the announced estimate. $\square$

In general the symbol $c = a \#_{\hbar} b$ is not compactly supported, but its *essential support* is contained in $\text{supp } a$. This generalizes the result of Prop. 3.19.

Remark 4.20. A slight modification of the proof of the Lemma shows that if $a = a(\hbar) \in S(\langle \rho \rangle^{-\infty})$ has its essential support contained in some bounded open set Ω (such that $a(\rho) = \mathcal{O}\left(\left(\frac{\hbar}{\text{dist}(\rho, \Omega)}\right)^\infty\right)$ for ρ outside Ω), then the same result applies to the symbol $a \#_{\hbar} b$ with $b \in S(m)$.

Let us now consider the Moyal product $a \#_{\hbar} b$ between two symbols $a, b \in C_c^\infty(\mathbb{R}^{2d})$, such that the supports of these two symbols are of diameters $\mathcal{O}(1)$, and distant from each other. To fix ideas, assume these supports have diameters ≤ 2 , and are centered on points $z_0, z_1 \in \mathbb{R}^{2d}$ with $|z_0 - z_1| \geq 10$. We already know from Prop. 3.16 that $a \#_{\hbar} b = \mathcal{O}(\hbar^\infty)_{\mathcal{S}}$. For future use, let us obtain a more precise estimate.

Lemma 4.21. *Two points $z_0, z_1 \in \mathbb{R}^{2d}$ at distance $|z_0 - z_1| \geq 10$. Consider $a_0, a_1 \in C_c^\infty(\mathbb{R}^{2d})$, such that $\text{supp } a_i \subset \{\rho \in \mathbb{R}^{2d}, |\rho - z_i| \leq 2\}$. Then the Moyal product $a_0 \#_{\hbar} a_1$ satisfies the*

¹⁵Here we are in performing an integration by parts in $\mathbb{R}^{4d}$, so the denominator $|y|^k$ in 2.44 should be replaced by $|(\rho_0, \rho_1)|^k$, where $|(\rho_0, \rho_1)|$ is the distance from the origin of the point (ρ_0, ρ_1) .

estimates

$$\forall \alpha \in \mathbb{N}^{2d}, \forall k \geq 0, \quad |\partial^\alpha (a_0 \#_{\hbar} a_1)(\rho)| \leq C_{\alpha,k} \hbar^{k-2d} \frac{1}{\left(|z_1 - z_0|^2 + \left|\rho - \frac{z_1 + z_0}{2}\right|^2\right)^{k/2}}.$$

Proof. We analyze the integral (4.5). The integrand is supported on points $(\rho_0, \rho_1) \in \{|z_0 - \rho_0| \leq 2, |z_1 - \rho_1| \leq 2\}$. Hence, using the estimate on the operator $({}^tL)^k$ as in (4.4), one can easily show (through some elementary planar geometry) that

$$|a_0 \#_{\hbar} a_1(\rho)| \leq C \hbar^{k-2d} \frac{1}{\left(|z_0 - \rho|^2 + |z_1 - \rho|^2\right)^{k/2}} \leq C' \hbar^{k-2d} \frac{1}{\left(|z_1 - z_0|^2 + \left|\rho - \frac{z_1 + z_0}{2}\right|^2\right)^{k/2}}.$$

As before, the same type of estimate holds for derivatives w.r.t. ρ . $\square$

Remark. Compared with the estimates of Prop. 3.16, we now have an explicit dependence in the distance $\sim |z_1 - z_0|$ between the two supports.

4.5. Action of pseudodifferential operators on L^2 . So far we have considered the action of operators $\text{Op}_{\hbar}(a)$ on $u \in \mathcal{S}(\mathbb{R}^d)$. However, in quantum mechanics the natural functional space is the Hilbert space $L^2(\mathbb{R}^d)$, or its Sobolev descendents $H^s(\mathbb{R}^d)$.

4.5.1. Symbols in the Schwartz space. Let us start with nice symbols $a \in \mathcal{S}(\mathbb{R}^{2d})$. We have seen in Proposition 3.13 that $\text{Op}_{\hbar}(a)$ acts on L^2 as a bounded operator, with an operator norm uniformly bounded w.r.t. $\hbar \in (0, 1]$. An alternative proof of the boundedness of $\text{Op}_{\hbar}(a)$ uses the fact that the Schwartz kernel $K_a(x, y) \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$, and the use of Schur's inequality (see the Lemma below). We will see below that we can get a sharper estimate on this bound in terms of the symbol a .

Lemma 4.22. (*Schur's inequality*) Assume that the Schwartz kernel $K(x, y)$ of an operator $A : \mathcal{S} \rightarrow \mathcal{S}'$ is a continuous function on $\mathbb{R}^d \times \mathbb{R}^d$, and satisfies

$$\sup_x \int_y |K(x, y)| < C_1, \quad \sup_y \int_x |K(x, y)| < C_2.$$

Then A can be extended to a bounded operator $L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$, and its norm $\|A\|_{L^2 \rightarrow L^2} \leq \sqrt{C_1 C_2}$.

Proof. We compute, for $u \in \mathcal{S}$:

$$\begin{aligned} |Au(x)|^2 &= \left| \int K(x, y) u(y) dy \right|^2 \\ &\leq \int |K(x, y)| |u(y)|^2 dy \int |K(x, y)| dy \\ &\leq C_1 \int |K(x, y)| |u(y)|^2 dy \end{aligned}$$

Integrating over x , we find

$$\begin{aligned} \|Au\|_{L^2}^2 &\leq C_1 \iint |K(x, y)| |u(y)|^2 dy dx \\ &\leq C_1 \int dy |u(y)|^2 \int |K(x, y)| dx \\ &\leq C_1 C_2 \|u\|_{L^2}^2. \end{aligned}$$

□

4.5.2. *Symbols in the class $S(1)$.* Let us now attack a less elementary task, which is to show that for any symbol a in the class $S(1)$, the operators $\text{Op}_h(a)$ are bounded on L^2 , and their norms are uniformly bounded w.r.t. h . We already know that this is the case for bounded symbols of the form $f(x)$ or $g(\xi)$, since the corresponding operators act by multiplication on L_x^2 , resp. on L_ξ^2 . The proof for a general symbols $a \in S(1)$ is more involved.

The idea is to split the symbol a into countably many symbols $a_{\mathbf{n}}$, each of them being supported in an $\mathcal{O}(1)$ neighbourhood of the lattice point $\mathbf{n} \in \mathbb{Z}^{2d}$ (as explained at the end of subsection 3.4.2).

Lemma 4.23. *(Partition of unity on $\mathbb{R}^d$). There exists a cutoff function $\chi \in C_c^\infty(\mathbb{R}^{2d})$ such that*

$$\sum_{\mathbf{n} \in \mathbb{Z}^{2d}} \chi(\rho - \mathbf{n}) \equiv 1.$$

Proof. Consider a cutoff function $\tilde{\chi} \in C_c^\infty(\mathbb{R}^{2d})$, supported in $\{|\rho| \leq R_d\}$, strictly positive in $\{|\rho| \leq R_d/2\}$. If $R_d \geq \sqrt{d}$, the function

$$S(\rho) = \sum_{\mathbf{n} \in \mathbb{Z}^{2d}} \tilde{\chi}(\rho - \mathbf{n})$$

is everywhere positive. It is also periodic. Hence, if we take $\chi(\rho) \stackrel{\text{def}}{=} \frac{\tilde{\chi}(\rho)}{S(\rho)}$, it defines a smooth partition of unity as stated. □

We then set $a_{\mathbf{n}}(\rho) \stackrel{\text{def}}{=} a(\rho)\chi(\rho - \mathbf{n})$, which is compactly supported in the ball $B(\mathbf{n}, R_d)$. The $S(1)$ seminorms of $a_{\mathbf{n}}$ are controlled by those of χ and a . By linearity, we can formally write

$$\text{Op}_{\hbar}(a) = \sum_{\mathbf{n} \in \mathbb{Z}^{2d}} \text{Op}_{\hbar}(a_{\mathbf{n}}).$$

Can we give a meaning to the sum on the RHS? In particular, how does it acts on $L^2(\mathbb{R}^d)$. Prop. 3.13 implies that all operators $\text{Op}_{\hbar}(a_{\mathbf{n}})$ are bounded on L^2 , uniformly w.r.t. $\hbar$ and $\mathbf{n}$. But all terms may have comparable operator norms, so we cannot apply the triangle inequality to the sum.

Yet, Lemma 4.21 shows that if $\mathbf{n}, \mathbf{n}'$ are distant from one another, the two operators $\text{Op}_{\hbar}(a_{\mathbf{n}})$, $\text{Op}_{\hbar}(a_{\mathbf{n}'})$ are “quasi-orthogonal” to each other. Translating this Lemma in the present notations, it implies that, for $|\mathbf{n} - \mathbf{n}'| \gg 1$, the norm $\|\text{Op}_{\hbar}(a_{\mathbf{n}}) \text{Op}_{\hbar}(a_{\mathbf{n}'})\|_{L^2 \rightarrow L^2}$ is of order $\mathcal{O}\left(\left(\frac{\hbar}{|\mathbf{n} - \mathbf{n}'|}\right)^{\infty}\right)$ (see eq. (4.11) for a more precise statement). Grossly speaking, this means that the image of $\text{Op}_{\hbar}(a_{\mathbf{n}'})$ is essentially in the kernel of $\text{Op}_{\hbar}(a_{\mathbf{n}})$, and vice-versa.

Remark 4.24. A simplified model for this quasi-orthogonality would be a (strictly) orthogonal decomposition $L^2 = \bigoplus_{\mathbf{n}} \mathcal{H}_{\mathbf{n}}$, such that $\mathcal{H}_{\mathbf{n}}^{\perp} \subset \ker(\text{Op}_{\hbar}(a_{\mathbf{n}}))$ and $\text{Ran}(\text{Op}_{\hbar}(a_{\mathbf{n}})) \subset \mathcal{H}_{\mathbf{n}}$. In that case, Pythagoras’s thm would give, for any $v = \bigoplus_{\mathbf{n}} v_{\mathbf{n}}$, $v_{\mathbf{n}} \in \mathcal{H}_{\mathbf{n}}$:

$$\|\text{Op}_{\hbar}(a)v\|^2 = \sum_{\mathbf{n}} \|\text{Op}_{\hbar}(a_{\mathbf{n}})v_{\mathbf{n}}\|^2 \leq \sum_{\mathbf{n}} \|\text{Op}_{\hbar}(a_{\mathbf{n}})\|^2 \|v_{\mathbf{n}}\|^2 \leq \left(\sup_{\mathbf{n}} \|\text{Op}_{\hbar}(a_{\mathbf{n}})\|^2\right) \|v\|^2.$$

To take into account the fact that the operators $\text{Op}_{\hbar}(a_{\mathbf{n}})$ are only quasi-orthogonal, we will use the **Cotlar-Stein Theorem**, an abstract operator theoretic result.

Theorem 4.25. (*Cotlar-Stein Theorem*) Let $(A_j)_{j \geq 1}$ be a family of bounded operators on some Hilbert space $\mathcal{H}$, and assume that the following bounds hold:

$$(4.7) \quad \sup_j \sum_k \|A_j^* A_k\|^{1/2} \leq C \quad \text{and} \quad \sup_j \sum_k \|A_j A_k^*\|^{1/2} \leq C.$$

Then the series $\sum_j A_j$ converges, in the strong operator topology¹⁶, to an operator A , which satisfies $\|A\| \leq C$.

Notice that the sum $\sum_j A_j$ does gnerally NOT converge in the operator norm topology, since the norms $\|A_k\|$ are not supposed to decay when $k \rightarrow \infty$ (they are only uniformly bounded).

¹⁶A family of bounded operators $(B_n)_n$ converges to a bounded operator B in the strong operator topology if, for any $v \in \mathcal{H}$, $\lim_{n \rightarrow \infty} B_n v = Bv$.

Proof. We truncate the sum to $A = A^{(J)} = \sum_{j=1}^J A_j$, so that the sum is well-defined. A is a bounded operator, so A^*A is a positive selfadjoint operator, which satisfies

$$\|(A^*A)^m\| = \|A^*A\|^m = \|A\|^{2m}.$$

We want to estimate the norm of $(A^*A)^m$ in a clever way. From the decomposition of A , we write

$$(A^*A)^m = \sum_{j_1, j_2, \dots, j_{2m}=1}^J A_{j_1}^* A_{j_2} A_{j_3}^* \cdots A_{j_{2m}} \stackrel{\text{def}}{=} \sum_{j_1, j_2, \dots, j_{2m}=1}^J A_{j_1 \dots j_{2m}}.$$

The trick is to find two bounds for the norm of $A_{j_1 \dots j_{2m}}$:

$$\begin{aligned} \|A_{j_1 \dots j_{2m}}\| &\leq \|A_{j_1}^* A_{j_2}\| \|A_{j_3}^* A_{j_4}\| \cdots \|A_{j_{2m-1}}^* A_{j_{2m}}\| \\ \|A_{j_1 \dots j_{2m}}\| &\leq \|A_{j_1}^*\| \|A_{j_2} A_{j_3}^*\| \cdots \|A_{j_{2m}}\|. \end{aligned}$$

Taking the *geometric mean* of these two bounds (and noticing that all $\|A_j\| \leq C$ from our assumptions), we get

$$\|A_{j_1 \dots j_{2m}}\| \leq C \|A_{j_1}^* A_{j_2}\|^{1/2} \|A_{j_2} A_{j_3}^*\|^{1/2} \|A_{j_3}^* A_{j_4}\|^{1/2} \cdots \|A_{j_{2m-1}}^* A_{j_{2m}}\|^{1/2}.$$

Through the triangular inequality, this gives:

$$\|(A^*A)^m\| \leq C \sum_{j_1, j_2, \dots, j_{2m}=1}^J \|A_{j_1}^* A_{j_2}\|^{1/2} \|A_{j_2} A_{j_3}^*\|^{1/2} \|A_{j_3}^* A_{j_4}\|^{1/2} \cdots \|A_{j_{2m-1}}^* A_{j_{2m}}\|^{1/2}.$$

If we first sum over j_1 using the assumption, we produce a factor C . Then we sum over j_2 , etc. In the end we sum over j_{2m} , which produces a factor J . This gives finally $\|(A^*A)^m\| \leq C C^{2m-1} J$, and therefore $\|A\| \leq C J^{1/2m}$. Since this estimate holds for any $m \geq 1$, we get

$$\|A^{(J)}\| \leq C,$$

a bound which is independent of the truncation order J .

Let us now prove the strong convergence when $J \rightarrow \infty$. Take $\psi \in \mathcal{H}$, and consider $\varphi = A_{k_0}^* \psi$. Then we may write formally

$$\sum_{j \geq 1} A_j \varphi = \sum_{j \geq 1} A_j A_{k_0}^* \psi,$$

and this series converges absolutely, since

$$\begin{aligned}
\sum_{j \geq 1} \|A_j A_{k_0}^* \psi\| &\leq \sum_{j \geq 1} \|A_j A_{k_0}^*\| \|\psi\| \\
&\leq \sum_{j \geq 1} \|A_j A_{k_0}^*\|^{1/2} \|A_j A_{k_0}^*\|^{1/2} \|\psi\| \\
&\leq \sum_{j, j' \geq 1} \|A_j A_{k_0}^*\|^{1/2} \|A_{j'} A_{k_0}^*\|^{1/2} \|\psi\| \\
&\leq C^2 \|\psi\|.
\end{aligned}$$

Hence the limit $A\varphi = \lim_{J \rightarrow \infty} A^{(J)}\varphi$ converges for any $\varphi \in \text{span}\{A_k^*(\mathcal{H}), k \geq 1\}$. On the other hand, we have proved that $\|A^{(J)}\| \leq C$ uniformly for all J . We thus deduce that $\|A\varphi\| \leq C\|\varphi\|$ for any $\varphi \in \text{span}\{A_k^*(\mathcal{H}), k \geq 1\}$. It is then possible to extend A to any φ in the closure of this subspace, keeping the same bound $\|A\varphi\| \leq C\|\varphi\|$. What is the orthogonal complement of that closure? It is the subspace $\bigcap_k \ker A_k$. For states in this subspace, we naturally take $A\varphi = 0$. Finally we have defined $A\varphi$ for all states $\varphi \in \mathcal{H}$, and showed that it satisfies the announced bound. $\square$

With this Cotlar-Stein theorem, we are now equipped to prove the L^2 continuity of pseudo-differential operators with symbols in $S(1)$, namely the following

Theorem 4.26. (*Calderón-Vaillancourt Theorem*) *Let $a = a(\hbar) \in S(1, \mathbb{R}^{2d})$. Then the operator $\text{Op}_\hbar^W(a)$ can be extended as a bounded operator on $L^2(\mathbb{R}^d)$, with a bound uniform w.r.t. $\hbar \in (0, 1]$.*

More precisely, there exists a constant $C_d > 0$ such that

$$(4.8) \quad \|\text{Op}_\hbar^W(a)\|_{L^2 \rightarrow L^2} \leq C_d \sum_{|\alpha| \leq 6d+2} \hbar^{|\alpha|/2} \|\partial^\alpha a\|_{L^\infty(\mathbb{R}^{2d})}.$$

The same estimate holds if we replace the Weyl quantization by any t -quantization.

Proof. As suggested above, we split the operator $\text{Op}_\hbar(a) = \sum_{\mathbf{n}} \text{Op}_\hbar(a_{\mathbf{n}})$. If we call $A_{\mathbf{n}} = \text{Op}_\hbar(a_{\mathbf{n}})$ the Cotlar-Stein theorem requires to compute the norms of the operators $\text{Op}_\hbar(a_{\mathbf{n}})^* \text{Op}_\hbar(a_{\mathbf{n}'}) = \text{Op}_\hbar(\bar{a}_{\mathbf{n}} \#_\hbar a_{\mathbf{n}'})$ and $\text{Op}_\hbar(a_{\mathbf{n}'}) \text{Op}_\hbar(a_{\mathbf{n}})^* = \text{Op}_\hbar(a_{\mathbf{n}'} \#_\hbar \bar{a}_{\mathbf{n}})$.

1) For $|\mathbf{n} - \mathbf{n}'| \leq 10R_d$ we apply the bounds of Lemma 3.5 for the seminorms of $\bar{a}_{\mathbf{n}} \#_\hbar a_{\mathbf{n}'}$. For ρ close to $\mathbf{n}$ we have

$$|\partial^\alpha (\bar{a}_{\mathbf{n}} \#_\hbar a_{\mathbf{n}'}) (\rho)| \leq C_{\gamma, \alpha} \|\langle D \rangle^{|\alpha|+2d+1} a_{\mathbf{n}}\|_{L^\infty} \|\langle D \rangle^{|\alpha|+2d+1} a_{\mathbf{n}'}\|_{L^\infty},$$

where we used the fact that the symbols $a_{\mathbf{n}}$ are compactly supported near $\mathbf{n}$. For ρ away from the support of $a_{\mathbf{n}}$ or $a_{\mathbf{n}'}$, the Lemma 4.18 implies that

$$|\partial^\alpha (\bar{a}_{\mathbf{n}} \#_{\hbar} a_{\mathbf{n}'}) (\rho)| \leq C \hbar^{k-2d} \frac{\|a_{\mathbf{n}}\|_{C^{k+|\alpha|}} \|a_{\mathbf{n}'}\|_{C^{k+|\alpha|}}}{(\text{dist}(\rho, \text{supp } a_{\mathbf{n}}) + \text{dist}(\rho, \text{supp } a_{\mathbf{n}'}))^k}.$$

We may apply Prop. 3.13 by taking all $|\alpha| \leq 2d+1$, and $k = 2d+1$ to have integrability in $\rho \in \mathbb{R}^{2d}$. We hence get the estimate

$$(4.9) \quad \|A_{\mathbf{n}}^* A_{\mathbf{n}'}\|_{L^2 \rightarrow L^2} \leq C_d \|a_{\mathbf{n}}\|_{C^{4d+2}} \|a_{\mathbf{n}'}\|_{C^{4d+2}} \leq C_d \|a\|_{C^{4d+2}}^2.$$

2) When $|\mathbf{n} - \mathbf{n}'| > 10R_d$, we use the Lemma 4.21 to show that the product symbol satisfies

$$(4.10) \quad |\partial^\alpha (\bar{a}_{\mathbf{n}} \#_{\hbar} a_{\mathbf{n}'}) (\rho)| \leq C_k \hbar^{k-2d} \frac{\|a_{\mathbf{n}}\|_{C^{k+|\alpha|}} \|a_{\mathbf{n}'}\|_{C^{k+|\alpha|}}}{\left(|\mathbf{n} - \mathbf{n}'|^2 + \left|\rho - \frac{\mathbf{n} + \mathbf{n}'}{2}\right|^2\right)^{k/2}}$$

(where the constants implicitly depend on the cutoff χ). Again, Prop. 3.13 used for all $|\alpha| \leq 2d+1$ and some $k \geq 2d+1$ leads to

$$(4.11) \quad \|A_{\mathbf{n}}^* A_{\mathbf{n}'}\|_{L^2 \rightarrow L^2} \leq C_k \hbar^{k-2d} \frac{\|a_{\mathbf{n}}\|_{C^{k+2d+1}} \|a_{\mathbf{n}'}\|_{C^{k+2d+1}}}{\langle \mathbf{n} - \mathbf{n}' \rangle^k} \leq C_{k,\chi} \hbar^{k-2d} \frac{\|a\|_{C^{k+2d+1}}^2}{\langle \mathbf{n} - \mathbf{n}' \rangle^k}, \quad k \geq 2d+1.$$

The same bound holds for the norms $\|A_{\mathbf{n}'} A_{\mathbf{n}}^*\|$. By taking $k \geq 4d+1$, we see that the expressions $\sum_{\mathbf{n}'} \|A_{\mathbf{n}}^* A_{\mathbf{n}'}\|^{1/2}$, $\sum_{\mathbf{n}'} \|A_{\mathbf{n}'} A_{\mathbf{n}}^*\|^{1/2}$ converge, and are bounded uniformly w.r.t. $\hbar$ and $\mathbf{n}'$:

$$\sup_{\mathbf{n}} \sum_{\mathbf{n}'} \|A_{\mathbf{n}}^* A_{\mathbf{n}'}\|^{1/2} \leq C_{d,\chi} \|a\|_{C^{6d+2}}, \quad \sup_{\mathbf{n}} \sum_{\mathbf{n}'} \|A_{\mathbf{n}'} A_{\mathbf{n}}^*\|^{1/2} \leq C_{d,\chi} \|a\|_{C^{6d+2}}.$$

We may thus apply the Cotlar-Stein Theorem. It shows that $\text{Op}_{\hbar}(a)$ is well-defined as a bounded operator on L^2 , with a norm

$$(4.12) \quad \|\text{Op}_{\hbar}^W(a)\|_{L^2 \rightarrow L^2} \leq C_d \|a\|_{C^{6d+2}} = C_d \sum_{|\alpha| \leq 6d+2} \|\partial^\alpha a\|_{L^\infty}, \quad \text{uniformly for } \hbar \in (0, 1].$$

We notice that the RHS does not depend on $\hbar$, in particular the above estimate holds in the case $\hbar = 1$. To improve this bound into the one stated in the Theorem when $\hbar < 1$, we use a simple scaling argument. Namely, the *unitary* rescaling operator

$$(4.13) \quad U_{\hbar} u(x) \stackrel{\text{def}}{=} \hbar^{d/4} u(\hbar^{1/2} x),$$

intertwines the quantization for “ $\hbar = \hbar$ ” and “ $\hbar = 1$ ”:

$$U_{\hbar} \text{Op}_{\hbar}^W(a) u = \text{Op}_1^W(a_{\hbar}) U_{\hbar} u,$$

where a_h is the rescaled symbol $a_h(\rho) = a(\hbar^{1/2}\rho)$. Indeed:

$$\begin{aligned} \hbar^{d/4} [\text{Op}_h^W(a)u](\hbar^{1/2}x) &= \hbar^{d/4} \int \frac{dyd\xi}{(2\pi\hbar)^d} e^{\frac{i}{\hbar}\xi \cdot (\hbar^{1/2}x - y)} a\left(\frac{\hbar^{1/2}x + y}{2}, \xi\right) u(y) \\ &= \int \frac{dYd\Xi}{(2\pi)^d} e^{\frac{i}{\hbar}\hbar^{1/2}\Xi \cdot (\hbar^{1/2}x - \hbar^{1/2}Y)} a\left(\frac{\hbar^{1/2}x + \hbar^{1/2}Y}{2}, \hbar^{1/2}\Xi\right) \hbar^{d/4} u(\hbar^{1/2}Y) \\ &= \int \frac{dYd\Xi}{(2\pi)^d} e^{\frac{i}{\hbar}\Xi \cdot (x - Y)} a_h\left(\frac{x + Y}{2}, \Xi\right) \hbar^{d/4} u(\hbar^{1/2}Y) \\ &= [\text{Op}_1^W(a_h)U_h u](x). \end{aligned}$$

This shows that the operators $\text{Op}_h^W(a)$, $\text{Op}_1^W(a_h)$ are unitarily conjugate, thus they have the same $L^2 \rightarrow L^2$ norm. Now, we can apply the estimate (4.12) to $\text{Op}_1^W(a_h)$, and notice that $\|\partial^\alpha a_h\|_{L^\infty} = \hbar^{|\alpha|/2} \|\partial^\alpha a\|_{L^\infty}$. $\square$

Remark 4.27. We will show below that the bound (4.8) can be slightly improved, namely the constant in front of the term $\|a\|_{L^\infty}$ can be taken to be unity.

The Calderón-Vaillancourt theorem is very important. It allows to transform remainder terms expressed in the topology of $S(1)$, into remainder terms in the topology of operators on L^2 , which is more natural when we study spectral questions or time evolution on L^2 . A first example is a direct corollary of the composition theorem 4.17:

Corollary 4.28. (*Pseudodifferential calculus on $L^2(\mathbb{R}^d)$*) Take two symbols $a, b \in S(1)$. The first statement from Thm 4.17 indicates that $a \#_\hbar b \in S(1)$. The asymptotic expansion of the same theorem translates into an expansion in L^2 :

$$\text{Op}_h^W(a) \text{Op}_h^W(b) = \sum_{j=0}^{N-1} \frac{(i\hbar/2)^j}{j!} \text{Op}_h^W\left(a\left(\omega(\overleftarrow{D}, \overrightarrow{D})\right)^j b\right) + \mathcal{O}(\hbar^N)_{\mathcal{L}(L^2)},$$

where the implied constant depends on a certain number of derivatives of a, b .

The two first terms:

$$\text{Op}_h^W(a) \text{Op}_h^W(b) = \text{Op}_h^W(ab) - \frac{i\hbar}{2} \text{Op}_h^W(\{a, b\}) + \mathcal{O}(\hbar^2)_{\mathcal{L}(L^2)},$$

are a manifestation of the quantum-classical correspondence, now in the L^2 framework.

For instance, for two symbols $a, b \in S(1)$ with *disjoint supports*, the above expansion shows that

$$\text{Op}_h^W(a) \text{Op}_h^W(b) = \mathcal{O}(\hbar^\infty)_{\mathcal{L}(L^2)}.$$

The symmetry of the Weyl quantization, stated in Prop. 2.11 for symbols $a \in \mathcal{S}$, can be generalized to all $a \in S(1)$.

Theorem 4.29. *For any real-valued symbol $a \in S(1)$, the operator $\text{Op}_h^W(a) : L^2 \rightarrow L^2$ is selfadjoint.*

4.6. Going in the reverse direction: from L^2 properties of the operator to those of its symbol. The Calderón-Vaillancourt theorem has a sort of “inverse”, namely we can deduce properties of the symbol $a \in \mathcal{S}'(\mathbb{R}^{2d})$ from the properties of the action of operator $\text{Op}_h(a)$ on L^2 . We first state without proof a result concerning the case $\hbar = 1$.

Proposition 4.30. *Let $a \in \mathcal{S}'(\mathbb{R}^{2d})$. We assume that the right quantization operators $\text{Op}_1^R(\partial^\alpha a)$ are bounded $L^2 \rightarrow L^2$ for all derivatives of order $|\alpha| \leq 2d+1$. Then $a \in L^\infty(\mathbb{R}^{2d})$, and we have the estimate*

$$\|a\|_{L^\infty} \leq C_d \sum_{|\alpha| \leq 2d+1} \|\text{Op}_1^R(\partial^\alpha a)\|_{\mathcal{L}(L^2)}.$$

Using the $\hbar^{1/2}$ -rescaling which connects $\text{Op}_h(a)$ with $\text{Op}_1(a_h)$, we obtain a more precise result in case of the $\hbar$ -quantization:

$$(4.14) \quad \|a\|_{L^\infty} \leq C_d \sum_{|\alpha| \leq 2d+1} \hbar^{|\alpha|/2} \|\text{Op}_h^R(\partial^\alpha a)\|_{L^2 \rightarrow L^2}.$$

The relations between the right symbol and the t -symbol lead to the following

Corollary 4.31. *Then there exists an integer $M_d > 0$ such that the following holds. For a given $t \in [0, 1]$, we assume that operators $\text{Op}_1^t(\partial^\alpha a)$ are bounded $L^2 \rightarrow L^2$ for all derivatives of order $|\alpha| \leq M_d$. Then $a \in L^\infty(\mathbb{R}^{2d})$, and we have the estimate*

$$\|a\|_{L^\infty} \leq C_d \sum_{|\alpha| \leq M_d} \|\text{Op}_1^t(\partial^\alpha a)\|_{L^2 \rightarrow L^2},$$

as well as the corresponding $\hbar$ -estimate.

Proof. For symbols a_t such that $\text{Op}_h^t(a_t) = \text{Op}_h^1(a_1)$, we have seen that $a_t = e^{i\hbar(t-1)D_x \cdot D_\xi} a_1$. Because all derivatives commute, we have $\partial^\alpha a_t = e^{i\hbar(t-1)D_x \cdot D_\xi} \partial^\alpha a_1$ for any $\alpha \in \mathbb{N}^{2d}$, and thus that $\text{Op}_h^t(\partial^\alpha a_t) = \text{Op}_h^1(\partial^\alpha a_1)$. The bounds on $\|\text{Op}_h^t(\partial^\alpha a_t)\|_{L^2}$ apply as well to $\|\text{Op}_h^1(\partial^\alpha a_1)\|_{L^2}$. The previous proposition hence delivers bounds on $\|a_1\|_{L^\infty}$, but as well to $\|\partial^\alpha a_1\|_{L^\infty}$ as long as $|\alpha| \leq M_d - (2d+1)$, so eventually we get a bound for $\|a_1\|_{C^{M_d-(2d+1)}}$.

On the other hand, the analysis of the convolution-type integral relating a_t with a_1 shows that, after sufficiently many integration by parts, we may control $\|a_t\|_{L^\infty}$ by a certain number of derivatives of a_1 :

$$\|a_t\|_{C^0} \lesssim \|a_1\|_{C^K}$$

for a certain $K = K(d)$. As a result, it suffices to take $M_d - (2d + 1) \geq K$ to control $\|a_t\|_{L^\infty}$. $\square$

From this estimate we deduce Beals's Theorem, which allows to characterize symbols in $S(1)$ from the properties of their quantization. This characterization uses the commutators of $A = \text{Op}_h^t(a)$ with the quantizations of linear symbols $\ell(x, \xi) = \xi_0 \cdot x - x_0 \cdot \xi$. The *adjoint action* of $\text{Op}_h(\ell)$ on some operator A is defined by the commutator

$$\text{ad}_{\text{Op}_h(\ell)} A = [\text{Op}_h(\ell), A].$$

Theorem 4.32. (*Beals's Theorem*) Let $a \in \mathcal{S}'(\mathbb{R}^{2d})$, possibly depending on $\hbar \in (0, 1]$, and for some $t \in [0, 1]$ take $A = \text{Op}_h^t(a)$. Then the two followings statements are equivalent:

1) $a \in S(1)$.

2) for every $N \geq 0$ and every sequence $\ell_1, \dots, \ell_N$ of linear symbols, the operator $\text{ad}_{\text{Op}_h(\ell_N)} \circ \dots \circ \text{ad}_{\text{Op}_h(\ell_1)} A$ is bounded on L^2 , with norm

$$(4.15) \quad \|\text{ad}_{\text{Op}_h(\ell_N)} \circ \dots \circ \text{ad}_{\text{Op}_h(\ell_1)} A\|_{\mathcal{L}(L^2)} = \mathcal{O}_N(\hbar^N).$$

Proof. We simply notice that $\text{ad}_{\text{Op}_h(\ell_1)} A$ involves derivatives of $a(\rho)$. The commutation with linear symbols is covariant with quantization, in the sense that the first-order expansion of the Moyal product is exact:

$$[\text{Op}_h(\ell), \text{Op}_h(a)] = -i\hbar \text{Op}_h(\{\ell, a\})$$

so the assumption implies that $\|\text{Op}_h(\partial a)\| = \mathcal{O}(1)$. Proceeding by iterations, we find that that $\|\text{Op}_h(\partial^\alpha a)\|_{\mathcal{L}(L^2)} = \mathcal{O}_\alpha(1)$ for all $\alpha \in \mathbb{N}^{2d}$. Injecting these estimates in (4.14) we get, for any $\beta \in \mathbb{N}^{2d}$,

$$\|\partial^\beta a\|_{L^\infty} \leq C_d \sum_{|\alpha| \leq 2d+1} \hbar^{|\alpha|/2} \|\text{Op}_h(\partial^{\beta+\alpha} a)\|_{\mathcal{L}(L^2)} = \mathcal{O}_\beta(1),$$

which shows that $a \in S(1)$. $\square$

4.7. Compact, Hilbert-Schmidt, Trace class pseudodifferential operators. We now study in more detail the pseudodifferential $\text{Op}_h(a)$ on $L^2(\mathbb{R}^d)$, with a view on their spectral properties.

One of our objectives is to find criteria for our operators to have discrete spectra. For this we will use a characterization of compact operators, since one way to prove discreteness of the spectrum of a symmetric operator A is to show that its resolvent $(A - i)^{-1}$ is compact. In a second step, we will be interested in counting the eigenvalues of A , and for this we will use the *functional calculus* of pseudodifferential operators.

We recall a few definitions relative to bounded operators $A : L^2 \rightarrow L^2$.

Definition 4.33. An operator $A : L^2 \rightarrow L^2$ is said to be *compact* if it maps any bounded subset of L^2 into a precompact set of L^2 . Equivalently, for any sequence $(\psi_j)_j$ bounded in L^2 , one can extract from the sequence $(A\psi_j)$ a subsequence converging in L^2 .

Proposition 4.34. *The spectrum of a compact operator A is made of eigenvalues $\mu_i \neq 0$ with finite multiplicities, which only possible accumulation point being the origin.*

If A is compact, then A^*A and AA^* are compact and selfadjoint, their nonzero eigenvalues can be called $(s_j^2)_{j \geq 1}$ (in decreasing order). The $(s_j)_{j \geq 1}$ are called the *singular values* of A .

Definition 4.35. A compact operator A is said to be *Hilbert-Schmidt* if $\sum_{j \geq 1} s_j^2 < \infty$. This condition defines the Hilbert-Schmidt norm $\|A\|_{HS}^2 \stackrel{\text{def}}{=} \sum_{j \geq 1} s_j^2$ of the operator A .

As we will see below, the space of H-S operators (also called the 2d Schatten class) admits a natural Hilbert structure.

Definition 4.36. A compact operator A is said to be *trace class* if $\sum_j s_j < \infty$. This condition defines a Banach norm $\|A\|_{tr} \stackrel{\text{def}}{=} \sum_j s_j$ on the space of trace class operators. This norm can be defined through a variational principle:

$$(4.16) \quad \|A\|_{tr} = \sup_{(e_j), (f_j)} \operatorname{Re} \sum_j \langle e_j, A f_j \rangle,$$

where the supremum is taken over all pairs of orthonormal bases.

The space of trace class operators (also called the 1st Schatten class) admits a linear functional, called the trace. It can be defined, for any orthonormal basis $(e_j)_{j \geq 1}$, by $\operatorname{tr} A \stackrel{\text{def}}{=} \sum_{j \geq 1} \langle e_j, A e_j \rangle$. This linear functional is continuous w.r.t. the trace norm: $|\operatorname{tr} A| \leq \|A\|_{tr}$.

Proposition 4.37. *i) A trace class $\Rightarrow$ A Hilbert-Schmidt.*

ii) For any A trace class (resp. HS) and B bounded, then AB and BA is trace class (resp. HS).¹⁷ The ideal of compact operators is closed for the operator norm: if $(A_n)_n$ are compact and $\|A_n - A\| \rightarrow 0$, then A is compact.

iii) If A, B are HS, then AB is trace-class, and $\|BA\|_{tr} \leq \|B\|_{HS} \|A\|_{HS}$. The HS scalar product is defined by $\langle A, B \rangle_{HS} = \operatorname{tr} A^ B$.*

iv) The trace enjoys the cyclic property $\operatorname{tr}(AB) = \operatorname{tr}(BA)$ (if A is trace-class and B bounded, or if A, B are HS).

¹⁷More formally, trace-class (resp. HS) operators forms a ideal of the space of bounded operators

On $L^2(\mathbb{R}^d)$, an operator A is Hilbert-Schmidt iff its Schwartz kernel $K_A \in L^2(\mathbb{R}^d \times \mathbb{R}^d)$, and one has

$$(4.17) \quad \|A\|_{HS} = \|K\|_{L^2}.$$

Corollary 4.38. *Take $a \in \mathcal{S}'(\mathbb{R}^{2d})$. Then the operator $\text{Op}_h^W(a)$ (which, a priori, acts $\mathcal{S} \rightarrow \mathcal{S}'$) can be extended to a Hilbert Schmidt operator $L^2 \rightarrow L^2$ iff its symbol $a \in L^2(\mathbb{R}^{2d})$. One then has the identity*

$$\|\text{Op}_h^W(a)\|_{HS}^2 = \int |a(x, \xi)|^2 \frac{dx d\xi}{(2\pi\hbar)^d} = \frac{1}{(2\pi\hbar)^d} \|a\|_{L^2(\mathbb{R}^{2d})}^2.$$

Proof. Let us start with symbols $a \in \mathcal{S}(\mathbb{R}^{2d})$. Start from the characterization (4.17), and recall the relationship between kernel and symbol:

$$K(x, y) = \int a\left(\frac{x+y}{2}, \xi\right) e^{i\frac{\xi \cdot (x-y)}{\hbar}} \frac{d\xi}{(2\pi\hbar)^d} = \frac{1}{(2\pi\hbar)^{d/2}} \left(\mathcal{F}_{\hbar|\xi \rightarrow z}^{-1} a\right)\left(\frac{x+y}{2}, z = x-y\right).$$

Using the fact that the change of variables $(x, y) \mapsto \left(\frac{x+y}{2}, x-y\right)$ has Jacobian unity, and the Parseval identity, we get

$$\int |K(x, y)|^2 dx dy = \frac{1}{(2\pi\hbar)^d} \int \left| \left(\mathcal{F}_{\hbar|\xi \rightarrow x_-}^{-1} a\right)(x_+, x_-) \right|^2 dx_+ dx_- = \frac{1}{(2\pi\hbar)^d} \int |a(x_+, \xi)|^2 dx_+ d\xi.$$

□

This identity can now be extended by density: $K \in L^2(\mathbb{R}^d \times \mathbb{R}^d)$ iff $a \in L^2(\mathbb{R}^{2d})$. We notice that symbols $a \in L^2(\mathbb{R}^{2d})$ are not necessarily in $S(1)$; nevertheless, we will mostly use the above characterization in cases where $a \in S(1) \cap L^2$. Since $HS \subset \text{compact}$, this corollary gives us a simple criterion to show the compactness of a PDO.

Corollary 4.39. *Assume the order function $m(\rho)$ belongs to $L^2(\mathbb{R}^{2d})$. Then for any symbol $a \in S(m)$, the operator $\text{Op}_h^W(a)$ is HS, hence compact. Besides, the HS norm of $\text{Op}_h^W(a)$ is bounded by $\mathcal{O}(\hbar^{-d/2})$.*

If the Schwartz kernel $K \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$, it is known that the operator $A_K : L^2 \rightarrow L^2$ is trace class, and its trace is given by

$$(4.18) \quad \text{tr} A_K = \int K(x, x) dx.$$

(this formula is the continuous analogue of the discrete sum $\text{tr} M = \sum_i M_{ii}$ for matrices). The relation between the symbol and the kernel of $\text{Op}_h^t(a)$ allows to prove the following Proposition.

Proposition 4.40. *Assume $a \in \mathcal{S}(\mathbb{R}^{2d})$. Then for any $t \in [0, 1]$ and any $\hbar \in (0, 1]$ the operator $\text{Op}_\hbar^t(a)$ is trace class, and its trace is given by*

$$\text{tr Op}_\hbar^t(a) = \frac{1}{(2\pi\hbar)^d} \int a(x, \xi) dx d\xi.$$

Proof. The relation between symbol and kernel is given in (2.3):

$$K(x, y) = (2\pi)^{-d/2} [\mathcal{F}_{\xi \rightarrow z} a](tx + (1-t)y, z = x - y).$$

Inserting this expression in the integral (4.18), we get

$$\text{tr Op}_\hbar^t(a) = \frac{1}{(2\pi\hbar)^{d/2}} \int [\mathcal{F}_{\xi \rightarrow z} a](x, 0) dx d\xi = \frac{1}{(2\pi\hbar)^d} \int a(x, \xi) dx d\xi.$$

□

Here is a more general criterion for a PDO to be compact on $L^2(\mathbb{R}^d)$.

Theorem 4.41. *If an order function m satisfies $m(\rho) \xrightarrow{|\rho| \rightarrow \infty} 0$, then for any $a \in S(m)$ and any $\hbar \in (0, 1]$, $t \in [0, 1]$, the operator $\text{Op}_\hbar^t(a)$ is a compact operator on $L^2(\mathbb{R}^d)$.*

Proof. We use the decomposition of $a(\rho)$ used in the proof of the Calderon-Vaillancourt Theorem, namely we split it into compactly supported symbols $a = \sum_{\mathbf{n} \in \mathbb{Z}^{2d}} a_{\mathbf{n}}$. We know that each $\text{Op}_\hbar(a_{\mathbf{n}})$ (we skip the superscript t) is H-S hence compact, therefore $A_M \stackrel{\text{def}}{=} \sum_{|\mathbf{n}| \leq M} A_{\mathbf{n}}$ is compact for any $M > 0$. The ideal of compact operators is closed w.r.t. the operator norm, so we only need to show that

$$(4.19) \quad \|A - A_M\|_{L^2 \rightarrow L^2} \xrightarrow{M \rightarrow \infty} 0.$$

To prove this limit we use the Cotlar-Stein Lemma, applied to the operator

$$B_M = A - A_M = \sum_{|\mathbf{n}| > M} A_{\mathbf{n}}.$$

Indeed, for $a \in S(m)$ the estimates (4.9, 4.10) are easily modified into

$$\begin{aligned} \|A_{\mathbf{n}}^* A_{\mathbf{n}'}\|_{L^2 \rightarrow L^2} &\leq C_{a,d} m(\mathbf{n}) m(\mathbf{n}') \quad |\mathbf{n} - \mathbf{n}'| \leq 10R_d, \\ \|A_{\mathbf{n}}^* A_{\mathbf{n}'}\|_{L^2 \rightarrow L^2} &\leq C_{a,k} \hbar^{k-2d} \frac{m(\mathbf{n}) m(\mathbf{n}')}{\langle \mathbf{n} - \mathbf{n}' \rangle^k}, \quad |\mathbf{n} - \mathbf{n}'| > 10R_d, \quad k \geq 2d + 1. \end{aligned}$$

Hence, for any $\mathbf{n} \in \mathbb{Z}^{2d}$ we may write

$$\sum_{|\mathbf{n}'| > M} \|A_{\mathbf{n}}^* A_{\mathbf{n}'}\|^{1/2} \leq C_{a,d} \sum_{|\mathbf{n}'| > M} \frac{\sqrt{m(\mathbf{n}) m(\mathbf{n}')}}{\langle \mathbf{n} - \mathbf{n}' \rangle^{k/2}} \leq C'_{a,d} m(\mathbf{n}),$$

where we used the defining property of an order function, and took k large enough to have the sum converge. As a result we get

$$\sup_{|\mathbf{n}| > M} \sum_{|\mathbf{n}'| > M} \|A_{\mathbf{n}}^* A_{\mathbf{n}'}\|^{1/2} \leq C'_{a,d} \sup_{|\mathbf{n}| > M} m(\mathbf{n}) \xrightarrow{M \rightarrow \infty} 0,$$

The same convergence holds for the sums $\sum_{\mathbf{n}'} \|A_{\mathbf{n}'} A_{\mathbf{n}}^*\|^{1/2}$. Applying the Cotlar-Stein Theorem proves the limit (4.19), hence the theorem. $\square$

4.7.1. Criteria for trace class operators. Let us now investigate criterions for a PDO to be trace-class. Let us first consider the case of an operator A with Schwartz kernel $K(x, y) \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$. If we consider a cutoff function $\psi \in C_c^\infty(\mathbb{R}^d)$ such that $\psi(x)\psi(y) \equiv 1$ on the support of K , we have

$$K(x, y) = \psi(x)\psi(y)K(x, y) = \int \hat{K}(\xi, \eta) e^{i(\xi \cdot x + y \cdot \eta)} \psi(x)\psi(y) \frac{d\xi d\eta}{(2\pi)^d}, \quad \text{with the notation } \hat{K} = \mathcal{F}_1 K.$$

For each ξ, η , the kernel $e^{i(\xi \cdot x + y \cdot \eta)} \psi(x)\psi(y)$ represents the rank-1 operator $u \mapsto \psi_\xi \langle \psi_{-\eta}, u \rangle$, where $\psi_\xi(x) = e^{i\xi \cdot x} \psi(x)$. The formula (4.16) shows that this operator has trace norm $\|\psi\|_{L^2}^2$, and a trace $\text{tr}(\psi_\xi \langle \psi_{-\eta}, \bullet \rangle) = \int e^{i(\xi + \eta) \cdot x} \psi(x)^2 dx$, so we get

$$(4.20) \quad \|A\|_{tr} \leq \|\psi\|_{L^2}^2 \int \left| \hat{K}(\xi, \eta) \right| \frac{d\xi d\eta}{(2\pi)^d} = \frac{\|\psi\|_{L^2}^2}{(2\pi)^d} \|\hat{K}\|_{L^1},$$

$$(4.21) \quad \text{tr} A = \int \int \hat{K}(\xi, \eta) e^{i(\xi + \eta) \cdot x} \psi(x)^2 \frac{dx d\xi d\eta}{(2\pi)^d} = \int K(x, x) dx.$$

A more general kernel K may be split using a partition of unity of $\mathbb{R}^d$, $1 = \sum_{\mathbf{n} \in \mathbb{Z}^d} \chi(\bullet - \mathbf{n})$, where $\chi \in C^\infty(\mathbb{R}^d, [0, 1])$ is supported in the box $[-1, 1]^d$:

$$(4.22) \quad K(x, y) = \sum_{\mathbf{n}, \mathbf{n}' \in \mathbb{Z}^d} K_{\mathbf{n}, \mathbf{n}'}(x, y), \quad K_{\mathbf{n}, \mathbf{n}'}(x, y) \stackrel{\text{def}}{=} K(x, y) \chi(x - \mathbf{n}) \chi(y - \mathbf{n}').$$

We may apply to each truncated kernel $K_{\mathbf{n}, \mathbf{n}'}$ the estimate (4.20), using the $\mathbb{Z}^d$ -translates of a fixed function ψ equal to unity in $[-1, 1]^d$ (note that all the translates share the same L^2 norm). If the $\|\widehat{K_{\mathbf{n}, \mathbf{n}'}}\|_{L^1}$ decay sufficiently fast so that $\sum_{\mathbf{n}, \mathbf{n}'} \|\widehat{K_{\mathbf{n}, \mathbf{n}'}}\|_{L^1} < \infty$, then by triangle inequality we deduce that A is trace class, with norm

$$\|A\|_{tr} \leq C_\psi \sum_{\mathbf{n}, \mathbf{n}'} \|\widehat{K_{\mathbf{n}, \mathbf{n}'}}\|_{L^1} < \infty, \quad \text{with} \quad C_\psi = \frac{\|\psi\|_{L^2}^2}{(2\pi)^d}.$$

By the standard Fourier transform estimate we have

$$\|\widehat{K_{\mathbf{n}, \mathbf{n}'}}\|_{L^1} \leq C_d \sum_{|\alpha| \leq 2d+1} \|\partial^\alpha K_{\mathbf{n}, \mathbf{n}'}\|_{L^1}.$$

Taking into account the partition of unity (4.22) and the fact that the derivatives of ψ are bounded, we find that

$$\|A\|_{tr} \leq C \sum_{|\alpha| \leq 2d+1} \sum_{\mathbf{n}, \mathbf{n}'} \|\partial^\alpha K_{\mathbf{n}, \mathbf{n}'}\|_{L^1} \leq C' \sum_{|\alpha| \leq 2d+1} \|\partial_{x,y}^\alpha K\|_{L^1(dx dy)}.$$

If the RHS is finite, the function $x \mapsto K(x, x)$ is then automatically continuous, bounded and integrable, and we have by linearity

$$\mathrm{tr} A = \int K(x, x) dx.$$

We have showed the following

Proposition 4.42. *Assume that Schwartz kernel $K(x, y)$ of an operator $A : L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$ satisfies*

$$\sum_{|\alpha| \leq 2d+1} \|\partial_{x,y}^\alpha K\|_{L^1(dx dy)} < \infty.$$

Then this operator is trace class on $L^2(\mathbb{R}^d)$, and its trace-norm is bounded by

$$(4.23) \quad \|A\|_{tr} \leq C_d \sum_{|\alpha| \leq 2d+1} \|\partial_{x,y}^\alpha K\|_{L^1(dx dy)}.$$

Furthermore, the restriction of the kernel on the diagonal is integrable, and

$$\mathrm{tr}(A) = \int K(x, x) dx.$$

Let us now search a criterion for a PDO $\mathrm{Op}_h(a)$ to be trace-class. For simplicity we start using the right quantization $\mathrm{Op}_1^R(a)$, which we may write as

$$\mathrm{Op}_1^R(a)u(x) = \int e^{i\xi \cdot x} a(x, \xi) \mathcal{F}_1 u(\xi) \frac{d\xi}{(2\pi)^{d/2}}.$$

Hence, $\mathrm{Op}_1^R(a)$ is the composition of the (unitary) Fourier transform, with the operator of kernel $K(x, \xi) = e^{i\xi \cdot x} a(x, \xi)$ (viewing ξ as the initial variable). These two operators share the same singular values, hence $\mathrm{Op}_1^R(a)$ is trace class iff A_K is so.

It is not possible to directly use the estimate (4.23) for the kernel $K(x, \xi)$, since we get a (bad) factor ξ each time we differentiate it w.r.t. x , and vice-versa. As we did before, we split this kernel using the smooth partition of unity $\sum_{\mathbf{n}} \chi(\bullet - \mathbf{n})$, to get elements

$$K_{\mathbf{n}, \mathbf{n}'}(x, \xi) = \chi(x - \mathbf{n}) \chi(\xi - \mathbf{n}') e^{i\xi \cdot x} a(x, \xi).$$

We then decompose the phase $\xi \cdot x = (\xi - \mathbf{n}') \cdot (x - \mathbf{n}) + \xi \cdot \mathbf{n} + \mathbf{n}' \cdot x - \mathbf{n} \cdot \mathbf{n}'$, so that the derivatives of the first term remains uniformly bounded in $\mathrm{supp} K_{\mathbf{n}, \mathbf{n}'}$. The terms $\xi \cdot \mathbf{n} + \mathbf{n}' \cdot x$

produce a shift in the Fourier transform:

$$\widehat{K_{\mathbf{n}, \mathbf{n}'}}(x^*, \xi^*) = e^{-i\mathbf{n} \cdot \mathbf{n}'} \widehat{a_{\mathbf{n}, \mathbf{n}'}}(x^* - \mathbf{n}', \xi^* - \mathbf{n}), \quad \text{where} \quad a_{\mathbf{n}, \mathbf{n}'}(x, \xi) \stackrel{\text{def}}{=} \chi(x - \mathbf{n}) \chi(\xi - \mathbf{n}') e^{i(\xi - \mathbf{n}') \cdot (x - \mathbf{n})} a(x, \xi)$$

We thus get a trace class operator provided

$$\sum_{\mathbf{n}', \mathbf{n}'} \|\widehat{K_{\mathbf{n}, \mathbf{n}'}}\|_{L^1} = \sum_{\mathbf{n}', \mathbf{n}'} \|\widehat{a_{\mathbf{n}, \mathbf{n}'}}\|_{L^1} < \infty$$

The advantage of this phase decomposition is that the derivatives of $a_{\mathbf{n}, \mathbf{n}'}$ are bounded uniformly in terms of those of the derivatives of $a(x, \xi)$ near $(\mathbf{n}, \mathbf{n}')$, because the factors $(\xi - \mathbf{n}')$, $(x - \mathbf{n})$ in the phase remain bounded. Hence, the above RHS is bounded above by

$$C \sum_{\mathbf{n}, \mathbf{n}'} \sum_{|\alpha| \leq 2d+1} \|\partial^\alpha a_{\mathbf{n}, \mathbf{n}'}\|_{L^1} \leq C' \sum_{|\alpha| \leq 2d+1} \|\partial^\alpha a\|_{L^1}.$$

We have thus proved that

$$\|\text{Op}^R(a)\|_{tr} \leq C_d \sum_{|\alpha| \leq 2d+1} \|\partial^\alpha a\|_{L^1(\mathbb{R}^{2d})}.$$

We may now restore the factors $\hbar$, using the unitary rescaling (4.13): $\text{Op}_\hbar^R(a) = U_\hbar \text{Op}_1^R(a_\hbar) U_\hbar^*$ imply that the two conjugate operators have same trace norm and trace. Analyzing the L^1 norms of $\partial^\alpha a_\hbar$, we obtain the following criteria for trace-class property:

Theorem 4.43. *Assume that the symbol $a \in S(1)$ satisfies $\sum_{|\alpha| \leq 2d+1} \|\partial^\alpha a\|_{L^1} \leq C$ uniformly for $\hbar \in (0, 1]$. Then the operator $\text{Op}_\hbar^R(a)$ is trace class, with the bound*

$$\|\text{Op}_\hbar^R(a)\|_{tr} \leq C_d \hbar^{-d} \sum_{|\alpha| \leq 2d+1} \hbar^{|\alpha|/2} \|\partial^\alpha a\|_{L^1(\mathbb{R}^{2d})}.$$

Its trace is explicitly given by

$$\text{tr Op}_\hbar^R(a) = \frac{1}{(2\pi\hbar)^d} \int a(x, \xi; \hbar) dx d\xi.$$

5. QUANTITATIVE STUDY OF SEMICLASSICAL PDOs

We now want to use the $\hbar$ -PDO toolbox to get informations on the spectral properties of $\text{Op}_\hbar(a)$ in terms of the properties of its symbol $a(x, \xi)$. We'll see that in some cases we can have access to a rather precise description of that spectrum.

5.1. Invertibility of elliptic PDOs and Gårding inequalities.

5.1.1. Ellipticity and invertibility. The first question is that of the *invertibility* of the operator $\text{Op}_\hbar(a)$, when the symbol a is invertible (that is, nonvanishing) on $\mathbb{R}^{2d}$.

Definition 5.1. A symbol $a \in S(1)$ is said to be (*semiclassically*) *elliptic* (in $S(1)$) if $|a(\rho; \hbar)| \geq \gamma > 0$ for all $\rho \in \mathbb{R}^{2d}$ and $\hbar \in (0, 1]$.

In that case, the pseudodifferential calculus of Cor. 4.28 will allow us to construct a *parametrix* for $\text{Op}_\hbar^W(a)$ (that is, a quasi-inverse), which is then easily transformed into a true inverse.

Theorem 5.2. Assume that $a \in S(1)$ is $\hbar$ -independent and elliptic. Then for $\hbar > 0$ small enough, $\text{Op}_\hbar(a)$ is invertible, and its inverse is a PDO with symbol $b = b(\hbar) \in S(1)$ admitting an asymptotic expansion

$$b \sim \sum_j \hbar^j b_j, \quad \text{with principal symbol } b_0 = \frac{1}{a}.$$

Proof. The construction is similar with the one in the proof of Proposition 3.22. We start by the trial function (Ansatz) $b_0 = 1/a$. From the ellipticity of a , one easily checks that this symbol is in $S(1)$. Then, the symbol calculus shows that

$$a \#_\hbar b_0 = 1 + r_1, \quad r_1 \in \hbar S(1).$$

From the Calderón-Vaillancourt theorem, for $\hbar$ small enough we'll have $\|\text{Op}_\hbar(r_1)\|_{L^2 \rightarrow L^2} \leq 1/2$, so we can invert $1 + \text{Op}_\hbar(r_1)$ by Neumann series¹⁸, to get

$$\text{Op}_\hbar(a) \text{Op}_\hbar(b_0) (I + \text{Op}_\hbar(r_1))^{-1} = I.$$

This produces a right inverse B^R for $\text{Op}_\hbar(a)$, with operator norm $\|B^R\|_{L^2 \rightarrow L^2} \leq C$. One may similarly construct a left inverse of the form $B^L = (I + \text{Op}_\hbar(r_2))^{-1} \text{Op}_\hbar(b_0)$. The existence of these two inverses shows that $\text{Op}_\hbar(a)$ is invertible, and that $B^L = B^L \text{Op}_\hbar(a) B^R = B^R \stackrel{\text{def}}{=} B$.

¹⁸The Neumann series is the expression $(I + R)^{-1} = \sum_{n \geq 0} (-1)^n R^n$, with norm $\|(I + R)^{-1}\| \leq (1 - \|R\|)^{-1}$, valid as soon as $\|R\| < 1$.

To prove that $B = \text{Op}_h(b)$ with $b \in S(1)$, one may use Beals's Theorem 4.32, and the following algebraic trick. For any linear symbols $\ell_1, \dots, \ell_N$, the commutator

$$(5.1) \quad \text{ad}_{\text{Op}_h(\ell_1)} B = -B (\text{ad}_{\text{Op}_h(\ell_1)} \text{Op}_h(a)) B = \mathcal{O}(\hbar)_{L^2 \rightarrow L^2}.$$

Applying the Leibniz rule to this expression, one shows by iteration that

$$\prod_{j=1}^N \text{ad}_{\text{Op}_h(\ell_j)} B = \mathcal{O}(\hbar^N)_{L^2 \rightarrow L^2}.$$

Beals's Lemma then states that $b \in S(1)$.

To get more information on the symbol b , we notice that $r_1 \in \hbar S(1)$, so we may partially cancel it by taking $b_1 = -r_1/a$, so that $a \# b_1 = -r_1 + \mathcal{O}(\hbar^2)_{S(1)}$. Continuing this way, we construct $b_2, b_3, \dots, b_N$ with $b_j \in \hbar^j S(1)$, such that $a \# (b_0 + \dots + b_N) = I + \mathcal{O}(\hbar^{N+1})_{S(1)}$. An equivalent way to obtain the expansion of b is to write:

$$b \sim b_0 \#_h (1 - r_1 + r_1 \#_h r_1 - r_1 \#_h r_1 \#_h r_1 + \dots)$$

□

This inversion property can be generalized to elliptic symbols in classes $S(m)$ for an arbitrary order function $m(\rho)$.

Definition 5.3. A symbol $a \in S(m)$ is said to be *elliptic* (in that class) if there exists $\gamma > 0$ such that $|a(\rho)| \geq \gamma m(\rho)$ for all $\rho \in \mathbb{R}^{2d}$ and $\hbar \in (0, 1]$.

Theorem 5.4. *If $a \in S(m)$ is elliptic, then for $\hbar \leq \hbar_0$ small enough, there exists $b \in S(m^{-1})$ such that $a \#_h b = b \#_h a = 1$.*

Proof. From the symbol $b_0 = a^{-1} \in S(m^{-1})$, we have $a \#_h b_0 = 1 + r_1(\hbar)$, with the symbol calculus showing that $r_1(\hbar) \in \hbar S(1)$. We can then use the preceding theorem in order (when $\hbar < \hbar_0$) to invert $\text{Op}_h(1 + r_1)$ into a PDO with symbol $\sim 1 - r_1 + r_1 \#_h r_1 - \dots$, and finally apply the Moyal product with $a^{-1} \in S(m^{-1})$ to get the exact inverse $b \in S(m^{-1})$. We notice that the formula for b is identical with the case $a \in S(1)$, the only change is in the symbol classes the various factors belong to. □

5.2. Domains of operators in $\Psi_h(m)$: semiclassical Sobolev spaces. Now that we know that symbols $a \in S(1)$ lead to bounded operators on $L^2 \rightarrow L^2$, what can be said of operators issued from symbols $a \in S(m)$ for a general order function m ? We will mostly consider the case when $m \geq 1$ and $m(\rho) \rightarrow \infty$ when $|\rho| \rightarrow \infty$, at least along certain directions in phase space.

Example 5.5. The semiclassical Laplacian $P = -\hbar^2 \Delta$ is the quantization of $p(x, \xi) = |\xi|^2$. This symbol belongs to the class $m(\rho) = \langle \xi \rangle^2$, which diverges in the limit $|\xi| \rightarrow \infty$. It is well-known that the Laplacian is unbounded on L^2 , and admits as natural domain the Sobolev space $H^2(\mathbb{R}^{2d}) = \{u \in L^2, \Delta u \in L^2\}$. This Sobolev space can be constructed as the image of L^2 by the resolvent $(1 - \Delta)^{-1}$, but also as the image of L^2 by the resolvent $(1 - \hbar^2 \Delta)^{-1}$:

$$H^2(\mathbb{R}^d) = (1 - \hbar^2 \Delta)^{-1} L^2(\mathbb{R}^d).$$

For a given $\hbar > 0$, we can equip this Sobolev space by the norm resulting from this construction, that is take, for any $u = (1 - \hbar^2 \Delta)^{-1} v \in H^2$,

$$\|u\|_{H^2} \stackrel{\text{def}}{=} \|v\|_{L^2} = \|(1 - \hbar^2 \Delta)u\|_{L^2}.$$

Of course, this norm is equivalent with the one constructed with $\hbar = 1$. Still, to emphasize the $\hbar$ -dependence of the norm, we denote the space H^2 equipped with this norm by $H_\hbar^2$.

In the above construction, the crucial object was the operator $1 - \hbar^2 \Delta = \text{Op}_\hbar(1 + |\xi|^2)$. The symbol $(1 + |\xi|^2)$ belongs to the class $S(m)$ for $m(x, \xi) = \langle \xi \rangle^2$, and also satisfies also $(1 + |\xi|^2) \geq m(\rho)$, so according to Definition 5.3, that symbol is *elliptic* in $S(m)$.

More generally, for an order function m , we may use an elliptic symbol in $S(m)$ to define a norm on $\mathcal{S}$, and then a functional space by completion.

Definition 5.6. Let m be an order function, and g_m be an elliptic symbol in $S(m)$. We then define the following norm on $\mathcal{S}(\mathbb{R}^d)$:

$$\forall u \in \mathcal{S}(\mathbb{R}^d), \quad \|u\|_{H_\hbar(m)} \stackrel{\text{def}}{=} \|\text{Op}_\hbar(g_m)u\|_{L^2}.$$

The completion of $\mathcal{S}(\mathbb{R}^d)$ w.r.t. this norm is denoted by $H_\hbar(m)$, it is called a generalized (semiclassical) Sobolev space.

Lemma 5.7. *If we choose another elliptic symbol g' in $S(m)$, then for $\hbar \leq \hbar_0$ small enough the corresponding norm is equivalent with the one above, with implied constants uniform w.r.t. $\hbar \in (0, \hbar_0]$.*

Proof. Let us call $\|u\|'_{H_\hbar(m)} \stackrel{\text{def}}{=} \|\text{Op}_\hbar(g')u\|_{L^2}$. From the ellipticity of $g \in S(m)$, for $\hbar$ small enough $\text{Op}_\hbar(g)$ is invertible and $\text{Op}_\hbar(g)^{-1} \in \Psi_\hbar(m^{-1})$, so that $\text{Op}_\hbar(g') \text{Op}_\hbar(g)^{-1} \in \Psi_\hbar(1)$. Hence

$$\begin{aligned} \|u\|'_{H_\hbar(m)} &= \|\text{Op}_\hbar(g') \text{Op}_\hbar(g)^{-1} \text{Op}_\hbar(g)u\|_{L^2} \\ &\leq \|\text{Op}_\hbar(g') \text{Op}_\hbar(g)^{-1}\|_{L^2 \rightarrow L^2} \|\text{Op}_\hbar(g)u\|_{L^2}, \end{aligned}$$

so $\|u\|'_{H_\hbar(m)} \leq C \|u\|_{H_\hbar(m)}$, with $C > 0$ uniform w.r.t. $\hbar$. Since g and g' play symmetric roles, we obtain the uniform norm equivalence for $\hbar \leq \hbar_0$. $\square$

Similarly, we may compare two generalized Sobolev spaces if the corresponding order functions are ordered:

Proposition 5.8. *Assume two order functions satisfy $m \leq m'$. We then have the inclusion $S(m) \subset S(m')$, and the opposite inclusion $H_h(m') \subset H_h(m)$. More quantitatively, there exists $C > 0$ such that, for any $u \in H_h(m')$ and any $\hbar \leq \hbar_0$,*

$$\|u\|_{H_h(m)} \leq C \|u\|_{H_h(m')}.$$

This bound generalizes the well-known estimates between Sobolev spaces of varying orders.

Proposition 5.9. *For any order function m , any symbol $a \in S(m)$ and $\hbar \leq \hbar_0$, the operator $\text{Op}_h(a) : \mathcal{S} \rightarrow \mathcal{S}$ can be extended to a bounded operator $H_h(m) \rightarrow L^2$.*

Proof. Let $g \in S(m)$ be an elliptic symbol, so $u \in H_h(m) \iff \text{Op}_h(g)u \in L^2$. For $\hbar \leq \hbar_0$ we have $\text{Op}_h(g)^{-1} \in \Psi_h(m^{-1})$ and $\text{Op}_h(a) \text{Op}_h(g)^{-1} \in \Psi_h(1)$. For any $u \in H_h(m)$, the action of $\text{Op}_h(a)$ on u reads:

$$\text{Op}_h(a)u = \text{Op}_h(a) \text{Op}_h(g)^{-1} \text{Op}_h(g)u.$$

In particular,

$$\|\text{Op}_h(a)u\|_{L^2} \leq \|\text{Op}_h(a) \text{Op}_h(g)^{-1}\|_{\mathcal{L}(L^2)} \|\text{Op}_h(g)u\|_{L^2} = \underbrace{\|\text{Op}_h(a) \text{Op}_h(g)^{-1}\|_{\mathcal{L}(L^2)}}_{\mathcal{O}(1)} \|u\|_{H_h(m)}.$$

□

Assume $m \geq 1$ so that $H_h(m) \subset L^2$ (see Prop. 5.8). If $a \in S(m)$ is real valued, we already know that $A \stackrel{\text{def}}{=} \text{Op}_h^W(a) : \mathcal{S} \rightarrow \mathcal{S}$ is symmetric w.r.t. the L^2 scalar product. In the case $m = 1$, $A : L^2 \rightarrow L^2$ is bounded and selfadjoint. If $m \geq 1$, we have just seen that we can take $H_h(m)$ as the domain of A . Is A essentially selfadjoint on this domain? We recall that one criterion for $A : D(A) \rightarrow L^2$ to be selfadjoint is that $\text{Ran}(A + i) = \text{Ran}(A - i) = L^2$. So we deduce the following

Proposition 5.10. *Consider an order function $m \geq 1$, assume that $a \in S(m)$ is real-valued, and is such that $a + i$ (which automatically belongs to $S(m)$) is elliptic in $S(m)$. Then for $\hbar$ small enough, the operator $\text{Op}_h^W(a) : H_h(m) \subset L^2 \rightarrow L^2$ is selfadjoint.*

Proof. From the reality of a , we already know that $\text{Op}_h^W(a)$ is symmetric. The ellipticity assumption implies that, for $\hbar$ small enough, $\text{Op}_h^W(a) \pm i : H_h(m) \rightarrow L^2$ are bijections, which is a necessary and sufficient criterion for self-adjointness. □

Another direct application of the calculus on $S(m)$ is a characterization of unbounded operators with discrete spectra.

Theorem 5.11. *Consider an order function $m(\rho) \xrightarrow{|\rho| \rightarrow \infty} \infty$. If $a \in S(m)$ is elliptic, then for $\hbar > 0$ small enough, the operator $\text{Op}_\hbar(a)$ is unbounded on L^2 with domain $H_\hbar(m)$, and it has a purely discrete spectrum.*

Proof. The ellipticity of a implies that $\text{Op}_\hbar(a)^{-1} \in \Psi_\hbar(m^{-1})$. From Theorem 4.41, the operator $\text{Op}_\hbar(a)^{-1} : L^2 \rightarrow L^2$ is compact, hence its spectrum consists in eigenvalues of finite multiplicities $\{\mu_j \in \mathbb{C}, |\mu_j| \leq C\}$ accumulating at zero (but different from zero). The spectrum of $\text{Op}_\hbar(a)$ is composed of the eigenvalues $\{\mu_j^{-1}\}$ such that $\mu_j \rightarrow \infty$ as $j \rightarrow \infty$. $\square$

Example 5.12. (Schrödinger operator with confining potential) If a potential function satisfies $V(x) \xrightarrow{|x| \rightarrow \infty} +\infty$ with polynomial growth (more precisely, V belongs to some class $S(\tilde{m})$ on $\mathbb{R}^d$ with $\tilde{m}(x) \rightarrow \infty$ and is elliptic), then the function $m(\rho) \stackrel{\text{def}}{=} \langle \xi \rangle^2 + \tilde{m}(x)$ is an order function which satisfies $m(\rho) \rightarrow \infty$. For $C > 0$ large enough the symbol $a(x, \xi) = |\xi|^2 + V(x) + C$ is obviously elliptic in $S(m)$. As a result, for $\hbar$ small enough the Schrödinger operator $\text{Op}_\hbar(a) = -\hbar^2 \Delta + V + C$ has discrete positive (and unbounded) spectrum. The spectrum of $-\hbar^2 \Delta + V$ is the same shifted by $-C$.

5.3. Resolvent operator and Gårding inequality.

5.3.1. *Weak Gårding inequality.* A major application of this invertibility will concern the study and manipulation of the **resolvent** of an operator $\text{Op}_\hbar(a) \in \Psi_\hbar(m)$, namely the family of bounded operators

$$R_\hbar(z) = (\text{Op}_\hbar(a) - z)^{-1},$$

for z in the resolvent set of $\text{Op}_\hbar(a)$, namely the subset of $\mathbb{C}$ where $\text{Op}_\hbar(a) - z : D(\text{Op}_\hbar(a)) \rightarrow L^2$ is invertible.

This family of operators is used to analyze the spectrum of $\text{Op}_\hbar(a)$, and to construct a functional calculus (at least when $\text{Op}_\hbar(a)$ is selfadjoint).

Corollary 5.13. *Take an order function $m \geq 1$, $a \in S(m)$, and $z \in \mathbb{C}$ is such that the symbol $(a - z)$ is elliptic in $S(m)$. Then for $\hbar > 0$ small enough, z belongs to the resolvent set of $\text{Op}_\hbar(a)$, and $(\text{Op}_\hbar(a) - z)^{-1}$ admits a symbol*

$$r(z; \hbar) = (a - z)^{-1} + \mathcal{O}(\hbar^2) \in S(m^{-1}).$$

Proof. The Moyal product

$$(5.2) \quad (a - z) \#_\hbar (a - z)^{-1} = 1 + 0 + r_2(z; \hbar)$$

with $r_2 \in \hbar^2 S(1)$. $\square$

A first use of the resolvent concerns the quasi-positivity of an operator Weyl-quantizing a positive symbol.

Proposition 5.14. (*Weak Gårding inequality*) *Assume that the symbol $a \in S(1)$ satisfies $a \geq 0$. Then for any $\epsilon > 0$, there exists $\hbar_\epsilon > 0$ such that, for any $0 < \hbar < \hbar_\epsilon$, the self-adjoint operator $\text{Op}_\hbar^W(a)$ satisfies*

$$\text{Op}_\hbar^W(a) \geq -\epsilon I.$$

Proof. For any fixed $z \leq -\epsilon$, $(a - z)$ is elliptic in $S(1)$, so according to the above Corollary we may invert $(\text{Op}_\hbar(a) - z)$ for $\hbar > 0$ small enough. We want to show that this “small enough $\hbar$ ” can be chosen uniformly for all $z \leq -\epsilon$. For this we need to show that the seminorms for the second-order symbol $r_2(z; \hbar)$ appearing in (5.2) are bounded uniformly w.r.t. $z \leq -\epsilon$. These seminorms involve a certain number of derivatives (w.r.t. ρ) of $(a - z)$ and $(a - z)^{-1}$. The derivatives of $(a(\rho) - z)$ are obviously independent of z ; on the other hand, the derivatives of $(a(\rho) - z)^{-1}$ are schematically of the form:

$$(5.3) \quad \partial^\alpha (a - z)^{-1} = (a - z)^{-1} \sum_{k=1}^{|\alpha|} \sum_{\beta^1 + \dots + \beta^k = \alpha} C_{\vec{\beta}} \prod_{j=1}^k \left((a - z)^{-1} \partial^{\beta^j} a \right),$$

so the RHS is bounded above by $\frac{|\partial^* a|}{(a-z)^2} + \frac{|\partial^* a| |\partial^* a|}{(a-z)^3} + \dots + \frac{|(\partial a)^k|}{(a-z)^{k+1}}$, uniformly for all $z \leq -\epsilon$. As a result, $\|\text{Op}_\hbar^W(r_2(z; \hbar))\|_{L^2 \rightarrow L^2} \leq C\hbar^2$ for all $z \leq -\epsilon$ and all $\hbar \in (0, 1]$. Hence, there exists $\hbar_\epsilon > 0$ such that $I + \text{Op}_\hbar^W(r_2(z; \hbar))$ is invertible, of uniformly bounded inverse for all $z \leq -\epsilon$ and $\hbar \in (0, \hbar_\epsilon)$. As a consequence, for any $\hbar \in (0, \hbar_\epsilon)$ and all $z \leq -\epsilon$, the operators $\text{Op}_\hbar^W(a) - z$ admit inverses of the form

$$(5.4) \quad (\text{Op}_\hbar^W(a) - z)^{-1} = \text{Op}_\hbar^W((a - z)^{-1}) \circ (I + \text{Op}_\hbar^W(r_2(z; \hbar)))^{-1},$$

showing that the half-line $(-\infty, -\epsilon]$ is in the resolvent set of $\text{Op}_\hbar^W(a)$. $\square$

Our next goal is to improve the above quasi-positivity result by trying to let the gap ϵ decay when $\hbar \searrow 0$. In such a situation the function $(a + \epsilon)^{-1}$ does not belong to $S(1)$ any longer, because it may grow like ϵ^{-1} , and its derivatives like $\epsilon^{-1-|\alpha|}$. For this reason, it is necessary to introduce classes of “singular” symbols, whose derivatives are allowed to grow when $\hbar \searrow 0$. Those symbol classes are called “exotic”.

5.3.2. Exotic symbol classes. Let us introduce the first classes of exotic symbols.

Definition 5.15. Take $\delta \in (0, 1/2)$ and an order function $m(\rho)$. We define the following exotic symbol class:

$$S_\delta(m) \stackrel{\text{def}}{=} \{a(\hbar) \in C^\infty(\mathbb{R}^{2d}), \forall \alpha \in \mathbb{N}^{2d}, \exists C_\alpha, \forall \hbar \in (0, 1]m, \forall \rho \in \mathbb{R}^{2d}, |\partial^\alpha a(\rho)| \leq C_\alpha m(\rho) \hbar^{-|\alpha|\delta}\}.$$

This class obviously extends the class $S(m)$, it contains symbols $a(\rho; \hbar)$ explicitly depending on $\hbar$, in a way which may be more and more singular as $\hbar \rightarrow 0$. For instance, this class contains functions of the type $a(\rho; \hbar) = \chi\left(\frac{\rho - \rho_0}{\hbar^\delta}\right)$, with $\chi \in C_c^\infty(\mathbb{R}^{2d})$ independent of $\hbar$: such symbols are microlocalized in a precise microscopic neighbourhood of ρ_0 when $\hbar \searrow 0$. Notice that $\hbar^\delta \gg \hbar^{1/2}$, hence the support of such an $a(\hbar)$ is much larger than a Planck cell.

Proposition 5.16. *In the case $m = 1$, the symbol calculus of Thm 4.17 and the Calderón-Vaillancourt Thm 4.26 naturally extend to the class $S_\delta(1)$, with the effective expansion parameter being $\hbar^{1-2\delta}$ instead of $\hbar$.*

Proof. If $a \in S_\delta(1)$, it is obvious that the rescaled function $\tilde{a}(\rho) \stackrel{\text{def}}{=} a(\hbar^\delta \rho)$ belongs to $S(1)$. A simple computation shows that the $\hbar^\delta$ -rescaling of the Moyal product $a_1 \#_\hbar a_2$ is exactly equal to $\tilde{a}_1 \#_{\hbar^{1-2\delta}} \tilde{a}_2$. Hence, applying Thm 4.17 to the latter product, we obtain an expansion for $a_1 \#_\hbar a_2$, with expansion parameter $\hbar^{1-2\delta}$.

Concerning the L^2 -boundedness, a slight modification of the scaling operator of eq.(4.13) shows that $U_{\hbar^\delta} \text{Op}_\hbar^W(a) = \text{Op}_{\hbar^{1-2\delta}}^W(\tilde{a}) U_{\hbar^\delta}$, so we may apply the Calderón-Vaillancourt Thm 4.26 to the operator $\text{Op}_{\hbar^{1-2\delta}}^W(\tilde{a})$, and translate it back to $\text{Op}_\hbar^W(a)$ by unitarity. $\square$

A more “pedestrian” way to understand the appearance of this modified parameter $\hbar^{1-2\delta}$ is the following: each term in the expansion of $a_1 \#_\hbar a_2$ is of order $\hbar^j \partial^j a \partial^j b \leq C \hbar^j \hbar^{-j\delta} \hbar^{-j\delta} = C \hbar^{j(1-2\delta)}$.

We notice that the value $\delta = 1/2$ is critical: for general symbols $a_i \in S_{1/2}(1)$, even though the symbol $a_1 \#_\hbar a_2$ is well defined, it cannot be expanded in an asymptotic expansion of a small parameter. There is nevertheless a way to consider symbols whose derivatives grow almost as fast as $\hbar^{-j/2}$, but for which we can maintain some form of asymptotic calculus. It consists of introducing a *second small parameter* (called $\tilde{\hbar}$), independent of $\hbar$, and to rescale symbols by $(\hbar/\tilde{\hbar})^{1/2}$.

Definition 5.17. [Critical symbol class] Consider the usual small parameter $\hbar \in (0, 1]$, and an independent small parameter $\tilde{\hbar} \in (0, 1]$, which we see as the inverse of a large constant. We may consider a symbol class depending on these two parameters:

$$\tilde{S}_{1/2}(1) \stackrel{\text{def}}{=} \left\{ a(\hbar, \tilde{\hbar}) \in C^\infty(\mathbb{R}^{2d}), \forall \alpha \in \mathbb{N}^{2d}, \|\partial^\alpha a\|_{L^\infty} \leq C_\alpha \left(\hbar/\tilde{\hbar} \right)^{-|\alpha|/2} \right\}.$$

One may straightforwardly adapt Prop. 5.16 to this critical class:

Proposition 5.18. *The symbol calculus of Thm 4.17 and the Calderón-Vaillancourt Thm 4.26 naturally extend to the class $\tilde{S}_{1/2}(1)$, with the effective expansion parameter being $\tilde{h}$. On the other hand, if $a_1 \in \tilde{S}_{1/2}(1)$ and $a_2 \in S(1)$, then $a_1 \#_h a_2 \in \tilde{S}_{1/2}(1)$ satisfies an expansion in the parameter $(h\tilde{h})^{1/2}$.*

Proof. The first statement is obtained through the rescaling $\tilde{a}(\rho) \stackrel{\text{def}}{=} a((h/\tilde{h})^{1/2}\rho) \in S(1)$. It satisfies

$$\widetilde{a_1 \#_h a_2} = \tilde{a}_1 \#_{\tilde{h}} \tilde{a}_2, \quad \text{and} \quad U_{(h/\tilde{h})^{1/2}} \text{Op}_h^W(a) = \text{Op}_{\tilde{h}}^W(\tilde{a}) U_{(h/\tilde{h})^{1/2}},$$

from where the proof proceeds as in Prop. 5.16. The second and third statements can be obtained by applying the asymptotic expansion for the Moyal product $a \#_h b$, and estimating the size of each term. Alternatively, for the second statement we may rescale as above, and use the expansion of the Moyal product $\tilde{a}_1 \#_{\tilde{h}} \tilde{a}_2$ in powers of $\tilde{h}$. $\square$

Claim 5.19. The semiclassical calculus of Thm 4.17 can also be extended to the classes $S_\delta(m)$ for any order function m , with the effective expansion parameter $\tilde{h}^{1-2\delta}$.

5.3.3. *Sharp Gårding inequality.* The first application of these exotic symbol calculi will be to improve the Gårding inequality:

Theorem 5.20. (*Sharp Gårding inequality*) *Assume that $a \in S(1)$ satisfies $a \geq 0$. Then there exists $C_0 > 0$ and $\hbar_0 > 0$ such that, for any $\hbar < \hbar_0$, the self-adjoint operator $\text{Op}_\hbar^W(a)$ satisfies, for $\hbar$ small enough:*

$$\text{Op}_\hbar^W(a) \geq -C_0 \hbar.$$

Proof. To obtain this inequality we will construct an inverse of $\text{Op}_\hbar^W(a - z)$ with $z \leq -C\hbar$ with $C > 0$ a large enough constant; equivalently, we will take $z \leq -\hbar/\tilde{h}$, where $\tilde{h} > 0$ will be a small parameter, independent of $\hbar$. This second notation is a hint that we will be using the critical exotic class of Def. 5.17.

As in the proof of the weak Gårding inequality, we need to study the trial function $(a - z)^{-1}$ and its derivatives. Since $a \geq 0$, the first bound is $\|(a - z)^{-1}\|_{L^\infty} \leq |z|^{-1}$. To estimate the derivatives we use the expansion (5.3). The simple bounds

$$(5.5) \quad (a - z)^{-1} |\partial^\beta a(x)| \leq C_\beta |z|^{-1}$$

leads to

$$(5.6) \quad |\partial^\alpha (a - z)^{-1}| \leq C_\alpha (a - z)^{-1} |z|^{-|\alpha|}.$$

However, we can take advantage of the positivity of a to improve this bound on the derivatives. Indeed, let us write the Taylor expansion up to second order:

$$a(x+y) = a(x) + \langle y, \partial a(x) \rangle + \int_0^1 (1-t) \langle \partial^2 a(x+ty) y, y \rangle,$$

and take $y = -\lambda \partial a(x)$ for some $\lambda > 0$. The positivity $a(x+y) \geq 0$ leads to

$$\lambda |\partial a(x)|^2 \leq a(x) + \frac{\lambda^2}{2} \|\partial^2 a\|_{L^\infty} |\partial a(x)|^2.$$

Selecting $\lambda = \|\partial^2 a\|_{L^\infty}^{-1}$, we obtain

$$|\partial a(x)| \leq (2 \|\partial^2 a\|_{L^\infty} a(x))^{1/2}.$$

This leads to

$$|z|^{1/2} |\partial a(x)| \leq C |z|^{1/2} a(x)^{1/2} \leq \frac{C}{2} (a + |z|), \quad \text{and then } (a + |z|)^{-1} |\partial a(x)| \leq \frac{C}{2} |z|^{-1/2},$$

which improves (5.5) for $|\beta| = 1$. For the terms with $|\beta| \geq 2$ we keep the bounds (5.5). Injecting these two estimates in the expansion (5.3) we see that the “worst term” is the term with all $|\beta^j| = 1$, which gives the bound

$$|\partial^\alpha (a - z)^{-1}| \leq C_\alpha (a - z)^{-1} |z|^{-|\alpha|/2},$$

which is sharper than (5.6). From this estimate, we check that if the spectral parameter $z \leq -\frac{\hbar}{\tilde{h}}$ the function $|z| (a - z)^{-1}$ belongs to the exotic symbol class $\tilde{S}_{1/2}(1)$ of Def. 5.17. Equipped with the corresponding calculus, we get

$$(a - z) \#_{\tilde{h}} (a - z)^{-1} = \underbrace{\frac{(a - z)}{|z|}}_{\frac{1}{|z|} S(1)} \#_{\tilde{h}} \underbrace{|z| (a - z)^{-1}}_{\tilde{S}_{1/2}} = 1 + 0 + r_2(z; \tilde{h}, \tilde{\tilde{h}}),$$

$$\text{with } r_2 \in \frac{1}{|z|} (\hbar \tilde{\tilde{h}}) \tilde{S}_{1/2} \subset \tilde{\hbar}^2 \tilde{S}_{1/2}.$$

As a result, applying the C-V theorem to the symbol $r_2(\tilde{h}, \tilde{\tilde{h}})$, we see that as long as $\tilde{\tilde{h}} \leq \tilde{\tilde{h}}_0$ and $\tilde{h} \leq 1$, the operator $I + \text{Op}_{\tilde{h}}^W(r_2(z; \tilde{h}, \tilde{\tilde{h}}))$ is invertible with a uniformly bounded inverse. Like in the proof of Prop. 5.14, this leads to the proof that $\text{Op}_{\tilde{h}}^W(a - z)$ is invertible. One can also check that the bound on $\text{Op}_{\tilde{h}}(r_2(z; \tilde{h}))$ is uniform w.r.t. $z \in (-\infty, -\hbar/\tilde{\tilde{h}}]$, which shows that $\text{Spec Op}_{\tilde{h}}^W(a) \subset (-\hbar/\tilde{\tilde{h}}, \infty)$. Calling $C_0 = 1/\tilde{\tilde{h}}_0$, we have thus shown that $\text{Op}_{\tilde{h}}^W(a) \geq -C_0 \tilde{h}$ for $\tilde{h} < \tilde{\tilde{h}}_0$. $\square$

Remark 5.21. The Weyl quantization maps a real symbol into a selfadjoint operator, but not a positive symbol to a positive operator. However, the above result shows that in the semiclassical limit, $\text{Op}_{\tilde{h}}^W(a)$ is “almost positive”. There exists an alternative quantization,

called the anti-Wick quantization, which automatically satisfies a strict positivity property: the quantization of a positive symbol is automatically a positive operator.

Corollary 5.22. (*Improved norm bound*) For $a \in S(1)$ real-valued, there exists $C_a > 0$ and $\hbar_0 > 0$ such that, for any $\hbar < \hbar_0$, the operator $\text{Op}_\hbar^W(a)$ satisfies

$$\inf_{\rho} a(\rho) - C_a \hbar \leq \text{Op}_\hbar^W(a) \leq \sup_{\rho} a(\rho) + C_a \hbar.$$

In particular,

$$\|\text{Op}_\hbar^W(a)\| \leq \|a\|_{L^\infty} + C_a \hbar.$$

Notice that this estimate is sharper than the bound we had obtained in the Calderon-Vaillancourt Thm 4.26.

Proof. The symbol $a_-(\rho) \stackrel{\text{def}}{=} a(\rho) - \inf a \geq 0$, so the sharp Gårding inequality implies that $\text{Op}_\hbar^W(a_-) \geq -C\hbar$, proving the lower bound on $\text{Op}_\hbar^W(a)$. In turn, the symbol $a_+(\rho) = \sup a - a(\rho) \geq 0$, so $\text{Op}_\hbar^W(a_+) \geq -C\hbar$, proving the upper bound. $\square$

5.4. Functional calculus on PDOs. In the previous section we have made use of the *resolvent* of a selfadjoint operator, namely the operator valued function $z \mapsto (z - \text{Op}_\hbar^W(a))$, for z outside the spectrum of $\text{Op}_\hbar^W(a)$. The holomorphy of this operator-valued function will allow us to manipulate it quite conveniently. In particular, through the resolvent one is able to adapt standard tools of complex analysis to the framework of operators. One such tool is the Cauchy formula, which allows to recover functions of the operator, from its resolvent.

We will especially consider selfadjoint operators $A = \text{Op}_\hbar^W(a)$, with $a \in S(m)$ a real valued symbol, not necessarily bounded. In this framework, the functions of A can be defined using the spectral theorem, as explained in the Appendix (see Corollaries A.2 and A.5). For a continuous, bounded function $f : \mathbb{R} \rightarrow \mathbb{R}$, the operator $f(A)$ is then a bounded selfadjoint operator on $L^2(\mathbb{R}^d)$, with norm $\|f(A)\|_{L^2 \rightarrow L^2} \leq \|f\|_{L^\infty}$. More precisely,

$$\|f(A)\|_{L^2 \rightarrow L^2} = \sup_{t \in \text{Spec } A} |f(t)|.$$

We want to investigate the operator $f(A)$ when $A = \text{Op}_\hbar^W(a)$ and $f : \mathbb{R} \rightarrow \mathbb{R}$ is a smooth, compactly supported function. We will show that $f(A)$ is a PDO in the class $\Psi_h(1)$, and compute the asymptotic expansion of its symbol in terms of the symbol a and the function f .

5.4.1. *A Cauchy formula for $f(A)$.* For this aim we will use a Cauchy formula (sometimes called the Helffer-Sjöstrand formula) to define the operator $f(A)$. This formula uses an auxiliary function $\tilde{f}$, which is *an almost analytic extension* of the function f .

Definition 5.23. Consider $f \in C_c^\infty(\mathbb{R}; \mathbb{C})$. An *almost analytic extension* of f is a function $\tilde{f} \in C_c^\infty(\mathbb{C}, \mathbb{C})$ which coincides with f on $\mathbb{R}$, and is “almost analytic” on $\mathbb{R}$, in the sense that¹⁹

$$\forall N \geq 0, \forall z \in \mathbb{C}, \quad \left| \bar{\partial} \tilde{f}(z) \right| \leq C_N |\operatorname{Im} z|^N.$$

A short way to write this almost analyticity is $\bar{\partial} \tilde{f}(z) = \mathcal{O}(|\operatorname{Im} z|^\infty)$. We will actually need this property only up to some fixed order N .

There are several ways to define such analytic extensions. One way uses the Fourier transform $\hat{f} = \mathcal{F}_1 f$ and two cutoff functions $\psi, \chi \in C_c^\infty(\mathbb{R})$ with $\psi = 1$ near $\operatorname{supp} f$, $\chi = 1$ near 0: the extension is then defined as

$$\tilde{f}(x + iy) \stackrel{\text{def}}{=} \chi(y) \psi(x) \int e^{i\xi(x+iy)} \chi(y\xi) \hat{f}(\xi) \frac{d\xi}{(2\pi)^{1/2}}.$$

Exercise 5.24. Check that this expression is an analytic extension of f (to infinite order).

Since we only need a finite order analytic extension, we may use a simpler definition, and take:

$$\tilde{f}(x + iy) = \left(\sum_{j=0}^N f^{(j)}(x) \frac{(iy)^j}{j!} \right) \tau \left(\frac{y}{\langle x \rangle} \right),$$

where $\tau \in C_c^\infty((-2, 2))$, $\tau(s) = 1$ on $[-1, 1]$.

Exercise 5.25. Check that the above function $\tilde{f}$ is almost analytic of f of order N .

We now use this almost analytic extension to state our Cauchy formula:

Proposition 5.26. Let $f \in C_c^\infty(\mathbb{R}; \mathbb{C})$ and $\tilde{f} \in C_c^\infty(\mathbb{C})$ an almost analytic extension²⁰ of f . Then for any $t \in \mathbb{R}$,

$$(5.7) \quad f(t) = -\frac{1}{\pi} \iint \bar{\partial} \tilde{f}(z) (z - t)^{-1} d^2 z.$$

(Notice that the integrand is smooth when $y \rightarrow 0$).

As a result, for any selfadjoint operator A , the function $f(A)$ can be written as

$$(5.8) \quad f(A) = -\frac{1}{\pi} \iint \bar{\partial} \tilde{f}(z) (z - A)^{-1} d^2 z.$$

¹⁹We remind the notation of holomorphic and anti-holomorphic derivatives. For $z = x + iy$, $\partial_z = \frac{1}{2}(\partial_x - i\partial_y)$, $\bar{\partial}_z = \frac{1}{2}(\partial_x + i\partial_y)$.

²⁰Actually it is sufficient to require that $\bar{\partial} \tilde{f}(x + iy) = \mathcal{O}(|y|)$.

Proof. To prove the scalar formula we integrate by parts to get $\frac{1}{\pi} \iint \tilde{f}(z) \bar{\partial}(z-t)^{-1} d^2z$, and we use the distributional formula²¹ $\bar{\partial} \frac{1}{z} = \pi \delta(z)$ to conclude. To prove the operator expression, we may write A using the projection valued decomposition

$$A = \int \lambda dP_\lambda,$$

where P_λ is the spectral projector of A on the interval $(-\infty, \lambda]$, so that for $z \notin \mathbb{R}$ we have $(z - A)^{-1} = \int (z - \lambda)^{-1} dP_\lambda$. We can then define

$$-\frac{1}{\pi} \iint \bar{\partial} \tilde{f}(z) (z - A)^{-1} d^2z = -\frac{1}{\pi} \iint \bar{\partial} \tilde{f}(z) \int (z - \lambda)^{-1} dP_\lambda d^2z,$$

noticing that the integrand of the LHS is well-defined in the limit $y \rightarrow 0$ thanks to the estimate

$$(5.9) \quad \|(z - A)^{-1}\| \leq \frac{1}{|\operatorname{Im} z|}$$

and the fact that $\tilde{f}$ is almost analytic. We may apply Fubini's theorem and for all $\lambda \in \mathbb{R}$ apply the expression (5.7) to recover $\int f(\lambda) dP_\lambda = f(A)$. $\square$

When $A = \operatorname{Op}_h^W(a)$, this expression for $f(A)$ will allow us to use our semiclassical analysis of the resolvent $(z - A)^{-1}$ to gather informations on the operator $f(A)$.

5.4.2. Refined estimates for the resolvent. Let us consider a real-valued symbol $a \in S(m)$, with the assumption $m \geq 1$, and assume that $(a + i)$ is *elliptic* in $S(m)$, that is, $|a(\rho) + i| \geq \gamma m(\rho)$ for some $\gamma > 0$ and all $\rho \in \mathbb{R}^{2d}$. In that case, the function $(a + i)^{-1} \in S(m^{-1})$. According to Thm 5.2 and the following Claim, for any given value of z away from the range of a , in particular for $\operatorname{Im} z > 0$ fixed, the symbol $b(z)$ of the resolvent $(z - \operatorname{Op}_h^W(a))^{-1}$ belongs to the class $S(m^{-1})$, and its principal symbol is the function $(z - a)^{-1}$. Yet, we will need to integrate the resolvent over $z \in \operatorname{supp} \tilde{f}$ which contains the real axis, so we need to understand how the estimates on $b(z)$ depend on z , in particular when $\operatorname{Im} z \rightarrow 0$.

Lemma 5.27. *Under the above conditions, the symbol $b(\rho; z, \hbar)$ of the resolvent $B(z) = (z - \operatorname{Op}_h^W(a))^{-1}$ satisfies the following bounds, uniformly for $\hbar \in (0, 1]$, $z \in \{|\operatorname{Re} z| \leq R, \operatorname{Im} z > 0\}$ and $\rho \in \mathbb{R}^{2d}$:*

$$(5.10) \quad |\partial^\alpha b(\rho; z; \hbar)| \leq C_{\alpha, a} \max \left(1, \frac{\hbar^{1/2}}{|\operatorname{Im} z|} \right)^{2d+1} |\operatorname{Im} z|^{-1-|\alpha|}.$$

Proof. We first treat the case of the order function $m = 1$. We use the inverse-CV result of Eq.(4.14) applied to the symbols $b(z)$ of $B(z) = (z - \operatorname{Op}_h^W(a))^{-1}$, slightly refining the proof

²¹Here $\delta(z)$ is the delta distribution at $0 \in \mathbb{C}$.

of Beals's Theorem. An easy computation, obtained by generalizing the trick (5.1), shows that

$$(5.11) \quad \left\| \text{ad}_{\text{Op}_h(\ell_N)} \circ \cdots \circ \text{ad}_{\text{Op}_h(\ell_1)} B(z) \right\|_{L^2 \rightarrow L^2} = \mathcal{O} \left(\frac{\hbar^N}{|\text{Im } z|^{N+1}} \right),$$

which implies $\text{Op}_h(\partial^\beta b(\rho; z; \hbar)) = \mathcal{O} \left(\frac{1}{|\text{Im } z|^{|\beta|+1}} \right)$. Applying the inverse C-V theorem (4.14) we find that for any $\alpha \in \mathbb{N}^{2d}$,

$$\|\partial^\alpha b(z)\|_{L^\infty} \leq C_\alpha \sum_{|\beta| \leq 2d+1} \hbar^{|\beta|/2} |\text{Im } z|^{-1-|\beta|-|\alpha|}.$$

Depending on the ratio $\frac{\hbar^{1/2}}{|\text{Im } z|}$, this sum is dominated either by the term $|\beta| = 0$, or by the terms $|\beta| = 2d + 1$, which gives the required result.

Now, let us assume that $a \in S(m)$ with $m(\rho) \rightarrow \infty$ and $(a + i)$ is elliptic in $S(m)$. As above we call $B(z) = (z - A)^{-1}$, $A = \text{Op}_h^W(a)$. We expand the commutator between $\ell^w = \text{Op}_h^W(\ell)$ and $B(z)$ in Beals's Theorem as:

$$\begin{aligned} [\ell^w, B(z)] &= -B(z) [\ell^w, A] B(z) \\ &= -B(z) [\ell^w, A] B(i) (i - A) B(z) \\ &= -B(z) [\ell^w, A] B(i) P(z), \end{aligned}$$

where the operator $P(z) = (i - A) B(z) = (i - A) (z - A)^{-1}$ satisfies $\|P(z)\| = \mathcal{O} \left(\frac{1}{|\text{Im } z|} \right)$. On the other hand, $[\ell^w, A] B(i) \in \hbar \Psi_h(1)$, so that $\|[\ell^w, A] B(i)\| = \mathcal{O}(\hbar)$. Using also the a priori bound $\|B(z)\| = \mathcal{O} \left(\frac{1}{|\text{Im } z|} \right)$ we obtain $\|[\ell^w, B(z)]\| = \mathcal{O} \left(\frac{\hbar}{|\text{Im } z|^2} \right)$. Proceeding by iterations we prove the estimate (5.11) for this case as well, which leads to the result. $\square$

We notice that if $|\text{Im } z|$ is too small, $b(\rho; z; \hbar)$ does not belong to any good symbol class. However, in the Cauchy integral we are interested in, this symbol is multiplied by $\bar{\partial} \tilde{f}(z)$, which tames its singularity.

Corollary 5.28. *For $m \geq 1$, $a \in S(m)$ with $(a + i)$ elliptic, and $f \in C_c^\infty(\mathbb{R}, \mathbb{C})$, the operator $f(\text{Op}_h^W(a))$ is a PDO with symbol $c \in S(m^{-\infty})$.*

Proof. If we apply the Cauchy formula (5.8) at the level of symbols, we get the explicit formula:

$$(5.12) \quad c(\rho; \hbar) = -\frac{1}{\pi} \iint \bar{\partial} \tilde{f}(z) b(\rho; z; \hbar) d^2 z.$$

The estimates on $\bar{\partial} \tilde{f}(z)$ and (5.10) show that $\bar{\partial} \tilde{f}(z) \partial_\rho^\alpha b(\rho; z; \hbar) = \mathcal{O}(|\text{Im } z|^\infty)$, uniformly w.r.t. $\rho \in \mathbb{R}^{2d}$, so that the symbol $c(\hbar) \in S(1)$. Another way to express this is to notice that the symbols $\bar{\partial} \tilde{f}(z) b(z; \hbar)$ belong to $S(1)$, uniformly w.r.t. $z \in \text{supp } \tilde{f}$.

For any $k \geq 0$ we may apply the above result to the function $f_k(t) = (i - t)^k f(t)$, so that $f(A) = (i - A)^{-k} f_k(A)$. Since $f_k(A)$ belongs to $\Psi_h(1)$, and $(a - i)$ is elliptic in $S(m)$, $f(A)$ belongs to $\Psi_h(m^{-k})$. $\square$

5.4.3. Computation of the symbol of $f(A)$. We now want to compute more explicitly the symbol $c(\rho; \hbar)$ of $f(A)$. For this aim, we will split the integral (5.12) between two regions. Fix some parameter $\delta \in (0, 1/2)$. The region “close to the real axis” is defined by $\{z \in \mathbb{C}, |\operatorname{Im} z| \leq \hbar^\delta\}$. Using the estimates (5.10) on the resolvent symbol and the almost analyticity of $\tilde{f}$, one sees that the contribution of this region to the integral (5.12) is $\mathcal{O}(\hbar^\infty)_{S(1)}$.

We are then lead to estimate the integral over the region “distant” from the real axis”,

$$\mathcal{R} \stackrel{\text{def}}{=} \{z \in \mathbb{C}, |\operatorname{Im} z| \geq \hbar^\delta\} \cap \{|z| \leq R_0\},$$

where R_0 will be taken large enough such that the disk $\{|z| \leq R_0\}$ contains the support of $\tilde{f}$. We call this truncated integral

$$c_{\mathcal{R}}(\rho) \stackrel{\text{def}}{=} -\frac{1}{\pi} \iint_{\mathcal{R}} \bar{\partial} \tilde{f}(z) b(\rho; z; \hbar) d^2 z,$$

and we have just shown that

$$(5.13) \quad c = c_{\mathcal{R}} + \mathcal{O}(\hbar^\infty)_{S(1)}.$$

In the region $\mathcal{R}$, using the expression (5.3) for the derivatives of $(z - a)^{-1}$, we get the simple bounds

$$(5.14) \quad \partial_\rho^\alpha (z - a(\rho))^{-1} \leq C_{\alpha,a} m(\rho)^{-1} |\operatorname{Im} z|^{-1-|\alpha|},$$

valid uniformly for $\rho \in \mathbb{R}^{2d}$ and $z \in \mathcal{R}$. Hence, for z in the region $\mathcal{R}$, the function $(z - a)^{-1}$ belongs to the symbol class $\hbar^{-\delta} S_\delta(m^{-1})$, where we use the exotic symbol class defined in Def. 5.15.

Lemma 5.29. *For $\hbar$ small enough and uniformly in $z \in \mathcal{R}$, the symbols $(z - a)^{-1}$ and $b(z; \hbar)$ both belong to the class $\hbar^{-\delta} S_\delta(m^{-1})$.*

Proof. The first part is contained in the estimate (5.14). The estimates (5.10) on derivatives of $b(z)$ show that $b(z) \in \hbar^{-\delta} S_\delta(1)$. We can easily adapt the proof of Corollary 5.4 to the setting of the exotic classe $S_\delta(m)$, namely by considering the expansion

$$(z - a) \#_\hbar (z - a)^{-1} = 1 + r_2(\hbar, z).$$

The symbol calculus in $S(m) \times S_\delta(m^{-1})$ shows that $r_2 \in \hbar^{2-3\delta} S_\delta(1)$. The Calderón-Vaillancourt theorem for the class $S_\delta(1)$ implies that for $\hbar$ small enough $\text{Op}_\hbar^W(1 + r_2)$ is invertible, of inverse in $S_\delta(1)$, so if we multiply the latter symbol on the left by $b_0(z) = (z - a)^{-1}$ we get the symbol $b(z) \in \hbar^{-\delta} S_\delta(m^{-1})$. $\square$

This proof also provides a way to compute the expansion for $b(z)$. From the identity

$$\text{Op}_\hbar^W(z - a) \text{Op}_\hbar^W(b_0(z)) (I + \text{Op}_\hbar^W(r_2(z)))^{-1} = I,$$

we get

$$(5.15) \quad b(z) = b_0(z) \# (1 - r_2(z) + r_2(z) \# r_2(z) - \dots).$$

We want to keep track of the z -dependence in the expansion for the remainder $r_2(\hbar, z)$. This expansion takes the following schematic form:

$$\begin{aligned} r_2(z) &\sim - \sum_{j \geq 2} \frac{(i\hbar/2)^j}{j!} a \left(\omega(\overleftarrow{D}, \overrightarrow{D}) \right)^j (z - a)^{-1} \\ &\sim \sum_{j \geq 2} \hbar^j (z - a)^{-1-j} D^j a \sum_{k=1}^j (z - a)^{j-k} \sum_{j_1 + \dots + j_k = j} \prod_{i=1}^k (D^{j_i} a), \end{aligned}$$

where we factorized by $(z - a)^{-j}$ so as to exhibit in the numerator polynomials $q_{j-1}(z, \rho)$ in the variable z , of degrees $\leq j - 1$:

$$r_2(z) \sim \sum_{j \geq 2} \hbar^j (z - a)^{-1-j} q_{j-1}(z).$$

The Moyal product $b_0 \# r_2$ then expands into

$$\begin{aligned} \sum_{\ell \geq 0} \hbar^\ell D^\ell (z - a)^{-1} D^\ell r_2 &= \sum_{\ell \geq 0} \hbar^\ell D^\ell (z - a)^{-1} D^\ell \left(\sum_{j \geq 2} \hbar^j (z - a)^{-1-j} q_{j-1}(z) \right) \\ &= \sum_{\ell \geq 0} \hbar^{\ell+j} (z - a)^{-1-\ell} Q_{\ell-1}(z) \sum_{j \geq 2} (z - a)^{-1-j-\ell} Q_{j,\ell}(z) \\ &= \sum_{\ell \geq 0, j \geq 2} \hbar^{\ell+j} (z - a)^{-(2\ell+j+2)} Q_{j,\ell}^{(1)}(z), \end{aligned}$$

with $\deg Q_{\ell-1} \leq \ell - 1$, $\deg Q_{j,\ell}(z) \leq j + \ell - 1$, so that $\deg Q_{j,\ell}^{(1)}(z) \leq 2\ell + j - 2$. If we group the terms of same order $k = \ell + j$, the denominators have orders $2 + 2\ell + j = 2 + 2k - j \leq 2k$, so we may write

$$b_0 \# r_2 \sim \sum_{k \geq 2} \hbar^k (z - a)^{-2k} Q_{2k-4}^{(1)}(z), \quad \deg Q_{2k-4}^{(1)} \leq 2k - 4.$$

In the region $\mathcal{R}$, this term is of order $\hbar^{2-4\delta} = \hbar^{2(1-2\delta)}$.

The next order $b_0 \# r_2 \# r_2$ has the form

$$\sum_{\ell \geq 0} \sum_{k \geq 2, j \geq 2} \hbar^{\ell+k+j} (z-a)^{-1-2(k+\ell)-j} Q_{k,j,\ell}(z),$$

with $\deg Q_{k,j,\ell}(z) \leq 2(k+\ell) + j - 5$. So at a given order $m = \ell + k + j$, the maximal power of the denominator is $1 + 2(k+\ell) + j = 1 + 2m - j \leq 2m - 1$, with $m \geq 4$:

$$b_0 \# (r_2)^{\#2} \sim \sum_{k \geq 4} \hbar^k (z-a)^{-2k+1} Q_{2k-7}^{(2)}(z), \quad \deg Q_{2k-7}^{(2)} \leq 2k-7.$$

This term is of order $\hbar^{4-7\delta} = \hbar^{4(1-2\delta)+\delta}$. Continuing the derivation by taking the Moyal product with r_2 , we find similarly

$$b_0 \# r_2^{\#3} \sim \sum_{k \geq 6} \hbar^k (z-a)^{-2k+2} Q_{2k-10}^{(3)}(z), \quad \deg Q_{2k-10}^{(3)} \leq 2k-10.$$

By induction, one can show that the higher powers satisfy the expansion

$$b_0 \# r_2^{\#n} \sim \sum_{k \geq 2n} \hbar^k (z-a)^{-2k+n-1} Q_{2k-3n-1}^{(n)}(z), \quad \deg Q_{2k-3n-1}^{(n)} \leq 2k-3n-1.$$

We see that at a given order $\hbar^k$, there will be finitely many terms $r_2^{\#n}$ involved (the ones such that $2n \leq k$), which can be grouped into a single asymptotic series for $b(z)$:

$$(5.16) \quad b(z) \sim (z-a)^{-1} + \sum_{k \geq 2} \hbar^k (z-a)^{-2k} Q_{2k-4}(z), \quad \deg Q_{2k-4} \leq 2k-4.$$

This expression will be of order $\hbar^{-\delta}$, uniformly for $z \in \mathcal{R}$.

The derivatives $\partial^\alpha b(z)$ can be analyzed similarly, they satisfy asymptotic expansions obtained by differentiating the above one. For $z \in \mathcal{R}$ one can check that the derivative $\partial^\alpha b(z)$ is dominated by the term $\partial^\alpha b_0(z) = \mathcal{O}(\hbar^{-\delta(1+|\alpha|)})$. This leads to the following

Lemma 5.30. *For $\hbar$ small enough and $z \in \mathcal{R}$, the symbol $b(z) \in \hbar^{-\delta} S_\delta(m^{-1})$ admits the expansion (5.16), uniformly w.r.t. $z \in \mathcal{R}$.*

By injecting the expansion for $b(z)$ in the Cauchy formula (5.12), we obtain the following expansion of $c_{\mathcal{R}}$:

$$c_{\mathcal{R}} \sim -\frac{1}{\pi} \iint_{\mathcal{R}} \bar{\partial} \tilde{f}(z) \left[(z-a)^{-1} + \sum_{k \geq 2} \hbar^k (z-a)^{-2k} Q_{2k-4}(z) \right] d^2 z.$$

Since $\bar{\partial} \tilde{f}(z) = \mathcal{O}(\hbar^\infty)$ when $|\operatorname{Im} z| \leq \hbar^\delta$, we may extend the integral to $z \in \mathbb{C}$, up to a term $\mathcal{O}(\hbar^\infty)_{S(1)}$. From (5.13), this full integral is also the expansion of the full symbol c :

$$c \sim -\frac{1}{\pi} \iint_{\mathbb{C}} \bar{\partial} \tilde{f}(z) \left[(z-a)^{-1} + \sum_{k \geq 2} \hbar^k (z-a)^{-2k} Q_{2k-4}(z) \right] d^2 z.$$

Fixing $\rho \in \mathbb{R}^{2d}$, each term of the expansion can be computed by using the Cauchy formula. The first term provides the principal symbol:

$$-\frac{1}{\pi} \iint \bar{\partial} \tilde{f}(z) (z - a(\rho))^{-1} d^2 z = f(a(\rho)),$$

by applying (5.7) with $t = a(\rho)$. The term of order $\hbar^k$, $k \geq 2$, can also be computed after some integration by parts in the variables $z, \bar{z}$:

$$\begin{aligned} -\frac{1}{\pi} \iint \bar{\partial} \tilde{f}(z) Q_k(z) (z - a)^{-2k} d^2 z &= -\frac{1}{\pi(2k-1)!} \iint \bar{\partial} \tilde{f}(z) Q_k(z) (-\partial)^{2k-1} [(z - a)^{-1}] d^2 z \\ &= \frac{1}{\pi(2k-1)!} \iint \partial^{2k-1} [\tilde{f}(z) Q_k(z)] \bar{\partial} [(z - a)^{-1}] d^2 z \\ &= \frac{1}{(2k-1)!} \partial_t^{2k-1} [f(t) Q_k(t)] \upharpoonright_{t=a(\rho)}. \end{aligned}$$

In the second line we integrated by parts ∂ and $\bar{\partial}$ separately, and used that $Q_k(z)$ is holomorphic, while in the last we used the fact that $\partial_z^j \tilde{f}(z) \upharpoonright_{z=t} = \partial_t^j f(t)$. We finally obtain the following

Theorem 5.31. *The symbol $c(\hbar)$ of the operator $f(\text{Op}_\hbar^W(a))$ admits an expansion in $S(1)$,*

$$c \sim \sum_{k \geq 0} \hbar^k c_k(\rho), \quad c_0 = f(a), \quad c_1 = 0.$$

Each $c_k(\rho) \in S(1)$, and is supported in the set

$$\text{supp } f(a) = \{\rho \in \mathbb{R}^{2d}, a(\rho) \in \text{supp } f\}.$$

5.5. Application of the functional calculus: Semiclassical Weyl's Law.

5.5.1. *Trace-class property of the operator $f(A)$.* We will now work under the following alternative assumptions on the order function m and the real-valued symbol $a \in S(m)$:

- (1) $m \rightarrow \infty$ as $|\rho| \rightarrow \infty$, and $(a + i)$ is elliptic in $S(m)$; take any $f \in C_c^\infty(\mathbb{R})$;
- (2) $m = 1$ and there exists an interval $I \Subset \mathbb{R}$ a compact set $\Omega \Subset \mathbb{R}^{2d}$ and $C > 0$ such that,

$$\forall \hbar \in (0, 1], \quad \forall \rho \in \mathbb{R}^{2d} \setminus \Omega, \quad \text{dist}(a(\rho; \hbar), I) \geq C.$$

In this case we assume that $f \in C_c^\infty(I)$.

In these two situations, the functions $c_k(\rho)$ appearing in the Thm 5.31 are all supported in a common compact set. Actually, the full symbol $c(\hbar)$ has a compact essential support:

Proposition 5.32. *If either of the above assumptions on m, a is satisfied, the symbol c of $f(\text{Op}_\hbar^W(a))$ belongs to $S(\langle \rho \rangle^{-\infty})$. Besides, $c(\hbar)$ is essentially supported in $\text{supp } f(a)$, with*

estimates

$$\partial^\alpha c(\rho; \hbar) = \mathcal{O} \left(\left(\frac{\hbar}{\text{dist}(\rho, \text{supp } f(a))} \right)^\infty \right), \quad \text{for any } \rho \text{ such that } \text{dist}(\rho, \text{supp } f(a)) \geq C.$$

Proof. Our general assumption is that there exists some bounded neighbourhood Ω of $\text{supp } f(a)$ and a constant $C > 0$, such that $\text{dist}(a(\rho), \text{supp } f) \geq C$ for all $\rho \notin \Omega$. Up to a trivial change of sign, we may assume that

$$a(\rho) \geq \max \text{supp } f + C, \quad \forall \rho \notin \Omega.$$

By smoothly modifying $a(\rho)$ inside Ω , we may construct an *auxiliary symbol* $\tilde{a} \in S(m)$, such that

$$\begin{cases} \tilde{a}(\rho) = a(\rho), & \rho \notin \Omega, \\ \tilde{a}(\rho) \geq \max \text{supp } f + C/2, & \rho \in \mathbb{R}^{2d}. \end{cases}$$

We then use the following resolvent identity, valid for any $z \notin \mathbb{R}$:

$$(5.17) \quad (z - \text{Op}_h^W(a))^{-1} = (z - \text{Op}_h^W(\tilde{a}))^{-1} + (z - \text{Op}_h^W(a))^{-1} \text{Op}_h^W(a - \tilde{a}) (z - \text{Op}_h^W(\tilde{a}))^{-1}.$$

We can now inject this decomposition into the Cauchy formula (5.8). Let us consider the first term on the RHS. Due to the range of $\tilde{a}$, we see that $(z - \text{Op}_h^W(\tilde{a}))$ is invertible if $\text{Re } z \leq \max \text{supp } f + C/4$, in particular we may assume that this is the case for $z \in \text{supp } \tilde{f}$, with uniform estimates. Besides, $(z - \text{Op}_h^W(\tilde{a}))^{-1}$ is a bounded operator, depending holomorphically on z in $\text{supp } \tilde{f}$, so that

$$\bar{\partial} (z - \text{Op}_h^W(\tilde{a}))^{-1} = 0, \quad \forall z \in \text{supp } \tilde{f}.$$

By integration by parts in the Cauchy formula, this shows that $f(\text{Op}_h^W(\tilde{a})) = 0$. We are now interested in integrating the second term over z in (5.17). Using the notation $b(z), \tilde{b}(z)$ for the symbols of the resolvents, the symbol c of the second term is given by

$$c = -\frac{1}{\pi} \int \bar{\partial} \tilde{f}(z) b(z) \#_h (a - \tilde{a}) \#_h \tilde{b}(z) d^2 z.$$

Since $(a - \tilde{a})$ is compactly supported, we know from the Quasilocality Lemma 4.18 that the symbol $b^{(2)}(z) \stackrel{\text{def}}{=} (a - \tilde{a}) \#_h \tilde{b}(z)$ is in $\mathcal{S}(\mathbb{R}^{2d})$ uniformly for $z \in \text{supp } \tilde{f}$, and admits estimates $\mathcal{O} \left(\left(\frac{\hbar}{\text{dist}(\rho, \Omega)} \right)^\infty \right)$ for ρ outside Ω . The Moyal product with the symbol $\bar{\partial} \tilde{f}(z) b(z)$, which is uniformly in $S(1)$, gives a symbol in $\mathcal{S}(\mathbb{R}^{2d})$ with the same estimates. Finally, integrating z over $\text{supp } \tilde{f}$ gives the Proposition. $\square$

Using Prop. 4.40 we obtain the following trace-class property of the operator $f(A)$:

Corollary 5.33. *Assume that either of the two assumptions on m, a are satisfied. Then, for any function $f \in C_c^\infty(\mathbb{R})$ (resp. for any $f \in C_c^\infty(I)$) and for $\hbar$ small enough, the operator*

$f(\text{Op}_h^W(a))$ is trace class on $L^2(\mathbb{R}^{2d})$. Besides, one has

$$(5.18) \quad \text{tr} f(\text{Op}_h^W(a)) = \frac{1}{(2\pi\hbar)^d} \int c(\rho) d\rho \sim \frac{1}{(2\pi\hbar)^d} \sum_{k \geq 0} \hbar^k \int c_k(\rho) d\rho.$$

In particular, the principal order term is $\frac{1}{(2\pi\hbar)^d} \int f(a(\rho)) d\rho$.

This corollary shows that for $\hbar > 0$ small enough, the spectrum of the selfadjoint operator $\text{Op}_h^W(a)$ inside $\text{supp } f$ is purely discrete, composed of eigenstates/values $(\varphi_j(\hbar), \lambda_j(\hbar))_{j \in J}$. In our semiclassical setting, we may try to estimate the density of these eigenvalues.

5.5.2. Semiclassical Weyl's Law. We now assume that the symbol a admits an expansion

$$a \sim \sum_{j \geq 0} \hbar^j a_j \quad a_j \in S(m) \text{ independent of } \hbar.$$

We are then able to prove the following bounds on the counting function.

Theorem 5.34. (*Semiclassical Weyl's law*) Fix some compact interval $[E_0, E_1] \Subset I$, and call $\mathcal{N}([E_0, E_1]; \hbar)$ the number of eigenvalues of $\text{Op}_h^W(a)$ in $[E_0, E_1]$, counted with multiplicities. Then we have the following estimates as $\hbar \rightarrow 0$:

$$\frac{1}{(2\pi\hbar)^d} (V_-([E_0, E_1]) + o(1)) \leq \mathcal{N}([E_0, E_1]; \hbar) \leq \frac{1}{(2\pi\hbar)^d} (V_+([E_0, E_1]) + o(1)),$$

where we define the phase space volumes

$$V_{\pm}([E_0, E_1]) = \lim_{\epsilon \searrow 0} \text{Vol} \{a_0^{-1}([E_0 \mp \epsilon, E_1 \pm \epsilon])\}.$$

Proof. For any $\epsilon > 0$, one can construct two smooth functions $f_{\pm} \in C_c^\infty(\mathbb{R})$, such that

$$\mathbb{1}_{[E_0+\epsilon, E_1-\epsilon]} \leq f_- \leq \mathbb{1}_{[E_0, E_1]} \leq f_+ \leq \mathbb{1}_{[E_0-\epsilon, E_1+\epsilon]}.$$

The standard functional calculus of selfadjoint operators shows the following inequalities:

$$\text{tr} f_-(A) \leq \mathcal{N}([E_0, E_1]; \hbar) \leq \text{tr} f_+(A).$$

We can apply the trace estimate (5.18) on both bounds, leading to

$$\int f_-(a_0(\rho)) d\rho - \mathcal{O}_{f_-}(\hbar) \leq (2\pi\hbar)^d \mathcal{N}([E_0, E_1]; \hbar) \leq \int f_+(a_0(\rho)) d\rho + \mathcal{O}_{f_+}(\hbar).$$

$$\text{Vol } a_0^{-1}([E_0 + \epsilon, E_1 - \epsilon]) - \mathcal{O}_{f_-}(\hbar) \leq (2\pi\hbar)^d \mathcal{N}([E_0, E_1]; \hbar) \leq \text{Vol } a_0^{-1}([E_0 - \epsilon, E_1 + \epsilon]) + \mathcal{O}_{f_+}(\hbar).$$

We can take a sequence $\epsilon = \epsilon_h \searrow 0$ slowly enough so that the remainders $\mathcal{O}_{f_{\pm}}(\hbar)$ still decay, and get the result. $\square$

Corollary 5.35. *If E_0 and E_1 are regular energies (meaning that $da_0(\rho)$ does not vanish on the energy shells $a_0^{-1}(E_i)$), then we have the asymptotics*

$$(5.19) \quad \mathcal{N}([E_0, E_1]; \hbar) = \frac{1}{(2\pi\hbar)^d} (\text{Vol } a_0^{-1}([E_0, E_1]) + o(1)), \quad \hbar \searrow 0.$$

Notice that from Sard's theorem, almost all values $E \in \mathbb{R}$ are regular values of a_0 .

Remark 5.36. This semiclassical Weyl's law is often interpreted in physics as the fact that each eigenstate “occupies” a volume $(2\pi\hbar)^d$ in phase space. More generally, that a region $U \subseteq \mathbb{R}^{2d}$ can “host” about $(2\pi\hbar)^{-d} \text{Vol } U$ orthogonal quantum states, or corresponds to a subspace of $L^2(\mathbb{R}^d)$ of dimension $\sim (2\pi\hbar)^{-d} \text{Vol } U$.

This counting is related with the idea of the uncertainty principle: the latter tells that a maximally localized quantum state occupies a “box” of volume $\sim Ch^d$. If we pave U with disjoint boxes of volumes $\sim Ch^d$, we can accomodate about $C^{-1}\hbar^{-d} \text{Vol } U$ maximally localized states (which can be hoped to generate a subspace of the same dimension).

Several improvements of Weyl's law are possible. We may want to let the interval $[E_0, E_1]$ depend explicitly on $\hbar$, for instance have it shrink at a certain speed when $\hbar \searrow 0$. The adaptation of the above method would consist in using $\hbar$ -dependent cutoff functions $f_{\pm}(\hbar)$, making sure that they belong to a good class $S_{\delta}(\mathbb{R})$ for some $\delta \in (0, 1/2)$; one then will need to extend the functional calculus presented above, to such $\hbar$ -dependent functions $f \in S_{\delta}(\mathbb{R})$. This method allows to take $\epsilon = \hbar^{\delta}$ in the above proof, which, for regular energies E_i , allows to get a remainder $\mathcal{O}(\hbar^{\delta})$ instead of $o(1)$ in (5.19). If E_0 is regular, this also shows that for any $C_0 > 0$ large enough,

$$\mathcal{N}([E_0, E_0 + C_0\hbar^{\delta}]; \hbar) = \frac{1}{(2\pi\hbar)^d} (\text{Vol } a_0^{-1}([E_0, E_0 + C_0\hbar^{\delta}]) + \mathcal{O}(\hbar^{\delta})),$$

where the implied constant on the RHS does not depend on the choice of the parameter C_0 . In particular, if $C_0 > 0$ is chosen large enough, then the above RHS is $\asymp \hbar^{\delta-d}$.

Exercise 5.37. Take some $\delta \in (0, 1/2)$. Show that the semiclassical functional calculus we have constructed above extends to compactly-supported functions $f \in S_{\delta}(\mathbb{R})$, and leads to a full symbol $c \in S_{\delta}(\mathbb{R}^{2d})$ for the operator $f(A)$.

Remark 5.38. Stronger improvements of the remainder estimate in (5.19) are possible, for instance replacing $o(1)$ by $\mathcal{O}(\hbar)$, but this requires to make stronger assumptions on the symbol a_0 , in particular dynamical assumptions on the Hamiltonian flow $\Phi_{a_0}^t$. The proofs involve different semiclassical techniques, typically one needs to use the propagator $e^{-it \text{Op}_{\hbar}^W(a)/\hbar}$, which is not a PDO but a different type of semiclassical beast (a semiclassical Fourier Integral Operator).

To connect this result with the usual Weyl's law for the Laplacian on a smooth compact Riemannian manifold, we would need to extend the semiclassical calculus to this manifold setting. This is feasible, but we will not do it in these notes (see e.g. Zworski's book).

Remark 5.39. In dimension $d = 1$ there are methods to get approximate values for the individual eigenvalues of $\text{Op}_h^W(a)$, in the limit $\hbar \rightarrow 0$. On the other hand, in higher dimension we have no such approximate expression for the eigenvalues. The above expression for the counting function is therefore very valuable. It gives global quantitative information on the spectrum, without any knowledge about individual eigenvalues.

6. MICROLOCAL PROPERTIES OF THE EIGENSTATES OF A PDO

We switch name for our real-valued symbol, and call it $p \sim \sum_{j \geq 0} \hbar^j p_j \in S(m)$. We suppose that p satisfies either of the two assumption of section 5.5.1, ensuring that the spectrum of $P_h = \text{Op}_h^W(p)$ is discrete in some interval $I \Subset \mathbb{R}$, for $\hbar > 0$ small enough.

Let us choose an energy $E_0 \in I$, such that $\text{Vol}[p_0^{-1}([E_0 - \epsilon, E_0 + \epsilon])] > 0$ for any $\epsilon > 0$. According to Weyl's law (5.19), each such interval $[E_0 - \epsilon, E_0 + \epsilon]$ contains many eigenvalues of P_h in the semiclassical limit. We are thus allowed to consider a sequence of eigenstates (φ_h, λ_h) , so that

$$(6.1) \quad (P_h - \lambda_h) \varphi_h = 0, \quad \lambda_h \rightarrow E_0 \quad \text{when} \quad \hbar \rightarrow 0.$$

For a general symbol P_h , we have no explicit, or even approximate expression for φ_h . What can we learn about these eigenstates φ_h from semiclassical methods? (we will always normalize our eigenstates as $\|\varphi_h\|_{L^2} = 1$).

Remark 6.1. From the assumptions on p , we have $|p_0(\rho) - E_0| \asymp m(\rho)$ for ρ outside a bounded region Ω .

6.1. Wavefront set properties.

Theorem 6.2. *The wavefront set of the family $(\varphi_h)_{h \rightarrow 0}$ is contained in $p_0^{-1}(E_0)$.*

Proof. The eigenstates satisfy $(P_h - \lambda_h)\varphi_h = 0$. Let $a \in S(1)$ be supported away from $p_0^{-1}(E_0)$. There exists some $\epsilon > 0$ such that $\text{supp } a$ is also disjoint from $p_0^{-1}([E_0 - \epsilon, E_0 + \epsilon])$. We want to show that $\|\text{Op}_h^W(a)\varphi_h\| = \mathcal{O}(\hbar^\infty)$. For this, we will construct a bounded operator $B_h = \text{Op}_h^W(b)$ such that

$$(6.2) \quad B_h(P_h - \lambda_h) = A_h + \mathcal{O}(\hbar^\infty)_{L^2 \rightarrow L^2}.$$

Once this is done, we will have

$$\begin{aligned} 0 &= B_h(P_h - \lambda_h)\varphi_h \\ &= A_h\varphi_h + \mathcal{O}(\hbar^\infty)_{L^2}, \end{aligned}$$

which will prove that $\text{supp } a$ is not in $\text{WF}_h(\varphi_h)$.

How to construct the operator B_h ? We will enlarge a bit the scope, and construct a family $B_h(\lambda)$ of operators, indexed by $\hbar$ and also by $\lambda \in [E_0 - \epsilon, E_0 + \epsilon]$. We want them to solve

$$(6.3) \quad B_h(\lambda)(P_h - \lambda) = A_h + \mathcal{O}(\hbar^\infty)_{L^2 \rightarrow L^2},$$

with implied constants uniform w.r.t. $\lambda \in [E_0 - \epsilon, E_0 + \epsilon]$. It is impossible to take $B_h(\lambda) = A_h(P_h - \lambda)^{-1}$, since $(P_h - \lambda)$ is not invertible for many such λ 's (for instance for $\lambda = \lambda_h$). However, the obstruction from being invertible comes from the phase space region surrounding $p_0^{-1}([E_0 - \epsilon, E_0 + \epsilon])$, which is away from $\text{WF}_h(A_h) = \text{supp } a$. At the principal symbol level, the equation $b_0(\lambda)(p_0 - \lambda) = a$ can be solved by

$$b_0(\rho; \lambda) \stackrel{\text{def}}{=} \begin{cases} (p_0(\rho) - \lambda)^{-1} a(\rho), & \rho \in \text{supp } a, \\ 0, & \rho \notin \text{supp } a. \end{cases}$$

which makes perfectly sense since $(p_0 - \lambda)$ does not vanish on $\text{supp } a$. Using the ellipticity assumptions of p (see Remark 6.1), the symbol $b_0(\lambda)$ belongs to $S(m^{-1})$, with uniform estimates w.r.t. λ . We will solve (6.3) by constructing the symbol $b(\lambda)$ of $B_h(\lambda)$ starting from the Ansatz $b(\lambda; \hbar) \sim \sum \hbar^j b_j(\lambda)$, and solving, order by order, the symbol equation $b(\lambda; \hbar) \#_h (p - \lambda) = a + \mathcal{O}(\hbar^\infty)$.

At order $\hbar^0$ we have already found the unique solution $b_0(\lambda)$.

At order $\hbar^1$ the equation reads

$$\begin{aligned} 0 &= \frac{1}{2i} \{b_0, p_0\} + b_0 p_1 + b_1 (p_0 - \lambda) \\ \implies b_1(\lambda) &= (p_0 - \lambda)^{-1} \left(b_0(\lambda) p_1 + \frac{1}{2i} \{b_0(\lambda), p_0\} \right). \end{aligned}$$

The expression on the RHS is well-defined, since $b_0(\lambda)$ is supported in $\text{supp } a$, away from $p_0^{-1}(\lambda)$. $b_1(\lambda)$ is in the class $S(m^{-1})$.

At any order $\hbar^j$, $j \geq 2$, the equation for $b_j(\lambda)$ will be of the form

$$b_j (p_0 - \lambda) + F(b_0, b_1, \dots, b_{j-1}; p_0, p_1, \dots, p_j) = 0,$$

where the function $F \in S(1)$ is supported in $\text{supp } a$. It is solved by $b_1 = (p_0 - \lambda)^{-1} F \in S(m^{-1})$. By Borel summation, we obtain a symbol $b(\lambda; \hbar) \in S(m^{-1})$, satisfying $b(\lambda) \#_h (p - \lambda) = a + \mathcal{O}(\hbar^\infty)_{S(1)}$. Its quantization $B_h(\lambda) = \text{Op}_h^W(b_h)$ therefore satisfies (6.3). Since all estimates are uniform w.r.t. $\lambda \in [E_0 - \epsilon, E_0 + \epsilon]$, we may particularize its values and take $B_h = B_h(\lambda_h)$, which solves (6.2). $\square$

Proposition 6.3. *The wavefront set $\text{WF}_h(\varphi_h)$ is not empty.*

Proof. We show it by reasoning *ab absurdo*. If each point $\rho \in p_0^{-1}(E_0)$ were outside $\text{WF}_h(\varphi_h)$, there would exist functions $\chi_\rho \in C_c^\infty$ with $\chi_\rho(\rho) = 1$, and such that

$$(6.4) \quad \text{Op}_h^W(\chi_\rho) \varphi_h = \mathcal{O}(\hbar^\infty).$$

Notice that for each ρ , $\chi_\rho(\rho') \geq 1/2$ in some ball $B(\rho, r_\rho)$. By compactness of $p_0^{-1}(E_0)$, one can extract a finite set of points $S \subset p_0^{-1}(E_0)$ such that $\chi \stackrel{\text{def}}{=} \sum_{\rho \in S} \chi_\rho \geq 1/2$ in some neighbourhood of $p_0^{-1}(E_0)$. By a slight modification of the χ_ρ , we may assume that $\chi \equiv 1$ near $p_0^{-1}(E_0)$. As a result, $a = 1 - \chi$ satisfies the properties in the proof of the above theorem, so that $\text{Op}_h^W(\chi)\varphi_h = \text{Op}_h^W(1 - a)\varphi_h = \varphi_h + \mathcal{O}(\hbar^\infty)$. This obviously contradicts (6.4). $\square$

6.2. Semiclassical measures. There is a more precise way to describe the microlocalization properties of the sequence of normalized states $(\varphi_h)_{h \rightarrow 0}$, by constructing *semiclassical measures* (sometimes called *semiclassical defect measures*) associated with that sequence.

Definition 6.4. Let $(u_h)_{h \rightarrow 0}$ be a sequence of normalized states. A semiclassical measure associated with this sequence is a *nonnegative Radon measure* μ on $\mathbb{R}^{2d}$ such that, after extracting a subsequence $(h_j \rightarrow 0)$, we have, for any observable $a \in C_c^\infty(\mathbb{R}^{2d})$,

$$\lim_{j \rightarrow \infty} \langle u_{h_j}, \text{Op}_{h_j}^W(a)u_{h_j} \rangle = \int a(\rho) d\mu(\rho).$$

If this limit holds without extracting a subsequence, we say that μ is *the* semiclassical measure associated with the sequence (u_h) .

The semiclassical measure indicates the region of phase space where the states (u_h) are microlocally significant (in the sense that they carry a positive L^2 weight in this region) in the semiclassical limit. It gives a more quantitative information than the wavefront set of the sequence.

Proposition 6.5. *Any semiclassical measure μ associated with (u_h) is necessarily supported in $\text{WF}_h(u_h)$.*

Proof. If $\rho \notin \text{WF}_h(u_h)$, then there is $\chi_\rho \in C_c^\infty(\mathbb{R}^{2d}, [0, 1])$ with $\chi_\rho(\rho) = 1$, and such that $\text{Op}_h^W(\chi_\rho)u_h = \mathcal{O}(\hbar^\infty)$. This implies that for any subsequence (h_j) , $\lim_{j \rightarrow \infty} \langle u_{h_j}, \text{Op}_{h_j}^W(\chi_\rho)u_{h_j} \rangle = 0$. Hence, for any semiclassical measure μ associated with the sequence, $\int \chi_\rho d\mu = 0$, which shows that $\rho \notin \text{supp } \mu$. $\square$

Do semiclassical measures always exist?

Theorem 6.6. *Any sequence $(u_h)_{h \rightarrow 0}$ of normalized states admits at least one semiclassical measure μ .*

Proof. Let us first fix an observable $a \in C_c^\infty(\mathbb{R}^{2d}, \mathbb{R})$. By the improved Calderon-Vaillancourt Thm (Cor. 5.22), we have

$$|\langle u_h, \text{Op}_h^W(a)u_h \rangle| \leq \|\text{Op}_h^W(a)\| \leq \|a\|_{L^\infty} + \mathcal{O}_a(\hbar).$$

As a consequence, we may extract a subsequence $(\hbar_j \rightarrow 0)$ s.t. $\lim_{j \rightarrow \infty} \langle u_{\hbar_j}, \text{Op}_{\hbar_j}^W(a) u_{\hbar_j} \rangle = \alpha$, with the limit $|\alpha| \leq \|a\|_{L^\infty}$.

To obtain a limit for any observable, we need to use the fact that the functional space $C_c^\infty(\mathbb{R}^{2d})$ is separable. Hence there is a sequence $(a_k)_{k \geq 1}$ of functions in $C_c^\infty(\mathbb{R}^{2d})$, which is dense in that space.

Let us consider the observable a_1 . From the above, we can extract a subsequence $(\hbar_j^1 \rightarrow 0)$ such that

$$\lim_{j \rightarrow \infty} \langle u_{\hbar_j^1}, \text{Op}_{\hbar_j^1}^W(a_1) u_{\hbar_j^1} \rangle = \alpha_1, \quad \text{with } |\alpha_1| \leq \|a_1\|_{L^\infty}.$$

Let us now consider the observable a_2 . We may extract from $(\hbar_j^1)$ a subsequence $(\hbar_j^2 \rightarrow 0)$ such that

$$\lim_{j \rightarrow \infty} \langle u_{\hbar_j^2}, \text{Op}_{\hbar_j^2}^W(a_2) u_{\hbar_j^2} \rangle = \alpha_2, \quad \text{with } |\alpha_2| \leq \|a_2\|_{L^\infty}.$$

By induction, when considering the observable a_k , we may extract from the sequence $(\hbar_j^{k-1} \rightarrow 0)$ a subsequence $(\hbar_j^k \rightarrow 0)$ such that

$$\lim_{j \rightarrow \infty} \langle u_{\hbar_j^k}, \text{Op}_{\hbar_j^k}^W(a_k) u_{\hbar_j^k} \rangle = \alpha_k, \quad \text{with } |\alpha_k| \leq \|a_k\|_{L^\infty}.$$

Notice that the subsequence $(\hbar_j^k)$ also “works” for the observables $a_1, a_2, \dots, a_{k-1}$. We cannot take for $\hbar_j$ the “ $k \rightarrow \infty$ limit” of the subsequences $(\hbar_j^k)$, because we may have $\lim_{k \rightarrow \infty} \hbar_1^k = 0$, in which case this limiting sequence would be trivial. Instead, we proceed by a *diagonal extraction argument*. Namely, we take $\hbar_j \stackrel{\text{def}}{=} \hbar_j^j$. One easily checks (from this diagonal extraction) that for any $k \geq 1$, this sequence satisfies

$$\lim_{j \rightarrow \infty} \langle u_{\hbar_j}, \text{Op}_{\hbar_j}^W(a_k) u_{\hbar_j} \rangle = \alpha_k.$$

The mapping $\Phi : a_k \rightarrow \alpha_k$ is obviously linear, and it is bounded as: $|\Phi(a_k)| \leq \|a_k\|_{L^\infty}$. This mapping is defined on a dense subset of $C_c^\infty(\mathbb{R}^{2d})$, so it can be extended continuously to the full space $C_c^\infty(\mathbb{R}^{2d})$. Now, if $a_{k_n} \rightarrow a$ in C_c^∞ , we have in particular $\|a_{k_n} - a\|_{L^\infty} \rightarrow 0$. Hence, for any $\epsilon > 0$, if $n \geq n(\epsilon)$ such that $\|a - a_{k_n}\|_{L^\infty} \leq \epsilon$, we have

$$\begin{aligned} \limsup_{j \rightarrow \infty} \left| \langle u_{\hbar_j}, \text{Op}_{\hbar_j}^W(a) u_{\hbar_j} \rangle - \langle u_{\hbar_j}, \text{Op}_{\hbar_j}^W(a_{k_n}) u_{\hbar_j} \rangle \right| &\leq \|a - a_{k_n}\|_{L^\infty} \leq \epsilon \\ \implies \limsup_{j \rightarrow \infty} \left| \langle u_{\hbar_j}, \text{Op}_{\hbar_j}^W(a) u_{\hbar_j} \rangle - \Phi(a) \right| &\leq 2\epsilon. \end{aligned}$$

We conclude that $\lim_{j \rightarrow \infty} \langle u_{\hbar_j}, \text{Op}_{\hbar_j}^W(a) u_{\hbar_j} \rangle = \Phi(a)$.

By the Riesz representation theorem, this bounded linear mapping defines a unique Radon measure on $\mathbb{R}^{2d}$, which we denote by μ :

$$\forall a \in C_c^\infty(\mathbb{R}^{2d}), \quad \Phi(a) = \int a(\rho) d\mu(\rho).$$

Since the scalar products $\langle u_h, \text{Op}_h^W(a)u_h \rangle$ are real, so are the limits $\Phi(a)$, so the measure μ is real valued. If $a \geq 0$, the sharp Gårding inequality (Thm 5.20) implies that

$$\Phi(a) = \lim_{j \rightarrow \infty} \langle u_{h_j}, \text{Op}_{h_j}^W(a)u_{h_j} \rangle \geq \liminf_j (-C_a \hbar_j) \geq 0,$$

which shows that the measure μ is nonnegative. $\square$

The bound $|\int a d\mu| \leq \|a\|_{L^\infty}$ immediately translates into the following property:

Proposition 6.7. *Any semiclassical measure μ associated with a family of normalized states $(u_h)_{h \rightarrow 0}$ satisfies $\mu(\mathbb{R}^{2d}) \leq 1$.*

Remark 6.8. For a general sequence (u_h) , the associated semiclassical measures can be strict subprobability measures, or even be trivial. For instance, if $f \in L^2$ is normalized and $0 \neq v_0 \in \mathbb{R}^d$, the sequence $(u_h = f(\bullet - \hbar^{-1}v_0))$ has a zero semiclassical measure, because the full mass of u_h escapes to $|x| \rightarrow \infty$.

Similarly, if $0 \neq \xi_0 \in \mathbb{R}^d$, the sequence $(u_h(x) = e^{i\xi_0 \cdot x / \hbar^2} f(x))$ has zero semiclassical measure, because the mass of u_h escapes to $|\xi| \rightarrow \infty$.

6.3. Semiclassical measures of eigenstates of P_h . Let us now specialize to the sequence of eigenstates (φ_h, λ_h) we had considered before. How do their semiclassical measures look like? By combining Thm 6.2 and Prop. 6.5 we obtain the following

Corollary 6.9. *Assume (φ_h, λ_h) are eigenstates of P_h so that $\lambda_h \rightarrow E_0$ as $\hbar \rightarrow 0$. Then any associated semiclassical measure is a probability measure supported in $p_0^{-1}(E_0)$.*

Proof. The Thm and Prop. directly imply that $\text{supp } \mu \subset p_0^{-1}(E_0)$. There remains to prove that any measure μ is a probability measure. From Prop. 6.7 μ is a subprobability measure, namely $\mu(\mathbb{R}^{2d}) \leq 1$. Let us show the converse inequality. Using the proof of Thm 6.2 we find that for any $\chi \in C_c^\infty(\mathbb{R}^{2d}, [0, 1])$ such that $\chi = 1$ in some neighbourhood U of $p_0^{-1}(E_0)$, we have $\text{Op}_h^W(\chi)\varphi_h = \varphi_h + \mathcal{O}(\hbar^\infty)$. As a result,

$$\mu(\text{supp } \chi) \geq \int \chi d\mu = \lim_{j \rightarrow \infty} \langle u_{h_j}, \text{Op}_{h_j}^W(\chi)u_{h_j} \rangle = 1.$$

$\square$

These properties of the semiclassical measures can actually be generalized to *quasimodes* of P_h , that is approximate eigenstates.

Proposition 6.10. *Assume that a sequence of normalized states $(u_h)_{h \rightarrow 0}$ satisfies the quasimode property*

$$\|(P_h - E_0)u_h\|_{L^2} = o(1) \quad \text{as } \hbar \rightarrow 0.$$

Then any semiclassical measure associated with (u_h) is a probability measure supported on $p_0^{-1}(E_0)$.

Proof. Let us go back to the proof of Thm 6.2. For $a \in S(1)$ supported away from $p_0^{-1}(E_0)$, we construct a bounded operator B_h satisfying (6.2), where λ_h has been replaced by E_0 . We then have

$$\begin{aligned} B_h(P_h - E_0)u_h &= A_h u_h + \mathcal{O}(\hbar^\infty) \\ \implies |\langle u_h, A_h u_h \rangle| &\leq \|B_h\| o(1) + \mathcal{O}(\hbar^\infty) \\ \implies \lim_{\hbar \rightarrow 0} \langle u_h, A_h u_h \rangle &= 0, \end{aligned}$$

so we find $\mu(a) = 0$.

For $\chi \in C_c^\infty$ equal to unity near $p_0^{-1}(E_0)$, we find for the same reason $\text{Op}_h^W(1 - \chi)u_h = o(1)$, hence $\text{Op}_h^W(\chi)u_h = u_h + o(1)$, and hence for any semiclassical measure associated with (u_h) , $\mu(\chi) = 1$. $\square$

Our last result is a refinement of this Proposition. For the first time it involves the Hamiltonian dynamics generated by p_0 .

Theorem 6.11. *Assume that a sequence of normalized states $(u_h)_{h \rightarrow 0}$ satisfies the sharper quasimode property*

$$\|(P_h - \lambda_h)u_h\|_{L^2} = o(\hbar) \quad \text{as } \hbar \rightarrow 0,$$

with $\lambda_h \rightarrow E_0$. Then any semiclassical measure associated with (u_h) is a probability measure supported on $p_0^{-1}(E_0)$, which is invariant w.r.t. the flow $\Phi_{p_0}^t$.

The invariance property of the measure is equivalent with the fact that for any $a \in C_c^\infty(\mathbb{R}^{2d})$,

$$(6.5) \quad \forall t \in \mathbb{R}, \quad \mu(a \circ \Phi_{p_0}^t) = \mu(a).$$

Proof. We will use the relation between commutator and Poisson bracket, mentioned in section 3.3, which can be easily extended to symbols $p \in S(m)$: for any $a \in C_c^\infty(\mathbb{R}^{2d})$ and $A_h = \text{Op}_h^W(a)$, we have

$$\frac{i}{\hbar} [P_h, A_h] = \text{Op}_h^W(\{p_0, a\}) + \mathcal{O}(\hbar)_{L^2 \rightarrow L^2}.$$

Injecting the commutator in the scalar product, we get (using the self-adjointness of P_h and A_h):

$$\langle u_h, [P_h - \lambda_h, A_h] u_h \rangle = \langle (P_h - \lambda_h) u_h, A_h u_h \rangle - \langle A_h u_h, (P_h - \lambda_h) u_h \rangle = o(\hbar).$$

Using the above identity, this gives

$$\langle u_h, \text{Op}_h^W(\{p, a\}) u_h \rangle = o(1),$$

which implies that any semiclassical measure μ satisfies $\mu(\{p_0, a\}) = 0$. This infinitesimal equation is actually equivalent with the invariance (6.5): since we may replace a by $a \circ \Phi_{p_0}^t$ in the above identity, we get:

$$\begin{aligned} \forall t \in [0, T], \quad 0 &= \mu(\{p_0, a \circ \Phi_{p_0}^t\}) = \mu\left(\frac{d}{dt} a \circ \Phi_{p_0}^t\right) = \frac{d}{dt} \mu(a \circ \Phi_{p_0}^t) \\ &\implies \mu(a \circ \Phi_{p_0}^T) - \mu(a \circ \Phi_{p_0}^0) = 0. \end{aligned}$$

□

APPENDIX A. APPENDIX: REMINDER ON OPERATOR AND SPECTRAL THEORY (ON HILBERT SPACE)

Below we describe a few properties of spectral theory on $\mathcal{H}$ a separable Hilbert space (we'll be mostly interested in the case $\mathcal{H} = L^2(\mathbb{R}^d)$).

A.1. Reminder: spectral theory of bounded operators. Let $A : \mathcal{H} \rightarrow \mathcal{H}$ be a *bounded* operator. Its resolvent set

$$\rho(A) = \{z \in \mathbb{C} : (A - z) \text{ is invertible on } \mathcal{H}, \text{ with bounded inverse}\}.$$

Its spectrum $\text{Spec}(A) = \mathbb{C} \setminus \rho(A)$. The spectrum can be composed of isolated eigenvalues of finite multiplicities (discrete spectrum) and essential spectrum (all the rest).

A bounded operator A admits an adjoint A^* , which is also bounded. A is selfadjoint iff $A = A^*$.

Theorem A.1. (*Spectral theorem*) For A a bounded selfadjoint operator, there exists a probability space $(X, \mathcal{M}, \mu)$, a unitary operator $U : \mathcal{H} \rightarrow L^2(X, \mu)$ and a function $f \in L^\infty(X, \mu)$ such that

$$(A.1) \quad A = U^* M_f U, \text{ where } M_f \text{ is the multiplication by } f.$$

Note that the pure point spectrum corresponds to the countable set $\{f(x_i), x_i \text{ an atom of } \mu\}$.

Corollary A.2. (*Functional calculus of bounded selfadjoint operators*) Take $\theta : \mathbb{R} \rightarrow \mathbb{R}$ a continuous function. Then, for A a bounded selfadjoint operator on $\mathcal{H}$, if we represent A as in (A.1), then the function $\theta \circ f \in L^\infty(\mu)$. We may then define the operator $\theta(A)$ as follows:

$$\theta(A) = U^* M_{\theta \circ f} U.$$

One can easily check that this definition is compatible with more obvious one, in the case where θ is a polynomial.

We remind that an operator $A : \mathcal{H} \rightarrow \mathcal{H}$ is compact iff it maps the unit ball $\{\|u\| \leq 1\}$ into a precompact set of $\mathcal{H}$ (that is, a set with compact closure). Compact operators are similar with operators of finite rank. In particular, their nonzero spectrum is exclusively made of eigenvalues of finite multiplicities, which may accumulate only at zero.

A.2. Reminder: unbounded selfadjoint operators. An unbounded operator P is defined by its domain $\mathcal{D}(P) \subset \mathcal{H}$, which is assumed to be dense in $\mathcal{H}$. This operator is closable if there exists a closed operator $\bar{P}$ which contains P (meaning that $\mathcal{D}(P) \subset \mathcal{D}(\bar{P})$ and they coincide on $\mathcal{D}(P)$).

The adjoint P^* (with its domain $\mathcal{D}(P^*)$) is defined by duality: $v \in \mathcal{D}(P^*)$ if

$$|\langle v, Pu \rangle| \leq C(v)\|u\|, \quad \text{for all } u \in \mathcal{D}(P).$$

Then, one may define P^*v by duality and density of $\mathcal{D}(P)$: due to the above inequality, there exists a unique state $P^*v \in \mathcal{H}$ such that $\langle v, Pu \rangle = \langle P^*v, u \rangle$ for all $u \in \mathcal{D}(P)$. This operator is always closed.

If P^* is densely defined, then P is closable, and its closure can be obtained as $\bar{P} = (P^*)^*$.

P is symmetric if $P \subset P^*$: for all $u, v \in \mathcal{D}(P)$, $\langle v, Pu \rangle = \langle Pv, u \rangle$.

P is essentially selfadjoint if $\bar{P} = P^*$.

P is selfadjoint if $P = P^*$.

Theorem A.3. (*Spectral theorem for unbounded selfadjoint operators*) Let $(A, \text{Dom}(A))$ be an unbounded selfadjoint operator on $\mathcal{H}$, with dense domain. There exists a measure space $(X, \mathcal{M}, \mu)$, a unitary operator $U : \mathcal{H} \rightarrow L^2(X, \mu)$ and a real valued measurable function f such that

- $\psi \in \text{Dom}(A)$ iff $U\psi \in \text{Dom}(M_f)$, meaning that $M_f U\psi \in L^2(X, \mu)$

- if this is the case, then $A\psi = U^* M_f U\psi$.

$$(A.2) \quad A = U^* M_f U.$$

The easiest example is that where A is already a multiplication operator. For instance, the operator of multiplication by x_1 , acting on $L^2(\mathbb{R}^d)$, admits as domain the subspace $\{u \in L^2(\mathbb{R}^d), x_1 u \in L^2(\mathbb{R}^d)\}$. We can take $X = \mathbb{R}^d$ and $f(x) = x_1$.

Example A.4. Consider the Schrödinger operator of a free particle on $\mathbb{R}^d$, $P_h = -\hbar^2 \Delta$. This operator is unbounded, its domain is the Sobolev space $H^2(\mathbb{R}^d)$. Through the (unitary) Fourier transform $\mathcal{F}_h$ it is mapped into the multiplication operator by $|\xi|^2$ acting on the space $L^2(\mathbb{R}^d, d\xi)$. So we may write

$$-\hbar^2 \Delta = \mathcal{F}_h^* M_{|\xi|^2} \mathcal{F}_h.$$

Corollary A.5. (*Functional calculus for unbounded selfadjoint operators*) Take $\theta : \mathbb{R} \rightarrow \mathbb{C}$ a continuous bounded function²². Then, for A an unbounded selfadjoint operator on $\mathcal{H}$, if we represent A as in (A.2), then the function $\theta \circ f \in L^\infty(\mu)$. We may then define the operator $\theta(A)$ as:

$$\theta(A) = U^* M_{\theta \circ f} U.$$

This operator can be extended to $\mathcal{H}$, where it is bounded, with $\|\theta(A)\|_{\mathcal{H} \rightarrow \mathcal{H}} \leq \|\theta\|_{C^0(\mathbb{R})} = \sup_{t \in \mathbb{R}} |\theta(t)|$.

Theorem A.6. (*Stone's theorem*) Suppose $(A, \text{Dom}(A) \subset \mathcal{H})$ is a selfadjoint (possibly unbounded) operator. Then the function $t \mapsto U(t) = e^{-itA}$ forms a strongly continuous unitary group on $\mathcal{H}$:

$$\begin{aligned} U(t)U(s) &= U(t+s), & U(t)^* &= U(-t), \\ \forall \psi \in \mathcal{H}, \quad \|U(t)\psi - \psi\| &\xrightarrow{t \rightarrow 0} 0. \end{aligned}$$

Furthermore, for any $\psi_0 \in \text{Dom}(A)$, the family of states $\psi(t) = U(t)\psi_0$ solves the Schrödinger equation

$$i\partial_t \psi(t) = A\psi(t), \quad \psi(0) = \psi_0,$$

and one has

$$\frac{U(t)\psi_0 - \psi_0}{t} \xrightarrow{t \rightarrow 0} -iA\psi_0.$$

Email address: `stephane.nonnenmacher@universite-paris-saclay.fr`

²²This calculus can be extended to bounded Borelian functions, which are functions $\theta : \mathbb{R} \rightarrow \mathbb{C}$.