Lecture Notes

Nalini Anantharaman

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Eigenfunctions of the laplacian on negatively curved manifolds : a semiclassical approach.

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Chapter 1

An introduction to semiclassical analysis.

1.1 Mechanics.

1.1.1 Three approaches to classical mechanics.

The variational approach. The Maupertuis or Euler principle [M1744, E1744] is the mechanical analogue of the Fermat principle in optics: a solid of mass $m = 1$, moving under the effect of a force $F = -\mathrm{grad}\, V$, with a total energy E, follows a trajectory γ which minimizes the action

$$S(\gamma) = \int \sqrt{2(E - V(\gamma))}\|d\gamma\| \tag{1.1}$$

among all curves with the same endpoints, and under the constraint that $\frac{\|\dot\gamma(t)\|^2}{2} + V(\gamma(t)) = E$ for all t. More precisely, we should look for *critical points* of S, among all paths with given endpoints, and constant total energy E. Say we work on a Riemannian manifold (X, g), and $\|.\|_x$ is the norm defined on T_xX by the riemannian metric : $\|v\|_x^2 = g_x(v, v)$. In other words, the Maupertuis principle says that the trajectories of energy E are geodesics for a new, degenerate metric, $2(E - V(x))g_x$.

The dual formulation, due to Lagrange [L1788], is to find the extrema of the functional

$$A(\gamma) = \int_0^T \left(\frac{\|\dot\gamma(t)\|^2_{\gamma(t)}}{2} - V(\gamma(t)) \right) dt \tag{1.2}$$

among all curves going from x to y in a given time T. Let us introduce the lagrangian $L(x, v) = \frac{\|v\|_x^2}{2} - V(x)$; the movement is described by the Euler-Lagrange equation

$$\frac{d}{dt}\left(\frac{\partial L}{\partial v}(\gamma, \dot\gamma)\right) = \frac{\partial L}{\partial x}(\gamma, \dot\gamma), \tag{1.3}$$

or more explicitly $D_{\dot\gamma}\dot\gamma = -\mathrm{grad}\, V(\gamma)$. This second order equation defines a local flow (ϕ^t_{EL}) on the tangent bundle TX, called the Euler-Lagrange flow.

Hamiltonian point of view. The hamiltonian is the Fenchel–Legendre transform of L with respect to the variable v :

$$H(x,\xi) = \xi.v - L(x,v)$$

with $\xi = \frac{\partial L}{\partial v}$; we are in a nice situation where the Legendre transformation

$$\mathcal{L}\mathrm{eg} : (x,v) \mapsto \left(x, \frac{\partial L}{\partial v}\right)$$

defines a diffeomorphism between the tangent bundle TX and the cotangent bundle T^*X. Its inverse is $\mathcal{L}\mathrm{eg}^{-1} : (x,\xi) \mapsto \left(x, \frac{\partial H}{\partial \xi}\right)$. In fact, in our case, $\mathcal{L}\mathrm{eg}$ is nothing else than the natural identification between TX and T^*X, provided by the riemannian metric. We can define a scalar product g^x on T^*_xX by $g^x(\xi,\xi) = g_x(v,v) = \|v\|^2_x$, with $\xi = \frac{\partial L}{\partial v}$. The vector ξ is called the momentum, and $H(x,\xi) = \frac{g^x(\xi,\xi)}{2} + V(x)$ is the total energy of the system (we will also denote $g^x(\xi,\xi) = \|\xi\|^2_x$, but do not confuse the norms $\|.\|_x$ on T^*_xX and T_xX !).

The Euler-Lagrange equation (1.3) is equivalent to Hamilton's system of equations,

$$\begin{cases} \dot x = \frac{\partial H}{\partial \xi} \\ \\ \dot\xi = -\frac{\partial H}{\partial x}\,, \end{cases} \tag{1.4}$$

which define a local flow (ϕ^t_H) on T^*X, called the hamiltonian flow. This flow is conjugate to (ϕ^t_{EL}) via the diffeomorphism $\mathcal{L}\mathrm{eg}$. It preserves the energy H, in the sense that $H(x(t),\xi(t))$ is constant for any trajecctory of the flow $(x(t),\xi(t))$. The hamiltonian flow also preserves the Liouville measure $dx\, d\xi$.

If a is a function on T^*X (an "observable quantity" in the language of Heisenberg), and if we denote $a_t = a \circ \phi^t_H$, we have

$$\frac{da}{dt} = \{H, a\},$$

where $\{.\,,.\}$ denotes the Poisson bracket, $\{H,a\} = \sum \partial_{\xi_j} H\, \partial_{x_j} a - \partial_{\xi_j} a\, \partial_{x_j} H$.

A more intrinsic way of writing the Hamilton equations (1.4) would be to see the vector field on the right hand side as the symplectic gradient of H, with respect to the *canonical symplectic form* on T^*X. Let us first define the Liouville 1-form on the cotangent bundle, defined by

$$\alpha_{(x,\xi)}(P) = \xi.d\pi(P) \text{ for all } P \in T_{(x,\xi)}(T^*X),$$

where $\pi : T^*X \longrightarrow X$ is the usual projection, and $d\pi$ its tangent map. The cotangent bundle T^*X can be endowed with the symplectic form

$$\omega = -d\alpha. \tag{1.5}$$

In local coordinates, $\alpha = p.dq$ and $\omega = dq \wedge dp$, if p and q denote respectively the "momentum" and "position" functions, $p(x, \xi) = \xi$, $q(x, \xi) = x$. Check that the right hand side of (1.4) is the expression in local coordinates of the symplectic gradient X_H of H, defined by $dH = \omega(X_H, .)$. Check also that the Poisson bracket is given by $\{f, g\} = -\omega(X_f, X_g) = dg(X_f)$, for f, g two functions on T^*X.

One can show that the flow ϕ_H preserves the symplectic form ω. In the language of symplectic geometry, a (local) diffeomorphism of T^*X which preserves ω is called a canonical transformation.

Hamilton–Jacobi equation, generating functions. The Hamilton–Jacobi point of view meets many technical difficulties, but it is the key tool to understand the semiclassical analysis of the Schrödinger equation.

Around 1830, Hamilton introduced a new point of view, by seeing the action as a function of the endpoints x and y [H1830, H1834]. Let $\gamma : [0, T] \longrightarrow X$ be a solution of the Euler–Lagrange equation, joining x to y in time T. For simplicity, we work in the nice, but usually unrealistic situation, where such a trajectory is unique. We can then consider the Lagrangian action $A(x, y; T) = \int_0^T L(\gamma, \dot\gamma)dt$ as a function of x, y, T, and check that

$$\frac{\partial A}{\partial x} = -\dot\gamma(0); \ \frac{\partial A}{\partial y} = \dot\gamma(T), \tag{1.6}$$

and

$$\frac{\partial A}{\partial T} = -E$$

where E is the energy $E = \frac{\|\dot\gamma\|^2}{2} + V(\gamma)$, constant along the trajectory γ.

According to Hamilton, being able to solve the equations (1.4) is equivalent to knowing the generating function A, solution of the Hamilton–Jacobi equation

$$\frac{\partial A}{\partial T} + H(x, \partial_x A) = 0, \tag{1.7}$$

for any initial condition (or even a large enough family of initial conditions). By this procedure, the ordinary differential equations (1.3) or (1.4) have been replaced by a single PDE. Quoting Hamilton, *"even if it should be thought that no practical facility is gained, yet an intellectual pleasure may result from the reduction of [...] all researches respecting the forces and motions of body, to the study of one characteristic function"*.

Let us also consider the Legendre transform of $A(x, y; T)$ with respect to the variable T,

$$S(x, y; E) = ET + A(x, y; T) \tag{1.8}$$

with

$$\frac{\partial S}{\partial E} = T \text{ and } \frac{\partial S}{\partial T} = -E.$$

This is nothing else as the Maupertuis action (1.1) of the trajectory γ joining x to y with energy E:

$$S(x, y; E) = \int \sqrt{2(E - V(\gamma))} \|\dot{\gamma}\| dt = \int_0^T \|\dot{\gamma}\|^2 dt.$$

To check it, note that

$$\int \sqrt{2(E - V(\gamma))} \|d\gamma\| = \int_0^T \|\dot{\gamma}\|^2 dt = ET + \int_0^T \left(\frac{\|\dot{\gamma}\|^2}{2} - V(\gamma) \right) dt.$$

We still have

$$\frac{\partial S}{\partial x} = -\dot{\gamma}(0); \ \frac{\partial S}{\partial y} = \dot{\gamma}(T). \tag{1.9}$$

The function S solves the stationary Hamilton–Jacobi equation,

$$H(x, \partial_x S) = E. \tag{1.10}$$

The solutions of the time–dependent Hamilton–Jacobi equation (1.7) and of the stationary equation (1.10) are related by the Legendre transform (1.8).

The Hamilton–Jacobi equation (1.7) has a simple geometrical intepretation. Consider a subset of the cotangent bundle T^*X, of the form $\mathcal{L}_0 = \{(x, d_x A_0), x \in \Omega_0\}$, with Ω_0 an open subset of X. This is a particular case of a *Lagrangian submanifold* in T^*X (see Chapter 4). Let $\mathcal{L}_0$ evolve under the Hamiltonian flow, and consider $\mathcal{L}_t = \phi_H^t \mathcal{L}_0$: because ϕ_H^t preserves the symplectic form ω, $\mathcal{L}_t$ is still a lagrangian manifold. Let us assume that, for $t \in [0, T]$, $\mathcal{L}_t$ still projects diffeomorphically on an open subset of $\Omega_t \subset X$. This means exactly that $\mathcal{L}_t$ is of the form $\mathcal{L}_t = \{(x, d_x A_t), x \in \Omega_t\}$ for some smooth function A_t. It can be shown that the relation $\mathcal{L}_t = \phi_H^t \mathcal{L}_0$ is equivalent to A_t solving the Hamilton–Jacobi equation (1.7), together with the condition that Ω_t is the image of $\mathcal{L}_0$ under the "exponential" map associated with $\mathcal{L}_0$:

$$\exp_{\mathcal{L}_0}^t : \mathcal{L}_0 \longrightarrow X, \tag{1.11}$$

$$\xi \mapsto \pi\big(\phi_H^t \xi\big) \tag{1.12}$$

(the notation π denotes the projection $T^*X \longrightarrow X$).

This approach suffers from the notorious problem of caustics. Usually, the exponential map will only be a diffeomorphism if the energy H is bounded on $\mathcal{L}_0$, and if t is small enough. For large times two kinds of problems arise,

– exp is not injective (two trajectories starting in $\mathcal{L}_0$ land at the same point in X)

– the tangent map $d\exp$ is not injective (focal points, conjugate points).

Geometrically, this means that after some time $\mathcal{L}_t$ will cease to project diffeomorphically on X. From a PDE point of view, this means that the equation (1.7) does not, in general, have globally defined smooth solutions.

Although the problem of caustics makes the Hamilton–Jacobi equation rather difficult to work with, it is, nevertheless, the key tool to understand Schrödinger's equation and its semiclassical analysis. Semiclassical methods often break down with the appearance of caustics, or little after.

We now review Schrödinger's view of mechanics, but also the work of Born, Heisenberg and Jordan, which lead to the idea of quantization.

1.1.2 Quantum/wave mechanics.

At the beginning of the twentieth century, it became clear that classical mechanics was not applicable to certain problems, like the study of energy radiation in atoms. People started looking for new physical laws, but it was not until 1925 that theories judged as satisfactory were elaborated. These theories involve Planck's constant $h = 2\pi\hbar = 6,626068.10^{-34} m^2.\mathrm{kg}/s$ (the "action quantum"), and one is supposed to recover classical mechanics when letting h tend to 0 in the equations.

Quantenmechanik. In 1925, Heisenberg, Born and Jordan gave some new laws of mechanics, supposed to replace the old Hamilton equations (1.4). Consider a hamiltonian system with d degrees of freedom (meaning that the manifold X has dimension d – in fact let us take $X = \mathbb{R}^d$). In classical mechanics the time evolution is given by equation (1.4), defining a flow on the phase space T^*X. According to the quantum mechanics of [BHJ25-II], the time evolution of the system is ruled by the five following principles :

(0) The "phase space" is a now Hilbert space $\mathcal{H}$.

(1) The "observable quantities" are described by linear operators (= infinite matrices). They used a boldface letter $\mathbf{a}$ to denote the quantum observable corresponding to the classical observable a; if a is a real–valued function on T^*X then the corresponding operator $\mathbf{a}$ is hermitian.

(2) Main rules : We consider, in particular, an algebra of operators generated by the momentum and position observables, $\mathbf{p} = (\mathbf{p}_1, \mathbf{p}_2, ..., \mathbf{p}_d)$ and $\mathbf{q} = (\mathbf{q}_1, ..., \mathbf{q}_d)$. They must obey the following commutation rules :

$$\begin{aligned}
\big[\mathbf{p}_k, \mathbf{q}_l\big] &= \frac{\hbar}{i}\delta_{kl}, && (1.13)\\
\big[\mathbf{p}_k, \mathbf{p}_l\big] &= 0, && (1.14)\\
\big[\mathbf{q}_k, \mathbf{q}_l\big] &= 0. && (1.15)
\end{aligned}$$

Assume now that the classical observable f is defined by a power series

$$f(p,q) = \sum \alpha_{sr} p^s q^r.$$

Then we should define the quantum observable $\mathbf{f}$ by

$$\mathbf{f}(\mathbf{p},\mathbf{q}) = \sum \alpha_{sr} \frac{1}{s+1} \sum_{l=0}^{s} \mathbf{p}^{s-l}\mathbf{q}^{r}\mathbf{p}^{l}.$$

This prehistoric "quantization rule" can be applied, in particular, to define the hamiltonian operator $\mathbf{H}$.

(3) A canonical transformation is a transformation that sends the observables $(\mathbf{p},\mathbf{q})$ to new observables $(\mathbf{P},\mathbf{Q})$ satisfying the same commutation relations. We ask that a canonical transformation preserves hermitian operators, and sends an observable of the form $\mathbf{f}(\mathbf{p},\mathbf{q})$ to $\mathbf{f}(\mathbf{P},\mathbf{Q})$. Such a transformation is of the form $\mathbf{P} = \mathbf{S}\mathbf{p}\mathbf{S}^{-1}$, $\mathbf{Q} = \mathbf{S}\mathbf{q}\mathbf{S}^{-1}$, where $\mathbf{S}$ is a unitary operator.

(4) The equations of motion are

$$\begin{cases} \dot{\mathbf{p}} = -\frac{\partial \mathbf{H}}{\partial \mathbf{q}} \\ \\ \dot{\mathbf{q}} = \frac{\partial \mathbf{H}}{\partial \mathbf{p}}\,, \end{cases} \tag{1.16}$$

where we define

$$\frac{\partial \mathbf{f}}{\partial \mathbf{x}_1} = \lim_{\varepsilon \longrightarrow 0} \frac{1}{\varepsilon}\big(\mathbf{f}(\mathbf{x}_1 + \varepsilon \mathbb{1}, \mathbf{x}_2, ..., \mathbf{x}_s) - \mathbf{f}(\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_s)\big)$$

for $\mathbf{f}(\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_s)$ a power series in the s observables $\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_s$ ($\mathbb{1}$ is the identity operator).

It can be shown from formula (1.13) that we have the identity

$$[\mathbf{f},\mathbf{g}] = \frac{\hbar}{i}\left(\frac{\partial \mathbf{f}}{\partial \mathbf{p}}\frac{\partial \mathbf{g}}{\partial \mathbf{q}} - \frac{\partial \mathbf{f}}{\partial \mathbf{q}}\frac{\partial \mathbf{g}}{\partial \mathbf{p}}\right)$$

holding for $\mathbf{f},\mathbf{g}$ power series in the operators $\mathbf{p}$ and $\mathbf{q}$.

In particular, the equations (1.16) can be reexpressed as

$$\dot{\mathbf{f}} = \frac{i}{\hbar}[\mathbf{H},\mathbf{f}]$$

for any observable $\mathbf{f}$.

(5) To integrate the equation of motion, we must find a unitary operator $\mathbf{S}$ such that

$$\mathbf{S}\mathbf{H}\mathbf{S}^{-1} = \mathbf{W} \tag{1.17}$$

is diagonal. In other words, we look for a canonical transformation which allows to express the solutions of (1.16) as a superposition of periodic motions[1].

In a basis where $\mathbf{H}$ is diagonal, we find, for any observable $\mathbf{f}$, that the matrix elements evolve according to

$$\mathbf{f}_{nm}(t) = \mathbf{f}_{nm}(0)e^{2i\pi\nu_{nm}t}; \tag{1.18}$$

where the radiation sprectrum ν_{nm} ("physical spectrum") is related to the eigenvalues (E_n) of $\mathbf{H}$ ("mathematical spectrum") by

$$\nu_{nm} = \frac{E_n - E_m}{h}.$$

Wellenmechanik. In 1926, Erwin Schrödinger, independently of the work of Heisenberg, Born and Jordan, proposed a new equation, supposed to describe the state of our system, when the value of the energy E is given (in a force field $-\operatorname{grad} V$, as above) : the "stationary" Schrödinger equation is a second order PDE,

$$-\frac{\hbar^2}{2}\triangle\psi + V\psi = E\psi, \tag{1.19}$$

where E is the energy. As we shall see, this equation is closely related to the stationary Hamilton–Jacobi equation (1.10). The evolution equation reads

$$i\hbar\frac{\partial\phi}{\partial t} = \left(-\frac{\hbar^2}{2}\triangle + V\right)\phi. \tag{1.20}$$

[1]The analogy with the theory of classical hamiltonian systems can be pushed further. In fact, equation (1.16) can is a linear hamiltonian flow, in an infinite dimensional space. Such systems are completely integrable, due to the fact that a unitary transformation diagonalizing $\mathbf{H}$ always exists. To be more explicit, let $(\mathcal{H}, \langle .,. \rangle)$ be a complex Hilbert space, seen as a real vector space endowed with the symplectic form $\omega(\phi,\psi) = \Im m\langle\phi,\psi\rangle$. If we use an orthonormal basis (e_n) to define coordinates, $\phi = \sum_n (x_n + i\xi_n)e_n$, then (x_n, ξ_n) are Darboux coordinates, meaning that $\omega = \sum_n dx_n \wedge d\xi_n$.

Let $\mathbf{H}$ be a self–adjoint operator; it can be used to define a quadratic hamiltonian $H(\psi) = \frac{1}{2}\langle\psi, \mathbf{H}\psi\rangle$. If we consider quadratic observables, $f(\psi) = \frac{1}{2}\langle\psi, \mathbf{f}\psi\rangle$, then the Poisson bracket defined by ω correspond to the usual commutator bracket,

$$\{f, g\}(\psi) = \frac{1}{2}\langle\psi, i[\mathbf{f}, \mathbf{g}]\psi\rangle.$$

The Hamilton equations defined by H read $\frac{d\psi}{dt} = -i\mathbf{H}\psi$. Finally, linear transformations preserving ω are of the form $\psi \mapsto \mathbf{S}\psi$ where $\mathbf{S}$ is unitary.

Thus, finding a unitary $\mathbf{S}$ such that $\mathbf{S}^{-1}\mathbf{H}\mathbf{S}$ is diagonal amounts to finding a linear canonical transformation $\psi \mapsto \mathbf{S}\psi$ which transforms the hamiltonian H into $H(\mathbf{S}\psi) = \frac{1}{2}\sum(2\pi\nu_n)^2(x_n^2 + \xi_n^2)$. This means that we can integrate the equation of motion by decomposing it into a superposition of infinitely many independent harmonic oscillators.

These two forms of the equation are related by a time/energy Fourier transform $\phi(t) = \int e^{-iEt/\hbar}\psi_E dE$, which recalls the relation (1.8).

According to Schrödinger's theory, the energy spectrum can be computed by finding the values of E for which equation (1.19) admits solutions which are *"single–valued, finite, and continuous throughout configuration space"*.

Schrödinger, motivated by the works of De Broglie, gives an interpretation of ψ as a "wave function". *"The true mechanical process is realised or represented in a fitting way by the* wave processes *in q–space, and not by the motion of* image points *in this space. The study of the motion of image points, which is the object of classical mechanics, is only an approximate treatment, and has, as such, just as much justification as geometrical or "ray" optics has, compared with the true optical process"*. This approximation is only justified when the dimensions of the system are very large compared to the wave length : *"we inevitably became involved in irremovable contradictions if we tried, as was very natural, to maintain also the idea of* paths of systems *in these processes; just as we find the tracing of the course of a* light ray *to be meaningless, in the neighbourhood of a diffraction phenomenon"*.

It is particularly interesting for us to note that Schrödinger derived the form of his equation from the desired behaviour of the solutions when $\hbar \longrightarrow 0$:

Assume that our mechanical phenomenon is described by a wave function ψ, and assume that this wave has the particular form : $\psi(x,0) = \exp\left(i\frac{A(x,0)}{\hbar} + C\right)$ at $t = 0$. Assume also that for $t > 0$ the wave ψ looks like

$$\psi(x,t) \sim \exp\left(i\frac{A(x,t)}{\hbar} + C\right) + \text{ small error.} \tag{1.21}$$

To find the form of the equation satisfied by ψ, Schrödinger postulates that the phase A must approximately satisfy the Hamilton-Jacobi equation (1.7), when the wave length is very small (semiclassical approximation). In other words, we must (almost) see the wave move according to the classical motion. Thus, the point is to find an equation, looking like a wave equation, and such that (1.21) is an approximate solution if $\frac{\partial A}{\partial t} + H(x, d_x A) = 0$ (1.7) and $\hbar \longrightarrow 0$.

To find such an equation, Schrödinger actually works with the stationary formulation : this means that $A(x,t)$ is of the form $A(x,t) = -Et + S(x)$ where S solves $H(x, d_x S) = E$ (1.10). If S satisfies (1.10), then the local speed of propagation of ψ is

$$u(x) = \frac{-\frac{\partial A}{\partial t}}{|\nabla A|} = \frac{E}{\sqrt{2(E - V(x))}}$$

and the wave length is $\lambda(x) = \frac{h}{\sqrt{2(E-V(x))}}$. This encourages Schrödinger to propose the equation

$$\frac{\partial^2\psi}{\partial t^2} = u^2 \triangle \psi.$$

From the expression of u, and the formula (1.21) supposed to give an approximate solution when $\lambda \longrightarrow 0$, we find $-\frac{\hbar^2}{2}\triangle\psi + V\psi = E\psi$.

The description of the semiclassical limit, yielding classical mechanics as a limiting case of wave mechanics, is the same as in optics; it is a phenomenon of constructive or destructive interferences (described in mathematics by the stationary phase method). Let us try to put Schrödinger's arguments into mathematical words : they already contain the seeds of semiclassical analysis. Every ψ can be written as

$$\psi(x) \sim \int a(x,\theta) \exp\left(\frac{i}{\hbar}A(x;\theta)\right) d\theta, \tag{1.22}$$

where θ varies in an open set of $\mathbb{R}^d$, and $\exp\left(\frac{i}{\hbar}A(x;\theta)\right)$ is a family parametrized by θ (for instance, the plane wave in $\mathbb{R}^d$, $\exp\left(\frac{i}{\hbar}\langle x,\theta\rangle\right)$), and a is a distribution. By linearity of the Schrödinger equation, and by the approximate form of the solutions (1.21), after time t the wave looks like

$$\psi(t,x) \sim \int a(x,\theta) \exp\left(\frac{i}{\hbar}A(t,x;\theta)\right) d\theta, \tag{1.23}$$

where $A(t,x;\theta)$ is the solution of (1.7) with initial condition $A(x;\theta)$. If the oscillations are very rapid (λ small) we expect all these waves to interfer destructively, except at those points x where the phase has a stationary point,

$$\partial_\theta A(t,x,\theta_0) = 0$$

(for some θ_0). At such a point, we see essentially the wave $\exp\left(\frac{i}{\hbar}A(t,x;\theta_0)\right)$, with the frequency vector $\xi = \partial_x A(t,x,\theta_0)$. Thus, the wave front at time t is the subset of the cotangent space

$$\mathcal{L}(t) = \{(x,\xi),\ \text{there exists } \theta_0, \partial_\theta A(t,x,\theta_0) = 0,\ \xi = \partial_x A(t,x,\theta_0)\}\,. \tag{1.24}$$

Assuming each $A(.,.,\theta)$ satisfies the Hamilton–Jacobi equation, check that $\mathcal{L}(t)$ is precisely the image of $\mathcal{L}(0)$ under the hamiltonian flow (1.4) at time t. In other words, the wave front is propagated according to the classical hamiltonian flow.

"The point of phase agreement for certain infinitesimal manifolds of wave systems, containing n parameters, moves according to the same laws as the image point of the mechanical system" [Schr26-II].

Recall that this is an approximation, valid when the wave length λ is very small; for mathematicians, this is the same as letting $\hbar$ tend to 0.

Schrödinger writes : *"I consider it a very difficult task to give an exact proof that the superposition of these wave systems really produces a noticeable disturbance in only a relatively small region surrounding the point of phase agreement, and that everywhere else they practically destroy one another through interference"* [Schr26-II]. As we shall see in Section 1.4.2, this problem can in fact be handled, imposing strong smoothness conditions on the distribution a.

1.2 Weyl quantization.

In [Schr26-III], Schrödinger realizes, in the case of $X = \mathbb{R}^d$, that his "wave mechanics" is equivalent to the "quantum mechanics" introduced by Born, Heisenberg and Jordan. A *quantization procedure* is a way to associate, to every function on the classical phase space $T^*X = \mathbb{R}^d \times \mathbb{R}^d$, an operator on the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^d)$, so that the commutation rules (1.13) are satisfied. Schrödinger suggests to associate the operator $\mathbf{q}_k =$ (multiplication by q_k) to the coordinate function q_k, and the operator $\mathbf{p}_k = \frac{\hbar}{i}\frac{\partial}{\partial q_k}$ to the function p_k.

One must then decide of a convention to define the operator $\mathbf{a}(\mathbf{q}, \mathbf{p})$ associated to an arbitrary function $a(q,p)$ of (q,p). For instance, the function $p_k q_k$ could be represented by the operator $\mathbf{p}_k\mathbf{q}_k$ or by $\mathbf{q}_k\mathbf{p}_k$. Schrödinger leaves this issue open, but recommends to quantize a hamiltonian of the form

$$H(q,p) = \frac{\|p\|^2}{2} + V(q),$$

where $\|.\|$ is a riemannian metric, by the operator $\mathbf{H} = -\frac{\hbar^2}{2}\triangle + V$, where $\triangle$ is the laplacian associated to the metric. In this representation, Heisenberg's equation (1.17), requiring to diagonalize the operator $\mathbf{H}$, can be written $-\frac{\hbar^2}{2}\triangle\psi + V\psi = E\psi$, which is exactly Schrödinger's equation (1.19). Thus, the two theories will give the same values of the energy spectrum. Schrödinger suggests, however, that two theories can be mathematically equivalent without being physically equivalent.

Weyl quantization. Hermann Weyl [Weyl27] proposed to quantize the observable $U_{p_0,q_0}(q,p) = e^{\frac{i}{\hbar}(p_0.q - q_0.p)}$ $(q_0, p_0 \in \mathbb{R}^d)$ by the operator $\mathbf{U}_{p_0,q_0}(\mathbf{q},\mathbf{p}) = e^{\frac{i}{\hbar}(p_0.\mathbf{q} - q_0.\mathbf{p})}$ (where $(\mathbf{q},\mathbf{p})$ are defined by Schrödinger's prescriptions). Then, the Fourier transform allows to quantize any observable : if a is decomposed into

$$a(q,p) = \int e^{\frac{i}{\hbar}(p_0.q - q_0.p)} \hat{a}_\hbar(q_0, p_0) \frac{dq_0 dp_0}{(2\pi\hbar)^d}$$

Weyl's quantization defines

$$\mathbf{a}(\mathbf{q},\mathbf{p}) = \int e^{\frac{i}{\hbar}(p_0.\mathbf{q} - q_0.\mathbf{p})} \hat{a}_\hbar(q_0, p_0) \frac{dq_0\, dp_0}{(2\pi\hbar)^d} =: \mathrm{Op}^W_\hbar(a),$$

also given by the formula

$$\mathrm{Op}_\hbar^W(a)f(x) = \frac{1}{(2\pi\hbar)^d}\int a\left(\frac{x+y}{2},\xi\right) e^{\frac{i}{\hbar}\xi.(x-y)} f(y)dy\,d\xi.$$

The Schrödinger representation. The family of operators $\mathbf{U}_{p,q}$ obeys the following composition rule,

$$\mathbf{U}_{p,q}.\mathbf{U}_{p',q'} = \mathbf{U}_{p+p',q+q'}e^{\frac{i}{\hbar}\frac{1}{2}(pq'-q'p)}. \tag{1.25}$$

Consider the Heisenberg group $\mathbf{H}_d$ with d degrees of freedom, defined as $\mathbb{R}^{2d+1}$ endowed with the composition rule

$$(p,q,t).(p',q',t') = \left(p+p', q+q', t+t' + \frac{1}{2}(pq'-qp')\right), \ (p,p',q,q' \in \mathbb{R}^d, t,t' \in \mathbb{R}).$$

Its Lie algebra is generated by $P_1,\ldots,P_d,Q_1,\ldots,Q_d,T$ with the relations

$$[P_j,P_k] = [Q_j,Q_k] = [P_j,T] = [Q_j,T] = 0;\ [P_j,Q_k] = \delta_{jk}T.$$

The identity (1.25) can be reinterpreted by saying that

$$\rho_h(p,q,t) = e^{\frac{it}{\hbar}}\mathbf{U}_{p,q}$$

defines a unitary representation from $\mathbf{H}_d$ into $L^2(\mathbb{R}^d)$, called the Schrödinger representation of parameter h. The associated infinitesimal representation is $P_k \mapsto \frac{\partial}{\partial q_k} = \frac{i}{\hbar}\mathbf{p}_k$, $Q_k \mapsto \frac{i}{\hbar}\mathbf{q}_k$, $T \mapsto \frac{i}{\hbar}I$.

Theorem 1.1. *(Stone–von Neumann 1930 [St30, vN31], see [Foll]) Every irreducible unitary representation of $\mathbf{H}_d$ is equivalent to exactly one of the following representations :*
(a) ρ_h ($h \in \mathbb{R}\setminus\{0\}$) acting on $L^2(\mathbb{R}^d)$;
(b) $\sigma_{ab}(p,q,t) = e^{2\pi i(ap+bq)}$, ($a,b \in \mathbb{R}^d$) acting on $\mathbb{C}$.

1.3 Born's probabilitic interpretation of the Schrödinger equation.

Born discovered that the square modulus $|\psi|^2$ of the wave functions (satisfying the Schrödinger equation) could be used to predict the probability of where the "particle" would be found. More precisely, if ψ is normalized so that $\int |\psi(t,x)|^2 dx = 1$, then $|\psi(t,x)|^2$ gives the probability density of finding, in an experiment, the particle at x (at time t). This was the beginning of a tense philosophical (or physical) debate on the correct interpretation of the wave/particle duality.

"Let me say at the outset, that in this discourse, I am opposing not a few special statements of quantum physics held today (1950s), I am opposing as it were the whole of it, I am opposing its basic views that have been shaped 25 years ago, when Max Born put forward his probability interpretation, which was accepted by almost everybody. (E. Schrödinger, The Interpretation of Quantum Physics. Ox Bow Press, Woodbridge, CN, 1995).

"I don't like it, and I'm sorry I ever had anything to do with it" (Erwin Schrödinger talking about quantum physics).

1.4 The semiclassical limit.

The main subject of these notes is to try to describe the localization of the probability density $|\psi(t,x)|^2 dx$, for a Schrödinger eigenfunction, in the semiclassical limit $\hbar \longrightarrow 0$. The quantum/classical correspondence tells us, intuitively, that the eigenfunctions, which correspond to stationary solutions of the Schrödinger equation, should look like invariant probability measures of the classical hamiltonian flow. In this section we give a quick survey of the mathematical tools used to study this question.

It is not really satisfactory, and usually practically impossible, to study the density $|\psi(t,x)|^2 dx$ itself. This is because, when taking the modulus of ψ, we lose some precious information on the frequency vector of ψ (related to its phase, or complex argument). We need to study simultaneously the Fourier transform of ψ. Of course, mathematically speaking, one cannot study at the same time the local property of a function and of its Fourier transform around some point $(x,\xi) \in T^*X$. In physics, this is expressed by Heisenberg's uncertainty principle, saying that one cannot measure the localization in position without perturbing a lot the momentum (and vice-versa). Microlocal analysis[2] is a collection of mathematical techniques allowing to study the joint localization of a function and its Fourier transform; because of the uncertainty principle, this can only be meaningful asymptotically, when $\hbar \longrightarrow 0$.

1.4.1 Fourier transform.

The Fourier transform

$$\mathcal{F}_\hbar(u)(\xi) = \hat{u}_\hbar(\xi) = (2\pi\hbar)^{-d/2} \int_{\mathbb{R}^d} e^{-\frac{i}{\hbar}\xi.x} u(x) \mathrm{d}x$$

allows to analyze a signal u in terms of its frequencies, at the scale $\hbar$. For $u \in C_o^\infty$, we have the decomposition

$$u(x) = (2\pi\hbar)^{-d/2} \int_{\mathbb{R}^d} e^{\frac{i}{\hbar}\xi.x} \hat{u}_\hbar(\xi) \mathrm{d}\xi \ .$$

[2]More precisely, we will present here its $\hbar$-dependent version, also called semiclassical analysis.

1.4.2 The stationary phase method.

It describes the asymptotic behaviour, as $\hbar \to 0$, of an integral of the form :

$$I(\hbar) = \int_{\mathbb{R}^D} e^{\frac{i}{\hbar}S(x)} a(x)\,\mathrm{d}x$$

where $a \in C_o^\infty(\mathbb{R}^D)$ and $S \in C^\infty(\mathbb{R}^D, \mathbb{R})$.

The interferences between the different terms $e^{\frac{i}{\hbar}S(x)}$ are destructive, except at the stationary points of the phase S. The precise statement is :

- If S has no critical/stationary point in the support of a, then $I(\hbar) = O(\hbar^\infty)$.
- If S has a unique critical point x_0, supposed to be non–degenerate, in the support of a, then there is an asymptotic development in powers of $\hbar$, up to any order,

$$I(\hbar) \sim (2\pi\hbar)^{D/2} \frac{e^{i\sigma\pi/4}}{|\det S''(x_0)|^{\frac{1}{2}}} e^{iS(x_0)/\hbar} \left(\sum_{j=0}^{\infty} \hbar^j a_j \right) \tag{1.26}$$

where $S''(x_0)$ is the hessian matrix of S at x_0, $\sigma = n_+ - n_-$ is the index of $S''(x_0)$ (the difference between the number of positive and negative eigenvalues), and $a_0 = a(x_0)$. More generally, a_j can be expressed in terms of the derivatives of a up to order $2j$, at the point x_0.

For technical applications, one usually needs to work with functions a which are not necessarily compactly supported, but have a well behaved behaviour at infinity, and can be allowed to depend on $\hbar$. The choice of a class of "symbols" is a technical issue, which depends on the aims, but also on the tastes of the authors. For the sake of completeness we give an example of a convenient class of symbols. However, it is not required to understand all technical issues to read the next sections.

Symbol spaces. Let $D, d > 0$ be two integers, and let U be an open subset of $\mathbb{R}^D$. Let us define *symbols of order* m (independent of $\hbar$) :

$$\begin{aligned}\Sigma^m(U \times \mathbb{R}^d) := \big\{ & a \in C^\infty(U \times \mathbb{R}^d; \mathbb{C}) / \\ & \text{for every compact } K \subset U, \text{ there exists } C, \\ & |D_z^\alpha D_\xi^\beta a(z,\xi))| \leq C(1+|\xi|)^{m-|\beta|} \text{ for all } (z,\xi) \in K \times \mathbb{R}^d \big\}.\end{aligned}$$

For instance, this class contains functions which are homogeneous in a neighbourhood of infinity. We denote $\Sigma^{-\infty} = \cap_{m\in\mathbb{Z}} \Sigma^m$ — this class contains the smooth compactly supported functions $C_o^\infty(U \times \mathbb{R}^d)$.

We also define *semiclassical symbols of order m and degree l* — thus called because they depend on a parameter $\hbar$:

$$\Sigma^{m,l} = \{a_\hbar(z,\xi) = \hbar^l \sum_{j=0}^{\infty} \hbar^j a_j(z,\xi),\ a_j \in \Sigma^{m-j}\} \tag{1.27}$$

This means that $a_\hbar(x,\xi)$ as an asymptotic development in powers of $\hbar$; in the sense that

$$a - \hbar^l \sum_{j=0}^{N-1} \hbar^j a_j \in \hbar^{l+N}\Sigma^{m-N}$$

for all N, uniformly in $\hbar$. In this context, we denote $\Sigma^{-\infty,+\infty} = \cap_{m\geq 0}\Sigma^{-m,m}$.

In these definitions, $U \times \mathbb{R}^d$ can be replaced by a fiber bundle of rank d on a D–dimensional manifold.

Fresnel integrals, generalized stationary phase method. We can now describe the asymptotic behaviour, as $h \to 0$, of the integral :

$$I_\hbar^S(a) = \int_{U\times\mathbb{R}^d} e^{\frac{i}{\hbar}S(z,\xi)} a(z,\xi)\, dz d\xi$$

where S is smooth, homogeneous of degree $n > 0$ near infinity with respect to ξ, and without critical points outside a compact subset of $U \times \mathbb{R}^d$. The integral $I_\hbar^S(a)$ is defined for $a \in \Sigma_o^{m,l}$, by continuation of the case $a \in C_o^\infty$. Here, the index $*_o$ in $\Sigma_o^{m,l}$ means that a is compactly supported with respect to z, with support independent on $\hbar$.

The method of stationary phase can still be applied in this setting.

1.4.3 Pseudodifferential operators.

A quantization procedure is a way to associate an operator to a classical observable $a(p,q)$. Recall Schrödinger's prescriptions, $\mathbf{q}_k =$ (multiplication by q_k), and $\mathbf{p}_k = \frac{\hbar}{i}\frac{\partial}{\partial q_k}$, compatible with Heisenberg's commutation relations (1.13). To extend this definition to an arbitrary function of (p,q), we meet an obvious problem : to quantize the function $p_k q_k^2$, for instance, we could propose the operators $\mathbf{p}_k\mathbf{q}_k^2$, $\mathbf{q}_k^2\mathbf{p}_k$, or $\mathbf{q}_k\mathbf{p}_k\mathbf{q}_k$. There are many quantization procedures. We already met the Weyl quantization, which combines several remarkable features, like the fact that it associates a symmetric operator to a real symbol. Later on, we shall also define the anti-Wick positive quantization, which associates a nonnegative operator to a nonnegative symbol.

The theory of pseudodifferential operators with small parameter allows to describe the passage from the quantum theory to the classical theory when $\hbar \longrightarrow 0$. This is also called $\hbar$-dependent microlocal analysis, microlocal analysis with small parameter, or semiclassical analysis. Pseudodifferential operators were first developed by Hörmander [Ho, Ho79] for the study of the regularizing properties of partial differential equations (without any small parameter). Pseudodifferential operators with small parameter, manipulated by Maslov [Masl65] in the framework of semiclassical analysis, developed by Voros in mathematical physics [Vor, Vor78], were perfectioned by Sjöstrand, Robert, Helffer, [DimSjo, Rob]... I advise to read [Helffer1] for a history of the first years of this theory in the seventies and an exhaustive bibliography; see also [Helffer2] for a survey of applications.

Symbol spaces depend on authors, and can be extremely sophisticated. Hörmander's definition has no $\hbar$ and involves symbols which are homogeneous near infinity, allowing to describe the regularizing properties of operators. The semiclassical symbol classes of [DimSjo] are rather aimed at describing the behaviour of operators when $\hbar \longrightarrow 0$, say in L^2 norm. The symbols we use here combine both approaches : taking $\hbar = 1$ we would find (one of) Hörmander's symbol spaces.

Pseudodifferential operators. Let Ω be an open subset of $\mathbb{R}^d$, and let $a = a_\hbar(x, y; \xi) \in \Sigma_o^{m,l}(\Omega \times \Omega \times \mathbb{R}^d)$. Here the index $_o$ means that for every compact $K \subset \Omega$, there exists a compact K' such that $a(x, y, \xi) = 0$ for $x \in K, y \notin K'$, $\xi \in \mathbb{R}^d$. Let u be a smooth function. We define :

$$\mathrm{OP}_\hbar(a)u(x) = (2\pi\hbar)^{-d} \int e^{\frac{i}{\hbar}\xi.(x-y)} a(x, y, \xi) u(y)\, \mathrm{d}y \mathrm{d}\xi,$$

the integral being well defined as a Fresnel integral. We denote $\Psi\mathrm{DO}^{m,l}(\Omega)$ these operators, called (proper) pseudodifferential operators of *degree* l and *order* m, on Ω. The intersection $\Psi\mathrm{DO}^{-\infty,\infty}$ of all the $\Psi\mathrm{DO}^{m,l}(\Omega)$ are the negligible operators : they are the operators with a smooth kernel $K_\hbar$, and such that all derivatives of $K_\hbar$ are $O(\hbar^\infty)$ uniformly on compact sets.[3]

Note that several symbols $a(x, y, \xi)$ can give the same operator $\mathrm{OP}_\hbar(a)$. As a simple example, we note that $a(x, y, \xi) = V(x)$ and $a(x, y, \xi) = V(y)$ both give the operator of multiplication by V. It is often convenient to choose special representatives :

Weyl quantization. Left and right quantizations.

Here $\Omega = \mathbb{R}^d$.

We already met the Weyl quantization[4], $\mathrm{Op}_\hbar^W(a) = \mathrm{OP}_\hbar\left(a(\frac{x+y}{2}, \xi)\right)$. If $a \in \Sigma_o^{m,l}(\mathbb{R}^d \times \mathbb{R}^d)$ is compactly supported with respect to the first variable, then $\mathrm{Op}_\hbar^W(a) \in \Psi\mathrm{DO}^{m,l}$.

[3] Usually, in this theory, all the assertions about operators hold *modulo negligible operators.* Likewise, the assertions about functions hold *modulo negligible functions.* These are the smooth functions $u_\hbar(x)$ such that all derivatives are $O(\hbar^\infty)$ uniformly on compact sets of X.

[4] I try to stick to the notation OP for symbols $a \in \Sigma(\Omega \times \Omega \times \mathbb{R}^d)$, and Op for symbols $a \in \Sigma(\Omega \times \mathbb{R}^d)$.

The inverse of Weyl quantization is explicit, given by the Wigner transform : if $K(x, y)$ is the kernel of the operator A, we let :

$$W_A(x,\xi) = (2\pi\hbar)^{-d/2} \int e^{\frac{iv\xi}{\hbar}} K\left(x + \frac{v}{2}, x - \frac{v}{2}\right) dv \ .$$

Then $A = \mathrm{Op}_\hbar^W(W_A)$. In particular, the Weyl symbol of an operator is unique.

Two other common quantizations are, the *left quantization*, defined by $\mathrm{Op}_\hbar^L(a) = \mathrm{OP}_\hbar\left(a(x,\xi)\right)$ where $a \in \Sigma_o^{m,l}(\mathbb{R}^d \times \mathbb{R}^d)$ and the *right quantization*, $\mathrm{Op}_\hbar^R(a) = \mathrm{OP}_\hbar\left(a(y,\xi)\right)$. The left and right symbols are both uniquely determined by the operator (there are explicit inversion formulas, too).

Example 1.2. *To quantize the observable* $a(p,q) = pq^2$*, the left quantization chooses* $\mathbf{q}^2\mathbf{p}$*, the right quantization chooses* $\mathbf{pq}^2$*, and the Weyl quantization forms the combination* $\frac{1}{4}(\mathbf{pq}^2 + 2\mathbf{qpq} + \mathbf{q}^2\mathbf{p}) = \frac{1}{2}(\mathbf{pq}^2 + \mathbf{q}^2\mathbf{p})$.

Exercise 1.3. *On* $\mathbb{R}^d \times \mathbb{R}^d$*, consider a lagrangian* $L(x,v)$ *defined by a riemannian metric,*

$$L(x,v) = \frac{1}{2} g_x(v,v) = \frac{1}{2} \sum_{i,j=1}^{d} g_{ij}(x) v_i v_j.$$

Check that the corresponding hamiltonian is

$$H(x,\xi) = \frac{1}{2} g^x(\xi,\xi) = \frac{1}{2} \sum_{i,j=1}^{d} g^{ij}(x) \xi_i \xi_j,$$

where $(g^{ij}(x))$ *is the inverse of the matrix* $(g_{ij}(x))$.

Write the explicit expression of the laplacian $\triangle$ *associated to the metric* g *(you may restrict yourself to* $d = 1$ *!).*

Choose a quantization procedure $\mathrm{Op}_\hbar = \mathrm{Op}_\hbar^W, \mathrm{Op}_\hbar^L$ *or* $\mathrm{Op}_\hbar^R$.

Show that

$$\mathrm{Op}_\hbar(H) = -\frac{1}{2}\hbar^2 \triangle + \hbar \left[\sum_{j=1}^{d} b_j(x) \frac{\hbar}{i} \frac{\partial}{\partial x_j} + c(x)\right]$$

for certain functions b_j, c*, the expression of which depends on your choice of* $\mathrm{Op}_\hbar$.

Show that there is a function d *such that*

$$-\frac{1}{2}\hbar^2 \triangle = \mathrm{Op}_\hbar\left(H(x,\xi) + \hbar\left(\sum_j b_j(x)\xi_j + c(x)\right) + \hbar^2 d(x)\right). \qquad (1.28)$$

Compare with (1.27) *to find the order and the degree of* $-\hbar^2\triangle$ *(of course, differential operators are pseudodifferential operators !).*

The expression of $b_j, c, d,$ *does depend on the choice of* $\mathrm{Op}_\hbar$*. The first term* $H(x,\xi)$ *does not, it is called the principal symbol of* $-\frac{1}{2}\hbar^2\triangle$*.*

Principal symbol. Let $a_\hbar \in \Sigma_o^{m,0}(\Omega\times\Omega\times\mathbb{R}^d)$. Applying the operator $A_\hbar = \mathrm{OP}_\hbar(a_\hbar) \in \Psi\mathrm{DO}^{m,0}$ to a function of the form $u(x)e^{iS(x)/\hbar}$, where u and S are smooth[5], the method of stationary phase gives the following asymptotics :

$$A_\hbar\left(u(x)e^{iS(x)/\hbar}\right) = a_0\left(x, x, S'(x)\right)\, u(x)e^{iS(x)/\hbar} + O(\hbar).$$

This shows that the function $a_0(x,x,\xi)$ on $\mathbb{R}^d\times\mathbb{R}^d = T^*\mathbb{R}^d$ does not depend on the choice of the symbol $a_\hbar(x,y,\xi)$, but only on the operator $A_\hbar$. It is called the principal symbol of $A_\hbar$, denoted $\sigma^0(A_\hbar)$. If $\sigma^0(A_\hbar)=0$, then $A_\hbar$ actually belongs to $\Psi\mathrm{DO}^{m-1,1}$ (and conversely).

Remark 1.4. *For* $a\in\Sigma_o^{m,0}$*, we note that* $\mathrm{Op}_\hbar^W(a)$*,* $\mathrm{Op}_\hbar^L(a)$*,* $\mathrm{Op}_\hbar^R(a)$ *all have the same principal symbol* $a_0(x,\xi)$*. In other words,*

$$\mathrm{Op}_\hbar^W(a) - \mathrm{Op}_\hbar^{R/L}(a) \in \Psi\mathrm{DO}^{m-1,+1}.$$

Continuity. Trace class and Hilbert-Schmidt operators. An operator in $\Psi\mathrm{DO}^{0,0}(\Omega)$ is bounded from $L^2(\Omega)$ to $L^2_{loc}(\Omega)$, uniformly with respect to $\hbar$.

An operator in $\Psi\mathrm{DO}^{m,0}(\Omega)$, where Ω is, as before, an open subset of $\mathbb{R}^d$, is

- trace class if $m<-d$
- Hilbert-Schmidt if $m<-d/2$

In this case, the trace of $OP(a)$ is given by the convergent integral,

$$\mathrm{Tr}\,\mathrm{OP}(a) = (2\pi\hbar)^{-d}\int_{\Omega\times\mathbb{R}^d} a(x,x,\xi)\mathrm{d}x\mathrm{d}\xi\ . \tag{1.29}$$

(This is the integral of the kernel of $OP(a)$ on the diagonal.)

Product. If $A_\hbar\in\Psi\mathrm{DO}^{m_1,0}$ and $B_\hbar\in\Psi\mathrm{DO}^{m_2,0}$, then the product $A_\hbar B_\hbar$ belongs to $\Psi\mathrm{DO}_o^{m_1+m_2-1,1}$, and the principal symbols are multiplied : $\sigma^0(A_\hbar B_\hbar) = \sigma^0(A_\hbar)\sigma^0(B_\hbar)$.

An equivalent statement : if $a\in\Sigma_o^{m_1,0}(\mathbb{R}^d\times\mathbb{R}^d)$ and $b\in\Sigma_o^{m_2,0}(\mathbb{R}^d\times\mathbb{R}^d)$, then $\mathrm{Op}_\hbar(a)\,\mathrm{Op}_\hbar(b)\in\Psi\mathrm{DO}^{m_1+m_2,0}(\mathbb{R}^d)$, and

$$\mathrm{Op}_\hbar(ab) - \mathrm{Op}_\hbar(a)\,\mathrm{Op}_\hbar(b) \in \Psi\mathrm{DO}^{m_1+m_2-1,1}(\mathbb{R}^d). \tag{1.30}$$

[5]Such a function is called a WKB state, see Chapter 4

(thanks to Remark 1.4, this statement does not depend on the choice of Op^W, Op^L or Op^R).

Brackets. If $A_\hbar \in \Psi\mathrm{DO}^{m_1,0}$ and $B_\hbar \in \Psi\mathrm{DO}^{m_2,0}$, then the bracket $[A_\hbar, B_\hbar]$ belongs to $\Psi\mathrm{DO}^{m_1+m_2-1,1}$, and

$$\sigma^0\left(\hbar^{-1}[A_\hbar, B_\hbar]\right) = \frac{1}{i}\left\{\sigma^0(A_\hbar), \sigma^0(B_\hbar)\right\};$$

where $\{.,.\}$ is the Poisson bracket.

Equivalently : if $a \in \Sigma_o^{m_1,0}(\mathbb{R}^d \times \mathbb{R}^d)$ and $b \in \Sigma_o^{m_2,0}(\mathbb{R}^d \times \mathbb{R}^d)$, we have

$$[\mathrm{Op}_\hbar(a), \mathrm{Op}_\hbar(b)] - \mathrm{Op}_\hbar\left(\frac{\hbar}{i}\{a,b\}\right) \in \Psi\mathrm{DO}^{m_1+m_2-2,2} \tag{1.31}$$

and again this statement does not depend on the choice of Op^W, Op^L or Op^R.

Remark 1.5. *There is also an integrated version of this result, called the Egorov Theorem. We will use it in the following form : assume the pseudodifferential operator $A_\hbar$ is self–adjoint. Define the Schrödinger flow $(U_\hbar^t) = (\exp -\frac{it}{\hbar}A_\hbar)$.*

Let $a \in C_c^\infty(T^*\mathbb{R}^d)$. Then, for any given t in $\mathbb{R}$,

$$\|U_\hbar^{-t}\,\mathrm{Op}_\hbar(a)U_\hbar^t - \mathrm{Op}_\hbar(a \circ \phi^t_{\sigma^0(A_\hbar)})\|_{L^2} = \mathcal{O}(\hbar), \qquad \hbar \to 0. \tag{1.32}$$

Here $\phi^t_{\sigma^0(A_\hbar)}$ is the Hamiltonian flow defined by the Hamiltonian $\sigma^0(A_\hbar)$.

Pseudodifferential operators on a compact manifold. Let X be a compact C^∞ manifold of dimension d. Let (Ω_i, φ_i) be a finite atlas of X ($X = \cup\Omega_i$, $\varphi_i : \Omega_i \longrightarrow \mathbb{R}^d$). Use the φ_i to define local coordinates $\Phi_i : T^*\Omega_i \longrightarrow \mathbb{R}^d \times \mathbb{R}^d$ on T^*X as follows :

$$\Phi_i(x,p) = (\varphi_i(x), (d\varphi_i(x))^{-1}p).$$

Check that these are symplectic coordinates on T^*X. Introduce a finite partition of unity $\chi_i \in C_o^\infty(\Omega_i)$ such that $\sum \chi_j^2 = 1$. For $a \in \Sigma_o^{m,l}(T^*X)$, we let :

$$\mathrm{Op}_\hbar(a)u = \sum_i \chi_i \left[\mathrm{OP}_\hbar\left(a \circ \Phi_i\right)\left(\chi_i u \circ \varphi_i^{-1}\right)\right] \circ \varphi_i\ . \tag{1.33}$$

The map $a \mapsto \mathrm{Op}_\hbar(a)$ thus defined depends on the partition of unity and of the local coordinates; but its range does not, modulo negligible operators. The algebra $\Psi\mathrm{DO}^{m,l}(X)$ of pseudodifferential operators on X (modulo negligible operators) is thus well defined.

All the properties stated above can be extended to this case.

1.5 Semiclassical measures, microlocal lifts.

A quantization procedure Op is said to be *nonnegative* if $\mathrm{Op}(a)$ is a nonnegative operator as soon as a is a nonnegative function. The usual quantization procedures do not have this property.

Positive quantization on $\mathbb{R}^d$.

Example 1.6. *(Coherent states) The coherent state (of size $\hbar$) centered at (x_0, ξ_0) is defined as the normalized gaussian state*

$$e_{x_0,\xi_0}(x) = \frac{1}{(\pi\hbar)^{d/4}} e^{\frac{i}{\hbar}\xi_0 . x} \exp\left(-\frac{\|x - x_0\|^2}{2\hbar}\right)$$

For $(x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d$, we shall denote $\Pi_{(x,\xi)}$ the orthogonal projector on $\mathbb{C}e_{(x,\xi)}$.

Theorem 1.7. *Let $a \in C_o^\infty(T^*\mathbb{R}^d)$. The operator defined by*

$$\mathrm{Op}^+(a) = (2\pi\hbar)^{-d} \int a(x, \xi)\, \Pi_{x,\xi}\, \mathrm{d}x\mathrm{d}\xi$$

belongs to the class $\Psi\mathrm{DO}^{-\infty,0}$, it is self–adjoint (resp. nonnegative) if a is real valued (resp. nonnegative). Its principal symbol is $a(x, \xi)$.

We have $\mathrm{Op}^+(1) = I$, which allows to extend the definition of Op^+ to the case when a is constant in a neighbourhood of infinity in T^*X.

This quantization is called the anti–Wick quantization.

To define a positive quantization procedure on a compact manifold X, we choose an atlas of X and a subordinate partition of unity, $\sum \chi_j^2 = 1$. For $a \in C_o^\infty(T^*X)$, we let $\mathrm{Op}_X^+(a) = \sum_j \chi_j \mathrm{Op}_{\mathbb{R}^d}^+(a)\chi_j$ — where $\mathrm{Op}_{\mathbb{R}^d}^+(a)$ is defined using local coordinates in the support of χ_j (see (1.33)). We can extend this definition to the case when a is constant in a neighbourhood of infinity in T^*X, by letting $\mathrm{Op}_X^+(1) = \mathrm{I}$.

Semiclassical measures. Let X be a compact riemannian manifold; we denote Vol the riemannian volume on X. To a family $(u_\hbar)$ of normalized elements of $L^2(X, \mathrm{Vol})$, we can associate the family of distributions $\mu_\hbar$ by the formula $\mu_\hbar(a) = \left\langle u_\hbar, \mathrm{Op}_\hbar^+(a)u_\hbar\right\rangle_{L^2(X,\mathrm{Vol})}$. They are in fact probability measures on T^*X. To be able to take weak limits when $\hbar \longrightarrow 0$, we see them as probability measures on the compactification $\overline{T^*X}$ of T^*X obtained by adding a sphere bundle a infinity. By convention, we will call the measures $\mu_\hbar$ the *Husimi measures*, associated to the family $(u_\hbar)$. The term *Wigner transform* will be exclusively used in the case $X = \mathbb{R}^d$, for the distributions $a \mapsto \left\langle u_\hbar, \mathrm{Op}_\hbar^W(a)u_\hbar\right\rangle$ defined thanks to the Weyl quantization. These distributions are also called *microlocal lifts* of the probability measures $|u_\hbar(x)|^2 d\mathrm{Vol}(x)$. This means that they project down to X to $|u_\hbar(x)|^2 d\mathrm{Vol}(x) + O(\hbar)$, but also contain information about the local frequency vector (Fourier transform) of $u_\hbar$.

Due to the uncertainty principle, these objects are not really meaningful for fixed $\hbar > 0$. In fact, their definition depends on a certain number of arbitrary choices, coming into play in the definition of Op : local coordinates, partition of unity, choice of the quantization procedure... However, the semiclassical limits of these distributions do not depend on all these arbitrary conventions. All of them give an operator $\mathrm{Op}(a)$ with principal symbol $a(x, \xi)$. In particular, if $a \in \Sigma_o^{0,0}(T^*X)$, two definitions of $\mathrm{Op}(a)$ only differ of $O(\hbar)$ in L^2 operator norm.

We shall call *semiclassical measure* associated to the family $(u_\hbar)$ any limit point of the sequence $(\mu_\hbar)$ in the weak topology.

Example 1.8. *(Coherent states)*

$$u_\hbar(x) = e_{x_0,\xi_0}(x) = \frac{1}{(\pi\hbar)^{d/4}} e^{\frac{i}{\hbar}\xi_0.x} \exp\left(-\frac{\|x - x_0\|^2}{2\hbar}\right)$$

Then there is a unique semiclassical measure, the Dirac mass at (x_0, ξ_0).

Example 1.9. *(Lagrangian states/WKB states) Let $u_\hbar(x) = b(x)e^{\frac{i}{\hbar}S(x)}$ where b and S are of class C^∞. In Chapter 4, we will call such functions* lagrangian states *associated to the lagrangian manifold $\mathcal{L} = \{(x, dS(x))\}$.*

There is a unique semiclassical measure associated to $(u_\hbar)$, it is carried by the lagrangian $\mathcal{L}$ and projects to X as the measure $|b(x)|^2\, d\mathrm{Vol}(x)$.

Exercise 1.10. *You have noted that we often omit to indicate the dependence on $\hbar$ in the definition of* Op *(which should be denoted* $\mathrm{Op}_\hbar$*). The choice of scaling is, nevertheless, very important, and the properties observed vary a lot according to the scaling.*

In the previous example, show that the measures defined by

$$\mu_{\hbar,\alpha}(a) = \langle u_\hbar, \mathrm{Op}^+_{\hbar^\alpha}(a)u_\hbar\rangle$$

concentrate to the 0-section in T^*X if $\alpha > 1$, to the sphere bundle at infinity $\overline{T^*X} \setminus T^*X$ if $\alpha < 1$.

When the $u_\hbar$ are the eigenfunctions of a hamiltonian operator as in (1.19), one can apply the following theorem :

Theorem 1.11. *Let P be a self–adjoint pseudodifferential operator, denote p_0 its principal symbol. Let $(u_\hbar)$ be a family of tamed[6] smooth functions, such that $Pu_\hbar = O(\hbar^\infty)$ and $\|u_\hbar\|_{L^2} = 1$. Let $\mu_\hbar$ be the Husimi measures associated to $(u_\hbar)$. Then, every weak limit μ_0 of the measures $\mu_\hbar$ on $\overline{T^*X}$*

[6] meaning that, for all $N \in \mathbb{N}$, for any compact K, there exists $k \in \mathbb{N}$ such that the C^N norm of $u_\hbar$ on K is $O(\hbar^{-k})$

1. *is a probability measure on* $\overline{T^*X}$*.*

2. *projects on* X *to a weak limit of the measures* $|u_\hbar(x)|^2 d\mathrm{Vol}(x)$*.*

3. *is invariant under the hamiltonian flow of* p_0*.*

4. *its restriction to* T^*X *is carried by the energy level* $\{p_0 = 0\}$*.*

5. *If* p_0 *is elliptic at infinity, then* μ_0 *is carried by* T^*X*.*

The first two items have already been proven.

Exercise 1.12. *Prove the third item by using the relation* $\sigma^0\left(\hbar^{-1}[P, \mathrm{Op}(a)]\right) = -i\{p_0, a\}$ *to show that* $\int \{p_0, a\} d\mu_0 = 0$ *for any* $a \in C_o^\infty(T^*X)$*.*

Prove the fourth item by using the relation $\sigma^0\left(\mathrm{Op}(a)P\right) = a\, p_0$ *to show that* $\int a\, p_0\, d\mu_0 = 0$ *for any* $a \in C_o^\infty(T^*X)$*.*

We do not give here the precise definition of "elliptic at infinity". It implies that P is invertible in a neighbourhood of infinity in the class of pseudodifferential operators. More precisely, there exists a smooth a, taking the constant value 1 in a neighbourhood of infinity in T^*X, and a pseudodifferential operator $\mathrm{Op}(b)$ such that

$$\mathrm{Op}(a) = \mathrm{Op}(b)P + R$$

where $R \in \Psi\mathrm{DO}^{-\infty,\infty}$ is a negligible operator. From this fact, the last item follows easily. The ellipticity criterion is satisfied by the Schrödinger operator $-\frac{\hbar^2 \triangle}{2} + V$ on a compact manifold X.

Eigenfunctions of the laplacian. Let (X, g) be a riemannian manifold, and $\triangle$ the laplacian on X associated to the metric. If $(-\hbar^2\triangle - 1)u_\hbar = 0$, and if we denote $\mu_\hbar$ the corresponding Husimi measures, then every limit point of the family $(\mu_\hbar)_{\hbar \longrightarrow 0}$ is a probability measure μ_0 carried by the unit cotangent bundle S^*X, invariant under the geodesic flow (apply Theorem 1.11 and remember Exercise 1.3). It is a widely open problem to find all the possible limits among the invariant measure on S^*X.

In the case of the round sphere or a flat torus, it is easy to construct families of eigenfunctions $(u_\hbar)$ for which $\mu_\hbar$ converges to the uniform measure on any given invariant lagrangian torus. On the flat torus $\mathbb{T}^d = \mathbb{R}^d/\mathbb{Z}^d$ for instance, the family $(e^{\frac{i}{\hbar}\xi_0 . x})$, where ξ_0 is a unitary vector (and of course $\frac{\xi_0}{\hbar} \in 2\pi\mathbb{Z}^d$), has a unique semiclassical measure, the uniform measure on the lagrangian torus $\{(x, \xi_0), x \in \mathbb{T}^d\}$. More generally, for a completely integrable system, one can use WKB methods [Brill26, Kr26, Wtz26, Kell58, Masl65] to build quasimodes, in other words solutions of $\|(-\hbar^2 \triangle - 1)u_\hbar\| = O(\hbar^\infty)$, the Husimi measures of which concentrate to any given invariant torus[7]. Historically, the case of completely integrable systems, or perturbations thereof,

[7]Note that $\|(-\hbar^2 \triangle - 1)u_\hbar\| \leq \varepsilon \|u_\hbar\|$ implies that 1 is an ε–neighbourhood of the spectrum of $-\hbar^2\triangle$, but does not imply that $u_\hbar$ is close to an eigenfunction of the laplacian.

was the most important, since it is related to the study of small atoms and ions. The "opposite" case of chaotic systems has been studied only more recently [Berr77, Vor77, Bo91], but the question of the localization of stationary motions in ergodic systems was already asked explicitly by Einstein [Ein17].

In these notes, we shall focus on the case where the geodesic flow has a very chaotic behaviour. When the geodesic flow is ergodic, the semiclassical measures are essentially described by the Snirelman theorem [Sn74, Ze87, CdV85] (see Chapter 2). Let X be a compact riemannian manifold; call $0 < \lambda_1 \leq \lambda_2 \leq \cdots$ the eigenvalues of the laplacian, and let (ψ_j) be an orthonormal basis of eigenfunctions : $-\triangle\,\psi_j = \lambda_j \psi_j$. Denote μ_j the corresponding Husimi measures (the semiclassical parameter is $\hbar = \lambda_j^{-1/2}$). We shall call L_E the desintegration of the Liouville measure $\mathrm{d}x\,\mathrm{d}\xi$ with respect to the value E of the hamiltonian $\frac{\|\xi\|^2}{2}$. We normalize L_E to be a probability measure on the energy layer $\{\frac{\|\xi\|^2}{2} = E\}$. If the geodesic flow on S^*X is ergodic with respect to $L_{\frac{1}{2}}$, then there is a "density 1" subsequence of te family (μ_j) converging to $L_{\frac{1}{2}}$:

Theorem 1.13 (Snirelman theorem)**.** *[Sn74, Ze87, CdV85] Assume that the action of S^*X is ergodic, with respect to the Liouville measure $L_{\frac{1}{2}}$. Then, there exists a subset $\mathcal{S} \subset \mathbb{N}$ of density 1, such that*

$$\mu_j \underset{j \longrightarrow +\infty, j \in \mathcal{S}}{\longrightarrow} L_{\frac{1}{2}}.$$

In specific examples, what we would like to know is whether the whole sequence μ_j converges to the Liouville measure, or if there can be exceptional subsequences converging to other invariant measures. In the case of nonpositively curved surfaces with flat cylinders, it is believed that certain sequences of eigenfunctions concentrate asymptotically on these cylinders. But in (strictly) negative curvature, it was conjectured by Rudnick and Sarnak [RudSa94] that the Liouville measure is the unique limit point of the μ_js. It would imply, in particular, that the sequence of probability measures $|\psi_j(x)|^2 d\mathrm{Vol}(x)$ on X converges weakly to the riemannian volume measure Vol.

Chapter 2

Entropy and localization of eigenfunctions.

2.1 Motivations

The field of *quantum chaos* tries to understand how the chaotic behaviour of a classical Hamiltonian system affects its quantum counterpart. For instance, let X be a compact Riemannian C^∞ manifold, with negative sectional curvatures. The geodesic flow has the Anosov property, which is considered as the ideal chaotic behaviour in the theory of dynamical systems. The corresponding quantum dynamics is the unitary flow generated by the Laplace-Beltrami operator on $L^2(X)$. One expects that the chaotic properties of the geodesic flow influence the spectral theory of the Laplacian. The Random Matrix conjecture [Bo91] asserts that the large eigenvalues should, after proper renormalization, statistically resemble those of a large random matrix, at least for a generic Anosov metric. The Quantum Unique Ergodicity conjecture [RudSa94] (see also [Berr77, Vor77]) deals with the corresponding eigenfunctions ψ: it claims that the probability density $|\psi(x)|^2 dx$ should approach (in a weak sense) the Riemannian volume, when the eigenvalue tends to infinity. In fact a stronger property should hold for the microlocal lift of this measure to the cotangent bundle T^*X, which describes the distribution of the wave function ψ on the classical phase space (position and momentum).

To describe the problem, we will adopt a semiclassical point of view, that is, consider the eigenstates of eigenvalue unity of the semiclassical Laplacian $-\hbar^2\triangle$, in the semiclassical limit $\hbar \to 0$. We denote by $(\psi_k)_{k\in\mathbb{N}}$ an orthonormal basis of $L^2(X)$ made of eigenfunctions of the Laplacian, and by $(-\frac{1}{\hbar_k^2})_{k\in\mathbb{N}}$ the corresponding eigenvalues:

$$-\hbar_k^2\,\triangle\psi_k = \psi_k, \quad \text{with} \quad \hbar_{k+1} \leq \hbar_k\,. \tag{2.1}$$

We are interested in the high-energy eigenfunctions of $-\triangle$, in other words the semiclassical limit $\hbar_k \to 0$.

To an eigenfunction ψ_k corresponds a distribution on T^*X defined by

$$\mu_k(a) = \langle \psi_k, \mathrm{Op}_{\hbar_k}(a)\psi_k \rangle_{L^2(X)}, \qquad a \in C_o^\infty(T^*X)\,.$$

Here $\mathrm{Op}_{\hbar_k}$ is a quantization procedure, set at the scale $\hbar_k$, which associates a bounded operator on $L^2(X)$ to any smooth phase space function a with nice behaviour at infinity. If a is a function on the manifold X, we have $\mu_k(a) = \int_X a(x)|\psi_k(x)|^2 dx + O(\hbar)$: the distribution μ_k is a *microlocal lift* of the probability measure $|\psi_k(x)|^2 dx$ into a phase space distribution. This means that it contains the information about the frequency vector of ψ_k (in other words, the momentum), in addition to the position distribution $|\psi_k(x)|^2 dx$. The definition of μ_k is not canonical, it depends on a certain number of choices, like the choice of local coordinates, or of the quantization procedure (Weyl, anti-Wick, "right" or "left" quantization...); this somehow reflects the fact that, for $\hbar > 0$, it does not really make sense to study simultaneously the position and frequency of the wave. Mathematically speaking, one cannot study at the same time the local property of a function and of its Fourier transform around some point $(x, \xi) \in T^*X$. But the asymptotic behaviour of μ_k when $\hbar_k \longrightarrow 0$ does not depend on the arbitrary conventions involved in its definition. We saw that it is possible to construct $\mathrm{Op}^+_{\hbar_k}$ so that the μ_k are probability measures, in which case we call them *Husimi measures* associated to the eigenfunctions ψ_k. We call *semiclassical measures* the limit points of the sequence $(\mu_k)_{k\in\mathbb{N}}$, in the distribution topology.

The quantum hamiltonian $-\frac{\hbar^2\triangle}{2}$ generates the Schrödinger flow $(U^t_\hbar) = (\exp(it\hbar\frac{\triangle}{2}))$ acting unitarily on $L^2(X)$. A solution of (2.1) is an invariant state of the flow $(U^t_\hbar)$, corresponding to the energy $\frac{1}{2}$ of the hamiltonian. In the semiclassical limit $\hbar \longrightarrow 0$, "quantum mechanics converges to classical mechanics". We will denote $|\cdot|_x$ the norm on $T^*_x M$ given by the metric. The geodesic flow $(g^t)_{t\in\mathbb{R}}$ is the Hamiltonian flow on T^*X generated by the Hamiltonian $H(x, \xi) = \frac{|\xi|_x^2}{2}$. In the previous chapter we saw :

Proposition 2.1. *Any semiclassical measure is a probability measure carried on the energy layer $S^*X = H^{-1}(\frac{1}{2})$. This measure is invariant under the geodesic flow.*

If the geodesic flow has the Anosov property — for instance if X has negative sectional curvature — then there exist many invariant probability measures on S^*X, in addition to the Liouville measure. The geodesic flow has countably many periodic orbits, each of them carrying an invariant probability measure. There are still many others, like the equilibrium states obtained by variational principles [KH].

For manifolds with an ergodic geodesic flow (with respect to the Liouville measure), it has been known for some time that *almost all* eigenfunctions become uniformly distributed over S^*X, in the semiclassical limit. This property is dubbed as Quantum Ergodicity :

Theorem 2.2. *[Sn74, Ze87, CdV85] Let X be a compact Riemannian manifold, assume that the action of the geodesic flow on S^*X is ergodic with respect to the Liouville measure $L_{\frac{1}{2}}$. Let $(\psi_k)_{k\in\mathbb{N}}$ be an orthonormal basis of $L^2(X)$ consisting of eigenfunctions of the Laplacian (2.1), and let (μ_k) be the associated distributions on T^*X.*

Then, there exists a subset $\mathcal{S} \subset \mathbb{N}$ of density 1, such that

$$\mu_k \underset{k\longrightarrow\infty, k\in\mathcal{S}}{\longrightarrow} L_{\frac{1}{2}}.$$

Proof: Let us recall the main lines of the argument, and see where the ergodicity comes into play. For all $a \in C_o^\infty(T^*X)$, one first shows, without using any assumption on the dynamics, that

$$\sum_{j,\,\lambda_j\leq E} \int a\, d\mu_j \underset{E\longrightarrow+\infty}{\sim} \frac{b_d}{(2\pi)^d} Vol(X) \int_{S^*X} a\, dL_{\frac{1}{2}} \times E^{d/2}. \tag{2.2}$$

The constant b_d is the volume of the euclidean d-dimensional ball. The idea is to express in two different ways the trace of $\mathrm{Op}_{\sqrt{E}}(a)$: the trace can be expressed either as a spectral sum $\sum_k \langle \mathrm{Op}(a)\psi_k, \psi_k\rangle$ or as the integral of the kernel on the diagonal (1.29). There are some technical details we skip here

From (2.2) one can deduce the Weyl asymptotics :

$$N(E) = \sharp\{j, \lambda_j \leq E\} \sim \frac{b_d}{(2\pi)^d} Vol(X)\, E^{d/2}$$

Thus, we have a Cesaro convergence :

$$\frac{1}{N(E)} \sum_{j,\,\lambda_j\leq E} \int a\, d\mu_j \underset{E\longrightarrow+\infty}{\longrightarrow} \int_{S^*X} a\, dL_{\frac{1}{2}}.$$

Using the ergodicity assumption, one can do better :

$$\frac{1}{N(E)} \sum_{j,\,\lambda_j\leq E} \left| \int a\, d\mu_j - \int_{S^*X} a\, dL_{\frac{1}{2}} \right|^2 \underset{E\longrightarrow+\infty}{\longrightarrow} 0. \tag{2.3}$$

We know from Theorem 1.11 (3.) that $|\int a\, d\mu_j - \int a \circ g^t\, d\mu_j| \longrightarrow 0$ as $j \longrightarrow +\infty$, for any fixed t. Thus, we can write, for any given T,

$$\begin{aligned}
&\limsup_{E\longrightarrow\infty} \frac{1}{N(E)} \sum_{j,\,\lambda_j\leq E} \left| \int a\, d\mu_j - \int_{S^*X} a\, dL_{\frac{1}{2}} \right|^2 \\
&\qquad = \limsup \frac{1}{N(E)} \sum_{j,\,\lambda_j\leq E} \left| \int M^T a\, d\mu_j - \int_{S^*X} a\, dL_{\frac{1}{2}} \right|^2 \\
&\qquad \leq \limsup \frac{1}{N(E)} \sum_{j,\,\lambda_j\leq E} \mu_j \left((M^T a - \int_{S^*X} a\, dL_{\frac{1}{2}})^2 \right) \\
&\qquad\qquad\qquad = L_{\frac{1}{2}} \left((M^T a - \int_{S^*X} a dL_{\frac{1}{2}})^2 \right).
\end{aligned}$$

We denoted $M^T a = T^{-1}\int_0^T a \circ g^t dt$ the time average of a on the interval $[0, T]$. We used the Cauchy-Schwartz inequality, which requires to know that the μ_j can be assumed to be *probability* measures (see §1.5. This was the missing argument in Snirelman's original paper). In the last line, we used the Cesaro convergence of the sequence (μ_j). Letting at the end T tend to $+\infty$, the ergodicity assumption means that

$$L_{\frac{1}{2}}\left((M^T a - \int_{S^*X} a\, dL_{\frac{1}{2}})^2\right) \underset{T\to\infty}{\longrightarrow} 0;$$

which proves (2.3).

Finally, the Snirelman theorem results from the classical lemma :

Lemma 2.3. *Let (a_n) be a sequence of nonnegative numbers. If*

$$\frac{1}{n}\sum_{k=0}^{n} a_k \longrightarrow 0$$

then there exists $\mathcal{S} \subset \mathbb{N}$ of density 1 such that $a_n \underset{n\in\mathcal{S}}{\longrightarrow} 0$.

□

Remark 2.4. *The result was subsequently extended to more general hamiltonians [HelMR87], to ergodic billiards [GL93, ZeZw96]; and to certain discrete time symplectic dynamical systems.*

The question of knowing, in particular cases, if there can exist "exceptional" subsequences with a different behaviour is widely open. On a negatively curved manifold, the geodesic flow satisfies the ergodicity assumption, and in fact much stronger properties : mixing, K–property,... In this case, the Quantum Unique Ergodicity conjecture [RudSa94] expresses the belief that there exists a unique semiclassical measure, namely the Liouville measure on S^*X : the whole sequence (μ_k) converges to $L_{\frac{1}{2}}$. In other words, in the semiclassical régime all eigenfunctions should become uniformly distributed over S^*X.

So far the most precise results on this question were obtained for manifolds X with constant negative curvature and *arithmetic* properties: see Rudnick–Sarnak [RudSa94], Wolpert [Wol01]. In that very particular situation, there exists a countable commutative family of self–adjoint operators commuting with the Laplacian : the Hecke operators. One may thus decide to restrict the attention to common bases of eigenfunctions, often called "arithmetic" eigenstates, or Hecke eigenstates. A few years ago, Lindenstrauss [Li06] proved that the arithmetic eigenstates become asymptotically equidistributed (Arithmetic Quantum Unique Ergodicity). If there is some degeneracy in the spectrum of the Laplacian, it could be possible that the Quantum Unique Ergodicity conjectured by Rudnick and Sarnak holds for one orthonormal basis but not for another. In the arithmetic case, it is believed that the spectrum of the Laplacian has bounded multiplicity, in which case it would be a harmless assumption to consider only Hecke eigenstates.

Nevertheless, one may be less optimistic about the general conjecture. Faure–Nonnenmacher–De Bièvre exhibited in [FNDB03] a simple example of a symplectic Anosov dynamical system, namely the action of the linear hyperbolic automorphism $\begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}$ on the 2-torus, the Weyl–quantization of which does not satisfy the Quantum Unique Ergodicity conjecture. In this model, it is known [KurRud00] that there is one orthonormal family of eigenfunctions satisfying Quantum Unique Ergodicity, but, due to high degeneracies in the spectrum, one can also construct eigenfunctions with a different behaviour. Precisely, [FNDB03] construct a family of eigenstates for which the semiclassical measure consists in two ergodic components: half of it is the Liouville measure, while the other half is a Dirac peak on a single unstable periodic orbit. It was also shown that this half-localization on a periodic orbit is *maximal* for this model [FN04] : a semiclassical measure cannot have more than half the mass carried by a finite union of closed orbits. Another type of semiclassical measure was recently obtained by Kelmer for a quantized automorphism on a higher-dimensional torus [Kelm05]: it consists in the Lebesgue measure on some invariant co-isotropic subspace of the torus. For these torus automorphisms, the existence of exceptional eigenstates is due to some nongeneric algebraic properties of the classical and quantized systems.

2.2 Main result.

We wish to consider the *Kolmogorov–Sinai* entropy of semiclassical measures. We work on a compact manifold X of arbitrary dimension, and assume that the geodesic flow has the Anosov property. In fact, our method is very general, and can without doubt be adapted to more general Anosov Hamiltonian systems.

The Kolmogorov–Sinai entropy, also called metric entropy, of a (g^t)-invariant probability measure μ is a nonnegative number $h_{KS}(\mu)$ that describes, in some sense, the complexity of a μ-typical orbit of the flow. The precise definition will be given later, but for the moment let us just give a few facts. A measure carried on a closed geodesic has zero entropy. In constant curvature, the entropy is known to be maximal for the Liouville measure. More generally, an upper bound on the entropy is given by the Ruelle inequality: since the geodesic flow has the Anosov property, the energy layer S^*X is foliated into unstable manifolds of the flow, and for any invariant probability measure μ one has

$$h_{KS}(\mu) \leq \left| \int_{S^*X} \log J^u(\rho) d\mu(\rho) \right| . \tag{2.4}$$

In this inequality, $J^u(\rho)$ is the *unstable Jacobian* of the flow at the point $\rho \in S^*X$, defined as the Jacobian of the map g^{-1} restricted to the unstable manifold at the point $g^1\rho$ (the average of $\log J^u$ over any invariant measure is negative). In fact, if μ is an invariant probability measure,

$$\int_{S^*X} \log J^u(\rho) d\mu(\rho) = -\int_{S^*X} \sum \lambda_j^+(\rho) d\mu(\rho)$$

where $\lambda_j^+(\rho)$ are the positive Lyapunov exponents of ρ. If X has dimension d and has constant sectional curvature -1, (2.4) just reads $h_{KS}(\mu) \leq d-1$. Besides, equality holds in (2.4) if and only if μ is the Liouville measure on S^*X [LY85].

Let μ be a (g^t)–invariant probability measure on S^*X. According to the Birkhoff ergodic theorem, for μ–almost every $\rho \in S^*X$, the weak limit

$$\mu^\rho = \lim_{|t| \longrightarrow \infty} \frac{1}{t} \int_0^t \delta_{g^s\rho} ds$$

exists, and is an ergodic probability measure. We can then write

$$\mu = \int_{S^*X} \mu^\rho d\mu(\rho),$$

which is called the ergodic decomposition of μ. Note that the ergodic probability measures are the extremal points of the compact convex set of (g^t)–invariant probability measures.

To understand the connection of our results with the previous discussion, it is important to know that the entropy if an *affine* functional on the convex set of (g^t)–invariant probability measures. In fact, we have

$$h_{KS}(\mu) = \int_{S^*X} h_{KS}(\mu^\rho) d\mu(\rho).$$

In what follows, we consider a certain subsequence of eigenstates $(\psi_{k_j})_{j\in\mathbb{N}}$ of the Laplacian, such that the corresponding sequence (μ_{k_j}) converges to a certain semiclassical measure μ (see the discussion preceding Proposition 2.1). The subsequence (ψ_{k_j}) will simply be denoted by $(\psi_\hbar)_{\hbar\to 0}$, using the slightly abusive notation $\psi_\hbar = \psi_{\hbar_{k_j}}$ for the eigenstate ψ_{k_j}. Each state $\psi_\hbar$ satisfies

$$(-\hbar^2 \triangle -1)\psi_\hbar = 0 . \tag{2.5}$$

Ii is proved in [A05] that the entropy of any semiclassical measure associated with eigenfunctions of the laplacian is strictly positive. In [AN07] more explicit lower bounds were obtained. We shall prove here the following lower bound :

Theorem 2.5. *Let μ be a semiclassical measure associated to the eigenfunctions of the Laplacian on X. Then its metric entropy satisfies*

$$h_{KS}(\mu) \geq \left| \int_{S^*X} \log J^u(\rho) d\mu(\rho) \right| - \frac{(d-1)}{2} \lambda_{\max} \,, \tag{2.6}$$

where $d = \dim M$ and $\lambda_{\max} = \lim_{t \to \pm\infty} \frac{1}{t} \log \sup_{\rho \in S^*X} |dg^t_\rho|$ is the maximal expansion rate of the geodesic flow on S^*X.

In particular, if X has constant sectional curvature -1, this means that

$$h_{KS}(\mu) \geq \frac{d-1}{2}. \tag{2.7}$$

The bound (2.7) in the above theorem is much sharper than the bound proved in [A05] in the case of constant curvature. On the other hand, if the curvature varies a lot (still being negative everywhere), the right hand side of (2.6) may be negative, in which case the above bound is trivial and the result of [A05] is better. We believe this to be but a technical shortcoming of our method, and would actually expect the following bound to hold:

$$h_{KS}(\mu) \geq \frac{1}{2} \left| \int_{S^*X} \log J^u(\rho) d\mu(\rho) \right| \,. \tag{2.8}$$

Our result is compatible with the kind of counter-examples obtained by Faure–Nonnenmacher–De Bièvre [FNDB03]. It allows certain ergodic components to be carried by closed geodesics, but says that others must have positive entropy. Compare with the much stronger result obtained in the arithmetic case by Bourgain and Lindenstrauss :

Theorem 2.6. *[BLi03] Let X be a congruence arithmetic surface, and (ψ_j) an orthonormal basis of eigenfunctions for the laplacian and the Hecke operators.*

Let μ be a corresponding semiclassical measure, with ergodic decomposition $\mu = \int_{S^*X} \mu^\rho d\mu(\rho)$, then for almost all ergodic components we have $h_{KS}(\mu^\rho) \geq \frac{1}{9}$.

Quantum Unique Ergodicity would mean that $h_{KS}(\mu) = \left| \int_{S^*X} \log J^u(\rho)\, d\mu(\rho) \right|$ [LY85]. We believe however that (2.8) is the optimal result that can be obtained without using more precise information, like for instance upper bounds on the multiplicities of eigenvalues. Indeed, in the above mentioned examples of Anosov systems where the Quantum Unique Ergodicity conjecture is wrong, the bound (2.8) is actually *sharp* [FNDB03, Kelm05, AN06]. In those examples, the spectrum has very high degeneracies, which allows for much freedom to select the eigenstates, and could be responsible for the failure of Quantum Unique Ergodicity. Such high degeneracies are not expected to happen in the case of the Laplacian on a negatively curved manifold. For the moment, however, there is no clear understanding of the precise relation between spectral degeneracies and failure of Quantum Unique Ergodicity.

2.3 Definition of entropy, and main idea of the proof.

Let μ be a probability measure on T^*X. Let $(P_1, \ldots, P_K)$ be a finite measurable partition of the unit tangent bundle : $T^*X = P_1 \sqcup ... \sqcup P_K$. The Shannon entropy of μ with respect to the partition P is

$$h_P(\mu) = -\sum_{k=1}^{K} \mu(P_k) \log \mu(P_k). \tag{2.9}$$

Assume now that μ is (g^t)–invariant. For any integer n, denote $P^{\vee n}$ the partition formed by the sets $P_{\alpha_0} \cap g^{-1}P_{\alpha_1} ... \cap g^{-n+1}P_{\alpha_{n-1}}$. Denote

$$\begin{aligned} &h_n(\mu, P) = h_{P^{\vee n}}(\mu) \\ &= -\sum_{(\alpha_j)\in\{1,\ldots,K\}^{\{0,\ldots,n-1\}}} \mu(P_{\alpha_0}\cap g^{-1}P_{\alpha_1}...\cap g^{-n+1}P_{\alpha_{n-1}}) \log \mu(P_{\alpha_0}\cap g^{-1}P_{\alpha_1}...\cap g^{-n+1}P_{\alpha_{n-1}}). \end{aligned} \tag{2.10}$$

If μ is (g^t)–invariant, it follows from the concavity of $x \mapsto -x \log x$ that

$$h_{n+m}(\mu, P) \leq h_n(\mu, P) + h_m(\mu, P), \tag{2.11}$$

in other words the sequence $(h_n(\mu, P))_{n\in\mathbb{N}}$ is subadditive. The entropy of μ with respect to the action of geodesic flow and to the partition P is defined by

$$h_{KS}(\mu, P) = \lim_{n\longrightarrow+\infty} \frac{h_n(\mu, P)}{n} = \inf_{n\in\mathbb{N}} \frac{h_n(\mu, P)}{n}. \tag{2.12}$$

Note that $\mu(P_{\alpha_0} \cap g^{-1}P_{\alpha_1} ... \cap g^{-n+1}P_{\alpha_{n-1}})$ measures the μ–probability to visit successively P_{α_0}, P_{α_1},..., $P_{\alpha_{n-1}}$ at times 1, 2,..., $n-1$ of the geodesic flow. Roughly speaking, the entropy measures the exponential decay of these probabilities when n gets large. It is easy to see that $h_{KS}(\mu, P) \geq \beta$ if there exists C such that $\mu(P_{\alpha_0} \cap g^{-1}P_{\alpha_1} ... \cap g^{-n}P_{\alpha_n}) \leq Ce^{-\beta n}$, for all n and all $\alpha_0, \ldots, \alpha_n$.

The entropy of μ with respect to the action of the geodesic flow is defined as

$$h_{KS}(\mu) = \sup_P h_{KS}(\mu, P), \tag{2.13}$$

the supremum running over all finite measurable partitions P. Assume μ is carried on the energy layer S^*X. Due to the Anosov property of the geodesic flow on S^*X, it is known that the supremum (2.13) is reached as soon as the maximum diameter of the sets $P_k \cap S^*X$ is small enough.

We will restrict our attention to partitions P which are actually partitions of the base X (lifted to T^*X) : $X = \sqcup_{k=1}^{K} P_k$. This choice is not crucial, but it simplifies certain aspects of the analysis.

The existence of the limit in (2.12), and the fact that it coincides with the inf follow from a standard subadditivity argument. A crucial consequence is that $h_{KS}(., P)$ has an upper semicontinuity property : if (μ_k) is a sequence of (g^t)–invariant probability measures converging weakly to μ, then

$$h_{KS}(\mu, P) \geq \limsup_k h_{KS}(\mu_k, P) \tag{2.14}$$

(provided μ does not charge the boundary of P). In particular : if (μ_k) converges weakly to μ, and if we have an estimate

$$\mu_k(P_{\alpha_0} \cap g^{-1}P_{\alpha_1} \ldots \cap g^{-n}P_{\alpha_n}) \leq C_k e^{-\beta n}$$

where β does not depend on k, we have $h_{KS}(\mu_k, P) \geq \beta$ for all k, and this estimate goes to the limit to yield $h_{KS}(\mu, P) \geq \beta$.

Since our semiclassical measure μ is defined as a limit of Husimi measures associated to $\psi_\hbar$, a naive idea would be to estimate from below the entropy of $\psi_\hbar$ and then take the limit.

A first problem is to decide how to define the $\psi_\hbar$–probability to visit successively P_{α_0}, P_{α_1},..., $P_{\alpha_{n-1}}$ at times 1, 2,..., $n-1$.

From the definition of the Husimi measures, a first idea could be to consider

$$\left\langle \psi_\hbar, \mathrm{Op}_\hbar \left((\mathbb{1}_{P_{\alpha_0}}) \, (\mathbb{1}_{P_{\alpha_1}} \circ g^1) \ldots (\mathbb{1}_{P_{\alpha_{n-1}}} \circ g^{n-1}) \right) \psi_\hbar \right\rangle . \tag{2.15}$$

To avoid dealing with characteristic functions (which are not quantized to pseudodifferential operators), we can smooth them by convolution and try replacing $\mathbb{1}_{P_k}$ by a smooth $\mathbb{1}^{sm}_{P_k}$. Even so, studying the large–n behaviour of (2.15) is very problematic. In fact, the derivatives of $(\mathbb{1}^{sm}_{P_{\alpha_0}}) \, (\mathbb{1}^{sm}_{P_{\alpha_1}} \circ g^1) \ldots (\mathbb{1}^{sm}_{P_{\alpha_{n-1}}} \circ g^{n-1})$ grow like e^n, so that when n reaches the size $|\log \hbar|$ this function no longer belongs to any reasonable symbol space (the operator is not a pseudodifferential operator).

We also note that an overlap of the form (2.15) is a *hybrid* expression: this is a *quantum* matrix element, but the operator is defined in terms of the *classical* flow ! From the point of view of quantum mechanics, it is more natural to consider, instead, the operator obtained as the product of Heisenberg-evolved quantized functions, namely

$$\hat{P}_{\alpha_{n-1}}(n-1)\hat{P}_{\alpha_{n-2}}(n-2) \ldots \hat{P}_{\alpha_1}(1)\hat{P}_{\alpha_0} . \tag{2.16}$$

Here we used the shorthand notation $\hat{P}_k \stackrel{\mathrm{def}}{=} \mathrm{Op}(\mathbb{1}^{sm}_{P_k})$, $k \in [1, K]$ (multiplication operators), and $\hat{P}_k(t) = U_\hbar^{-t} \hat{P}_k U_\hbar^t$. Instead of (2.15), a second idea would be to consider

$$\left\langle \psi_\hbar, \hat{P}_{\alpha_{n-1}}(n-1) \ldots \hat{P}_{\alpha_1}(1) \hat{P}_{\alpha_0} \psi_\hbar \right\rangle . \tag{2.17}$$

as the $\psi_\hbar$–probability to visit successively P_{α_0}, P_{α_1},..., $P_{\alpha_{n-1}}$ at times 1, 2,..., $n-1$. However, the scalar product is a complex number, and can not be directly manipulated as a probability.

Our third and final try is to consider

$$\|\hat{P}_{\alpha_{n-1}}(n-1)\ldots\hat{P}_{\alpha_1}(1)\hat{P}_{\alpha_0}\psi_\hbar\|^2. \tag{2.18}$$

In fact, if we do the smoothing of $\mathbb{1}_{P_k}$ so that

$$\sum_k (\mathbb{1}_{P_k})^2 \equiv 1$$

then the norms (2.18) can actually be manipulated like probability measures :

$$\sum_{\alpha_0,\ldots,\alpha_{n-1}} \|\hat{P}_{\alpha_{n-1}}(n-1)\hat{P}_{\alpha_{n-2}}(n-2)\ldots\hat{P}_{\alpha_1}(1)\hat{P}_{\alpha_0}\psi_\hbar\|^2 = 1,$$

and

$$\sum_{\alpha_{n-1}} \|\hat{P}_{\alpha_{n-1}}(n-1)\hat{P}_{\alpha_{n-2}}(n-2)\ldots\hat{P}_{\alpha_1}(1)\hat{P}_{\alpha_0}\psi_\hbar\|^2$$
$$= \|\hat{P}_{\alpha_{n-2}}(n-2)\ldots\hat{P}_{\alpha_1}(1)\hat{P}_{\alpha_0}\psi_\hbar\|^2.$$

Finally, using the Egorov theorem (1.32), we see that, for fixed n,

$$\|\hat{P}_{\alpha_{n-1}}(n-1)\ldots\hat{P}_{\alpha_1}(1)\hat{P}_{\alpha_0}\psi_\hbar\|^2 \underset{\hbar\longrightarrow 0}{\longrightarrow} \mu\left((\mathbb{1}^{sm}_{P_{\alpha_0}})^2\,(\mathbb{1}^{sm}_{P_{\alpha_1}}\circ g^1)^2\ldots(\mathbb{1}^{sm}_{P_{\alpha_{n-1}}}\circ g^{n-1})^2\right)$$

if the Husimi measures of $\psi_\hbar$ converge to μ. Apart from the smoothing, this is the quantity we are interested in when computing entropy of μ (2.10).

We actually proved in [A05] that

$$\|\hat{P}_{\alpha_{n-1}}(n-1)\ldots\hat{P}_{\alpha_1}(1)\hat{P}_{\alpha_0}\psi_\hbar\|^2 \leq \frac{C}{\hbar^d}e^{-(d-1)n},$$

say, in dimension d and constant curvature -1, and assuming the diameter of the P_k is small enough[1]. From this, it would be tempting to deduce that the entropy of the $\psi_\hbar$–Husimi measures is bounded below by $d-1$, then use the semicontinuity property (2.14) to deduce that $h_{KS}(\mu) \geq d-1$ (thus proving quantum unique ergodicity).

Of course, we can not apply (2.14), since we are not in the situation of a sequence (μ_k) of g^t–invariant probability measures converging to μ. To use (2.14) we need to know if a similar property holds in our quantum framework, using expressions such as (2.18) to evaluate entropies. This is, in fact, NOT the case : a factor of 2 is lost somewhere in the proof, and we will end up proving

$$h_{KS}(\mu) \geq \frac{d-1}{2}.$$

[1]To prove this estimate, we assume, without any loss of generality, that the injectivity radius of X is larger than 1.

Chapter 3

The entropic uncertainty principle.

In this chapter, we start proving our main theorem, (2.6). To simplify the notations we restrict ourselves to the case of constant curvature $\equiv -1$.

We start with a functional inequality called the "entropic uncertainty principle".

3.1 The abstract result...

We consider a complex Hilbert space $(\mathcal{H}, \langle .,. \rangle)$, and denote $\|\psi\| = \sqrt{\langle \psi, \psi \rangle}$ the associated norm. The same notation $\|.\|$ will also be used for the operator norm on $\mathcal{L}(\mathcal{H})$.

We define the following family of l_p norms on $\mathcal{H}^N$: for $\Psi = (\Psi_1, \ldots, \Psi_N) \in \mathcal{H}^N$, we let

$$\|\Psi\|_p \stackrel{\text{def}}{=} \left(\sum_{k=1}^{N} \|\Psi_k\|^p \right)^{1/p}, \quad 1 \leq p < \infty\,, \text{ and } \quad \|\Psi\|_\infty \stackrel{\text{def}}{=} \max_k \|\Psi_k\|\,. \quad (3.1)$$

For $p = 2$, this norm coincides with the Hilbert norm deriving from the scalar product

$$\langle \Psi, \Phi \rangle_{\mathcal{H}^N} = \sum_k \langle \Psi_k, \Phi_k \rangle_{\mathcal{H}}.$$

We can define similarly a family of l_p norms on $\mathcal{H}^M \ni \Phi = (\Phi_1, \ldots, \Phi_M)$:

$$\|\Phi\|_p \stackrel{\text{def}}{=} \left(\sum_{j=1}^{M} \|\Phi_j\|^p \right)^{1/p}, \quad 1 \leq p < \infty\,, \text{ and } \quad \|\Phi\|_\infty \stackrel{\text{def}}{=} \max_j \|\Phi_j\|\,. \quad (3.2)$$

For $\Psi \in \mathcal{H}^N$ with $\|\Psi\|_2 = 1$, we define its entropy,

$$h(\Psi) = -\sum_{k=1}^{N} \|\Psi_k\|^2 \log \|\Psi_k\|^2\,;$$

(and we define similarly the entropy of a normalized vector $\Phi \in \mathcal{H}^M$).

Consider the action of a bounded operator $T : \mathcal{H}^N \to \mathcal{H}^M$, which we present as a $M \times N$ matrix $(T_{j\,k})$ of bounded operators on $\mathcal{H}$. We denote $\|T\|_{p,q}$ the norm of T from $l_p(\mathcal{H}^N)$ to $l_q(\mathcal{H}^M)$, for $1 \le p, q \le \infty$.

Theorem 3.1 (Riesz interpolation theorem)**.** *[DunSchw, Section VI.10] The function* $\log \|T\|_{1/a,1/b}$ *is a convex function of* (a, b) *in the square* $0 \le a, b \le 1$*.*

From this theorem, Maassen and Uffink derived a new form of uncertainty relations [MaaUff88].

Theorem 3.2. *Assume that* $\|T\|_{2,2} = 1$*, which implies in particular that* $\|T_{jk}\| \le 1$ *for all* k, j*. Introduce the real number* $c(T) = \max_{j,k}\|T_{jk}\|$ *, where the norm is the operator norm in* $\mathcal{L}(\mathcal{H})$*.*

For all $\Psi \in \mathcal{H}$ *such that* $\|\Psi\|_2 = 1$ *and* $\|T\Psi\|_2 = 1$*, we have*

$$h(T\Psi) + h(\Psi) \ge -2 \log c(T) \,.$$

Proof: In the case $a = 1, b = 0$, we have for any Ψ,

$$\|T\Psi\|_\infty = \sup_j \|(T\Psi)_j\| \le \sup_{j,k} \|T_{j,k}\| \sum_{k'} \|\Psi_{k'}\| = \sup_{j,k} \|T_{j,k}\| \; \|\Psi\|_1 \ ,$$

which can be written as $\|T\|_{1,\infty} \le \sup_{j,k} \|T_{j,k}\| \stackrel{\text{def}}{=} c(T)$.

Let us assume that T is contracting on l_2 : $\|T\|_{2,2} \le 1$. We take $t \in [0, 1]$ and $a_t = \frac{1+t}{2}$, $b_t = \frac{1-t}{2}$ to interpolate between $(1/2, 1/2)$ and $(1, 0)$; Theorem 3.2 implies that

$$\|T\|_{1/a_t,1/b_t} \le c(T)^t \,.$$

This is equivalent to the following

Corollary 3.3. *Let the operator* $T : \mathcal{H}^N \longrightarrow \mathcal{H}^M$ *satisfy* $\|T\|_{2,2} \le 1$ *and call* $c(T) \stackrel{\text{def}}{=} \sup_{j,k} \|T_{j,k}\|$*. Then, for all* $t \in [0, 1]$*, for all* $\Psi \in \mathcal{H}^N$*,*

$$\|T\Psi\|_{\frac{2}{1-t}} \le c(T)^t \; \|\Psi\|_{\frac{2}{1+t}} \ .$$

We define for any $r > 0$ or $-1 < r < 0$ the "moments"

$$M_r(\Psi) \stackrel{\text{def}}{=} \left(\sum_j \|\Psi_j\|^{2+2r} \right)^{1/r} .$$

Corollary 3.3 leads to the following family of "uncertainty relations":

$$\forall t \in (0, 1),\ \forall \Psi \in \mathbb{C}^N, \qquad M_{\frac{t}{1-t}}(T\Psi)\, M_{\frac{-t}{1+t}}(\Psi) \le c(T)^2 \,. \tag{3.3}$$

In the case $\|\Psi\|_2 = 1$, we notice that the moments converge to the same value when $r \to 0$ from above or below:

$$\lim_{r\to 0} M_r(\Psi) = \mathrm{e}^{-h(\Psi)}\,, \quad \text{where} \quad h(\Psi) = -\sum_j \|\Psi_j\|^2 \log \|\Psi_j\|^2 \,.$$

If, furthermore, $\|T\Psi\|_2 = 1$, then the limit $t \to 0$ of the inequalities (3.3) yield the Entropic Uncertainty Principle stated in Theorem 3.2. □

We shall use Theorem 3.2 in the following particular case :

Example 3.4. *Suppose we have two partitions of unity $(\pi_k)_{k=1}^N$ and $(\tau_j)_{j=1}^M$, that is, two families of operators on $\mathcal{H}$ such that*

$$\sum_{k=1}^{N} \pi_k \pi_k^* = Id, \qquad \sum_{j=1}^{M} \tau_j \tau_j^* = Id. \tag{3.4}$$

Let U be a unitary operator on $\mathcal{H}$. We can take $T_{j\,k} = \tau_j^* U \pi_k$.

Lemma 3.5. *Let $T_{jk} = \tau_j^* U \pi_k$, for some bounded operator $U : \mathcal{H} \to \mathcal{H}$. Then we have the identity*

$$\|T\|_{2,2} = \|U\|_{\mathcal{L}(\mathcal{H})}\,.$$

Proof. The operator T may be described as follows. Consider a line and column vectors of operators on $\mathcal{H}$:

$$L \stackrel{\text{def}}{=} (\pi_1, \ldots, \pi_N)\,, \quad \text{as well as } C = \begin{pmatrix} \tau_1^* \\ \ldots \\ \tau_M^* \end{pmatrix}.$$

We can write $T = CUL$. We insert this formula in the identity

$$\|T\|_{2,2}^2 = \|T^*T\|_{\mathcal{L}(\mathcal{H}^N)} = \left\| L^\dagger U^* C^\dagger C U L \right\|_{\mathcal{L}(\mathcal{H}^N)}$$

Using (3.4) for the τ_j, we notice that $C^\dagger C = Id_{\mathcal{H}}$, so that the norm above reads

$$\left\| L^\dagger U^* U L \right\|_{\mathcal{L}(\mathcal{H}^N)}\,.$$

Then, we use the identities

$$\left\|(UL)^\dagger (UL)\right\|_{\mathcal{L}(\mathcal{H}^N)} = \left\|(UL)(UL)^\dagger\right\|_{\mathcal{L}(\mathcal{H})} = \left\|(UL)L^\dagger U^*\right\|_{\mathcal{L}(\mathcal{H})} = \|UU^*\|_{\mathcal{L}(\mathcal{H})}\,,$$

where we used (3.4) for the π_k. □

Therefore, if U is contracting (resp. $\|U\|_{\mathcal{L}(\mathcal{H})} = 1$) one has $\|T\|_{2,2} \leq 1$ (resp. $\|T\|_{2,2} = 1$).

We also specify the vector Ψ by taking $\Psi_k = \pi_k^* \psi$ for some normalized $\psi \in \mathcal{H}$. From (3.4), we check that $\|\Psi\|_2 = \|\psi\|$, and also that $(T\Psi)_j = \tau_j^* U\psi$. Thus, if $\|U\psi\| = 1$, the relation (3.4) also implies $\|T\Psi\|_2 = \|U\psi\| = 1$. With this choice for T and Ψ, Theorem 3.2 reads as follows:

Theorem 3.6. *Let U be an isometry on $\mathcal{H}$, and let π, τ be two quantum partitions of unity as in* (3.4).
Define $c_{\tau,\pi}(U) \stackrel{\text{def}}{=} \sup_{j,k} \|\tau_j^* \, U \, \pi_k\|_{\mathcal{L}(\mathcal{H})}$.

Then, for any normalized $\psi \in \mathcal{H}$, we have

$$h_\tau(U\psi) + h_\pi(\psi) \geq -2 \log c_{\tau,\pi}(U)$$

where $h_\pi(\psi) = -\sum_{k=1}^N \|\pi_k^*\psi\|^2 \log \|\pi_k^*\psi\|^2$ and $h_\tau(\psi) = -\sum_{j=1}^M \|\tau_j^*\psi\|^2 \log \|\tau_j^*\psi\|^2$.

Note that the definition $h_\pi(\psi) = -\sum_{k=1}^N \|\pi_k^*\psi\|^2 \log \|\pi_k^*\psi\|^2$ is somewhat analogous to (2.9), π playing the role of the partition P and ψ the role of the measure μ. We will call $h_\pi(\psi)$ the Shannon entropy of the state ψ with respect to the partition π.

3.2 ... applied to eigenfunctions of the laplacian...

In this section we define the data to input in Theorem 3.6, in order to obtain informations on the eigenstates $\psi_\hbar$ and the semiclassical measures μ considered in the previous chapters. Only the Hilbert space is fixed, $\mathcal{H} \stackrel{\text{def}}{=} L^2(X)$. All other data depend on the semiclassical parameter $\hbar$: the quantum partitions π, τ, the unitary operator U. Besides we will need yet another technical variant of Theorem 3.6.

3.2.1 Smooth partition of unity

To evaluate the Kolmogorov–Sinai entropy, we start by decomposing T^*X into a finite partition. We actually specify the form of the partition we want to use. We work with a measurable partition $(P_k)_{k=1,\ldots,K}$ of the base X : $X = \sqcup P_k$, that we lift to a partition of the phase space T^*X.

For semiclassical methods we actually need to work with smooth functions, so that we introduce a smooth partition of unity $(\mathbb{1}_{P_k}^{sm})$, obtained by smoothing the characteristic functions $(\mathbb{1}_{P_k})$ with a convolution kernel. We require that the smoothing be done so that $\sum_{k=1}^K (\mathbb{1}_{P_k}^{sm})^2 = 1$.

We finally denote $\hat{P}_k = \mathrm{Op}(\mathbb{1}_{P_k}^{sm})$ (it is just the operator of multiplication by $\mathbb{1}_{P_k}^{sm}$). We have

$$\forall x \in M, \qquad \sum_{k=1}^K \hat{P}_k^2 = I\,, \tag{3.5}$$

which means that they form a quantum partition of unity as in (3.4), which we will call $\mathcal{P}^{(0)}$.

3.2.2 Refinement of the partition under the Schrödinger flow.

We denote by $U^t = \exp(it\hbar \triangle /2)$ the quantum propagator. With no loss of generality, we will assume that the injectivity radius of X is much greater than 1, and work with the propagator at time one, $U = U^1$. This propagator quantizes the geodesic flow at time one, g^1. The $\hbar$-dependence of U will be implicit in our notations.

As one does to compute the Kolmogorov–Sinai entropy of an invariant measure, we define a new quantum partition of unity by evolving and refining the initial partition $\mathcal{P}^{(0)}$ under the quantum evolution. For each time $n \in \mathbb{N}$ and any sequence of symbols $\boldsymbol{\alpha} = (\alpha_0 \cdots \alpha_{n-1})$, $\alpha_i \in [1, K]$ (we say that the sequence $\boldsymbol{\alpha}$ is of *length* $|\boldsymbol{\alpha}| = n$), we define the operators

$$\hat{P}_{\boldsymbol{\alpha}} = \hat{P}_{\alpha_{n-1}}(n-1)\hat{P}_{\alpha_{n-2}}(n-2)\dots\hat{P}_{\alpha_0}\,. \tag{3.6}$$

We keep using the notation $A(t) = U^{-t}AU^t$ for the quantum evolution of an operator A. From (3.5) and the unitarity of U, the family of operators $\left\{\hat{P}_{\boldsymbol{\alpha}}\right\}_{|\boldsymbol{\alpha}|=n}$ obviously satisfies the relation $\sum_{|\boldsymbol{\alpha}|=n} \hat{P}_{\boldsymbol{\alpha}}\,\hat{P}_{\boldsymbol{\alpha}}^* = Id_{L^2}$, and therefore forms a quantum partition which we call $\mathcal{P}^{(n)}$. We also have $\sum_{|\boldsymbol{\alpha}|=n} \hat{P}_{\boldsymbol{\alpha}}^*\,\hat{P}_{\boldsymbol{\alpha}} = Id_{L^2}$, and we denote $\mathcal{T}^{(n)}$ the partition of unity given by the family of operators $\left\{\hat{P}_{\boldsymbol{\alpha}}^*\right\}_{|\boldsymbol{\alpha}|=n}$.

3.2.3

In the entropic uncertainty principle, Theorem 3.6, we shall input the following data :

- the quantum partition $\pi = \mathcal{P}^{(n)}$ is given by the family of operators $\{\hat{P}_{\boldsymbol{\alpha}},\ |\boldsymbol{\alpha}| = n\}$. The quantum partition $\tau = \mathcal{T}^{(n)}$ is given by the family of operators $\{\hat{P}_{\boldsymbol{\alpha}}^*,\ |\boldsymbol{\alpha}| = n\}$. The integer n will always be of order $\mathcal{K}|\log\hbar|$, where $\mathcal{K}$ will be determined later.
- the isometry will be $\mathcal{U} = U^n$.

To apply Theorem 3.6 we would need an upper bound on $c_{\mathcal{T}^{(n)},\mathcal{P}^{(n)}}(\mathcal{U}) = \max_{|\boldsymbol{\alpha}|=|\boldsymbol{\alpha}'|=n} \|\hat{P}_{\boldsymbol{\alpha}'}\,U^n\,\hat{P}_{\boldsymbol{\alpha}}\|$. We remark that $\hat{P}_{\boldsymbol{\alpha}'}\,U^n\,\hat{P}_{\boldsymbol{\alpha}}$ can be developed as

$$U^{-n+1}\hat{P}_{\alpha'_{n-1}}U\cdots U\hat{P}_{\alpha'_1}U\hat{P}_{\alpha'_0}U\hat{P}_{\alpha_{n-1}}\cdots U\hat{P}_{\alpha_1}U\hat{P}_{\alpha_0}$$

or equivalently

$$U^{n+1}\hat{P}_{\alpha'_n}(2n)\cdots\hat{P}_{\alpha'_1}(n+1)\hat{P}_{\alpha'_0}(n)\hat{P}_{\alpha_{n-1}}(n-1)\cdots\hat{P}_{\alpha_1}(1)\hat{P}_{\alpha_0}.$$

The best bound we can hope for on the norm of these operators is certainly the trivial one : $c_{\mathcal{T}^{(n)},\mathcal{P}^{(n)}}(\mathcal{U}) \leq 1$. On the other hand, if we add an energy cutoff $\mathrm{Op}_\hbar(\chi)$ we can prove an interesting bound : see Theorem 3.9 below.

3.2.4 The main estimate

Let us assume (without loss of generality) that the injectivity radius of X is greater than 1; and that the diameter of each P_k is small enough so that, for every j, k, for every $x, y \in P_j, P_k$, there is at most one unit speed geodesic joining x and y in time 1.

The estimate essentially proven in [A05] is :

Theorem 3.7. *Let χ be an energy cut-off, that is, a smooth compactly supported function vanishing outside $H^{-1}([1/2-\varepsilon, 1/2+\varepsilon])$.*

Given $\mathcal{K} > 0$ and a partition $\mathcal{P}^{(0)}$, there exists $\hbar_{\mathcal{K},\mathcal{P}^{(0)},\chi}$ such that, for any $\hbar \leq \hbar_{\mathcal{K},\mathcal{P}^{(0)},\chi}$, for any positive integer $n \leq \mathcal{K}|\log\hbar|$, and any pair of sequences $\boldsymbol{\alpha}$, $\boldsymbol{\alpha}'$ of length n,

$$\|\hat{P}_{\boldsymbol{\alpha}'}\, U^n\, \hat{P}_{\boldsymbol{\alpha}}\, \mathrm{Op}(\chi)\| \leq C\, \hbar^{-\frac{d}{2}}\, e^{-(d-1)n}(1+O(\varepsilon))^n\,. \qquad (3.7)$$

The constant C only depends on the Riemannian manifold.

Remark 3.8. *If we were in variable curvature, instead of the exponent $d-1$ we would have a variable exponent depending on the local Lyapunov exponents.*

The idea in Theorem 3.7 is rather simple, although the technical implementation becomes cumbersome. We first show that any state in the image of $\mathrm{Op}(\chi)$ can be decomposed as a superposition of essentially $\hbar^{-\frac{d}{2}}$ normalized lagrangian states, supported on lagrangian manifolds transverse to the stable leaves of the flow. In fact the lagrangian states we work with are truncated δ–functions, supported on spheres $S^*_z X$. The action of the operator $U^{n-1}\hat{P}_{\boldsymbol{\alpha}'}\, U^n\, \hat{P}_{\boldsymbol{\alpha}} = \hat{P}_{\alpha'_{n-1}} U \cdots U \hat{P}_{\alpha'_0} U \hat{P}_{\alpha_{n-1}} \cdots U \hat{P}_{\alpha_0}$ on such lagrangian states is described by the theory of Fourier integral operators (WKB methods), and is intuitively simple to understand : each application of U stretches the lagrangian in the unstable direction whereas each multiplication by $\hat{P}_\alpha$ chops a small piece of lagrangian. This iteration of stretching and cutting accounts for the exponential decay. The proof is developed in Chapter 4.

In [AN07] the estimate of Theorem 3.7 was modified by optimizing the shape of the cutoff χ : we considered a smooth function $\chi \in C^\infty(\mathbb{R}; [0,1])$, with $\chi(t) = 1$ for $|t| \leq 1$ and $\chi_\delta(t) = 0$ for $|t| \geq 1$. Then, for some fixed $\delta \in (0,1)$, we rescale that function to obtain an $\hbar$-dependent cutoff near S^*X:

$$\forall \hbar \in (0,1),\ \forall n \in \mathbb{N},\ \forall \rho \in T^*X, \qquad \chi_\delta(\rho;\hbar) \stackrel{\mathrm{def}}{=} \chi\big(\hbar^{-1+\delta}(H(\rho)-1/2)\big)\,. \qquad (3.8)$$

The cutoff χ_δ is localized in a tubular neighbourhood of S^*X of width $2\hbar^{1-\delta}$

Theorem 3.9. *[AN07] Given $\mathcal{K} > 0$ a partition $\mathcal{P}^{(0)}$ and $\delta > 0$ small enough, there exists $\hbar_{\mathcal{K},\mathcal{P}^{(0)},\delta}$ such that, for any $\hbar \leq \hbar_{\mathcal{K},\mathcal{P}^{(0)},\delta}$, for any positive integer $n \leq \mathcal{K}|\log \hbar|$, and any pair of sequences $\boldsymbol{\alpha}$, $\boldsymbol{\alpha}'$ of length n,*

$$\|\hat{P}_{\boldsymbol{\alpha}'}\, U^n\, \hat{P}_{\boldsymbol{\alpha}}\, \mathrm{Op}(\chi_\delta)\| \leq C\, \hbar^{-\frac{d-1}{2}-\delta}\, e^{-(d-1)n}(1+O(h^\delta))^n\,. \tag{3.9}$$

The constant C only depends on the Riemannian manifold (M, g).

Theorem 3.9 essentially improves the prefactor $\hbar^{-\frac{d}{2}}$ of Theorem 3.7. Its proof is similar, the main difficulty being to define $\mathrm{Op}(\chi_\delta)$ — the function χ_δ does not fall into one of the usual "nice" classes of symbols, since its derivatives explode quite fast when $\hbar \longrightarrow 0$. To define $\mathrm{Op}(\chi_\delta)$ would be much beyond the scope of these notes (see [SZ99, AN07]).

3.2.5 Technical variant of the entropic uncertainty principle.

It must have become clear now that we cannot apply Theorem 3.6 directly, because we need to insert our energy cut-off $\mathrm{Op}(\chi)$. On the other hand, this frequency cut–off does not really bother us, since it hardly modifies the eigenfunctions (see later (3.10)).

We generalize the statement of Theorem 3.6 by introducing an auxiliary operator $\mathcal{O}$.

Theorem 3.10. *[AN07] Let $\mathcal{O}$ be a bounded operator on $\mathcal{H}$. Let $\mathcal{U}$ be an isometry on $\mathcal{H}$.*
Define $c_{\mathcal{O}}^{\tau,\pi}(\mathcal{U}) \stackrel{\text{def}}{=} \sup_{j,k}\|\tau_j^*\, \mathcal{U}\, \pi_k\, \mathcal{O}\|_{\mathcal{L}(\mathcal{H})}$.

Then, for any $\theta \geq 0$, for any normalized $\psi \in \mathcal{H}$ satisfying

$$\forall k = 1, \ldots, \mathcal{N}, \qquad \|(Id - \mathcal{O})\pi_k^*\psi\| \leq \theta\,,$$

the entropies $h_\tau\big(\mathcal{U}\psi\big)$, $h_\pi\big(\psi\big)$ satisfy

$$h_\tau\big(\mathcal{U}\psi\big) + h_\pi\big(\psi\big) \geq -2\log\big(c_{\mathcal{O}}^{\pi,\tau}(\mathcal{U}) + \mathcal{N}\,\theta\big).$$

3.2.6 Applying the entropic uncertainty principle

We now precise all the data we will use in the entropic uncertainty principle, Theorem 3.10:

- the quantum partition $\pi = \mathcal{P}^{(n)}$, $\tau = \mathcal{T}^{(n)}$ have already been defined. The integer n will be of order $\mathcal{K}|\log \hbar|$, where the choice of $\mathcal{K}$ will be determined later. In the semiclassical limit, these partitions have cardinality $\mathcal{N} = K^n \asymp \hbar^{-K_0}$ for some fixed $K_0 > 0$.

- the isometry will be $\mathcal{U} = U^n$.

- the operator $\mathcal{O}$ is $\mathcal{O} = \mathrm{Op}(\chi_\delta)$. Since we are, at the end, interested in eigenfunctions of the laplacian, we need to know that this operator hardly modifies them. In fact, for any $L > 0$, there exists $\hbar_L$ such that, for any $\hbar \leq \hbar_L$, the Laplacian eigenstate satisfies

$$\forall \boldsymbol{\alpha}, |\boldsymbol{\alpha}| = n \leq \mathcal{K}|\log \hbar|, \ \|\big(\mathrm{Op}(\chi_\delta) - Id\big)\hat{P}^*_{\boldsymbol{\alpha}}\psi_\hbar\| \leq \hbar^L \|\psi_\hbar\| \,. \quad (3.10)$$

These means that, for an eigenfunction $\psi_\hbar$, all the states $\hat{P}^*_{\boldsymbol{\alpha}}\psi_\hbar$ are very sharply microlocalized near the energy layer S^*X.

- $\theta = \hbar^L$, and L will be chosen very large.

  All these quantities are defined for $n = \mathcal{K}|\log \hbar|$, $\mathcal{K}$ will be determined later, but fixed.

As in Theorem 3.10, the entropy associated with a state $\psi \in \mathcal{H}$ are given by

$$h_{\mathcal{P}^{(n)}}(\psi) = -\sum_{|\boldsymbol{\alpha}|=n} \|\hat{P}^*_{\boldsymbol{\alpha}}\psi\|^2 \log\big(\|\hat{P}^*_{\boldsymbol{\alpha}}\psi\|^2\big).$$

Similarly,

$$h_{\mathcal{T}^{(n)}}(\psi) = -\sum_{|\boldsymbol{\alpha}|=n} \|\hat{P}_{\boldsymbol{\alpha}}\psi\|^2 \log\big(\|\hat{P}_{\boldsymbol{\alpha}}\psi\|^2\big).$$

We may apply Theorem 3.10 to any sequence of states satisfying (3.10).

Corollary 3.11. *Define*

$$c_{\mathrm{Op}\,\chi_\delta}(U^n) \stackrel{\mathrm{def}}{=} \max_{|\boldsymbol{\alpha}|=|\boldsymbol{\alpha}'|=n} \|\hat{P}_{\boldsymbol{\alpha}'}\, U^n\, \hat{P}_{\boldsymbol{\alpha}}\, \mathrm{Op}(\chi_\delta)\| \,. \quad (3.11)$$

Then for any normalized state ϕ satisfying (3.10),

$$h_{\mathcal{T}^{(n)}}(U^n\,\phi) + h_{\mathcal{P}^{(n)}}(\phi) \geq -2\log\big(c_{\mathrm{Op}\,\chi_\delta}(U^n) + h^{L-K_0}\big)\,.$$

We now apply Corollary 3.11 to the particular case of the eigenstates $\psi_\hbar$. The estimate (3.9) can be rewritten as

$$c_{\mathrm{Op}\,\chi_\delta}(U^n) \leq C\,\hbar^{-\frac{d-1}{2}-\delta} e^{-(d-1)n}(1 + O(\hbar^\delta))^n \,.$$

We choose L large enough such that $\hbar^{L-K_0}$ is negligible in comparison with $\hbar^{-\frac{d-1}{2}-\delta}e^{-(d-1)n}$.

Proposition 3.12. *Let $(\psi_\hbar)_{\hbar\to 0}$ be any sequence of eigenstates* (2.5)*. Then, in the semiclassical limit, the entropies of $\psi_\hbar$ satisfy*

$$h_{\mathcal{T}^{(n)}}(\,\psi_\hbar) + h_{\mathcal{P}^{(n)}}(\psi_\hbar) \geq 2(d-1)n + (d-1+2\delta)\log\hbar + \mathcal{O}(1) \,. \quad (3.12)$$

This holds for $n \leq \mathcal{K}|\log\hbar|$ ($\mathcal{K}$ arbitrary) and $\hbar \leq \hbar_{\mathcal{K},\mathcal{P}^{(0)},\delta}$.

3.3 ...and the conclusion.

Before taking the limit $\hbar \to 0$, we prove that a similar lower bound holds if we replace $n \asymp |\log \hbar|$ by some fixed n_o, and $\mathcal{P}^{(n)}$ by the corresponding partition $\mathcal{P}^{(n_o)}$. Proposition 3.13 is the semiclassical analogue of the classical subadditivity of entropy for invariant measures.

We introduce the Ehrenfest time $n_E(\hbar) = \frac{(1-\delta')|\log \hbar|}{\lambda_{\max}}$ (δ' fixed, arbitrarily small). In constant curvature -1, the expansion rate of the geodesic flow on S^*X is $\lambda_{\max} = 1$. The Ehrenfest time is the main limitation to use semiclassical methods to understand the large time behaviour of the Schrödinger flow : roughly speaking, we have $U^{-t}\operatorname{Op}_\hbar(a)U^t \sim \operatorname{Op}(a \circ g^t)$ for $|t| \leq \frac{n_E(\hbar)}{2}$, but for larger t we can no longer refer to the geodesic flow to understand $U^{-t}\operatorname{Op}_\hbar(a)U^t$. In other words, we can use our methods of classical ergodic theory for $|t| \leq \frac{n_E(\hbar)}{2}$, and not afterwards.

Proposition 3.13 (Subadditivity)**.** *Let $\delta' > 0$. There is a function $R(n_o, \hbar)$ such that, for all integer n_o,*

$$\lim_{\hbar \longrightarrow 0} |R(n_o, \hbar)| = 0$$

and such that, for all n_o, $n \in \mathbb{N}$ with $n_o + n \leq n_E(\hbar) = \frac{(1-\delta')|\log \hbar|}{\lambda_{\max}}$, for any $(\psi_\hbar)$ normalized eigenstates satisfying (2.5), *the following inequality holds:*

$$h_{\mathcal{P}^{(n_o+n)}}(\psi_\hbar) \leq h_{\mathcal{P}^{(n_o)}}(\psi_\hbar) + h_{\mathcal{P}^{(n)}}(\psi_\hbar) + R(n_o, \hbar)\,.$$

The non–commutative dynamical system formed by (U^t) acting on pseudodifferential operators is (approximately) commutative on time intervals of length $n_E(\hbar)$:

$$\|[\operatorname{Op}_\hbar(a)(t), \operatorname{Op}_\hbar(b)(-t)]\|_{L^2(X)} = \mathcal{O}(\hbar^{c\delta'}),$$

for any time $|t| \leq \frac{n_E(\hbar)}{2}$, or equivalently (using the unitarity of U^t)

$$\|[\operatorname{Op}_\hbar(a)(t), \operatorname{Op}_\hbar(b)]\|_{L^2(X)} = \mathcal{O}(\hbar^{c\delta'}),$$

for any time $|t| \leq n_E(\hbar)$. On such a time interval, we almost have a commutative dynamical system, up to small errors tending to 0 with $\hbar$. This roughly explains why the quantum entropy $h_{\mathcal{P}^{(n_o+n)}}(\psi_\hbar)$ has the same subadditivity property as the classical entropy (2.11), up to small errors, as long as $n_o + n$ remains bounded by the Ehrenfest time.

Thanks to this subadditivity, we may finish the proof of Theorem 2.5. Although Proposition 3.12 held for $n \leq \mathcal{K}|\log \hbar|$ and $\mathcal{K}$ arbitrary, we are now limited by Proposition 3.13 to $\mathcal{K} = \frac{1-\delta'}{\lambda_{\max}}$. For $n = n_E(\hbar)$, Proposition 3.12 can be written

$$h_{\mathcal{P}^{(n)}}(\psi_\hbar) + h_{\mathcal{T}^{(n)}}(\psi_\hbar) \geq 2(d-1)n - \frac{(d-1+2\delta)\lambda_{\max}}{(1-\delta')}\, n + \mathcal{O}(1)\,. \quad (3.13)$$

Let $n_o \in \mathbb{N}$ be fixed and $n = n_E(\hbar)$. Using the Euclidean division $n = qn_o + r$ (with $r \leq n_o$), Proposition 3.13 implies that for $\hbar$ small enough,

$$\frac{h_{\mathcal{P}^{(n)}}(\psi_\hbar)}{n} \leq \frac{h_{\mathcal{P}^{(n_o)}}(\psi_\hbar)}{n_o} + \frac{h_{\mathcal{P}^{(r)}}(\psi_\hbar)}{n} + \frac{R(n_o, \hbar)}{n_o}.$$

Of course a similar inequality holds with $\mathcal{P}$ replaced by $\mathcal{T}$.

Using (3.12) and the fact that $h_{\mathcal{P}^{(r)}}(\psi_\hbar)$ stays uniformly bounded (by a quantity depending on n_o) when $\hbar \to 0$, we find

$$\frac{1}{2}\left[\frac{h_{\mathcal{P}^{(n_o)},}(\psi_\hbar)}{n_o} + \frac{h_{\mathcal{T}^{(n_o)},}(\psi_\hbar)}{n_o}\right] \geq (d-1) - \frac{(d-1+2\delta)\lambda_{\max}}{2(1-\delta')}\, n \\ + \mathcal{O}(1) - \frac{R(n_o,\hbar)}{2n_o} + \mathcal{O}_{n_o}(1/n)\,. \quad (3.14)$$

We are now dealing with the partition $\mathcal{P}^{(n_o)}$, n_0 being fixed.

3.3.1 End of the proof

Let us take a subsequence of $(\psi_{\hbar_k})$ such that the Husimi measures $\mu_k = \mu_{\psi_{\hbar_k}}$ converge to a semiclassical measure μ on S^*X, invariant under the geodesic flow (see Prop. 2.1). We may take the limit $\hbar_k \to 0$ (so that $n \to \infty$) in the expression above. The norms appearing in the definition of $h_{\mathcal{P}^{(n_o)}}(\psi_{\hbar_k})$ and $h_{\mathcal{T}^{(n_o)}}(\psi_{\hbar_k})$can be written as

$$\|\hat{P}_{\boldsymbol{\alpha}}\,\psi_{\hbar_k}\| = \|\hat{P}_{\alpha_{n_o}}(n_o)\cdots\hat{P}_{\alpha_1}(1)\hat{P}_{\alpha_0}\,\psi_{\hbar_k}\| \quad (3.15)$$

$$\|\hat{P}^*_{\boldsymbol{\alpha}}\,\psi_{\hbar_k}\| = \|\hat{P}_{\alpha_0}\hat{P}_{\alpha_1}(1)\cdots\hat{P}_{\alpha_{n_o}}(n_o)\,\psi_{\hbar_k}\|\,. \quad (3.16)$$

For any sequence $\boldsymbol{\alpha}$ of length n_o, the laws of pseudodifferential calculus imply the convergence of $\|\hat{P}^*_{\boldsymbol{\alpha}}\,\psi_{\hbar_k}\|^2$ and $\|\hat{P}_{\boldsymbol{\alpha}}\,\psi_{\hbar_k}\|^2$ to the same quantity $\mu(\{\boldsymbol{\alpha}\})$, where $\{\boldsymbol{\alpha}\}$ is the function $(\mathbb{1}^{sm}_{P_{\alpha_0}})^2\,(\mathbb{1}^{sm}_{P_{\alpha_1}})^2\circ g^1\ldots(\mathbb{1}^{sm}_{P_{\alpha_{n_o-1}}})^2\circ g^{n_o-1}$ on T^*X. Thus $h_{\mathcal{P}^{(n_o)}}(\psi_{\hbar_k})$ and $h_{\mathcal{T}^{(n_o)}}(\psi_{\hbar_k})$ both semiclassically converge to the classical entropy

$$h_{n_o}(\mu) \stackrel{\text{def}}{=} h_{n_o}(\mu, (\mathbb{1}^{sm2}_{P_k})) = -\sum_{|\boldsymbol{\alpha}|=n_o}\mu(\{\boldsymbol{\alpha}\})\log\mu(\{\boldsymbol{\alpha}\})\,.$$

We have thus obtained the lower bound

$$\frac{h_{n_o}(\mu)}{n_o} \geq (d-1) - \frac{(d-1+2\delta)\lambda_{\max}}{2(1-\delta')}\,. \quad (3.17)$$

δ and δ' could be taken arbitrarily small, and at this stage they can be let vanish. Remember also that $\lambda_{\max} = 1$.

The Kolmogorov–Sinai entropy of μ (with respect to the partition $X = \sqcup P_k$) is by definition the limit of the first term $\frac{h_{n_o}(\mu)}{n_o}$ when n_o goes to infinity

(2.10) (2.12), with the notable difference that the smooth functions $(\mathbb{1}_{P_k}^{sm})^2$ should be replaced by the characteristic functions $(\mathbb{1}_{P_k})$. We note, however, that the lower bound (3.17) does not depend on the derivatives of $(\mathbb{1}_{P_k}^{sm})^2$: as a result, the same bound carries over to the characteristic functions $(\mathbb{1}_{P_k})$.

We can finally let n_o tend to $+\infty$, to obtain (2.7).

$\square$

Chapter 4

WKB methods.

To prove our main estimate (Theorem 3.7), we need to describe the action of the operator $U^t = \exp(it\hbar\frac{\triangle}{2})$ on "rapidly oscillating" functions, in the limit $\hbar \longrightarrow 0$. The idea, already used by Schrödinger, is first to describe the action of $\exp(it\hbar\frac{\triangle}{2})$ on functions of the form $e^{\frac{i}{\hbar}S(x)}$, called WKB functions or lagrangian functions; and then to use the fact that all the functions we consider are integral combinations of lagrangian functions.

4.1 Lagrangian submanifolds of T^*X and generating functions.

We have seen that T^*X is endowed with a "canonical" symplectic form ω, defined as follows. Let $\Omega \subset X$ be an open subset of X, endowed with a coordinate chart $\phi : X \longrightarrow \mathbb{R}^d$. Then $T^*\Omega \subset T^*X$ can be endowed with the coordinate chart

$$\Phi : T^*\Omega \longrightarrow \mathbb{R}^d \times (\mathbb{R}^d)^* \tag{4.1}$$

$$(x, p) \mapsto (\phi(x), (T\phi_x^*)^{-1}p). \tag{4.2}$$

On $T^*\Omega$, ω is defined as the pullback by Φ of the symplectic form $\sum_{i=1}^d dq_i \wedge dp_i$ of $\mathbb{R}^d \times (\mathbb{R}^d)^*$. We leave it to the reader to check that this definition does not depend on the choice of local coordinates. Thus, by choosing an atlas of X, one can define ω on T^*X, and the definition does not depend on the atlas. In fact, ω can also be defined in a intrinsic way by formula (1.5).

Definition 4.1. *A lagrangian submanifold, in the $2d$-dimensional symplectic manifold (T^*X, ω), is a d-dimensional submanifold on which ω vanishes.*

Equivalently, a submanifold $\mathcal{L}$ is lagrangian if and only if, for all $z \in \mathcal{L}$, $T_z\mathcal{L}$ is its own ω-orthogonal in $T_z(T^*X)$.

Example 4.2. *On $T^*\mathbb{R}^d = \mathbb{R}^d \times (\mathbb{R}^d)^*$ endowed with the symplectic form $\sum_{i=1}^d dq_i \wedge dp_i$, affine subspaces of the form $\mathbb{R}^d \times \{\xi_0\}$ or $\{x_0\} \times \mathbb{R}^d$ are* *examples of lagrangian submanifolds. More generally, for any manifold X, the zero section $\{(x,0), x \in X\} \subset T^*X$ is a lagrangian submanifold of T^*X. For any $x \in X$, the fiber T^*_xX is also lagrangian.*

Generating functions.

Exercise 4.3. *In $\mathbb{R}^d \times (\mathbb{R}^d)^*$ endowed with the symplectic form $\sum_{i=1}^d dq_i \wedge dp_i$, consider an linear subspace of the form* $\mathrm{Graph}A = \{(x, Ax)\}$ *where A is a linear operator from $\mathbb{R}^d$ to itself. Show that* $\mathrm{Graph}A$ *is lagrangian if and only if A is symmetric for the canonical euclidean structure on $\mathbb{R}^d$: $\langle Ax, y\rangle = \langle x, Ay\rangle$. Of course, not all linear lagrangian subspaces of $\mathbb{R}^d \times (\mathbb{R}^d)^*$ are of this form : for instance, $\{0\} \times \mathbb{R}^d$ is not a graph.*

Exercise 4.4. *Generalization : let X be a smooth manifold and consider T^*X endowed with its usual symplectic structure. Let $\Omega \subset X$ be an open subset of X, and let a be a smooth 1–form on Ω. Consider the graph* $\mathrm{Graph}\, a = \{(x, a_x)\} \subset T^*\Omega$. *Show that* $\mathrm{Graph}\, a$ *is lagrangian if and only if the 1–form a is closed : $da = 0$.*

In particular, if Ω is simply connected, this implies the existence of a smooth function $S : \Omega \longrightarrow \mathbb{R}$ such that $a = dS$. The function S is called a generating function of the lagrangian manifold $\mathrm{Graph}\, a$.

This gives us more examples of lagrangian submanifolds !

We denote $\pi : T^*X \longrightarrow X$ the canonical projection.

Definition 4.5. *Let $\mathcal{L} \subset T^*X$ be a lagrangian submanifold. The* caustic *of $\mathcal{L}$ is the set of points $z \in \mathcal{L}$ such that the restriction of π to $\mathcal{L}$ is not a local diffeomorphism at z.*

If z does not belong to the caustic, Exercise 4.4 shows there is a neighbourhood of z in $\mathcal{L}$ which is the graph of the differential of a function S (defined up to an additive constant). We say S is a generating function of $\mathcal{L}$ near z.

What happens on the caustic ?

Let $S(x,\theta)$ be a real–valued function on $\Omega_X \times \Omega_{\mathbb{R}^N}$ where Ω_X is an open subset of X and $\Omega_{\mathbb{R}^N}$ an open subset of $\mathbb{R}^N$. Let $C_S = \big\{(x,\theta), \frac{\partial S}{\partial \theta} = 0\big\}$. On C_S we assume that all the differentials $d_{(x,\theta)}\frac{\partial S}{\partial \theta_i}$ $(i = 1, \ldots, N)$ are linearly independent : then C_S is a smooth d–dimensional submanifold of $\Omega_X \times \Omega_{\mathbb{R}^N}$ (recall $d = dim\, X$). Define $j_S : C_S \longrightarrow T^*X$ by $j_S(x,\theta) = (x, \partial_x S(x,\theta))$.

Proposition 4.6. *The map j_S is an immersion. Its image,*

$$\mathcal{L}_S = \{(x,\xi) \in T^*X,\ \textit{there exists } \theta/\partial_\theta S(x,\theta) = 0 \textit{ and } \xi = \partial_x S(x,\theta)\}$$

is a lagrangian submanifold of T^*X.

One calls $S(.,\theta)$ a generating family (or generating function) of $\mathcal{L}_S$. Compare with (1.24).

Theorem 4.7. *Every lagrangian submanifold $\mathcal{L}$ of T^*X admits, locally, a generating family. More precisely : for $z_0 \in \mathcal{L}$, let $N = dim\, Ker\, d\pi_{z_0}$. There is a neighbourhood Ω of z_0 in T^*X, an open subset Ω_X of X and an open subset $\Omega_{\mathbb{R}^N}$ of $\mathbb{R}^N$, and finally a function $S : \Omega_X \times \Omega_{\mathbb{R}^N} \longrightarrow \mathbb{R}$ satisfying all the required conditions, such that*

$$\mathcal{L} \cap \Omega = \mathcal{L}_S.$$

Proof: Using (4.1) we see it is enough to consider the case $X = \mathbb{R}^d$. Let $z_0 = (x_0, \xi_0) \in T^*\mathbb{R}^d = \mathbb{R}^d \times (\mathbb{R}^d)^*$ and let $L = T_{z_0}\mathcal{L}$. It is a lagrangian linear subspace of $\mathbb{R}^d \times (\mathbb{R}^d)^*$. Let $p : \mathbb{R}^d \times (\mathbb{R}^d)^* \longrightarrow \mathbb{R}^d$ be the projection on the first coordinate. By assumption, $F = p(L)$ is a linear subspace of $\mathbb{R}^d$ of dimension $d - N$. Let G be a supplementary subspace of F in $\mathbb{R}^d$: $\mathbb{R}^d = F \oplus G$. We have a corresponding decomposition of the dual space, $\mathbb{R}^*_d = G^\circ \oplus F^\circ$, where F° is the space of linear forms vanishing on F, and similarly for G°. We leave it to the reader to check that the projection $P : L \longrightarrow F \times F^\circ$ is an isomorphism.

Since L is tangent to $\mathcal{L}$ at z_0, there is a neighbourhood Ω of z_0 such that $P : \mathcal{L} \longrightarrow F \times F^\circ$ is a diffeomorphism. In other words, there is a smooth map $\varphi : (F \times F^\circ) \cap \Omega \longrightarrow G \times G^\circ$ such that $\mathcal{L} \cap \Omega$ is the graph of φ. Writing $\varphi = (f, g)$ we have

$$\mathcal{L} \cap \Omega = \{(x_F, f(x_F, \xi_{F^\circ}), g(x_F, \xi_{F^\circ}), \xi_{F^\circ}), x_F \in F, \xi_{F^\circ} \in F^\circ\}.$$

For $\mathcal{L}$ to be lagrangian we must have $df \wedge d\xi_{F^\circ} + dx_F \wedge dg = 0$, in other words $d(fd\xi_{F^\circ} - gdx_F) = 0$. This means there exists, in a neighbourhood of z_0, a function $S(x_F, \xi_{F^\circ})$ such that $dS = fd\xi_{F^\circ} - gdx_F$ (equivalently, $f = \partial_{\xi_{F^\circ}} S, g = -\partial_{x_F} S$). Consider the function

$$\mathcal{S}(x_F, x_G, \xi_{F^\circ}) = \xi_{F^\circ}.x_G - S(x_F, \xi_{F^\circ})$$

defined on an open subset of $F \times G \times F^\circ = \mathbb{R}^d \times F^\circ$. It is now straightforward to check this is a generating function of $\mathcal{L} \cap \Omega$, and $dim\, F^\circ = N$ as announced. $\square$

Example 4.8. *Here is a fundamental example : in $T^*\mathbb{R}^d = \mathbb{R}^d \times (\mathbb{R}^d)^*$ endowed with the canonical symplectic form $\sum_{i=1}^d dq_i \wedge dp_i$, a generating function for $T^*_x\mathbb{R}^d = \{x\} \times (\mathbb{R}^d)^*$ is $S(y, \theta) = \sum_{i=1}^d \theta_i(y_i - x_i) = \langle \theta, y - x\rangle$ (here $N = d$ and θ varies in $\mathbb{R}^d$).*

Exercise 4.9. *A crucial thing : (i) Show that a (connected) lagrangian submanifold $\mathcal{L}$ is invariant under the hamiltonian flow of H if and only if it is contained in some fixed energy layer $\{H = E\}$.*

(ii) As a particular case, deduce that if $H(x, d_xS(x, \theta)) = E$ for any (x, θ), then the lagrangian manifold $\mathcal{L}_S$ generated by S is invariant under the hamiltonian flow.

(iii) Assume now that S is a smooth function of (t, x, θ), and assume that

$$\frac{\partial S}{\partial t} + H(x, d_x S) = 0$$

for all (t, x, θ). Denote $S_t(x, \theta) = S(t, x, \theta)$. Show that the lagrangian manifold $\mathcal{L}_{S_t}$ is the image of $\mathcal{L}_{S_0}$ under g^t. Hint : reduce the problem to the previous one by considering the hamiltonian $\overline{H}(x, t, \xi, E) = H(x, \xi) + E$ on $T^*(X \times \mathbb{R})$.

4.2 Lagrangian distributions.

Let $\mathcal{L}$ be a lagrangian submanifold of T^*X. For our applications we shall only be interested in the case where $\mathcal{L}$ is relatively compact and where it has a global generating function S : $\mathcal{L} = \mathcal{L}_S$, S being defined on $\Omega_X \times \Omega_{\mathbb{R}^N}$. In this case we define the notion of a lagrangian function associated to $\mathcal{L}$ as follows :

Definition 4.10. *We denote $O^m(X, \mathcal{L}_S)$ the space of functions of the form*

$$u_\hbar(x) = \frac{e^{i\alpha(\hbar)}}{(2\pi\hbar)^{N/2}} \int_{\Omega_{\mathbb{R}^N}} e^{i\frac{S(x,\theta)}{\hbar}} a_\hbar(x, \theta) d\theta$$

where

– *$\alpha(\hbar)$ is a real number depending on $\hbar$,*

– *the function a defined on $\Omega_X \times \Omega_{\mathbb{R}^N}$ is smooth and has an asymptotic development when $\hbar \longrightarrow 0$,*

$$a \sim \sum_{j=0}^{\infty} \hbar^{j+m} a_{j+m},$$

the asymptotic development holds in all C^k–norms on compact subsets,

– *we assume that a is compactly supported with respect to the variable θ.*

As usual, the class $O^m(X, \mathcal{L}_S)$ should actually be defined *modulo negligible functions,* which, we recall, are smooth functions $u_\hbar$ for which all the C^k–norms on compact sets are $O(\hbar^\infty)$. Then, one can prove [GS94] that the definition of $O^m(X, \mathcal{L}_S)$ does not depend on the choice of the generating function S :

Theorem 4.11. *If $\mathcal{L}_S = \mathcal{L}_{S'}$ then $O^m(X, \mathcal{L}_S) = O^m(X, \mathcal{L}_{S'})$.*

Example 4.12. *On $X = \mathbb{R}^d$, the Dirac mass at x*

$$\delta_x(y) = \frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^d} e^{\frac{\langle \xi, y-x \rangle}{\hbar}} d\xi$$

can be seen as a lagrangian distribution associated with the lagrangian submanifold $T_x^*\mathbb{R}^d$ ($S(y,\xi) = \langle \xi, y-x\rangle$), but note that the symbol $a(y,\xi) \equiv 1$ is not compactly supported. Let $\chi(y,\xi)$ be a smooth, positive, compactly supported function, call Ω a bounded open set containing the support of χ. Then the function

$$\delta_x^\chi(y) = \frac{1}{(2\pi\hbar)^d}\int \mathrm{e}^{\frac{\langle \xi, y-x\rangle}{\hbar}}\chi(y,\xi)d\xi$$

falls into the class $O^{-d/2}(\mathbb{R}^d, T_x^*\mathbb{R}^d \cap \Omega)$. Assume χ takes the constant value 1 in a neighbourhood of a certain compact subset $\mathcal{E} \subset T^*\mathbb{R}^d$. Then δ_x^χ is often called a "delta–function truncated away from $\mathcal{E}$" : it is a Dirac mass whose frequencies near $\mathcal{E}$ have not been touched, while the frequencies out of Ω have been removed.

4.3 WKB description of the operator $U^t = \exp(it\hbar\frac{\triangle}{2})$.

Remark 4.13. *The initials WKB stand for Wentzel, Kramers and Brillouin, who independently proposed this method to find approximate solutions of a 1-d* stationary *Schrödinger equation — in other words, to find approximate eigenfunctions [Wtz26, Kr26, Brill26]. The method was later generalized by Keller and Maslov to higher dimension, but it only works for completely integrable systems [Kell58, Masl65].*

Here we present the WKB method applied to the evolutive *Schrödinger equation. It was first used by Van Vleck [VV28].*

Consider an initial state $u(0)$ of the form $u(0,x) = a_\hbar(0,x)\,\mathrm{e}^{\frac{i}{\hbar}S(0,x)}$, where $S(0,\bullet)$, $a_\hbar(0,\bullet)$ are smooth functions defined on a subset of $\Omega \subset X$, $a_\hbar$ has a fixed compact support in Ω and has an asymptotic development $a_\hbar \sim \sum_k \hbar^k\, a_k$, valid in all C^n–norms. This represents a WKB (or Lagrangian) state, supported on the Lagrangian manifold $\mathcal{L}(0) = \{(x, d_xS(0,x)),\ x \in \Omega\}$.

The WKB method consists in looking for an approximate expression[1] for the state $\tilde{u}(t) \stackrel{\text{def}}{=} U^t u(0)$, in the form

$$u(t,x) = \mathrm{e}^{\frac{iS(t,x)}{\hbar}}\, a_\hbar(t,x) = \mathrm{e}^{\frac{iS(t,x)}{\hbar}} \sum_{k=0}^{N-1} \hbar^k a_k(t,x) \tag{4.3}$$

where N is a fixed, arbitrarily large integer. We want $u(t)$ to solve $\frac{\partial u}{\partial t} = i\hbar\frac{\triangle_x u}{2}$ up to a remainder of order $\hbar^N$. Computing explicitly both sides of the equation, and identifying the successive powers of $\hbar$, we see that the

[1] often called an Ansatz

functions S and a_k must satisfy the following partial differential equations:

$$\begin{cases} \frac{\partial S}{\partial t} + H(x, d_x S) = 0 \quad \text{(Hamilton-Jacobi equation)} \\ \\ \frac{\partial a_0}{\partial t} = -\langle d_x a_0, d_x S(t,x)\rangle - a_0 \frac{\triangle_x S(t,x)}{2} \quad \text{(0-th transport equation)}\,, \\ \\ \frac{\partial a_k}{\partial t} = \frac{i \triangle a_{k-1}}{2} - \langle da_k, dS\rangle - a_k \frac{\triangle S}{2} \quad (k\text{-th transport equation})\,. \end{cases} \tag{4.4}$$

Assume that, on a certain time interval — say $s \in [0,1]$ — the above equations have a well defined smooth solution $S(s,x)$, meaning that the transported Lagrangian manifold $\mathcal{L}(s) = \phi_H^s \mathcal{L}(0)$ is of the form $\mathcal{L}(s) = \{(x, d_x S(s,x))\}$, where $S(s)$ is a smooth function on the open set $\pi\mathcal{L}(s)$. Under these conditions, we denote as follows the induced flow on X:

$$G_s^t : x \in \pi\mathcal{L}(s) \mapsto \pi g^{t-s}\big(x, d_x S(s,x)\big) \in \pi\mathcal{L}(t)\,, \tag{4.5}$$

In the first chapter we introduced the *exponential map* associated to $\mathcal{L}_s$: we have $G_s^t = \exp_{\mathcal{L}_s}^{t-s} \circ \pi^{-1}$. Note that $G_s^s = I$ and that the following composition rule holds : $G_{t_1}^{t_2} \circ G_{t_0}^{t_1} = G_{t_0}^{t_2}$.

We then introduce the following (unitary) operator T_s^t, which transports functions on $\pi\mathcal{L}(s)$ into functions on $\pi\mathcal{L}(t)$:

$$T_s^t(a)(x) = a \circ G_t^s(x)\ J_t^s(x)^{1/2}\,. \tag{4.6}$$

Here $J_t^s(x)$ is the Jacobian of the map G_t^s at the point x (measured with respect to the Riemannian volume on X). It is given by

$$J_s^t(x) = \exp\Big\{ \int_s^t \triangle S\big(\tau, G_s^\tau(x)\big)\, d\tau \Big\}\,. \tag{4.7}$$

We leave it as an exercise to check this formula, and to deduce that the 0-th transport equation in (4.4) is explicitly solved by

$$a_0(t) = T_0^t\, a_0\,, \quad t \in [0,1]\,. \tag{4.8}$$

The higher-order terms $k \geq 1$ are given by

$$a_k(t) = T_0^t a_k + \int_0^t T_s^t \left(\frac{i \triangle a_{k-1}}{2}(s) \right) ds\,. \tag{4.9}$$

The function $u(t,x)$ defined by (4.3) satisfies the approximate equation

$$\frac{\partial u}{\partial t} = i\hbar \frac{\triangle u}{2} - i\hbar^N\, \mathrm{e}^{\frac{i}{\hbar} S(t,x)} \frac{\triangle a_{N-1}}{2}(t,x)\,.$$

From Duhamel's principle and the unitarity of U^t, the difference between $u(t)$ and the exact solution $\tilde{u}(t)$ is bounded, for $t \in [0,1]$, by

$$\|u(t) - \tilde{u}(t)\|_{L^2} \leq \frac{\hbar^N}{2} \int_0^t \|\triangle a_{N-1}(s)\|_{L^2}\, ds \leq C\, t\, \hbar^N \Big(\sum_{k=0}^{N-1} \|a_k(0)\|_{C^{2(N-k)}} \Big)\,. \tag{4.10}$$

The constant C is controlled by the volumes of the sets $\pi\mathfrak{L}(s)$ $(0 \leq s \leq t \leq 1)$, and by a certain number of derivatives of the flow G_t^s $(0 \leq s \leq t \leq 1)$.

Remark 4.14. *Elaborating on these methods, one proves the following : if u is a lagrangian state in $O^m(X, \mathfrak{L})$, then $U^t u$ is a lagrangian state in $O^m(X, g^t\mathfrak{L})$. We have proved it in the particular case when $g^t\mathfrak{L}$ is a graph over X for all t. The operator U^t is called a* Fourier Integral Operator *associated with the transformation g^t.*

This is the property Schrödinger had looked for when introducing his equation. We have, in addition, found the explicit formula for all the $a_k(t)$. For $k = 0$, equation (4.8) *is called the Van Vleck formula.*

Exercise 4.15. *Check the equations* (4.4)*, and note they also hold in the presence of a potential V.*

4.4 Proof of the main estimate.

4.4.1 Decomposition of $\mathrm{Op}(\chi)u$ into truncated delta–functions.

We prove Theorem 3.7 about the norm of the operator

$$\hat{P}_{\alpha_n}(n)\hat{P}_{\alpha_{n-1}}(n-1)...\hat{P}_{\alpha_0}\,\mathrm{Op}(\chi) = U^{-n}\hat{P}_{\alpha_n}U\hat{P}_{\alpha_{n-1}}...U\hat{P}_{\alpha_0}\,\mathrm{Op}(\chi)$$

(where we denote $U^t = \exp(ith\frac{\triangle}{2})$ and $U = U^1$). Since U^t is unitary, the norm of this operator is also the same as the norm of $\hat{P}_{\alpha_n}U\hat{P}_{\alpha_{n-1}}...U\hat{P}_{\alpha_0}\,\mathrm{Op}(\chi)$.

The pseudo-differential operator $\mathrm{Op}(\chi)$ is defined in §1.4.3 :

$$\mathrm{Op}(\chi) = \sum_l \varphi_l\; \mathrm{OP}(\chi)\; \varphi_l$$

where (φ_l) is an auxiliary partition of unity on X $(\sum_l \varphi_l(x)^2 \equiv 1)$ such that the support of each φ_l is endowed with local coordinates in $\mathbb{R}^d$. In local coordinates in the support of φ_l, $\mathrm{OP}(\chi)$ is then defined by the usual formula,

$$\mathrm{OP}(\chi)u(x) = (2\pi\hbar)^{-d} \int u(z) e^{i\frac{\langle \xi, x-z\rangle}{\hbar}} \chi(z,\xi) dz d\xi. \tag{4.11}$$

The function χ will be chosen of the form $\chi(z,\xi) = \chi_1(|\xi|_z)$ where χ_1 is a smooth function on $\mathbb{R}_+$ supported in $[1-\varepsilon/2, 1+\varepsilon/2]$ with $\chi_1 \equiv 1$ in a neighbourhood of 1. For $x \in \Omega_{\alpha_0}$, we can write

$$\mathrm{Op}(\chi)u(x) = \sum_l \int u(z)\delta_z^l(x) dz, \tag{4.12}$$

where we denote δ_z^l the truncated δ-function

$$\delta_z^l(x) = \varphi_l(x)\varphi_l(z) \int e^{\frac{i\langle \xi, x-z\rangle}{\hbar}} \chi(z,\xi) \frac{d\xi}{(2\pi\hbar)^d}. \tag{4.13}$$

Each δ_z^l is a lagrangian state associated with the lagrangian manifold $T_z^* X \cap H^{-1}\left((\frac{1}{2}-\varepsilon, \frac{1}{2}+\varepsilon)\right)$. Equation (4.12) means that every state in the image of $\mathrm{Op}(\chi)$ can be decomposed as an integral combination of the lagrangian states δ_z^l. If we can estimate the norm of $\hat{P}_{\alpha_n} U \hat{P}_{\alpha_{n-1}} \ldots U \hat{P}_{\alpha_0} \delta_z^l$ for any z, we can use (4.12) to estimate the norm of $\hat{P}_{\alpha_n} U \hat{P}_{\alpha_{n-1}} \ldots U \hat{P}_{\alpha_0} \mathrm{Op}(\chi) u$ for arbitrary u, by writing

$$\begin{aligned} \|\hat{P}_{\alpha_n} U \hat{P}_{\alpha_{n-1}} \ldots U \hat{P}_{\alpha_0} \mathrm{Op}(\chi) u\| &\leq \sum_l \sup_z \|\hat{P}_{\alpha_n} U \hat{P}_{\alpha_{n-1}} \ldots U \hat{P}_{\alpha_0} \delta_z^l\| \int_X |u(y)| dy \\ &\leq \sum_l \sup_z \|\hat{P}_{\alpha_n} U \hat{P}_{\alpha_{n-1}} \ldots U \hat{P}_{\alpha_0} \delta_z^l\| \sqrt{\mathrm{Vol}\, X} \|u\|_{L^2(X)} \end{aligned}$$

The estimates will be done by induction on n: we will propose an Ansatz – that is, an approximate expression – for $\hat{P}_{\alpha_n} U \hat{P}_{\alpha_{n-1}} \ldots U \hat{P}_{\alpha_0} \delta_z^l$, valid for "large" n. In what follows we omit the ^{l} superscript and just consider δ_z.

4.4.2 The Ansatz for $n = 1$.

At $n = 0$ we know that $\hat{P}_{\alpha_0} \delta_z(x)$ is a lagrangian state associated with the lagrangian manifold $\mathcal{L}^0 = T_z^* X \cap H^{-1}\left((\frac{1}{2}-\varepsilon, \frac{1}{2}+\varepsilon)\right)$, a union of spheres $H^{-1}(\frac{1}{2}+\eta) \cap T_z^* X$.

From Remark 4.14, we know that $U^t \hat{P}_{\alpha_0} \delta_z$ is a lagrangian state associated to

$$\mathcal{L}^0(t) = g^t \left(T_z^* X \cap H^{-1}\left((\frac{1}{2}-\varepsilon, \frac{1}{2}+\varepsilon) \right) \right).$$

If we assume that the injectivity radius of X is greater than $1+100\varepsilon$, then this is a graph over X for $0 < t < 1+\varepsilon$. This is just saying that the exponential map $\exp_z^t$ is a diffeormorphism from $T_z^* X \cap H^{-1}\left((\frac{1}{2}-\varepsilon, \frac{1}{2}+\varepsilon)\right)$ onto its image, for $0 < t < 1+\varepsilon$.

This means we have an Ansatz

$$U^t \hat{P}_{\alpha_0} \delta_z \sim (2\pi\hbar)^{-d/2} e^{\frac{iS^0(t,x|z)}{\hbar}} \big(\sum_{k=0}^{\infty} \hbar^k b_k^0(t,x|z) \big). \tag{4.14}$$

The function $S^0(t,x)$ is a generating function of the lagrangian manifold $\mathcal{L}^0(t)$.

Taking $t = 1$, we denote

$$v^0(1;x|z) = e^{\frac{iS^0(t,x|z)}{\hbar}} b_\hbar^0(1,x|z), \tag{4.15}$$

$$b_\hbar^0(1,x|z) \stackrel{\text{def}}{=} \big(\textstyle\sum_{k=0}^{N-1} \hbar^k b_k^0(1,x|z) \big) \tag{4.16}$$

It gives us an approximation to $U \hat{P}_{\alpha_0} \delta_z$, the difference being bounded in L^2–norm by $O(\hbar^{N-\frac{d}{2}})$.

4.4.3 Iteration of the WKB Ansätze

In this section we will obtain an approximate Ansatz for $\hat{P}_{\alpha_n} \dots U\hat{P}_{\alpha_1} U\hat{P}_{\alpha_0}\delta_z$. Above we have already performed the first step, obtaining an approximation $v^0(1|z)$ of $U\hat{P}_{\alpha_0}\delta_z$. Until Lemma 4.16 we will fix the base point z, and omit it in our notations when no confusion may arise; at the end we will obtain an estimate which is uniform in z.

Applying the multiplication operator $\hat{P}_{\alpha_1}$ to the state $v^0(1) := v^0(1|z)$, we obtain another WKB state which we denote as follows:

$$v^1(0,x) = b^1_\hbar(0,x)\,\mathrm{e}^{\frac{i}{\hbar}S^1(0,x)}\,,\qquad \text{with}\qquad \begin{cases} S^1(0,x) := S^0(1,x|z)\,,\\ b^1_\hbar(0,x) := \hat{P}_{\alpha_1}(x)\, b^0_\hbar(1,x|z)\,. \end{cases}$$

This state is associated with the lagrangian manifold

$$\mathcal{L}^1(0) = \mathcal{L}^0(1) \cap T^*\Omega_{\alpha_1}\,.$$

If this intersection is empty, then $v^1(0) = 0$, which means that $\hat{P}_{\alpha_1} U\, v(0|z) = \mathcal{O}(\hbar^N)$ in L^2 norm. In the opposite case, we can evolve $v^1(0)$ following the procedure described in §4.3. For $t \in [0,1]$, and up to an error $\mathcal{O}_{L^2}(\hbar^N)$, the evolved state $U^t v^1(0)$ is given by the WKB Ansatz

$$v^1(t,x) = b^1_\hbar(t,x)\,\mathrm{e}^{\frac{i}{\hbar}S^1(t,x)}\,,\qquad b^1_\hbar(t) = \sum_{k=0}^{N-1} b^1_k(t)\,.$$

The state $v^1(t)$ is associated with the Lagrangian $\mathcal{L}^1(t) = g^t\,\mathcal{L}^1(0)$, and the function $b^1_\hbar(t)$ is supported inside $\pi\mathcal{L}^1(t)$.

Evolved Lagrangians

We can iterate this procedure, obtaining a sequence of approximations

$$v^j(t) = U^t\,\hat{P}_{\alpha_j} v^{j-1}(1) + \mathcal{O}(\hbar^N)\,,\quad \text{where}\quad v^j(t,x) = v^j(t,x|z) = b^j_\hbar(t,x|z)\,\mathrm{e}^{\frac{i}{\hbar}S^j(t,x|z)}\,. \tag{4.17}$$

(Again, z is fixed for the moment, and we will not always indicate in the notations the z-dependence). To show that this procedure is consistent, we must check that the Lagrangian manifold $\mathcal{L}^j(t)$ supporting $v^j(t)$ does not develop caustics through the evolution ($t \in [0,1]$), and that the projection $\pi : \mathcal{L}^j(t) \to X$ remains injective. These were the conditions required to apply the WKB method.

We now show that these properties hold, due to the assumptions on the classical flow.

The manifolds $\mathcal{L}^j(t)$ are obtained by the following procedure. Knowing $\mathcal{L}^{j-1}(1)$, which is generated by the phase function $S^{j-1}(1)$, we take for $\mathcal{L}^j(0)$ the intersection

$$\mathcal{L}^j(0) = \mathcal{L}^{j-1}(1) \cap T^*\Omega_{\alpha_j}\,.$$

If this set is empty, we then stop the construction. Otherwise, this Lagrangian is evolved into $\mathcal{L}^j(t) = g^t \mathcal{L}^j(0)$ for $t \in [0,1]$. Notice that the Lagrangian $\mathcal{L}^j(t)$ corresponds to evolution at time $j+t$ of a piece of $\mathcal{L}^0(0)$: it is made up of the image under the geodesic flow of a compact piece of the fiber T_z^*X. If the geodesic flow is Anosov, the geodesic flow has no conjugate points — by a result of Klingenberg [Kl74]. This means precisely that $g^t\mathcal{L}^0(0)$ will not develop caustics.

Because the injectivity radius is $\geq 1+100\varepsilon$, any point $x \in \Omega_{\alpha_j}$ can be connected to another point $x' \in X$ by at most one geodesic of length $\leq 1+\varepsilon$. This ensures that, for any $j \geq 1$, $0 \leq t \leq 1$, the manifold $\mathcal{L}^j(t)$ projects injectively to $\pi\mathcal{L}^j$.

Finally, we recall that $\mathcal{L}^0(0)$ was obtained by propagating a piece of $T_z^*X \cap H^{-1}(\frac{1}{2}-\varepsilon, \frac{1}{2}+\varepsilon)$. Since the geodesic flow on each energy layer $H^{-1}(1/2+\eta)$ is Anosov, the sphere bundle $H^{-1}(1/2+\eta) \cap T_z^*X$ is uniformly transverse to the strong stable foliation in $H^{-1}(1/2+\eta)$ — also a result of [Kl74].

As a result, under the geodesic flow a piece of sphere $H^{-1}(1/2+\eta)\cap T_z^*X$ becomes exponentially close to an unstable leaf of $H^{-1}(1/2+\eta)$ when $t \to +\infty$. This transversality of spheres with the stable foliation is crucial in our choice of the "basis" δ_z.

Exponential decay.

We now analyze the behaviour of the symbols $b_\hbar^j(t,x)$ appearing in (4.17), when $j\to\infty$. These symbols are constructed iteratively: starting from the function $b_\hbar^{j-1}(1) = \sum_{k=0}^{N-1} b_k^{j-1}(1)$ supported inside $\pi\mathcal{L}^{j-1}(0)$, we define

$$b_\hbar^j(0,x) = \hat{P}_{\alpha_j}(x)\, b_\hbar^{j-1}(1,x)\,, \qquad x \in \pi\mathcal{L}^j(0)\,. \tag{4.18}$$

The WKB procedure of §4.3 shows that for any $t\in[0,1]$,

$$U^t\, v^j(0) = v^j(t) + R_N^j(t)\,, \tag{4.19}$$

where the transported symbol $b_\hbar^{j-1}(t) = \sum_{k=0}^{N-1} \hbar^k\, b_k^{j-1}(t)$ is supported inside $\pi\mathcal{L}^j(t)$. The remainder satisfies

$$\|R_N^j(t)\| \leq C\, t\, \hbar^N \Big(\sum_{k=0}^{N-1} \|b_k^j(0)\|_{C^{2(N-k)}} \Big)\,. \tag{4.20}$$

To control this remainder when $j\to\infty$, we need to bound from above the derivatives of $b_\hbar^j$. Lemma 4.16 below shows that all terms $b_k^j(t)$ and their derivatives decay exponentially when $j\to\infty$, due to the Jacobian appearing in (4.6).

To understand the reasons of the decay, we first look at the principal symbol $b_0^j(1,x)$. It satisfies the following recurrence:

$$b_0^j(1,x) = T_j^{j+1}(\hat{P}_{\alpha_j} \times b_0^{j-1}(1))(x) = (\hat{P}_{\alpha_j} \times b_0^{j-1}(1)) \circ G_{j+1}^j(x)\sqrt{J_{j+1}^j(x)}\,; \tag{4.21}$$

using similar notations as above, the transport map $G_{s,t}$ is defined, for $j \leq s,\ t \leq j+1$, by $G_{s,t} := \exp_{\mathcal{L}^j(s-j)}^{t-s} \circ \pi^{-1}$, and maps $\pi\mathcal{L}^j(s-j)$ to $\pi\,\mathcal{L}^j\,(t-j)$. We denote J_s^t the jacobian of G_s^t. We recall that $G_{n-1}^n G_{n-2}^{n-1} \dots G_1^2 = G_1^n$, where both sides are defined.

Iterating this expression, and using the fact that $0 \leq \hat{P}_{\alpha_j} \leq 1$, we get at time n and for any $x \in \pi\mathcal{L}^n(0)$:

$$|b_0^n(0,x)| \leq |b_0^0(1, G_n^1(x))| \times \Big(J_n^{n-1}(x) J_{n-1}^{n-2}(G_n^{n-1}x) \dots J_2^1(G_3^2(x))\Big)^{1/2}. \tag{4.22}$$

By the chain rule, this product of jacobians is simply $J_n^1(x)^{1/2} = J_1^n(G_n^1(x))^{-1/2}$.

Recall that $\mathcal{L}^0(0)$ intersected with each energy layer $S^{1+\eta}X := \{\xi \in T^*X, \|\xi\| = 1+\eta\}$ is just a piece of the sphere $S_z^{1+\eta}X$. Thus, if $d(x,z) = 1+\eta$, the jacobian $J_1^n(G_n^1(x))$ measures the expansion rate of the sphere $g^n(S_z^{1+\eta}X)$: in dimension d and curvature $\equiv -1$, it grows asymptotically like $e^{(d-1)(1+\eta)n}$ when $n \to \infty$. If $x \in \pi\mathcal{L}^1(0)$ (and if this last set is non-empty) we have $d(x,z) \leq 1+\varepsilon$ (because $\mathcal{L}^0(0)$ is contained in $H^{-1}(\frac{1}{2}-\varepsilon, \frac{1}{2}+\varepsilon)$). We obtain the following estimate on the principal symbol $b_0^n(0)$:

$$\forall n \geq 1 \quad \|b_0^n(0)\|_\infty \leq \|b_0^0(1)\|_\infty \,[\exp(-n(d-1-\varepsilon))]^{1/2} \tag{4.23}$$

The following lemma, which we shall not prove here, shows that the upper bound extends to the full symbol $b_\hbar^n(0,x)$ and its derivatives.

Lemma 4.16. *Take any index $0 \leq k \leq N$ and $m \leq 2(N-k)$. Then there exists a constant $C(k,m)$ such that*

$$\forall n \geq 1,\ \forall x \in \pi\mathcal{L}^n(0), \qquad |d^m b_k^n(0,x|z)| \leq C(k,m)\, n^{m+3k}\,[\exp(-n(d-1-\varepsilon))]^{1/2}. \tag{4.24}$$

This bound is uniform with respect to the initial point z. For $(k,m) \neq (0,0)$, the constant $C(k,m)$ depends on the partition $\mathcal{P}^{(0)}$, while $C(0,0)$ does not.

Taking into account the fact that the remainders $R_N^j(1)$ are dominated by the derivatives of the b_k^j (see (4.20)), the above statement translates into

$$\forall j \geq 1, \qquad \|R_N^j(1)\|_{L^2} \leq C(N)\, j^{3N}\,[\exp(-n(d-1-\varepsilon))]^{1/2}\,\hbar^N.$$

A crucial fact for us is that the above bound also holds for the propagated remainder $\hat{P}_{\alpha_n} U \cdots U \hat{P}_{\alpha_{j+1}} R_N^j(1)$, due to the fact that the operators $\hat{P}_{\alpha_j} U$ have norms less than 1. As a result, the total error at time n is bounded from above by the sum of the errors $\|R_N^j(1)\|$. We obtain the following estimate for any $n > 0$:

$$\|\hat{P}_{\alpha_n} U \hat{P}_{\alpha_{n-1}} \cdots \hat{P}_{\alpha_1} v^0(1|z) - v^n(0|z)\| \leq C(N)\, \hbar^N \sum_{j=0}^{n} j^{3N} \left[\exp(-n(d-1-\varepsilon))\right]^{1/2}. \tag{4.25}$$

The last term is bounded by $C(N)\hbar^N$. This bound is uniform with respect to the initial point z.

4.4.4 Conclusion.

From (4.25), to estimate the norm of the vector $\hat{P}_{\alpha_n} U \hat{P}_{\alpha_{n-1}} \cdots \hat{P}_{\alpha_1} v^0(1|z)$ up to $O(\hbar^N)$, we can use our Ansatz $v^n(0|z)$. From (4.24) and the definition (4.17) of $v^n(0|z)$, we see that

$$\|v^n(0|z)\|_{L^2(X)} \leq \left[\exp(-n(d-1-\varepsilon))\right]^{1/2} \sum_{k=0}^{N-1} C(k,0)\hbar^k n^{3k}. \tag{4.26}$$

As required in Theorem 3.7, let us now take an arbitrary large $\mathcal{K}$, and $n = \mathcal{K}|\log \hbar|$. In the inequalities (4.23) and (4.26), the right hand term is bounded *below* by a fixed power of $\hbar$ (more precisely, $\hbar^{-\frac{1}{2}\mathcal{K}(d-1-\varepsilon)}$). Thus, we will choose N, the order of our WKB expansion, so that the remainder (4.25) is negligible compared to $\hbar^{-\frac{1}{2}\mathcal{K}(d-1-\varepsilon)}$.

Now, remember the relation (4.14) between $v^0(1|z)$ and $U\hat{P}_{\alpha_0}\delta_z$: note in particular the normalization factor $(2\pi\hbar)^{-d/2}$. The combination of (4.25) and (4.26) gives us

$$\|\hat{P}_{\alpha_n} U \hat{P}_{\alpha_{n-1}} \cdots \hat{P}_{\alpha_1} U\, \hat{P}_{\alpha_0}\delta_z\|_{L^2(X)} \leq \frac{2}{(2\pi\hbar)^{d/2}} \left[\exp(-n(d-1-\varepsilon))\right]^{1/2} \tag{4.27}$$

for $n = \mathcal{K}|\log \hbar|$ and $\hbar \leq \hbar_{\mathcal{K}}$.

Combined with (4.12) and the subsequent discussion, we find

$$\|\hat{P}_{\alpha_n} U \hat{P}_{\alpha_{n-1}} ... U \hat{P}_{\alpha_0}\, \mathrm{Op}(\chi) u\| \leq \frac{2l\sqrt{\mathrm{Vol}\, X}}{(2\pi\hbar)^{d/2}} \|u\|_{L^2(X)} \left[\exp(-n(d-1-\varepsilon))\right]^{1/2}$$

which is the announced result.

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