The Semi-Classical Egorov Theorem on Riemannian Manifolds

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1 Introduction

The mechanics of our everyday world are accurately described by the laws of Newton's classical mechanics, whereas on the much smaller scale of atoms and molecules such a description can only be achieved in the framework of quantum mechanics. Of course the physical laws on the small scale completely determine those on a larger one. So the question that naturally arises is if and how classical mechanics can be regarded as a certain scaling limit of quantum mechanics.
The answer to this question should also shed some light on the circumstances under which classical mechanics provide a valid description of a system.

Let us now review the mathematical framework in that this question can be precisely formulated and answered. We will formulate both theories in terms of their observables, i.e. quantities of the system that can be measured by an observer.

In classical mechanics we can represent the state of a system by the current positions x and momenta p of the particles in the system, which corresponds to a point in phase space. The dynamics of this system are determined by the Hamiltonian total energy function h, for example $h = \frac{p^2}{2m} + V(x)$ for particles of mass m moving in a potential V. An observable a is represented by a real valued function on phase space and its equation of motion is the Liouville equation

(1.1) $$\frac{da}{dt} = -\{h, a\} = \frac{\partial h}{\partial p}\frac{\partial a}{\partial x} - \frac{\partial h}{\partial x}\frac{\partial a}{\partial p}$$

where $\{\ ,\ \}$ is called the Poisson bracket.
By contrast in quantum mechanics a state ψ is a vector in the Hilbert space of square integrable functions on configuration space X, that is the space of the particles' positions only. Its evolution in time is determined by the Schrï¿½dinger equation

(1.2) $$i\hbar\frac{\partial \psi}{\partial t} = H\psi$$

where H is a self-adjoint linear operator on $L^2(X)$ called the Hamiltonian. For N particles with equal masses moving in a potential V and Euclidean space we would have $H = -\frac{\hbar^2}{2m}\Delta + V(x)$ where Δ is the Laplace operator on $\mathbb{R}^{3N}$. The observables of quantum mechanics are the self-adjoint operators on $L^2(X)$. They obey the Heisenberg equation

(1.3) $$\frac{dA}{dt} = \frac{i}{\hbar}[H, A] = \frac{i}{\hbar}(HA - AH)$$

Observe that in these equations $\hbar$ fixes an energy scale. So the limit of high energies, where one expects classical mechanics to be valid, is mathematically described by the limit $\hbar \to 0$. This is called the semi-classical limit.
There are cases where the equations have this structure but the scaling-parameter is actually not $\hbar$. For example it could be the mass-ratio of electrons versus nuclei as in the Born-Oppenheimer approximation. In section 3.2 we present the example of constraint quantum dynamics which somewhat generalises this approximation.
To avoid confusion we now introduce the semi-classical parameter ε and consider $\varepsilon \to 0$ as the semi-classical limit .

In order to compare these theories we need to find a correspondence between their respective observables. Since there may be quantum observables that do not correspond to any classical quantity this means we want to find a 'quantisation' map taking functions on phase space to self-adjoint operators. This allows us to identify classical and quantum systems when quantisation maps the respective Hamiltonians to one another. Given this map and the identification of the systems we can compare the dynamics on both levels.

The Egorov Theorem states that they are close in the sense that the difference of the time evolutions of an observable is of order ε. To put this more precisely let Op() be the quantisation map, then there is a constant C_T such that for all $t \in [0, T]$

(1.4) $\|\mathrm{Op}(a)(t) - \mathrm{Op}(a(t))\|_{\mathcal{L}(L^2(X))} \leq C_T \varepsilon$

To prove this theorem of course one needs to specify the quantisation map as well as the classes of observables and spaces for which it is supposed to hold. A simple proof for the case $X = \mathbb{R}^d$ can be found in the book by Robert [Rob]. This result was extended to compact Riemannian manifolds by Schubert [Sch] and to observables on an extended phase space by Uribe and Paul [PU]. Here we will present a detailed proof in the setting where the configuration space X is a Riemannian manifold of bounded geometry (see 1.2 for a definition) and phase space is the cotangent bundle T^*X. To get a quantisation formula we will develop a (semi-classical) calculus of pseudodifferential operators based on the work of Pflaum [Pfl1, Pfl2] and Safarov [Saf]. From this we will get an explicit dependence of the error on the curvature, showing in particular that the approximation is one order better if the curvature is zero.
An important field of application for the Egorov Theorem is quantum chaos, the study of quantum systems whose corresponding classical systems have some 'chaotic' property like ergodicity, mixing or unstable fixed points. A survey of this field can be found in the article by Zelditch [Zel].

1.1 Notation

First of all let us introduce some notation: Let $\alpha = (\alpha_1, \dots, \alpha_d) \in \mathbb{N}^d$ be a multiindex and $x = (x_1, \dots, x_d) \in \mathbb{R}^d$. We put

$$(1.5)\quad |\alpha| = \sum_{j=1}^{d} \alpha_j \qquad \alpha! = \prod_{j=1}^{d} \alpha_j! \qquad x^\alpha = \prod_{j=1}^{d} x_j^{\alpha_j}$$

Let (X, g) be a Riemannian manifold of dimension d, $p : TX \to X$ its tangent and $\pi : T^*X \to X$ its cotangent bundle.
When $\xi \in T_x^*X$, $v \in T_xX$ we write $v^2 = |v|^2 = g(v, v)$, $\xi^2 = g(\xi, \xi)$ and denote by $\langle v, \xi \rangle = \xi(v)$ the duality bracket.

We define the L^2 product of $f, g \in \mathcal{C}_0^\infty(X)$ by $\langle f, g \rangle = \int_X \overline{f(x)} g(x) dx$, where dx denotes the canonical volume density.
The space $L^2(X)$ is the completion of $\mathcal{C}_0^\infty(X)$ under the norm $\|f\|_{L^2} = \sqrt{\langle f, f \rangle}$.
The formal adjoint of a linear operator A is the operator A^* such that $\langle f, Ag \rangle = \langle A^* f, g \rangle$ for all $f, g \in \mathcal{C}_0^\infty(X)$ and the transpose A^T is the operator that satisfies this equation for all $f, g \in \mathcal{C}_0^\infty(X, \mathbb{R})$.
An unbounded linear operator on $L^2(X)$ is a tuple $(A, D(A))$ where the domain $D(A)$ is a linear subspace of $L^2(X)$ and $A : D(A) \to L^2(X)$. Such an operator is called symmetric if $D(A)$ is dense and $\langle f, Ag \rangle = \langle Af, g \rangle$ for all $f, g \in D(A)$. If additionally $D(A^*) := \{f \in L^2(X) : \exists h \ \forall g \in D(A) : \ \langle f, Ag \rangle = \langle h, g \rangle\} = D(A)$ then A is called self-adjoint.

The capital letter C will be used to denote various constants that may differ even in a single equation.

1.2 Normal Coordinates and Manifolds of Bounded Geometry

On a Riemannian manifold we have a set of natural coordinates, called geodesic or normal coordinates, that can be calculated from the metric. Here we will introduce these coordinates and derive some identities for later use. In this context we also define manifolds of bounded geometry on which we have a natural way to define functions with globally bounded derivatives.

For every $x \in X$ there exists a neighbourhood U_x such that for all $y \in U_x$ there is a unique geodesic of minimal length $\gamma_{x,y}$ in U_x joining x and y. If we take $\gamma_{x,y}(1) = y$ then $|\dot\gamma_{x,y}(0)|$ is the length of the geodesic. Identification of y and $z_x(y) := \dot\gamma_{x,y}(0)$ gives rise to a diffeomorphism $\exp_x : V \subset T_xX \to U_x$, $\exp_x z_x(y) = \gamma_{x,y}(1) = y$.
Let $\rho(x)$ be the supremum of all $r > 0$ for which $\exp_x : B_x(0, r) \to U_{x,r}$ is a diffeomorphism and define the injectivity radius of X as $\rho_X = \inf_{x \in X} \rho(x)$.

Clearly for $r < \rho_X$ $\exp_x : B_x(0,r) \to U_{x,r}$ is a diffeomorphism for every $x \in X$.
Choosing an orthonormal basis $(e_j)_{j\leq d}$ of T_xX gives us normal (also called canonical or geodesic) coordinates z_x on U_x via

$$(1.6)\quad z_x^k(y) = g\left(\exp_x^{-1} y, e_k\right) = g(\dot{\gamma}_{x,y}(0), e_k)$$

Obviously $z_x(x) = 0$ and $\frac{\partial}{\partial z_x^k}\Big|_x = e_k$ in these coordinates so the coefficients of the metric tensor in x are $g_{kl}(x) = g(e_k, e_l) = \delta_{kl}$.

The coordinate functions z_x^k of course depend on the choice of orthonormal basis $(e_j)_{j\leq d}$, but we can compare normal coordinte systems based at different (sufficiently close) points x, y by choosing such a basis in one of them (say x) and the basis induced by the orthonormal frame (1.10) in y.

Definition 1.1. A Riemannian manifold X is of *bounded geometry* if

1. $\rho_X > 0$
2. The transition functions between normal coordinate charts have bounded derivatives to any order, i.e. if $r < \rho_X$ and $U_{y,r} \cap U_{x,r} \neq \emptyset$, then for every multiindex α there is a constant $C_{\alpha,r}$ (independent of x and y) such that:

   $$(1.7)\quad \left|\frac{\partial^{|\alpha|} z_x}{\partial z_y^\alpha}\right| \leq C_{\alpha,r}$$

   on $U_{y,r} \cap U_{x,r}$.

This definition is discussed in more detail in [Shu]. Examples are compact manifolds or covering manifolds thereof and Lie groups, which of course include $\mathbb{R}^d$.
$\rho_X > 0$ implies that every geodesic can be extended indefinetely, so X is geodesically complete and by the Hopf-Rinow theorem (see [Jos]) the closed and bounded sets $K \subset M$ are compact.
Bounded geometry provides a notion of $\mathcal{C}^k$-bounded functions

Definition 1.2. Let X be of bounded geometry. $f \in \mathcal{C}^k(X)$ has *bounded derivatives up to order* k, write $f \in \mathcal{C}_b^k(X)$, if for every multiindex α with $|\alpha| \leq k$ and $r < \rho_X$ there is a constant $C_{\alpha,r}$ for which

$$(1.8)\quad \left|\frac{\partial^{|\alpha|}}{\partial z_x^\alpha} f\right| \leq C_{\alpha,r}$$

on every patch of normal coordinates $z_x : U_{x,r} \to \mathbb{R}^d$.

Of course this definition can also be given without bounded geometry but it would not be as natural since the derivatives $\frac{\partial^{|\alpha|}}{\partial z_x^\alpha}\Big|_x f$ would have to decay in regions where the derivatives of coordinate changes are large.

Normal coordinates also induce bundle coordinates (z_x, ζ_x) on T^*U_x by

$$(1.9)\quad \xi_y = \sum_k \zeta_{x,k}(\xi) dz_x^k(y)$$

Now let $\Psi_{x,y}(t) : T_xX \to T_{\gamma_{x,y}(t)}X$ and $\Phi_{x,y}(t) : T_x^*X \to T^*_{\gamma_{x,y}(t)}X$ be parallel transport along $\gamma_{x,y}$ with respect to the Levi-Civita connection, where the latter is defined by identification of T_x^*X with T_xX through g. $g(\Psi_{x,y}v, \Psi_{x,y}w)$ and $\langle \dot\gamma_{x,y}, \Phi_{x,y}\xi\rangle$ are constant along $\gamma_{x,y}$ because the connection is metric and therefore $\Psi_{x,y}$ and $\Phi_{x,y}$ are orthogonal maps.
We define an orthonormal frame E of TU_x by

$$(1.10)\quad e_k(y) = \Psi_{x,y} e_k$$

and see that this gives us $z_x^k(y) = g(\dot\gamma_{x,y}(1), e_k(y)) = -z_y^k(x)$ because $\dot\gamma_{x,y}(1) = -\dot\gamma_{y,x}(0)$. Let R be the curvature tensor. In local coordinates $x = (x^1, \dots, x^d)$ with $\partial_k = \frac{\partial}{\partial x^k}$ we put

$$(1.11)\quad g\left(R(\partial_k, \partial_l)\partial_m, \partial_n\right) = R_{klmn} = \sum_j g_{jk} R^j_{lmn}$$

and define the Ricci- and scalar curvatures by

$$(1.12)\quad \mathrm{Ric}_{kl}(x) = \sum_m R^m_{kml}(x) \qquad \text{and} \qquad \kappa(x) = \sum_{k,l} g^{kl}(x) R_{kl}(x)$$

We have the identities (see for example [dC, p. 93])

$$(1.13)\quad \begin{aligned} R^k_{lmn} + R^k_{nlm} + R^k_{mnl} &= 0 \\ R_{klmn} &= R_{mnkl} \\ R_{klmn} &= -R_{klnm} \\ \mathrm{Ric}_{kl} &= \mathrm{Ric}_{lk} \end{aligned}$$

If X is of bounded geometry the coeffecients of the curvature and metric tensors and their derivatives are bounded by global constants when written in normal coordinates on patches $U_{x,r}$ with $r < \rho_X$. To calculate some important geometric quantities we now make use of the expansion of the metric in normal coordinates around x derived in the book of Berline, Getzler and Vergne [BGV, p. 36].

$$(1.14)\quad g_{kl}(y) = \delta_{kl} - \frac{1}{3}\sum_{m,n} R_{kmln}(x) z_x^m(y) z_x^n(y) + \mathcal{O}(|z_x(y)|^3)$$

First of all we compute the Christoffel symbols

$$(1.15)\quad \Gamma^k_{lm}(x) = \frac{1}{2}\sum_n \left[\frac{\partial}{\partial z_x^l} g_{mn} + \frac{\partial}{\partial z_x^m} g_{nl} - \frac{\partial}{\partial z_x^n} g_{lm}\right] g^{nk} = 0$$

Then put $G(y) = \sqrt{\det g_{kl}(y)}$ and see that the Laplace-Beltrami Operator takes the form

$$(1.16)\quad \Delta f(x) = G^{-1}(x) \sum_{k,l} \frac{\partial}{\partial z_x^l} \left[G(x) g^{lk}(x) \frac{\partial}{\partial z_x^k} f(x) \right] = \sum_k \frac{\partial^2}{\partial (z_x^k)^2} f(x)$$

Next we introduce $\Theta_x(y) : T_y X \to T_y X$ as the change of basis

$$(1.17)\quad \left.\frac{\partial}{\partial z_x^k}\right|_y = \sum_{j=1}^d \Theta_k^j e_j(y)$$

We have (see [BGV]) $|\Theta_x(y)| := |\det \Theta_x(y)| = |\det(D_{z_x} \exp_x)| = G(y)$ and thus write $|\Theta_x(v)| = |\det(D_v \exp_x)|$. Θ_x has the local expansion:

$$(1.18)\quad \Theta_l^k = \delta_l^k - \frac{1}{6} \sum_{m,n} R_{mln}^k z_x^m(y) z_x^n(y) + \mathcal{O}(|z_x|^3)$$

from which we see that

(1.19)

$$\begin{aligned} \left.\frac{\partial^2 |\Theta_x|}{\partial z_x^k \partial z_x^l}\right|_x &= \sum_{\sigma \in S_d} \operatorname{sgn} \sigma \left[\underbrace{\sum_{m \neq n} \left.\frac{\partial \Theta_{\sigma(m)}^m}{\partial z_x^k}\right|_x \left.\frac{\partial \Theta_{\sigma(n)}^n}{\partial z_x^l}\right|_x}_{=0} \prod_{j \neq m,n} \Theta_{\sigma(j)}^j + \sum_m \left.\frac{\partial^2 \Theta_{\sigma(m)}^m}{\partial z_x^k \partial z_x^l}\right|_x \prod_{j \neq m} \underbrace{\Theta_{\sigma(j)}^j}_{=\delta_{\sigma(j)}^j} \right] \\ &= -\frac{1}{6} \sum_{m=1}^d \left(R_{lmk}^m(x) + R_{kml}^m(x) \right) = -\frac{1}{3} \operatorname{Ric}_{kl}(x) \end{aligned}$$

Now $\Theta_x(\tilde{y})$ is invertible for $\tilde{y} \in U_x$ so we can use the equation

$$(1.20)\quad \left.\frac{\partial}{\partial z_y^k}\right|_{\tilde{y}} = \sum_{l,m} (\Theta_y)_k^l \left(\Theta_x^{-1}\right)_l^m \left.\frac{\partial}{\partial z_x^m}\right|_{\tilde{y}}$$

together with (1.18) to calculate the derivatives of coordinate changes

$$(1.21)\quad \begin{aligned} \left.\frac{\partial z_x^j}{\partial z_y^k}\right|_{\tilde{y}} &= \sum_{l,m} (\Theta_y)_k^l \left(\Theta_x^{-1}\right)_l^m \delta_m^j \\ &= \delta_k^j + \frac{1}{6} \sum_{l,m} \left[R_{lkm}^j(x) z_x^l(\tilde{y}) z_x^m(\tilde{y}) - R_{lkm}^j(y) z_y^l(\tilde{y}) z_y^m(\tilde{y}) \right] + \mathcal{O}(|z_x + z_y|^3) \end{aligned}$$

$$(1.22)\quad \begin{aligned} \left.\frac{\partial^2 z_x^j}{\partial z_y^l z_y^k}\right|_{\tilde{y}} = \frac{1}{6} \sum_m \Big[&\left(R_{lkm}^j(x) + R_{mkl}^j(x) \right) z_x^m(\tilde{y}) - \left(R_{lkm}^j(y) + R_{mkl}^j(y) \right) z_y^m(\tilde{y}) \Big] \\ &+ \mathcal{O}(|z_x + z_y|^2) \end{aligned}$$

2 Pseudodifferential Operators on Manifolds

In this chapter we introduce a semi-classical (with parameter ε) pseudodifferential calculus on manifolds of bounded geometry as the main tool for the proof of the Egorov Theorem. We will start by specifying classes of (complex valued) observables, called symbols, for which we then define a quantisation map and its inverse, the symbol map. We will also establish the relationship between bounded symbols and bounded operators that we need to get the estimate (1.4) in the operator norm. For this we will need global bounds on symbols and their derivatives, so it will be convenient to restrict ourselves to manifolds of bounded geometry.
In the following sections we study products of pseudodifferential operators to be able to express the Heisenberg equation on the level of symbols and introduce another quantisation formula, Weyl quantisation, mapping real valued symbols to symmetric operators and thus giving the desired relation for the physical observables.

We want results that do not depend on some choice of coordinates so we try to formulate everything in a coordinate-free way and whenever we need to do a calculation in local coordinates we use normal coordinates as these are intrinsically defined. Our results will then only depend on the geodesics on X. They are consequently independent of the representation in coordinates but depend of course on the metric.
Safarov [Saf] treats the more general case of manifolds with a linear connection and gets similar results depending on that connection.

The calculus we get is a slightly modified version of that described by Pflaum in [Pfl2], from where we have also taken most of the ideas for the proofs. The formulas for Weyl quantisation and the Weyl symbol are due to Safarov [Saf] and similar formulas can be found in [Pfl1].

2.1 Spaces of Symbols and Asymptotic Expansions

From now on let (X, g) be a Riemannian manifold of bounded geometry and, for simplicity, connected.

Definition 2.1. A function $a \in \mathcal{C}^\infty(T^*X)$ is called a *symbol of order* $\mu \in \mathbb{R}$ if for every $r < \rho_X$ and multiindices α, β there are constants $C_{r,\alpha,\beta}$ such that for every normal coordinate chart $z_y : U_{y,r} \to \mathbb{R}^d$ we have

$$\left|\frac{\partial^{|\alpha|}}{\partial z_y^\alpha}\frac{\partial^{|\beta|}}{\partial \zeta_y^\beta} a(x,\xi)\right| \le C_{r,\alpha,\beta}(1+|\xi|)^{\mu-|\beta|} \tag{2.1}$$

for every $(x, \xi) \in T^*U_{y,r}$.

We denote the space of symbols of order μ by $S^\mu(T^*X)$ (or just S^μ) and define $S^{-\infty}(T^*X) = \bigcap_{\mu\in\mathbb{R}} S^\mu(T^*X)$ as well as $S^\infty(T^*X) = \bigcup_{\mu\in\mathbb{R}} S^\mu(T^*X)$.

To check if a function $a \in \mathcal{C}^\infty(T^*X)$ is a symbol of order μ it suffices to check this in normal coordinates centered at $x = \pi(\xi)$ for every $x \in X$.

Proposition 2.2. *Let $a \in \mathcal{C}^\infty(T^*X)$. If for all multiindices α, β there are constants $C_{\alpha,\beta}$ such that*

$$\left|\frac{\partial^{|\alpha|}}{\partial z_x^\alpha}\right|_{\pi(\xi)=x}\frac{\partial^{|\beta|}}{\partial \zeta_x^\beta} a(\pi(\xi),\xi)\right| \le C_{\alpha,\beta}(1+|\xi|)^{\mu-|\beta|} \tag{2.2}$$

then $a \in S^\mu$.

Proof. Let $r < \rho_X$ and $z_y : U_{y,r} \to \mathbb{R}^d$ be a normal coordinate chart. For $x \in U_{y,r}$ we have $\zeta_{x,k} = \sum_l \zeta_{y,l}\frac{\partial z_y^l}{\partial z_x^k}$, so

$$\begin{aligned}\frac{\partial a(x,\xi)}{\partial \zeta_{y,k}} &= \sum_l \frac{\partial z_y^k}{\partial z_x^l}\frac{\partial a(x,\xi)}{\partial \zeta_{x,l}}\\ \frac{\partial a(x,\xi)}{\partial z_y^k} &= \sum_{l,m} \frac{\partial z_x^l}{\partial z_y^k}\frac{\partial a(x,\xi)}{\partial z_x^l} + \frac{\partial a(x,\xi)}{\partial \zeta_{x,l}}\frac{\partial}{\partial z_y^k}\frac{\partial z_y^m}{\partial z_x^l}\zeta_{x,m}\end{aligned} \tag{2.3}$$

Observe that in the last term the growth coming from ζ_x is cancelled by the derivative in the same variable. Now by the definition of bounded geometry 1.1 the derivatives of coordinate changes are bounded by a constant that depends only on r and the order of differentiation. This gives us the required estimate for first order derivatives and those for higher orders follow inductively. □

Example 2.3.

a) If $a \in \mathcal{C}_b^\infty(X)$ then $a \circ \pi \in S^0(T^*X)$.

b) Let $V \in \mathcal{C}_b^\infty(X)$, then $a(x,\xi) = \xi^2 + V(x) \in S^2(T^*X)$.

c) For $a \in S^\mu$ and $b \in S^\nu$ we obviously have $a + b \in S^{\max(\mu,\nu)}$ and $ab \in S^{\mu+\nu}$ by Leibniz' rule.

Later on we will be interested in expansions of symbols with respect to a parameter ε. We say that a function $f \in \mathcal{C}^\infty(T^*X)$ is of order ε^n in $S^\mu(X)$ and write $f = \mathcal{O}^\mu(\varepsilon^n)$ if there is $\varepsilon_0 > 0$ such that $\varepsilon^{-n} f \in S^\mu(X)$ (with constants independent of ε) for all $\varepsilon \in (0, \varepsilon_0]$. A symbol is $\mathcal{O}^\mu(\varepsilon^\infty)$ if it is $\mathcal{O}^\mu(\varepsilon^k)$ for every k.
Next we define the notion of asymptotic expansion.

Definition 2.4. A symbol $a \in S^\mu$ has the asymptotic expansion

$$(2.4)\quad a \sim \sum_{k=0}^{\infty} \varepsilon^k a_k$$

if $a_k \in S^\mu$ for every k and

$$(2.5)\quad a - \sum_{k=0}^{N} \varepsilon^k a_k = \mathcal{O}^\mu(\varepsilon^{N+1})$$

It is a standard result (see the lecture notes by Evans and Zworski [EZ]) that an expansion of this form always defines a symbol in S^μ that is unique up to $\mathcal{O}^\mu(\varepsilon^\infty)$.

The symbols we have just defined have global bounds, i.e. the constants in (2.1) are independent of the coordinate neighbourhood in which we take the estimate. Usually this is only required locally, so our symbol classes are subclasses of those defined for example in [Hör, Pfl2, Saf]. These classes coincide when X is compact.
We could also consider more general symbol classes as done in [Pfl2, Saf]. For example they could take values in vector bundles over X or differentiation could have a modified influence on decay. Most of these generalisations do not change much in the theory but may overburden the presentation, so we will stick to our simple case here.

2.2 Quantisation by Oscillatory Integrals

The basic idea of the quantisation map is that on $\mathbb{R}^{3N}$ the kinetic energy operator $H_0 := -\frac{\hbar^2}{2m}\Delta$ has the 'Fourier-representation' $\frac{p^2}{2m}$ which is just the classical kinetic energy if we interpret p as momentum. More precisely if $\mathcal{F}$ is the Fourier transform with inverse $\mathcal{F}^{-1}$ then for $f \in D(H_0)$

$$(2.6)\quad -\frac{\hbar^2}{2m}\Delta f = \mathcal{F}^{-1}\left[\frac{p^2}{2m}\left(\mathcal{F}f\right)(p)\right]$$

First we define the Fourier transform for symbols of order $-\infty$, which are functions that decrease rapidly in every fibre.

$$\begin{aligned} &\mathcal{F} : S^{-\infty}(TX) \to S^{-\infty}(T^*X) \\ &(\mathcal{F}a)(x,\xi) = \int_{T_xX} e^{-i\langle v,\xi\rangle/\varepsilon} a(x,v) dv \end{aligned} \tag{2.7}$$

and

$$\begin{aligned} &\mathcal{F}^{-1} : S^{-\infty}(T^*X) \to S^{-\infty}(TX) \\ &\left(\mathcal{F}^{-1}a\right)(x,v) = \frac{1}{(2\pi\varepsilon)^d} \int_{T_xX} e^{i\langle v,\xi\rangle/\varepsilon} a(x,\xi) d\xi \end{aligned} \tag{2.8}$$

Here dv and $d\xi$ denote the volume densities induced by g on T_xX and T_x^*X, i.e. integration is with respect to the Lebesgue measure with lengths measured by g. Since integration is only over $T_xX \cong \mathbb{R}^d$ all the standard results for the Fourier transform are valid. In particular $\mathcal{F}^{-1}$ is the inverse of $\mathcal{F}$. This is expressed by the formula

$$\frac{1}{(2\pi\varepsilon)^d} \int_{T_xX} \int_{T_x^*X} e^{-i\langle v-w,\xi\rangle/\varepsilon} a(x,v) dv d\xi = a(x,w) \tag{2.9}$$

Let $a \in S^\mu(X)$ with $\mu < -d$. Then the integral

$$I_a(x,v) = \frac{1}{(2\pi\varepsilon)^d} \int_{T_x^*X} e^{-i\langle v,\xi\rangle/\varepsilon} a(x,\xi) d\xi \tag{2.10}$$

exists in the sense of Lebesgue for every $v \in T_xX$.
In particular if $y \in V_x$ for a normal coordinate neighbourhood of x we can put $I_a(x,y) = I_a(x, z_x(y))$ and interpret this as a (x-dependent) distribution on $\mathcal{C}_0^\infty(V_x)$ by

$$I_a(x)f = \int_{V_x} I_a(x,y) f(y) dy \tag{2.11}$$

We generalise this idea to define an operator associated to a symbol by using suitable cutoffs.

Definition 2.5. Let $r < \rho_X$ and $W \subset V \subset \{(x,v) \in TX : |v| < r\}$ be neighbourhoods of the zero section.
Let $\psi : TX \to [0,1]$ be a smooth cutoff function with $\mathrm{supp}\psi \subset V$ and $\psi|_W \equiv 1$. Then the map $(\pi, \exp) : V \to U \subset X \times X$ is a diffeomorphism and $\exp_x(V_x) \subset U_{x,r}$ is a normal coordinate neighbourhood of x. Let $\psi_x(y) = \psi(x, z_x(y)) \in \mathcal{C}_b^\infty(X \times X)$.

Define the phase function $\varphi : X \times T^*X|_U \to \mathbb{C}$ by $\varphi(y,(x,\xi)) = \langle z_x(y), \xi\rangle$.

Then the *quantisation of* $a \in S^\mu(X)$ (with cutoff ψ) is a linear map $\mathcal{C}_0^\infty(X) \to \mathcal{C}^\infty(X)$ given by

$$(2.12)\quad \begin{aligned}(\mathrm{Op}_\psi(a) f)(x) &= \frac{1}{(2\pi\varepsilon)^d}\int_X \int_{T_x^*X} \psi_x(y) e^{-i\varphi(y,(x,\xi))/\varepsilon} a(x,\xi) f(y) d\xi dy \\ &= \frac{1}{(2\pi\varepsilon)^d}\int_{T_xX}\int_{T_x^*X} |\Theta_x(v)| \psi(x,v) e^{-i\langle v,\xi\rangle/\varepsilon} a(x,\xi) f(\exp_x v) d\xi dv\end{aligned}$$

This is clearly a linear map, but at first this definition only makes sense when $\mu < -d$.

For better understanding let us examine this definition in the case $X = \mathbb{R}^d$. The phase function reads $\varphi(y,(x,\xi)) = \langle y - x, \xi\rangle$, where it is instructive to note that $y - x$ is the vector pointing straightly from x to $y = \exp_x(y-x)$, where we evaluate f.
Furthermnore $|\Theta_x(v)| \equiv 1$ so the formula simplifies to

$$(2.13)\quad (\mathrm{Op}_\psi(a) f)(x) = \frac{1}{(2\pi\varepsilon)^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \psi(x, y-x) e^{-i\langle y-x,\xi\rangle/\varepsilon} a(x,\xi) f(y) d\xi dy$$

This is just the usual quantisation formula for $X = \mathbb{R}^d$ apart from the introduction of the cutoff function. We will see later that this is only a minor diffenerence.
Now we can view (2.12) as the natural geometric generalisation of the usual definition by replacing vectors that 'point' somewhere by the tangent vectors to the geodesics ending in that point (and restricting ourselves to neighbourhoods where this makes unambiguous sense).

In order to extend the definition we take $a \in S^\mu(X)$ and approximate it by $a_n(x,\xi) = \chi(\xi/n) a(x,\xi) \in S^{-\infty}(X)$, where χ is a smooth cutoff function with $\chi \equiv 1$ on $B_{\pi(\xi)}(0,1)$,and make use of the following

Lemma 2.6. *Let $U_{x,r}$ be a normal coordinate neighbourhood of x with $r < \rho_X$, then there is a first order differential operator L on $U_{x,r} \times T^*U_{x,r}$ for which*

i) $Le^{-i\varphi/\varepsilon} = e^{-i\varphi/\varepsilon}$

ii) $(L^T)^k\,[a(x,\xi)f(y)] \in S^{\mu-k}(T^*U_{x,r})$ *for* $a \in S^\mu$, $f \in \mathcal{C}_0^\infty(U_{x,r})$ *and every* $y \in U_{x,r}$

Proof. Take

$$(2.14)\quad L = \frac{1}{1+\xi^2}\sum_{j=1}^d \left(1 + i\varepsilon\zeta_{x,j}\frac{\partial}{\partial z_x^j}\right)$$

in normal coordinates around x, which clearly satisfies the first equation. Now writing the integral in these coordinates and integrating by parts gives

$$(2.15)\quad L^T\phi = \frac{1}{|\Theta_x|\,(1+\xi^2)}\sum_{j=1}^d \left(1 - i\varepsilon\zeta_{x,j}\frac{\partial}{\partial z_x^j}\right)(|\Theta_x|\,\phi)$$

then we have $(L^T)^k(af) \in S^{\mu-k}(T^*U_x)$ for every $y \in U_{x,r}$ because X is of bounded geometry and example 2.3c). □

Now put $f^\psi(x,v) = \psi(x,v) f(\exp_x v)$ and calculate

$$\begin{aligned}
\operatorname{Op}_\psi(a_n) &= \frac{1}{(2\pi\varepsilon)^d} \int_X \int_{T_x^*X} \psi_x(y) a_n(x,\xi) f(y) e^{-i\varphi(y,(x,\xi))/\varepsilon} d\xi dy \\
&= \frac{1}{(2\pi\varepsilon)^d} \int_X \int_{T_x^*X} \psi_x(y) a_n(x,\xi) f(y) L^k e^{-i\varphi(y,(x,\xi))/\varepsilon} d\xi dy \\
&= \frac{1}{(2\pi\varepsilon)^d} \int_X \int_{T_x^*X} \chi(\xi/n) e^{-i\varphi(y,(x,\xi))/\varepsilon} (L^T)^k \left[\psi_x(y) a(x,\xi) f(y)\right] d\xi dy
\end{aligned} \tag{2.16}$$

which does not depend on k by equality to the first line.
Now $\left|\chi(\xi/n)(L^T)^k(af^\psi)\right| \leq \left|(L^T)^k(af^\psi)\right|$ which is an integrable function when $\mu - k < -d$ by lemma 2.6. So we can apply the dominated convergence theorem to find that the limit for $n \to \infty$ of the integral equals

$$\frac{1}{(2\pi\varepsilon)^d} \int_X \int_{T_x^*X} e^{-i\varphi(y,(x,\xi))/\varepsilon} (L^T)^k \left[\psi_x(y) a(x,\xi) f(y)\right] d\xi dy \tag{2.17}$$

and take this as the definition of $\operatorname{Op}_\psi(a) f$ for arbitrary μ.
Finally the bounds on the derivatives of a and the fact that f has compact support ensure that $\operatorname{Op}_\psi(a) f \in \mathcal{C}^\infty(X)$.

Now that we have shown that $I_a(x)f$ makes sense we formally write $I_a(x,v)$ for the (distribution valued) ξ integral.
As direct consequences of this definition we can firstly change the order of integration by

$$\begin{aligned}
&\int_X \int_{T_x^*X} \psi_x(y) e^{-i\varphi(y,(x,\xi))/\varepsilon} a(x,\xi) f(y) d\xi dy \\
&:= \int_X \int_{T_x^*X} e^{-i\varphi(y,(x,\xi))/\varepsilon} (L^T)^k \left[\psi_x(y) a(x,\xi) f(y)\right] d\xi dy \\
&= \int_{T_x^*X} \int_X e^{-i\varphi(y,(x,\xi))/\varepsilon} (L^T)^k \left[\psi_x(y) a(x,\xi) f(y)\right] dy d\xi \\
&= \int_{T_x^*X} \int_X \psi_x(y) e^{-i\varphi(y,(x,\xi))/\varepsilon} a(x,\xi) f(y) dy d\xi
\end{aligned} \tag{2.18}$$

where the last step is integration by parts in the (absolutely convergent) inner integral. The iterated integral exists in this order because f and ψ are smooth with compact supports whereas $a \in S^\mu$ grows at most polinomially. Secondly we can 'integrate by parts', i.e. if $D = \sum_{j=1}^d b_j \partial_{\xi_j} + c_j$ with $b_j \in S^0$, $c_j \in S^{-1}$, then as distibutions:

$$\frac{1}{(2\pi\varepsilon)^d} \int_{T_x^*X} a(x,\xi) D e^{-i\langle v,\xi\rangle/\varepsilon} d\xi = \frac{1}{(2\pi\varepsilon)^d} \int_{T_x^*X} e^{-i\langle v,\xi\rangle/\varepsilon} D^T a(x,\xi) d\xi \tag{2.19}$$

The quantisation of a symbol $a \in S^\mu$ is called a pseudodifferential operator (of order μ), we denote the space of these operators by Ψ^μ. This means that the elements of Ψ^μ are those linear maps $A : \mathcal{C}_0^\infty(X) \to \mathcal{C}^\infty(X)$ for which there is a cutoff ψ and $a \in S^\mu$ with $A = \mathrm{Op}_\psi(a)$.
$\Psi^{-\infty}$ is also called the space of smoothing operators because its elements map distributions with compact support to smooth functions. A pseudodifferential operator A is smoothing if and only if it's Kernel is smooth with bounded derivatives of any order, that is $Af(x) = \int_X K_A(x,y)f(y)dy$ with $K_A \in \mathcal{C}_b^\infty(X \times X)$. We will prove this in section 2.3.

Example 2.7.

a) For $a \in \mathcal{C}_b^\infty(X)$ the operator $\mathrm{Op}_\psi(a \circ \pi)$ is just pointwise multiplication by a.

b) The operator associated to a polynomial symbol that is locally of the form $a = \sum_{|\alpha|\le N} \zeta_x^\alpha (c_\alpha \circ \pi) \in S^N$ for some functions $c_\alpha \in \mathcal{C}^\infty(V_x)$ can easily be calculated in normal coordinates using $\zeta_x^\alpha e^{-i\langle v,\xi\rangle/\varepsilon} = i\varepsilon \frac{\partial^{|\alpha|}}{\partial v^\alpha} e^{-i\langle v,\xi\rangle/\varepsilon}$ and integration by parts:

(2.20)
$$\begin{aligned}(\mathrm{Op}_\psi(a)f)(x) &= \frac{1}{(2\pi\varepsilon)^d}\int_{T_xX}\int_{T_x^*X}\sum_{|\alpha|\le N}|\Theta_x|\,\psi(x,v)\zeta_x^\alpha e^{-i\langle v,\xi\rangle/\varepsilon}c_\alpha(x)f(\exp_x v)d\xi dv\\ &= \sum_{|\alpha|\le N}(-i\varepsilon)^{|\alpha|}c_\alpha(x)\mathcal{F}^{-1}\mathcal{F}\left[\frac{\partial^{|\alpha|}}{\partial v^\alpha}\left(|\Theta_x|\,\psi(x,v)f(\exp_x v)\right)\right](x,0)\\ &= \sum_{|\alpha|\le N}(-i\varepsilon)^{|\alpha|}c_\alpha(x)\frac{\partial^{|\alpha|}}{\partial z_x^\alpha}\left(|\Theta_x|\,f\right)\end{aligned}$$

So quantisation of a polynomial symbol defines a differential operator. In particular for $a = \xi^2$ we have

$$\mathrm{Op}(a)f(x) = -\varepsilon^2\sum_k\left(\frac{\partial^2}{(\partial z_x^k)^2} - \frac{1}{3}\mathrm{Ric}_{kk}(x)\right)f(x) = -\varepsilon^2\left(\Delta - \frac{\kappa(x)}{3}\right)f(x) \tag{2.21}$$

In these examples the quantisation is independent of the cutoff ψ. We will now show that this is true in general, at least up to an error of order ε^∞.

Proposition 2.8. *Let ψ and $\tilde\psi$ be two cutoff functions as in definition 2.5 and supported in V, $\tilde V$. If $a \in S^\mu$, then $Op_\psi(a) - Op_{\tilde\psi}(a)$ is $\mathcal{O}(\varepsilon^\infty)$ in $\Psi^{-\infty}$.*

Proof. First notice that $\psi - \tilde\psi$ vanishes in a neighbourhood of $\{v = 0\}$, therefore we have

$$(\psi-\tilde\psi)\left(\sum_{j=1}^d\frac{i\varepsilon v^j}{v^2}\frac{\partial}{\partial\zeta_{x,j}}\right)e^{-i\langle v,\xi\rangle/\varepsilon} = (\psi-\tilde\psi)\varepsilon De^{-i\langle v,\xi\rangle/\varepsilon} = (\psi-\tilde\psi)e^{-i\langle v,\xi\rangle/\varepsilon} \tag{2.22}$$

By (2.19) we then have for every $k \in \mathbb{N}$

$$
\begin{aligned}
&(\mathrm{Op}_{\psi}(a) - \mathrm{Op}_{\tilde{\psi}}(a))f \\
&= \frac{1}{(2\pi\varepsilon)^d} \int_{T_xX} \int_{T_x^*X} |\Theta_x| \, (\psi - \tilde{\psi}) a(x,\xi) f(exp_x v)(\varepsilon D)^k e^{-i\langle v,\xi\rangle/\varepsilon} d\xi dv \\
&= \frac{\varepsilon^k}{(2\pi\varepsilon)^d} \int_{T_xX} \int_{T_x^*X} |\Theta_x| \, (\psi - \tilde{\psi}) e^{-i\langle v,\xi\rangle/\varepsilon} f(exp_x v)(D^T)^k a(x,\xi) d\xi dv
\end{aligned} \tag{2.23}
$$

Now obviously $(D^T)^k a \in S^{\mu-k}$, so the ξ integral defining the kernel

$$
I_a(x,v) = \frac{\varepsilon^k}{(2\pi\varepsilon)^d} [\psi - \tilde{\psi}](x,v) \int_{T_x^*X} e^{-i\langle v,\xi\rangle/\varepsilon} (D^T)^k a(x,\xi) d\xi \tag{2.24}
$$

exists in the sense of Lebesgue and defines an n-times differentiable function of v if $\mu + n - k < -d$. The derivatives in x and v of this function are clearly bounded independently of (x,v) because those of $(D^T)^k a$, $\psi - \tilde{\psi}$ and any coordinate changes are. This shows that $I_a(x, z_x(y)) \in \mathcal{C}_b^\infty(X \times X)$ and thus $\mathrm{Op}_{\psi}(a) - \mathrm{Op}_{\tilde{\psi}}(a) = \mathcal{O}(\varepsilon^\infty)$ in $\Psi^{-\infty}$. □

Remark 2.9. The key point in the proof of the last proposition was that $\psi - \tilde{\psi}$ vanishes near the critical point $\{v = \xi = 0\}$ of the phase function φ. From this we can see that the properties of $I_a(x,v)$ are determined, up to an error of $\mathcal{O}(\varepsilon^\infty)$, by those of the integrand in a neighbourhood of this point.
Let us also note that a function $u(\xi)$ with the same property would have allowed for introduction of $D = \sum \frac{i\varepsilon}{\xi^2} \zeta_j \partial_v^j$ and given the same result.
We could even use an ε dependent cutoff function ψ_ε as long as differentiation with respekt to v does not loose a full order of ε, for example if $\varepsilon^k \partial_{v^j}^k \psi = \mathcal{O}(\sqrt{\varepsilon}^k)$. In the following we will often use this argument without elaborating on the calculations.

As we have just proven that the dependence of the quantisation on ψ is negligible we will write $\mathrm{Op}_{\psi}(a) = \mathrm{Op}(a)$ from now on and sometimes adjust cutoff functions as needed.

There is some freedom to choose a different quantisation map than the one defined in (2.12) and get a slightly different calculus. For example we could have written the y integral in normal coordinates straight away and without the factor $|\Theta_x|$. In this calculus the quantisation of ξ^2 is just $-\varepsilon^2\Delta$. We will see that this difference is irrelevant for the Egorov Theorem because it is of the same order as the error terms. We have chosen this version because it behaves well under coordinate changes as we will see in section 2.4.

2.3 The Symbol Map

In this section we introduce the symbol of a pseudodifferential operator as the inverse (modulo ε^∞) of the quantisation map. This is an improvement in comparison with pseudodifferential calculus defined in local coordinates, where in general only the leading order $\sigma_p \in S^\mu/S^{\mu-1}$ of a symbol can be recovered from the pseudodifferential operator.

Definition 2.10. Let $A \in \Psi^\mu$ be a pseudodifferential operator and ψ a cutoff function. The ψ-cut *symbol of* A is the function on T^*X defined by

$$\sigma_{\psi,A}(x,\xi) = A\left[\left|\Theta_x(\cdot)\right|^{-1}\psi_x(\cdot)e^{i\varphi(\cdot,(x,\xi))/\varepsilon}\right](x) \tag{2.25}$$

where A acts on the variables denoted by $(\cdot)$.

Theorem 2.11. *The map $\sigma_\psi : \Psi^\infty \to S^\infty$ is the inverse of quantisation up to an error which is asymptotically close to zero, that is*

$$\sigma_\psi(Op(a)) = a + \mathcal{O}^{-\infty}(\varepsilon^\infty) \quad \textit{and} \quad Op(\sigma_{\psi,A}) = A + \mathcal{O}(\varepsilon^\infty) \ \textit{in}\ \Psi^{-\infty} \tag{2.26}$$

Consequently σ is order-preserving and the dependence on ψ is asymptotically close to zero.

Proof. We first prove that σ is the left inverse.
Let $A = \mathrm{Op}_{\tilde\psi}(a)$ with $a \in S^\mu$. Note that $\psi' = \psi\tilde\psi$ is also a cutoff function and calculate

$$\begin{aligned}
\sigma_{\psi,A}(x,\xi) &= \frac{1}{(2\pi\varepsilon)^d}\int_X\int_{T_x^*X} e^{-i\varphi(y,(x,\zeta))/\varepsilon}a(x,\zeta)\psi_x'(y)\left|\Theta_x(y)\right|^{-1}e^{i\varphi(y,(x,\xi))/\varepsilon}d\zeta dy\\
&= \frac{1}{(2\pi\varepsilon)^d}\int_{T_xX}\int_{T_x^*X} a(x,\zeta)\psi'(x,v)e^{-i\langle v,\zeta-\xi\rangle/\varepsilon}d\zeta dv\\
&= a(x,\xi) - \frac{1}{(2\pi\varepsilon)^d}\int_{T_xX}\int_{T_x^*X}(1-\psi'(x,v))a(x,\zeta)e^{-i\langle v,\zeta-\xi\rangle/\varepsilon}d\zeta dv
\end{aligned} \tag{2.27}$$

where we have used the Fourier inversion formula (2.9). To complete the proof we need to show that the second summand is $\mathcal{O}^{-\infty}(\varepsilon^\infty)$. Since $(1-\psi')$ vanishes near $v=0$ we can proceed as in the proof of proposition 2.8 and use the differential operator $D = \sum_j \frac{i\varepsilon}{v^2}v^j\partial_{\zeta_j}$ together with integration by parts to improve the decay of a. Now check that because of $\left(D^T\right)^k a = \mathcal{O}^{\mu-k}(\varepsilon^k)$ the function

$$\widehat{\left(D^T\right)^k}a(x,v) := \int_{T_x^*X}\left(D^T\right)^k a(x,\zeta)e^{-i\langle v,\zeta\rangle/\varepsilon}d\zeta \tag{2.28}$$

is rapidly decreasing and $(k-d-\mu-1)$-times differentiable in v. Therefore

$$\frac{1}{(2\pi\varepsilon)^d}\int_{T_xX}(1-\psi'(x,v))\widehat{\left(D^T\right)^k}a(x,v)e^{i\langle v,\xi\rangle/\varepsilon} \tag{2.29}$$

is convergent and defines a smooth function b for which $\varepsilon^{-l}(1+\xi^2)^l b(x,\xi)$ is bounded when $2l < k-d-\mu-1$, so $b = \mathcal{O}^{-\infty}(\varepsilon^\infty)$.
Now by our definition of Ψ^μ every element $A \in \Psi^\infty$ is of the form $A = \mathrm{Op}_\psi(a)$ for some ψ and $a \in S^\infty$. So because σ is left inverse we have $\mathrm{Op}(\sigma_A) = \mathrm{Op}(a + \mathcal{O}^{-\infty}(\varepsilon^\infty)) = A + \mathcal{O}(\varepsilon^\infty)$ in $\Psi^{-\infty}$. □

Example 2.12.

a) We have $\frac{\partial^2 |\Theta_x(\cdot)|^{-1}}{\partial (z_x^k)^2} = -\frac{\partial^2 |\Theta_x(\cdot)|}{\partial (z_x^k)^2}$ because $\frac{\partial |\Theta_x(\cdot)|}{\partial z_x^k} = 0$, so we can calculate the symbol of the Laplace-Beltrami operator:

$$\sigma_{\psi,\varepsilon^2\Delta}(x,\xi) = \varepsilon^2 \sum_k \frac{\partial^2}{\partial (z_x^k)^2}\left[|\Theta_x(\cdot)|^{-1}\psi_x(\cdot)e^{i\varphi(\cdot,(x,\xi))/\varepsilon}\right] = -\xi^2 + \frac{\varepsilon^2}{3}\kappa(x) \tag{2.30}$$

from which we see that $\sigma_\psi(\mathrm{Op}(\xi^2)) = \xi^2$ independently of ψ.

b) Let $\mathcal{A}$ be a vector field, $\mathcal{A}_y = \sum_k g^k(y)\frac{\partial}{\partial z_x^k}$ with $g^k \in \mathcal{C}^\infty(U_{x,r})$ in normal coordinates centered at x. Let A be the operator given by: $Af = i\varepsilon df(\mathcal{A})$. The symbol of A is

$$\begin{aligned}\sigma_{\psi,A}(x,\xi) &= i\varepsilon \sum_k g^k(x)\frac{\partial}{\partial z_x^k}\left[|\Theta_x(\cdot)|^{-1}\psi_x(\cdot)e^{i\varphi(\cdot,(x,\xi))/\varepsilon}\right] \\ &= -\sum_k g^k(x)\zeta_{x,k}(\xi) = -\langle \mathcal{A}_x, \xi\rangle\end{aligned} \tag{2.31}$$

Lemma 2.13. *An operator $A : \mathcal{C}_0^\infty(X) \to \mathcal{C}^\infty(X)$ is an element of $\Psi^{-\infty}$ if and only if $Af(x) = \int_X K_A(x,y)f(y)dy$ for some $K_A \in \mathcal{C}_b^\infty(X\times X)$.*

Proof. First let $A = \mathrm{Op}_\psi(a)$ with $a \in S^{-\infty}$. Then

$$K_A(x,y) = \frac{1}{(2\pi\varepsilon)^d}\int_{T_x^*X} \psi_x(y)e^{-i\varphi(y,(x,\xi))/\varepsilon}a(x,\xi)d\xi \tag{2.32}$$

is smooth because a is rapidly decreasing and the bounds on the derivatives can easily be calculated using those for the derivatives of a, $\psi_x(y)$ and changes between normal coordinate charts.

Now let $K_A \in \mathcal{C}_b^\infty(X\times X)$. We have

$$\sigma_A(x,\xi) = \int_{T_xX} K_A(x,\exp_x v)\psi(x,v)e^{i\langle v,\xi\rangle/\varepsilon}dv \tag{2.33}$$

Because $\psi(x,v)$ has compact support in $B_x(0,r)$ we have the estimate

$$|\sigma_A(x,\xi)| \le \|K_A\|_\infty \operatorname{vol} B_x(0,r) \tag{2.34}$$

and similar estimates for the derivatives.
Furthermore we can use $\zeta_x^\alpha e^{-i\langle v,\xi\rangle/\varepsilon} = i\varepsilon\frac{\partial^{|\alpha|}}{\partial v^\alpha}e^{-i\langle v,\xi\rangle/\varepsilon}$ together with integration by parts to see that

$$\left|(1+\xi^2)^k\frac{\partial^{|\alpha|}}{\partial z_x^\alpha}\frac{\partial^{|\beta|}}{\partial \zeta_x^\beta}\sigma_A(x,\xi)\right| \le C_{k,\alpha,\beta} \tag{2.35}$$

for every k,α,β, so $\sigma_A \in S^{-\infty}$. □

2.4 Weyl-Quantisation

In this section we will introduce Weyl quantisation as a tool which directly relates the observables of classical and quantum mechanics, that are real functions on phase space and self-adjoint operators respectively.
We also recover the main results of section 2.2 for this quantisation by giving a formula expressing one quantisation in terms of the other.

Definition 2.14. Let $\gamma(t,y) = \exp_x(tz_x(y))$ and $\Phi_{x,y}(t) : T_x^*X \to T_{\gamma(t,y)}^*X$ be parallel transport along γ. Define the *Weyl quantisation* of $a \in S^\mu$ by

(2.36)
$$\begin{aligned}(\mathrm{Op}^W(a)\, f)(x) &:= \frac{1}{(2\pi\varepsilon)^d} \int_X \int_{T_x^*X} \psi_x(y) e^{-i\varphi(y,(x,\xi))/\varepsilon} a\left(\gamma(\tfrac{1}{2}, y), \Phi_{x,y}(\tfrac{1}{2})\xi\right) f(y) d\xi dy \\ &= \frac{1}{(2\pi\varepsilon)^d} \int_{T_xX} \int_{T_x^*X} |\Theta_x|\, e^{-i\langle v,\xi\rangle/\varepsilon} a\left(\exp_x(\tfrac{v}{2}), \Phi_{x,y}(\tfrac{1}{2})\xi\right) f^\psi(x,v) d\xi dv\end{aligned}$$

Proposition 2.15. *Let $a \in S^\mu$. There is $\sigma_A \in S^\mu$ such that $Op^W(a) = Op(\sigma_A)$ and vice versa. We call a the Weyl symbol of $A = Op(\sigma_A)$ and write $a = \sigma_A^W$.*

Proof. Use Taylor's formula in the normal coordinates around x to see that

$$(2.37)\quad a\left(\gamma(t,y), \Phi_{x,y}(t)\xi\right) = \sum_{|\alpha|\le N} \frac{t^{|\alpha|}}{\alpha!} z_x(y)^\alpha \frac{d^{|\alpha|}}{dz_x^\alpha}\bigg|_{x=y} a\left(y, \Phi_{x,y}\xi\right) + r_{N+1}$$

with the remainder

$$(2.38)\quad r_{N+1} = \frac{t^{N+1}}{(N+1)!} \sum_{|\alpha|=N+1} z_x(y)^\alpha \int_0^1 \frac{d^{|\alpha|}}{dz_x^\alpha}\bigg|_{y=\gamma(\tau)} a\left(y, \Phi_{x,y}\xi\right) d\tau$$

Next, substitute this expansion for a in (2.36) and use

$$(2.39)\quad z_x(y)^\alpha e^{-i\langle z_x(y),\xi\rangle/\varepsilon} = (i\varepsilon)^{|\alpha|} \partial_\xi^\alpha e^{-i\langle z_x(y),\xi\rangle/\varepsilon}$$

together with integration by parts to get

$$(2.40)\quad \sigma_A(x,\xi) = \sum_{|\alpha|\le N} \frac{1}{\alpha!} \left(\frac{-i\varepsilon}{2}\right)^{|\alpha|} \frac{\partial^{|\alpha|}}{\partial\zeta_x^\alpha} \frac{d^{|\alpha|}}{dz_x^\alpha}\bigg|_{y=x} a\left(y, \Phi_{x,y}\xi\right) + r_{N+1}$$

with $r_{N+1} = \mathcal{O}^{\mu-N-1}\left(\varepsilon^{N+1}\right)$, so $b \in S^\mu$ is obvious.
In the other direction just do the same calculation in normal coordinates around $\gamma(\frac{1}{2})$ and with $\exp_{\gamma(0.5)}\left(-\frac{1}{2}\dot\gamma\left(\frac{1}{2}\right)\right) = x$ we get

$$(2.41)\quad \sigma_A^W(x,\xi) = \sum_{|\alpha|\le N} \frac{1}{\alpha!} \left(\frac{i\varepsilon}{2}\right)^{|\alpha|} \frac{\partial^{|\alpha|}}{\partial\zeta_x^\alpha} \frac{d^{|\alpha|}}{dz_x^\alpha}\bigg|_{y=x} \sigma_A\left(y, \Phi_{x,y}\xi\right) + r_{N+1}$$

□

Example 2.16.

a) The function $\xi^2 = g(\xi,\xi)$ is invariant under parallel transport along γ, so we have $\sigma^W\left(-\varepsilon^2\Delta + \frac{\varepsilon^2}{3}\kappa(x)\right) = \sigma(\mathrm{Op}(\xi^2)) = \xi^2$.

b) Let A be the operator $Af = i\varepsilon df(\mathcal{A})$ of example 2.12b), then we have

(2.42)
$$\sigma_A^W(x,\xi) = -\langle \mathcal{A}_x, \xi\rangle - \frac{i\varepsilon}{2}\sum_{j,k}\frac{\partial}{\partial\zeta_{x,k}}\frac{\partial}{\partial z_x^k}\bigg|_{y=x} g^j(y)\zeta_{x,j}(\Phi_{x,y}\xi) = -\langle \mathcal{A}_x,\xi\rangle - \frac{i\varepsilon}{2}\operatorname{div}(\mathcal{A})$$

since $\frac{\partial}{\partial z_x^k}\Big|_{y=x}(\Phi_{x,y})^l_m = \Gamma^l_{km}(x) = 0$.

c) From the previous example we can see that

$$\text{(2.43)}\quad \mathrm{Op}^W(\langle \mathcal{A}_x,\xi\rangle) f = -Af - \frac{i\varepsilon}{2}\operatorname{div}(\mathcal{A})f = -\frac{i\varepsilon}{2}\left(d[\mathcal{A}(f)] + df(\mathcal{A})\right)$$

We get the results 2.8 and 2.26 as corollaries of Proposition 2.15

Corollary 2.17. *The dependence of $Op^W(a)$ on ψ is $\mathcal{O}(\varepsilon^\infty)$ in $\Psi^{-\infty}$.*

Corollary 2.18. *If $a \in S^0$ then $Op^W(a)$ is a bounded operator on $L^2(X)$.*

Theorem 2.19. *Let $a \in S^\mu$, then $Op^W(a)^* = Op^W(\overline{a})$ up to an error of $\mathcal{O}(\varepsilon^\infty)$ in $\Psi^{-\infty}$ coming from a change of cutoff.*

Proof. In the proof we make use of the following properties of geodesics:

$$\text{(2.44)}\quad \gamma(\tfrac{1}{2}) = \exp_x\Big(\frac{z_x(y)}{2}\Big) = \exp_y\Big(-\frac{\dot\gamma(1)}{2}\Big) = \exp_y\Big(\frac{z_y(x)}{2}\Big)$$

$$\text{(2.45)}\quad \Phi_{x,y}\left(\tfrac{1}{2}\right) = \Phi_{y,x}\left(\tfrac{1}{2}\right)\Phi_{x,y}(1)$$

Now let $f, g \in \mathcal{C}_0^\infty(X)$. Keeping in mind the formulas above we change variables with $\Phi_{x,y} : T_x^*X \to T_y^*X$, $\xi \to \Phi_{x,y}\xi := \eta$ (remember that Φ is orthogonal, so it's determinant has absolute value 1).

$$\text{(2.46)}\quad \begin{aligned}
\left\langle g, \mathrm{Op}^W(a) f\right\rangle &= \int_X \overline{g(x)}\mathrm{Op}^W(a) f(x) dx \\
&= \int_X\int_X\int_{T_y^*X} \psi_x(y) a\left(\gamma(\tfrac{1}{2}), \Phi_{y,x}(\tfrac{1}{2})\eta\right) e^{-i\langle z_x(y),\eta\rangle/\varepsilon}\overline{g(x)} f(y) d\eta dy dx \\
&= \int_X\int_X\int_{T_y^*X} f(y)\overline{\psi_x(y) a\left(\gamma(\tfrac{1}{2}), \Phi_{y,x}(\tfrac{1}{2})\eta\right) e^{-i\langle z_y(x),\eta\rangle/\varepsilon}} g(x) d\eta dx dy \\
&= \left\langle \mathrm{Op}^W(\overline{a}) g, f\right\rangle
\end{aligned}$$

where we have used $z_x(y) = -z_y(x)$ and the last equality holds if $\psi(x, z_x(y))$ behaves like an appropriate cutoff function $\tilde{\psi}(y, w)$ at y. To get a ψ with this property just let $\mathrm{supp}\psi_x \subset U_{x,\rho_X/3}$, which is a normal coordinate neighbourhood for every $y \in U_{x,\rho_X/3} \subset U_{y,2\rho_X/3}$. So if we put $w = \exp_y^{-1}(x) \in B_y(0, 2\rho_X/3) \subset T_yX$ the function $\tilde{\psi}(y, w) = \psi(x, z_x(y))$ has the required properties.

□

In this calculation we can see the benefit of defining quantisation in the way we have, with the functional determinant Θ in the integral over T_xX. However this is not the only way of defining a Weyl-quantisation such that this theorem holds, a slightly different version can be found in the paper by Pflaum [Pfl1].

Remark 2.20. The theorem just proved together with theorem 2.26 shows that if $a \in S^0$ is real, then $\mathrm{Op}^W(a)$ is formally self-adjoint in the sense that $\mathrm{Op}^W(a)^* = \mathrm{Op}^W(a)$ in $\Psi^\infty/\Psi^{-\infty}$. For symbols whose quantisations are unbounded the question of self-adjointness depends on the domains of $A = \mathrm{Op}^W(a)$ and A^* and is far more complicated. Here we have only shown that A with domain $\mathcal{C}_0^\infty(X)$ (we will see in section 2.5 that this is really a domain for A if we choose ψ right) is symmetric. In the case $X = \mathbb{R}^d$ and with some additional conditions on a Robert [Rob, chap. 3] proves that A with domain $\mathcal{S}(\mathbb{R}^d)$ has a unique self-adjoint extension.

2.5 Products of Pseudodifferential Operators and their Symbols

To prove the Egorov Theorem we will need an expression for the symbol of the commutator $[A, B]$. For this we need to understand the meaning of the operator product on the level of symbols, i.e. we want to find a composition rule '#' such that $\mathrm{Op}(a\#b) = \mathrm{Op}(a)\mathrm{Op}(b)$.

Now first of all a pseudodifferential operator is a map $\mathcal{C}_0^\infty(X) \to \mathcal{C}^\infty(X)$ so the product may not even be well defined. If we look at the quantisation formulas (2.12) and (2.36) we can observe that if for some $x \in X$ we have $f|_{U_{x,r}} \equiv 0$ then the integrands are always zero, so we have $\mathrm{Op}(a)f(x) = \mathrm{Op}^W(a)f(x) = 0$ for every $a \in S^\infty$ if $\mathrm{dist}(x, \mathrm{supp}f) > r$. Because the support of f is compact it must be bounded, i.e. if we take $x \in X$ then the function $\mathrm{dist}(x, y)$ is bounded by a constant C_x on $\mathrm{supp}f$. Therefore for y in the support of $\mathrm{Op}(a)f$ or $\mathrm{Op}^W(a)f$ we have $\mathrm{dist}(x, y) \le C_x + r$, so these supports are also compact because X is of bounded geometry. Thus the product is well defined. Let us now consider the symbol of this product:

$$\begin{aligned} \sigma_{AB}(x,\xi) &= \left[AB\left(|\Theta_x(\cdot)|^{-1}\psi_x(\cdot)e^{i\varphi(\cdot,(x,\xi))/\varepsilon}\right)\right](x) \\ &= \left[A\left(|\Theta_x|^{-1}\psi_x e^{i\varphi(\cdot,(x,\xi))/\varepsilon}\sigma_B^{ext}(\cdot,(x,\xi))\right)\right](x) + \mathcal{O}^{-\infty}(\varepsilon^\infty) \end{aligned} \tag{2.47}$$

where

$$\sigma_B^{ext}(y,(x,\xi)) = \psi_x(y)\,|\Theta_x(y)|\,e^{-i\varphi(y,(x,\xi))/\varepsilon}\left[B\left(|\Theta_x|^{-1}\,\psi_x e^{i\varphi(\cdot,(x,\xi))/\varepsilon}\right)\right](y) \tag{2.48}$$

since $1-\psi_x(\cdot)$ vanishes near the diagonal.

Lemma 2.21. *Let $a \in S^\mu$ and $A = Op(a)$. Then for any $f \in \mathcal{C}_b^\infty$ the symbol*

$$\sigma_{A,f}(x,\xi) = \left[A\left(|\Theta_x(\cdot)|^{-1}\,\psi_x(\cdot)e^{i\varphi(\cdot,(x,\xi))/\varepsilon}f(\cdot)\right)\right](x) \tag{2.49}$$

has the asymptotic expansion

$$\sigma_{A,f}(x,\xi) \sim \sum_{\alpha\in\mathbb{N}^d} \frac{(-i\varepsilon)^{|\alpha|}}{\alpha!}\left[\left.\frac{\partial^{|\alpha|}}{\partial\zeta_x^\alpha}\right|_\xi a\right]\left[\left.\frac{\partial^{|\alpha|}}{\partial z_x^\alpha}\right|_x f\right] \tag{2.50}$$

Proof. Using Taylor's formula and integrating by parts we get

(2.51)

$$\begin{aligned}
\sigma_{A,f}(x,\xi) &= \frac{1}{(2\pi\varepsilon)^d}\int_{T_xX}\int_{T_x^*X}\psi(x,v)e^{i\langle v,\xi-\zeta\rangle/\varepsilon}a(x,\zeta)f(\exp_x v)d\zeta dv\\
&= \frac{1}{(2\pi\varepsilon)^d}\int_{T_x^*X}\int_{T_xX}\psi(x,v)e^{-i\langle v,\zeta\rangle/\varepsilon}a(x,\xi+\zeta)f(\exp_x v)dvd\zeta\\
&= \frac{1}{(2\pi\varepsilon)^d}\sum_{|\alpha|\le N}\frac{1}{\alpha!}\int_{T_x^*X}\int_{T_xX}\psi(x,v)f(\exp_x v)e^{-i\langle v,\zeta\rangle/\varepsilon}\zeta^\alpha\left[\left.\frac{\partial^{|\alpha|}}{\partial\zeta_x^\alpha}\right|_\xi a\right]dvd\zeta + r_N\\
&= \frac{1}{(2\pi\varepsilon)^d}\sum_{|\alpha|\le N}\frac{1}{\alpha!}\int_{T_x^*X}\int_{T_xX}f^\psi(x,v)(i\varepsilon)^{|\alpha|}\frac{\partial^{|\alpha|}}{\partial v^\alpha}e^{-i\langle v,\zeta\rangle/\varepsilon}\left[\left.\frac{\partial^{|\alpha|}}{\partial\zeta_x^\alpha}\right|_\xi a\right]dvd\zeta + r_N\\
&= \frac{1}{(2\pi\varepsilon)^d}\sum_{|\alpha|\le N}\frac{(-i\varepsilon)^{|\alpha|}}{\alpha!}\left[\left.\frac{\partial^{|\alpha|}}{\partial\zeta_x^\alpha}\right|_\xi a\right]\int_{T_xX}\int_{T_x^*X}e^{-i\langle v,\zeta\rangle/\varepsilon}\frac{\partial^{|\alpha|}}{\partial v^\alpha}f^\psi(x,v)d\zeta dv + r_N\\
&= \sum_{|\alpha|\le N}\frac{(-i\varepsilon)^{|\alpha|}}{\alpha!}\left[\left.\frac{\partial^{|\alpha|}}{\partial\zeta_x^\alpha}\right|_\xi a\right]\left[\left.\frac{\partial^{|\alpha|}}{\partial z_x^\alpha}\right|_x f\right] + r_N
\end{aligned}$$

with the remainder

$$r_N(x,\xi) = \frac{(-i\varepsilon)^{N+1}}{(2\pi\varepsilon)^d}\sum_{|\beta|=N+1}\frac{N+1}{\beta!}\int_{T_x^*X}\int_0^1(1-t)^N\left.\frac{\partial^{|\beta|}}{\partial\zeta_x^\beta}\right|_{\xi+t\eta}a \int_{T_xX}e^{-i\langle v,\eta\rangle/\varepsilon}\frac{\partial^{|\beta|}}{\partial v^\beta}f^\psi(x,v)dvdtd\eta \tag{2.52}$$

The integral defines the value of r_N for fixed ξ, so first let $|\xi|\ge 1$. Split the integral in $r_N = r_N^\chi + r_N^{1-\chi}$ using a cutoff $\chi(\eta)$ equal to 1 where $|\eta|\le|\xi/3|$ and with $\chi=0$ for

$|\eta| \geq |\xi/2|$.
By the Schwartz inequality and Plancherel's formula the first part has the bound

(2.53)
$$|r_N^\chi| \leq C\varepsilon^{N+1-d/2} \sum_{|\beta|=N+1} \frac{N+1}{\beta!} \left\| \int_0^1 (1-t)^N \chi(\eta) \frac{\partial^{|\beta|}}{\partial \zeta_x^\beta}\bigg|_{\xi+t\eta} a dt \right\|_{L^2(T_x^*X)} \left\| \frac{\partial^{|\beta|}}{\partial v^\beta} f^\psi \right\|_{L^2(T_xX)}$$

where the second expression is clearly bounded independently of $x \in X$. Now for $a \in S^\mu$ and $N \geq \mu$ we have by definition

$$\left| \chi(\eta) \frac{\partial^{|\beta|}}{\partial \zeta_x^\beta}\bigg|_{\xi+t\eta} a \right| \leq C\chi(\eta) \left(1 + |\xi + t\eta|\right)^{\mu-(N+1)} \leq C\chi(\eta) \left(1 + |\xi| - |\eta|\right)^{\mu-(N+1)} \tag{2.54}$$

where the second inequality holds because $\mu - (N+1) < 0$ and $|\eta| < |\xi|$ on suppχ. We use this to calculate the norm in polar coordinates and get

$$\begin{aligned} \left\| \int_0^1 (1-t)^N \chi(\eta) \frac{\partial^{|\beta|}}{\partial \zeta_x^\beta}\bigg|_{\xi+t\eta} a dt \right\|_{L^2(T_x^*X)} &\leq C \left\| \chi(\cdot) \left(1 + |\xi| - |\cdot|\right)^{\mu-(N+1)} \right\|_{L^2(T_x^*X)} \\ &\leq C \left(1 + |\xi|\right)^{d/2+\mu-(N+1)} \end{aligned} \tag{2.55}$$

In the second part $r_N^{1-\chi}$ we introduce $D = \sum \frac{i\varepsilon}{\eta^2} \zeta_{x,j}(\eta) \partial_v^j$ k-times and then integrate by parts. Since $N \geq \mu$ we have $\left|\partial_\xi^\beta a\right| \leq C$ and we can use (2.53) and polar coordinates with $s = |\eta|$ to get

$$\left|r_N^{1-\chi}\right| \leq C\varepsilon^{N+1-d/2+k} \left(\int_{|\xi|/3}^\infty s^{d-1-2k} ds \right)^{1/2} \leq C\varepsilon^{N+1-d/2+k} \left|\xi\right|^{d/2-k} \tag{2.56}$$

for every $k > d/2$, so $r_N^{1-\chi} = \mathcal{O}^{-\infty}(\varepsilon^\infty)$.
In the case $|\xi| < 1$ we choose our cutoff to be 1 for $|\eta| \leq 1/2$ and 0 for $|\eta| \geq 1$. A calculation similar to the one just carried through then shows that r_N is bounded.
Together these two cases prove that $|r_N| \leq C\varepsilon^{N+1-d/2} \left(1 + |\xi|\right)^{\mu-k+d/2}$ and repetition of these arguments for the derivatives of r_N proves that r_N is $\mathcal{O}(\varepsilon^{N+1-d/2})$ in $S^{d/2+\mu-(N+1)}$ and the expansion for $\sigma_{A,f}$. □

It is important to note that the function σ_B^{ext} appearing in (2.47) depends on ε, so merely taking lemma 2.21 and substituting this for f may not give a proper expansion in powers of ε. To find this we must first expand σ_B^{ext} using essentially the same technique as in lemma 2.21.

Lemma 2.22. *Let $b \in S^\mu$ with $B = Op(b)$. Then if we define $\sigma_B^{ext} : X \times T^*X \to \mathbb{C}$ by*

$$\sigma_B^{ext}(y, (x,\xi)) = \psi_x(y) \left|\Theta_x(y)\right| e^{-i\varphi(y,(x,\xi))/\varepsilon} \left[B\left(\left|\Theta_x\right|^{-1} \psi_x e^{i\varphi(\cdot,(x,\xi))/\varepsilon}\right)\right](y) \tag{2.57}$$

for every $\alpha \in \mathbb{N}^d$ we have the asymptotic expansion

$$\frac{\partial^{|\alpha|}}{\partial z_x^\alpha}\bigg|_{y=x} \sigma_B^{ext}(y,(x,\xi)) \sim \frac{\partial^{|\alpha|}}{\partial z_x^\alpha}\bigg|_{y=x} |\Theta_x| \sum_{\beta\in\mathbb{N}^d} \sum_{k\leq\frac{|\beta|}{2}} \sum_{\substack{\beta_1+\ldots+\beta_k=\beta \\ |\beta_j|\geq 2}} \frac{(-i\varepsilon)^{|\beta|-k}}{k!} \left[\frac{\partial^{|\beta|}}{\partial \zeta_y^\beta}\bigg|_{d\varphi_y} b\right] \prod_{j=1}^k \frac{1}{\beta_j!}\left[\frac{\partial^{|\beta_j|}}{\partial z_y^{\beta_j}}\bigg|_y \varphi(\cdot,(x,\xi))\right] \tag{2.58}$$

Proof. First let us note that differentiation in $d\varphi$ is with respect to the first variable, that is

$$d\varphi_y = \sum_k \frac{\partial\varphi(\cdot,(x,\xi))}{\partial z_x^k} dz_x^k\bigg|_y = \sum_k \zeta_{x,k} dz_x^k\bigg|_y = \sum_{j,k} \zeta_{x,k}\frac{\partial z_x^k}{\partial z_y^j}\bigg|_y dz_y^j \tag{2.59}$$

in normal coordinates around x and y respectively.
For x, y and $\tilde{y}$ close enough define

$$\eta(y,\tilde{y},(x,\xi)) = \varphi(\tilde{y},(x,\xi)) - \varphi(y,(x,\xi)) - \langle z_y(\tilde{y}), d\varphi_y\rangle \tag{2.60}$$

and take note that η is linear in the ξ variable and that $\eta(y,y,(x,\xi)) = 0$. Now we calculate

$$\frac{\partial}{\partial z_y^k}\bigg|_{\tilde{y}} \eta(y,\cdot,(x,\xi)) = \sum_j \left(\frac{\partial z_x^j}{\partial z_y^k}\bigg|_{\tilde{y}} - \frac{\partial z_x^j}{\partial z_y^k}\bigg|_y\right)\zeta_{x,j} \tag{2.61}$$

which is obviously zero when $y = \tilde{y}$.
Then we write

$$\sigma_B^{ext}(y,(x,\xi)) = \psi_x(y)\,|\Theta_x(y)|\left[B\left(|\Theta_x|^{-1}\psi_x e^{i\eta(y,\cdot,(x,\xi))/\varepsilon} e^{i\langle z_y(\cdot),d\varphi_y\rangle/\varepsilon}\right)\right](y) \tag{2.62}$$

and proceed with Taylor's formula as in (2.51) to get

$$\sigma_B^{ext}(y,(x,\xi)) = \psi_x(y)\,|\Theta_x(y)| \sum_{|\beta|\leq N} \frac{(-i\varepsilon)^{|\beta|}}{\beta!}\left[\frac{\partial^{|\beta|}}{\partial\zeta_y^\alpha}\bigg|_{d\varphi_y} b\right]\left[\frac{\partial^{|\beta|}}{\partial z_y^\beta}\bigg|_y F(y,\cdot,(x,\xi))\right] + R_N(y,(x,\xi)) \tag{2.63}$$

with $F(y,\cdot,(x,\xi)) = \psi_x(y)e^{i\eta(y,\cdot,(x,\xi))/\varepsilon}$. Of course both F and R_N still depend on ε so to complete the proof we must show that this is really an asymptotic expansion.
First use Leibniz' rule and (2.61) to compute

$$\frac{\partial^{|\beta|}}{\partial z_y^\beta}\bigg|_y F(y,\cdot,(x,\xi)) = \sum_{0\leq k\leq\frac{|\beta|}{2}} \sum_{\substack{\beta_0+\ldots+\beta_k=\beta \\ |\beta_j|\geq 2}} \frac{(-i\varepsilon)^{-k}}{k!\beta_0!}\left[\frac{\partial^{|\beta_0|}}{\partial z_y^{\beta_0}}\bigg|_y \psi_x\right]\prod_{j=1}^k \frac{1}{\beta_j!}\left[\frac{\partial^{|\beta_j|}}{\partial z_y^{\beta_j}}\bigg|_y \varphi(\cdot,(x,\xi))\right] \tag{2.64}$$

If we evaluate this expression or its derivatives at $y = x$ all the summands with $\beta_0 \neq 0$ will be 0 because ψ_x is equal to 1 in a neighbourhood of x, so this gives exactly the claimed expansion.
The form of the remainder can be seen from lemma 2.21, but now the estimate of the term

$$\text{(2.65)} \quad \left\| \frac{\partial^{|\beta|}}{\partial v^\beta} \psi^2(y,\cdot) F\left(y, \exp_y(\cdot), (x,\xi)\right) \right\|_{L^2(T_y X)}$$

depends on ξ and ε, while the estimate on the part containing b is completely analogous. In order to compute the order of $\partial^\alpha|_{y=x} R_N$ we only need to calculate that of expressions of the form

$$\text{(2.66)} \quad \left.\frac{\partial^{|\alpha|}}{\partial z_x^\alpha}\right|_{y=x} \left.\frac{\partial^{|\beta|}}{\partial z_y^\beta}\right|_{\tilde{y}} F\left(y, \cdot, (x,\xi)\right) =: \partial^\alpha F^\beta$$

and then proceed as in the proof of lemma 2.21. For this we will need the identities

$$\text{(2.67)} \quad \left.\frac{\partial}{\partial z_x^k}\right|_{y=x} \eta(y, \tilde{y}, (x,\xi)) = 0 \qquad \text{and} \qquad \left.\frac{\partial^{|\alpha|}}{\partial z_x^\alpha}\right|_{y=x} \left.\frac{\partial}{\partial z_y^k}\right|_{\tilde{y}} \eta(y,\cdot,(x,\xi)) = 0 \text{ for } |\alpha| < 2$$

that can easily be derived from (2.61) and the formulas for coordinate changes (1.21) and (1.22).
Now let us consider a single summand $S_{\alpha\beta}$ of $\partial^\alpha F^\beta$. Since η is linear in ξ it is clear that

$$\text{(2.68)} \quad \left| \frac{i}{\varepsilon} \left.\frac{\partial^{|\beta|}}{\partial z_y^\beta}\right|_y \eta(y,\cdot,(x,\xi)) \right| \leq C \varepsilon^{-1} |\xi|$$

so if a summand $S_{\beta,m}$ of F^β has m factors with $|\beta_m| = 1$, then in the worst case it grows like $\left(\varepsilon^{-1}|\xi|\right)^{m+(|\beta|-m)/2}$. By (2.67) for $S_{\alpha\beta}$ coming from derivation of $S_{\beta,m}$ to be nonzero there have to be at least $|\alpha_1| \geq 2m$ derivatives acting on those factors with $|\beta_m| = 1$. So we can have at most $\alpha_2 = \alpha - \alpha_1$ derivatives acting on F. Then the exponent of $\varepsilon^{-1}|\xi|$ can be at most $(|\beta| + m + \alpha_2)/2 \leq (|\beta| + |\alpha|)/2$. So if we look at (2.53) we see from the proof of lemma 2.21 that for every derivative we gain one order in the first part and loose at most half an order in the second part. Therefore

$$\text{(2.69)} \quad \left.\frac{\partial^{|\alpha|}}{\partial z_x^\alpha}\right|_{y=x} R_N = \mathcal{O}(\varepsilon^{(N+1-d-|\alpha|)/2}) \text{ in } S^{\mu+(d+|\alpha|-N-1)/2}$$

□

Theorem 2.23. *Let $a \in S^\mu$ and $b \in S^\nu$, with $A = Op(a)$, $B = Op(b)$. Then the symbol*

σ_{AB} *of the operator product* AB *has the asymptotic expansion.*

$$\sigma_{AB} \sim \sum_{\alpha\in\mathbb{N}^d}\sum_{\beta\in\mathbb{N}^d}\sum_{k\leq\frac{|\beta|}{2}}\sum_{\substack{\beta_1+\ldots+\beta_k=\beta\\|\beta_j|\geq 2}} \frac{(-i\varepsilon)^{|\alpha|+|\beta|-k}}{\alpha!k!}\left[\left.\frac{\partial^{|\alpha|}}{\partial\zeta_x^\alpha}\right|_\xi a\right] \left.\frac{\partial^{|\alpha|}}{\partial z_x^\alpha}\right|_{y=x}\left\{|\Theta_x|\left[\left.\frac{\partial^{|\beta|}}{\partial\zeta_y^\beta}\right|_{d\varphi_y} b\right]\prod_{j=1}^k\frac{1}{\beta_j!}\left[\left.\frac{\partial^{|\beta_j|}}{\partial z_y^{\beta_j}}\right|_y\varphi(\cdot,(x,\xi))\right]\right\} \tag{2.70}$$

Proof. To get the form of the expansion we start from (2.47) and use lemma 2.21 where we insert for σ_B^{ext} and its derivatives the expansion proved in lemma 2.22.
It remains to be shown that the error is really $\mathcal{O}^{-\infty}(\varepsilon^\infty)$. Take from the proof of lemma 2.21 the remainder r_N, inserting for f the M-th order expansion (2.63) of σ_B^{ext}. The terms (2.64) grow at most like $(\varepsilon^{-1}|\xi|)^{|\beta|/2}$, so the only problematic term is $r_N(R_M)$ where we need to estimate the order of $\partial^\alpha|_y R_N$. Now for $y\neq x$ the argument from the proof of lemma 2.22 is not valid, but because of (2.67) we can choose a cutoff function $\chi(x,y)$, equal to zero away from the diagonal, with

$$\left|\chi^\varepsilon(x,y)\left.\frac{\partial^{|\alpha|}}{\partial z_x^\alpha}\right|_y\left.\frac{\partial}{\partial z_y^k}\right|_{\tilde{y}}\eta(y,\cdot,(x,\xi))\right|\leq C\sqrt{\varepsilon\,(1+|\xi|)^{-1}} \tag{2.71}$$

for $|\alpha|<2$.
We use this to split the integrand in two and get $r_N=r_N^\chi+r_N^{1-\chi}$ with $r_N^{1-\chi}=\mathcal{O}^{-\infty}(\varepsilon^\infty)$ since $1-\chi^\varepsilon$ vanishes near the diagonal (see remark 2.9). Then by definition of χ^ε we get

$$\left|\chi^\varepsilon(x,y)\frac{\partial^{|\alpha|}}{\partial z_x^\alpha}\frac{\partial^{|\beta|}}{\partial z_y^\beta}F(y,\cdot,(x,\xi))\right|\leq C(|\xi|/\varepsilon)^{(|\alpha|+|\beta|)/2} \tag{2.72}$$

so we have $r_N(R_M)=\mathcal{O}(\varepsilon^{(N+M+2)/2})$ in $S^{\mu+\nu+d-(N+M+2)/2}$. □

The expansion just proved clearly defines a symbol that is unique in $S^\infty/S^{-\infty}$, so it gives us the composition rule # known as the Moyal product and $S^\infty/S^{-\infty}$ as well as $S^0/S^{-\infty}$ are Algebras with this product.

Corollary 2.24. *The second order expansion of* σ_{AB} *is explicitly given by*

$$\begin{aligned}\sigma_{AB}(x,\xi) = \sum_{|\alpha|\leq 2}\frac{(-i\varepsilon)^{|\alpha|}}{\alpha!}&\left[\left.\frac{\partial^{|\alpha|}}{\partial\zeta^\alpha}\right|_\xi a\right]\left[\left.\frac{\partial^{|\alpha|}}{\partial z_x^\alpha}\right|_x b\right]\\ &-\frac{\varepsilon^2}{12}\sum_{k,l,m,n}\left[\left.\frac{\partial}{\partial\zeta_n}\right|_\xi a\right]\left[\left.\frac{\partial^2}{\partial\zeta_l\partial\zeta_m}\right|_\xi b\right]R^k_{mln}(x)\zeta_k\\ &+\frac{\varepsilon^2}{6}\sum_{k,l}\left[\left.\frac{\partial^2}{\partial\zeta_k\partial\zeta_l}\right|_\xi a\right]b(x,\xi)\,\mathrm{Ric}_{kl}(x)+\mathcal{O}^{\mu+\nu-3}(\varepsilon^3)\end{aligned} \tag{2.73}$$

Proof. The form of the expansion is clear from theorem 2.23, where the order of a summand is of course $|\alpha| + |\beta| - k$. In order to determine the coefficients we have to calculate for $|\alpha|, |\beta| \le 2$

$$\varphi_{\alpha\beta} = \frac{\partial^{|\alpha|}}{\partial z_x^\alpha}\bigg|_{y=x} \frac{\partial^{|\beta|}}{\partial z_y^\beta} \varphi(\cdot, (x, \xi)) = \sum_k \zeta_{x,k} \frac{\partial^{|\alpha|}}{\partial z_x^\alpha}\bigg|_{y=x} \frac{\partial^{|\beta|} z_x^k}{\partial z_y^\beta} \tag{2.74}$$

From (1.22) we see that $\varphi_{0\beta} = 0$ when $|\beta| \le 2$, so the only nonzero coefficients with $k \ne 0$ are

$$\frac{\partial}{\partial z_x^n}\bigg|_{y=x} \frac{\partial^2 z_x^k}{\partial z_y^l \partial z_y^m} = \frac{1}{6}\left(R^k_{mln}(x) + R^k_{nlm})(x)\right) \tag{2.75}$$

and because $R^k_{nlm} = -R^k_{nml}$ we have $\sum_{l,m} R^k_{nlm} \partial^{m,l} b = 0$ which gives us the second summand. The only case in which $\partial^\alpha |\Theta_x|$ is nonzero is $|\alpha| = 2$ and consequently $|\beta| = 0$. We then have

$$\frac{\partial^2 |\Theta_x|}{\partial z_x^k \partial z_x^l}\bigg|_x = -\frac{1}{6} \sum_{m=1}^d (R^m_{lmk}(x) + R^m_{kml}(x)) = -\frac{1}{3} \operatorname{Ric}_{kl}(x) \tag{2.76}$$

as calculated in (1.19). □

The ideas of the proofs of this section are all from [Pfl2] but we have corrected a sign in the estimate (2.54) and the proof of lemma 2.22 is much longer because (2.64) only holds in the point $\tilde{y} = y$ and not in a neighbourhood as stated in [Pfl2] (otherwise $\eta \equiv 0$ in this neighbourhood).

2.6 L^2 bounds for Pseudodifferential Operators

In this section we prove a version of the Calderon-Vallaincourt theorem for the calculus we have just defined. This will allow us to extend the operators in Ψ^0 to operators on $L^2(X)$.

The proof follows that of Hörmander ([Hör], Lemma 18.1.11 and Lemma 18.1.12.)

Lemma 2.25. *If $K \in \mathcal{C}(X \times X)$ and*

$$\sup_{y \in X} \int_X |K(x,y)|\, dx \le C \qquad \sup_{x \in X} \int_X |K(x,y)|\, dy \le C \tag{2.77}$$

then the integral operator $\hat{K}$ with kernel K is a bounded operator on $L^2(X)$ with norm bounded by C.

Proof. Let $f \in L^2(X)$, using Cauchy-Schwarz' inequility gives us

$$(2.78)\quad |\hat{K}f(x)|^2 \leq \left(\int_X |K(x,y)f(y)|\,dy\right)^2 \leq \int_X |K(x,y)|\,|f(y)|^2\,dy \int_X |K(x,z)|\,dz$$

so, estimating the last integral by C, we get

$$(2.79)\quad \int_X |\hat{K}f(x)|^2 dx \leq C \int_X \int_X |K(x,y)|\,|f(y)|^2\,dydx \leq C^2 \int |f(y)|^2\,dy$$

□

Theorem 2.26. *Let $a \in S^0$, then $Op(a)$ is a bounded operator on $L^2(X)$.*

Proof. For $a \in S^\mu$ with $\mu < -d$ the Operator $A = \mathrm{Op}_\psi(a)$ is an integral operator with kernel

$$(2.80)\quad K_A(x,y) = \frac{1}{(2\pi\varepsilon)^d} \int_{T_x^*X} \psi_x(y) e^{-i\varphi(y,(x,\xi))/\varepsilon} a(x,\xi) d\xi$$

and K_A is obviously continuous and bounded by

$$(2.81)\quad |K_A(x,y)| \leq \frac{1}{(2\pi\varepsilon)^d} \int_{T_x^*X} C(1+|\xi|)^\mu d\xi \leq C$$

Now for $n \in \mathbb{N}$, $(1 + |\exp_x^{-1}(y)|^{2n})K_A(x,y)$ (which is well defined because of the cutoff) is also bounded and continuous since for $n = 1$

(2.82)

$$(1+\exp_x^{-1}(y)^2)K_A(x,y) = \frac{\psi_x(y)}{(2\pi\varepsilon)^d} \int_{T_x^*X} e^{-i\varphi(y,(x,\xi))/\varepsilon} \left(a(x,\xi) + \varepsilon^2 \sum_{j\leq d} \partial_{\xi_j}^2 a(x,\xi)\right) d\xi$$

and in general it is the kernel of an operator associated to a symbol in S^μ consisting of a and its derivatives.
Therefore K_A satsifies the conditions of lemma 2.25 and we have proven that A is bounded if $\mu < -d$.
Next we extend this result to all $\mu < 0$ by looking at the quadratic form

$$(2.83)\quad \|Af\|^2 = \langle Af, Af\rangle = \langle A^*Af, f\rangle \leq \|A^*A\|\,\|f\|^2$$

and observing that the results of section 2.4 imply that $A^*A \in \Psi^{2\mu}$, and eventually $2^k\mu < -d$ for any $\mu < 0$.

Finally take $a \in S^0$, $M = 2\,\|a^2\|_\infty$ and define

$$(2.84)\quad b(x,\xi) = \left(M - |a(x,\xi)|^2\right)^{\frac{1}{2}} \in S^0$$

since $M/2 \leq \left(M - |a(x,\xi)|^2\right) \leq M$ and the square root ist smooth and bounded in this region.
Now the product expansion 2.23 implies that

$$(2.85)\quad C^*C = \mathrm{Op}(M - |a(x,\xi)|^2) + \varepsilon R_1$$

and the results (2.15, 2.19) of section 2.4 show that

$$(2.86)\quad \mathrm{Op}(|a(x,\xi)|^2) = A^*A + \varepsilon R_2$$

with $R_1, R_2 \in \Psi^{-1}$. Consequently $R = R_1 + R_2$ is bounded because it is in Ψ^{-1}. This gives us the estimate for the norm of A

$$(2.87)\quad \|Af\|^2 \leq \langle A^*Af, f\rangle + \langle C^*Cf, f\rangle \leq (M + \varepsilon \|R\|) \|f\|^2$$

□

3 The Egorov Theorem

3.1 Proof of the Egorov Theorem

In the previous sections we have established a correspondence between classical and quantum mechanical observables through the Weyl calculus. Here we want to use this to show that the respective time evolutions of these observables differ only by a small amount when ε is small.

By the standard theory of ordinary differential equations the Hamiltonian vector field $X_H = -\{h, \cdot\}$ generates a local flow $\phi_t : T^*X \to T^*X$. This means that there is $T > 0$ such that for $t \in [0, T]$ the solutions of the Liouville equation $\frac{d}{dt}a = X_H(a)$ are given by $a(t) = a \circ \phi_t$.
A self-adjoint operator H generates a strongly continuous unitary group $U(t) = e^{-iHt/\varepsilon}$, this means that the solutions of the the Schrödinger equation (1.2) are $\psi(t) = U(t)\psi_0$ where $\psi_0 \in D(H)$ is the initial state. The Heisenberg equation (1.3) for the observables is then solved by $A(t) = U^*(t)AU(t)$. We want to compare this time evolution to the classical flow ϕ_t via the quantisation and symbol maps. Since it is determined by the commutator $[H, A]$ we start by calculating the corresponding symbol $\sigma^W_{[A,H]}$

Lemma 3.1. *Let $a \in S^\mu$, $b \in S^\nu$ and $A = Op^W(a)$, $B = Op^W(b)$. Then we have*

$$\begin{aligned}\sigma^W_{[A,B]}(x,\xi) =& i\varepsilon\,\{a,b\} \\ &+ \frac{\varepsilon^2}{12}\sum_{k,l,m,n} R^k_{mnl}(x)\zeta_{x,k}\frac{\partial^3 ab}{\partial\zeta_{x,m}\partial\zeta_{x,n}\partial\zeta_{x,l}} \\ &+ \frac{\varepsilon^2}{6}\sum_{k,l}\mathrm{Ric}_{kl}(x)\left(b\frac{\partial^2 a}{\partial\zeta_{x,k}\partial\zeta_{x,l}} - a\frac{\partial^2 b}{\partial\zeta_{x,k}\partial\zeta_{x,l}}\right) + \mathcal{O}^{\mu+\nu-3}(\varepsilon^3)\end{aligned} \tag{3.1}$$

where $\{\cdot,\cdot\}$ is the Poisson-bracket induced by the canonical symplectic form on T^*X.

Proof. We use the expansion (2.73) for σ_{AB}, get the Weyl symbol from proposition 2.15 and then calculate $\sigma^W_{[A,B]} = \sigma^W_{AB} - \sigma^W_{BA}$. Here it is important to note that any expression appearing in σ^W_{AB} that is invariant if we swap a and b will dissapear in $\sigma^W_{[A,B]}$.
Let α and β be the multiindices of theorem 2.23 and γ that of proposition 2.15. The the zeroth order expression corresponds to $|\alpha| = |\beta| = |\gamma| = 0$, so it is equal to $\sigma_A\sigma_B$

and clearly dissapears in $\sigma^W_{[A,B]}$. Now to first order in σ^W_{AB} we have the cases $|\alpha| = 1$, $|\beta| = |\gamma| = 0$ and $|\gamma| = 1$, $|\beta| = |\alpha| = 0$ and get

$$\text{(3.2)}\quad i\varepsilon\left(\sum_k \frac{1}{2}\frac{\partial}{\partial\zeta_{x,k}}\frac{\partial\sigma_A\sigma_B}{\partial z_x^k} - \frac{\partial\sigma_A}{\partial\zeta_{x,k}}\frac{\partial\sigma_B}{\partial z_x^k}\right) = \frac{i\varepsilon}{2}\left\{\sigma_A, \sigma_B\right\}$$

and use $\sigma_A = a - \frac{i\varepsilon}{2}\partial_\zeta\partial_z a + \mathcal{O}^{\mu-2}(\varepsilon^2)$ to find

$$\text{(3.3)}\quad \frac{i\varepsilon}{2}\left\{\sigma_A, \sigma_B\right\} = \frac{i\varepsilon}{2}\{a, b\} + \frac{\varepsilon^2}{4}\left(\{\partial_\zeta\partial_z a, b\} + \{a, \partial_\zeta\partial_z b\}\right) + \mathcal{O}^{\mu+\nu-3}(\varepsilon^3)$$

From this we already see that the first order expansion is given by

$$\text{(3.4)}\quad \sigma^W_{[A,B]} = i\varepsilon\{a, b\} + \mathcal{O}^{\mu+\nu-2}(\varepsilon^2)$$

To find the expressions of order ε^2 we proceed as above and start by calculating the expressions for $\beta = 0$ and different α and γ.

$$\text{(3.5)}\quad |\alpha| = 0,\ |\gamma| = 2: \quad -\frac{\varepsilon^2}{4}\sum_{k,l}\frac{\partial^2}{\partial\zeta_{x,l}\partial\zeta_{x,k}}\frac{\partial^2\sigma_A\sigma_B}{\partial z_x^l\partial z_x^k}$$

which is of course symmetric in a and b.

$$\text{(3.6)}\quad |\alpha| = 2,\ |\gamma| = 0: \quad -\frac{\varepsilon^2}{2}\sum_{k,l}\frac{\partial^2\sigma_A}{\partial\zeta_{x,l}\partial\zeta_{x,k}}\frac{\partial^2\sigma_B}{\partial z_x^l\partial z_x^k}$$

$$\begin{aligned}
|\alpha| = 1,\ |\gamma| = 1: \quad & \frac{\varepsilon^2}{2}\sum_{k,l}\frac{\partial}{\partial\zeta_{x,k}}\frac{\partial}{\partial z_x^k}\left(\frac{\partial\sigma_A}{\partial\zeta_{x,l}}\frac{\partial\sigma_B}{\partial z_x^l}\right)\\
\text{(3.7)}\quad & = \frac{\varepsilon^2}{2}\sum_{k,l}\Bigg(\underbrace{\frac{\partial}{\partial z_x^k}\frac{\partial\sigma_A}{\partial\zeta_{x,l}}\frac{\partial}{\partial z_x^l}\frac{\partial\sigma_B}{\partial\zeta_{x,k}}}_{\text{symmetric}} + \underbrace{\frac{\partial^2\sigma_A}{\partial\zeta_{x,l}\partial\zeta_{x,k}}\frac{\partial^2\sigma_B}{\partial z_x^l\partial z_x^k}}_{\text{negative of (3.6)}}\\
& \quad + \frac{\partial}{\partial\zeta_{x,l}}\left[\frac{\partial}{\partial\zeta_{x,k}}\frac{\partial\sigma_A}{\partial z_x^k}\right]\frac{\partial\sigma_B}{\partial z_x^l} + \frac{\partial\sigma_A}{\partial z_x^l}\frac{\partial}{\partial z_x^l}\left[\frac{\partial}{\partial\zeta_{x,k}}\frac{\partial\sigma_B}{\partial z_x^k}\right]\Bigg)
\end{aligned}$$

As we can see from (2.73) the terms with $|\beta| \neq 0$ are just those in the second order expansion of σ_{AB} that contain the curvature. Now we use $\sigma_A = a + \mathcal{O}^{\mu-1}(\varepsilon)$ and calculate $\sigma^W_{[A,B]} = \sigma^W_{AB} - \sigma^W_{BA}$. The last two summands of (3.7) combined with their counterparts from σ^W_{BA} exactly cancel with the ε^2 part of (3.3), so the only remaining summands of order ε^2 are those containing the curvature. They can be simplified to those of (3.1) using the symmetries of R^k_{mln}. □

Theorem 3.2. *Let $h \in S^\mu$ with $H = Op^W(h)$ self adjoint and $U(t) := e^{-iHt/\varepsilon}$. Let ϕ_t, $t \in [0, T]$ be the Hamiltonian flow generated by h. If $a \in \mathcal{C}_0^\infty(T^*X)$ then*

$$\text{(3.8)}\quad \left\|U^*(t)\,Op^W(a)\,U(t) - Op^W(a \circ \phi_t)\right\|_{\mathcal{L}(L^2(X))} \leq C_T\left(\varepsilon\,\|R\| + \varepsilon^2\right)$$

where

$$\|R\| = \sup_{x\in X} \max_{k,l,m,n} \left|R^k_{lmn}(x)\right| \tag{3.9}$$

Proof. Define $A(t) = U^*(t)\mathrm{Op}^W(a)\, U(t)$ and $A_t = \mathrm{Op}^W(a\circ\phi_t)$ and check that

$$\frac{d}{dt}(A_t f) = \mathrm{Op}^W\left(\frac{d}{dt}[a\circ\phi_t]\right) f = \mathrm{Op}^W\left(-\{h, a\circ\phi_t\}\right) f \tag{3.10}$$

because a has compact support, and that

$$\frac{d}{dt}A(t)f = \frac{i}{\varepsilon}[H, A(t)]\, f = \frac{i}{\varepsilon}U^*(t)\,[H, A(0)]\, U(t) f \tag{3.11}$$

when $f \in D(H)$, which is just the property of the unitary group. We use this together with the expansion $\sigma^W_{[H,A_{t-\tau}]} = i\varepsilon\{h, a\circ\phi_{t-\tau}\} + \varepsilon^2 r(t-\tau) + \varepsilon^3 c(t-\tau)$ from lemma 3.1 to calculate for $f \in D(H)$

$$\begin{aligned}
[A(t) - A_t]\, f &= \int_0^t \frac{d}{d\tau}U^*(\tau)A_{t-\tau}U(\tau) f d\tau \\
&= \int_0^t U^*(\tau)\left(\frac{i}{\varepsilon}[H, A_{t-\tau}] + \mathrm{Op}^W\left(\{h, a\circ\phi_{t-\tau}\}\right)\right) U(\tau) f d\tau \\
&= -\int_0^t U^*(\tau)\mathrm{Op}^W\left(\varepsilon r(t-\tau) + \varepsilon^2 c(t-\tau)\right) U(\tau) f d\tau
\end{aligned} \tag{3.12}$$

Now because a has compact support so does $a\circ\phi_t$, so $r(t)$ and $c(t)$ are in $S^{-\infty}$ for every $t \le T$. The dependence of these remainders on t is obviously continuous. Since $D(H)$ is dense in $L^2(X)$ we can estimate the norm

(3.13)
$$\|A(t) - A_t\|_{\mathcal{L}(L^2(X))} \le CT \sup_{t\in[0,T]} \left(\varepsilon \left\|\mathrm{Op}^W(r(t))\right\|_{\mathcal{L}(L^2(X))} + \varepsilon^2 \left\|\mathrm{Op}^W(c(t))\right\|_{\mathcal{L}(L^2(X))}\right)$$

This gives us (3.8) if we take into account the dependence of r on the curvature from 3.1. □

Remark 3.3. We see that the approximation is of order ε^2 if $R = 0$. If X is not flat there cannot be a second order approximation of U by a Hamiltonian flow since the remainder r contains derivatives of the observable a of order greater than one and therefore the map $X(a) = \{h, a\} + \varepsilon r$ does not satisfy the Leibniz rule and is consequently not a vector field.

Remark 3.4. The condition $a \in \mathcal{C}_0^\infty(T^*X)$ is of course very restrictive. From the proof we can see that the Egorov Theorem will hold for $h \in S^\mu$, $a \in S^\nu$ with $\mu + \nu - 2 \le 0$ if we can prove $a\circ\phi_t \in S^\nu$ and (3.10). This of course depends strongly on h.

Remark 3.5. We would like to emphasise that the growth of $A(t) - A_t$ is not linear in time because the remainders depend on $a \circ \phi_t$ and it's derivatives. To get an estimate on the time dependence of the error one needs additional assumptions on h to prove bounds for ϕ_t and it's derivatives. If all the relevant derivatives of ϕ_t can be bounded by e^{cT} the error is bounded by $\varepsilon T C e^{cT}$ so the approximation is valid up to times of the order of the Ehrenfest time $-\log \varepsilon$. Estimates of this kind are proved for Hamiltonians growing at most quadratically in ξ in [BGP] and [BR].

3.2 Example: Constraint Quantum Dynamics

In this section we will apply the Egorov Theorem 3.2 and the pseudodifferential calculus developed in chapter 2 to a recent result by Teufel and Wachsmuth [WT] on the dynamics of quantum systems constrained to submanifolds.

Let (M, g) be a Riemannian mainfold of bounded geometry and consider the Schrödinger equation with the Hamiltonian $H = -\Delta + V_\varepsilon$. Let V_ε be a potential that localises a certain class of states in an ε-tube around a submanifold $X \subset M$. If X is also of bounded geometry and the embedding $X \hookrightarrow M$ has bounded derivatives of any order, then under suitable assumptions on V_ε the result [WT, theorem 1] is that we can equip X with an effective metric G_{eff} and define an effective Hamiltonian H_{eff} with $D(H_{\text{eff}}) \subset L^2(X)$ (with measure induced by G_{eff}) such that the effective time evolution $e^{-iH_{\text{eff}}t/\varepsilon}$ on X is a good approximation of the original one in the following sense: there is a mapping U satisfying $UU^* = 1$ from a space of suitable initial conditions $\mathcal{H}_0 \subset L^2(M)$, with associated projection P_0, to $L^2(X)$ so that

$$\text{(3.14)} \quad \left\| \left[e^{-iHt/\varepsilon} - U^* e^{-iH_{\text{eff}}t/\varepsilon} U \right] P_0 \right\|_{\mathcal{L}(L^2(M))} \leq C t \varepsilon^2$$

The effective Hamiltonian is:

$$\text{(3.15)} \quad H_{\text{eff}} f = -\varepsilon^2 \left[\Delta_{G_{\text{eff}}} + i(d^* \mathcal{A}(x)) - \mathcal{A}^2(x) \right] f - 2i\varepsilon^2 G_{\text{eff}}(\mathcal{A}, df) + E_0(x) f$$

The objects in this equation are:

- the effective metric

  $$\text{(3.16)} \quad G_{\text{eff}} = G + \varepsilon B$$

  where G is the metric induced on X by g and $B : TM \times TM \to \mathbb{R}$ is a symmetric bilinear map depending on the second fundamental form of the embedding $X \hookrightarrow M$. It is with respect to this metric that the objects in (3.15) are to be understood.
- the connection 1-form $\mathcal{A}$ of the generalised Berry connection (see [WT, theorem 2] for a definition).

- the codifferential operator d^* which on 1-forms is defined by

$$\int_X f d^*\mathcal{A} = \int_X G_{\text{eff}}(\mathcal{A}, df) \tag{3.17}$$

  for every function $f \in \mathcal{C}_0^\infty(X)$.

- the effective potential E_0 that also accounts for the energy of the motion in the direction normal to X.

Now suppose $H_{\text{eff}} \in \Psi^2$. Then we can use the pseudodifferential calculus on (X, G_{eff}) to determine the Weyl-symbol $h_{\text{eff}} = \sigma^W(H_{\text{eff}})$ as in the examples 2.12 and 2.16. We get:

- $\sigma[-\varepsilon^2\Delta_{G_{\text{eff}}}](x,\xi) = G_{\text{eff}}(\xi,\xi) - \frac{\varepsilon^2}{3}\kappa(x) = \xi^2 + \mathcal{O}^0(\varepsilon^2) = \sigma^W[-\varepsilon^2\Delta_{G_{\text{eff}}}](x,\xi)$
- $d^*\mathcal{A}$ and $\mathcal{A}^2$ are multiplication operators, so they are equal to their symbols.
- $\sigma[i\varepsilon G_{\text{eff}}(\mathcal{A}, d)](x,\xi) = -G_{\text{eff}}(\mathcal{A},\xi)$ by a calculation similar to that of example 2.12b) and $\sigma^W\left[i\varepsilon G_{\text{eff}}(\mathcal{A}, d)\right](x,\xi) = -G_{\text{eff}}(\mathcal{A},\xi) - \frac{i\varepsilon}{2}d^*\mathcal{A}$

Adding these up we get

$$\begin{aligned} h_{\text{eff}}(x,\xi) &= \xi^2 + 2\varepsilon G_{\text{eff}}(\mathcal{A}(x),\xi) + \varepsilon^2\mathcal{A}^2(x) + E_0(x) - \frac{\varepsilon^2}{3}\kappa(x) \\ &= (\xi + \varepsilon\mathcal{A}(x))^2 + E_0(x) + \mathcal{O}^0(\varepsilon^2) \end{aligned} \tag{3.18}$$

which is the classical Hamiltonian for a particle interacting with a potential $E_0(x)$ and a weak magnetic field $B = \varepsilon d\mathcal{A}$. It is in S^2 if E_0 and the components of $\mathcal{A}$ are in $\mathcal{C}_b^\infty(X)$. Now we can apply the Egorov Theorem 3.2 and get:

Corollary 3.6. *Put $h^0_{\mathit{eff}} = \xi^2 + E_0(x)$ and let $a \in \mathcal{C}_0^\infty(T^*X)$. If $h^0_{\mathit{eff}} \in S^2$, then $E_0(x)$ and its derivatives are bounded and the flow ϕ^0_t exists globally in time. By* (3.14) *and the Egorov Theorem we have for all $t \leq T$*

$$\left\|P_0\left[e^{iHt/\varepsilon}U^*\,Op^W(a)\,Ue^{-iHt/\varepsilon} - U^*\,Op^W\left(a\circ\phi^0_t\right)U\right]P_0\right\|_{\mathcal{L}(L^2(M))} \leq C_T\varepsilon \tag{3.19}$$

Proof. To see that ϕ^0_t exists globally start with some initial value (x,ξ) and write the differential equations in normal coordinates at x:

$$\begin{aligned} \frac{dz^k_x}{dt} &= 2\zeta_{x,k} \\ \frac{d\zeta_{x,k}}{dt} &= -\frac{\partial E_0}{\partial z^k_x} \end{aligned} \tag{3.20}$$

Because E_0 and its derivatives are bounded there is a Lipschitz constant for the right hand side that does not depend on the point (x,ξ). The Picard-Lindelöf theorem then gives existence of ϕ^0_t up to a time T which is also independent of (x,ξ). We can now apply the same argument to the initial value $\phi^0_T(x,\xi)$ and see that ϕ^0_t must exist for every $t \geq 0$.

To complete the proof observe that $\mathrm{Op}^W(a \circ \phi_t^0)$ approximates $e^{iH_{\mathrm{eff}}t/\varepsilon}\mathrm{Op}^W(a)\,e^{-iH_{\mathrm{eff}}t/\varepsilon}$ up to order ε by the Egorov Theorem 3.2 and that this still holds after applying UP_0 and P_0U^* because their norm is 1. The unitary groups $e^{iH_{\mathrm{eff}}t/\varepsilon}$ and $e^{iHt/\varepsilon}$ are close by (3.14) and $\mathrm{Op}^W(a)$ is a bounded operator so we can deduce the result with a standard 3ε-argument. □

Since the error in 3.6 is of order ε we could also have used the induced metric G instead of G_{eff} for quantisation without changing the result. The case where we can see additional geometric effects, like the Berry connection and the correction to the metric, in the semi-classical approximation is when the induced metric is flat.

Corollary 3.7. *Let $h_{\mathit{eff}} \in S^2$ and ϕ_t^ε be the flow generated by this function (which exists globally in time). Let $a \in \mathcal{C}_0^\infty(T^*X)$ and assume the induced metric G on X to be flat, then for all $t \leq T$*

$$\left\| P_0 \left[e^{iHt/\varepsilon} U^* Op^W(a)\, U e^{-iHt/\varepsilon} - U^* Op^W(a \circ \phi_t^\varepsilon)\, U \right] P_0 \right\|_{\mathcal{L}(L^2(M))} \leq C_T \varepsilon^2 \tag{3.21}$$

Proof. If G is flat, then the curvature of G_{eff} is of order ε, so in (3.8) the curvature terms in the error are of order ε^2. The arguments used in the previous corollary then prove the result. □

These corollaries show that there is a class of observables on M, namely those that are equal to $P_0U^*\mathrm{Op}^W(a)\,UP_0$ for $a \in \mathcal{C}_0^\infty(T^*X)$, that behave in this sense semi-classically as $\varepsilon \to 0$. A more detailed discussion of semi-classical observables on the different spaces for the case $M = \mathbb{R}^d$, $X = \mathbb{R}^{d-k}$ can be found in [Teu].

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Index of Notation

Symbol	Explanation	Page
$\mathbb{N}$	natural numbers including 0	
X	connected Riemannian manifold of bounded geometry with metric g and dimension d	
TX, T^*X	tangent and cotangent bundle of X	5
ρ_X	injectivity radius of X	5
$B_x(0,r)$	open ball of radius r around $0 \in T_xX$	5
$U_{x,r}$	neighbourhood of radius r of $x \in X$	5
R^k_{lmn}	coefficients of the curvature tensor	7
Ric_{kl}	coefficients of the Ricci tensor	7
κ	scalar curvature	7
$\mathcal{C}^\infty(X)$	smooth functions $X \to \mathbb{C}$	
$\mathcal{C}^\infty(X,\mathbb{R})$	smooth functions $X \to \mathbb{R}$	
$\mathcal{C}^\infty_0(X)$	smooth functions with compact support	
$\mathcal{C}^k_b(X)$	k-times continuously differentiable functions with bounded derivatives	6
$\mathcal{S}(\mathbb{R}^d)$	Schwartz functions on $\mathbb{R}^d$	
$L^2(X)$	square integrable functions $X \to \mathbb{C}$	5
$S^\mu(T^*X)(= S^\mu)$	symbols of order μ	10
$\mathrm{Op}(a)$	quantisation of a	12
$\mathrm{Op}^W(a)$	Weyl-quantisation of a	19
$\Psi^\mu(X)$	quantisations of symbols of order μ	14
σ_A	symbol of A	17
σ^W_A	Weyl-symbol of A	19
$\mathcal{O}^\mu(\varepsilon^k)$	order ε^k in S^μ	11