Introduction to Quantization

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1 Introduction

1.1 Basic classical mechanics

Basic classical mechanics takes place in *phase space* $\mathbb{R}^d \oplus \mathbb{R}^d$. The variables are the *positions* x^i, $i = 1, \dots, d$, and the *momenta* p_i, $i = 1, \dots, d$. Real-valued functions on $\mathbb{R}^d \oplus \mathbb{R}^d$ are called *observables*. (For example, positions and momenta are observables). The space of observables is equipped with the (commutative) product bc and with the *Poisson bracket*

$$\{b, c\} = \partial_{x^i} b \partial_{p_i} c - \partial_{p_i} b \partial_{x^i} c.$$

(We use the summation convention of summing wrt repeated indices). Thus in particular

$$\{x^i, x^j\} = \{p_i, p_j\} = 0, \quad \{x^i, p_j\} = \delta^i_j. \tag{1.1}$$

The dynamics is given by a real function on $\mathbb{R}^d \oplus \mathbb{R}^d$ called the *(classical) Hamiltonian* $H(x, p)$. The equations of motion are

$$\begin{aligned} \frac{\mathrm{d}x(t)}{\mathrm{d}t} &= \partial_p H(x(t), p(t)), \\ \frac{\mathrm{d}p(t)}{\mathrm{d}t} &= -\partial_x H(x(t), p(t)). \end{aligned}$$

We treat $x(t), p(t)$ as the functions of the initial conditions

$$x(0) = x, \qquad p(0) = p.$$

More generally, the evolution of an observable $b(x,p)$ is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}b(x(t),p(t)) = \{b,H\}(x(t),p(t)).$$

The dynamics preserves the product (this is obvious) and the Poisson bracket:

$$bc(x(t),p(t)) = b(x(t),p(t))c(x(t),p(t)),$$

$$\{b,c\}(x(t),p(t)) = \{b(x(t),p(t)),c(x(t),p(t))\},$$

Examples of classical Hamitonians:

particle in electrostatic and magnetic potentials	$\frac{1}{2m}(p-A(x))^2+V(x)$,
particle in curved space	$\frac{1}{2}p_i g^{ij}(x)p_j$,
harmonic oscillator	$\frac{1}{2}p^2+\frac{\omega^2}{2}x^2$,
particle in constant magnetic field	$\frac{1}{2}(p_1-Bx_2)^2+\frac{1}{2}(p_2+Bx_1)^2$,
general quadratic Hamiltonian	$\frac{1}{2}a^{ij}p_ip_j+b_i^jx^ip_j+\frac{1}{2}c_{ij}x^ix^j$.

1.2 Basic quantum mechanics

Let $\hbar$ be a positive parameter, typically small.

Basic quantum mechanics takes place in the Hilbert space $L^2(\mathbb{R}^d)$. Self-adjoint operators on $L^2(\mathbb{R}^d)$ are called observables. For a pair of such operators A,B we have their *product* AB. (Note that we disregard the issues that arise with unbounded operators for which the product is problematic). From the product one can derive their commutative *Jordan product* $\frac{1}{2}(AB+BA)$ and their *commutator* $[A,B]$. The dynamics is given by a self-adjoint operator H called the Hamiltonian. On the level of the Hilbert space the evolution equation is

$$\mathrm{i}\hbar\frac{\mathrm{d}\Psi}{\mathrm{d}t} = H\Psi(t), \quad \Psi(0)=\Psi,$$

so that $\Psi(t)=\mathrm{e}^{-\frac{\mathrm{i}t}{\hbar}H}\Psi$. On the level of observables,

$$\hbar\frac{\mathrm{d}A(t)}{\mathrm{d}t} = \mathrm{i}[H,A(t)], \quad A(0)=A,$$

so that $A(t)=\mathrm{e}^{\frac{\mathrm{i}t}{\hbar}H}A\mathrm{e}^{-\frac{\mathrm{i}t}{\hbar}H}$. The dynamics preserves the product:

$$(AB)(t) = A(t)B(t).$$

We have distinguished observables: the *positions* $\hat{x}^i$, $i=1,\dots,n$, and the *momenta* $\hat{p}_i := \frac{\hbar}{\mathrm{i}}\partial_{x^i}$, $i=1,\dots,n$. They satisfy

$$[\hat{x}^i,\hat{x}^j] = [\hat{p}_i,\hat{p}_j] = 0, \quad [\hat{x}^i,\hat{p}_j] = \mathrm{i}\hbar\delta^i_j.$$

Examples of quantum Hamiltonians

$$\begin{array}{rl}
\text{particle in electrostatic and} & \\
\text{magnetic potentials} & \dfrac{1}{2m}(\hat{p}-A(\hat{x}))^2+V(\hat{x}), \\
\text{particle in curved space} & \dfrac{1}{2}g^{-1/4}(\hat{x})\hat{p}_i g^{ij}(\hat{x})g^{1/2}(\hat{x})\hat{p}_j g^{-1/4}(\hat{x}), \\
\text{harmonic oscillator} & \dfrac{1}{2}\hat{p}^2+\dfrac{\omega^2}{2}\hat{x}^2, \\
\text{particle in constant magnetic field} & \dfrac{1}{2}(\hat{p}_1-B\hat{x}_2)^2+\dfrac{1}{2}(\hat{p}_2+B\hat{x}_1)^2, \\
\text{general quadratic Hamiltonian} & \dfrac{1}{2}a^{ij}\hat{p}_i\hat{p}_j+b_i^j\hat{x}^i\hat{p}_j+\dfrac{1}{2}c_{ij}\hat{x}^i\hat{x}^j.
\end{array}$$

1.3 Concept of quantization

Quantization usually means a linear transformation, which to a function on phase space $b:\mathbb{R}^{2d}\to\mathbb{C}$ associates an operator $\mathrm{Op}^\bullet(b)$ acting on the Hilbert space $L^2(\mathbb{R}^d)$, and in addition has various good properties. (The superscript $\bullet$ stands for a possible decoration indicating the type of a given quantization).

(Sometimes we will write $\mathrm{Op}^\bullet(b(x,p))$ for $\mathrm{Op}^\bullet(b)$–in this notation x, p play the role of coordinate functions on the phase space and not concrete points).

Here are desirable properties of a quantization:

(1) $\mathrm{Op}^\bullet(1)=\mathbb{1}$, $\mathrm{Op}^\bullet(x^i)=\hat{x}^i$, $\mathrm{Op}^\bullet(p_j)=\hat{p}_j$.

(2) $\frac{1}{2}\big(\mathrm{Op}^\bullet(b)\mathrm{Op}^\bullet(c)+\mathrm{Op}^\bullet(c)\mathrm{Op}^\bullet(b)\big)\approx\mathrm{Op}^\bullet(bc)$.

(3) $[\big(\mathrm{Op}^\bullet(b),\mathrm{Op}^\bullet(c)]\approx\mathrm{i}\hbar\mathrm{Op}^\bullet(\{b,c\})$.

Above, $\approx$ denotes equality modulo terms small in terms of $\hbar$. The function b will be called the *symbol* (or *dequantization*) of the operator B.

Note that (1) implies that (3) is true with $\approx$ replaced with $=$ if b is a 1st degree polynomial.

1.4 The role of the Planck constant

Recall that the position operator $\hat{x}_i$, is the multiplication by x_i and the momentum operator is $\hat{p}_i:=\frac{\hbar}{\mathrm{i}}\partial_{x_i}$. Thus we treat the position $\hat{x}$ as the distinguished physical observable, which is the same in the classical and quantum formalism. The momentum is scaled by the Planck constant. This is the usual convention in physics.

Let $\mathrm{Op}^\bullet(b)$ stand for the quantization with $\hbar=1$. The quantization with any $\hbar$ will be denoted by $\mathrm{Op}_\hbar^\bullet(b)$. Note that we have the relationship

$$\mathrm{Op}_\hbar^\bullet(b)=\mathrm{Op}^\bullet(b_\hbar),\quad b_\hbar(x,p)=b(x,\hbar p).$$

However this convention breaks the symplectic invariance of the phase space. In some situations it is more natural to use the Planck constant differently and to use the position operator $\tilde{x}_i$ which is the multiplication operator by $\sqrt{\hbar}x_i$, and the momentum operator $\tilde{p} := \frac{\sqrt{\hbar}}{\mathrm{i}}\partial_{x_i}$. Note that they satisfy the usual commutation relations

$$[\tilde{x}_i, \tilde{p}_j] = \mathrm{i}\hbar\delta_{ij}.$$

The corresponding quantization of a function b is

$$\widetilde{\mathrm{Op}}_\hbar^\bullet(b) := \mathrm{Op}^\bullet(\tilde{b}_\hbar), \quad \tilde{b}_\hbar(x,p) = b(\sqrt{\hbar}x, \sqrt{\hbar}p). \tag{1.2}$$

so that

$$\widetilde{\mathrm{Op}}_\hbar^\bullet(x_i) = \tilde{x}_i, \quad \widetilde{\mathrm{Op}}_\hbar^\bullet(p_i) = \tilde{p}_i.$$

The advantage of (1.2) is that positions and momenta are treated on the equal footing. This approach is typical when we consider coherent states.

Of course, both approaches are unitary equivalent. Indeed, introduce the unitary scaling

$$\tau_\lambda \Phi(x) = \lambda^{-d/2}\Phi\big(\lambda^{-1/2}x\big).$$

Then

$$\widetilde{\mathrm{Op}}_\hbar^\bullet(b_\hbar) = \tau_{\hbar^{1/2}}\mathrm{Op}^\bullet(b_\hbar)\tau_{\hbar^{-1/2}}.$$

1.5 Aspects of quantization

Quantization has many aspects in contemporary mathematics and physics.

1. *Fundamental formalism*
   – used to define a quantum theory from a classical theory;
   – underlying the emergence of classical physics from quantum physics (Weyl-Wigner-Moyal, Wentzel-Kramers-Brillouin).

2. *Technical parametrization*
   – of operators used in PDE's (Maslov, 4 volumes of Hörmander);
   – of observables in quantum optics (Nobel prize for Glauber);
   – signal encoding.

3. *Subject of mathematical research*
   – geometric quantization;
   – deformation quantization (Fields medal for Kontsevich!);

4. *Harmonic analysis*
   – on the Heisenberg group;
   – special approach for more general Lie groups and symmetric spaces.

We will not discuss (3), where the starting point is a symplectic or even a Poison manifold. We will concentrate on (1) and (2), where the starting point is a (linear) symplectic space, or sometimes a cotangent bundle.

A seperate subject is quantization of systems with an infinite number of degrees of freedom, as in QFT, where it is even nontrivial to quantize linear dynamics.

2 Preliminaries

2.1 Integral kernel of an operator

Every linear operator A on $\mathbb{C}^n$ can be represented by a matrix $[A_i^j]$.

One would like to generalize this concept to infinite dimensional spaces (say, Hilbert spaces) and continuous variables instead of a discrete variables i, j. Suppose that a given vector space is represented, say, as $L^2(X)$, where X is a certain space with a measure. One often uses the representation of an operator A in terms of its *integral kernel* $X \times X \ni (x, y) \mapsto A(x, y)$, so that

$$A\Psi(x) = \int A(x, y)\Psi(y)\mathrm{d}y.$$

Note that strictly speaking $A(\cdot, \cdot)$ does not have to be a function. E.g. in the case $X = \mathbb{R}^d$ it could be a distribution, hence one often says the *distributional kernel* instead of the *integral kernel*. Sometimes $A(\cdot, \cdot)$ is ill-defined anyway. Below we will describe some situations where there is a good mathematical theory of integral/distributional kernels.

At least formally, we have

$$AB(x, y) = \int A(x, z)B(z, y)\mathrm{d}z,$$

$$A^*(x, y) = \overline{A(y, x)}.$$

Example 2.1. *Let $\Phi, \Psi \in L^2(\mathbb{R}^d)$. Consider the operator A*

$$Av := \Psi(\Phi|v), \qquad v \in L^2(\mathbb{R}^d). \tag{2.1}$$

Then the integral kernel of A is

$$A(x, y) := \Psi(x)\overline{\Phi(y)}. \tag{2.2}$$

Note that often (especially in physics) A is written in the bra-ket notation:

$$A = |\Psi)(\Phi|. \tag{2.3}$$

Example 2.2. *Let the variable in $\mathbb{R}^d$ be called x. Usually, we will denote by the same symbol the operator of multiplication by the variable x. If it causes confusion, and then we use the notation $\hat{x}$ for this operator. Thus*

$$(\hat{x}\Psi)(x) = x\Psi(x). \tag{2.4}$$

Then $f(\hat{x})$ is the operator of the multiplication by $f(x)$.

$$(f(\hat{x})\Psi)(x) = f(x)\Psi(x). \tag{2.5}$$

Here are the integral kernels of some operators:

$$f(\hat{x})(x, y) = f(x)\delta(x - y), \tag{2.6}$$

$$\Big(f(\hat{x})Ag(\hat{x})\Big)(x, y) = f(x)A(x, y)g(y). \tag{2.7}$$

Note that we will usually write x for $\hat{x}$.

2.2 Distributions

Distributions are linear functionals on $\mathcal{D}(\mathbb{R}^d) := C_{\mathrm{c}}^{\infty}(\mathbb{R}^d)$ satisfying some continuity relations. Thus they are functions

$$\mathcal{D}(\mathbb{R}^d) \ni \Psi \mapsto \langle T|\Psi\rangle \in \mathbb{C}. \tag{2.8}$$

The set of distributions is denoted $\mathcal{D}'(\mathbb{R}^d)$. Elements of $\mathcal{D}(\mathbb{R}^d)$ are often called test functions,

If where $f \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$, then the following is a distribution:

$$\int f(x)\Psi(x)\mathrm{d}x. \tag{2.9}$$

Distributions given by locally integrable functions, as in (2.9), are called regular. We will typically use the integral notation also for non-regular distributions:

$$\langle T|\Psi\rangle = \int T(x)\Psi(x)\mathrm{d}x.$$

Here are some examples of non-regular distributions:

$$\int \delta(t)\Phi(t)\mathrm{d}t := \Phi(0), \tag{2.10}$$

$$\int (t \pm \mathrm{i}0)^{\lambda}\Phi(t)\mathrm{d}t := \lim_{\epsilon\searrow 0}\int (t \pm \mathrm{i}\epsilon)^{\lambda}\Phi(t)\mathrm{d}t. \tag{2.11}$$

2.3 Tempered distributions

The space of *Schwartz functions on* $\mathbb{R}^n$ is defined as

$$\mathcal{S}(\mathbb{R}^n) := \big\{\Psi \in C^{\infty}(\mathbb{R}^n) \ :\ \int |x^{\alpha}\nabla_x^{\beta}\Psi(x)|^2\mathrm{d}x < \infty, \quad \alpha, \beta \in \mathbb{N}^n\big\}. \tag{2.12}$$

Remark 2.3. *The definition (2.12) is equivalent to*

$$\mathcal{S}(\mathbb{R}^n) = \big\{\Psi \in C^{\infty}(\mathbb{R}^n) \ :\ |x^{\alpha}\nabla_x^{\beta}\Psi(x)| \le c_{\alpha,\beta}, \quad \alpha, \beta \in \mathbb{N}^n\big\}. \tag{2.13}$$

$\mathcal{S}'(\mathbb{R}^n)$ denotes the space of continuous functionals on $\mathcal{S}(\mathbb{R}^n)$, ie. $\mathcal{S}(\mathbb{R}^n) \ni \Psi \mapsto \langle T|\Psi\rangle \in \mathbb{C}$ belongs to $\mathcal{S}'$ iff there exists N such that

$$|\langle T|\Psi\rangle| \le \Big(\sum_{|\alpha|+|\beta|<N}\int |x^{\alpha}\nabla_x^{\beta}\Psi(x)|^2\mathrm{d}x\Big)^{\frac{1}{2}}.$$

The Fourier transformation is a continuous map from $\mathcal{S}'$ into itself. We have continuous inclusions

$$\mathcal{S}(\mathbb{R}^n) \subset L^2(\mathbb{R}^n) \subset \mathcal{S}'(\mathbb{R}^n).$$

Theorem 2.4 (The Schwartz kernel theorem)**.** *B is a continuous linear transformation from $\mathcal{S}(\mathbb{R}^d)$ to $\mathcal{S}'(\mathbb{R}^d)$ iff there exists a distribution $B(\cdot,\cdot) \in \mathcal{S}'(\mathbb{R}^d \oplus \mathbb{R}^d)$ such that*

$$(\Psi|B\Phi) = \int \overline{\Psi(x)}B(x,y)\Phi(y)\mathrm{d}x\mathrm{d}y, \quad \Psi, \Phi \in \mathcal{S}(\mathbb{R}^d).$$

Note that $\Leftarrow$ is obvious. The distribution $B(\cdot,\cdot) \in \mathcal{S}'(\mathbb{R}^d \oplus \mathbb{R}^d)$ is called the *distributional kernel of the transformation* B. All bounded operators on $L^2(\mathbb{R}^d)$ satisfy the Schwartz kernel theorem.

Examples:

(1) $\mathrm{e}^{-\mathrm{i}xy}$ is the kernel of the Fourier transformation

(2) $\delta(x-y)$ is the kernel of identity.

(3) $\partial_x\delta(x-y)$ is the kernel of ∂_x. .

2.4 Fourier tranformation

Let $\mathbb{R}^d \ni x \mapsto f(x)$. We adopt the following definition of the *Fourier transform.*

$$\mathcal{F}f(\xi) := \int \mathrm{e}^{-\mathrm{i}\xi x} f(x)\mathrm{d}x.$$

The inverse Fourier transform is given by

$$\mathcal{F}^{-1}g(x) = (2\pi)^{-d}\int \mathrm{e}^{\mathrm{i}x\xi} g(\xi)\mathrm{d}\xi.$$

Formally, $\mathcal{F}^{-1}\mathcal{F} = 1\!\!1$ can be expressed as

$$(2\pi)^{-d}\int \mathrm{e}^{\mathrm{i}(x-y)\xi}\mathrm{d}\xi = \delta(x-y).$$

Hence

$$(2\pi)^{-d}\int\int \mathrm{e}^{\mathrm{i}x\xi}\mathrm{d}\xi\mathrm{d}x = 1.$$

$\mathcal{F}$ maps $\mathcal{S}(\mathbb{R}^d)$ and $\mathcal{S}'(\mathbb{R}^d)$ into itself.

Suppose the variable has a generic name, say x. Then we set

$$D_x := \frac{1}{\mathrm{i}}\partial_x.$$

Clearly,

$$\mathrm{e}^{\mathrm{i}tD_x}\Phi(x) = \Phi(x+t), \tag{2.14}$$

$$g(D_x)(x,y) = \frac{\mathcal{F}g(y-x)}{(2\pi)^d}, \quad \text{or} \quad \big(g(D_x)f\big)(x) = \frac{1}{(2\pi)^d}\int (\mathcal{F}g)(x-y)f(y)\mathrm{d}y. \tag{2.15}$$

Proposition 2.5. *The Fourier transform of* $\mathbb{R}^d \oplus \mathbb{R}^d \ni (\eta,\xi) \mapsto \mathrm{e}^{-\mathrm{i}t\eta\xi}$ *is* $\frac{(2\pi)^d}{t^d}\mathrm{e}^{\frac{\mathrm{i}xp}{t}}$. *Hence*

$$\left(\mathrm{e}^{-\mathrm{i}tD_xD_p}f\right)(x,p) = \frac{1}{(2\pi t)^d}\int \mathrm{e}^{\frac{\mathrm{i}(x-x')(p-p')}{t}} f(x',p')\mathrm{d}x'\mathrm{d}p'. \tag{2.16}$$

Proof.

$$\int \mathrm{e}^{-\mathrm{i}t\eta\xi-\mathrm{i}p\eta-\mathrm{i}x\xi}\mathrm{d}\eta\mathrm{d}\xi \quad = \quad \mathrm{e}^{\frac{\mathrm{i}xp}{t}}\int\int \mathrm{e}^{-\mathrm{i}t(\eta+\frac{x}{t})(\xi+\frac{p}{t})}\mathrm{d}\eta\mathrm{d}\xi.$$

□

2.5 Semiclassical Fourier transformation

If we use the parameter $\hbar$, it is natural to use the semiclassical Fourier tranformation

$$\mathcal{F}_\hbar f(p) := \int \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}px} f(x)\mathrm{d}x.$$

Its inverse is given by

$$\mathcal{F}_\hbar^{-1} g(x) = (2\pi\hbar)^{-d} \int \mathrm{e}^{\frac{\mathrm{i}}{\hbar}xp} g(p)\mathrm{d}p.$$

Recall that we defined $\hat{p}_i := \frac{\hbar}{\mathrm{i}}\partial_{x^i}$, $i = 1, \dots, n$.

Proposition 2.6. *The semiclassical Fourier transformation swaps the position and momentum:*

$$\begin{aligned} \mathcal{F}_\hbar^{-1}\hat{x}\mathcal{F}_\hbar &= \hat{p}, \\ \mathcal{F}_\hbar^{-1}\hat{p}\mathcal{F}_\hbar &= -\hat{x}. \end{aligned}$$

Proof.

$$\big(\mathcal{F}_\hbar^{-1}\hat{x}\mathcal{F}_\hbar\Psi\big)(p) = \frac{1}{(2\pi\hbar)^d}\int \mathrm{d}x \int \mathrm{d}k \mathrm{e}^{\frac{\mathrm{i}}{\hbar}px} x \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}kx}\Psi(k) \tag{2.17}$$

$$= \frac{1}{(2\pi\hbar)^d}\int \mathrm{d}x \int \mathrm{d}k \hbar\mathrm{i}\partial_k \mathrm{e}^{\frac{\mathrm{i}}{\hbar}px} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}kx}\Psi(k) \tag{2.18}$$

$$= -\frac{1}{(2\pi\hbar)^d}\int \mathrm{d}x \int \mathrm{d}k \mathrm{e}^{\frac{\mathrm{i}}{\hbar}px} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}kx}\hbar\mathrm{i}\partial_k\Psi(k) \quad = \quad \hat{p}\Psi(p). \tag{2.19}$$

$$\big(\mathcal{F}_\hbar^{-1}\hat{p}\mathcal{F}_\hbar\Psi\big)(x) = \frac{1}{(2\pi\hbar)^d}\int \mathrm{d}x \int \mathrm{d}k \mathrm{e}^{\frac{\mathrm{i}}{\hbar}px} \frac{\hbar}{\mathrm{i}}\partial_p \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}py}\Psi(y) \tag{2.20}$$

$$= -\frac{1}{(2\pi\hbar)^d}\int \mathrm{d}x \int \mathrm{d}k \mathrm{e}^{\frac{\mathrm{i}}{\hbar}px} y \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}py}\Psi(y) \quad = \quad -\hat{x}\Psi(x). \tag{2.21}$$

□

Hence, for Borel functions f, g

$$\mathcal{F}_\hbar^{-1} f(\hat{x})\mathcal{F}_\hbar = f(\hat{p}), \tag{2.22}$$

$$\mathcal{F}_\hbar^{-1} g(\hat{p})\mathcal{F}_\hbar = g(-\hat{x}). \tag{2.23}$$

(2.23) can be rewritten as

$$\big(g(\hat{p})\big)(x,y) = \frac{1}{(2\pi\hbar)^d}\int\int \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(x-y)p} g(p)\mathrm{d}p \tag{2.24}$$

$$= \frac{1}{(2\pi\hbar)^d}\big(\mathcal{F}_\hbar g\big)(y-x). \tag{2.25}$$

2.6 Hilbert-Schmidt operators

We say that an operator B is Hilbert-Schmidt if

$$\infty > \mathrm{Tr} B^*B = \sum_{i\in I}(e_i|B^*Be_i) = \sum_{i\in I}(Be_i|Be_i),$$

where $\{e_i\}_{i\in I}$ is an arbitrary basis and the RHS does not depend on the choice of the basis. Hilbert-Schmidt are bounded.

Proposition 2.7. *Suppose that $\mathcal{H} = L^2(X)$ for some measure space X. The following conditions are equivalent*

(1) *B is Hilbert-Schmidt.*

(2) *The distributional kernel of B is $L^2(X \times X)$.*

Moreover, if B, C are Hilbert-Schmidt, then

$$\mathrm{Tr} B^*C = \int \overline{B(x,y)}C(x,y)\mathrm{d}x\mathrm{d}y.$$

2.7 Trace class operators

B is trace class if

$$\infty > \mathrm{Tr}\sqrt{B^*B} = \sum_{i\in I}(e_i|\sqrt{B^*B}e_i).$$

If B is trace class, then we can define its trace:

$$\mathrm{Tr} B := \sum_{i\in I}(e_i|Be_i).$$

where again $\{e_i\}_{i\in I}$ is an arbitrary basis and the RHS does not depend on the choice of the basis.

Trace class operators are Hilbert-Schmidt:

$$B^*B = (B^*B)^{1/4}(B^*B)^{1/2}(B^*B)^{1/4} \leq (B^*B)^{1/4}\|B\|(B^*B)^{1/4} = \|B\|(B^*B)^{1/2}.$$

Hence

$$\mathrm{Tr} B^*B \leq \|B\|\mathrm{Tr}\sqrt{B^*B}.$$

Consider a trace class operator C and a bounded operator B. On the formal level we have the formula

$$\mathrm{Tr} BC = \int B(y,x)C(x,y)\mathrm{d}x\mathrm{d}y. \tag{2.26}$$

In particular by setting $B = 1\!\!1$, we obtain formally

$$\mathrm{Tr} C = \int C(x,x)\mathrm{d}x.$$

3 x,p- and Weyl-Wigner quantizations

3.1 x,p-quantization

Suppose we look for a linear transformation that to a function b on phase space associates an operator $\mathrm{Op}^\bullet(b)$ such that

$$\mathrm{Op}^\bullet(f(x)) = f(\hat{x}), \quad \mathrm{Op}^\bullet(g(p)) = g(\hat{p}).$$

The so-called x,p*-quantization*, often used in the PDE community, is determined by the additional condition

$$\mathrm{Op}^{x,p}(f(x)g(p)) = f(\hat{x})g(\hat{p}).$$

Note that

$$\big(f(\hat{x})g(\hat{p})\big)\Psi(x) = (2\pi\hbar)^{-d}\int \mathrm{d}p \int \mathrm{d}y f(x)g(p)\mathrm{e}^{\frac{\mathrm{i}(x-y)p}{\hbar}}\Psi(y). \tag{3.1}$$

Hence we can generalize (3.1) for a general function on the phase space b

$$\big(\mathrm{Op}^{x,p}(b)\Psi\big)(x) = (2\pi\hbar)^{-d}\int \mathrm{d}p \int \mathrm{d}y b(x,p)\mathrm{e}^{\frac{\mathrm{i}(x-y)p}{\hbar}}\Psi(y). \tag{3.2}$$

In the PDE-community one writes

$$\mathrm{Op}^{x,p}(b) = b(x,\hbar D). \tag{3.3}$$

We also have the closely related p,x*-quantization*, which satisfies

$$\mathrm{Op}^{p,x}(f(x)g(p)) = g(\hat{p})f(\hat{x}).$$

It is given by the formula

$$\big(\mathrm{Op}^{p,x}(b)\Psi\big)(x) = (2\pi\hbar)^{-d}\int \mathrm{d}p \int \mathrm{d}y b(y,p)\mathrm{e}^{\frac{\mathrm{i}(x-y)p}{\hbar}}\Psi(y). \tag{3.4}$$

Thus the kernel of the operator as x,p- and p,x-quantization is given by:

$$\mathrm{Op}^{x,p}(b_{x,p}) = B, \quad B(x,y) = (2\pi\hbar)^{-d}\int \mathrm{d}p b_{x,p}(x,p)\mathrm{e}^{\frac{\mathrm{i}(x-y)p}{\hbar}}, \tag{3.5}$$

$$\mathrm{Op}^{p,x}(b_{p,x}) = B, \quad B(x,y) = (2\pi\hbar)^{-d}\int \mathrm{d}p b_{p,x}(y,p)\mathrm{e}^{\frac{\mathrm{i}(x-y)p}{\hbar}}. \tag{3.6}$$

Proposition 3.1. *We can compute the symbol from the kernel: If (3.5), then*

$$b_{x,p}(x,p) = \int B(x,x-z)\mathrm{e}^{-\frac{\mathrm{i}zp}{\hbar}}\mathrm{d}z. \tag{3.7}$$

Proof. We set $y = x - z$ in (3.5):

$$B(x,x-z) = (2\pi\hbar)^{-d}\int \mathrm{e}^{\frac{\mathrm{i}zp}{\hbar}} b_{x,p}(x,p)\mathrm{d}p.$$

Thus $z \mapsto B(x,x-z)$ is obtained from $b_{x,p}(x,p)$ by $\mathcal{F}_\hbar^{-1}$ in the second variable. We apply $\mathcal{F}_\hbar$. □

Proposition 3.2. $\big(\mathrm{Op}^{x,p}(b)\big)^* = \mathrm{Op}^{p,x}(\bar{b})$.

Proposition 3.3. *We can go from x,p- to p,x-quantization: If (3.5) and (3.6) hold, then*

$$\mathrm{e}^{-\mathrm{i}\hbar D_x D_p} b_{x,p}(x,p) = b_{p,x}(x,p). \tag{3.8}$$

Proof.

$$\begin{aligned} b_{x,p}(x,p) &= \int B(x, x-z)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}zp}\mathrm{d}z \\ &= (2\pi\hbar)^{-d}\int\int b_{p,x}(x-z,w)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}z(w-p)}\mathrm{d}z\mathrm{d}w \\ &= (2\pi\hbar)^{-d}\int\int b_{p,x}(y,w)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(x-y)(w-p)}\mathrm{d}y\mathrm{d}w \\ &= \mathrm{e}^{-\mathrm{i}\hbar D_x D_p} b_{p,x}(x,p). \end{aligned}$$

□

Therefore, formally,

$$\mathrm{Op}^{x,p}(b) = \mathrm{Op}^{p,x}(b) + O(\hbar).$$

3.2 Weyl-Wigner quantization

The definition of the *Weyl-Wigner quantization* looks like a compromise between the x,p and p,x-quantizations:

$$\big(\mathrm{Op}(b)\Psi\big)(x) = (2\pi\hbar)^{-d}\int \mathrm{d}p\int \mathrm{d}y b\Big(\frac{x+y}{2},p\Big)\mathrm{e}^{\frac{\mathrm{i}(x-y)p}{\hbar}}\Psi(y). \tag{3.9}$$

In the PDE-community it is usually called the *Weyl quantization* and denoted by

$$\mathrm{Op}(b) = b^w(x,\hbar D).$$

If $\mathrm{Op}(b) = B$, the kernel of B is given by:

$$B(x,y) \quad = \quad (2\pi\hbar)^{-d}\int \mathrm{d}p b\Big(\frac{x+y}{2},p\Big)\mathrm{e}^{\frac{\mathrm{i}(x-y)p}{\hbar}}. \tag{3.10}$$

Proposition 3.4. *We can compute the symbol from the kernel:*

$$b(x,p) = \int B\Big(x+\frac{z}{2}, x-\frac{z}{2}\Big)\mathrm{e}^{-\frac{\mathrm{i}zp}{\hbar}}\mathrm{d}z. \tag{3.11}$$

Proof.

$$B\Big(x+\frac{z}{2}, x-\frac{z}{2}\Big) = (2\pi\hbar)^{-d}\int \mathrm{e}^{\frac{\mathrm{i}zp}{\hbar}} b(x,p)\mathrm{d}p,$$

which is $\mathcal{F}_\hbar{-1}$ applied to $b(x,\cdot)$. We apply $\mathcal{F}_\hbar$. □

b is usually called in the PDE community the *Weyl symbol* and in the quantum physics community the *Wigner function*.

Example 3.5. *Let P_0 be the orthogonal projection onto the normalized vector $\pi^{-\frac{d}{4}}\mathrm{e}^{-\frac12 x^2}$. The integral kernel of P_0 equals*

$$P_0(x,y) = \pi^{-\frac{d}{2}}\mathrm{e}^{-\frac12 x^2 - \frac12 y^2}.$$

Its various symbols equal

$$\begin{array}{rl} x,p\text{-symbol:} & 2^{\frac{d}{2}}\mathrm{e}^{-\frac12 x^2-\frac12 p^2 - \mathrm{i}x\cdot p}, \\ p,x\text{-symbol:} & 2^{\frac{d}{2}}\mathrm{e}^{-\frac12 x^2-\frac12 p^2 + \mathrm{i}x\cdot p}, \\ \text{Weyl-Wigner symbol:} & 2^{\frac{d}{2}}\mathrm{e}^{-\frac12 x^2-\frac12 p^2}. \end{array}$$

Proposition 3.6. *We can go from the x,p- to the Weyl quantization:*

$$\text{if} \quad \mathrm{Op}^{x,p}(b_{x,p}) = \mathrm{Op}(b), \quad \text{then}$$

$$\mathrm{e}^{\frac{\mathrm{i}}{2}\hbar D_x D_p} b(x,p) = b_{x,p}(x,p). \tag{3.12}$$

Consequently,

$$b_{x,p} = b + O(\hbar).$$

3.3 Weyl operators

Proposition 3.7 (Baker-Campbell-Hausdorff formula)**.** *Suppose that*

$$\big[[A,B],A\big] = \big[[A,B],B\big] = 0.$$

Then

$$\mathrm{e}^{A+B} = \mathrm{e}^{A}\mathrm{e}^{B}\mathrm{e}^{-\frac12 [A,B]}.$$

Proof. We will show that for any $t \in \mathbb{R}$

$$\mathrm{e}^{t(A+B)} = \mathrm{e}^{tA}\mathrm{e}^{tB}\mathrm{e}^{-\frac12 t^2[A,B]}. \tag{3.13}$$

First, using the Lie formula, we obtain

$$\begin{array}{rcl} \mathrm{e}^{tA}B\mathrm{e}^{-tA} & = & \sum\limits_{n=0}^{\infty}\frac{t^n}{n!}\mathrm{ad}_A^n(B) \\ & = & B + t[A,B]. \end{array}$$

Now

$$\begin{array}{rcl} \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{tA}\mathrm{e}^{tB}\mathrm{e}^{-\frac12 t^2[A,B]} & = & A\mathrm{e}^{tA}\mathrm{e}^{tB}\mathrm{e}^{-\frac12 t^2[A,B]} \\ & & +\mathrm{e}^{tA}B\mathrm{e}^{tB}\mathrm{e}^{-\frac12 t^2[A,B]} \\ & & -\mathrm{e}^{tA}\mathrm{e}^{tB}t[A,B]\mathrm{e}^{-\frac12 t^2[A,B]} \\ & = & (A+B)\mathrm{e}^{tA}\mathrm{e}^{tB}\mathrm{e}^{-\frac12 t^2[A,B]}. \end{array}$$

Besides, (3.13) is true for $t = 0$. $\Box$

Let $\xi = (\xi_1, \dots, \xi_d)$, $\eta = (\eta_1, \dots, \eta_d) \in \mathbb{R}^d$. Clearly,

$$[\xi_i \hat{x}_i, \eta_j \hat{p}_j] = \mathrm{i}\hbar \xi_i \eta_i.$$

Therefore,

$$\begin{aligned} \mathrm{e}^{\mathrm{i}\xi_i \hat{x}_i} \mathrm{e}^{\mathrm{i}\eta_i \hat{p}_i} &= \mathrm{e}^{-\frac{\mathrm{i}\hbar}{2}\xi_i\eta_i} \mathrm{e}^{\mathrm{i}(\xi_i \hat{x}_i + \eta_i \hat{p}_i)} \\ &= \mathrm{e}^{-\mathrm{i}\hbar\xi_i\eta_i} \mathrm{e}^{\mathrm{i}\eta_i \hat{p}_i} \mathrm{e}^{\mathrm{i}\xi_i \hat{x}_i}. \end{aligned}$$

The operators $\mathrm{e}^{\mathrm{i}(\xi_i \hat{x}_i + \eta_i \hat{p}_i)}$ are sometimes called *Weyl operators*. They satisfy the relations that involve the symplectic form:

$$\mathrm{e}^{\mathrm{i}(\xi_i \hat{x}_i + \eta_i \hat{p}_i)} \mathrm{e}^{\mathrm{i}(\xi_i' \hat{x}_i + \eta_i' \hat{p}_i)} = \mathrm{e}^{-\frac{\mathrm{i}\hbar}{2}(\xi_i \eta_i' - \eta_i \xi_i')} \mathrm{e}^{\mathrm{i}\left((\xi_i + \xi_i')\hat{x}_i + (\eta_i + \eta_i')\hat{p}_i\right)} \tag{3.14}$$

They translate the position and momentum:

$$\begin{aligned} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(-y\hat{p} + w\hat{x})} \hat{x} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(y\hat{p} - w\hat{x})} &= \hat{x} - y, \\ \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(-y\hat{p} + w\hat{x})} \hat{p} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(y\hat{p} - w\hat{x})} &= \hat{p} - w. \end{aligned}$$

3.4 Weyl-Wigner quantization in terms of Weyl operators

Note that

$$\mathrm{e}^{\mathrm{i}(\xi_i \hat{x}_i + \eta_i \hat{p}_i)} = \mathrm{e}^{\frac{\mathrm{i}}{2}\xi_i \hat{x}_i} \mathrm{e}^{\mathrm{i}\eta_i \hat{p}_i} \mathrm{e}^{\frac{\mathrm{i}}{2}\xi_i \hat{x}_i}. \tag{3.15}$$

Hence the integral kernel of $\mathrm{e}^{\mathrm{i}(\xi_i \hat{x}_i + \eta_i \hat{p}_i)}$ is

$$(2\pi\hbar)^{-d} \int \mathrm{d}p \mathrm{e}^{\mathrm{i}(\frac{1}{2}\xi_i x_i + \eta_i p_i + \frac{1}{2}\xi_i y_i) + \frac{\mathrm{i}}{\hbar}(x_i - y_i)p_i}.$$

Therefore,

$$\mathrm{Op}(\mathrm{e}^{\mathrm{i}(\xi_i x_i + \eta_i p_i)}) = \mathrm{e}^{\mathrm{i}(\xi_i \hat{x}_i + \eta_i \hat{p}_i)}. \tag{3.16}$$

Every function b on $\mathbb{R}^d \oplus \mathbb{R}^d$ can be written in terms of its Fourier transform:

$$b(x, p) = (2\pi)^{-2d} \int\int\int\int \mathrm{e}^{\mathrm{i}(x_i - y_i)\xi_i + \mathrm{i}(p_i - w_i)\eta_i} b(y, w) \mathrm{d}y \mathrm{d}w \mathrm{d}\xi \mathrm{d}\eta. \tag{3.17}$$

Applying Op to both sides of (3.17), and then using (3.16), we obtain

$$\mathrm{Op}(b) = (2\pi)^{-2d} \int\int\int\int \mathrm{e}^{\mathrm{i}(\hat{x}_i - y_i)\xi_i + \mathrm{i}(\hat{p}_i - w_i)\eta_i} b(y, w) \mathrm{d}y \mathrm{d}w \mathrm{d}\xi \mathrm{d}\eta, \tag{3.18}$$

which can be treated as an alternative definition of the Weyl-Wigner quantization.

3.5 Weyl-Wigner quantization and functional calculus

Let $(\xi, \eta) \in \mathbb{R}^d \oplus \mathbb{R}^d$). Let f be a function on $\mathbb{R}$, say, $f \in L^\infty(\mathbb{R})$. Then $f(\xi x + \eta p)$ belongs to $L^\infty(\mathbb{R}^d \oplus \mathbb{R}^d)$. By functional calculus of selfadjoint operators, $f(\xi\hat{x} + \eta\hat{p}) \in B\big(L^\infty(\mathbb{R}^d)\big)$ We have

$$\mathrm{Op}\big(f(\xi x + \eta p)\big) = f(\xi\hat{x} + \eta\hat{p}). \tag{3.19}$$

To see this we just use the Fourier transform of f, denoted $\mathcal{F}f$ and the property (3.16):

$$\begin{aligned} f(\xi\hat{x} + \eta\hat{p}) &= (2\pi)^{-1} \int \mathcal{F}f(t) \mathrm{e}^{\mathrm{i}(\xi\hat{x}+\eta\hat{p})t} \mathrm{d}t, \\ f(\xi_i x_i + \eta_i p_i) &= (2\pi)^{-1} \int \mathcal{F}f(t) \mathrm{e}^{\mathrm{i}(\xi x+\eta p)t} \mathrm{d}t. \end{aligned}$$

Suppose that we have functionals $\xi^{(j)}, \eta^{(j)} \in \mathbb{R}^d \oplus \mathbb{R}^d$, $j = 1, \dots, m$, satisfying

$$\{\xi^{(j)}\hat{x} + \eta^{(j)}\hat{p}, \xi^{(k)}\hat{x} + \eta^{(k)}\hat{p}\} = 0, \quad j, k = 1, \dots, m. \tag{3.20}$$

Then

$$[\xi^{(j)}\hat{x} + \eta^{(j)}\hat{p}, \xi^{(k)}\hat{x} + \eta^{(k)}\hat{p}] = 0, \quad j, k = 1, \dots, m \tag{3.21}$$

Therefore, by the functional calculus for commuting self-adjoint operators, for a function $F \in L^\infty(\mathbb{R}^m)$ we have

$$F(\xi^{(1)}\hat{x} + \eta^{(1)}\hat{p}, \dots, \xi^{(m)}\hat{x} + \eta^{(m)}\hat{p}) = \mathrm{Op}\big(F(\xi^{(1)}x + \eta^{(1)}p, \dots, \xi^{(m)}x + \eta^{(m)}p)\big). \tag{3.22}$$

Note that the maximal number of linearly independent functionals satisfying (3.20) is d. Here is an example in $\mathbb{R}^2 \oplus \mathbb{R}^2$:

$$\cos(\alpha_1)x_1 + \sin(\alpha_1)p_1 = 0, \quad \cos(\alpha_2)x_2 + \sin(\alpha_2)p_2 = 0. \tag{3.23}$$

3.6 Classical and quantum mechanics over a symplectic vector space

A *symplectic form* is a nondegenerate antisymmetric form. A vector space equipped with a symplectic form is called a *symplectic vector space*. It has to have an even dimension.

Let $\mathbb{R}^{2d}$ be an even dimensional vector space. Let ϕ^j, $j = 1, \dots, 2d$ denote the canonical coordinates in $\mathbb{R}^{2d}$. Let $\omega = [\omega_{ij}]$ be a symplectic form. We will denote by $[\omega^{ij}]$ the inverse of $[\omega_{ij}]$.

On every symplectic vector space we have a natural Poisson bracket for functions b, c on $\mathbb{R}^{2d}$:

$$\{b, c\} = \partial_{\phi^i} b \omega^{ij} \partial_{\phi^j} c.$$

Proposition 3.8. *In every symplectic space we can choose a basis $\phi^i = x_i$, $\phi^{d+i} = p_i$ so that the Poisson bracket has the form (1.1), that is*

$$\omega_{i,i+d} = 1, \quad \omega_{i+d,i} = -1.$$

Thus every symplectic space is isomorphic to the space $\mathbb{R}^d \oplus \mathbb{R}^d$ with the usual structure.

We say that a linear transformation $r = [r_i^j]$ is symplectic if it preserves the symplectic form. Explicitly, $r^{\#}\omega r = \omega$, or

$$r_i^p \omega_{pq} r_j^q = \omega_{ij}$$

The set of such transformations is denoted $Sp(\mathbb{R}^{2d})$. It is a Lie group.

We say that a linear transformation $b = [b_i^j]$ is infinitesimally symplectic if it infinitesimally preserves the symplectic form. In other words, $\mathbb{1} + \epsilon b$ is for small ϵ approximately symplectic. Explicitly, $b^{\#}\omega + \omega b = 0$, or

$$b_i^p \omega_{pj} + \omega_{ip} b_j^p = 0.$$

The set of such transformations is denoted $sp(\mathbb{R}^{2d})$. It is a Lie algebra.

In parallel with the *classical system* described by functions on the phase space $\mathbb{R}^{2d}$ we also consider a *quantum system* described by operators on a certain Hilbert space equipped with distinguished operators $\hat{\phi}^j$, $j = 1, \dots, 2d$ satisfying (formally)

$$[\hat{\phi}^j, \hat{\phi}^k] = \mathrm{i}\omega^{jk}\mathbb{1}. \tag{3.24}$$

Proposition 3.9. *b is an infinitesimally symplectic transformaton iff $c = \omega^{-1}b$ is symmetric, so that $b_j^i = \omega^{ik}c_{kj}$. Then*

$$H = \frac{1}{2}c_{jk}\phi^j\phi^k, \quad \hat{H} = \mathrm{Op}(H) = \frac{1}{2}c_{jk}\hat{\phi}^j\hat{\phi}^k$$

is the corresponding classical and quantum Hamiltonian. Let $[r_i^j(t)]$ be the corresponding dynamics, which is a 1-parameter group in $Sp(\mathbb{R}^{2d})$. Then the classical and quantum dynamics generated by this Hamiltonian are given by the flow $r(t)$:

$$\phi^j(t) = r_k^j(t)\phi^k(0), \quad \hat{\phi}^j(t) = r_k^j(t)\hat{\phi}^k(0),$$

3.7 Weyl quantization for a symplectic vector space

Let $\hat{\phi}_i$ satisfy the relations (3.24). For $\zeta = (\zeta_1, \dots, \zeta_{2d}) \in \mathbb{R}^{2d}$ set

$$\hat{\phi}\cdot\zeta := \sum_i \hat{\phi}_i\zeta_i, \quad W(\zeta) := \mathrm{e}^{\mathrm{i}\zeta\cdot\hat{\phi}}.$$

Then

$$W(\zeta)W(\theta) = \mathrm{e}^{-\frac{\mathrm{i}}{2}\zeta\cdot\omega\theta}W(\zeta + \theta).$$

For a function b on $\mathbb{R}^{2d}$ we can define its Weyl-Wigner quantization:

$$\mathrm{Op}(b) := (2\pi)^{-2d}\int\int \mathrm{e}^{\mathrm{i}(\hat{\phi}_i - \psi_i)\cdot\zeta^i} b(\psi)\mathrm{d}\psi\mathrm{d}\zeta.$$

Note that

$$\mathrm{Op}\big(\mathrm{e}^{\mathrm{i}\phi\cdot\zeta}\big) = \mathrm{e}^{\mathrm{i}\hat{\phi}\cdot\zeta}. \tag{3.25}$$

More generally, for any Borel function f

$$\mathrm{Op}\big(f(\phi\cdot\zeta)\big) = f(\hat{\phi}\cdot\zeta). \tag{3.26}$$

Proposition 3.10.

$$\mathrm{Op}\big(\phi\zeta_1\cdots\phi\zeta_n\big)=\frac{1}{n!}\sum_{\sigma\in S_n}\hat{\phi}\zeta_{\sigma(i)}\cdots\hat{\phi}\zeta_{\sigma(n)}. \tag{3.27}$$

Proof. We have

$$\mathrm{Op}\big((\phi\zeta)^n\big)=(\hat{\phi}\zeta)^n. \tag{3.28}$$

This is a special case of (3.27), it is also seen directly from (3.25) by expanding into a power series. Let $t_1,\dots,t_n\in\mathbb{R}$. By (3.28),

$$\mathrm{Op}\big((t_1\phi{\cdot}\zeta_1+\cdots+t_n\phi{\cdot}\zeta_n)^n\big)=(t_1\hat{\phi}{\cdot}\zeta_1+\cdots+t_n\hat{\phi}{\cdot}\zeta_n)^n. \tag{3.29}$$

The coefficient at $t_1\cdots t_n$ on both sides is

$$\mathrm{Op}(n!\phi{\cdot}\zeta_1\cdots\phi{\cdot}\zeta_n)=\sum_{\sigma\in S_n}\hat{\phi}{\cdot}\zeta_{\sigma^{-1}(1)}\cdots\hat{\phi}{\cdot}\zeta_{\sigma^{-1}(n)}.$$

□

3.8 Positivity

Clearly,

$$\mathrm{Op}(b)^*=\mathrm{Op}(\bar{b}).$$

Therefore, b is real iff $\mathrm{Op}(b)$ is Hermitian. What about positivity? We will see that there is no implication in either direction between the positivity of b and of $\mathrm{Op}(b)$.

We have

$$(\hat{x}-\mathrm{i}\hat{p})(\hat{x}+\mathrm{i}\hat{p})=\hat{x}^2+\hat{p}^2-\hbar\geq 0.$$

Therefore

$$\mathrm{Op}(x^2+p^2-\hbar)\geq 0, \tag{3.30}$$

even though $x^2+p^2-\hbar$ is not everywhere positive.

The converse is more complicated. Consider the generator of dilations

$$A:=\frac{1}{2}(\hat{x}\hat{p}+\hat{p}\hat{x})=\hat{x}\hat{p}-\frac{\mathrm{i}}{2}=\mathrm{Op}(xp).$$

Its name comes from the 1-parameter group it generates:

$$\mathrm{e}^{\mathrm{i}tA}\Phi(x)=\mathrm{e}^{t/2}\Phi(\mathrm{e}^{t}x).$$

Note that $\mathrm{sp}\,A=\mathbb{R}$. Indeed, A preserves the direct decomposition $L^2(\mathbb{R})=L^2(0,\infty)\oplus L^2(-\infty,0)$. We will show that the spectrum of A restricted to each of these subspaces is $\mathbb{R}$. Consider the unitary operator $U:L^2(0,\infty)\to L^2(\mathbb{R})$ given by $U\Phi(s)=\mathrm{e}^{s/2}\Phi(\mathrm{e}^s)$ with the inverse $U^*\Psi(x)=x^{-1/2}\Psi(\log x)$. Then $U^*\hat{p}U=A$. But $\mathrm{sp}\,\hat{p}=\mathbb{R}$. Therefore, $\mathrm{sp}\,A^2=(\mathrm{sp}\,A)^2=[0,\infty[$.

We have $A^2 = \mathrm{Op}(xp)^2 = \mathrm{Op}(b)$, where

$$\begin{aligned}
b(x,p) &= \mathrm{e}^{\frac{\mathrm{i}\hbar}{2}(D_{p_1}D_{x_2}-D_{x_1}D_{p_2})}x_1p_1x_2p_2\Big|_{\substack{x:=x_1=x_2,\\ p:=p_1=p_2.}} \\
&= x^2p^2 + \frac{\hbar^2}{4\cdot 2}2D_{p_1}D_{x_2}D_{x_1}D_{p_2}x_1p_1x_2p_2\Big|_{\substack{x:=x_1=x_2,\\ p:=p_1=p_2,}} \\
&= x^2p^2 + \frac{\hbar^2}{4}.
\end{aligned}$$

Hence

$$\mathrm{Op}(x^2p^2) = A^2 - \frac{\hbar^2}{4}.$$

Therefore $\mathrm{Op}(x^2p^2)$ is not a positive operator even though its symbol is positive

3.9 Parity operator

Define the parity operator

$$I\Psi(x) = \Psi(-x). \tag{3.31}$$

More generally, set

$$I_{(y,w)} := \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(-y\hat{p}+w\hat{x})}I\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(y\hat{p}-w\hat{x})}. \tag{3.32}$$

Clearly,

$$I_{(y,w)}\Psi(x) = \mathrm{e}^{\frac{2\mathrm{i}}{\hbar}w\cdot(x-y)}\Psi(2y-x).$$

Let $\delta_{(y,w)}$ denote the delta function at $(y,w) \in \mathbb{R}^d \oplus \mathbb{R}^d$.

Proposition 3.11.

$$\mathrm{Op}\big((\pi\hbar)^d\delta_{(0,0)}\big) = I. \tag{3.33}$$

More generally,

$$\mathrm{Op}\big((\pi\hbar)^d\delta_{(y,w)}\big) = I_{(y,w)}. \tag{3.34}$$

Proof.

$$\begin{aligned}
\mathrm{Op}\big((\pi\hbar)^d\delta_{(0,0)}\big)(x,y) &= 2^{-d}\int\delta\Big(\frac{x+y}{2},\xi\Big)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(x-y)\cdot\xi}\mathrm{d}\xi \\
&= 2^{-d}\delta\Big(\frac{x+y}{2}\Big) = \delta(x+y).
\end{aligned}$$

To see the last step we substitute $\frac{y}{2} = \tilde{y}$ below and evaluate the delta function:

$$\int\delta\Big(\frac{x+y}{2}\Big)\Phi(y)\mathrm{d}y = \int\delta\Big(\frac{x}{2}+\tilde{y}\Big)\Phi(2\tilde{y})2^d\mathrm{d}\tilde{y} = 2^d\Phi(-x). \tag{3.35}$$

□

Theorem 3.12. *Let* $\mathrm{Op}(b) = B$.

(1) *If* $b \in L^1(\mathbb{R}^d \oplus \mathbb{R}^d)$, *then* B *is a compact operator. In terms of an absolutely norm convergent integral, we can write*

$$B = (\pi\hbar)^{-d} \int I_{(x,p)} b(x,p) \mathrm{d}x\mathrm{d}p. \tag{3.36}$$

Hence,

$$\|B\| \leq (\pi\hbar)^{-d} \|b\|_1. \tag{3.37}$$

(2) *If* B *is trace class, then* b *is continuous, vanishes at infinity and*

$$b(x,p) = 2^d \mathrm{Tr} I_{(x,p)} B. \tag{3.38}$$

Hence

$$|b(x,p)| \leq 2^d \mathrm{Tr}|B|.$$

Proof. Obviously,

$$b = \int b(x,p) \delta_{x,p} \mathrm{d}x\mathrm{d}p.$$

Hence

$$\begin{aligned} \mathrm{Op}(b) &= \int b(x,p) \mathrm{Op}(\delta_{x,p}) \mathrm{d}x\mathrm{d}p \\ &= (\pi\hbar)^{-d} \int b(x,p) I_{(x,p)} \mathrm{d}x\mathrm{d}p. \end{aligned}$$

Next,

$$\begin{aligned} b(x,p) &= \int \delta_{(x,p)}(y,w) b(y,w) \mathrm{d}y\mathrm{d}w \\ &= (2\pi\hbar)^d \mathrm{Tr} \mathrm{Op}(\delta_{(x,p)}) \mathrm{Op}(b) \\ &= 2^d \mathrm{Tr} I_{(x,p)} \mathrm{Op}(b). \end{aligned}$$

□

3.10 Special classes of symbols

Proposition 3.13. *The following conditions are equivalent*

(1) B *is continuous from* $\mathcal{S}$ *to* $\mathcal{S}'$.

(2) *The* x,p*-symbol of* B *is Schwartz.*

(3) *The* p,x*-symbol of* B *is Schwartz.*

(4) *The Weyl-Wigner symbol of* B *is Schwartz.*

Proof. By the Schwartz kernel theorem (1) is equivalent to B having the kernel in $\mathcal{S}'$. The formulas (3.5), (3.6) and (3.10) involve only partial Fourier transforms and some constant coefficients. □

Proposition 3.14. *The following conditions are equivalent*

(1) *B is Hilbert-Schmidt.*

(2) *The x,p-symbol of B is L^2.*

(3) *The p,x-symbol of B is L^2.*

(4) *The Weyl-Wigner symbol of B is L^2.*

Moreover, if b, c are L^2, then

$$\mathrm{Tr}\mathrm{Op}^{x,p}(b)^*\mathrm{Op}^{x,p}(c) = \mathrm{Tr}\mathrm{Op}(b)^*\mathrm{Op}(c) = (2\pi\hbar)^{-d}\int \overline{b(x,p)}c(x,p)\mathrm{d}x\mathrm{d}p. \tag{3.39}$$

3.11 Trace and quantization

Let us rewrite (3.39) as

$$\mathrm{Tr}\mathrm{Op}^{px}(a)\mathrm{Op}^{xp}(b) = (2\pi\hbar)^{-d}\int a(x,p)b(x,p)\mathrm{d}x\mathrm{d}p, \tag{3.40}$$

$$\mathrm{Tr}\mathrm{Op}(a)\mathrm{Op}(b) = (2\pi\hbar)^{-d}\int a(x,p)b(x,p)\mathrm{d}x\mathrm{d}p. \tag{3.41}$$

Setting $a(x,p) = 1$ we formally obtain

$$\mathrm{Tr}\mathrm{Op}(b) = \mathrm{Tr}\mathrm{Op}^{x,p}(b) = (2\pi\hbar)^{-d}\int b(x,p)\mathrm{d}x\mathrm{d}p. \tag{3.42}$$

One can try to use (3.41) and (3.41) when $A = \mathrm{Op}(a)$ is, say, bounded and describes an observable, and $B = \mathrm{Op}(b)$ is trace class, and describes a density matrix, so that it expresses the expectation value of the state B in an observable A. The left hand sides are then well defined. Usually there are no problems with the integrals on the right hand sides, and (3.41) and (3.41) give the epectation value by a "classical" formula.

For instance, consider a function of the position $f(x)$ and a function of the momentum $g(p)$. Their p,x quantizations are obvious

$$f(\hat{x}) = \mathrm{Op}^{px}\big(f(x)\big), \quad g(\hat{p}) = \mathrm{Op}^{px}\big(g(p)\big).$$

Inserting this into (3.41) we obtain

$$\mathrm{Tr}f(\hat{x})\mathrm{Op}^{x,p}(b) = (2\pi\hbar)^{-d}\int f(x)b(x,p)\mathrm{d}x\mathrm{d}p,$$

$$\mathrm{Tr}g(\hat{p})\mathrm{Op}^{x,p}(b) = (2\pi\hbar)^{-d}\int g(p)b(x,p)\mathrm{d}x\mathrm{d}p.$$

Thus with help of the x,p-quantization we can compute the so-called marginals involving (separately) the position and momentum.

With the Weyl-Wigner quantization we have much more possibilities. E.g. for any α we have

$$f(\xi\hat{x}+\eta\hat{p}) = \mathrm{Op}\big(f(\xi x+\eta p)\big).$$

Therefore,

$$\mathrm{Tr} f(\xi\hat{x}+\eta\hat{p})\mathrm{Op}(b) = (2\pi\hbar)^{-d}\int f(\xi x+\eta p) b(x,p)\mathrm{d}x\mathrm{d}p.$$

3.12 Star product for the x,p and p,x quantization

Proposition 3.15. *Suppose that b,c, say, belong to $\mathcal{S}(\mathbb{R}^d\oplus\mathbb{R}^d)$ We have the following formula for the symbol of the product: If*

$$\mathrm{Op}^{x,p}(b)\mathrm{Op}^{x,p}(c) = \mathrm{Op}^{x,p}\big(b \star^{x,p} c\big), \tag{3.43}$$

then

$$\big(b\star^{x,p} c\big)(x,p) = \mathrm{e}^{-\mathrm{i}\hbar D_{p_1} D_{x_2}} b(x_1,p_1)c(x_2,p_2)\Big|_{\substack{x:=x_1=x_2,\\ p:=p_1=p_2.}}. \tag{3.44}$$

Similarly, we have

$$\mathrm{Op}^{p,x}(b)\mathrm{Op}^{p,x}(c) = \mathrm{Op}^{p,x}\big(b \star^{p,x} c\big), \tag{3.45}$$

then

$$\big(b\star^{p,x} c\big)(x,p) = \mathrm{e}^{-\mathrm{i}\hbar D_{x_1} D_{p_2}} b(x_1,p_1)c(x_2,p_2)\Big|_{\substack{x:=x_1=x_2,\\ p:=p_1=p_2.}}.$$

Proof.

$$\begin{aligned}
&\mathrm{Op}^{x,p}(b)\mathrm{Op}^{x,p}(c)(x,y)\\
=\;& (2\pi\hbar)^{-2d}\int\int\int b(x,p_1)c(x_2,p_2)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\big((x-x_2)p_1+(x_2-y)p_2\big)}\mathrm{d}p_1\mathrm{d}x_2\mathrm{d}p_2\\
=\;& (2\pi\hbar)^{-d}\int \mathrm{d}p_2\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(x-y)p_2}\\
&\times(2\pi\hbar)^{-d}\int\int b(x,p_1)c(x_2,p_2)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(x_2-x)(p_2-p_1)}\mathrm{d}p_1\mathrm{d}x_2\\
=\;& (2\pi\hbar)^{-d}\int \mathrm{d}p_2\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(x-y)p_2}\mathrm{e}^{-\mathrm{i}\hbar D_{p_1}D_{x_2}} b(x_1,p_1)c(x_2,p_2)\Big|_{\substack{x:=x_1=x_2,\\ p:=p_1=p_2.}},
\end{aligned}$$

which proves (3.44). □

Note that with the assumption $b,c\in\mathcal{S}(\mathbb{R}^d\oplus\mathbb{R}^d)$, (3.44) is well defined. However, one can expect that the above formula has a much wider range of validity. For instance, it makes sense and is valid if either $b\in\mathcal{S}(\mathbb{R}^d\oplus\mathbb{R}^d)$ and c is a polynomial or the other way around. Obviously,

$$\begin{aligned}
[\hat{x},\mathrm{Op}^{x,p}(b)] &= \mathrm{i}\hbar\mathrm{Op}^{x,p}(\partial_p b) = \mathrm{i}\hbar\mathrm{Op}^{x,p}(\{x,b\}),\\
[\hat{p},\mathrm{Op}^{x,p}(b)] &= -\mathrm{i}\hbar\mathrm{Op}^{x,p}(\partial_x b) = \mathrm{i}\hbar\mathrm{Op}^{x,p}(\{p,b\}).
\end{aligned}$$

Note that

$$\begin{aligned}\big(b \star^{x,p} c\big)(x,p) &= b(x,p)c(x,p) - \mathrm{i}\hbar\partial_p b(x,p)\partial_x c(x,p) + O(\hbar^2),\\ \big(c \star^{x,p} b\big)(x,p) &= b(x,p)c(x,p) - \mathrm{i}\hbar\partial_x b(x,p)\partial_p c(x,p) + O(\hbar^2).\end{aligned}$$

Hence,

$$\begin{aligned}\mathrm{Op}^{x,p}(b)\mathrm{Op}^{x,p}(c) &= \mathrm{Op}^{x,p}(bc) + O(\hbar),\\ [\mathrm{Op}^{x,p}(b), \mathrm{Op}^{x,p}(c)] &= \mathrm{i}\hbar\mathrm{Op}^{x,p}(\{b,c\}) + O(\hbar^2),\end{aligned}$$

or in other words,

$$b \star^{x,p} c = bc + O(\hbar),$$
$$b \star^{x,p} c - c \star^{x,p} b = \mathrm{i}\hbar\{b,c\} + O(\hbar^2).$$

3.13 Star product for the Weyl-Wigner quantization

Proposition 3.16. *Suppose that b, c, say, belong to $\mathcal{S}(\mathbb{R}^d \oplus \mathbb{R}^d)$ We have the following formula for the symbol of the product:*

$$\text{if} \qquad \mathrm{Op}(a)\mathrm{Op}(b) = \mathrm{Op}(a \star b), \quad \text{then} \tag{3.46}$$

$$a \star b(x,p) = \mathrm{e}^{\frac{\mathrm{i}}{2}\hbar(D_{p_1}D_{x_2} - D_{x_1}D_{p_2})} a(x_1,p_1)b(x_2,p_2)\Big|_{\substack{x := x_1 = x_2,\\ p := p_1 = p_2.}}.$$

Proof. Let

$$A = \mathrm{Op}(a), \quad B = \mathrm{Op}(b), \quad AB =: C = \mathrm{Op}(c).$$

Then

$$\begin{aligned}C(x_1,x_2) &= \frac{1}{(2\pi\hbar)^{2d}} \int\int\int a\Big(\frac{x_1+y}{2}, p_1\Big) b\Big(\frac{y+x_2}{2}, p_2\Big) \mathrm{e}^{\mathrm{i}\frac{(x_1-y)}{\hbar}p_1} \mathrm{e}^{\mathrm{i}\frac{(y-x_2)}{\hbar}p_2} \mathrm{d}y\mathrm{d}p_1\mathrm{d}p_2,\\ c(z,p) &= \int C\Big(x + \frac{u}{2}, x - \frac{u}{2}\Big)\mathrm{e}^{-\mathrm{i}\frac{up}{\hbar}}\mathrm{d}u\\ &= \frac{1}{(2\pi\hbar)^{2d}} \int\int\int\int a\Big(\frac{x+2^{-1}u+y}{2}, p_1\Big) b\Big(\frac{y+x-2^{-1}u}{2}, p_2\Big)\\ &\quad \times \mathrm{e}^{\mathrm{i}\frac{x+2^{-1}u-y}{\hbar}p_1} \mathrm{e}^{\mathrm{i}\frac{y-x+2^{-1}u}{\hbar}p_2} \mathrm{e}^{-\mathrm{i}\frac{up}{\hbar}} \mathrm{d}u\mathrm{d}y\mathrm{d}p_1\mathrm{d}p_2\\ &= \frac{1}{(\pi\hbar)^{2d}} \int\int\int\int a(z_1,p_1)b(z_2,p_2)\mathrm{e}^{2\mathrm{i}\frac{(z-z_1)(p-p_2)-(p-p_1)(z-z_2)}{\hbar}} \mathrm{d}z_1\mathrm{d}z_2\mathrm{d}p_1\mathrm{d}p_2,\end{aligned}$$

where we substituted

$$z_1 = \frac{x+2^{-1}u+y}{2}, \quad z_2 = \frac{x-2^{-1}u+y}{2}, \tag{3.47}$$

□

Proposition 3.17. *If h is a polynomial of degree ≤ 1, then*

$$\frac{1}{2}\big(\mathrm{Op}(h)\mathrm{Op}(b) + \mathrm{Op}(b)\mathrm{Op}(h)\big) \quad = \quad \mathrm{Op}(bh),$$

Proof. Consider for instance $h = x$.

$$\begin{aligned}
\mathrm{e}^{\frac{\mathrm{i}}{2}\hbar(D_{p_1}D_{x_2} - D_{x_1}D_{p_2})} x_1 b(x_2,p_2)\Big|_{\substack{x:=x_1=x_2,\\ p:=p_1=p_2.}} &= xb(x,p) + \frac{\mathrm{i}\hbar}{2}\partial_p b(x,p),\\
\mathrm{e}^{\frac{\mathrm{i}}{2}\hbar(D_{p_1}D_{x_2} - D_{x_1}D_{p_2})} b(x_1,p_1)x_2\Big|_{\substack{x:=x_1=x_2,\\ p:=p_1=p_2.}} &= xb(x,p) - \frac{\mathrm{i}\hbar}{2}\partial_p b(x,p).
\end{aligned}$$

□

Consequently,

$$\begin{aligned}
\big(\hat{p} - A(\hat{x})\big)^2 &= \mathrm{Op}\Big(\big(p - A(x)\big)^2\Big),\\
\mathrm{Op}\big(a_{ij}x_ix_j + 2b_{ij}x_ip_j + c_{ij}p_ip_j\big) &= a_{ij}\hat{x}_i\hat{x}_j + b_{ij}\hat{x}_i\hat{p}_j + b_{ij}\hat{p}_j\hat{x}_i + c_{ij}\hat{p}_i\hat{p}_j.
\end{aligned}$$

Proposition 3.18. *Let h be a polynomial of degree ≤ 2. Then*

(1)
$$[\mathrm{Op}(h), \mathrm{Op}(b)] = \mathrm{i}\hbar\mathrm{Op}(\{h,b\}). \tag{3.48}$$

(2) *Let $x(t), p(t)$ solve the Hamilton equations with the Hamiltonian h. Then the affine symplectic transformation*

$$r_t\big(x(0),p(0)\big) = \big(x(t),p(t)\big)$$

satisfies

$$\mathrm{e}^{\frac{\mathrm{i}t}{\hbar}\mathrm{Op}(h)}\mathrm{Op}(b)\mathrm{e}^{-\frac{\mathrm{i}t}{\hbar}\mathrm{Op}(h)} = \mathrm{Op}(b \circ r_t^{-1}).$$

Proof.

$$\begin{aligned}
&\mathrm{e}^{\frac{\mathrm{i}}{2}\hbar(D_{p_1}D_{x_2} - D_{x_1}D_{p_2})} h(x_1,p_1)b(x_2,p_2)\Big|_{\substack{x:=x_1=x_2,\\ p:=p_1=p_2.}}\\
= \quad & h(x,p)b(x,p) + \frac{\mathrm{i}\hbar}{2}\big(D_p h(x,p)D_x b(x,p) - D_p h(x,p) D_x b(x,p)\big),\\
&+\frac{(\mathrm{i}\hbar)^2}{8}(D_{p_1}D_{x_2} - D_{x_1}D_{p_2})^2 h(x_1,p_1)b(x_2,p_2)\Big|_{\substack{x:=x_1=x_2,\\ p:=p_1=p_2.}}
\end{aligned}$$

When we swap h and b, we obtain the same three terms except that the second has the opposite sign. This proves (1).

To prove (2) note that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t} b\circ r_t &= \{h, b\circ r_t\}\\ [\mathrm{Op}(h), \mathrm{Op}(b\circ r_t)] &= \mathrm{i}\hbar \mathrm{Op}(\{h, b\circ r_t\}).\end{aligned}$$

Now, $\mathrm{e}^{-\frac{\mathrm{i}t}{\hbar}\mathrm{Op}(h)}\mathrm{Op}(b\circ r_t)\mathrm{e}^{\frac{\mathrm{i}t}{\hbar}\mathrm{Op}(h)}\Big|_{t=0} = \mathrm{Op}(b)$ and

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{\frac{-\mathrm{i}t}{\hbar}\mathrm{Op}(h)}\mathrm{Op}(b\circ r_t)\mathrm{e}^{\frac{\mathrm{i}t}{\hbar}\mathrm{Op}(h)}\\ =\ & \mathrm{e}^{\frac{-\mathrm{i}t}{\hbar}\mathrm{Op}(h)}\Big(-\frac{\mathrm{i}}{\hbar}[\mathrm{Op}(h), \mathrm{Op}(b\circ r_t)] + \mathrm{Op}\big(\frac{\mathrm{d}}{\mathrm{d}t} b\circ r_t\big)\Big)\mathrm{e}^{\frac{\mathrm{i}t}{\hbar}\mathrm{Op}(h)} \ =\ 0\end{aligned}$$

□

Note that

$$\begin{aligned}\frac{1}{2}\big(\mathrm{Op}(b)\mathrm{Op}(c) + \mathrm{Op}(c)\mathrm{Op}(b)\big) &= \mathrm{Op}(bc) + O(\hbar^2), &(3.49)\\ [\mathrm{Op}(b), \mathrm{Op}(c)] &= \mathrm{i}\hbar\mathrm{Op}(\{b,c\}) + O(\hbar^3), &(3.50)\\ \text{if}\ \ \mathrm{supp}b\cap\mathrm{supp}c = \emptyset,\quad \text{then}\quad \mathrm{Op}(b)\mathrm{Op}(c) &= O(\hbar^\infty). &(3.51)\end{aligned}$$

4 Coherent states and Wick ordering

4.1 General coherent states

Fix a normalized vector $\Psi\in L^2(\mathbb{R}^d)$. The family of *coherent vectors associated with the vector* Ψ is defined by

$$\Psi_{(y,w)} := \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(-y\hat{p}+w\hat{x})}\Psi,\quad (y,w)\in\mathbb{R}^d\oplus\mathbb{R}^d.$$

The orthogonal projection onto $\Psi_{(y,w)}$, called the *coherent state*, will be denoted

$$P_{(y,w)} := |\Psi_{(y,w)})(\Psi_{(y,w)}| = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(-y\hat{p}+w\hat{x})}|\Psi)(\Psi|\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(y\hat{p}-w\hat{x})}.$$

It is natural to assume that

$$\big(\Psi|\hat{x}\Psi\big) = 0,\quad \big(\Psi|\hat{p}\Psi\big) = 0.$$

This assumption implies that

$$\big(\Psi_{(y,w)}|\hat{x}\Psi_{(y,w)}\big) = y,\quad \big(\Psi_{(y,w)}|\hat{p}\Psi_{(y,w)}\big) = w.$$

Note however that we will not use the above assumption in this section.

Explicitly,

$$\begin{aligned}\Psi_{(y,w)}(x) &= \mathrm{e}^{\frac{i}{\hbar}(w\cdot x-\frac{1}{2}y\cdot w)}\Psi(x-y),\\ P_{(y,w)}(x_1,x_2) &= \Psi(x_1-y)\overline{\Psi(x_2-y)}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(x_1-x_2)\cdot w}.\end{aligned}$$

Theorem 4.1.

$$(2\pi\hbar)^{-d}\int P_{(y,w)}\mathrm{d}y\mathrm{d}w = 1\!\!1. \tag{4.1}$$

Proof. Let $\Phi\in L^2(\mathbb{R}^d)$. Then

$$\begin{aligned}
&\int\int(\Phi|P_{(y,w)}\Phi)\mathrm{d}y\mathrm{d}w\\
=\ &\int\int\int\int\overline{\Phi(x_1)}\Psi(x_1-y)\overline{\Psi(x_2-y)}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(x_1-x_2)\cdot w}\Phi(x_2)\mathrm{d}x_1\mathrm{d}x_2\mathrm{d}y\mathrm{d}w\\
=\ &(2\pi\hbar)^d\int\int\overline{\Phi(x)}\Psi(x-y)\overline{\Psi(x-y)}\Phi(x)\mathrm{d}x\mathrm{d}y=(2\pi\hbar)^d\|\Phi\|^2\|\Psi\|^2.
\end{aligned}$$

4.2 Contravariant quantization

Let b be a function on te phase space. We define its *contravariant quantization* by

$$\mathrm{Op}^{\mathrm{ct}}(b):=(2\pi\hbar)^{-d}\int P_{(x,p)}b(x,p)\mathrm{d}x\mathrm{d}p. \tag{4.2}$$

If $B=\mathrm{Op}^{\mathrm{ct}}(b)$, then b is called the *contravariant symbol* of B.

We have

(1) $|\mathrm{Tr}\mathrm{Op}^{\mathrm{ct}}(b)|\le(2\pi\hbar)^{-d}\int|b(x,p)|\mathrm{d}x\mathrm{d}p$;

(2) $\|\mathrm{Op}^{\mathrm{ct}}(b)\|\le\sup_{x,p}|b(x,p)|$;

(3) $\mathrm{Op}^{\mathrm{ct}}(1)=1\!\!1$;

(4) $\mathrm{Op}^{\mathrm{ct}}(b)^*=\mathrm{Op}^{\mathrm{ct}}(\bar{b})$.

(5) Let $b\ge0$. Then $\mathrm{Op}^{\mathrm{ct}}(b)\ge0$.

4.3 Covariant quantization

The covariant quantization is the operation dual to the contravariant quantization. Strictly speaking, the operation that has a natural definition and good properties is not the covariant quantization but the covariant symbol of an operator.

Let $B\in B(\mathcal{H})$. Then we define its *covariant symbol* by

$$b(x,p):=\mathrm{Tr}P_{(x,p)}B=\big(\Psi_{(x,p)}|B\Psi_{(x,p)}\big).$$

B is then called the *covariant quantization* of b and is denoted by

$$\mathrm{Op}^{\mathrm{cv}}(b)=B.$$

(1) $\mathrm{Op}^{\mathrm{cv}}(1)=1\!\!1$,

(2) $\mathrm{Op}^{\mathrm{cv}}(b)^*=\mathrm{Op}^{\mathrm{cv}}(\bar{b})$.

(3) $\|\mathrm{Op}^{\mathrm{cv}}(b)\|\ge\sup_{x,p}|b(x,p)|$.

(4) Let $\mathrm{Op}^{\mathrm{cv}}(b)\ge0$. Then $b\ge0$.

(5) $\mathrm{Tr}\mathrm{Op}^{\mathrm{cv}}(b)=(2\pi\hbar)^{-d}\int b(x,p)\mathrm{d}x\mathrm{d}p$.

4.4 Connections between various quantizations

Let us compute various symbols of $P_{(y,w)}$:

$$\begin{aligned}
\text{covariant symbol}(x,p) &= |(\Psi|\Psi_{(y-x,w-p)})|^2,\\
\text{Weyl symbol}(x,p) &= 2^d(\Psi_{(y-x,w-p)}|I\Psi_{(y-x,w-p)}),\\
\text{contravariant symbol}(x,p) &= (2\pi\hbar)^d\delta(x-y)\delta(p-w).
\end{aligned}$$

Let us now show how to pass between the covariant, Weyl-Wigner and contravariant quantization. Note that there is a preferred direction: from contravariant to Weyl, and then from Weyl-Wigner to covariant. Going back is less natural.

Proposition 4.2. *Let*

$$\mathrm{Op}^{\mathrm{ct}}(b^{\mathrm{ct}}) = \mathrm{Op}(b) = \mathrm{Op}^{\mathrm{cv}}(b^{\mathrm{cv}}).$$

Then

$$\begin{aligned}
b(x,p) &= (\pi\hbar)^{-d}\int b^{\mathrm{ct}}(y,w)(\Psi_{(y-x,w-p)}|I\Psi_{(y-x,w-p)})\mathrm{d}y\mathrm{d}w,\\
b^{\mathrm{cv}}(x,p) &= (\pi\hbar)^{-d}\int b(y,w)(\Psi_{(-y+x,-w+p)}|I\Psi_{(-y+x,-w+p)})\mathrm{d}y\mathrm{d}w,\\
b^{\mathrm{cv}}(x,p) &= (2\pi\hbar)^{-d}\int b^{\mathrm{ct}}(y,w)\big|(\Psi|\Psi_{(y-x,w-p)})\big|^2\mathrm{d}y\mathrm{d}w.
\end{aligned}$$

Proof. We use

$$\begin{aligned}
\mathrm{Op}(b) &= (\pi\hbar)^{-d}\int I_{(x,p)}b(x,p)\mathrm{d}x\mathrm{d}p,\\
b(x,p) &= 2^d\mathrm{Tr}I_{(x,p)}\mathrm{Op}(b),\\
\mathrm{Op}^{\mathrm{ct}}(b^{\mathrm{ct}}) &= (2\pi\hbar)^{-d}\int P_{(x,p)}b^{\mathrm{ct}}(x,p)\mathrm{d}x\mathrm{d}p,\\
b^{\mathrm{cv}}(x,p) &= \mathrm{Tr}P_{(x,p)}\mathrm{Op}^{\mathrm{ct}}(b^{\mathrm{cv}}) = \big(\Psi_{(x,p)}|\mathrm{Op}^{\mathrm{ct}}(b^{\mathrm{cv}})\Psi_{(x,p)}\big)
\end{aligned}$$

□

Proposition 4.3. *We have*

$$\mathrm{Tr}\mathrm{Op}^{\mathrm{cv}}(a)\mathrm{Op}^{\mathrm{ct}}(b) = (2\pi\hbar)^{-d}\int a(x,p)b(x,p)\mathrm{d}x\mathrm{d}p. \tag{4.3}$$

Proof. Indeed, let $A = \mathrm{Op}^{\mathrm{cv}}(a)$. Then the lhs of (4.3) is

$$\begin{aligned}
&\mathrm{Tr}A(2\pi\hbar)^{-d}\int b(x,p)|\Psi_{(x,p)})(\Psi_{(x,p)}|\mathrm{d}x\mathrm{d}p\\
=\ &(2\pi\hbar)^{-d}\int(\Psi_{(x,p)}|A|\Psi_{(x,p)})b(x,p)\mathrm{d}x\mathrm{d}p,
\end{aligned}$$

which is the rhs of (4.3). □

4.5 Gaussian coherent vectors

Consider the normalized Gaussian vector scaled appropriately with the Planck constant

$$\Omega(x) = (\pi\hbar)^{-\frac{d}{4}} \mathrm{e}^{-\frac{1}{2\hbar}x^2}. \tag{4.4}$$

The corresponding coherent vectors are equal to

$$\Omega_{(y,w)}(x) = (\pi\hbar)^{-\frac{d}{4}} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}w\cdot x - \frac{\mathrm{i}}{2\hbar}y\cdot w - \frac{1}{2\hbar}(x-y)^2}. \tag{4.5}$$

In the literature, when one speaks about coherent states, one has usually in mind (4.5). They are also called *Gaussian or Glauber's coherent states.* In the case of Gaussian states, there are several alternative names of the covariant and contravariant symbol of an operator:

(1) For contravariant symbol:
   - (i) upper symbol,
   - (ii) anti-Wick symbol,
   - (iii) Glauber-Sudarshan function,
   - (iv) P-function;

(2) For covariant symbol:
   - (i) lower symbol,
   - (ii) Wick symbol,
   - (iii) Husimi or Husimi-Kano function,
   - (iv) Q-function.

We will use the terms *Wick/anti-Wick quantization/symbol.*

Proposition 4.2 specified to Gaussian coherent states becomes

Proposition 4.4. *Let* $\mathrm{Op}^{\mathrm{ct}}(b^{\mathrm{ct}}) = \mathrm{Op}(b) = \mathrm{Op}^{\mathrm{cv}}(b^{\mathrm{cv}})$. *Then*

$$\begin{aligned}
b(x,p) &= \int\int b^{\mathrm{ct}}(y,w)(\pi\hbar)^{-d}\mathrm{e}^{-\frac{1}{\hbar}(x-y)^2-\frac{1}{\hbar}(p-w)^2}\mathrm{d}y\mathrm{d}w, \quad b = \mathrm{e}^{-\frac{\hbar}{4}(D_x^2+D_p^2)}b^{\mathrm{ct}};\\
b^{\mathrm{cv}}(x,p) &= \int\int b(y,w)(\pi\hbar)^{-d}\mathrm{e}^{-\frac{1}{\hbar}(x-y)^2-\frac{1}{\hbar}(p-w)^2}\mathrm{d}y\mathrm{d}w, \quad b^{\mathrm{cv}} = \mathrm{e}^{-\frac{\hbar}{4}(D_x^2+D_p^2)}b;\\
b^{\mathrm{cv}}(x,p) &= \int\int b^{\mathrm{ct}}(y,w)(2\pi\hbar)^{-d}\mathrm{e}^{-\frac{1}{2\hbar}(x-y)^2-\frac{1}{2\hbar}(p-w)^2}\mathrm{d}y\mathrm{d}w, \quad b^{\mathrm{cv}} = \mathrm{e}^{-\frac{\hbar}{2}(D_x^2+D_p^2)}b^{\mathrm{ct}}.
\end{aligned}$$

4.6 Creation and annihilation operator

Set

$$\begin{aligned}
a_i &= (2\hbar)^{-1/2}(x_i + \mathrm{i}p_i),\\
a_i^* &= (2\hbar)^{-1/2}(x_i - \mathrm{i}p_i).
\end{aligned}$$

We have

$$\{a_i, a_j^*\} = -\frac{\mathrm{i}}{\hbar}\delta_{ij}.$$

$$x_i = \frac{\hbar^{1/2}}{2^{1/2}}(a_i + a_i^*), \quad p_i = \frac{\hbar^{1/2}}{\mathrm{i}2^{1/2}}(a_i - a_i^*). \tag{4.6}$$

In this way, the classical phase space $\mathbb{R}^d \oplus \mathbb{R}^d$ has been identified with the complex space $\mathbb{C}^d$. The Lebesgue measure has also a complex notation:

$$\frac{\hbar^d}{\mathrm{i}^d}\mathrm{d}a^*\mathrm{d}a = \mathrm{d}x\mathrm{d}p. \tag{4.7}$$

To justify the notation (4.7) we write in terms of differential forms:

$$\mathrm{d}a_j^* \wedge \mathrm{d}a_j = \frac{1}{2\hbar}\big(\mathrm{d}x - \mathrm{i}\mathrm{d}p\big) \wedge \big(\mathrm{d}x + \mathrm{i}\mathrm{d}p\big) = \mathrm{i}\hbar^{-1}\mathrm{d}x \wedge \mathrm{d}p.$$

On the quantum side we introduce the operators

$$\begin{array}{rcl} \hat{a}_i &=& (2\hbar)^{-1/2}(\hat{x}_i + \mathrm{i}\hat{p}_i), \\ \hat{a}_i^* &=& (2\hbar)^{-1/2}(\hat{x}_i - \mathrm{i}\hat{p}_i). \end{array}$$

We have

$$[\hat{a}_i, \hat{a}_j^*] = \delta_{ij}.$$

$$\hat{x}_i = \frac{\hbar^{1/2}}{2^{1/2}}(\hat{a}_i + \hat{a}_i^*), \quad \hat{p}_i = \frac{\hbar^{1/2}}{\mathrm{i}2^{1/2}}(\hat{a}_i - \hat{a}_i^*). \tag{4.8}$$

Let $y, w \in \mathbb{R}^d \oplus \mathbb{R}^d$. We introduce classical complex variables

$$\begin{array}{rcl} b &:=& (2\hbar)^{-\frac{1}{2}}(y + \mathrm{i}w), \\ b^* &:=& (2\hbar)^{-\frac{1}{2}}(y - \mathrm{i}w). \end{array}$$

Note that

$$\frac{\mathrm{i}}{\hbar}(-y\hat{p} + w\hat{x}) = -b^*\hat{a} + b\hat{a}^*. \tag{4.9}$$

We have

$$\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(-y\hat{p}+w\hat{x})}\hat{x} = (\hat{x}+y)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(-y\hat{p}+w\hat{x})}, \qquad \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(-y\hat{p}+w\hat{x})}\hat{p} = (\hat{p}+w)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(-y\hat{p}+w\hat{x})}, \tag{4.10}$$

$$\mathrm{e}^{(-b^*\hat{a}+b\hat{a}^*)}\hat{a}^* = (\hat{a}^*+b^*)\mathrm{e}^{(-b^*\hat{a}+b\hat{a}^*)}, \qquad \mathrm{e}^{(-b^*\hat{a}+b\hat{a}^*)}\hat{a} = (\hat{a}+b)\mathrm{e}^{(-b^*\hat{a}+b\hat{a}^*)}. \tag{4.11}$$

Recall that in the real notation we had coherent vectors

$$\Omega_{y,w} := \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(-y\hat{p}+w\hat{x})}\Omega. \tag{4.12}$$

In the complex notation they become

$$\Omega_b := \mathrm{e}^{(-b^*\hat{a}+b\hat{a}^*)}\Omega. \tag{4.13}$$

Using $\Omega(x) = \mathrm{e}^{-\frac{x^2}{2\hbar}}$ and $\hat{a}_i = (2\hbar)^{-\frac{1}{2}}(\hat{x}_i + \hbar\partial_{x_i})$ we obtain

$$\hat{a}_i\Omega = 0.$$

This justifies the name "annihilation operators" for $\hat{a}_i$. More generally, by (4.11),

$$\hat{a}_j\Omega_b = b_j\Omega_b,$$

Note that the identity (4.1) can be rewritten as

$$\mathbb{1} = (2\pi\mathrm{i})^{-d}\int |\Omega_a)(\Omega_a|\mathrm{d}a^*\mathrm{d}a. \tag{4.14}$$

4.7 Quantization by an ordering prescription

Consider a polynomial function on the phase space:

$$w(x,p) = \sum_{\alpha,\beta} w_{\alpha,\beta} x^\alpha p^\beta. \tag{4.15}$$

It is easy to describe the x,p and p,x quantizations of w in terms of ordering the positions and momenta:

$$\begin{aligned} \mathrm{Op}^{x,p}(w) &= \sum_{\alpha,\beta} w_{\alpha,\beta} \hat{x}^\alpha \hat{p}^\beta, \\ \mathrm{Op}^{p,x}(w) &= \sum_{\alpha,\beta} w_{\alpha,\beta} \hat{p}^\beta \hat{x}^\alpha. \end{aligned}$$

The Weyl quantization amounts to the full symmetrization of $\hat{x}_i$ and $\hat{p}_j$, as described in (3.27).

We can also rewrite the polynomial (4.15) in terms of a_i, a_i^* by inserting (4.6). Thus we obtain

$$w(x,p) = \sum_{\gamma,\delta} \tilde{w}_{\gamma,\delta} a^{*\gamma} a^\delta =: \tilde{w}(a^*, a). \tag{4.16}$$

Then we can introduce the *Wick quantization*

$$\mathrm{Op}^{a^*,a}(w) = \sum_{\gamma,\delta} \tilde{w}_{\gamma,\delta} \hat{a}^{*\gamma} \hat{a}^\delta \tag{4.17}$$

and the *anti-Wick quantization*

$$\mathrm{Op}^{a,a^*}(w) = \sum_{\gamma,\delta} \tilde{w}_{\gamma,\delta} \hat{a}^\delta \hat{a}^{*\gamma}. \tag{4.18}$$

Theorem 4.5. (1) *The Wick quantization coincides with the covariant quantization for Gaussian coherent states.*

(2) *The anti-Wick quantization coincides with the contravariant quantization for Gaussian coherent states.*

Proof. (1)

$$\begin{aligned} (\Omega_{(x,p)} | \mathrm{Op}^{a^*,a}(w) \Omega_{(x,p)}) &= \big(\Omega_a | \sum_{\gamma,\delta} \tilde{w}_{\gamma,\delta} \hat{a}^{*\gamma} \hat{a}^\delta \Omega_a) \\ &= \sum_{\gamma,\delta} \tilde{w}_{\gamma,\delta} a^{*\gamma} a^\delta \\ &= w(x,p). \end{aligned}$$

(2)

$$\begin{aligned}
\mathrm{Op}^{a,a^*}(w) &= \sum_{\gamma,\delta} \tilde{w}_{\gamma,\delta}\hat{a}^\delta (2\pi\mathrm{i})^{-d} \int |\Omega_a)(\Omega_a|\mathrm{d}a^*\mathrm{d}a\hat{a}^{*\gamma} \\
&= (2\pi\mathrm{i})^{-d} \sum_{\gamma,\delta} \int \tilde{w}_{\gamma,\delta} a^\delta a^{*\gamma} |\Omega_a)(\Omega_a|\mathrm{d}a^*\mathrm{d}a \\
&= (2\pi\hbar)^{-d} \int w(x,p)|\Omega_{(x,p)})(\Omega_{(x,p)}|\mathrm{d}x\mathrm{d}p.
\end{aligned}$$

□

The Wick quantization is widely used, especially for systems with an infinite number of degrees of freedom. Note the identity

$$\left(\Omega|\mathrm{Op}^{a^*,a}(w)\Omega\right) = \tilde{w}(0,0). \tag{4.19}$$

4.8 Connection between the Wick and anti-Wick quantization

As described in equation (4.15), there are two natural ways to write the symbol of the Wick (or anti-Wick) quantization. We can either write it in terms of x, p, or in terms of a^*, a. In the latter notation we decorate the symbol with a tilde.

Let

$$\mathrm{Op}^{a,a^*}(w^{a,a^*}) = \mathrm{Op}^{a^*,a}(w^{a^*,a}).$$

Then

$$\begin{aligned}
w^{a^*,a}(x,p) &= \mathrm{e}^{\frac{\hbar}{2}(\partial_x^2+\partial_p^2)} w^{a,a^*}(x,p) \\
&= (2\pi\hbar)^{-d} \int\int \mathrm{e}^{-\frac{1}{2\hbar}\left((x-y)^2+(p-w)^2\right)} w^{a,a^*}(y,w)\mathrm{d}y\mathrm{d}w, \qquad (4.20) \\
\tilde{w}^{a^*,a}(a^*,a) &= \mathrm{e}^{\partial_{a^*}\partial_a} \tilde{w}^{a,a^*}(a^*,a) \\
&= (2\pi\mathrm{i})^{-d} \int\int \mathrm{e}^{-(a^*-b^*)(a-b)} \tilde{w}^{a,a^*}(b^*,b)\mathrm{d}b^*\mathrm{d}b.. \qquad (4.21)
\end{aligned}$$

(4.20) was proven before. To see that (4.21) and (4.20) are equivalent we note that

$$\begin{aligned}
\partial_a &= \frac{\hbar^{1/2}}{2^{1/2}}(\partial_x + \mathrm{i}\partial_p), \\
\partial_{a^*} &= \frac{\hbar^{1/2}}{2^{1/2}}(\partial_x - \mathrm{i}\partial_p),
\end{aligned}$$

hence

$$\partial_{a^*}\partial_a = \frac{\hbar}{2}(\partial_x^2 + \partial_p^2).$$

One can also see (4.21) directly. To this end it is enough to consider $a^{*n}a^m$ (a and a^* are now single variables). To perform Wick ordering we need to make all possible contractions.

Each contraction involves a pair of two elements: one from $\{1, \dots, n\}$ and the other from $\{1, \dots, m\}$. The number of possible k-fold contractions is

$$\frac{n!}{k!(n-k)!} \frac{m!}{k!(m-k)!} k! = \frac{1}{k!} \frac{n!}{(n-k)!} \frac{m!}{(m-k)!}.$$

But

$$\mathrm{e}^{\partial_{a^*} \partial_a} a^{*n} a^m = \sum_{k=0}^{\infty} \frac{1}{k!} \frac{n!}{(n-k)!} a^{*(n-k)} \frac{m!}{(m-k)!} a^{m-k}.$$

4.9 Wick symbol of a product

Let us use the complex notation for the Wick quantization. Suppose that

$$\mathrm{Op}^{a^*,a}(w) = \mathrm{Op}^{a^*,a}(w_2)\mathrm{Op}^{a^*,a}(w_1).$$

Then

$$\tilde{w}(a^*, a) = \mathrm{e}^{\partial_{a_2} \partial_{a_1^*}} \tilde{w}_2(a_2^*, a_2)\tilde{w}_1(a_1^*, a_1)\Big|_{a = a_2 = a_1}. \tag{4.22}$$

(Clearly $a = a_2 = a_1$ implies $a^* = a_2^* = a_1^*$). This follows essentially by the same argument as the one used to show (4.21). Using (**??**), one can rewrite (4.22) as an integral:

$$\tilde{w}(a^*, a) = \int \int \mathrm{e}^{-b^* b} \tilde{w}_2(a^*, a + b)\tilde{w}_1(a^* + b^*, a) \frac{\mathrm{d}b^* \mathrm{d}b}{(2\pi \mathrm{i})^d}. \tag{4.23}$$

Note that in (4.23) we treat $\tilde{w}_1$ and $\tilde{w}_2$ as functions of two independent variables obtained by analytic continuation: a and b do not have to coincide. For the product we will prefer however it is more convenient to use the Bargmann kernel instead of the Wick symbol, which will be described in the next subsection.

4.10 Berezin diagram

One can distinguish 5 most natural quantizations. Their respective relations are nicely described by the following diagram, called sometimes the *Berezin diagram*:

$$\begin{tikzcd}
 & \begin{array}{c}\text{anti-Wick}\\ \text{quantization}\end{array} \arrow[d, "\mathrm{e}^{-\frac{\hbar}{4}(D_x^2+D_p^2)}"] & \\
\begin{array}{c}p,x\\ \text{quantization}\end{array} \arrow[r, "\mathrm{e}^{\frac{\mathrm{i}\hbar}{2} D_x \cdot D_p}"] & \begin{array}{c}\text{Weyl-Wigner}\\ \text{quantization}\end{array} \arrow[r, "\mathrm{e}^{\frac{\mathrm{i}\hbar}{2} D_x \cdot D_p}"] \arrow[d, "\mathrm{e}^{-\frac{\hbar}{4}(D_x^2+D_p^2)}"] & \begin{array}{c}x,p\\ \text{quantization}\end{array} \\
 & \begin{array}{c}\text{Wick}\\ \text{quantization}\end{array} &
\end{tikzcd}$$

All these five quantizations assign to a function b on $\mathbb{R}^d \oplus \mathbb{R}^d$ an operator $\mathrm{Op}^\bullet(b)$ (where we $\bullet$ stands for the appropriate name). They have the properties:

(1) $\mathrm{Op}^\bullet(1) = 1\!\!1$, $\mathrm{Op}^\bullet(x^i) = \hat{x}^i$, $\mathrm{Op}^\bullet(p_j) = \hat{p}_j$.

(2) $\frac{1}{2}\big(\mathrm{Op}^\bullet(b)\mathrm{Op}^\bullet(c) + \mathrm{Op}^\bullet(c)\mathrm{Op}^\bullet(b)\big) = \mathrm{Op}^\bullet(bc) + O(\hbar)$.

(3) $[\big(\mathrm{Op}^\bullet(b), \mathrm{Op}^\bullet(c)] = \mathrm{i}\hbar\mathrm{Op}^\bullet(\{b,c\}) + O(\hbar^2)$.

(4) $[\big(\mathrm{Op}^\bullet(b), \mathrm{Op}^\bullet(c)] = \mathrm{i}\hbar\mathrm{Op}^\bullet(\{b,c\})$ if b is a 1st degree polynomial.

(5) $\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(-y\hat{p}+w\hat{x})}\mathrm{Op}^\bullet(b)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(y\hat{p}-w\hat{x})} = \mathrm{Op}^\bullet\big(b(x-y, p-w)\big)$.

In the case of the Weyl quantization some of the above properties can be strengthened:

(2)' $\frac{1}{2}\big(\mathrm{Op}(b)\mathrm{Op}(c) + \mathrm{Op}(c)\mathrm{Op}(b)\big) = \mathrm{Op}(bc) + O(\hbar^2)$.

(3)' $[\big(\mathrm{Op}(b), \mathrm{Op}(c)] = \mathrm{i}\hbar\mathrm{Op}(\{b,c\}) + O(\hbar^3)$.

(4)' $[\big(\mathrm{Op}(b), \mathrm{Op}(c)] = \mathrm{i}\hbar\mathrm{Op}(\{b,c\})$ if b is a 2nd degree polynomial.

4.11 Symplectic invariance of quantization

The phase space $\mathbb{R}^d \oplus \mathbb{R}^d$ is equipped with the symplectic form $\omega = \begin{pmatrix} 0 & -1\!\!1 \\ 1\!\!1 & 0 \end{pmatrix}$. Recall that a linear transformation r is called symplectic if $r^\# \omega r = \omega$. If we write

$$r = \begin{pmatrix} a & b \\ c & d \end{pmatrix},$$

then this is equivalent to

$$\begin{array}{ll} d^\# a - b^\# c & = 1\!\!1, \\ c^\# a - a^\# c & = 0, \\ d^\# b - b^\# d & = 0. \end{array} \tag{4.24}$$

They form a group, denoted $Sp(\mathbb{R}^d \oplus \mathbb{R}^d)$.

Symplectic transformations preserving the decomposition $\mathbb{R}^d \oplus \mathbb{R}^d$ satisfy $b = c = 0$ and $d = a^{\#-1}$. Thus they have the form

$$r = \begin{pmatrix} a & 0 \\ 0 & a^{\#-1} \end{pmatrix},$$

where $a \in GL(\mathbb{R}^d)$. We will denote this group by $GL(\mathbb{R}^d)$.

$\mathbb{R}^d \oplus \mathbb{R}^d$ can be identified with $\mathbb{C}^d$ by $(x,p) \mapsto 2^{-\frac{1}{2}}\hbar^{-\frac{1}{2}}(x + \mathrm{i}p)$. Suppose that $\mathbb{R}^d$ is equipped with a scalar product $x \cdot x'$. Then we equip $\mathbb{C}^d$ with a (sesquilinear) scalr product

$$(x + \mathrm{i}p|x' + \mathrm{i}p') := x \cdot x' + p \cdot p' + \mathrm{i}(x \cdot p' - p \cdot x'). \tag{4.25}$$

Transformations preserving this scalar product are called unitary and form a group denoted $U(\mathbb{C}^d)$. Elements of $U(\mathbb{C}^d)$ have the form

$$r = \begin{pmatrix} a & b \\ -b & a \end{pmatrix},$$

where

$$\begin{array}{ll} a^{\#}a + b^{\#}b & = \mathbb{1}, \\ b^{\#}a - a^{\#}b & = 0 \end{array}. \tag{4.26}$$

Note that unitary transformations are symplectic. This follows e.g. from the fact that the imaginary part of the scalar product is the symplectic form.

Thus we defined two subgroups of $Sp(\mathbb{R}^d \oplus \mathbb{R}^d)$: $GL(\mathbb{R}^d)$ and $U(\mathbb{C}^d)$.

Theorem 4.6. (1) *Let $r \in Sp(\mathbb{R}^d \oplus \mathbb{R}^d)$. Then there exists a unitary transformation U_r on $L^2(\mathbb{R}^d)$ such that for any symbol m*

$$\mathrm{Op}\big(m \circ r^{-1}\big) = U_r \mathrm{Op}(m) U_r^*. \tag{4.27}$$

The operator U_r is defined uniquely up to a phase factor. It yields a projective representation: for some phase factors c_{r_1,r_2} we have

$$U_{r_1} U_{r_2} = c_{r_1,r_2} U_{r_1 r_r}. \tag{4.28}$$

(2) *If $r \in GL(\mathbb{R}^d)$, then*

$$\mathrm{Op}^\bullet\big(m \circ r^{-1}\big) = U_r \mathrm{Op}^\bullet(m) U_r^* \tag{4.29}$$

where $\mathrm{Op}^\bullet$ stands for the xp and px quantization.

(3) *If $r \in U(\mathbb{C}^d)$, then*

$$\mathrm{Op}^\bullet\big(m \circ r^{-1}\big) = U_r \mathrm{Op}^\bullet(m) U_r^* \tag{4.30}$$

where $\mathrm{Op}^\bullet$ stands for the Wick and anti-Wick quantization.

Proof. (1) Every element of the symplectic group is a product of e^a, where a is infinitesimally symplectic. For such transformations we can apply Prop. 3.18.

(2) is follows by a change of variables.

To prove (3) we note that the coherent state $P_{0,0} = \mathrm{Op}(p_{0,0})$ has the symbol

$$p_{0,0} = 2^{\frac{d}{2}} \mathrm{e}^{-\frac{1}{2}x^2 - \frac{1}{2}p^2},$$

which is invariant under the group $U(\mathbb{C}^d)$. $\Box$

4.12 Bargmann-Segal representation

Recall that for $b \in \mathbb{C}^n$ the coherent state Ω_b is given by

$$\Omega_b = \mathrm{e}^{-b^*\hat{a} + b\hat{a}^*}\Omega = \mathrm{e}^{-\frac{|b|^2}{2}} \mathrm{e}^{ba^*}\Omega. \tag{4.31}$$

Hence (4.14) can be rewritten as

$$\mathbb{1} = (2\pi \mathrm{i})^{-d} \int \big|\mathrm{e}^{b\hat{a}^*}\Omega\big)\big(\mathrm{e}^{b\hat{a}^*}\Omega\big| \mathrm{e}^{-|b|^2} \mathrm{d}b^* \mathrm{d}b. \tag{4.32}$$

We introduce the complex wave or Bargmann(-Segal) transformation

$$U_{\mathrm{cw}} F(b^*) := \big(\mathrm{e}^{b\hat{a}^*}\Omega | F\big). \tag{4.33}$$

$U_{\rm cw}$ maps $L^2(\mathbb{R}^d)$ onto the Bargmann(-Segal) space, that is the space of antiholomorphic functions on $\mathbb{C}^d$ with the scalar product given by

$$(F|G)_{\rm cw} := (2\pi{\rm i})^{-d}\int \overline{F(b^*)}G(b^*){\rm e}^{-|b|^2}{\rm d}b^*{\rm d}b. \tag{4.34}$$

We have

$$U_{\rm cw}\Omega = 1, \tag{4.35}$$
$$(U_{\rm cw}\hat{a}_i^*F)(b^*) = b_i^*(U_{\rm cw}F)(b^*), \tag{4.36}$$
$$(U_{\rm cw}\hat{a}_iF)(b^*) = \frac{\partial}{\partial b_i^*}(U_{\rm cw}F)(b^*). \tag{4.37}$$

4.13 Bargmann kernel

Let W be an operator. We define its Bargmann kernel

$$W^{\rm cw}(b_1^*, b_2) := \big({\rm e}^{b_1\hat{a}^*}\Omega|W{\rm e}^{b_2\hat{a}}\Omega\big) = {\rm e}^{\frac{|b_1|^2}{2}}{\rm e}^{\frac{|b_2|^2}{2}}(\Omega_{b_1}|W\Omega_{b_2}). \tag{4.38}$$

The Bargmann kernel is closely related to the Wick symbol. Indeed, when we restrict it to $b_1 = b_2$ we retrieve the Wick symbol:

$$\text{if} \quad W = \sum_{\gamma,\delta}\tilde{w}_{\gamma,\delta}\hat{a}^{*\gamma}\hat{a}^{\delta}, \tag{4.39}$$
$$\text{then} \quad W^{\rm cw}(b^*, b) = {\rm e}^{|b|^2}\sum_{\gamma,\delta}\tilde{w}_{\gamma,\delta}b^{*\gamma}b^{\delta}. \tag{4.40}$$

The advantage of the Bargmann kernel is its analyticity wrt its arguments. In fact, analytically continuing the Wick symbol and multiplying it by an appropriate factor we obain the Bargmann kernel:

$$W^{\rm cw}(b_1^*, b_2) = {\rm e}^{b_1^*b_2}\sum_{\gamma,\delta}\tilde{w}_{\gamma,\delta}b_1^{*\gamma}b_2^{\delta}, \tag{4.41}$$

$$\tag{4.42}$$

The name “Bargmann kernel” comes from the identity

$$\big(\Phi|W\Psi\big) = \int\int \overline{(U_{\rm cw}\Phi)(b_1^*)}W^{\rm cw}(b_1^*, b_2)(U_{\rm cw}\Psi)(b_2^*)\frac{{\rm e}^{-|b_1|^2}{\rm d}b_1^*{\rm d}b_1}{(2\pi{\rm i})^d}\frac{{\rm e}^{-|b_2|^2}{\rm d}b_2^*{\rm d}b_2}{(2\pi{\rm i})^d}. \tag{4.43}$$

Here is the formula for the Bargman kernel, which is essentially a different presentation of the identity (4.23):

$$(W_1W_2)^{\rm cw}(b_1^*, b_2) = \int W_1(b_1^*, b)W_2(b^*, b_2)\frac{{\rm e}^{-|b|^2}{\rm d}b^*{\rm d}b}{(2\pi{\rm i})^d}. \tag{4.44}$$

5 Formal semiclassical calculus

5.1 Algebras with a filtration/gradation

Let Ψ^∞ be an (associative) algebra (over $\mathbb{C}$).

We say that it is an algebra with filtration $\{\Psi^m \ : \ m \in \mathbb{Z}\}$ iff Ψ^m are linear subspaces of Ψ^∞ such that

$$\Psi^\infty = \bigcup_{m\in\mathbb{Z}} \Psi^m, \tag{5.1}$$

$$\Psi^m \subset \Psi^{m'}, \quad m \leq m', \tag{5.2}$$

$$\Psi^m . \Psi^{m'} \subset \Psi^{m+m'}. \tag{5.3}$$

We write $\Psi^{-\infty} := \bigcap\limits_m \Psi^m$. Clearly, $\Psi^{-\infty}$ is an ideal and so are Ψ^m with $m \leq 0$.

Let Ψ^∞ be an algebra with filtration. We say that it is an algebra with a gradation if there exist linear subspaces $\Psi^{(m)}$ such that

$$\Psi^m = \Psi^{m-1} \oplus \Psi^{(m)}, \tag{5.4}$$

$$\Psi^{(m)} . \Psi^{(m')} \subset \Psi^{(m+m')}. \tag{5.5}$$

Let $\mathfrak{B}$ be an algebra. Let $\hbar$ be a real variable. Then we can consider the algebra of formal power series

$$\sum_{j=-\infty}^{m} \hbar^{-j} b_j, \quad b_j \in \mathfrak{B}. \tag{5.6}$$

We will denote it by $\mathfrak{B}[[\hbar]]$. if it is equipped with the usual multiplication, that is

$$\sum_{j=-\infty}^{m} \hbar^{-j} b_j \sum_{k=-\infty}^{m'} \hbar^{-k} c_k = \sum_{n=-\infty}^{m+m'} \hbar^{-n} \sum_{i=n-m'}^{m} b_i c_{n-i} \tag{5.7}$$

Set $\mathfrak{B}^m[[\hbar]]$ to be the space of formal power series of degree $\leq m$ and $\mathfrak{B}^{(m)}[[\hbar]] = \hbar^{-m}\mathfrak{B}$.

Clearly, $\mathfrak{B}[[\hbar]]$ is an algebra with a gradation and filtration.

An example of a commutative algebra is $C^\infty(\mathbb{R}^d \oplus \mathbb{R}^d)$. Clearly, $C^\infty(\mathbb{R}^d \oplus \mathbb{R}^d)[[\hbar]]$ is a commutative algebra with a gradation and filtration. We will later equip it with other noncommutative multiplications.

5.2 The x, p star product on the formal semiclassical algebra

It is natural to interpret the $\star^{x,p}$ star product on the space of formal power series with coefficients in $C^\infty(\mathbb{R}^d \oplus \mathbb{R}^d)$. Clearly, if

$$b(x,p) = \sum_{j=-\infty}^{m} \hbar^{-j} b_j(x,p), \quad b_j \in C^\infty(\mathbb{R}^d \oplus \mathbb{R}^d), \tag{5.8}$$

$$c(x,p) = \sum_{k=-\infty}^{m'} \hbar^{-k} c_k(x,p), \quad c_k \in C^\infty(\mathbb{R}^d \oplus \mathbb{R}^d), \tag{5.9}$$

then

$$\big(b \star^{x,p} c\big)(x,p) = \sum_{n=0}^{\infty} \frac{(-\mathrm{i}\hbar D_{p_1} D_{x_2})^n}{n!} b(x_1,p_1)c(x_2,p_2)\Big|_{\substack{x := x_1 = x_2, \\ p := p_1 = p_2.}}$$

equips $C^\infty(\mathbb{R}^d \oplus \mathbb{R}^d)[[\hbar]]$ with a noncommutative product, so that it becomes an algebra which will be denoted $\Psi(\mathbb{R}^d \oplus \mathbb{R}^d)[[\hbar]] = \Psi[[\hbar]]$. Clearly, we have a filtration given by the space of formal power series of degree at most m, denoted $\Psi^m[[\hbar]]$. However, $\hbar^m C^\infty(\mathbb{R}^d \oplus \mathbb{R}^d)$ is not a gradation of our algebra: If $b, c \in C^\infty(\mathbb{R}^d \oplus \mathbb{R}^d)$, then

$$b \star^{x,p} c = \sum_{j=0}^{\infty} \hbar^j d_{-j}, \tag{5.10}$$

where in general $d_{-j} \neq 0$ for $j > 0$.

We will use two notations for elements of $\Psi[[\hbar]]$. Either we will use *symbols*, and then the multiplication will be denoted by the appropriately decorated star:

$$b \star^{x,p} c = d$$

or we will use the *operator notation*

$$\mathrm{Op}^{x,p}(b)\mathrm{Op}^{x,p}(c) = \mathrm{Op}^{x,p}(d)$$

The passage between these two notations is obtained by applying $\mathrm{Op}^{x,p}$ to a symbol.

Now if $b \in \Psi^m[[\hbar]]$, $c \in \Psi^{m'}[[\hbar]]$, then

$$\begin{aligned} b \star^{x,p} c \in \Psi^{k+m}[[\hbar]], &\qquad b \star^{x,p} c = bc \quad \mathrm{mod}(\Psi^{k+m-1}[[\hbar]]), \\ b \star^{x,p} c - c \star^{x,p} b \in \Psi^{k+m-1}[[\hbar]], &\qquad b \star^{x,p} c - c \star^{x,p} b = \mathrm{i}\hbar\{b,c\} \quad \mathrm{mod}(\Psi^{k+m-2}[[\hbar]]). \end{aligned}$$

5.3 The Moyal star product on the formal semiclassical algebra

Again, we can interpret the star product on the space of formal power series with coefficients in $C^\infty(\mathbb{R}^d \oplus \mathbb{R}^d)$:

$$a \star b(x,p) := \sum_{n=0}^{\infty} \frac{\big(\frac{\mathrm{i}}{2}\hbar(D_{p_1}D_{x_2} - D_{x_1}D_{p_2})\big)^n}{n!} a(x_1,p_1)b(x_2,p_2)\Big|_{\substack{x := x_1 = x_2, \\ p := p_1 = p_2.}} .$$

Again, we have two notations for elements and the product: using *symbols*,

$$b \star c = d,$$

or in the *operator notation*

$$\mathrm{Op}(b)\mathrm{Op}(c) = \mathrm{Op}(d).$$

$b * c$ is called the *star product* or the *Moyal product* of b and c.

Note that this star product is just a different representation of the algebra $\Psi[[\hbar]]$. We can pass from one representation to the other by the operators described in the Berezin diagram:

$$b \star c = \mathrm{e}^{-\mathrm{i}\frac{\hbar}{2}D_xD_p}\Big(\big(\mathrm{e}^{\mathrm{i}\frac{\hbar}{2}D_xD_p}b\big)\star^{x,p}\big(\mathrm{e}^{\mathrm{i}\frac{\hbar}{2}D_xD_p}c\big)\Big) \tag{5.11}$$

Now if $b \in \Psi^m[[\hbar]]$, $c \in \Psi^{m'}[[\hbar]]$, then

$$\begin{aligned} b\star c &\in \Psi^{k+m}[[\hbar]], & b\star c &= bc \mod(\Psi^{k+m-2}[[\hbar]]),\\ b\star c - c\star b &\in \Psi^{k+m-1}[[\hbar]], & b\star c - c\star b &= \mathrm{i}\hbar\{b,c\} \mod(\Psi^{k+m-3}[[\hbar]]). \end{aligned}$$

$$\text{if } \ \mathrm{supp} b \cap \mathrm{supp} c = \emptyset, \quad \text{then} \quad b\star c \ = \ 0. \tag{5.12}$$

5.4 Principal and extended principal symbols

We have equipped $\Psi[[\hbar]]$ with 5 products, as in the Berezin diagram. They yield isomorphic algebras—we can pass from one representation to another using the transformations given in the Berezin diagram.

Let

$$A = \mathrm{Op}^\bullet\Big(\sum_{n=-\infty}^{m} a_n\hbar^{-n}\Big), \qquad \sum_{n=-\infty}^{m} a_n\hbar^{-n} \in \Psi^m[[\hbar]]. \tag{5.13}$$

Then

$$\mathrm{s}_{\mathrm{p}}^m(A) := \hbar^{-m}a_m$$

does not depend on the quantization. It is called the *principal symbol* of the operator A (wrt $\Psi^m[[\hbar]]$).

Let $A \in \Psi^m[[\hbar]], \quad B \in \Psi^k[[\hbar]]$. Then

$$\begin{aligned} &AB \in \Psi^{m+k}[[\hbar]],\\ &\mathrm{s}_{\mathrm{p}}^{m+k}(AB) = \mathrm{s}_{\mathrm{p}}^m(A)\mathrm{s}_{\mathrm{p}}^k(B),\\ &[A,B] \in \Psi^{m+k-1}[[\hbar]],\\ &\mathrm{s}_{\mathrm{p}}^{m+k-1}([A,B]) = \mathrm{i}\hbar\{\mathrm{s}_{\mathrm{p}}^m(A), \mathrm{s}_{\mathrm{p}}^k(B)\}. \end{aligned}$$

If we use the Weyl quantization in (5.13) holds, then

$$\mathrm{s}_{\mathrm{sp}}^m(A) := \hbar^{-m+1}a_{m-1}$$

is called the *subprincipal symbol.* The sum of the principal and subprincipal symbol, which we will denote

$$\mathrm{s}_{\mathrm{p+sp}}^m(A) := \hbar^{-m}a_m + \hbar^{-m+1}a_{m-1}$$

has remarkable properties:

$$\begin{aligned} \mathrm{s}_{\mathrm{p+sp}}^{m+k}\Big(\frac{1}{2}(AB+BA)\Big) &= \mathrm{s}_{\mathrm{p+sp}}^m(A)\mathrm{s}_{\mathrm{p+sp}}^k(B) + O(\hbar^{-m-k+2}),\\ \mathrm{s}_{\mathrm{p+sp}}^{m+k-1}([A,B]) &= \mathrm{i}\hbar\big\{\mathrm{s}_{\mathrm{p+sp}}^m(A), \mathrm{s}_{\mathrm{p+sp}}^k(B)\big\} + O(\hbar^{-m-k+3}). \end{aligned}$$

5.5 Inverses

Let $A \in \Psi^m[[\hbar]]$. We say that A is *elliptic* if it has an everywhere non-zero principal symbol, that is

$$\mathrm{s}_{\mathrm{p}}^m(A)(x,p) \neq 0, \quad x,p \in \mathbb{R}^d \oplus \mathbb{R}^d. \tag{5.14}$$

Theorem 5.1. *Let $A \in \Psi^m[[\hbar]]$ be elliptic. Then there exists a unique $B \in \Psi^{-m}[[\hbar]]$ such that*

$$AB = BA = \mathbb{1}. \tag{5.15}$$

Besides,

$$\mathrm{s}_{\mathrm{p}}^{-m}(B) = \frac{1}{\mathrm{s}_{\mathrm{p}}^m(A)}. \tag{5.16}$$

Proof. Let $\mathrm{s}_{\mathrm{p}}^m(A) = \hbar^{-m} a_m$. Set

$$B_0 := \hbar^m \mathrm{Op}\Big(\frac{1}{a_m}\Big) \in \Psi^{-m}[[\hbar]].$$

Then $AB_0 \in \Psi^0[[\hbar]]$ and

$$\mathrm{s}_{\mathrm{p}}(AB_0) = 1.$$

Hence

$$AB_0 = \mathbb{1} + C$$

where $C \in \Psi^{-1}[[\hbar]]$. Now

$$(\mathbb{1} + C)^{-1} = \sum_{n=0}^{\infty} (-1)^n C^n$$

is a well defined element of $\Psi^0[[\hbar]]$, because $C^n \in \Psi^{-n}[[\hbar]]$. We set

$$B := B_0(1 + C)^{-1} \in \Psi^{-m}[[\hbar]],$$

which is an inverse of A. $\square$

5.6 More about star product

The star product can be written in the following asymmetric form:

$$\begin{aligned} b * c(x,p) &= b\Big(x - \frac{\hbar}{2}D_p, p + \frac{\hbar}{2}D_x\Big)c(x,p) & (5.17)\\ &= c\Big(x + \frac{\hbar}{2}D_p, p - \frac{\hbar}{2}D_x\Big)b(x,p). & (5.18) \end{aligned}$$

Note that the operators $b(\cdots)$ in (5.17) and (5.18) can be understood as the quantization with "x,p to the left and D_x, D_p to the right", written in the PDE notation, see (3.3).

There is another way to interpret these formulas. Note that the operators $x \mp \frac{\hbar}{2}D_p$ and $p \pm \frac{\hbar}{2}D_x$ commute. Thus we can understand the operators $b(\cdots)$ as a function of two commuting operators.

Alternatively (and we will do it in the sequel) the operators $b(\cdots)$ can be interpreted in terms of the Weyl quantization. Indeed, define the following symbols on the doubled phase space

$$\begin{aligned} b_{\rm l}(x,p,\xi_p,\xi_p) &:= b\Big(x - \frac{1}{2}\xi_p, p + \frac{1}{2}\xi_x\Big), \\ c_{\rm r}(x,p,\xi_p,\xi_p) &:= c\Big(x + \frac{1}{2}\xi_p, p - \frac{1}{2}\xi_x\Big). \end{aligned}$$

Then (5.17) and (5.18) can be rewritten as

$$\begin{aligned} b * c(x,p) &= \mathrm{Op}(b_{\rm l})c(x,p) && (5.19) \\ &= \mathrm{Op}(c_{\rm r})b(x,p) && (5.20) \end{aligned}$$

Let us prove (5.17). We start from

$$b * c(x,p) = \mathrm{e}^{\frac{\mathrm{i}}{2}\hbar(D_{p_1}D_{x_2} - D_{x_1}D_{p_2})} b(x_1,p_1)c(x_2,p_2)\Big|_{\substack{x := x_1 = x_2, \\ p := p_1 = p_2.}} . \tag{5.21}$$

We treat $b(x,p)$ as the operator of multiplication. We move $\mathrm{e}^{\frac{\mathrm{i}}{2}\hbar(D_{p_1}D_{x_2} - D_{x_1}D_{p_2})}$ to the right obtaining

$$b\Big(x_1 - \frac{\hbar}{2}D_{p_2}, p_1 + \frac{\hbar}{2}D_{x_2}\Big)c(x_2,p_2)\Big|_{\substack{x := x_1 = x_2, \\ p := p_1 = p_2.}} ,$$

which equals the RHS of (5.17) (using the first interpretation).

We have similar formulas for the product in the x,p-quantization.

$$\begin{aligned} b \star^{x,p} c(x,p) &= b\big(x, p + \hbar D_x\big)c(x,p) \\ &= c\big(x + \hbar D_p, p\big)b(x,p). \end{aligned}$$

5.7 The exponential

The formulas (5.17) and (5.18) are a good starting point for the formal functional calculus. For a function f let us write

$$f(\mathrm{Op}(g)) = \mathrm{Op}\big(f_\star(g)\big).$$

For instance

$$\exp\big(\mathrm{i}\mathrm{Op}(g)\big) = \mathrm{Op}\big(\exp_\star(\mathrm{i}g)\big).$$

We then have

Proposition 5.2.

$$\exp_\star(\mathrm{i}g) = \exp_\star\Big(\frac{\mathrm{i}}{2}g\Big)\exp_\star\Big(\frac{\mathrm{i}}{2}g\Big) = \exp\Big(\frac{\mathrm{i}}{2}\mathrm{Op}(g_{\rm l} + g_{\rm r})\Big)1, \tag{5.22}$$

$$\exp_\star\Big(\frac{\mathrm{i}}{\hbar}g\Big) \star b \star \exp_\star\Big(-\frac{\mathrm{i}}{\hbar}g\Big) = \exp\Big(\frac{\mathrm{i}}{\hbar}\mathrm{Op}(g_{\rm l} - g_{\rm r})\Big)b. \tag{5.23}$$

In other words,

$$\exp\Big(\mathrm{iOp}(g)\Big) = \mathrm{Op}\Big(\exp\Big(\frac{\mathrm{i}}{2}\mathrm{Op}(g_{\mathrm{l}} + g_{\mathrm{r}})\Big)1\Big), \tag{5.24}$$

$$\exp\Big(\frac{\mathrm{i}}{\hbar}\mathrm{Op}(g)\Big)\mathrm{Op}(b)\exp\Big(-\frac{\mathrm{i}}{\hbar}\mathrm{Op}(g)\Big) = \mathrm{Op}\bigg(\exp\Big(\frac{\mathrm{i}}{\hbar}\mathrm{Op}(g_{\mathrm{l}} - g_{\mathrm{r}})\Big)b\bigg). \tag{5.25}$$

To see (5.22) we first note that

$$\exp_\star\Big(\frac{\mathrm{i}}{2}g\Big)\star b = \exp\Big(\frac{\mathrm{i}}{2}\mathrm{Op}(g_{\mathrm{l}})\Big)b,$$
$$b\star\exp_\star\Big(\frac{\mathrm{i}}{2}g\Big) = \exp\Big(\frac{\mathrm{i}}{2}\mathrm{Op}(g_{\mathrm{r}})\Big)b,$$

and then

$$\exp_\star(\mathrm{i}g) = \exp_\star\Big(\frac{\mathrm{i}}{2}g\Big)\star 1\star\exp_\star\Big(\frac{\mathrm{i}}{2}g\Big) \tag{5.26}$$

□

To see the usefulness of (5.22) and (5.23), introduce the "Taylor tails" of g_{l} and g_{r} at $\xi_x, \xi_p = 0$:

$$g_{\mathrm{l},n}(x,p,\xi_x,\xi_p) := \sum_{n\le|\alpha|+|\beta|}\partial_x^\alpha\partial_p^\beta g(x,p)\frac{(-1)^{|\alpha|}}{2^{|\alpha|+\beta|}}\xi_p^\alpha\xi_x^\beta, \tag{5.27}$$

$$g_{\mathrm{r},n}(x,p,\xi_x,\xi_p) := \sum_{n\le|\alpha|+|\beta|}\partial_x^\alpha\partial_p^\beta g(x,p)\frac{(-1)^{|\beta|}}{2^{|\alpha|+\beta|}}\xi_p^\alpha\xi_x^\beta. \tag{5.28}$$

Note that $\mathrm{Op}(g_{\mathrm{l},n})$ and $\mathrm{Op}(g_{\mathrm{l},n})$ are $O(\hbar^n)$. We can rewrite (5.22) and (5.23) as

$$\exp_\star(\mathrm{i}g) = \exp\Big(\mathrm{i}g(x,p) + \frac{\mathrm{i}}{2}\mathrm{Op}(g_{\mathrm{l},2} + g_{\mathrm{r},2})\Big)1, \tag{5.29}$$

$$\exp_\star\Big(\frac{\mathrm{i}}{\hbar}g\Big)\star b\star\exp_\star\Big(-\frac{\mathrm{i}}{\hbar}g\Big) = \exp\Big(g_{,x}(x,p)\partial_p - g_{,p}(x,p)\partial_x + \frac{\mathrm{i}}{\hbar}\mathrm{Op}(g_{\mathrm{l},3} - g_{\mathrm{r},3})\Big)b. \tag{5.30}$$

6 Uniform symbol class

6.1 The boundedness of quantized uniform symbols

Let us set $\hbar = 1$.

In practice quantization is applied to symbols that belong to certain classes with good properties. Hörmander introduced the following class of symbols: $f \in S^m_{\rho,\delta}(\mathbb{R}^d\oplus\mathbb{R}^d)$ if $f \in C^\infty(\mathbb{R}^d\oplus\mathbb{R}^d)$ and the following estimate holds:

$$|\partial_x^\beta\partial_p^\alpha f(x,p)| \le C_{\alpha,\beta}\langle p\rangle^{m-|\alpha|\rho+|\beta|\delta}, \qquad \alpha,\beta. \tag{6.1}$$

There are some deep reasons for considering such symbol classes, however for the moment we will use only the simplest one, corresponding to $m = \delta = \rho = 0$.

Thus we will denote by $S_{00}^0(\mathbb{R}^d \oplus \mathbb{R}^d)$ the space of $b \in C^\infty(\mathbb{R}^d \oplus \mathbb{R}^d)$ such that

$$|\partial_x^\beta \partial_p^\alpha b| \leq C_{\alpha,\beta}, \qquad \alpha, \beta.$$

We will often write S_{00}^0 for $S_{00}^0(\mathbb{R}^d \oplus \mathbb{R}^d)$.

Here is one of the classic results about the pseudodifferential calculus:

Theorem 6.1 (The Calderon-Vaillancourt Theorem)**.** *If* $a \in S_{00}^0$, *then* $\mathrm{Op}^{x,p}(a)$ *and* $\mathrm{Op}(a)$ *are bounded.*

We will present a proof of the above theorem in the following subsections.

6.2 Quantization of Gaussians

Consider the harmonic oscillator

$$H = \hat{x}^2 + \hat{p}^2. \tag{6.2}$$

The quantization of Gaussians can be expressed in terms of the harmonic oscillator.

Proposition 6.2.

$$\mathrm{Op}\big(\mathrm{e}^{-\lambda(x^2+p^2)}\big) = \begin{cases} (1-\lambda^2)^{-d/2} \exp\Big(-\frac{1}{2}\log\frac{(1+\lambda)}{(1-\lambda)}H\Big), & 0 < \lambda < 1, \\ 2^{-d}1\!\!1_{\{d\}}(H), & \lambda = 1, \\ (\lambda^2-1)^{-d/2}(-1)^{(H-d)/2} \exp\Big(-\frac{1}{2}\log\frac{(1+\lambda)}{(\lambda-1)}H\Big), & 1 < \lambda. \end{cases} \tag{6.3}$$

Proof. It is enough to consider $d = 1$. Let us make an ansatz

$$\mathrm{e}^{-tH} = \mathrm{Op}(c\mathrm{e}^{\lambda(x^2+p^2)}). \tag{6.4}$$

We have

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{-tH} =& \frac{1}{2}(H\mathrm{e}^{-tH} + \mathrm{e}^{-tH}H) \\ =& \frac{1}{2}\mathrm{Op}\Big((x^2+p^2) \star c\mathrm{e}^{-\lambda(x^2+p^2)} + c\mathrm{e}^{-\lambda(x^2+p^2)} \star (x^2+p^2)\Big) \\ \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Op}(c\mathrm{e}^{\lambda(x^2+p^2)}) =& \mathrm{Op}\Big(\big(\dot{c} - c\dot{\lambda}(x^2+p^2)\big)\mathrm{e}^{-\lambda(x^2+p^2)}\Big). \end{aligned}$$

Now

$$\begin{aligned} &\frac{1}{2}\Big((x^2+p^2) \star c\mathrm{e}^{-\lambda(x^2+p^2)} + c\mathrm{e}^{-\lambda(x^2+p^2)} * (x^2+p^2)\Big) \\ =&(x^2+p^2)c\mathrm{e}^{-\lambda(x^2+p^2)} - \frac{1}{8}\Big(\partial_{x_1}\partial_{p_2} - \partial_{p_1}\partial_{x_2}\Big)^2 (x_1^2+p_1^2)c\mathrm{e}^{-\lambda(x_2^2+p_2^2)}\Big|_{\substack{x = x_1 = x_2, \\ p = p_1 = p_2,}} \\ =&c\Big((x^2+p^2)(1-\lambda^2) + \frac{\lambda}{2}\Big)\mathrm{e}^{-t(x^2+p^2)} \end{aligned}$$

We obtain the system of equations

$$\dot{\lambda} = -1 + \lambda^2, \qquad \dot{c} = \frac{c\lambda}{2},$$

solved by $\lambda = \tanh t$, $c = (\cosh t)^{\frac{1}{2}}$. Therefore,

$$\mathrm{e}^{-tH} = (\cosh t)^{\frac{1}{2}} \mathrm{Op}\Big(\mathrm{e}^{\tanh(t)(x^2+p^2)}\Big). \tag{6.5}$$

Expressing t in terms of λ we obtain the case $0 < \lambda < 1$. Taking the limit at $\lambda = 1$ we obtain the second case. Then, by analytic continuation in λ we obtain $1 < \lambda < \infty$. □

There are 3 distinct regimes of the parameter λ: For $0 < \lambda < 1$, the quantization of the Gaussian is proportional to a thermal state of H. As λ increases to 1, it becomes "less mixed"–its "temperature" decreases. At $\lambda = 1$ it becomes pure—its "temperature" becomes zero and it is the ground state of H. For $1 < \lambda < \infty$, when we compress the Gaussian, it is no longer positive—due to the factor $(-1)^{(H-d)/2}$ it has eigenvalues with alternating signs. Besides, it becomes "more and more mixed", contrary to the naive classical picture.

Thus, at $\lambda = 1$ we observe a kind of a "phase transition": For $0 \leq \lambda < 1$ the quantization of a Gaussian behaves more or less according to the classical intuition. For $1 < \lambda$ the classical intuition stops to work—compressing the classical symbol makes its quantization more "diffuse".

It is easy to compute the trace and the tracial norm of (8.18):

Proposition 6.3.

$$\mathrm{Tr}\mathrm{Op}\big(\mathrm{e}^{-\lambda(x^2+p^2)}\big) = \frac{1}{2^d\lambda^d}. \tag{6.6}$$

$$\mathrm{Tr}\left|\mathrm{Op}\big(\mathrm{e}^{-\lambda(x^2+p^2)}\big)\right| = \begin{cases} \frac{1}{2^d\lambda^d} & \lambda \leq 1, \\ \frac{1}{2^d}, & 1 \leq \lambda. \end{cases} \tag{6.7}$$

Proof. Let us restrict ourselves to $d = 1$, using that $\mathrm{sp}\,(H) = \{1 + 2n \mid n = 0, 1, 2, \dots\}$. Let us prove (6.7):

$$\begin{aligned}
\mathrm{Tr}\left|\mathrm{Op}\big(\mathrm{e}^{-\lambda(x^2+p^2)}\big)\right| &= \sum_{n=0}^{\infty}(1-\lambda^2)^{-\frac{1}{2}}\Big(\frac{1-\lambda}{1+\lambda}\Big)^{\frac{1}{2}(1+2n)} \\
&= \frac{1}{2\lambda}, \qquad 0 < \lambda \leq 1, \\
&= \sum_{n=0}^{\infty}(\lambda^2-1)^{-\frac{1}{2}}\Big(\frac{\lambda-1}{1+\lambda}\Big)^{\frac{1}{2}(1+2n)} \\
&= \frac{1}{2}, \qquad 1 \leq \lambda.
\end{aligned}$$

Evidently, the trace (6.6) does not see the "phase transition" at $\lambda = 1$. However, if we consider the trace norm, this phase transition appears—(6.7) is differentiable except at $\lambda = 1$. Note that (6.7) can be viewed as a kind of quantitative "uncertainty principle".

6.3 Proof of the Calderon-Vaillancourt Theorem

We start with the following proposition.

Proposition 6.4. *For $s > \frac{d}{2}$, define the functions*

$$\psi_s(\xi) := (2\pi)^{-d} \int \mathrm{d}\zeta\, (1+\zeta^2)^{-s} \mathrm{e}^{\mathrm{i}\zeta\xi}, \tag{6.8}$$

$$P_s(x,p) := \psi_s(x)\psi_s(p). \tag{6.9}$$

Then $\mathrm{Op}(P_s)$ *is trace class and*

$$\mathrm{Tr}\Big|\mathrm{Op}(P_s)\Big| \leq \frac{\Gamma(s)^2 + \Gamma(s-\frac{d}{2})^2}{(2\pi)^d \Gamma(s)^2}. \tag{6.10}$$

Proof. Let us use the so-called Schwinger parametrization

$$X^{-s} = \frac{1}{\Gamma(s)} \int_0^\infty \mathrm{e}^{-tX} t^{s-1}\, \mathrm{d}t \tag{6.11}$$

to get

$$\begin{aligned} \psi_s(\xi) &= \frac{1}{\Gamma(s)(2\pi)^d} \int_0^\infty \mathrm{d}t \int \mathrm{d}\zeta\, \mathrm{e}^{-t(1+\zeta^2)} t^{s-1} \mathrm{e}^{\mathrm{i}\zeta\xi} \\ &= \frac{1}{\pi^{\frac{d}{2}} 2^d \Gamma(s)} \int_0^\infty \mathrm{d}t\, t^{s-\frac{d}{2}-1} \mathrm{e}^{-t-\frac{\xi^2}{4t}}. \end{aligned} \tag{6.12}$$

Now

$$P_s(x,p) = \frac{1}{\pi^d 2^{2d} \Gamma^2(s)} \int_0^\infty \mathrm{d}u \int_0^\infty \mathrm{d}v \mathrm{e}^{-u-v-\frac{x^2}{4u}-\frac{p^2}{4v}} (uv)^{s-\frac{d}{2}-1}. \tag{6.13}$$

By (6.7), we have

$$\mathrm{Tr}\left|\mathrm{Op}\big(\mathrm{e}^{-\alpha x^2 - \beta p^2}\big)\right| = \begin{cases} \frac{1}{(2\sqrt{\alpha\beta})^d}, & \alpha\beta \leq 1, \\ \frac{1}{2^d}, & 1 \leq \alpha\beta. \end{cases} \tag{6.14}$$

Hence,

$$\begin{aligned} &\mathrm{Tr}\Big|\mathrm{Op}(P_s)\Big| \\ \leq &\frac{1}{2^{2d}\pi^d\Gamma^2(s)} \int_0^\infty \mathrm{d}u \int_0^\infty \mathrm{d}v \mathrm{e}^{-u-v} \mathrm{Tr}\left|\mathrm{Op}\left(\mathrm{e}^{-\frac{x^2}{4u}-\frac{p^2}{4v}}\right)\right| (uv)^{s-\frac{d}{2}-1} \\ \leq &\frac{1}{2^d\pi^d\Gamma^2(s)} \left(\int\limits_{4\leq uv,\ u,v>0} \mathrm{d}u \int \mathrm{d}v\ \ \mathrm{e}^{-u-v} (uv)^{s-1} + \int\limits_{uv\leq 4,\ u,v>0} \mathrm{d}u \int \mathrm{d}v\ \ \mathrm{e}^{-u-v} (uv)^{s-\frac{d}{2}-1} \right) \\ \leq &\frac{\Gamma(s)^2 + \Gamma(s-\frac{d}{2})^2}{2^d \pi^d \Gamma^2(s)}. \end{aligned}$$

□

Proposition 6.5. *Let B be a self-adjoint trace class operator and $h \in L^\infty(\mathbb{R}^{2d})$. Then*

$$A := \frac{1}{(2\pi)^d} \int \mathrm{d}y \int \mathrm{d}w h(y,w) \mathrm{e}^{-\mathrm{i}y\hat{p}+\mathrm{i}w\hat{x}} B \mathrm{e}^{\mathrm{i}y\hat{p}-\mathrm{i}w\hat{x}} \tag{6.15}$$

is bounded and

$$\|A\| \leq \mathrm{Tr}|B| \, \|h\|_\infty. \tag{6.16}$$

Proof. Define $T_\Phi : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^{2d})$ by

$$T_\Phi \Theta(y,w) := (2\pi)^{-\frac{d}{2}} (\Phi | \mathrm{e}^{\mathrm{i}y\hat{p}-\mathrm{i}w\hat{x}} \Theta), \quad \Theta \in L^2(\mathbb{R}^{2d}). \tag{6.17}$$

We check that T_Φ is an isometry. This implies that for $\Phi, \Psi \in L^2(\mathbb{R}^d)$ of norm one

$$\frac{1}{(2\pi)^d} \int \mathrm{d}y \int \mathrm{d}w h(y,w) \mathrm{e}^{-\mathrm{i}y\hat{p}+\mathrm{i}w\hat{x}} |\Phi)(\Psi| \mathrm{e}^{\mathrm{i}y\hat{p}-\mathrm{i}w\hat{x}} \tag{6.18}$$

is bounded and its norm is less than $\|h\|_\infty$. Indeed, (6.18) can be written as the product of three operators

$$T_\Phi^* h T_\Psi, \tag{6.19}$$

(Note that the proof of the boundedness of the contravariant quantizatio for bounded symbols is essentially the same. The transformation T is sometimes called the FBI transformation, for Fourier-Bros-Iagolnitzer).

Now it suffices to write

$$B = \sum_{i=1}^\infty \lambda_i |\Phi_i)(\Psi_i|, \tag{6.20}$$

where Φ_i, Ψ_i are normalized, $\lambda_i \geq 0$ and $\mathrm{Tr}|B| = \sum_{i=1}^\infty \lambda_i$.

□

Proof of Theorem 6.1. Set

$$h := (1 - \Delta_x)^s (1 - \Delta_p)^s a. \tag{6.21}$$

Then

$$\begin{aligned} a(x,p) &= (1 - \Delta_x)^{-s} (1 - \Delta_p)^{-s} h(x,p) &(6.22)\\ &= \int \mathrm{d}y \int \mathrm{d}w \, P_s(x-y, p-w) h(y,w). &(6.23) \end{aligned}$$

Hence

$$\begin{aligned} \mathrm{Op}(a) &= \int \mathrm{d}y \int \mathrm{d}w \, \mathrm{Op}\big(P_s(x-y,p-w)\big) h(y,w) &(6.24)\\ &= \frac{1}{(2\pi)^d} \int \mathrm{d}y \int \mathrm{d}w \, h(y,w) \mathrm{e}^{-\mathrm{i}y\hat{p}+\mathrm{i}w\hat{x}} \mathrm{Op}(P_s) \mathrm{e}^{\mathrm{i}y\hat{p}-\mathrm{i}w\hat{x}}. &(6.25) \end{aligned}$$

Therefore, by Proposition 6.5,

$$\|\mathrm{Op}(a)\| \leq \mathrm{Tr}\big|\mathrm{Op}(P_s)\big| \|h\|_\infty. \tag{6.26}$$

□

6.4 Beals criterion

We will write $\mathrm{ad}_B(A) := [B, A]$.

$|y, q)$ will denote the Gaussian coherent state centered at $y, q \in \mathbb{R}^{\oplus}\mathbb{R}^d$.

Remark 6.6. *The implication (2)⇒(3) in the following theorem is called the* Beals Criterion.

The function

$$\mathbb{R}^{2d} \times \mathbb{R}^{2d} \ni (y, q, y'q') \mapsto (y, q|B|y'q')$$

is called the phase space correlation function.

Theorem 6.7. *The following conditions are equivalent:*

(1) *For any n there exists C_n such that $|(y, q|B|y'q')| \leq C_n \langle (y, q) - (y'q') \rangle^{-n}$.*

(2) $\mathrm{ad}_{\hat{x}}^{\alpha} \mathrm{ad}_{\hat{p}}^{\beta} B \in B(L^2(\mathbb{R}^d)), \quad \alpha, \beta.$

(3) $B = \mathrm{Op}(b), \quad b \in S_{00}^0(\mathbb{R}^d \oplus \mathbb{R}^d).$

(4) $B = \mathrm{Op}^{x,p}(b), \quad b \in S_{00}^0(\mathbb{R}^d \oplus \mathbb{R}^d),$

Proof. We will prove (1)⇒(3)⇒(2)⇒(1). We omit (4).

(1)⇒(3): We have

$$\begin{aligned} b(x,p) &= 2^d \mathrm{Tr} I_{(x,p)} B \\ &= \frac{2^d}{(2\pi)^{2d}} \mathrm{Tr} \int \int \mathrm{d}y \mathrm{d}q \mathrm{d}y' \mathrm{d}q' \, |y, q)(y, q|I_{(x,p)}|y', q')(y', q'|B \\ &= \frac{1}{2^d \pi^{2d}} \int \int \mathrm{d}y \mathrm{d}q \mathrm{d}y' \mathrm{d}q' \, (y, q|I_{(x,p)}|y', q')(y', q'|B|y, q). \end{aligned}$$

Now

$$(y, q|I_{(x,p)}|y', q') = \mathrm{e}^{\frac{\mathrm{i}}{2}(yq' - qy')} \mathrm{e}^{\mathrm{i}(x(q-q') - p(y-y'))} \mathrm{e}^{-(x - \frac{y+y'}{2})^2 - (p - \frac{q+q'}{2})^2}.$$

Therefore,

$$\left| \partial_x^{\alpha} \partial_p^{\beta} (y, q|I_{(x,p)}|y', q') \right| \leq C_{\alpha,\beta} \langle q - q' \rangle^{|\alpha|} \langle y - y' \rangle^{|\beta|}.$$

Hence

$$\begin{aligned} &|b(x,p)| \\ \leq &C'_{\alpha,\beta} \int \int \mathrm{d}y \mathrm{d}q \mathrm{d}y' \mathrm{d}q' \, \langle q - q' \rangle^{|\alpha|} \langle y - y' \rangle^{|\beta|} |(y', q'|B|y, q)|. \end{aligned}$$

(3)⇒(2): Let $b \in S_{00}^0$. We have

$$\mathrm{ad}_{\hat{x}}^{\alpha} \mathrm{ad}_{\hat{p}}^{\beta} \mathrm{Op}(b) = \mathrm{i}^{|\alpha| - |\beta|} \mathrm{Op}\big(\partial_p^{\alpha} \partial_x^{\beta} b\big). \tag{6.27}$$

Now $\partial_p^{\alpha} \partial_x^{\beta} b \in S_{00}^0$. Hence the Calderon-Vaillancourt Theorem implies that (6.27) is bounded.

(2)⇒(1): Iterating

$$\begin{aligned}&(y-y')(y,q|B|y'q')\\ =&-(y,q|(\hat{x}-y)B|y'q')+(y,q|[\hat{x},B]|y'q')+(y,q|B(\hat{x}-y')|y'q')\end{aligned}$$

we obtain

$$\begin{aligned}&(y-y')^n(y,q|B|y'q')\\ =&\sum_{k,m}C_{k,m}\left(y,q|(\hat{x}-y)^k\mathrm{ad}_{\hat{x}}^{n-k-m}(B)(\hat{x}-y')^m|y',q'\right).\end{aligned}$$

Similarly, we get

$$\begin{aligned}&(q-q')^n(y,q|B|y'q')\\ =&\sum_{k,m}C_{k,m}\left(y,q|(\hat{p}-q)^k\mathrm{ad}_{\hat{p}}^{n-k-m}(B)(\hat{p}-q')^m|y',q'\right).\end{aligned}$$

Cearly,

$$(\hat{x}-y)^n|y,q),\quad (\hat{p}-q)^n|y,q)\in L^2(\mathbb{R}^d).$$

Therefore,

$$(y-y')^n(y,q|B|y'q'),\quad (q-q')^n(y,q|B|y'q')$$

are bounded. □

6.5 The algebra Ψ_{00}^0

Let us denote by Ψ_{00}^0 the set of operators described in Theorem 6.7.

Theorem 6.8. Ψ_{00}^0 *is a* $*$*-algebra.*

Proof. We use repeatedly the Leibnitz rule and then the Beals criterion:

$$\mathrm{ad}_{\hat{x}}(AB)=\mathrm{ad}_{\hat{x}}(A)B+A\mathrm{ad}_{\hat{x}}(B),$$

and similarly with $\hat{p}$. □

Theorem 6.9. *Let* $B\in\Psi_{00}^0$ *be boundedly invertible. Then* $B^{-1}\in\Psi_{00}^0$.

Proof. Similarly as above, using

$$\mathrm{ad}_{\hat{x}}(A^{-1})=-A^{-1}\mathrm{ad}_{\hat{x}}(A)A^{-1}.$$

□

Theorem 6.10.

1. *Let f be a function holomorphic on a neighborhood of* $\mathrm{sp}\, B$*, where* $B \in \Psi^0_{00}$*. Then* $f(B) \in \Psi^0_{00}$*.*
2. *Let f be a function smooth on* $\mathrm{sp}\, B$*, where* $B \in \Psi^0_{00}$ *and B is self-adjoint. Then* $f(B) \in \Psi^0_{00}$*.*

Proof. (1): We write

$$f(A) = \frac{1}{2\pi \mathrm{i}} \int_\gamma (z - A)^{-1} f(z) \mathrm{d}z$$

and use

$$\mathrm{ad}_{\hat{x}} (z - A)^{-1} = (z - A)^{-1} \mathrm{ad}_{\hat{x}}(A)(z - A)^{-1}.$$

(2) We write

$$f(A) = \frac{1}{2\pi} \int \mathrm{d}t \mathrm{e}^{-\mathrm{i}tA} \hat{f}(t),$$

noting that $\mathrm{sp}\,(A)$ is compact and we can assume that $f \in C^\infty_{\mathrm{c}}(\mathbb{R})$. Then we apply

$$\mathrm{ad}_{\hat{x}} \mathrm{e}^{-\mathrm{i}tA} = \int_0^1 \mathrm{d}\tau \mathrm{e}^{-\mathrm{i}t\tau A} \mathrm{ad}_{\hat{x}}(A) \mathrm{e}^{-\mathrm{i}t(1-\tau)A}.$$

□

For example, if $H \in \Psi^0_{0,0}$, then $\mathrm{e}^{\mathrm{i}tH} \in \Psi^0_{0,0}$. Therefore, if also $B \in \Psi^0_{0,0}$, then $\mathrm{e}^{\mathrm{i}tH} B \mathrm{e}^{-\mathrm{i}tH} \in \Psi^0_{0,0}$.

Without much difficulty, we can show that if H is a 2nd order polynomial plus an element of $\Psi^0_{0,0}$ and $B \in \Psi^0_{0,0}$, then $\mathrm{e}^{\mathrm{i}tH} B \mathrm{e}^{-\mathrm{i}tH} \in \Psi^0_{0,0}$. However, without a small Planck constant this does not sound very interesting.

6.6 Gaussian dynamics on uniform symbol class

We will denote by $S^0_0(\mathbb{R}^n)$ the space of $b \in C^\infty(\mathbb{R}^n)$ such that

$$|\partial^\alpha_x b| \leq C_\alpha.$$

Note that $S(\mathbb{R}^n)$ has the structure of a Frechet space with an ascending sequence of seminotma

$$\|b\|_N := \sum_{|\alpha| \leq N} \|\partial^\alpha b\|_\infty.$$

Clearly, our main example of $S^0_0(\mathbb{R}^n)$ is $S^0_{00}(\mathbb{R}^{2d})$, where $\mathbb{R}^{2d}$ is the phase space, however it is convenient to be more general.

Let us describe some continuous linear operations between spaces $S^0_0(\mathbb{R}^n)$.

Proposition 6.11. *Let* $\mathbb{R}^{m+k} = \mathbb{R}^m \oplus \mathbb{R}^k$*. Then*

$$f \mapsto f\Big|_{\mathbb{R}^m \oplus \{0\}}$$

is a continuous map from $S^0_0(\mathbb{R}^{m+k})$ *to* $S^0_0(\mathbb{R}^m)$*.*

Proposition 6.12. *Let ν be a quadratic form. Then $\mathrm{e}^{\frac{\mathrm{i}}{2}D\nu D}$ is bounded on $S_0^0(\mathbb{R}^n)$ and depends continuously on ν.*

Proof. It is enough to show that, there exist C and N such that

$$\sup|\mathrm{e}^{\frac{\mathrm{i}}{2}D\nu D}b(x)| \leq C \sup_{|\beta|\leq N} |\partial_x^\beta b(x)|. \tag{6.28}$$

We can diagonalize the form η:

$$D\nu D = t_1 D_1^2 + \cdots t_k D_k^2 - t_{k+1}D_{k+1}^2 - \cdots - t_{k+m}D_{k+m}^2.$$

We will actually assume that the dimension is 1–it is easy to generalize the argument to any dimension.

Now

$$\mathrm{e}^{\pm\frac{\mathrm{i}}{2}tD^2}f(x) = \int \frac{1}{\sqrt{\pm\mathrm{i}2\pi t}}\mathrm{e}^{\pm\frac{\mathrm{i}}{2t}z^2}f(x-z)\mathrm{d}z. \tag{6.29}$$

Changing the variables, up to a constant, we can rewrite this as

$$\int \mathrm{e}^{\pm\frac{\mathrm{i}}{2}y^2}f(x-\sqrt{t}y)\mathrm{d}y. \tag{6.30}$$

Define the operator

$$\mathcal{L} := (1+y^2)^{-1}\left(\mp\mathrm{i}y\frac{\mathrm{d}}{\mathrm{d}y}+1\right). \tag{6.31}$$

Then $\mathcal{L}\mathrm{e}^{\pm\frac{\mathrm{i}}{2}y^2} = \mathrm{e}^{\pm\frac{\mathrm{i}}{2}y^2}$, and hence, integrating by parts we obtain

$$\int \mathrm{e}^{\pm\frac{\mathrm{i}}{2}y^2}f(x-\sqrt{t}y)\mathrm{d}y = \int\left(\mathcal{L}^2\mathrm{e}^{\pm\frac{\mathrm{i}}{2}y^2}\right)f(x-\sqrt{t}y)\mathrm{d}y \tag{6.32}$$

$$= \int \mathrm{e}^{\pm\frac{\mathrm{i}}{2}y^2}\mathcal{L}^{\#2}f(x-\sqrt{t}y)\mathrm{d}y, \tag{6.33}$$

where

$$\mathcal{L}^{\#} = \left(\mp\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}y}y+1\right)(1+2y^2)^{-1} \tag{6.34}$$

is the transpose of $\mathcal{L}$. Now

$$\left|\mathcal{L}^{\#2}f(\sqrt{t}y)\right| \leq C\langle y\rangle^{-2},$$

which is integrable. □

Later on we will need a more elaborate estimate. Consider space $\mathbb{R}^n \oplus \mathbb{R}^k$ with variables x, ξ. We consider the space

$$S_{00}^m := \{f \in C^\infty(\mathbb{R}^n \oplus \mathbb{R}^k) \mid |\partial_x^\alpha \partial_\xi^\beta f| \leq C_{\alpha,\beta}\langle\xi\rangle^m\}. \tag{6.35}$$

Proposition 6.13. *Let ν be a quadratic form on $\mathbb{R}^n \oplus \mathbb{R}^k$. Then $\mathrm{e}^{\frac{\mathrm{i}}{2}D\nu D}$ is bounded on (6.35) and depends continuously on ν.*

Proof. We need to show that, there exist C and N such that

$$\sup|\langle\xi\rangle^{-m}\mathrm{e}^{\frac{\mathrm{i}}{2}D\nu D}b(x,\xi)| \leq C \sup_{|\alpha|+|\beta|\leq N} |\langle\xi\rangle^{-m}\partial_x^\alpha\partial_\xi^\beta b(x,\xi)|. \tag{6.36}$$

This follows by similar arguments as in the proof of Proposition 6.12. □

6.7 Semiclassical calculus

We go back to $\hbar$. We will write $\mathrm{Op}_\hbar$ for the quantization depending on $\hbar$, that is

$$\mathrm{Op}(b)(x,y) = (2\pi\hbar)^{-d}\int \mathrm{d}p b\Big(\frac{x+y}{2},p\Big)\mathrm{e}^{\frac{\mathrm{i}(x-y)p}{\hbar}}. \tag{6.37}$$

Theorem 6.14. *Let $a,b\in S_{00}^0$. Then there exist $c_0,\dots,c_n\in S_{0,0}^0$ and $\hbar\mapsto r_\hbar\in S_{00}^0$ such that*

$$\mathrm{Op}_\hbar(a)\mathrm{Op}_\hbar(b)=\sum_{j=0}^n \hbar^j\mathrm{Op}_\hbar(c_j)+\hbar^{n+1}\mathrm{Op}_\hbar(r_\hbar),$$

$$\big|\partial_x^\alpha\partial_p^\beta\partial_\hbar^k r_\hbar\big|\leq C_{\alpha,\beta,k}.$$

Besides,

$$c_0=ab,\quad c_1=\frac{\mathrm{i}}{2}\{a,b\}.$$

If in addition a or b is 0 on an open set $\Theta\subset\mathbb{R}^d\oplus\mathbb{R}^d$, then so are $c_0,\dots,c_n$.

Proof. We Taylor expand the Moyal product:

$$a\star b(x,p) := \sum_{j=0}^n\frac{\big(\frac{\mathrm{i}}{2}\hbar(D_{p_1}D_{x_2}-D_{x_1}D_{p_2})\big)^j}{j!}a(x_1,p_1)b(x_2,p_2)\Big|_{\substack{x:=x_1=x_2,\\ p:=p_1=p_2.}} \tag{6.38}$$

$$+\int_0^1\mathrm{d}\tau\frac{\big(\frac{\mathrm{i}}{2}\hbar(D_{p_1}D_{x_2}-D_{x_1}D_{p_2})\big)^{n+1}(1-\tau)^n}{n!}\mathrm{e}^{\frac{\mathrm{i}}{2}\hbar\tau(D_{p_1}D_{x_2}-D_{x_1}D_{p_2})}a(x_1,p_1)b(x_2,p_2)\Big|_{\substack{x:=x_1=x_2,\\ p:=p_1=p_2.}}$$

Then we use Proposition 6.12 to estimate the remainder. □

Theorem 6.15. *Let $b\in S_{0,0}^0$ and $b(x,p)\neq 0$, $(x,p)\in\mathbb{R}^{2d}$. Then for small enough $\hbar$ the operator $\mathrm{Op}_\hbar(b)$ is invertible and there exist $c_0,c_2,\dots,c_{2n}\in S$ and $\hbar\mapsto r_\hbar\in S$ such that*

$$\mathrm{Op}_\hbar(b)^{-1}=\sum_{j=0}^m\hbar^{2j}\mathrm{Op}_\hbar(c_{2j})+\hbar^{2m+2}\mathrm{Op}_\hbar(r_\hbar),$$

$$\big|\partial_x^\alpha\partial_p^\beta\partial_\hbar^k r_\hbar\big|\leq C_{\alpha,\beta,k}.$$

Besides,

$$c_0=b^{-1}.$$

As a corollary of the above theorem, for any neighborhood of the image of b there exists $\hbar_0$ such that, for $|\hbar|\leq\hbar_0$, $\mathrm{sp}\,\big(\mathrm{Op}_\hbar(b)\big)$ is contained in this neighborhood.

Theorem 6.16. *1. Let $b \in S^0_{00}$ and f be a function holomorphic on a neighborhood of the image of b. Then for small enough $\hbar$ the function f is defined on* $\mathrm{sp}\left(\mathrm{Op}_\hbar(b)\right)$ *and there exist $c_0, c_2, \dots, c_{2n} \in S$ and $\hbar \mapsto r_\hbar \in S$ such that*

$$f\Big(\mathrm{Op}_\hbar(b)\Big) = \sum_{j=0}^{n} \hbar^{2j} \mathrm{Op}_\hbar(c_{2j}) + \hbar^{2n+2} \mathrm{Op}_\hbar(r_\hbar),$$

$$\left|\partial_x^\alpha \partial_p^\beta \partial_\hbar^k r_\hbar\right| \leq C_{\alpha,\beta,k}.$$

Besides,

$$c_0 = f \circ b.$$

2. *The same conclusion holds if f is smooth and b is real, and we use the functional calculus for self-adjoint operators.*

6.8 Inequalities

Lemma 6.17. (1) *Let $b \in S^0_{00}$ and $\mathrm{Op}(b) = \mathrm{Op}^{a^*,a}(b^+)$. Then $b^+ \in S^0_{00}$ and $b - b^+ = O(\hbar)$ in S^0_{00}*

(2) *Let $b^- \in S^0_{00}$ and $\mathrm{Op}^{a,a^*}(b^-) = \mathrm{Op}(b)$. Then $b \in S^0_{00}$ and $b^- - b = O(\hbar)$ in S^0_{00}.*

Proof. We use

$$b^+ = \mathrm{e}^{\frac{\hbar}{4}(\partial_x^2 + \partial_p^2)} b, \tag{6.39}$$

$$b = \mathrm{e}^{\frac{\hbar}{4}(\partial_x^2 + \partial_p^2)} b^-, \tag{6.40}$$

and the fact that

$$\mathrm{e}^{\frac{\hbar}{4}(\partial_x^2 + \partial_p^2)} b - b = \frac{\hbar}{4} \int_0^1 \mathrm{e}^{\frac{\hbar}{4}\tau(\partial_x^2 + \partial_p^2)} (\partial_x^2 + \partial_p^2) b \mathrm{d}\tau$$

is of the order $\hbar$ as a map on S^0_{00}. □

Theorem 6.18 (Sharp Gaarding Inequality)**.** *Let $b \in S^0_{00}$ be positive. Then*

$$\mathrm{Op}(b) \geq -C\hbar.$$

Proof. Let b_0 be the Wick symbol of $\mathrm{Op}(b)$, that is,

$$\mathrm{Op}^{a^*,a}(b_0) = \mathrm{Op}(b). \tag{6.41}$$

Then, by Thm 6.17 (1), we have $b_0 \in S^0_{00}$ and $b_0 - b = O(\hbar)$ in S^0_{00}. Besides,

$$\mathrm{Op}(b_0) = \mathrm{Op}^{a,a^*}(b). \tag{6.42}$$

Now

$$\mathrm{Op}(b) = \mathrm{Op}(b_0) + \mathrm{Op}(b - b_0) = \mathrm{Op}^{a,a^*}(b) + O(\hbar). \tag{6.43}$$

The first term on the right of (6.43) is positive, because it is the anti-Wick quantization of a positive symbol. □

Theorem 6.19 (Fefferman-Phong Inequality)**.** *Let $b \in S_{00}^0$ be positive. Then*

$$\mathrm{Op}_\hbar(b) \geq -C\hbar^2.$$

We will not give a complete proof. We will only note that the inequality follows by basic calculus if we assume that

$$b = \sum_{j=1}^{k} c_j^2$$

for real $c_j \in S_{00}^0$. We note also that the Sharp Gaarding inequality is true for matrix valued symbols, with the same proof. This is not the case of the Fefferman-Phong Inequality.

6.9 Semiclassical asymptotics of the dynamics

Theorem 6.20 (Egorov Theorem)**.** *Let h be the sum of a polynomial of second order and a S_{00}^0 function.*

(1) *Let $x(t), p(t)$ solve the Hamilton equations with the Hamiltonian h and the initial conditions $x(0), p(0)$. Then*

$$\gamma_t(x(0), p(0)) = \big(x(t), p(t)\big)$$

defines a symplectic (in general, nonlinear) transformation which preserves S_{00}^0.

(2) *Let $b \in S_{00}^0$. Then there exist $b_{t,2j} \in S_{00}^0$, $j = 0, 1, \dots,$ such that for $|t| \leq t_0$*

$$\mathrm{e}^{\frac{\mathrm{i}t}{\hbar}\mathrm{Op}(h)}\mathrm{Op}(b)\mathrm{e}^{-\frac{\mathrm{i}t}{\hbar}\mathrm{Op}(h)} - \sum_{j=0}^{n} \mathrm{Op}\big(\hbar^{2j} b_{t,2j}\big) = O(\hbar^{2n+2}). \tag{6.44}$$

Moreover,

$$b_{t,0}(x, p) = b\big(\gamma_t^{-1}(x, p)\big) \tag{6.45}$$

and $\mathrm{supp} b_{t,2j} \subset \gamma_t \mathrm{supp} b$*, $j = 0, 1, \dots$.*

Proof. Let us prove (2). We make an ansatz

$$\mathrm{e}^{\frac{\mathrm{i}t}{\hbar}\mathrm{Op}(h)}\mathrm{Op}(b)\mathrm{e}^{-\frac{\mathrm{i}t}{\hbar}\mathrm{Op}(h)} = \sum_{j=0}^{n} \mathrm{Op}\big(\hbar^{2j} b_{t,2j}\big) + \hbar^{2n+2}\mathrm{Op}(r_{t,2n+2,\hbar}), \tag{6.46}$$

$$b_{t,0}\Big|_{t=0} = b, \quad b_{t,2j}\Big|_{t=0} = 0, \quad j = 1, \dots, n; \quad r_{t,2n+2,\hbar}\Big|_{t=0} = 0. \tag{6.47}$$

We have

$$\begin{aligned}
& -\frac{\mathrm{d}}{\mathrm{d}t}\hbar^{2n+2}\mathrm{e}^{\frac{-\mathrm{i}t}{\hbar}\mathrm{Op}(h)}\mathrm{Op}\big(r_{t,2n+2,\hbar}\big)\mathrm{e}^{\frac{\mathrm{i}t}{\hbar}\mathrm{Op}(h)} \\
= \quad & \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Op}\big(b\big) - \frac{\mathrm{d}}{\mathrm{d}t}\hbar^{2n+2}\mathrm{e}^{\frac{-\mathrm{i}t}{\hbar}\mathrm{Op}(h)}\mathrm{Op}\big(r_{t,2n+2,\hbar}\big)\mathrm{e}^{\frac{\mathrm{i}t}{\hbar}\mathrm{Op}(h)} \\
= \quad & \frac{\mathrm{d}}{\mathrm{d}t}\sum_{j=0}^{n}\hbar^{2j}\mathrm{e}^{\frac{-\mathrm{i}t}{\hbar}\mathrm{Op}(h)}\mathrm{Op}\big(b_{t,2j}\big)\mathrm{e}^{\frac{\mathrm{i}t}{\hbar}\mathrm{Op}(h)} \\
= \quad & \sum_{j=0}^{n}\hbar^{2j}\mathrm{e}^{\frac{-\mathrm{i}t}{\hbar}\mathrm{Op}(h)}\Big(-\frac{\mathrm{i}}{\hbar}\big[\mathrm{Op}(h), \mathrm{Op}\big(b_{t,2j}\big)\big] + \mathrm{Op}\big(\frac{\mathrm{d}}{\mathrm{d}t}b_{t,2j}\big)\Big)\mathrm{e}^{\frac{\mathrm{i}t}{\hbar}\mathrm{Op}(h)}
\end{aligned}$$

The $j$the term in the above sum is expanded up to the order $\hbar^{2n+2}$:

$$\hbar^{2j}\mathrm{e}^{\frac{-\mathrm{i}t}{\hbar}\mathrm{Op}(h)}\mathrm{Op}\Big(\{h,b_{t,2j}\}+\sum_{k=1}^{n-j}\hbar^{2k}c_{t,2j,2k}+\hbar^{2n+2-2j}d_{t,2j,2n+2-2j,\hbar}+\frac{\mathrm{d}}{\mathrm{d}t}b_{t,2j}\Big)\mathrm{e}^{\frac{\mathrm{i}t}{\hbar}\mathrm{Op}(h)}.$$

Collecting terms of the order $\hbar^{2j}$ we obtain equations

$$\frac{\mathrm{d}}{\mathrm{d}t}b_{t,2j}=\{b_{t,2j},h\}+f_{t,2j},\quad j=0,\dots,n \tag{6.48}$$

where

$$f_{t,0}:=0, \tag{6.49}$$

$$f_{t,2j}:=-\sum_{i=0}^{j-1}c_{t,2i,2j-2i},\quad j=1,\dots,n, \tag{6.50}$$

are given by differential operators acting on $b_{t,0},\dots,b_{t,2j-2}$. (6.48) with initial conditions (6.47) are solved by

$$b_{t,0}(x,p):=b\big(\gamma_t^{-1}(x,p)\big), \tag{6.51}$$

$$b_{t,2j}(x,p):=\int_0^t f_{t-s,2j}\big(\gamma_s^{-1}(x,p)\big)\mathrm{d}s. \tag{6.52}$$

Thus

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{\frac{-\mathrm{i}t}{\hbar}\mathrm{Op}(h)}\mathrm{Op}\big(r_{t,2n+2,\hbar}\big)\mathrm{e}^{\frac{\mathrm{i}t}{\hbar}\mathrm{Op}(h)}\quad=\quad\mathrm{Op}(g_{t,2n+2,\hbar}),$$

where $g_{t,2n+2,\hbar}$ is an explicit function of $b_{t,0},\dots,b_{t,2n}$ of order 0 in $\hbar$. Integrating (6.53) from 0 to t we obtain the estimate (6.44). □

6.10 Algebra of semiclassical operators

We say that $]0,1[\ni\hbar\mapsto b_\hbar\in S_{00}^0$ is an *admissible semiclassical symbol* of order m if for any n there exist $b_m,b_{m-1},\dots,b_{-n}\in S_{00}^0$ and $\hbar\mapsto r_\hbar\in S_{00}^0$ is such that for any n

$$b_\hbar=\sum_{j=-n}^{m}\hbar^{-j}b_j+r_{\hbar,-n-1}$$

$$\big|\partial_x^\alpha\partial_p^\beta\partial_\hbar^k r_{\hbar,-n-1}\big|\leq\hbar^{n+1}C_{\alpha,\beta,k}.$$

Note that the sequence $b_m,,b_{m-1},\dots$ is uniquely defined by $b_\hbar$ (does not depend on n).

Let $\Theta\subset\mathbb{R}^d\oplus\mathbb{R}^d$ be closed. We say that $b_\hbar$ is $O(\hbar^\infty)$ outside Θ if $b_m,b_{m-1},\dots=0$ outside Θ.

Let $S_{00,\mathrm{sc}}^{0,m}$ denote the space of admissible semiclassical symbols and $\Psi_{00,\mathrm{sc}}^{0,m}$ the set of their semiclassical quantizations. We write $S_{00,\mathrm{sc}}^{0,m}(\Theta)$ for the space of symbols that vanish outside Θ and $\Psi_{00,\mathrm{sc}}^{0,m}(\Theta)$ for their quantizations.

Note that if $a, b \in S^0_{00}$ are symbols that do not depend on $\hbar$, then $a \star b$ depends on $\hbar$ and is an admissible symbol of order 0.

Clearly,

$$\Psi^{0,\infty}_{00,\mathrm{sc}} := \bigcup_{m=-\infty}^{\infty} \Psi^{0,m}_{00,\mathrm{sc}}$$

is a $*$-algebra with gradation closed wrt taking inverses of elliptic elements and functional calculus in the sense described in Theorem 6.16. $\Psi^{0,\infty}_{00,\mathrm{sc}}(\Theta)$ are ideals in $\Psi^{0,\infty}_{00,\mathrm{sc}}$.

The ideal

$$\Psi^{0,-\infty}_{00,\mathrm{sc}} := \bigcap_{m=-\infty}^{\infty} \Psi^{0,m}_{00,\mathrm{sc}}$$

consists of operators of the order $O(\hbar^\infty)$. Note that $\Psi^0_{00,\mathrm{sc}}/\Psi^{0,-\infty}_{00,\mathrm{sc}}$ is isomorphic to a subalgebra of the formal semiclassical algebra $\Psi[[\hbar]]$.

6.11 Frequency set

Let $\hbar \mapsto \psi_\hbar \in L^2(\mathcal{X})$. Let $(x_0, p_0) \in \mathbb{R}^d \oplus \mathbb{R}^d$.

Theorem 6.21. *The following conditions are equivivlent:*

(1) *There exists $\chi \in C^\infty_\mathrm{c}$ with $\chi(x_0) \neq 0$ and a neighborhood $\mathcal{W}$ of p_0 such that*

$$\big(\mathcal{F}_\hbar(\chi\psi_\hbar)\big)(p) = O(\hbar^\infty), \quad p \in \mathcal{W}.$$

(2) *There exists $b \in C^\infty_\mathrm{c}(\mathbb{R}^d \oplus \mathbb{R}^d)$ such that $b(x_0, p_0) \neq 0$ and*

$$\|\mathrm{Op}_\hbar(b)\psi_\hbar\| = O(\hbar^\infty).$$

(3) *There exists a neighborhood $\mathcal{V}$ of (x_0, p_0) such that for all $c \in C^\infty_\mathrm{c}(\mathcal{U})$*

$$\|\mathrm{Op}_\hbar(c)\psi_\hbar\| = O(\hbar^\infty).$$

The set of points in $\mathbb{R}^d \oplus \mathbb{R}^d$ that do not satisfy the conditions of Theorem 6.21 is called the frequency set of $\hbar \mapsto \psi_\hbar$ and denoted $\mathrm{FS}(\psi_\hbar)$.

Note that we can replace the Weyl quantization by the x, p or p, x quantization in the definition of the frequency set.

6.12 Properties of the frequency set

Theorem 6.22. *Let $a \in S^0_{00}$. Then*

$$\mathrm{FS}\left(\mathrm{Op}_\hbar(a)\psi_\hbar\right) = \mathrm{supp}(a) \cap FS(\psi_\hbar).$$

Theorem 6.23. *Let $h \in S^0_{00} + \mathrm{Pol}^{\leq 2}$ be real. Let $t \mapsto \gamma_t$ be the Hamiltonian flow generated by h. Then*

$$\mathrm{FS}(\mathrm{e}^{\mathrm{i}t\mathrm{Op}_\hbar(h)}\psi_\hbar) = \gamma_t\left(FS(\psi_\hbar)\right).$$

Theorem 6.24. *Let*

$$\psi_\hbar(x) = a(x)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)}.$$

Then

$$\mathrm{FS}(\psi_\hbar) \subset \{x \in \mathrm{supp}a,\ p = \nabla S(x)\}. \tag{6.53}$$

Proof. We apply the *nonstationary method*. Let $p \neq \partial_x S(x)$ on the support of $b \in C_\mathrm{c}^\infty(\mathbb{R}^d \oplus \mathbb{R}^d)$. Let $(2\pi\hbar)^{-\frac{d}{2}}\mathcal{F}_\hbar$ denote the unitary semiclassical Fourier transformation. Then

$$\Big((2\pi\hbar)^{-\frac{d}{2}}\mathcal{F}_\hbar\mathrm{Op}_\hbar^{p,x}(b)\psi_\hbar\Big)(p) \quad = \quad (2\pi\hbar)^{-\frac{d}{2}}\int \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}xp}b(p,x)a(x)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)}\mathrm{d}x. \tag{6.54}$$

Let

$$T := (p - \partial_x S(x))^{-2}(p - \partial_x S(x))\partial_x.$$

Let

$$T^\# = \partial_x(p - \partial_x S(x))^{-2}(p - \partial_x S(x))$$

be the transpose of T. Clearly,

$$-\mathrm{i}\hbar T\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(S(x)-xp)} = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(S(x)-xp)}. \tag{6.55}$$

Therefore, (6.54) equals

$$(-\mathrm{i}\hbar)^n(2\pi\hbar)^{-\frac{d}{2}}\int b(p,x)a(x)T^n\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(S(x)-xp)}\mathrm{d}x \tag{6.56}$$

$$= \quad (-\mathrm{i}\hbar)^n(2\pi\hbar)^{-\frac{d}{2}}\int \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(S(x)-xp)}T^{\#n}b(p,x)a(x)\mathrm{d}x = O(\hbar^{n-\frac{d}{2}}). \tag{6.57}$$

Thus (6.53) holds. □

In practice, we usually have the equality in (6.53), because by the stationary phase method we can compute its leading behavior.

7 Spectral asymptotics

7.1 Trace of functions of operators in the pseudodifferential setting

We have already seen that for smooth functions f and symbols $b \in S_{00}^0$ we have

$$f\big(\mathrm{Op}(b)\big) = \mathrm{Op}(f \circ b) + O(\hbar^2). \tag{7.1}$$

Note that this is especially easy to see for polynomials: It follows from (3.49) that

$$\mathrm{Op}(b)^n = \mathrm{Op}(b^n) + O(\hbar^2).$$

One can extend (7.1) to more general classes of symbols and unbounded operators by using the resolvent.

Recall that

$$\mathrm{Tr}\mathrm{Op}(a) \quad = \quad (2\pi\hbar)^{-d} \int a(x,p)\mathrm{d}x\mathrm{d}p.$$

Therefore, we can expect that under appropriate assumptions

$$\begin{aligned} \mathrm{Tr} f\big(\mathrm{Op}(b)\big) &= \mathrm{Tr}\Big(\mathrm{Op}(f\circ b) + O(\hbar^2)\Big) \\ &= (2\pi\hbar)^{-d}\int f\big(b(x,p)\big)\mathrm{d}x\mathrm{d}p + O(\hbar^{-d+2}). \end{aligned} \tag{7.2}$$

7.2 Weyl asymptotics from pseudodifferential calculus

For a bounded from below self-adjoint operator H set

$$N_\mu(H) := \#\{\text{eigenvalues of } H \text{ counted with multiplicity } \leq \mu\} \tag{7.3}$$

$$= \mathrm{Tr}\mathbb{1}_{]-\infty,\mu]}(H). \tag{7.4}$$

In particular, we can try to use $f = \mathbb{1}_{]-\infty,\mu]}$ in (7.2). It is too optimistic to expect

$$\mathbb{1}_{]-\infty,\mu]}(\mathrm{Op}(h)) = \mathrm{Op}\big(\mathbb{1}_{]-\infty,\mu]}(h)\big) + O(\hbar^2). \tag{7.5}$$

After all the step function is not nice – it is not even continuous. If there is a gap in the spectrum around μ, one can try to smooth it out. Therefore, there is a hope at least for some weaker error term instead of $O(\hbar^2)$. If (7.5) were true, then we could expect

$$N_\mu\big(\mathrm{Op}(h)\big) \quad = \quad (2\pi\hbar)^{-d}\int_{h(x,p)\leq\mu} \mathrm{d}x\mathrm{d}p + O(\hbar^{-d+2}). \tag{7.6}$$

Define

$$(E)_+ := \begin{cases} E, & E > 0, \\ 0, & E < 0. \end{cases}, \qquad (E)_- := \begin{cases} 0, & E > 0, \\ -E, & E < 0. \end{cases}.$$

For instance, if V satisfies $V - \mu > 0$ outside a compact set then

$$\begin{aligned} N_\mu(-\hbar^2\Delta + V(x)) &\simeq (2\pi\hbar)^{-d} \int\limits_{p^2+V(x)\leq\mu} \mathrm{d}x\mathrm{d}p + O(\hbar^{-d+2}) \\ &= (2\pi\hbar)^{-d} \int\limits_{|p|\leq\sqrt{(V(x)-\mu)_-}} \mathrm{d}x\mathrm{d}p + O(\hbar^{-d+2}) \\ &= (2\pi\hbar)^{-d} c_d \int (V(x)-\mu)_-^{\frac{d}{2}}\mathrm{d}x + O(\hbar^{-d+2}), \end{aligned} \tag{7.7}$$

where the volume of the ball of radius r in d dimensions is $c_d r^d$.

Asymptotics of the form (7.7) are called the *Weyl asymptotics*. In practice the error term $O(\hbar^{-d+2})$ is too optimistic and one gets something worse (but hopefully at least $o(\hbar^{-d})$).

7.3 Weyl asymptotics by the Dirichlet/Neumann bracketing

We will show that if V is continuous potential with $V-\mu>0$ outside a compact set then

$$N_\mu(-\hbar^2\Delta+V(x))\simeq(2\pi\hbar)^{-d}c_d\int_{V(x)\le\mu}(V(x)-\mu)_-^{\frac{d}{2}}\mathrm{d}x+o(\hbar^{-d}).\tag{7.8}$$

This is an old result of Weyl.

Here are the tools that we will use:

$$A\le B\ \Rightarrow\ N_\mu(A)\ge N_\mu(B),$$

$$N_\mu(A\oplus B)=N_\mu(A)+N_\mu(B).$$

To simplify we will assume that $d=1$.

Let $\Delta_D=\Delta_{[0,L],D}$, resp. $\Delta_N=\Delta_{[0,L],N}$ denote the Dirichlet, resp. Neumann Laplacian on $L^2[0,L]$. This means both Δ_D and Δ_N equal ∂_x^2 on their domains:

$$\mathcal{D}(\Delta_D):=\{f\in L^2[0,L]\mid f''\in L^2[0,L],\ f(0)=f(L)=0\},\tag{7.9}$$
$$\mathcal{D}(\Delta_N):=\{f\in L^2[0,L]\mid f''\in L^2[0,L],\ f'(0)=f'(L)=0\}.\tag{7.10}$$

For $\alpha\in\mathbb{R}$ let $[\alpha]$ denote the largest integer $\le\alpha$,

Lemma 7.1. *Δ_D and Δ_N are selfadjoint operators such that*

$$\begin{aligned}N_\mu\big(-\hbar^2\Delta_D\big)&=[L(\pi\hbar)^{-1}(\mu)_+^{1/2}],\\ N_\mu\big(-\hbar^2\Delta_N\big)&=[L(\pi\hbar)^{-1}(\mu)_+^{1/2}]+\theta(\mu).\end{aligned}$$

Proof. The eigenfunctions and the spectrum of Δ_D, resp. Δ_N are

$$\begin{aligned}&\sin\frac{\pi nx}{L},\qquad \frac{\hbar^2\pi^2n^2}{L^2},\quad n=1,2,\dots;\\ &\cos\frac{\pi nx}{L},\qquad \frac{\hbar^2\pi^2n^2}{L^2},\quad n=0,1,2,\dots.\end{aligned}$$

Thus the last eigenvalue has the number $n=[L(\hbar\pi)^{-1}(\mu)_+^{1/2}]$. $\square$

Lemma 7.2. *Both $-\Delta_D$ and $-\Delta_N$ are positive operators. More precisely, let $f\in L^2[0,L]$. Then*

$$-(f|\Delta_Df)=\begin{cases}\int_0^L|f'(x)|^2\mathrm{d}x, & f(0)=f(L)=0,\\ \infty, & f(0)\ne0\quad \text{or } f(L)\ne0;\end{cases}\tag{7.11}$$

$$-(f|\Delta_Nf)=\int_0^L|f'(x)|^2\mathrm{d}x.\tag{7.12}$$

Consequently, if $(f|\Delta_Df)<\infty$, then $(f|\Delta_Df)=(f|\Delta_Nf)$. Hence

$$-\Delta_N\le-\Delta_D.\tag{7.13}$$

Proof. We check that this is true for finite linear combinations of elements of the respective bases. Then we use an approximation argument. □

Divide $\mathbb{R}$ into intervals

$$I_{m,j} := \Big[(j-1/2)m^{-1}, (j+1/2)m^{-1}\Big].$$

Put at the borders of the intervals the Neumann/Dirichlet boundary conditions. The Neumann conditions lower the expectation value and the Dirichlet conditions increase them. Set

$$\begin{aligned}\overline{V}_{m,j} &= \sup\{V(x) \ : \ x \in I_{m,j}\},\\ \underline{V}_{m,j} &= \inf\{V(x) \ : \ x \in I_{m,j}\}.\end{aligned}$$

We have

$$\begin{aligned} & \bigoplus_{j\in\mathbb{Z}} \Big(-\hbar^2\Delta_{I_{m,j},N} + \underline{V}_{m,j}\Big) \\ \leq \ -\hbar^2\Delta + V(x) \ \leq \ & \bigoplus_{j\in\mathbb{Z}} \Big(-\hbar^2\Delta_{I_{m,j},D} + \overline{V}_{m,j}\Big).\end{aligned}$$

Hence,

$$\begin{aligned} & \sum_{j\in\mathbb{Z}} N_\mu\Big(-\hbar^2\Delta_{I_{m,j},N} + \underline{V}_{m,j}\Big) \\ \geq \ N_\mu\Big(-\hbar^2\Delta + V(x)\Big) \ \geq \ & \sum_{j\in\mathbb{Z}} N_\mu\Big(-\hbar^2\Delta_{I_{m,j},D} + \overline{V}_{m,j}\Big).\end{aligned}$$

Therefore,

$$\begin{aligned} & \sum_{j\in\mathbb{Z}} m^{-1}(\hbar\pi)^{-1}(\underline{V}_{m,j}-\mu)_-^{1/2} + \sum_{j\in\mathbb{Z}} \theta\big(\mu - \underline{V}_{m,j}\big) \\ \geq \ N_\mu\Big(-\hbar^2\Delta + V(x)\Big) \ \geq \ & \sum_{j\in\mathbb{Z}} m^{-1}(\hbar\pi)^{-1}(\overline{V}_{m,j}-\mu)_-^{1/2}.\end{aligned}$$

Using the fact that $(V-\mu)_-$ has a compact support, we can estimate

$$\sum_{j\in\mathbb{Z}} \theta\big(\mu - \underline{V}_{m,j}\big) \ \leq \ mC.$$

By properties of Riemann sums we can find m_ϵ such that for $m \geq m_\epsilon$

$$\Big|\sum_{j\in\mathbb{Z}} m^{-1}(\underline{V}_{m,j}-\mu)_-^{1/2} - \int (V(x)-\mu)_-^{1/2}\mathrm{d}x\Big| \ < \ \epsilon/3, \tag{7.14}$$

$$\Big|\sum_{j\in\mathbb{Z}} m^{-1}(\overline{V}_{m,j}-\mu)_-^{1/2} - \int (V(x)-\mu)_-^{1/2}\mathrm{d}x\Big| \ < \ \epsilon/3. \tag{7.15}$$

Therefore,

$$\left|N_\mu\Big(-\hbar^2\Delta+V(x)\Big)-\frac{1}{\hbar\pi}\int(V(x)-\mu)_-^{1/2}\mathrm{d}x\right| \quad < \quad \frac{2\epsilon}{\hbar\pi3}+\frac{Cm_\epsilon}{\pi}. \tag{7.16}$$

Hence the right hand side of (7.16) is $o(\hbar^{-1})$. This proves (7.8)

If we assume that V is differentiable, then m_ϵ can be assumed to be $C_0\epsilon^{-1}$. Then we can optimize and set $\epsilon=\sqrt{\hbar}$. This allows us to replace $o(\hbar^{-1})$ by $O(\hbar^{-1/2})$.

7.4 Energy of many fermion systems

Consider fermions with the 1-particle space $\mathcal{H}$ is spanned by an orthonormal basis $\Phi_1,\Phi_2,\dots$. The n-particle fermionic space $\wedge^n\mathcal{H}$ is spanned by Slater determinants

$$\Psi_{i_1,\dots,i_n}:=\frac{1}{\sqrt{n!}}\Phi_{i_1}\wedge\cdots\wedge\Phi_{i_n},\quad i_1<\cdots<i_n.$$

Suppose that we have noninteracting fermions with the 1-particle Hamiltonian H. Then the Hamiltonian on the N-particle space is

$$\mathrm{d}\Gamma^n(H)=H\otimes\mathbb{1}\cdots\otimes\mathbb{1}+\cdots+\mathbb{1}\otimes\cdots\otimes\mathbb{1}\otimes H\Big|_{\Lambda^n\mathcal{H}}.$$

Suppose that $E_1<E_2<\dots$ are the eigenvalues of H in the ascending order and $\Phi_1,\Phi_2,\dots$ are the corresponding normalized eigenvectors. This means that the full Hamiltonian $\mathrm{d}\Gamma^n(H)$ acts on Slater determinants as

$$\mathrm{d}\Gamma^n(H)\Psi_{i_1,\dots,i_n}=(E_{i_1}+\cdots+E_{i_1})\Psi_{i_1,\dots,i_n}.$$

For simplicity we assume that eigenvalues are nondegenerate. Then the ground state of the system is the Slater determinant

$$\Psi_{1,\dots,n}=\frac{1}{\sqrt{n!}}\Phi_1\wedge\cdots\wedge\Phi_n. \tag{7.17}$$

The ground state energy is $E_1+\cdots+E_n$.

If B is a 1-particle observable, then on the n-particle space it is given by

$$\mathrm{d}\Gamma^n(B)=B\otimes\mathbb{1}\cdots\otimes\mathbb{1}+\cdots+\mathbb{1}\otimes\cdots\otimes\mathbb{1}\otimes B\Big|_{\Lambda^n\mathcal{H}}.$$

Let $\Psi\in\Lambda^n\mathcal{H}$. The expectation value of $\mathrm{d}\Gamma^n(B)$ in the n-fermionic state Ψ is given by

$$\big(\Psi\big|\mathrm{d}\Gamma^n(B)\Psi\big)=\mathrm{Tr}B\gamma_\Psi$$

where γ_Ψ is the so-called *reduced 1-particle density matrix*. Note that $0\le\gamma_\Psi\le\mathbb{1}$ and $\mathrm{Tr}\gamma_\Psi=n$. The reduced 1-particle density matrix of the Slater determinant (7.17) $\Psi_{1,\dots,n}$ is the projection onto the space spanned by $\Phi_1,\dots,\Phi_n$. Hence, the reduced 1-particle density matrix of the ground state is $\gamma=\mathbb{1}_{]-\infty,\mu]}(H)$.

In practice it is often more convenient as the basic parameter to use the chemical potential μ instead of the number of particles n. Then we can expect that the 1-particle density matrix of the ground state is given by $1\!\!1_{]-\infty,\mu]}(H)$, where we find μ from the relation

$$\mathrm{Tr} 1\!\!1_{]-\infty,\mu]}(H) = n.$$

Suppose that the 1-particle space is $L^2(\mathbb{R}^d)$. Then the 1-particle reduced density matrix can be represented by its kernel $\gamma_\Psi(x,y)$. Explicitly,

$$\gamma_\Psi(x,y) = \int \mathrm{d}x_2 \cdots \int \mathrm{d}x_n \overline{\Psi(x,x_2,\cdots,x_n)}\Psi(y,x_2,\cdots,x_n). \tag{7.18}$$

We are particularly interested in expectation values of the position. For position independent observables we do not need to know the full reduced density matrix, but only the density:

$$\mathrm{Tr}\gamma_\Psi f(\hat{x}) = \int \rho_\Psi(x) f(x),$$

where

$$\rho_\Psi(x) := \gamma_\Psi(x,x).$$

Note that

$$\int \rho_\Psi(x)\mathrm{d}x = n. \tag{7.19}$$

If $\gamma = \mathrm{Op}(g)$, then

$$\mathrm{Tr}\gamma_\Psi f(\hat{x}) = (2\pi\hbar)^{-d} \int\int g(x,p) f(x)\mathrm{d}x\mathrm{d}p.$$

Hence

$$\rho_\Psi(x) = (2\pi\hbar)^{-d} g(x,p)\mathrm{d}p.$$

Suppose now that the 1-particle Hamiltonian is $H = \mathrm{Op}(h)$. Remember that then the symbol of $1\!\!1_{]-\infty,\mu]}(H)$ is approximately given by

$$1\!\!1_{]-\infty,\mu]}\big(h(x,p)\big).$$

The corresponding density is

$$\rho(x) \approx (2\pi\hbar)^{-d} \int 1\!\!1_{]-\infty,\mu]}\big(h(x,p)\big)\mathrm{d}p = (2\pi\hbar)^{-d} \int\limits_{h(x,p)\leq\mu} \mathrm{d}p.$$

Let $c_d r^d$ be the volume of the ball of radius r. If $h(x,p) = p^2 + v(x)$, then

$$\rho(x) \quad\approx\quad (2\pi\hbar)^{-d} \int\limits_{p^2+v(x)\leq\mu} \mathrm{d}p = (2\pi\hbar)^{-d} c_d (v(x)-\mu)_-^{\frac{d}{2}}.$$

Let us compute the kinetic energy

$$\begin{aligned}
\mathrm{Tr}\hat{p}^2 1\!\!1_{]-\infty,\mu]}(H) &\approx (2\pi\hbar)^{-d} \int\int_{p^2+v(x)<\mu} p^2 \mathrm{d}x\mathrm{d}p \\
&= (2\pi\hbar)^{-d} \int \mathrm{d}x \int_{|p|<(v(x)-\mu)_-^{\frac{1}{2}}} dc_d |p|^{d+1} \mathrm{d}|p| \\
&= (2\pi\hbar)^{-d} \int \mathrm{d}x \frac{dc_d}{d+2} (v(x)-\mu)_-^{\frac{d+2}{2}} \\
&\approx (2\pi\hbar)^{-d} \frac{d}{d+2} c_d^{-2/d} \int \rho^{\frac{d+2}{d}}(x)\mathrm{d}x.
\end{aligned}$$

Thus if we know that ρ is the density of a ground state of a Schrödinger Hamiltonian, then we expect that the kinetic energy is given by the functional

$$E_{\mathrm{kin}}(\rho) := (2\pi\hbar)^{-d} \frac{d}{d+2} c_d^{-2/d} \int \rho^{\frac{d+2}{d}}(x)\mathrm{d}x. \tag{7.20}$$

Consider quantum fermions in an external potential V and interacting addition with the potential W. That is, we consider the Hamiltonian

$$\sum_{i=1}^{n} \left(p_i^2 + V(x_i)\right) + \sum_{1\leq i<j\leq n} W(x_i - x_j) \tag{7.21}$$

on the n-particle antisymmetric space $\wedge^n L^2(\mathbb{R}^d)$ (we drop the hats).

Let $\Psi \in \wedge^n L^2(\mathbb{R}^d)$. Clearly, the potential energy of a state with density ρ in the potential V is given by

$$\Big(\Psi | \sum_{1\leq i\leq n} V(x_i)\Psi\Big) = \int V(x)\rho_\Psi(x)\mathrm{d}x =: E_{\mathrm{pot}}(\rho_\Psi). \tag{7.22}$$

We can expect by classical arguments that for a state Ψ

$$\Big(\Psi | \sum_{1\leq i<j\leq n} W(x_i - x_j)\Psi\Big) \simeq \int\int W(x-y)\rho_\Psi(x)\rho_\Psi(y)\mathrm{d}x\mathrm{d}y =: E_{\mathrm{int}}(\rho_\Psi). \tag{7.23}$$

The Thomas-Fermi functional is given by the sum of (7.20), (7.22) and ((7.23) applied to an arbitrary positive ρ satisfying $\int \rho(x)\mathrm{d}x = n$:

$$\begin{aligned}
E_{\mathrm{TF}}(\rho) &:= E_{\mathrm{kin}}(\rho) + E_{\mathrm{pot}}(\rho) + E_{\mathrm{int}}(\rho) \qquad (7.24)\\
&= (2\pi\hbar)^{-d} \frac{d}{d+2} c_d^{-2/d} \int \rho^{\frac{d+2}{d}}(x)\mathrm{d}x \\
&\quad + \int V(x)\rho(x)\mathrm{d}x + \int\int W(x-y)\rho(x)\rho(y)\mathrm{d}x\mathrm{d}y. \qquad (7.25)
\end{aligned}$$

We expect that

$$\inf\Big\{E_{\mathrm{TF}}(\rho) \mid \rho \geq 0, \quad \int \rho(x)\mathrm{d}x = n\Big\} \tag{7.26}$$

approximates the ground state energy of (7.21).

8 Standard pseudodifferential calculus on $\mathbb{R}^d$

8.1 Comparison of algebras introduced so far

So far we introduced three kinds of "pseudodifferential algebras".

1. The algebra Ψ_{00}^0. It consists of operators on $L^2(\mathbb{R}^d)$ with symbols in $S_{00}^0(\mathbb{R}^d \oplus \mathbb{R}^d)$, that is, satisfying
$$|\partial_x^\beta \partial_p^\alpha b| \leq C_{\alpha,\beta}, \qquad \alpha, \beta.$$

2. The algebra $\Psi_{00,\mathrm{sc}}^{0,\infty}$. It consists of $\hbar$-dependent families of elements of Ψ_{00}^0, asymptotic to power series in $\hbar$ with coefficients in Ψ_{00}^0.

3. The algebra $\Psi^\infty[[\hbar]]$, that is formal power series in $\hbar$ with coefficients in $C^\infty(\mathbb{R}^d \oplus \mathbb{R}^d)$.

The algebra Ψ_{00}^0 consists of true operators on $L^2(\mathbb{R}^d)$. It is closed not only wrt the multiplication (as any algebra), but it is closed wrt several other operations. It is closed wrt various functional calculi, it is invariant wrt the symplectic group, and also wrt the dynamics generated by elements of this algebra. It has one drawback: it has no "small Planck constant". Therefore its utility is limited—the point of quantization is to use classical arguments for quantum operators, but this can be done only if the Planck constant is small.

The algebra $\Psi_{00,\mathrm{sc}}^{0,\infty}$ consists of true operators that depend on a Planck constant. It is closed wrt the multiplication, is closed wrt to taking various functions and wrt a dynamics of the form described in Egorov Theorem 6.20. Using this algebra we can make various interesting statements about true operators of the sort: "there exists $\hbar_0 > 0$ such that for $0 < \hbar < \hbar_0$ something happens". For instance: if the principal symbol is invertible, then for small $\hbar$ the operator is invertible. On the other hand, the definition of this algebra is quite ugly: we have the "remainder term" which has to be taken into account, even though it is "semiclassically small".

The algebra $\Psi^\infty[[\hbar]]$ is much "cleaner" than $\Psi_{00,\mathrm{sc}}^{0,\infty}$, at least from the purely algebraic point of view. You do not have an ugly remainder, you do not worry about estimates. However, it does not consist of true operators, only of "caricatures of operators". Nevertheless, it retains the essential structure of $\Psi_{00,\mathrm{sc}}^{0,\infty}$. Besides, it is probably useful as a pedagogical object.

There are some mathematicians who care only about formal algebras–for them algebras of the form $\Psi^\infty[[\hbar]]$ are OK. We prefer to think about true operators and use various algebras as tools.

The disadvantage of algebras 2. and 3. is that the Planck constant is external. In what follows we will describe algebras that possess a "natural effective Planck constant". These algebras come from the theory of partial differential operators. They are appropriate extentions of the algebra of differential operators with smooth coefficients.

8.2 Classes of symbols

In this section as a rule we will set $\hbar = 1$. The variable conjugate to x will be generically denoted ξ. We will not put hats on classical variabes to denote operators—thus x will denote both classical variable and the corresponding multiplication operator. The quantization of ξ will be denoted $D = -\mathrm{i}\partial_x$.

Let $m \in \mathbb{N}$. We define $S^m_{\mathrm{pol}}(\mathrm{T}^\# \mathbb{R}^d)$ to be the set of functions of the form

$$a(x, \xi) = \sum_{|\beta| \le m} a_\beta(x) \xi^\beta, \tag{8.1}$$

where for any α, β

$$|\partial_x^\alpha a_\beta| \le c_{\alpha,\beta}. \tag{8.2}$$

The subscript pol stands for *polynomial*.

Let $m \in \mathbb{R}$. We define $S^m(\mathrm{T}^\# \mathbb{R}^d)$ to be the set of functions $a \in C^\infty(\mathrm{T}^\# \mathbb{R}^d)$ such that for any α, β

$$|\partial_x^\alpha \partial_\xi^\beta a(x, \xi)| \le c_{\alpha,\beta} \langle \xi \rangle^{m - |\beta|}. \tag{8.3}$$

We say that a function $a(x, \xi)$ is homogeneous in ξ of degree m if $a(x, \lambda\xi) = \lambda^m a(x, \xi)$ for any $\lambda > 0$. Note that there are many such functions smooth outside of $\xi = 0$, for instance $|\xi|^m$, however they are rarely smooth at $\xi = 0$.

We set $S^m_{\mathrm{ph}}(\mathrm{T}^\# \mathbb{R}^d)$ to be the set of functions $a \in S^m(\mathrm{T}^\# \mathbb{R}^d)$ such that for any n there exist functions a_{m-k}, $k = 0, \dots, n$, homogeneous in ξ of degree $m - k$ such that

$$\begin{aligned}
|\partial_x^\alpha \partial_\xi^\beta a_{m-k}(x, \xi)| &\le c_{\alpha,\beta} |\xi|^{m-k-|\beta|}, \ |\xi| > 1, \\
\left| \partial_x^\alpha \partial_\xi^\beta \Big(a(x, \xi) - \sum_{k=0}^{n} a_{m-k}(x, \xi) \Big) \right| &\le c_{\alpha,\beta,n} |\xi|^{m-n-1}, \ |\xi| > 1.
\end{aligned}$$

We then write $a \simeq \sum_{k=0}^{\infty} a_{m-k}$, where a_{m-k} are uniquely determined. The subscript ph stands for *polyhomogeneous*.

We introduce also

$$S^{-\infty} := \bigcap_m S^m = \bigcap_m S^m_{\mathrm{ph}},$$

$$S^\infty := \bigcup_m S^m, \quad S^\infty_{\mathrm{ph}} := \bigcup_m S^m_{\mathrm{ph}}, \quad S^\infty_{\mathrm{pol}} := \bigcup_m S^m_{\mathrm{pol}}.$$

$S^\infty_{\mathrm{pol}}(\mathrm{T}^\# \mathbb{R}^d)$ is called the space of *symbols polynomial in* ξ.

$S^\infty_{\mathrm{ph}}(\mathrm{T}^\# \mathbb{R}^d)$ is called the space of *step* 1 *polyhomogeneous symbols*. Some mathematicians call them *classical symbols*, which has nothing to do with classical mechanics, and is related to the fact that this symbol class was used in "classic papers" from the 60's or 70's.

Elements of $S^m(\mathrm{T}^\# \mathbb{R}^d)$ are often just called *symbols of order* m, since this class is often regarded as the "most natural".

Clearly, for $m \in \mathbb{N}$, $S^m_{\mathrm{pol}} \subset S^m_{\mathrm{ph}}$. In fact, if $a(x, \xi)$ is of the form (8.1), then

$$a(x, \xi) = \sum_{n=0}^{m} a_{m-n}(x, \xi), \tag{8.4}$$

$$a_k(x, \xi) := \sum_{|\alpha| = k} a_\alpha(x) \xi^\alpha. \tag{8.5}$$

For any $m \in \mathbb{R}$, $S^m_{\mathrm{ph}} \subset S^m$.

Clearly, S^∞, S^∞_{ph} and S^∞_{pol} are commutative algebras with gradation.

$a \in S^m$ iff $a\langle\xi\rangle^k \in S^{m+k}$. Likewise, $a \in S^m_{\mathrm{ph}}$ iff $a\langle\xi\rangle^k \in S^{m+k}_{\mathrm{ph}}$.

The algebra S^∞_{ph} appears naturally if we want to compute $(1+\xi^2)^{-1}$, or $\sqrt{1+\xi^2}$. Clearly, we cannot do it inside S^∞_{pol}, however we can do it in the larger algebra S^∞_{ph}. We will discuss it further in the subsection about ellipticity.

8.3 Classes of pseudodifferential operators

We introduce the following classes of operators from $\mathcal{S}(\mathbb{R}^d)$ to $\mathcal{S}'(\mathbb{R}^d)$:

$$\Psi^m := \{\mathrm{Op}(a) \mid a \in S^m\}, \tag{8.6}$$
$$\Psi^m_{\mathrm{ph}} := \{\mathrm{Op}(a) \mid a \in S^m_{\mathrm{ph}}\}, \tag{8.7}$$
$$\Psi^m_{\mathrm{pol}} := \{\mathrm{Op}(a) \mid a \in S^m_{\mathrm{pol}}\}. \tag{8.8}$$

Lemma 8.1. $\mathrm{e}^{\frac{\mathrm{i}}{2}D_xD_\xi}$ *is bounded on* S^m.

Proof. Recall that in (6.35) we defined

$$S^k_{00} := \{f \in C^\infty(\mathbb{R}^n \oplus \mathbb{R}^k) \mid |\partial_x^\alpha \partial_\xi^\beta f| \leq C_{\alpha,\beta}\langle\xi\rangle^k\}. \tag{8.9}$$

By Proposition 6.13 $\mathrm{e}^{\frac{\mathrm{i}}{2}D_xD_\xi}$ is bounded on $S^k_{0,0}$. In particular,

Let $a \in S^m$. Then $\partial_x^\alpha \partial_\xi^\beta a \in S^{m-|\beta|} \subset S^{m-|\beta|}_{0,0}$. Now

$$\partial_x^\alpha \partial_\xi^\beta \mathrm{e}^{\frac{\mathrm{i}}{2}D_xD_\xi} a = \mathrm{e}^{\frac{\mathrm{i}}{2}D_xD_\xi} \partial_x^\alpha \partial_\xi^\beta a \in S^{m-|\beta|}_{00}. \tag{8.10}$$

Hence

$$|\partial_x^\alpha \partial_\xi^\beta \mathrm{e}^{\frac{\mathrm{i}}{2}D_xD_\xi} a| \leq C_{\alpha,\beta}\langle\xi\rangle^{m-|\beta|}. \tag{8.11}$$

□

Proposition 8.2.

$$\Psi^m := \{\mathrm{Op}^{x,\xi}(a) \mid a \in S^m\}, \tag{8.12}$$
$$\Psi^m_{\mathrm{ph}} := \{\mathrm{Op}^{x,\xi}(a) \mid a \in S^m_{\mathrm{ph}}\}, \tag{8.13}$$
$$\Psi^m_{\mathrm{pol}} := \{\mathrm{Op}^{x,\xi}(a) \mid a \in S^m_{\mathrm{pol}}\}. \tag{8.14}$$

Proof. Recall the transformation from the Weyl symbol to the Kohn-Nirenberg symbol:

$$\begin{aligned}\mathrm{e}^{\frac{\mathrm{i}}{2}D_\xi D_x} a(x,\xi) = &\sum_{j=0}^{n} \frac{\left(\frac{\mathrm{i}}{2}D_\xi D_x\right)^j}{j!} a(x,\xi) \\ &+ \int_0^1 \mathrm{d}\tau \frac{\left(\frac{\mathrm{i}}{2}D_\xi D_x\right)^{n+1}(1-\tau)^n}{n!} \mathrm{e}^{\frac{\mathrm{i}}{2}\tau D_\xi D_x} a(x,\xi).\end{aligned} \tag{8.15}$$

We need to show that $\mathrm{e}^{\frac{\mathrm{i}}{2}D_x D_\xi}$ is bounded on S^m, S^m_{ph} and S^m_{pol}. In the case of polynomial symbols the statement is obvious. For S^m it is proven in Lemma 8.1. For S^m_{ph} we can use the expansion (8.15). We note that the jth term of this expansion belongs to S^{m-j}_{ph} and the remainder using Lemma 8.1 can be proven to belong to S^{m-n-1}. □

8.4 Multiplication of pseudodifferential operators

The following lemma is proven in a similar way as the lemma 8.1:

Lemma 8.3. $\mathrm{e}^{\frac{\mathrm{i}}{2}(D_{\xi_1}D_{x_2}-D_{x_1}D_{\xi_2})}$ *is bounded on the space*

$$\{c \in C^\infty(\mathbb{R}^{4d}) \mid |\partial_{x_1}^{\delta_1}\partial_{\xi_1}^{\gamma_1}\partial_{x_2}^{\delta_2}\partial_{\xi_2}^{\gamma_2} c| \leq C\langle\xi_1\rangle^{m-|\beta_1|}\langle\xi_2\rangle^{k-|\beta_2|}\}. \tag{8.16}$$

Theorem 8.4. Ψ^∞, $\Psi^\infty_{\mathrm{ph}}$ *and* $\Psi^\infty_{\mathrm{pol}}$ *are algebras with gradation.*

Proof. Let us prove that $\Psi^m \cdot \Psi^k \subset \Psi^{m+k}$. Let $a \in S^m$ and $b \in S^k$.

$$a \star b(x,p) := \mathrm{e}^{\frac{\mathrm{i}}{2}(D_{\xi_1}D_{x_2}-D_{x_1}D_{\xi_2})} a(x_1,\xi_1) b(x_2,\xi_2)\Big|_{\substack{x := x_1 = x_2, \\ \xi := \xi_1 = \xi_2.}}$$

By Lemma 8.3,

$$|\partial_{x_1}^{\alpha_1}\partial_{\xi_1}^{\beta_1}\partial_{x_2}^{\alpha_2}\partial_{\xi_2}^{\beta_2}\mathrm{e}^{\frac{\mathrm{i}}{2}(D_{\xi_1}D_{x_2}-D_{x_1}D_{\xi_2})} a(x_1,\xi_1) b(x_2,\xi_2)| \leq C\langle\xi_1\rangle^{m-|\beta_1|}\langle\xi_2\rangle^{k-|\beta_2|}. \tag{8.17}$$

Restricting to $\begin{matrix} x := x_1 = x_2, \\ \xi := \xi_1 = \xi_2. \end{matrix}$ yields the estimate

$$|\partial_x^\alpha\partial_\xi^\beta a \star b(x,p)| \leq C\langle\xi\rangle^{m+k-|\beta|}. \tag{8.18}$$

Thus $a \star b \in S^{m+k}$.

If $a \in S^m_{\mathrm{ph}}$ and $b \in S^k_{\mathrm{ph}}$, we use the expansion

$$a \star b(x,p) := \sum_{j=0}^{n} \frac{\left(\frac{\mathrm{i}}{2}(D_{\xi_1}D_{x_2} - D_{x_1}D_{\xi_2})\right)^j}{j!} a(x_1,\xi_1) b(x_2,\xi_2)\Big|_{\substack{x := x_1 = x_2, \\ \xi := \xi_1 = \xi_2.}} \tag{8.19}$$

$$+ \int_0^1 \mathrm{d}\tau \frac{\left(\frac{\mathrm{i}}{2}(D_{\xi_1}D_{x_2} - D_{x_1}D_{\xi_2})\right)^{n+1}(1-\tau)^n}{n!} \mathrm{e}^{\frac{\mathrm{i}}{2}\tau(D_{\xi_1}D_{x_2}-D_{x_1}D_{\xi_2})} a(x_1,\xi_1) b(x_2,\xi_2)\Big|_{\substack{x := x_1 = x_2, \\ \xi := \xi_1 = \xi_2.}}$$

The jth term of this expansion is in S^{m+k-j}_{ph} and the remainder by Lemma 8.3 is in $S^{m+k-n-1}$. □

In the usual semiclassical quantization of a function $a(x,p)$ we insert the Planck constant in the second variable, that is after quantization we use the function $a(x,\hbar\xi)$. Thus it satisfies the estimates

$$|\partial_x^\alpha \partial_\xi^\beta a| \le C_{\alpha,\beta}\hbar^{|\beta|}. \tag{8.20}$$

If we compare (8.20) with (8.3), that is

$$|\partial_x^\alpha \partial_\xi^\beta a(x,\xi)| \le c_{\alpha,\beta}\langle\xi\rangle^{m-|\beta|}, \tag{8.21}$$

we see that in the class S^m the function $\langle\xi\rangle^{-1}$ plays the role of the Planck constant.

Let $a \in S^m$ and $b \in S^k$. We then have Clearly, the jth term in the above sum belongs to S^{m+k-j}. Thus we have an analog of the semiclassical expansion of the star product.

8.5 Sobolev spaces

For $k \in \mathbb{R}$, the kth Sobolev space is defined as

$$L^{2,k}(\mathbb{R}^d) := \{f \in \mathcal{S}'(\mathbb{R}^d) \mid (1+\xi^2)^{k/2}\hat{f} \in L^2(\mathbb{R}^d)\}.$$

We equip $L^{2,k}(\mathbb{R}^d)$ with the scalar product

$$(f|g)_k := (\hat{f}|(1+\xi^2)^k\hat{g}).$$

Clearly, $L^{2,k}(\mathbb{R}^d)$ is a family of Hilbert spaces such that

$$L^{2,k}(\mathbb{R}^d) \subset L^{2,k'}(\mathbb{R}^d), \quad k \ge k'.$$

The following operator is unitary:

$$\langle D\rangle^k = (1-\Delta)^{k/2} : L^{2,k}(\mathbb{R}^d) \to L^2(\mathbb{R}^d).$$

We also write

$$L^{2,\infty} := \bigcap_k L^{2,k}(\mathbb{R}^d), \quad L^{2,-\infty} := \bigcup_k L^{2,k}(\mathbb{R}^d).$$

Clearly, $S^0 \subset S^0_{00}$. Therefore, by the Calderon-Vaillancourt Theorem all elements of Ψ^0 are bounded on $L^2(\mathbb{R}^d)$. The following proposition generalizes this to other Sobolev spaces and to Ψ^m for all m.

Proposition 8.5. *For any $k, m \in \mathbb{R}$, $A \in \Psi^m$ extends to a bounded operator*

$$A : L^{2,k}(\mathbb{R}^d) \to L^{2,k-m}(\mathbb{R}^d),$$

and also to a continuous operator on $L^{2,\infty}$ and $L^{2,-\infty}$.

Proof. It is enough to show that if $A = \mathrm{Op}(a)$ with $a \in S^m$, then

$$(1-\Delta)^{-\frac{m}{2}+\frac{k}{2}}A(1-\Delta)^{-\frac{k}{2}} \tag{8.22}$$

is bounded on $L^2(\mathbb{R}^d)$. But $(1-\Delta)^{-\frac{k}{2}} \in \Psi^{-k}$, $(1-\Delta)^{-\frac{m}{2}+\frac{k}{2}} \in \Psi^{-m+k}$. Hence (8.22) belongs to Ψ^0, so it is bounded. □

Corollary 8.6. *$A \in \Psi^{-\infty}$ maps $L^{2,-\infty}(\mathbb{R}^d)$ to $L^{2,\infty}(\mathbb{R}^d)$.*

Note that $L^{2,\infty}(\mathbb{R}^d) \subset C^\infty(\mathbb{R}^d)$. Therefore, elements of $\Psi^{-\infty}$ are called *smoothing operators.*

Proposition 8.7. *The following statements are equivalent:*

1. *$A \in \Psi^m$.*
2. *$\mathrm{ad}_x^\alpha \mathrm{ad}_D^\beta(A)\langle D\rangle^{-m+|\alpha|}$ is bounded for any α, β.*

Proof. (1)⇒(2) Let $A = \mathrm{Op}^{x,\xi}(a)$. Fix α, β. We have

$$\partial_x^\gamma \partial_\xi^\delta \Big((\partial_x^\alpha \partial_\xi^\beta a)\langle\xi\rangle^{-m+|\beta|}\Big) \tag{8.23}$$

$$= \sum_{\delta_1+\delta_2=\delta} C_{\delta_1,\delta_2}(\partial_x^{\alpha+\gamma}\partial_\xi^{\beta+\delta_1} a)\partial_\xi^{\delta_2}\langle\xi\rangle^{-m+|\beta|}. \tag{8.24}$$

This is clearly bounded. Hence by the x, ξ version of the Calderon-Vaillancourt Theorem

$$\begin{aligned} \mathrm{Op}^{x,\xi}\big((\partial_x^\alpha \partial_\xi^\beta a)\langle\xi\rangle^{-m+|\beta|}\big) &= \mathrm{Op}^{x,\xi}\big(\partial_x^\alpha \partial_\xi^\beta a\big)\langle D\rangle^{-m+|\beta|} \\ &= \mathrm{i}^{|\alpha|-|\beta|}\mathrm{ad}_D^\alpha \mathrm{ad}_x^\beta(A)\langle D\rangle^{-m+|\beta|} \end{aligned} \tag{8.25}$$

is bounded.

(1)⇐(2) Fix α, β again. We have

$$\mathrm{ad}_D^\gamma \mathrm{ad}_x^\delta \Big((\mathrm{ad}_D^\alpha \mathrm{ad}_x^\beta A)\langle D\rangle^{-m+|\beta|}\Big) \tag{8.26}$$

$$= \sum_{\delta_1+\delta_2=\delta} C_{\delta_1,\delta_2}(\mathrm{ad}_D^{\alpha+\gamma}\mathrm{ad}_x^{\beta+\delta_1} A)\mathrm{ad}_x^{\delta_2}\langle D\rangle^{-m+|\beta|}. \tag{8.27}$$

Using $\mathrm{ad}_x^\alpha\langle D\rangle^k = (-\mathrm{i})^{|\alpha|}\partial_\xi^\alpha\langle D\rangle^k$, it is easy to see that (8.57) is bounded. By the x, ξ version of the Beals criterion

$$(\mathrm{ad}_D^\alpha \mathrm{ad}_x^\beta A)\langle D\rangle^{-m+|\beta|} = \mathrm{Op}^{x,\xi}(b_{\alpha,\beta}),$$

where $b_{\alpha,\beta}$ is bounded. But

$$b_{\alpha,\beta} = \mathrm{i}^{-|\alpha|+|\beta|}\partial_x^\alpha \partial_\xi^\beta a\langle\xi\rangle^{-m+|\beta|}.$$

□

8.6 Principal and extended principal symbols

Recall that if $A = \mathrm{Op}(a)$, then a is called the symbol (or the full symbol) of A and sometimes is denoted $\mathrm{s}(A)$.

Suppose first that $a = \sum\limits_{|\beta|\leq m} a_\beta(x)\xi^\beta \in S^m_{\mathrm{pol}}$ and $A = \mathrm{Op}(a)$. Then

$$\begin{aligned} \mathrm{s}^m_{\mathrm{pr}}(A) &:= \sum_{|\beta|=m} a_\beta(x)\xi^\beta, \\ \mathrm{s}^m_{\mathrm{sub}}(A) &:= \sum_{|\beta|=m-1} a_\beta(x)\xi^\beta \end{aligned}$$

are called resp. the *principal symbol* and the *subprincipal symbol* of A. It is natural to combine them into the *extended principal symbol of* A

$$\mathrm{s}^m_{\mathrm{ep}}(A) := \mathrm{s}^m_{\mathrm{pr}}(A) + \mathrm{s}^m_{\mathrm{sub}}(A).$$

The above definition has a natural extension to step 1 polyhomogeneos operators. If $a \simeq \sum\limits_{k=0}^{\infty} a_{m-k} \in S^m_{\mathrm{ph}}$, as a decomposition of the symbol into homogeneous terms, then

$$\begin{aligned} \mathrm{s}^m_{\mathrm{pr}}(A) &:= a_m(x,\xi), \\ \mathrm{s}^m_{\mathrm{sub}}(A) &:= a_{m-1}(x,\xi). \end{aligned}$$

Note that if $A = \mathrm{Op}^{x,\xi}(b)$ and $b \simeq \sum_{k=0}^{\infty} b_{m-k}$, then the principal symbol is b_m and the subprincipal symbol is $b_{m-1} + \frac{\mathrm{i}}{2}\partial_x\partial_\xi b_m$.

If $A = \mathrm{Op}(a) \in \Psi^m$, then we do not have such a clean definition of the principal and subprincipal symbol. The principal and extended symbol are then defined as elements of $\mathrm{s}^m_{\mathrm{pr}}(A) \in S^m/S^{m-1}$, resp. $\mathrm{s}^m_{\mathrm{ep}}(A) \in S^m/S^{m-2}$ by

$$\mathrm{s}^m_{\mathrm{pr}}(A) := \mathrm{s}(A) \pmod{S^{m-1}}, \tag{8.28}$$

$$\mathrm{s}^m_{\mathrm{ep}}(A) := \mathrm{s}(A) \pmod{S^{m-2}}. \tag{8.29}$$

Let $A \in \Psi^m$ and $B \in \Psi^k$. Then

$$\begin{aligned} AB \in \Psi^{m+k} &\quad \text{and} \\ \mathrm{s}^{m+k}_{\mathrm{pr}}(AB) &= \mathrm{s}^m_{\mathrm{pr}}(A)\mathrm{s}^k_{\mathrm{pr}}(B), \\ \mathrm{s}^{m+k}_{\mathrm{ep}}\Big(\frac{1}{2}[A,B]_+\Big) &= \mathrm{s}^m_{\mathrm{ep}}(A)\mathrm{s}^k_{\mathrm{ep}}(B) \pmod{S^{m+k-2}}; \\ [A,B] \in \Psi^{m+k-1} &\quad \text{and} \\ \mathrm{s}^{m+k-1}_{\mathrm{pr}}([A,B]) &= \{\mathrm{s}^m_{\mathrm{pr}}(A), \mathrm{s}^k_{\mathrm{pr}}(B)\}, \\ \mathrm{s}^{m+k-1}_{\mathrm{ep}}([A,B]) &= \{\mathrm{s}^m_{\mathrm{ep}}(A), \mathrm{s}^k_{\mathrm{ep}}(B)\} \pmod{S^{m+k-3}}. \end{aligned}$$

8.7 Cotangent bundle

In this subsection $\mathcal{X}$ is a manifold. In our subsequent applications we will usually assume that $\mathcal{X} = \mathbb{R}^d$, however the material of this subsection is more general.

The cotangent bundle of $\mathcal{X}$ will be denoted by $\mathrm{T}^\#\mathcal{X}$.

Let $F : \mathcal{X} \ni x \mapsto \tilde{x} \in \mathcal{X}$ be a diffeomorphism. We can define its prolongation to the cotangent bundle $\mathrm{T}^{\#}\mathcal{X}$. If we choose coordinates on $\mathcal{X}$, then the prolongation of F and its inverse are given by

$$\begin{aligned} x^i &\mapsto \tilde{x}^j(x) & \qquad \tilde{x}^j &\mapsto x^i(\tilde{x}) \\ \xi_i &\mapsto \tilde{\xi}_j(x,\xi) = \frac{\partial x^i}{\partial \tilde{x}^j}(x)\xi_i & \qquad \tilde{\xi}_j &\mapsto \xi_i(\tilde{x},\tilde{\xi}) = \frac{\partial \tilde{x}^j}{\partial x^i}(\tilde{x})\tilde{\xi}_j. \end{aligned}$$

Note that $\mathrm{T}^{\#}\mathcal{X}$ is a symplectic manifold with the symplectic form $\mathrm{d}x^j \wedge \mathrm{d}\xi_j$ and the prolongation of F preserves this symplectic form:

$$\begin{aligned} \mathrm{d}\tilde{x}^i \wedge \mathrm{d}\tilde{\xi}_i &= \frac{\partial \tilde{x}^i}{\partial x^j}\mathrm{d}x^j \wedge \Big(\frac{\partial \tilde{\xi}_i}{\partial x^k}\mathrm{d}x^k + \frac{\partial \tilde{\xi}_i}{\partial \xi_k}\mathrm{d}\xi_k\Big) & (8.30) \\ &= \frac{\partial \tilde{x}^i}{\partial x^j}\mathrm{d}x^j \wedge \Big(\frac{\partial \tilde{x}^n}{\partial x^k}\frac{\partial^2 x^m}{\partial \tilde{x}^n \partial \tilde{x}^i}\xi_m \mathrm{d}x^k + \frac{\partial x^k}{\partial \tilde{x}^i}\mathrm{d}\xi_k\Big) & (8.31) \\ &= \mathrm{d}x^j \wedge \mathrm{d}\xi_j. & (8.32) \end{aligned}$$

8.8 Diffeomorphism invariance

The action of a diffeomorphism F on functions on $\mathcal{X}$ will be denoted $F_{\#}$:

$$F_{\#}f(\tilde{x}) := f\big(x(\tilde{x})\big).$$

Proposition 8.8. *Suppose that A is an operator with the integral kernel $A(x_1,x_2)$. Then the integral kernel of $F_{\#}^{-1}AF_{\#}$ is $A(\tilde{x}(x_1),\tilde{x}(x_2))\Big|\frac{\partial \tilde{x}}{\partial x}(x_2)\Big|$.*

Proof. We have

$$\begin{aligned} AF_{\#}f(\tilde{x}_1) &= \int A(\tilde{x}_1,\tilde{x}_2)f(x(\tilde{x}_2))\mathrm{d}\tilde{x}_2 & (8.33) \\ &= \int A(\tilde{x}_1,\tilde{x}(x_2))f(x_2)\Big|\frac{\partial \tilde{x}}{\partial x}(x_2)\Big|\mathrm{d}x_2 & (8.34) \\ F_{\#}^{-1}AF_{\#}f(\tilde{x}_1) &= \int A(\tilde{x}(x_1),\tilde{x}(x_2))f(x_2)\Big|\frac{\partial \tilde{x}}{\partial x}(x_2)\Big|\mathrm{d}x_2. & (8.35) \end{aligned}$$

□

We will use the same notation $F_{\#}$ for the action of the prolongation of F on $C^\infty(T^{\#}\mathcal{X})$ given by

$$F_{\#}a(\tilde{x},\tilde{\xi}) = a\Big(x(\tilde{x}), \frac{\partial \tilde{x}}{\partial x}(\tilde{x})\tilde{\xi}\Big).$$

Theorem 8.9. *Let $F : \mathbb{R}^d \to \mathbb{R}^d$ be a diffeomorphism that moves only a bounded part of $\mathbb{R}^d$. Then the following holds.*

(1) *The spaces $S^m_{\mathrm{pol}}(\mathrm{T}^{\#}\mathbb{R}^d)$, $S^m_{\mathrm{ph}}(\mathrm{T}^{\#}\mathbb{R}^d)$, $S^m(\mathrm{T}^{\#}\mathbb{R}^d)$ are invariant wrt $F_{\#}$.*

(2) *The operators $F_{\#}$ are bounded invertible on spaces $L^{2,m}$.*

(3) *The algebras* $\Psi_{\rm pol}(\mathbb{R}^d)$, $\Psi_{\rm ph}(\mathbb{R}^d)$ *and* $\Psi(\mathbb{R}^d)$ *are invariant wrt* $F_\#$.

Proof. (1) The invariance of $S_{\rm pol}^m$ and $S_{\rm ph}^m$ is obvious. In fact, functions on $\mathrm{T}^\#\mathbb{R}^d$ homogeneous in ξ of any degree are invariant wrt difeeomorphisms.

To check the invariance of S^m we note that

$$\frac{\partial}{\partial\tilde{x}} = \Big(\frac{\partial}{\partial\tilde{x}}\frac{\partial\tilde{x}}{\partial x}\Big)\tilde{\xi}\frac{\partial}{\partial\xi} + \frac{\partial\tilde{x}}{\partial x}\frac{\partial}{\partial x}, \tag{8.36}$$

$$\frac{\partial}{\partial\tilde{\xi}} = \frac{\partial\tilde{x}}{\partial x}\frac{\partial}{\partial\xi}. \tag{8.37}$$

Now

$$\partial_{\tilde{x}}^\alpha\partial_{\tilde{\xi}}^\beta a(x,\xi) = \sum_{\substack{\beta\leq\gamma\leq\alpha+\beta,\\ \delta\leq\alpha;}} c_{\gamma,\delta}\tilde{\xi}^{\delta-\beta}\partial_x^\gamma\partial_\xi^\delta a(x,\xi). \tag{8.38}$$

Now the term on the right can be estimated by

$$C|\tilde{\xi}|^{|\delta|-|\beta|}\langle\xi\rangle^{m-|\delta|} \leq C_1\langle\xi\rangle^{m-|\beta|}.$$

(2) Let us first compute $F_\#^{-1}\Delta F_\#$. We have

$$\begin{aligned}\Delta F_\# f(\tilde{x}) &= \delta^{ij}\frac{\partial}{\partial\tilde{x}^i}\frac{\partial}{\partial\tilde{x}^j}f\big(x(\tilde{x})\big)\\ &= \delta^{ij}\frac{\partial x^k}{\partial\tilde{x}^i}\frac{\partial}{\partial x^k}\frac{\partial x^l}{\partial\tilde{x}^j}\frac{\partial}{\partial x^l}f\big(x(\tilde{x})\big)\\ F_\#^{-1}\Delta F_\# f(x) &= \delta^{ij}\frac{\partial x^k}{\partial\tilde{x}^i}\frac{\partial}{\partial x^k}\frac{\partial x^l}{\partial\tilde{x}^j}\frac{\partial}{\partial x^l}f(x).\end{aligned}$$

Assume first that m is a positive integer.

$$\big(1-F_\#^{-1}\Delta F_\#)^m(1-\Delta)^{-m} = \sum_{|\beta|\leq m} c_\beta(x)\partial_{x^{\beta_1}}\cdots\partial_{x^{\beta_k}}(1-\Delta)^{-m}, \tag{8.39}$$

where $c_\beta(x)$ are bounded. $\partial_{x^{\beta_1}}\cdots\partial_{x^{\beta_k}}(1-\Delta)^{-m}$ is also bounded for $|\beta|\leq m$ on $L^2(\mathbb{R}^d)$ by the Fourier transformation. Hence (8.39) is bounded.

By interpolation one obtains the boundedness of (8.39) for any positive m.

Exchanging the role of Δ and $F_\#^{-1}\Delta F_\#$ we obtain the result also for negative m.

(3) We use the Beals criterion. Set

$$\tilde{x} := F_\#^{-1}xF, \tag{8.40}$$

$$\tilde{D} := F_\#^{-1}DF \;=\; \frac{\partial x}{\partial\tilde{x}}D \tag{8.41}$$

Here, $\tilde{x}$ is the multiplication operator by the variable $\tilde{x}(x)$, and clearly by assumption $\tilde{x}-x\in C_{\rm c}^\infty$. Similarly, $\tilde{D}-D=\big(1-\frac{\partial x}{\partial\tilde{x}}\big)D$, where $\big(1-\frac{\partial x}{\partial\tilde{x}}\big)\in C_{\rm c}^\infty$.

Let $A \in \Psi^m$. To check the Beals criterion for $F_\# A F_\#^{-1}$ it is enough to prove the boundedness of

$$\begin{aligned} & F_\#^{-1} \mathrm{ad}_x^\alpha \mathrm{ad}_D^\beta (F_\# A F_\#^{-1}) \langle D\rangle^{-m+|\beta|} F_\# \\ = & \mathrm{ad}_{\tilde{x}}^\alpha \mathrm{ad}_{\tilde{D}}^\beta (A) \langle \tilde{D}\rangle^{-m+|\beta|}. \end{aligned} \tag{8.42}$$

Now $\langle D\rangle^{m-|\beta|}\langle \tilde{D}\rangle^{-m+|\beta|}$ is bounded by (2) and

$$\mathrm{ad}_{\tilde{x}}^\alpha \mathrm{ad}_{\tilde{D}}^\beta (A) \langle D\rangle^{-m+|\beta|}$$

is bounded by Lemma 8.10 below. This proves the boundedness of (8.42). □

Lemma 8.10. *Let $A \in \Psi^m$. Let $f_1', \dots, f_n' \in C_\mathrm{c}^\infty$. Then*

$$[f_1(x), \dots [f_n(x), A] \cdots]\langle D\rangle^{-m+n} \tag{8.43}$$

is bounded.

Proof. Let us write

$$f_i(x) = (2\pi)^{-d} \int \hat{f}_i(\xi) \mathrm{e}^{\mathrm{i}x\xi_i} \mathrm{d}\xi_i.$$

Then (8.43) can be rewritten as

$$\begin{aligned} & (2\pi)^{-dn} \int \mathrm{d}\xi_1 \int_0^1 \mathrm{d}\tau_1 \cdots \int \mathrm{d}\xi_n \int_0^1 \mathrm{d}\tau_n \\ & \times \mathrm{e}^{\mathrm{i}((1-\tau_1)\xi_1 + \cdots + (1-\tau_n)\xi_n)x} [\xi_1 x \cdots [\xi_n x, A] \cdots]\langle D\rangle^{-m+n} \mathrm{e}^{\mathrm{i}(\tau_1\xi_1 + \cdots + \tau_n \xi_n)x} && (8.44) \\ & \times \hat{f}_1(\xi_1) \cdots \hat{f}_n(\xi_n) \langle D + \tau_1\xi_1 + \cdots + \tau_n\xi_n\rangle^{m-n} \langle D\rangle^{-m+n}. && (8.45) \end{aligned}$$

Now (8.44) is bounded because $A \in \Psi^m$. Besides, the whole integral is bounded because

$$\begin{aligned} \|\langle D + \tau_1\xi_1 + \cdots + \tau_n\xi_n\rangle^{m-n} \langle D\rangle^{-m+n}\| &\leq \langle \tau_1\xi_1 + \cdots + \tau_n\xi_n\rangle^{|-m+n|}, && (8.46) \\ |\xi_1 \hat{f}_1(\xi_1) \cdots \xi_n \hat{f}_n(\xi_n)| &\leq c_N \langle \xi_1\rangle^N \cdots\cdots \langle \xi_n\rangle^N. && (8.47) \end{aligned}$$

□

8.9 Ellipticity

Proposition 8.11. 1. *If $a \in S_\mathrm{ph}^m$ and $|a(x,\xi)| \geq c\langle\xi\rangle^m$, $c > 0$, then $a(x,\xi)^{-1}$ belongs to S_ph^{-m}. More generally, for any $p \in \mathbb{C}$, $a(x,\xi)^p$ belongs to $S_\mathrm{ph}^{-\mathrm{Re}(p)m}$.*

2. *The same is true if we replace S_ph with S.*

Proof. Let $a \in S_\mathrm{ph}^m$. Let $a_m(x,\xi)$ be its principal symbol Set

$$r(x,\xi) = a(x,\xi) - a_m(x,\xi).$$

Then $|a_m(x,\xi)| \geq c|\xi|^m$, $c > 0$, and for large $|\xi|$ we have a convergent power series expansion

$$a(x,\xi)^{-1} = \frac{1}{a_m(x,\xi)\Big(1 + \frac{r(x,\xi)}{a_m(x,\xi)}\Big)} = \sum_{n=0}^{\infty} (-1)^n \frac{r(x,\xi)^n}{a_m(x,\xi)^{n+1}}. \tag{8.48}$$

Now the nth term on the right of (8.48) belongs to S_{ph}^{-m-n}. Hence the whole sum belongs to S_{ph}^{-m}.

The proof for the pth power is similar, except that we use the Taylor expansion of $a(x,\xi)^p = a_m(x,\xi)^p \big(1 + \frac{r(x,\xi)}{a_m(x,\xi)}\big)^p$.

Next, assume that $a \in S^m$. The Faa di Bruno formula implies

$$\partial_x^\alpha \partial_\xi^\beta a^p = \sum_{\substack{\alpha_1 + \cdots + \alpha_n = \alpha, \\ \beta_1 + \cdots + \beta_n = \beta.}} C_{\alpha_1,\beta_1\dots,\alpha_n,\beta_n} a^{p-n} \partial_x^{\alpha_1} \partial_\xi^{\beta_1} a \cdots \partial_x^{\alpha_n} \partial_\xi^{\beta_n} a. \tag{8.49}$$

The term in the above sum can be estimated by

$$C\langle\xi\rangle^{pm-nm} \langle\xi\rangle^{m-|\gamma_1|} \cdots \langle\xi\rangle^{m-|\gamma_n|} = C\langle\xi\rangle^{pm-|\beta|}. \tag{8.50}$$

Hence $a^p \in S^{mp}$. □

We say that $b \in S^m(\mathbb{R}^d)$ is *elliptic* if for some r, $c_0 > 0$

$$|b(x,\xi)| \geq c_0|\xi|^m, \quad |\xi| > r.$$

Proposition 8.12. *Let $m > 0$. Let $b \in S^m(\mathbb{R}^d)$ be elliptic and $z - b(x,\xi)$ invertible. Then there exists $c > 0$ such that*

$$|z - b(x,\xi)| \geq c\langle\xi\rangle^m, \tag{8.51}$$

so that the statements of Proposition 8.11 are true.

Proof. We have

$$\begin{aligned} |z - b(x,\xi)| &\geq c_0|\xi|^m - |z|, \quad |\xi| > r, \\ |z - b(x,\xi)| &\geq c_R, \quad |\xi| < R, \quad \text{(by compactness)}. \end{aligned}$$

This clearly implies (8.51). □

Quantizations of elliptic symbols of a positive degree are unbounded. Therefore, their theory involves various technicalities that we would like to avoid and we will develop it only under restrictive assumptions.

Theorem 8.13. *1. Let $m > 0$. Let $b \in S^m$ be positive and elliptic, that is, for some r, $c_0 > 0$*

$$b(x,\xi) \geq c_0|\xi|^m, \quad |\xi| > r.$$

Then $\mathrm{Op}(b)$ with domain $L^{2,m}$ is self-adjoint and if $z \notin \mathrm{sp}\,(\mathrm{Op}(b)$, then

$$(z - \mathrm{Op}(b))^{-1} \in \Psi^{-m}. \tag{8.52}$$

2. If in addition $b \in S^{m}_{\mathrm{ph}}$, then

$$(z - \mathrm{Op}(b))^{-1} \in \Psi^{-m}_{\mathrm{ph}}. \tag{8.53}$$

Proof. We know that $\mathrm{Op}(b)$ is well defined as an operator $L^{2,m} \to L^2$. We will show that for z with $|\arg(z)| \geq \epsilon > 0$ and $|z|$ big enough the operator $z - \mathrm{Op}(b)$ is invertible.

Suppose that $z - b(x, \xi)$ is invertible. Then

$$(z - b) \star (z - b)^{-1} = 1 + r, \tag{8.54}$$

where $r \in S^{-2}$. We check that the seminorms of r as an element of S^0_{00} go to zero for $|\arg(z)| \geq \epsilon > 0$ and $|z|$ large enough. Hence $\|\mathrm{Op}(r)\| \to 0$. We rewrite (8.54) as

$$\big(z - \mathrm{Op}(b)\big)\mathrm{Op}\big((z - b)^{-1}\big) = \mathbb{1} + \mathrm{Op}(r). \tag{8.55}$$

Then we can write for $\|\mathrm{Op}(r)\| < 1$

$$\big(z - \mathrm{Op}(b)\big)\mathrm{Op}\big((z - b)^{-1}\big)\big(\mathbb{1} + \mathrm{Op}(r)\big)^{-1} = \mathbb{1}. \tag{8.56}$$

Thus $z - \mathrm{Op}(b)$ is right invertible. An analogous reasoning shows that it is left invertible. Hence it is invertible and

$$\big(z - \mathrm{Op}(b)\big)^{-1} = \mathrm{Op}\big((z - b)^{-1}\big)\big(\mathbb{1} + \mathrm{Op}(r)\big)^{-1}, \tag{8.57}$$

belongs to Ψ^{-m}. In particular, the range of (8.57) is contained in $L^{2,m}$.

Let $z \notin \mathrm{sp}\,\mathrm{Op}(b)$. Let z_1 satisfies $|\arg(z_1)| \geq \epsilon > 0$ and $|z_1|$ big enough, so that the above construction applies.

$$(z - \mathrm{Op}(b))^{-1} = (z_1 - \mathrm{Op}(b))^{-1} + (z - z_1)(z_1 - \mathrm{Op}(b))^{-1}(z - \mathrm{Op}(b))^{-1},$$

hence the range of $\big(z - \mathrm{Op}(b)\big)^{-1}$ is $L^{2,m}$ as well. We will show that for any k

$$\big(z - \mathrm{Op}(b)\big)^{-1} : L^{2,k} \to L^{2,m+k}. \tag{8.58}$$

We have

$$\begin{aligned} \big[D, \big(z - \mathrm{Op}(b)\big)^{-1}\big] &= \big(z - \mathrm{Op}(b)\big)^{-1}[D, \mathrm{Op}(b)]\big(z - \mathrm{Op}(b)\big)^{-1} \\ &= \big(z - \mathrm{Op}(b)\big)^{-1}[D, \mathrm{Op}(b)]\langle D\rangle^{-m}\langle D\rangle^{m}\big(z - \mathrm{Op}(b)\big)^{-1}. \end{aligned} \tag{8.59}$$

Thus (8.59) is bounded. We can iterate (8.59) obtaining the boundedness of

$$\mathrm{ad}^{\alpha}_{D}\big(z - \mathrm{Op}(b)\big)^{-1}.$$

This easily implies (8.58).

Now $\big(z - \mathrm{Op}(b)\big)^{-1} \in \Psi^{-m}$ follows by the Beals criterion.

(8.57) does not tell us much about the resolvent of $\mathrm{Op}(b)$. One can try to improve it as follows. Let $z \in \mathbb{C}$, not necessarily in $\mathrm{sp}\,\mathrm{Op}(b)$. Modifying b for ξ in a bounded set, so that $|z - b_0| \geq c\langle\xi\rangle$ and $b - b_0 \in S^{-\infty}$, we can rewrite (8.54) as

$$(z - b) \star (z - b_0)^{-1} = 1 + r_0, \tag{8.60}$$

where $r_0 \in S^{-2}$. Multiplying this by $1 - r_0 + \cdots + (-r_0)^{\star n}$, we obtain

$$(z - b) \star (z - b_0)^{-1} \star (1 - r_0 + \cdots + (-r_0)^{\star n}) = 1 - (-r)^{\star(n+1)}.$$

Hence if we set

$$c_{2n}(z) := (z - b)^{-1} \star \big(1 - r_0 + \cdots + (-r_0)^{\star n}\big),$$

then $c_{2n} \in S^{-m}$ and

$$(z - \mathrm{Op}(b))\mathrm{Op}\big(c_{2n}(z)\big) - \mathbb{1} \in \Psi^{-m-2n-2}. \tag{8.61}$$

Thus if $z - \mathrm{Op}(b)$ is invertible, then

$$\mathrm{Op}(c_{2n}(z)) - (z - \mathrm{Op}(b))^{-1} \in \Psi^{-m-2n-2}.$$

This can be used to prove that if b is polyhomogeneous, then so is $(z - \mathrm{Op}(b))^{-1}$. $\square$

Let us state a corollary of the above constructions, which goes under the name of *elliptic regularity.*

Corollary 8.14. *Assume the hypotheses of Theorem 8.13. Let*

$$\mathrm{Op}(b)f = g, \tag{8.62}$$

where $g \in L^{2,\infty}$ and $f \in L^{2,-\infty}$. Then $f \in L^{2,\infty}$.

Proof. We can assume that $f \in L^{2,k}$ for some k. Let $c_{2n} \in S^{-m}$ and $r_{2n+2} \in S^{-2n-2}$ such that

$$\mathrm{Op}\big(c_{2n}\big)\mathrm{Op}(b) - \mathbb{1} = \mathrm{Op}(r) \in \Psi^{-2n-2}, \tag{8.63}$$

see the proof above. We multiply (8.62) by $\mathrm{Op}(c_{2n})$, obtaining

$$f = \mathrm{Op}(c_{2n})g - \mathrm{Op}(r_{2n+2})f. \tag{8.64}$$

Now $\mathrm{Op}(c_{2n})g \in L^{2,\infty}$, $\mathrm{Op}(r_{2n+2})f \in L^{2,k+2n+2}$. Since n was arbitrary, $f \in L^{2,\infty}$. $\square$

Remark 8.15. *Using the Beals criterion, under the assumptions of Theorem 8.13, we can show that $\mathrm{Op}(b)^p \in \Psi^{mp}$, at least for $p \in \mathbb{Z}$, presumably also for $p \in \mathbb{C}$.*

Remark 8.16. *An easy argument involving the so-called Borel summation allows us to construct $c_\infty(z) \in S^m$ such that*

$$(z - \mathrm{Op}(b))\mathrm{Op}\big(c_\infty(z)\big) - \mathbb{1} \in \Psi^{-\infty}. \tag{8.65}$$

Such an operator is called a parametrix of $z - \mathrm{Op}(b)$.

8.10 Asymptotics of the dynamics

The following version of the Egorov Theorem is to a large extent analogous to its semiclassical version, that is Theorem 6.20. Compare the Hamiltonian in Theorem 6.20, which was $\frac{1}{\hbar}\mathrm{Op}(h)$, and the Hamiltonian in the following theorem:

Theorem 8.17 (Egorov Theorem). *Let $h \in S^1_{\mathrm{ph}}$ be real and elliptic. Let h_1 be its principal symbol.*

(1) *Let $x(t), \xi(t)$ solve the Hamilton equations with the Hamiltonian h_1 and the initial conditions $x(0), \xi(0)$. Then*

$$\gamma_t(x(0), \xi(0)) = \big(x(t), \xi(t)\big)$$

defines a symplectic transformation homogeneous in ξ.

(2) *Let $b \in S^m_{\mathrm{ph}}$ be homogeneous in ξ of degree m. Then there exist $b_t \simeq \sum\limits_{n=0}^{\infty} b_{t,m} \in S^m_{\mathrm{ph}}$ such that*

$$\mathrm{e}^{\mathrm{i}t\mathrm{Op}(h)}\mathrm{Op}(b)\mathrm{e}^{-\mathrm{i}t\mathrm{Op}(h)} = \mathrm{Op}\big(b_t\big). \tag{8.66}$$

Moreover,

$$b_{t,m}(x,\xi) = b_m\big(\gamma_t^{-1}(x,\xi)\big) \tag{8.67}$$

and $\mathrm{supp} b_{t,m-n} \subset \gamma_t(\mathrm{supp} b)$*,* $n = 0, 1, \dots$*.*

We skip the proof of the above theorem, because it is very similar to the proof of Theorem 6.20.

8.11 Singular support

Proposition 8.18. *Let f be a distribution of compact support. Then*

$$f \in C^\infty_{\mathrm{c}} \ \Leftrightarrow\ |\hat{f}(\xi)| \leq c_n \langle\xi\rangle^{-n}, \quad n \in \mathbb{N}. \tag{8.68}$$

Proof. $\Leftarrow$. We can differentiate

$$f(x) := (2\pi)^{-d}\int \mathrm{e}^{\mathrm{i}x\xi}\hat{f}(\xi)\mathrm{d}\xi \tag{8.69}$$

any number of times.

$\Rightarrow$ We integrate by parts:

$$(\mathrm{i}\xi)^\alpha \hat{f}(\xi) := (2\pi)^{-d}\int(\partial_x^\alpha \mathrm{e}^{-\mathrm{i}x\xi})f(x)\mathrm{d}x = (2\pi)^{-d}(-1)^{|\alpha|}\int \mathrm{e}^{-\mathrm{i}x\xi}\partial_x^\alpha f(x)\mathrm{d}x. \tag{8.70}$$

□

For $f \in \mathcal{D}'(\mathbb{R}^d)$, we say that is *smooth near* $x_0 \in \mathbb{R}^d$ if if there exists a neighborhood $\mathcal{U}$ of x_0 such that f is C^∞ on $\mathcal{U}$. We say that x_0 beongs to the *singular support of* f, denoted $\mathrm{Sing}(f)$, if f is not smooth near x_0. The singular support is a closed subset of $\mathbb{R}^d$.

In the following proposition we give three equivalent characterizations of the complement of the singular support.

Proposition 8.19. *Let f be a distribution on $\mathbb{R}^d$ and $x_0 \in \mathbb{R}^d$. The following are equivalent:*

(1) *f is smooth near x_0.*

(2) *There exists $\chi_0 \in C_{\mathrm{c}}^\infty(\mathbb{R}^d)$, $\chi_0(x_0) \neq 0$, such that*

$$|\widehat{\chi_0 f}(\xi)| \leq c_n \langle \xi \rangle^{-n}, \quad n \in \mathbb{N}. \tag{8.71}$$

(3) *There exists a neighborhood $\mathcal{U}$ of x_0 such that for any $\chi \in C_{\mathrm{c}}^\infty(\mathcal{U})$,*

$$|\widehat{\chi f}(\xi)| \leq c_n \langle \xi \rangle^{-n}, \quad n \in \mathbb{N}. \tag{8.72}$$

Proof. (1)$\Rightarrow$(3) follows by Proposition 8.18 $\Rightarrow$. (3)$\Rightarrow$(2) is obvious.

Let us prove (2)$\Rightarrow$(1). $\chi_0 f$ is smooth by Proposition 8.18 $\Leftarrow$. Let $\mathcal{U} := \{x \mid |\chi_0(x)| > \frac{1}{2}|\chi_0(x_0)|\}$. Then $\mathcal{U}$ is an open neighborhood of x_0 on which χ_0^{-1} is smooth. Hence $f = \chi_0^{-1}(\chi_0 f)$ is also smooth on $\mathcal{U}$. □

We say that $b \in S^m$ is elliptic near x_0 iff there exist $c > 0$, r and a neighborhood $\mathcal{U}$ of x_0 such that

$$|b(x,\xi)| \geq c|\xi|^m, \quad x \in \mathcal{U}, \quad |\xi| > r. \tag{8.73}$$

Theorem 8.20. *Let $f \in L^{2,-\infty}$ and $a \in S^\infty$. Then*

(1) *If $a \in S^{-\infty}$, then*

$$\mathrm{Sing}(\mathrm{Op}(a)f) = \emptyset. \tag{8.74}$$

(2) *Let Ω be a closed subset of $\mathbb{R}^d$. If $\mathrm{supp} a \subset \mathrm{T}^\#\Omega$, then*

$$\mathrm{Sing}(\mathrm{Op}(a)f) \subset \mathrm{Sing}(f) \cap \Omega. \tag{8.75}$$

(3) *Let Ω_0 be a closed subset of $\mathbb{R}^d$. If a is elliptic near Ω_0, then*

$$\mathrm{Sing}(\mathrm{Op}(a)f) \supset \mathrm{Sing}(f) \cap \Omega_0. \tag{8.76}$$

Proof. (1) is obvious. Let us prove (2).

Let $f \in L^{2,k}$ and $a \in S^m$. Let $x_0 \not\in \mathrm{Sing}(f)$. Let $\chi, \chi_1, \in C_{\mathrm{c}}^\infty$, $\chi_0\chi_1 = \chi_0$, $\chi_0(x_0) \neq 0$ and $\mathrm{supp}\chi_1 \cap \mathrm{Sing}(f) = \emptyset$. We will write χ_0, χ_1 for $\chi_0(x), \chi_1(x)$.

$$\begin{aligned}\chi_0 \mathrm{Op}(a) f = \chi_0\chi_1 \mathrm{Op}(a) f &= \chi_0[\chi_1, \mathrm{Op}(a)] + \chi_0 \mathrm{Op}(a)\chi_1 f \\ &= \sum_{k=0}^n \binom{n}{k} \chi_0 \mathrm{ad}_{\chi_1}^k\big(\mathrm{Op}(a)\big)\chi_1^{n-k} f.\end{aligned} \tag{8.77}$$

But $\mathrm{ad}_{\chi_1}^k(A) \in \Psi^{m-k}$ and $\chi_1^{n-k} f \in L^{2,\infty}$. Thus all terms in (8.77) with $k < n$ belong to $L^{2,\infty}$. The term $\chi_0 \mathrm{ad}_{\chi_1}^n\big(\mathrm{Op}(a)\big) f \in L^{k-m+n}$. Since n was arbitrary, (8.77)$\in L^{2,\infty}$. This proves

$$\mathrm{Sing}(\mathrm{Op}(a)f) \subset \mathrm{Sing}(f). \tag{8.78}$$

Now let $x_0 \not\in \Omega$. We can find $\chi \in C_{\mathrm{c}}^\infty$ such that $\chi(x_0) \neq 0$ and $\chi a = 0$. Then $\chi \star a \in S^{-\infty}$. Hence $\chi \mathrm{Op}(a) f \in L^{2,\infty}$. Therefore,

$$\mathrm{Sing}(\mathrm{Op}(a)f) \subset \Omega. \tag{8.79}$$

This proves (2). □

8.12 Wave front

Let

$$\mathrm{T}^{\#}_{\neq 0}\mathbb{R}^d := \{(x,\xi) \in \mathrm{T}^{\#}\mathbb{R}^d \;\mid\; \xi \neq 0\}$$

denote the cotangent bundle of $\mathbb{R}^d$ with the zero section removed. We equip $\mathrm{T}^{\#}_{\neq 0}\mathbb{R}^d$ with an action of $\mathbb{R}_+$ as follows:

$$(x,\xi) \mapsto (x, t\xi), \quad t \in \mathbb{R}_+ \tag{8.80}$$

We say that a subset of $\mathrm{T}^{\#}_{\neq 0}\mathbb{R}^d$ is *conical* iff it is invariant with respect to this action. Conical subsets can be identified with $\mathrm{T}^{\#}_{\neq 0}\mathbb{R}^d/\mathbb{R}_+$.

Proposition 8.21. *Let $f \in \mathcal{D}'(\mathbb{R}^n)$ and $(x_0,\xi_0) \in \mathrm{T}^{\#}_{\neq 0}\mathbb{R}^d$. The following are equivalent:*

(1) *There exists $\chi \in C_{\mathrm{c}}^{\infty}(\mathcal{X})$ with $\chi(x_0) \neq 0$ and a conical neighborhood $\mathcal{W}$ of ξ_0 such that*

$$|\widehat{\chi f}(\xi)| \leq c_n \langle \xi \rangle^{-n},\ \xi \in \mathcal{W},\ n \in \mathbb{N}. \tag{8.81}$$

(2) *There exists a neighborhood $\mathcal{U}$ of x_0 and a conical neighborhood $\mathcal{W}$ of ξ_0 such that if $\chi \in C_{\mathrm{c}}^{\infty}(\mathcal{U})$, then*

$$|\widehat{\chi f}(\xi)| \leq c_n \langle \xi \rangle^{-n},\ \xi \in \mathcal{W},\ n \in \mathbb{N}. \tag{8.82}$$

We say that f is smooth in a conical neighborhood of (x_0,ξ_0) iff the equivalent conditions of Proposition 8.21 hold. Clearly, f is smooth in a neighborhood of x_0 iff it is smooth in a conical neighborhood of (x_0,ξ_0) for all nonzero $\xi_0 \in \mathrm{T}^{\#}_{x_0}\mathbb{R}^d$.

The complement in $\mathrm{T}^{\#}_{\neq 0}\mathbb{R}^d$ of points where f is smooth is called the *wave front set of* f and denoted $\mathrm{WF}(f)$. The wave front set is a closed conical subset of $\mathrm{T}^{\#}_{\neq 0}\mathbb{R}^d$. Clearly, $\mathrm{Sing}(f)$ is the projection of $\mathrm{WF}(f)$ onto the first variable.

We say that $b \in S^m$ is elliptic in a conical neighborhood of (x_0,ξ_0) iff there exist $c > 0$, r, a neighborhood $\mathcal{U}$ of x_0 and a conical neighborhood $\mathcal{W}$ of ξ_0 such that

$$|b(x,\xi)| \geq c|\xi|^m, \quad (x,\xi) \in \mathcal{U} \times \mathcal{W}, \quad |\xi| > r. \tag{8.83}$$

The following theorem gives two possible alternative definitions of microlocal smoothness.

Theorem 8.22. *Let $f \in L^{2,-\infty}$ and $(x_0,\xi_0) \in \mathrm{T}^{\#}_{\neq 0}\mathbb{R}^d$. The following conditions are equivalent:*

(1) *f is smooth in a conical neighborhood of (x_0,ξ_0).*

(2) *There exists m and $b \in S^m_{\mathrm{ph}}$ elliptic in a conical neighborhood of (x_0,ξ_0) such that*

$$\mathrm{Op}(b)u \in L^{2,\infty}.$$

(3) *There exists a neighborhood $\mathcal{U}$ of x_0 and a conical neighborhood $\mathcal{W}$ of ξ_0 such that for all $b \in S^{\infty}$ supported in $\mathcal{U} \times \mathcal{W}$ we have*

$$\mathrm{Op}(b)u \in L^{2,\infty}.$$

Proof. (1)⇒(3). Let $\mathcal{U}$, $\mathcal{W}$ be as in Prop. 8.21 (2). Let $\mathcal{U}_0$ be a neighborhood of x_0 whose closure is contained in $\mathcal{U}$. Likewise, let $\mathcal{W}_0$ be a conical neighborhood of ξ_0 whose closure is contained in $\mathcal{W}$. We will show that (3) is satisfied for $\mathcal{U}_0, \mathcal{W}_0$.

Let $\chi \in C_{\mathrm{c}}^\infty(\mathcal{U})$ such that $\chi = 1$ on $\mathcal{U}_0$. Let $\kappa \in C^\infty(\mathcal{W})$ be homogeneous of degeree 0 for $|\xi| > 1$ such that $\kappa = 1$ on $\mathcal{W}_0$ for $|\xi| > 2$. Then $\chi(x), \kappa(\xi) \in S^0$, and

$$b = b \star \kappa(\xi) \star \chi(x) + r, \quad r \in S^{-\infty}.$$

Hence

$$\mathrm{Op}(b)f = \mathrm{Op}(b)\kappa(D)\chi(x)f + \mathrm{Op}(r)f.$$

Now $\kappa(D)\chi(x)f \in L^{2,\infty}$ by the condition (8.82) and $\mathrm{Op}(r)f \in L^{2,\infty}$ because $\mathrm{Op}(r) \in \Psi^{-\infty}$. Hence $\mathrm{Op}(b)f \in \Psi^{-\infty}$.

(3)⇒(2) is obvious.

(2)⇒(1). We can assume that $\mathcal{U}$ and $\mathcal{W}$ are open such that $|b(x,\xi)| > |\xi|^m$ on $\mathcal{U} \times \mathcal{W}$ for $|\xi| > 1$. Let $b_0 \in S^{-m}$ such that $b_0 = b^{-1}$ there. Set $b_1 := b_0 \star b$. Then $b_1 = 1 + S^{-\infty}$ inside $\mathcal{U} \times \mathcal{W}$.

Let $\chi \in C_{\mathrm{c}}^\infty(\mathcal{U})$. Let $\kappa \in C^\infty$ be homogeneous of degree 0 for $|\xi| > 2$ and supported in $\mathcal{W}$. Then

$$\kappa(\xi) \star \chi(x) \star b_1 = \kappa(\xi) \star \chi(x) + r, \quad r \in S^{-\infty}.$$

Therefore,

$$\kappa(D)\chi(x) = \kappa(D)\chi(x)\mathrm{Op}(b_0)\mathrm{Op}(b) + \mathrm{Op}(r_1), \quad r_1 \in S^{-\infty}$$

We apply this to f. Using $\mathrm{Op}(b)f \in L^{2,\infty}$ we see that

$$\kappa(D)\chi(x)f \in L^{2,\infty},$$

which means that (1) holds. □

8.13 Properties of the wave front set

Example 8.23. *Let $\mathcal{Y}$ be a k-dimensional submanifold of $\mathbb{R}^d$ with a k-form β. Then the distribution*

$$\langle F|\psi\rangle := \int_{\mathcal{Y}} \phi\beta$$

has the wave front set in the conormal bundle to $\mathcal{Y}$:

$$WF(F) \subset \mathcal{N}^\#\mathcal{Y} := \{(x,\xi) \ : \ x \in \mathcal{Y}, \quad \langle\xi|v\rangle = 0, \ v \in \mathrm{T}\mathcal{Y}\}.$$

Example 8.24. *For $\mathcal{X} = \mathbb{R}$,*

$$WF((x + \mathrm{i}0)^{-1}) = \{(0,\xi) \ : \ \xi > 0\}.$$

Example 8.25. *Let H be a homogeneous function of degree 1 smooth away from the origin and $v \in C^\infty$,*

$$|\partial_\xi^\beta v(\xi)| \le c_\beta \langle\xi\rangle^{m-|\beta|}$$

Then

$$\int \mathrm{e}^{\mathrm{i}x\xi - \mathrm{i}H(\xi)} v(\xi) \mathrm{d}\xi = u(x)$$

satisfies

$$WF(u) = \{(\nabla_\xi H(\xi), \xi) \ : \ \xi \in \mathrm{supp} v\}.$$

Theorem 8.26. *Let $u \in L^{2,\infty}$ and $a \in S^\infty$.*

(1) *If $a \in S^{-\infty}$, then*

$$WF(\mathrm{Op}(a)u) = \emptyset. \tag{8.84}$$

(2) *Let Γ be a conical subset of $\mathrm{T}^\#\mathbb{R}^d$. If $\mathrm{supp} a \subset \Gamma$, then*

$$WF(\mathrm{Op}(a)u) \subset WF(u) \cap \Gamma.$$

(3) *Let Γ_0 be a conical subset of $\mathrm{T}^\#\mathbb{R}^d$. If $a \in S^m$ is elliptic on Γ_0, then*

$$WF(\mathrm{Op}(a)u) \supset WF(u) \cap \Gamma_0.$$

Theorem 8.27 (Theorem about propagation of singularities)**.** *Let $h \in S^1_{\mathrm{ph}}$ be real and elliptic. Let γ_t be the Hamiltonian flow generated by h_1, the principal symbol of h. Then*

$$WF(\mathrm{e}^{\mathrm{i}t\mathrm{Op}(h)}u) = \gamma_t\left(WF(u)\right).$$

9 Operators on manifolds

9.1 Invariant measure

Let M be a (pseudo-)Riemannian manifold with coordinates $[x^i]$ and a metric tensor $[g^{ij}]$. The coordinates for every point p determine the basis $\mathrm{d}x^i$, $i = 1, \dots, d$, of $T_p^\# M$ and ∂_{x^i}, $i = 1, \dots, d$, of $T_p M$. We have

$$g_{ij} = (\partial_{x^i} | \partial_{x^j}), \quad g^{ij} = (\mathrm{d}x^i | \mathrm{d}x^j),$$

where $[g^{ij}]$ is the inverse of $[g_{ij}]$. When we change the coordinates $x \to \tilde{x}$, then

$$\tilde{g}_{nm} = \frac{\partial x^i}{\partial \tilde{x}^n} \frac{\partial x^j}{\partial \tilde{x}^m} g_{ij}.$$

Therefore,

$$\det \tilde{g} = \Big(\det \frac{\partial x}{\partial \tilde{x}}\Big)^2 \det g.$$

Hence

$$\int f(x) |\det g|^{\frac{1}{2}}(x) \mathrm{d}x = \int f(\tilde{x}) |\det \tilde{g}|^{\frac{1}{2}}(\tilde{x}) \mathrm{d}\tilde{x}. \tag{9.1}$$

Thus if we set $|g| := \det g$, then $|g|^{\frac{1}{2}}(x)\mathrm{d}x$ is an invariant measure on M. It defines a natural Hilbert space with the scalar product

$$(u|w) := \int \overline{u(x)} w(x) |g|^{\frac{1}{2}}(x)\mathrm{d}x. \tag{9.2}$$

Here u, w are scalar functions on M, that is their values do not depend on the coordinates.

Instead of scalars one can use *half densities*, that is functions on M that depend on coordinates: if we change the coordinate from x to $\tilde{x}$ it transforms as $u \to |\sqrt{\frac{\partial \tilde{x}}{\partial x}}|u$.

Every scalar function can be *half-densitized*. More precisely, the following map associates to a scalar function u a half-density:

$$u \mapsto u_{\frac{1}{2}} := |g|^{\frac{1}{4}} u.$$

The scalar product between two half-densities is

$$(u|w) = \int \overline{u_{\frac{1}{2}}(x)} w_{\frac{1}{2}}(x)\mathrm{d}x. \tag{9.3}$$

9.2 Geodesics

Let M be a Riemannian manifold and $p_0, p_1 \in M$, then a geodesics joining p_0 and p_1 is a map $[0,1] \ni t \overset{\gamma}{\mapsto} x(t) \in M$ such that $x(0) = p_0$ and $x(1) = p_1$, which is a stationary point of the length

$$\int_0^1 \sqrt{g_{ij}(x(t))\dot{x}^i(t)\dot{x}^j(t)}\mathrm{d}t. \tag{9.4}$$

The Euler-Lagrange equations yield

$$\begin{aligned} 0 \;=\; \Big(\frac{\mathrm{d}}{\mathrm{d}t}\partial_{\dot{x}^k} - \partial_{x^k}\Big)\sqrt{g_{ij}\dot{x}^i\dot{x}^j} &= \frac{1}{2\sqrt{g_{ij}\dot{x}^i\dot{x}^j}}\Big(2g_{ik}\ddot{x}^i + g_{kj,l}\dot{x}^j\dot{x}^l + g_{ik,l}\dot{x}^i\dot{x}^l - g_{ij,k}\dot{x}^i\dot{x}^j\Big) \\ &\quad + g_{kj}\dot{x}^j \frac{\mathrm{d}}{\mathrm{d}t}\frac{1}{\sqrt{g_{ij}\dot{x}^i\dot{x}^j}}. \end{aligned} \tag{9.5}$$

Introducing the Christoffel symbol

$$\Gamma^i_{kl} = \frac{1}{2} g^{im}(g_{mk,l} + g_{ml,k} - g_{kl,m}) \tag{9.6}$$

we rewrite this as

$$\ddot{x}^i + \Gamma^i_{kl}\dot{x}^k\dot{x}^l = f(t)\dot{x}^i, \tag{9.7}$$

where $f(t)$ is arbtrary.

There exists another variational principle for geodesics based on the functional

$$\int_0^1 g_{ij}(x(\tau))\dot{x}^i(\tau)\dot{x}^j(\tau)\mathrm{d}\tau. \tag{9.8}$$

Here the Euler-Lagrange equations yield simply

$$0 = \Big(\frac{\mathrm{d}}{\mathrm{d}\tau}\partial_{\dot{x}^k} - \partial_{x^k}\Big) g_{ij}\dot{x}^i\dot{x}^j = \ddot{x}^k + \Gamma_{ij}^k \dot{x}^i\dot{x}^j.$$

We obtain a unique canonical parametrization by the so-called *affine parameter*. Note that (9.8) can be used also in the pseudo-Riemannian case.

Using the Lagrangian

$$L(x, \dot{x}) = g_{ij}(x)\dot{x}^i\dot{x}^j$$

we introduce the momentum

$$\xi_i := \frac{\partial \mathcal{L}}{\partial \dot{x}^i} = g_{ij}\dot{x}^j$$

and after the Legendre transformation we obtain the Hamiltonian

$$H = \dot{x}^i\xi_i - L = g^{ij}(x)\xi_i\xi_j. \tag{9.9}$$

Note that the same trajectories as for (13.5) one obtains with the Hamiltonian

$$\sqrt{H} = \sqrt{g^{ij}(x)\xi_i\xi_j}. \tag{9.10}$$

In fact, the Hamilton equations for (9.10) are

$$\begin{aligned} \dot{x}^i &= \frac{g^{ij}(x)\xi_j}{\sqrt{g^{ij}(x)\xi_i\xi_j}}, \\ \dot{\xi}_k &= -\frac{g^{ij}_{,k}(x)\xi_i\xi_j}{2\sqrt{g^{ij}(x)\xi_i\xi_j}}, \end{aligned}$$

Besides $\sqrt{g^{ij}(x)\xi_i\xi_j}$ is preserved along the trajectories. The advantage of the Hamilton equations for (9.10) is that they preserve conical sets—they are invariant wrt the scaling in ξ.

9.3 2nd order operators

Suppose that we have an operator on $C^\infty(M)$, which in coordinates has the form

$$L := g^{ij}(x)\partial_i\partial_j + b^i(x)\partial_i + c(x). \tag{9.11}$$

We will assume that g^{ij} is real and nondegenerate. When we change the coordinates, the principal symbol $g^{ij}\xi^i\xi^j$ does not change. Therefore, it can be interpreted as the metric tensor, so that M becomes a pseudo-Riemannian manifold.

Clearly, b_i and c depend on the choice of coordinates. To interpret (9.11) geometrically, choose a 1-form $A_i\mathrm{d}x^i$ and a 0-form V. Let u, w be (scalar) functions on M. The following expression does not depend on the coordinates:

$$\int |g|^{\frac{1}{2}}\Big(\overline{(-\mathrm{i}\partial_i u + A_i u)} g^{ij}(-\mathrm{i}\partial_j w + A_j w) + V\overline{u}w\Big)\mathrm{d}x. \tag{9.12}$$

After integrating by parts, (9.12) becomes

$$\int \overline{u}\Big(|g|^{-\frac12}(-\mathrm{i}\partial_i + A_i)|g|^{\frac12}g^{ij}(-\mathrm{i}\partial_j + A_j) + V\Big)w|g|^{\frac12}\mathrm{d}x. \tag{9.13}$$

Therefore, the geometric form of (9.11) on scalars, resp. on half-densities are

$$L := |g|^{-\frac12}(-\mathrm{i}\partial_i + A_i)|g|^{\frac12}g^{ij}(-\mathrm{i}\partial_j + A_j) + V, \tag{9.14}$$

$$L_{\frac12} := |g|^{-\frac14}(-\mathrm{i}\partial_i + A_i)|g|^{\frac12}g^{ij}(-\mathrm{i}\partial_j + A_j)|g|^{-\frac14} + V. \tag{9.15}$$

9.4 Equations second order in time

Consider the equation

$$r(t) = (\partial_t^2 + L)f(t), \tag{9.16}$$

where L is positive. Given $f(0)$, $f'(0)$ it can be solved as follows:

$$\begin{aligned} f(t) =& \frac{\mathrm{e}^{\mathrm{i}t\sqrt{L}}}{2\sqrt{L}}\Big(\sqrt{L}f(0) - \mathrm{i}f'(0) - \mathrm{i}\int_0^t \mathrm{e}^{-\mathrm{i}u\sqrt{L}}r(u)\mathrm{d}u\Big) \\ &+ \frac{\mathrm{e}^{-\mathrm{i}t\sqrt{L}}}{2\sqrt{L}}\Big(\sqrt{L}f(0) + \mathrm{i}f'(0) + \mathrm{i}\int_0^t \mathrm{e}^{\mathrm{i}u\sqrt{L}}r(u)\mathrm{d}u\Big). \end{aligned} \tag{9.17}$$

9.5 Wave equation–static case

Assume that g_{ij} is positive definite metric tensor on a manifold Σ. Consider the static wave (or Klein-Gordon) equation on $\mathbb{R}\times\Sigma$:

$$\Big(\partial_t^2 + |g|^{-\frac14}(-\mathrm{i}\partial_i + A_i)|g|^{\frac12}g^{ij}(-\mathrm{i}\partial_j + A_j)|g|^{-\frac14} + Y\Big)f = r. \tag{9.18}$$

It is of the form (9.16) with L given by (9.15). If L is positive, then we can apply (9.17) directly. If not, we can split it as

$$L = L_0 + Y,$$

where

$$L_0 := |g|^{-\frac14}(-\mathrm{i}\partial_i + A_i)|g|^{\frac12}g^{ij}(-\mathrm{i}\partial_j + A_j)|g|^{-\frac14} \tag{9.19}$$

is positive. Then we can rewrite (9.17) as

$$\begin{aligned} f(t) =& \frac{\mathrm{e}^{\mathrm{i}t\sqrt{L_0}}}{2\sqrt{L_0}}\Big(\sqrt{L_0}f(0) - \mathrm{i}f'(0) - \mathrm{i}\int_0^t \mathrm{e}^{-\mathrm{i}u\sqrt{L_0}}\big(r(u) - Y\big)f(u)\mathrm{d}u\Big) \\ &+ \frac{\mathrm{e}^{-\mathrm{i}t\sqrt{L_0}}}{2\sqrt{L_0}}\Big(\sqrt{L_0}f(0) + \mathrm{i}f'(0) + \mathrm{i}\int_0^t \mathrm{e}^{\mathrm{i}u\sqrt{L_0}}\big(r(u) - Yf(u)\big)\mathrm{d}u\Big). \end{aligned} \tag{9.20}$$

Theorem 9.1. *Suppose that $f, r \in L^{2,-\infty}$. Suppose that g, A, Y are smooth, $[g^{ij}]$ is positive. Let γ_t be the geodesic flow, that is, the flow on $\mathrm{T}^\#\mathbb{R}^d$ given by the Hamiltonian $\sqrt{g^{ij}(x)\xi_i\xi_j}$. Then*

$$\mathrm{WF}(f(t)) = \gamma_t\big(\mathrm{WF}(f(0)\big) \cup \bigcup_{0<s<t}\gamma_{t-s}\mathrm{WF}\big(r(s)\big). \tag{9.21}$$

Proof. If L is positive, we can use directly Theorem 8.27. If not, we can use (9.20). We note that $\frac{1}{\sqrt{L_0}}Y \in \Psi^{-1}$. Therefore, the statement follows by iterating (9.20). □

9.6 Wave equation—generic case

Suppose that M is a Lorentzian manifold. Consider the Klein-Gordon equation on M:

$$\Big(|g|^{-\frac14}(-\mathrm{i}\partial_\mu + A_\mu)|g|^{\frac12}g^{\mu\nu}(-\mathrm{i}\partial_\nu + A_\nu)|g|^{-\frac14} \; + Y\Big)f = r. \tag{9.22}$$

We say that a hypersurface $\mathcal{S}$ is Cauchy if it is spatial and every geodesics intersects $\mathcal{S}$ exactly once. We say that M is globally hyperbolic if it possesses a Cauchy surface.

For a geodesic γ given by $\mathbb{R} \ni t \mapsto x^\mu(t)$, we define its lift to $T^\#_{\neq 0}M$ by

$$\tilde\gamma := \big\{\big(x^\mu(t), \lambda\dot x^\mu(t) g_{\mu\nu}\big(x(t)\big)\ \mid\ t\in\mathbb{R},\quad \lambda\neq 0\big\}.$$

Introduce the *characteristic set of the equation (9.22)*

$$\mathrm{Char} := \{(x,\xi)\in T^\#_{\neq 0}M \mid \xi_\mu\xi_\nu g(x) = 0\}.$$

Note that Char is a closed conical set. It is a disjoint union of lifts of null geodesics.

Theorem 9.2. *We assume that M is globally hyperbolic. Suppose that $f, r \in L^{2,-\infty}$ satisfy (9.22). Then*

$$\mathrm{WF}(f) \subset \mathrm{Char} \cup \mathrm{WF}(r).$$

Besides, if $\tilde\gamma$ is a null geodesic lifted to the cotangent bundle $T^\#_{\neq 0}M$, then $\mathrm{WF}(f)\cap\tilde\gamma$ *is a union of intervals whose ends are contained in* $\mathrm{WF}(r)$ *or are infinite.*

In order to analyse (9.22) it is useful to identify (at least locally) M with $\mathbb{R}\times\Sigma$, such that the metric $g = [g_{\mu\nu}]$ restricted to Σ, denoted g_Σ, was spatial. Equivalently, $\mathrm{d}t$ is timelike. Thus M is foliated by Cauchy surfaces. (It is a nontrivial fact that you can do it on a globally hyperbolic manifold).

10 Path integrals

In this section $\hbar = 1$ and we do not put hats on p and x. We will be not very precise concerning the limits – often lim may mean the strong limit.

10.1 Evolution

Suppose that we have a family of operators $t\mapsto B(t)$ depending on a real variable. Typically, we will assume that $B(t)$ are generators of 1-parameter groups (eg. i times a self-adjoint operator). Under certain conditions on the continuity that we will not discuss there exists a unique operator function that in appropriate sense satisfies

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t_+}U(t_+,t_-) &= B(t_+)U(t_+,t_-),\\ U(t,t) &= 1\!\!1.\end{aligned}$$

It also satisfies

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t_-}U(t_+,t_-) &= -U(t_+,t_-)B(t_-),\\ U(t_2,t_1)U(t_1,t_0) &= U(t_2,t_0).\end{aligned}$$

If $B(t)$ are bounded then

$$U(t_+,t_-)=\sum_{n=0}^{\infty}\ \underset{t_+>t_n>\cdots>t_1>t_-}{\int\cdots\int} B(t_n)\cdots B(t_1)\mathrm{d}t_n\cdots\mathrm{d}t_1.$$

We will write

$$\mathrm{Texp}\left(\int_{t_-}^{t_+}B(t)\mathrm{d}t\right):=U(t_+,t_-).$$

In particular, if $B(t)=B$ does not depend on time, then $U(t_+,t_-)=\mathrm{e}^{(t_+-t_-)B}$.

In what follows we will restrict ourselves to the case $t_-=0$ and $t_+=t$ and we will consider

$$U(t):=\mathrm{Texp}\left(\int_0^t B(s)\mathrm{d}s\right). \tag{10.1}$$

Note that the whole evolution can be retrieved from (10.1) by

$$U(t_+,t_-)=U(t_+)U(t_-)^{-1}.$$

We have

$$U(t)=\lim_{n\to\infty}\prod_{j=1}^{n}\mathrm{e}^{\frac{t}{n}B(\frac{jt}{n})}. \tag{10.2}$$

(In multiple products we will assume that the factors are ordered from the right to the left).

Now suppose that $F(s,u)$ is an operator function such that uniformly in s

$$\begin{aligned}\mathrm{e}^{uB(s)}-F(s,u) &= o(u),\\ \|F(s,u)\| &\leq C.\end{aligned}$$

Then

$$U(t)=\lim_{n\to\infty}\prod_{j=1}^{n}F\Big(\frac{jt}{n},\frac{t}{n}\Big). \tag{10.3}$$

Indeed,

$$\begin{aligned}&\prod_{j=1}^{n}\mathrm{e}^{\frac{t}{n}B(\frac{jt}{n})}-\prod_{j=1}^{n}F\Big(\frac{jt}{n},\frac{t}{n}\Big)\\ =\ &\sum_{k=1}^{n}\prod_{j=k+1}^{n}F\Big(\frac{jt}{n},\frac{t}{n}\Big)\left(\mathrm{e}^{\frac{t}{n}B(\frac{kt}{n})}-F\Big(\frac{kt}{n},\frac{t}{n}\Big)\right)\prod_{j=1}^{k-1}\mathrm{e}^{\frac{t}{n}B(\frac{jt}{n})}\\ =\ &no(n^{-1})\underset{n\to\infty}{\to}0.\end{aligned}$$

Example 10.1. (1) $F(s,u) = \mathbb{1} + uB(s)$. *Thus*

$$U(t) = \lim_{n\to\infty} \prod_{j=1}^{n} \left(\mathbb{1} + \frac{t}{n} B\Big(\frac{jt}{n}\Big) \right).$$

Strictly speaking, this works only if $B(t)$ is uniformly bounded.

In particular,

$$\mathrm{e}^{tB} = \lim_{n\to\infty} \Big(\mathbb{1} + \frac{t}{n} B \Big)^{n}.$$

(2) $F(s,u) = \big(\mathbb{1} - uB(s)\big)^{-1}$. *Then*

$$U(t) := \lim_{n\to\infty} \prod_{j=1}^{n} \left(\mathbb{1} - \frac{t}{n} B\Big(\frac{jt}{n}\Big) \right)^{-1}.$$

This should work also if $B(t)$ is unbounded.

In particular,

$$\mathrm{e}^{tB} = \lim_{n\to\infty} \Big(\mathbb{1} - \frac{t}{n} B \Big)^{-n}.$$

(3) *Suppose that $B(t) = A(t) + C(t)$, where both $A(t)$ and $C(t)$ are generators of semigroups. Set $F(s,u) = \mathrm{e}^{uA(t)}\mathrm{e}^{uC(t)}$. Thus*

$$U(t) = \lim_{n\to\infty} \prod_{j=1}^{n} \mathrm{e}^{\frac{t}{n}A(\frac{jt}{n})}\mathrm{e}^{\frac{t}{n}C(\frac{jt}{n})}. \tag{10.4}$$

In particular, we obtain the Lie-Trotter formula

$$\mathrm{e}^{t(A+C)} = \lim_{n\to\infty} \Big(\mathrm{e}^{\frac{t}{n}A}\mathrm{e}^{\frac{t}{n}C} \Big)^{n}.$$

10.2 Scattering operator

We will usually assume that the dynamics is generated by $\mathrm{i}H(t)$ where $H(t)$ is a self-adjoint operator. Often,

$$H(t) = H_0 + V(t),$$

where H_0 is a fixed self-adjoint operator. The evolution in the interaction picture is

$$S(t_+, t_-) \quad := \quad \mathrm{e}^{\mathrm{i}t_+ H_0} \mathrm{Texp}\Big(- \mathrm{i} \int_{t_-}^{t_+} H(t)\mathrm{d}t \Big) \mathrm{e}^{-\mathrm{i}t_- H_0}.$$

The scattering operator is defined as

$$S \quad := \quad \lim_{t_+, -t_- \to\infty} S(t_+, t_-).$$

Introduce the Hamiltonian in the interaction picture

$$H_{\mathrm{Int}}(t) := \mathrm{e}^{\mathrm{i}tH_0} V(t) \mathrm{e}^{-\mathrm{i}tH_0}.$$

Note that

$$\begin{aligned}
\partial_{t_+} S(t_+, t_-) &= -\mathrm{i} H_{\mathrm{Int}}(t_+) S(t_+, t_-), \\
\partial_{t_-} S(t_+, t_-) &= \mathrm{i} S(t_+, t_-) H_{\mathrm{Int}}(t_+), \\
S(t, t) &= \mathbb{1}.
\end{aligned}$$

Therefore,

$$\begin{aligned}
S(t_+, t_-) &= \mathrm{Texp}\Big(-\mathrm{i} \int_{t_-}^{t_+} H_{\mathrm{Int}}(t) \mathrm{d}t \Big), \\
S &= \mathrm{Texp}\Big(-\mathrm{i} \int_{-\infty}^{\infty} H_{\mathrm{Int}}(t) \mathrm{d}t \Big)
\end{aligned}$$

10.3 Bound state energy

Suppose that Φ_0 and E_0, resp. Φ and E are eigenvectors and eigenvalues of H_0, resp H, so that

$$H_0 \Phi_0 = E_0 \Phi_0, \qquad H\Phi = E\Phi.$$

We assume that Φ, E are small perturbations of Φ_0, E_0 when the coupling constant λ is small enough.

The following heuristic formulas can be sometimes rigorously proven:

$$E - E_0 = \lim_{t \to \pm\infty} (2\mathrm{i})^{-1} \frac{\mathrm{d}}{\mathrm{d}t} \log(\Phi_0 | \mathrm{e}^{-\mathrm{i}tH_0} \mathrm{e}^{\mathrm{i}2tH} \mathrm{e}^{-\mathrm{i}tH_0} \Phi_0). \tag{10.5}$$

To see why we can expect (10.5) to be true, we write

$$(\Phi_0 | \mathrm{e}^{-\mathrm{i}tH_0} \mathrm{e}^{\mathrm{i}2tH} \mathrm{e}^{-\mathrm{i}tH_0} \Phi_0) = |(\Phi_0|\Phi)|^2 \mathrm{e}^{\mathrm{i}2t(E-E_0)} + C(t).$$

Then, if we can argue that for large t the term $C(t)$ does not play a role, we obtain (10.5).

10.4 Path integrals for Schrödinger operators

We consider

$$\begin{aligned}
h(t, x, p) &:= \frac{1}{2} p^2 + V(t, x), \\
H(t) := \mathrm{Op}(h(t)) &= -\frac{1}{2} \Delta + V(t, x), \\
U(t) &:= \mathrm{Texp}\left(-\mathrm{i} \int_0^t H(s) \mathrm{d}s \right).
\end{aligned} \tag{10.6}$$

We have

$$\mathrm{e}^{-\frac{\mathrm{i}}{2} t\Delta}(x, y) = (2\pi \mathrm{i}t)^{-d/2} \mathrm{e}^{\frac{\mathrm{i}}{2t}(x-y)^2}.$$

From

$$U(t) \quad = \quad \lim_{n\to\infty} \prod_{j=1}^{n} \mathrm{e}^{-\mathrm{i}\frac{t}{n}V(\frac{jt}{n},x)}\mathrm{e}^{\mathrm{i}\frac{t}{2n}\Delta}$$

we obtain

$$\begin{aligned}
U(t,x,y) &= \lim_{n\to\infty}\int \mathrm{d}x_{n-1}\cdots\int \mathrm{d}x_1 \prod_{j=1}^{n}\Big(\frac{2\pi\mathrm{i}t}{n}\Big)^{-\frac{d}{2}} \mathrm{e}^{\frac{\mathrm{i}n(x_{j-1}-x_j)^2}{2t}-\mathrm{i}\frac{t}{n}V(\frac{jt}{n},x_j)}\Big|_{\substack{y=x_0,\\ x=x_n.}} \\
&= \lim_{n\to\infty}\Big(\frac{2\pi\mathrm{i}t}{n}\Big)^{-\frac{dn}{2}}\int \mathrm{d}x_{n-1}\cdots\int \mathrm{d}x_1 \\
&\quad\times\exp\left(\frac{\mathrm{i}t}{n}\sum_{j=1}^{n}\Big(\frac{n^2(x_{j-1}-x_j)^2}{2t^2}-V\Big(\frac{jt}{n},x_j\Big)\Big)\right)\Big|_{\substack{y=x_0,\\ x=x_n.}} .
\end{aligned}$$

Heuristically, this is written as

$$U(t,x,y) = \int \exp\Big(\mathrm{i}\int_0^t L\big(s,x(s),\dot{x}(s)\big)\mathrm{d}s\Big)\mathcal{D}_{x,y}\big(x(\cdot)\big),$$

where

$$L(s,x,\dot{x}) := \frac{1}{2}\dot{x}^2 - V(s,x)$$

is the Lagrangian and

$$\mathcal{D}_{x,y}\big(x(\cdot)\big) := \lim_{n\to\infty}\Big(\frac{2\pi\mathrm{i}t}{n}\Big)^{-\frac{dn}{2}}\mathrm{d}x\Big(\frac{(n-1)t}{n}\Big)\cdots\mathrm{d}x\Big(\frac{t}{n}\Big) \tag{10.7}$$

is some kind of a limit of the Lebesgue measure on paths $[0,t]\ni s\mapsto x(s)$ such that $x(0)=y$ and end up at $x(t)=x$.

10.5 Example–the harmonic oscillator

Let

$$H = \frac{1}{2}p^2 + \frac{1}{2}x^2.$$

It is well-known that for $t\in]0,\pi[$,

$$\mathrm{e}^{-\mathrm{i}tH}(x,y) = (2\pi\mathrm{i}\sin t)^{-\frac{1}{2}}\exp\Big(\frac{-(x^2+y^2)\cos t + 2xy}{2\mathrm{i}\sin t}\Big). \tag{10.8}$$

(10.8) is called the Mehler formula.

We will derive (10.8) from the path integral formalism. We will use the explicit formula for the free dynamics with $H_0 = \frac{1}{2}p^2$:

$$\mathrm{e}^{-\mathrm{i}tH_0}(x,y) = (2\pi\mathrm{i}t)^{-\frac{1}{2}}\exp\Big(\frac{-(x-y)^2}{2\mathrm{i}t}\Big). \tag{10.9}$$

For $t \in]0,\pi[$, there exists a unique trajectory for H starting from y and ending at x. Similarly (with no restriction on time) there exists a unique trajectory for H_0:

$$x_{\rm cl}(s) = \frac{\cos(s-\frac{t}{2})}{\cos\frac{t}{2}}(x+y) + \frac{\sin(s-\frac{t}{2})}{\sin\frac{t}{2}}(x-y), \tag{10.10}$$

$$x_{0,\rm cl}(s) = x\frac{s}{t} + y\frac{(t-s)}{t}. \tag{10.11}$$

Now we set $x(s) = x_{\rm cl}(s) + z(s)$ and obtain

$$\int_0^t L\big(x(s),\dot{x}(s)\big){\rm d}s = \int_0^t \frac{1}{2}\big(\dot{x}^2(s) - x^2(s)\big){\rm d}s \tag{10.12}$$

$$= \int_0^t L\big(x_{\rm cl}(s),\dot{x}_{\rm cl}(s)\big){\rm d}s + \int_0^t L\big(z(s),\dot{z}(s)\big){\rm d}s \tag{10.13}$$

$$= \frac{(x^2+y^2)\cos t - 2xy}{2\sin t} + \int_0^t \frac{1}{2}\big(\dot{z}^2(s) - z^2(s)\big){\rm d}s. \tag{10.14}$$

Similarly, setting $x(s) = x_{0,\rm cl}(s) + z(s)$ we obtain

$$\int_0^t L_0\big(x(s),\dot{x}(s)\big){\rm d}s = \int_0^t \frac{1}{2}\dot{x}^2(s){\rm d}s \tag{10.15}$$

$$\tag{10.16}$$

$$= \frac{(x-y)^2}{2t} + \int_0^t \frac{1}{2}\dot{z}^2(s){\rm d}s. \tag{10.17}$$

Therefore,

$$\frac{{\rm e}^{-{\rm i}tH}(x,y)}{{\rm e}^{-{\rm i}tH_0}(x,y)} = \frac{\int \exp\Big({\rm i}\int_0^t L\big(x(s),\dot{x}(s)\big){\rm d}s\Big)\mathcal{D}_{x,y}\big(x(\cdot)\big)}{\int \exp\Big({\rm i}\int_0^t L_0\big(x(s),\dot{x}(s)\big){\rm d}s\Big)\mathcal{D}_{x,y}\big(x(\cdot)\big)} \tag{10.18}$$

$$= \frac{\int \exp\Big({\rm i}\frac{(x^2+y^2)\cos t-2xy}{2\sin t} + {\rm i}\int_0^t \frac{1}{2}\big(\dot{z}^2(s)-z^2(s)\big){\rm d}s\Big)\mathcal{D}_{0,0}\big(z(\cdot)\big)}{\int \exp\Big({\rm i}\frac{(x-y)^2}{2t} + {\rm i}\int_0^t \frac{1}{2}\dot{z}^2(s){\rm d}s\Big)\mathcal{D}_{0,0}\big(z(\cdot)\big)} \tag{10.19}$$

$$= \det\left(\frac{\frac{\rm i}{2}(-\Delta)}{\frac{\rm i}{2}(-\Delta-1)}\right)^{\frac{1}{2}} \frac{\exp\Big({\rm i}\frac{(x^2+y^2)\cos t-2xy}{2\sin t}\Big)}{\exp\Big({\rm i}\frac{(x-y)^2}{2t}\Big)} \tag{10.20}$$

Here $-\Delta$ denotes the minus Laplacian with the Dirichlet boundary conditions on the interval $[0,t]$. Its spectrum is $\Big\{\frac{\pi^2k^2}{t^2} \mid k=1,2,\dots\Big\}$. Therefore, at least formally,

$$\det\left(\frac{\frac{\rm i}{2}(-\Delta)}{\frac{\rm i}{2}(-\Delta-1)}\right) = \frac{1}{\det\Big(1\!\!1 + \Delta^{-1}\Big)} \tag{10.21}$$

$$= \prod_{k=1}^{\infty}\Big(1 - \frac{t^2}{\pi^2k^2}\Big) = \frac{t}{\sin t}. \tag{10.22}$$

Now (10.9) implies (10.8).

10.6 Path integrals for Schrödinger operators with the imaginary time

Let us repeat the same computation for the evolution generated by

$$-H(t) = -\big(-\Delta + V(t,x)\big).$$

We add the superscript E for "Euclidean":

$$U^{\mathrm{E}}(t) := \mathrm{Texp}\left(-\int_0^t H(s)\mathrm{d}s\right) \quad = \quad \lim_{n\to\infty}\prod_{j=1}^n \mathrm{e}^{-\frac{t}{n}V(\frac{jt}{n},x)}\mathrm{e}^{\frac{t}{n}\Delta}.$$

Using

$$\mathrm{e}^{\frac12 t\Delta}(x,y) = (2\pi t)^{-d/2}\mathrm{e}^{-\frac{1}{2t}(x-y)^2}.$$

we obtain

$$\begin{aligned} U^{\mathrm{E}}(t,x,y) \quad &= \quad \lim_{n\to\infty}\Big(\frac{2\pi t}{n}\Big)^{-\frac{dn}{2}}\int \mathrm{d}x_{n-1}\cdots\int \mathrm{d}x_1 \\ &\times\exp\left(\frac{t}{n}\sum_{j=1}^n\Big(\frac{-n^2(x_j-x_{j-1})^2}{2t^2} - V\Big(\frac{jt}{n},x_j\Big)\Big)\right)\Bigg|_{\substack{y=x_0,\\ x=x_n.}} . \end{aligned}$$

Heuristically, this is written as

$$U^{\mathrm{E}}(t,x,y) = \int \exp\Big(-\int_0^t L^{\mathrm{E}}\big(s,x(s),\dot{x}(s)\big)\mathrm{d}s\Big)\mathcal{D}^{\mathrm{E}}_{x,y}\big(x(\cdot)\big),$$

where

$$L^{\mathrm{E}}(s,x,\dot{x}) := \frac12\dot{x}^2 + V\big(s,x\big)$$

is the "Euclidean Lagrangian" and

$$\mathcal{D}^{\mathrm{E}}_{x,y}(x(\cdot)) := \lim_{n\to\infty}\Big(\frac{2\pi t}{n}\Big)^{-\frac{dn}{2}}\mathrm{d}x\Big(\frac{(n-1)t}{n}\Big)\cdots\mathrm{d}x\Big(\frac{t}{n}\Big)$$

is similar to (10.7).

10.7 Wiener measure

$$\mathrm{d}W_y\big(x(\cdot)\big) = \exp\Big(-\int_0^t \frac12\dot{x}^2(s)\Big)\mathrm{d}s\mathcal{D}^{\mathrm{E}}_{x(t),y}\big(x(\cdot)\big)\mathrm{d}x(t)$$

can be interpreted as a measure on paths, functions $[0,t]\ni s\mapsto x(s)$ such that $x(0)=y$—the Wiener measure.

Let us fix $t_n > \cdots > t_1 > 0$, and F is a function on the space of paths depending only on $x(t_n), \dots, x(t_1)$ (such a function is called a cylinder function). Thus

$$F\big(x(\cdot)\big) = F_{t_n,\dots,t_1}\big(x(t_n), \dots, x(t_1)\big).$$

Then we set

$$\begin{aligned}
&\int \mathrm{d}W_y\big(x(\cdot)\big)F\big(x(\cdot)\big) \qquad (10.23)\\
&= \int F_{t_n,\dots,t_1}(x_n,\dots,x_1)\frac{\mathrm{e}^{-\frac{(x_n-x_{n-1})^2}{2(t_n-t_{n-1})}}}{\big(2\pi(t_n-t_{n-1})\big)^{\frac{d}{2}}}\mathrm{d}x_n \cdots \frac{\mathrm{e}^{-\frac{(x_2-x_1)^2}{2(t_2-t_1)}}}{\big(2\pi(t_2-t_1)\big)^{\frac{d}{2}}}\mathrm{d}x_2\frac{\mathrm{e}^{-\frac{(x_1-y)^2}{2t_1}}}{\big(2\pi t_1\big)^{\frac{d}{2}}}\mathrm{d}x_1.
\end{aligned}$$

We easily check the correctness of the definition on all cylinder functions. Then we extend the measure to a larger space of paths–there are various possibilities.

We can use the Wiener measure to (rigorously) express the integral kernel of $U^{\mathrm{E}}(t)$. Let $\Phi, \Psi \in L^2(\mathbb{R}^d)$. Then the so-called Feynman-Katz formula says

$$\begin{aligned}
&(\Phi|U^{\mathrm{E}}(t)\Psi) \qquad (10.24)\\
&= \int \mathrm{d}x(0)\int \mathrm{d}W_{x(0)}\big(x(\cdot)\big)\overline{\Phi\big(x(t)\big)}\Psi\big(x(0)\big)\exp\Big(-\int_0^t V\big(s,x(s)\big)\mathrm{d}s\Big).
\end{aligned}$$

Theorem 10.2. *Let $t, t_1, t_2 > 0$. Then*

$$\int x(t)\mathrm{d}W_0\big(x(\cdot)\big) = 0, \qquad (10.25)$$

$$\int x_i(t_2)x_j(t_1)\mathrm{d}W_0\big(x(\cdot)\big) = \delta_{ij}\min(t_2,t_1), \qquad (10.26)$$

$$\int \big(x(t_2)-x(t_1)\big)^2\mathrm{d}W_0\big(x(\cdot)\big) = d|t_2-t_1|. \qquad (10.27)$$

Proof. Let us prove (10.26). Let $t_2 > t_1$. Then

$$\int x(t_2)x(t_1)\mathrm{d}W_0\big(x(\cdot)\big) = \int\int x_2\frac{\mathrm{e}^{-\frac{(x_2-x_1)^2}{2(t_2-t_1)}}}{(2\pi(t_2-t_1))^{\frac{d}{2}}}x_1\frac{\mathrm{e}^{-\frac{x_1^2}{2t_1}}}{(2\pi t_1)^{\frac{d}{2}}}\mathrm{d}x_1\mathrm{d}x_2 \qquad (10.28)$$

$$= \int x_1^2\frac{\mathrm{e}^{-\frac{x_1^2}{2t_1}}}{(2\pi t_1)^{\frac{d}{2}}}\mathrm{d}x_1 \quad = \quad t_1. \qquad (10.29)$$

□

Recall the formula (**??**)

$$\mathrm{e}^{\frac{1}{2}\partial_x\cdot\nu\partial_x}\Psi(0) \quad = \quad (\det 2\pi\nu)^{-\frac{1}{2}}\int \Psi(x)\mathrm{e}^{-\frac{1}{2}x\cdot\nu^{-1}x}\mathrm{d}x, \qquad (10.30)$$

which says that for Gaussian measures you can "integrate by differentiating". The Wiener measure is Gaussian, and in this case (10.30) has the form

$$\int \mathrm{d}W_0\big(x(\cdot)\big)F\big(x(\cdot)\big) = \exp\Big(\frac{1}{2}\partial_{x(s_2)}\min(s_2,s_1)\partial_{x(s_1)}\Big)F\big(x(\cdot)\big). \qquad (10.31)$$

Indeed, the operator whose quadratic form appears in the Wiener measure is the Laplacian on $[0,t]$, which is Dirichlet at 0 and Neumann at t. Now the operator with the integral kernel $\min(t_2,t_1)$ is the inverse of this Laplacian.

10.8 General Hamiltonians – Weyl quantization

Let $[0,t]\ni s\mapsto h(s,x,p)\in\mathbb{R}$ be a time dependent classical Hamiltonian. Set

$$H(s):=\mathrm{Op}\big(h(s)\big)$$

and $U(t)$ as in (10.6).

Lemma 10.3.

$$\mathrm{e}^{-\mathrm{i}u\mathrm{Op}\left(h(s)\right)}-\mathrm{Op}\big(\mathrm{e}^{-\mathrm{i}uh(s)}\big)=O(u^3). \tag{10.32}$$

Proof. Let us drop the reference to s in $h(s)$. We have

$$\frac{\mathrm{d}}{\mathrm{d}u}\mathrm{e}^{\mathrm{i}u\mathrm{Op}(h)}\mathrm{Op}\big(\mathrm{e}^{-\mathrm{i}uh}\big) = \mathrm{i}\mathrm{e}^{\mathrm{i}u\mathrm{Op}(h)}\Big(\mathrm{Op}(h)\mathrm{Op}\big(\mathrm{e}^{-\mathrm{i}uh}\big)-\mathrm{Op}\big(h\mathrm{e}^{-\mathrm{i}uh}\big)\Big). \tag{10.33}$$

Now

$$\mathrm{Op}(h)\mathrm{Op}(\mathrm{e}^{-\mathrm{i}uh})=\mathrm{Op}\big(h\mathrm{e}^{-\mathrm{i}uh}\big)+\frac{\mathrm{i}}{2}\mathrm{Op}\big(\{h,\mathrm{e}^{-\mathrm{i}uh}\}\big)+O(u^2). \tag{10.34}$$

The second term on the right of (10.34) is zero. Therefore, (10.33) is $O(u^2)$. Clearly, $\mathrm{e}^{\mathrm{i}u\mathrm{Op}(h)}\mathrm{Op}\big(\mathrm{e}^{-\mathrm{i}uh}\big)\big|_{u=0}=1\!\!1$. Integrating $O(u^2)$ from 0 we obtain $O(u^3)$. □

Thus we can use $F(s,u):=\mathrm{Op}\big(\mathrm{e}^{-\mathrm{i}uh(s)}\big)$ in (10.3), so that

$$U(t) = \lim_{n\to\infty}\prod_{j=1}^{n}\mathrm{Op}\Big(\mathrm{e}^{-\mathrm{i}\frac{t}{n}h\left(\frac{jt}{n}\right)}\Big)$$

Thus

$$\begin{aligned}U(t,x,y) &= \lim_{n\to\infty}\int\cdots\int\prod_{j=1}^{n}\exp\left(-\tfrac{\mathrm{i}t}{n}h\left(\tfrac{jt}{n},\tfrac{x_j+x_{j-1}}{2},p_j\right)+\mathrm{i}(x_j-x_{j-1})p_j\right)\\ &\quad\times\prod_{j=1}^{n-1}\mathrm{d}x_j\prod_{j=1}^{n}\frac{\mathrm{d}p_j}{(2\pi)^d}\Big|_{\substack{y=x_0,\\ x=x_n.}}\end{aligned} \tag{10.35}$$

$$\begin{aligned}&= \lim_{n\to\infty}\int\cdots\int\exp\left(\tfrac{\mathrm{i}t}{n}\sum_{j=0}^{n}\left(\tfrac{(x_j-x_{j-1})p_j}{\frac{t}{n}}-h\left(\tfrac{jt}{n},\tfrac{x_j+x_{j-1}}{2},p_j\right)\right)\right)\\ &\quad\times\prod_{j=1}^{n-1}\mathrm{d}x_j\prod_{j=1}^{n}\frac{\mathrm{d}p_j}{(2\pi)^d}\Big|_{\substack{y=x_0,\\ x=x_n.}}\;.\end{aligned} \tag{10.36}$$

Heuristically, this is written as follows:

$$U(t,x,y) \quad = \quad \int \mathrm{D}_{x,y}\left(x(\cdot)\right)\mathrm{D}\left(p(\cdot)\right)\exp\left(\mathrm{i}\int_0^t\left(\dot{x}(s)p(s)-h(s,x(s),p(s)\right)\mathrm{d}s\right),$$

where $[0,t]\ni s\mapsto(x(s),p(s))$ is an arbitrary phase space trajectory with $x(0)=y$, $x(t)=x$ and the "measure on the phase space paths" is

$$\mathrm{D}_{x,y}\left(x(\cdot)\right)=\lim_{n\to\infty}\prod_{j=1}^{n-1}\mathrm{d}x\Big(\frac{jt}{n}\Big),\quad \mathrm{D}\big(p(\cdot)\big)=\prod_{j=1}^{n}\frac{\mathrm{d}p\Big((j-\frac{1}{2})\frac{t}{n}\Big)}{(2\pi)^d}.$$

10.9 Hamiltonians quadratic in momenta I

Assume in addition that

$$h(t,x,p)=\frac{1}{2}(p-A(t,x))^2+V(t,x). \tag{10.37}$$

Then

$$\mathrm{Op}\big(h(t)\big) \quad = \quad \frac{1}{2}(p_i-A_i(t,x))^2+V(t,x).$$

Introduce

$$v=p-A(t,x).$$

The Lagrangian for (10.37) is

$$L(t,x,v)=\frac{1}{2}v^2+vA(t,x)-V(t,x).$$

Consider the phase space path integral (10.36). The exponent depends quadratically on p. Therefore, we can integrate it out, obtaining a configuration space path integral. More precisely, first we make the change of variables

$$v_j=p_j-A\big(\tfrac{jt}{n},\tfrac{x_j+x_{j-1}}{2}\big),$$

and then we do the integration wrt v:

$$\begin{aligned}
U(t,x,y) \quad &= \quad \lim_{n\to\infty}\int\cdots\int\exp\left(\tfrac{\mathrm{i}t}{n}\sum_{j=1}^{n}\Big(\tfrac{(x_j-x_{j-1})}{\frac{t}{n}}\big(v_j+A(\tfrac{jt}{n},\tfrac{x_j+x_{j-1}}{2})\big)\right.\\
&\qquad \left.-\frac{1}{2}v_j^2-V\big(\tfrac{jt}{n},\tfrac{x_j+x_{j-1}}{2}\big)\Big)\right)\prod_{j=1}^{n-1}\mathrm{d}x_j\prod_{j=1}^{n}\frac{\mathrm{d}v_j}{(2\pi)^d}\Bigg|_{\substack{y=x_0,\\ x=x_n}}\\
&= \quad \lim_{n\to\infty}\int\cdots\int\exp\left(\tfrac{\mathrm{i}t}{n}\sum_{j=1}^{n}L\left(\frac{jt}{n},\frac{x_j+x_{j-1}}{2},\frac{(x_j-x_{j-1})}{\frac{t}{n}}\right)\right)\\
&\qquad\times(2\pi\tfrac{\mathrm{i}t}{n})^{-n\frac{d}{2}}\prod_{j=1}^{n-1}\mathrm{d}x_j\Bigg|_{\substack{y=x_0,\\ x=x_n}}.
\end{aligned} \tag{10.38}$$

Heuristically, this is written as

$$U(t,x,y) \quad = \quad \int \mathcal{D}_{x,y}\left(x(\cdot)\right) \exp\left(\mathrm{i}\int_0^t L(s,x(s),\dot{x}(s))\mathrm{d}s\right),$$

where $[0,t] \ni s \mapsto x(s)$ is a configuration space trajectory with $x(0) = y$, $x(t) = x$ and the formal "measure on the configuration space paths" is the same as in (10.7)

10.10 Hamiltonians quadratic in momenta II

Suppose, more generally, that

$$h(t,x,p) = \frac{1}{2}(p_i - A_i(t,x))g^{ij}(t,x)(p_j - A_j(t,x)) + V(t,x). \tag{10.39}$$

Then

$$\begin{aligned}\mathrm{Op}\big(h(t)\big) \quad &= \quad \frac{1}{2}(p_i - A_i(t,x))g^{ij}(t,x)(p_j - A_j(t,x)) + V(t,x) \\ &\quad -\frac{1}{4}\sum_{ij}\partial_{x^i}\partial_{x^j}g^{ij}(t,x).\end{aligned}$$

(For brevity, $[g^{ij}]$ will be denoted g^{-1} and $[g_{ij}]$ is denoted g)

Introduce

$$v = g^{-1}(t,x)\big(p - A(t,x)\big)$$

The Lagrangian for (10.39) is

$$L(t,x,v) = \frac{1}{2}v^i g_{ij}(t,x)v^j + v^j A_j(t,x) - V(t,x).$$

Consider the phase space path integral (10.36). The exponent depends quadratically on p. Therefore, we can integrate it out, obtaining a configuration space path integral. More precisely, first we do the integration wrt $p(\cdot)$:

$$\begin{aligned}U(t,x,y) \quad &= \quad \int \mathrm{D}_{x,y}\big(x(\cdot)\big)\mathrm{D}\big(p(\cdot)\big)\exp\Bigg(\mathrm{i}\int_0^t \Big(\dot{x}(s)p(s) \\ &\quad -\frac{1}{2}\big(p(s) - A(s,x(s)\big)g^{-1}\big(s,x(s)\big)\big(p(s) - A\big(s,x(s)\big) - V\big(s,x(s)\big)\Big)\mathrm{d}s\Bigg) \\ &= \quad \int \mathcal{D}_{x,y}\big(x(\cdot)\big)\exp\Bigg(\mathrm{i}\int_0^t \Big(\frac{1}{2}\dot{x}(s)g\big(s,x(s)\big)\dot{x}(s) + \dot{x}(s)A\big(s,x(s)\big) - V\big(s,x(s)\big)\Big)\mathrm{d}s \\ &\quad +\frac{1}{2}\int_0^t \mathrm{Tr}g\big(s,x(s)\big)\mathrm{d}s\Bigg) \\ &= \quad \int \mathcal{D}_{x,y}\left(x(\cdot)\right)\exp\left(\int_0^t \Big(\mathrm{i}L(s,x(s),\dot{x}(s)) + \frac{1}{2}\mathrm{Tr}g\big(s,x(s)\big)\Big)\mathrm{d}s\right).\end{aligned} \tag{10.40}$$

10.11 Semiclassical path integration

Let us repeat the most important formulas in the presence of a Planck constant $\hbar$.

$$U(t) \quad := \quad \mathrm{Texp}\left(-\frac{\mathrm{i}}{\hbar}\int_0^t H(s)\mathrm{d}s\right). \tag{10.41}$$

$$U(t,x,y) \quad = \quad \int \mathrm{D}_{x,y}\left(x(\cdot)\right)\mathrm{D}\left(\hbar^{-1}p(\cdot)\right)\exp\left(\frac{\mathrm{i}}{\hbar}\int_0^t \left(\dot{x}(s)p(s) - h(s,x(s),p(s))\right)\mathrm{d}s\right),$$

We assume in addition that the Hamiltonian has the form (10.39), and we set

$$x(s) = x_{\mathrm{cl}}(s) + \sqrt{\hbar}z(s),$$

where x_{cl} is the classical solution such that $x_{\mathrm{cl}}(0) = y$ and $x_{\mathrm{cl}}(t) = x$.

$$\begin{aligned}
U(t,x,y) \quad &= \quad \hbar^{-\frac{d}{2}}\int \mathcal{D}_{x,y}\left(\hbar^{-\frac{1}{2}}x(\cdot)\right)\exp\left(\frac{\mathrm{i}}{\hbar}\int_0^t L(s,x(s),\dot{x}(s))\mathrm{d}s\right) \\
&= \quad \hbar^{-\frac{d}{2}}\exp\left(\frac{\mathrm{i}}{\hbar}\int_0^t L(s,x_{\mathrm{cl}}(s),\dot{x}_{\mathrm{cl}}(s))\mathrm{d}s\right) \\
&\quad \times\int \mathcal{D}_{0,0}\left(z(\cdot)\right)\exp\Bigg(\frac{\mathrm{i}}{2}\int_0^t \Big(\partial_{x(s)}^2 L\big(s,x_{\mathrm{cl}}(s),x_{\mathrm{cl}}(s)\big)z(s)z(s) \\
&\quad\quad +2\partial_{x(s)}\partial_{\dot{x}(s)}L\big(s,x_{\mathrm{cl}}(s),x_{\mathrm{cl}}(s)\big)z(s)\dot{z}(s) \\
&\quad\quad +\partial_{\dot{x}(s)}^2 L\big(s,x_{\mathrm{cl}}(s),x_{\mathrm{cl}}(s)\big)\dot{z}(s)\dot{z}(s) + O(\sqrt{\hbar})\Big)\mathrm{d}s\Bigg) \\
&= \hbar^{-\frac{d}{2}}\det\left(\frac{1}{2\pi}\begin{bmatrix} \int_0^t \partial_{x(s)}^2 L\big(s,x_{\mathrm{cl}}(s),x_{\mathrm{cl}}(s)\big) & \int_0^t \partial_{x(s)}\partial_{\dot{x}(s)}L\big(s,x_{\mathrm{cl}}(s),x_{\mathrm{cl}}(s)\big) \\ \int_0^t \partial_{x(s)}\partial_{\dot{x}(s)}L\big(s,x_{\mathrm{cl}}(s),x_{\mathrm{cl}}(s)\big) & \int_0^t \partial_{\dot{x}(s)}^2 L\big(s,x_{\mathrm{cl}}(s),x_{\mathrm{cl}}(s)\big)\end{bmatrix}\right)^{-\frac{1}{2}} \\
&\quad \times\exp\left(\frac{\mathrm{i}}{\hbar}\int_0^t L(s,x_{\mathrm{cl}}(s),\dot{x}_{\mathrm{cl}}(s))\mathrm{d}s\right)\big(1+O(\sqrt{\hbar})\big).
\end{aligned}$$

10.12 General Hamiltonians – Wick quantization

Let $[0,t]\ni s\mapsto h(s,a^*,a)\in\mathbb{R}$ be a time dependent classical Hamiltonian expressed in terms of the complex coordinates. Set

$$H(t) := \mathrm{Op}^{a^*,a}\big(h(t)\big)$$

and $U(t)$ as in (10.41). (We drop the tilde from $\tilde{h}$ and $\tilde{u}$, as compared with the notation of (4.15).)

Following Lemma 10.3 we prove that

$$\mathrm{e}^{-\mathrm{i}u\mathrm{Op}^{a^*,a}\left(h(s)\right)} - \mathrm{Op}^{a^*,a}\big(\mathrm{e}^{-\mathrm{i}uh(s)}\big) = O(u^2). \tag{10.42}$$

Thus we can use $F(s,u) := \mathrm{Op}^{a^*,a}\big(\mathrm{e}^{-\mathrm{i}uh(s)}\big)$ in (10.3), so that

$$\mathrm{Op}^{a^*,a}\big(u(t)\big) \;:=\; U(t) \;=\; \lim_{n\to\infty}\prod_{j=1}^{n}\mathrm{Op}^{a^*,a}\big(\mathrm{e}^{-\mathrm{i}\frac{t}{n}h\left(\frac{jt}{n}\right)}\big).$$

Thus, by (**??**),

$$u(t,a^*,a) \;=\; \lim_{n\to\infty}\exp\Big(\sum_{k>j}\partial_{a_k}\partial_{a_j^*}\Big)\prod_{j=1}^{n}\exp\left(-\tfrac{\mathrm{i}t}{n}h\left(\tfrac{jt}{n},a_j^*,a_j\right)\right)\Big|_{\;a=a_n=\cdots=a_1.}\;.$$

Heuristically, this can be rewritten as

$$\begin{aligned} u(t,a^*,a) \;&=\; \exp\left(\int_0^t \mathrm{d}s_+\int_0^t \mathrm{d}s_-\theta(s_+-s_-)\partial_{a^*(s_+)}\partial_{a(s_-)}\right)\\ &\quad\times\exp\left(-\mathrm{i}\int_0^t h\left(s,a^*(s),a(s)\right)\mathrm{d}s\right)\Big|_{a=a(s),t>s>0}. \end{aligned} \tag{10.43}$$

Alternatively, we can use the integral formula (**??**), and rewrite (10.43) as

$$\begin{aligned} u(t,a^*,a) = \int\cdots\int\exp\Big(\sum_{j=1}^{n-1}\Big(-\frac{(b_{j+1}-b_j)b_j^*}{2}+\frac{b_{j+1}(b_{j+1}^*-b_j^*)}{2}\Big)\\ \times\prod_{j=1}^{n}\exp\left(-\tfrac{\mathrm{i}t}{n}h\left(\tfrac{jt}{n},a^*+b_j^*,a+b_j\right)\right)\prod_{j=1}^{n-1}\frac{\mathrm{d}b_{j+1}\mathrm{d}b_j^*}{(2\pi\mathrm{i})^d}\Big|_{b_n^*=0,\,b_1=0}. \end{aligned} \tag{10.44}$$

Heuristically, it can be rewritten as

$$u(t,a^*,a) \tag{10.45}$$

$$= \frac{\int\mathcal{D}\big(b^*(\cdot),b(\cdot)\big)\exp\Big(\int_0^t\Big(-\frac{b^*(s)\partial_s b(s)}{2}+\frac{\partial_s b^*(s)b(s)}{2}-\mathrm{i}h\left(s,a^*+b^*(s),a+b(s)\right)\Big)\mathrm{d}s\Big)}{\int\mathcal{D}\big(b^*(\cdot),b(\cdot)\big)\exp\Big(\int_0^t\big(-\frac{b^*(s)\partial_s b(s)}{2}+\frac{\partial_s b^*(s)b(s)}{2}\big)\mathrm{d}s\Big)}.$$

Here, $\mathcal{D}\big(b^*(\cdot),b(\cdot)\big)$ is a "measure" on the complex trajectories satisfying $b^*(t)=0$, $b(0)=0$.

Let us describe another derivation of (10.45), which starts from (10.43). Consider the operator G on $L^2([0,t])$ with the integral kernel $G(s_+,s_-):=\theta(s_+-s_-)$ Note that

$$\partial_{s_+}\theta(s_+-s_-)=\delta(s_+-s_-).$$

Besides, $\theta f(0)=0$. Therefore, $\partial_s G=\mathbb{1}$. Thus G is the inverse ("Green's operator") of the operator ∂_s with the boundary condition $f(0)=0$. It is an unbounded operator with empty resolvent. It is not antiselfadjoint – its adjoint is ∂_x with the boundary condition $f(t)=0$. The corresponding sesquilinear form can be written as

$$\int_0^t a^*(s)\partial_s a(s)\mathrm{d}s.$$

Using (**??**), (10.43) can be rewritten formally as (10.45).

10.13 Vacuum expectation value

In particular, we have the following expression for the vacuum expectation value:

$$\begin{aligned}
&\big(\Omega|U(t)\Omega\big)\\
=\quad&\frac{\int\mathcal{D}\big(a(\cdot)\big)\exp\Big(\int_0^t\left(a^*(s)\partial_s a(s)-\mathrm{i}h\left(s,a^*(s),a(s)\right)\right)\mathrm{d}s\Big)}{\int\mathcal{D}\big(a(\cdot)\big)\exp\big(\int_0^t a^*(s)\partial_s a(s)\mathrm{d}s\big)}.
\end{aligned}\tag{10.46}$$

For $f,g\in\mathbb{C}^d$ we will write

$$a^*(f)=a_if_i,\quad a(g)=a_i\overline{g}_i.$$

One often tries to express everything in terms of vacuum expectation values. To this end introduce functions

$$[0,t]\ni s\mapsto F(s),G(s)\in\mathbb{C}^d,$$

and a (typically, nonphysical) Hamiltonian

$$H(s)+a^*\big(F(s)\big)+a\big(G(s)\big).$$

The vacuum expectation value for this Hamiltonian is called the *generating function*:

$$Z(F,\overline{G})=\left(\Omega|\mathrm{Texp}\left(-\mathrm{i}\int_0^t\Big(H(s)+a^*\big(F(s)\big)+a\big(G(s)\big)\Big)\mathrm{d}s\right)\Omega\right).$$

Note that we can retrieve full information about $U(t)$ from $Z(F,\overline{G})$ by differentiation. Indeed let

$$F_i(s)=f_i\delta(s-t),\quad G_i(s)=g_i\delta(s),\quad f_i,g_i\in\mathbb{C}^d.$$

Then

$$\begin{aligned}
&F_1\cdots F_n\overline{G}_1\cdots\overline{G}_m\partial_F^n\partial_{\overline{G}}^m Z(F,\overline{G})\Big|_{F=0,\overline{G}=0}\\
=\quad&\mathrm{i}^{n-m}\Big(a^*(f_1)\cdots a^*(f_n)\Omega|U(t)a^*(g_1)\cdots a^*(g_m)\Omega\Big)
\end{aligned}$$

To see this, assume for simplicity that

$$F_1(s)=\cdots=F_n(s)=f\delta(s-t),\quad G_1(s)=\cdots=G_m(s)=g\delta(s),$$

and approximate the delta function:

$$\delta(s)\approx\begin{cases}1/\epsilon & 0<s<\epsilon;\\ 0 & \epsilon<s<t;\end{cases},\quad \delta(s-t)\approx\begin{cases}0 & 0<s<t-\epsilon;\\ 1/\epsilon & t-\epsilon<s<t;\end{cases}.$$

Using these approximations, we can write

$$\begin{aligned}
Z(sF,u\overline{G})\quad&=\quad\lim_{\epsilon\to 0}\Big(\Omega|\mathrm{e}^{-\mathrm{i}s\frac{\epsilon}{\epsilon}a(f)}U(t)\mathrm{e}^{-\mathrm{i}u\frac{\epsilon}{\epsilon}a^*(g)}\Omega\Big)\\
&=\quad\Big(\mathrm{e}^{\mathrm{i}sa^*(f)}\Omega|U(t)\mathrm{e}^{-\mathrm{i}ua^*(g)}\Omega\Big).
\end{aligned}$$

Now

$$
\begin{aligned}
& F_1\cdots F_1\overline{G}_1\cdots\overline{G}_1\partial_F^n\partial_{\overline{G}}^m Z(F,\overline{G})\Big|_{F=0,\overline{G}=0} \\
= \; & \partial_s^n\partial_u^m\Big(\mathrm{e}^{\mathrm{i}sa^*(f)}\Omega|U(t)\mathrm{e}^{-\mathrm{i}ua^*(g)}\Omega\Big)\Big|_{s=0,\ u=0} \\
= \; & \mathrm{i}^{n-m}\Big(a^*(f_1)^n\Omega|U(t)a^*(g_1)^m\Omega\Big).
\end{aligned}
$$

10.14 Scattering operator for Wick quantized Hamiltonians

Assume now that the Hamiltonian is defined for all times and is split into a time-independent quadratic part and a perturbation:

$$h(t,a^*,a)=a^*\varepsilon a+\lambda q(t,a^*,a).$$

Set

$$
\begin{aligned}
H_0 &= \mathrm{Op}^{a^*,a}(a^*\varepsilon a)=\hat{a}^*\varepsilon\hat{a}=\sum_i \hat{a}_i^*\varepsilon_i\hat{a}_i \\
Q(t) &= \mathrm{Op}^{a^*,a}(q(t)),
\end{aligned}
$$

so that $H(t)=H_0+\lambda Q(t)$. The scattering operator is

$$S \;=\; \mathrm{Texp}\Big(-\mathrm{i}\int_{-\infty}^{\infty}H_{\mathrm{Int}}(t)\mathrm{d}t\Big),$$

where the interaction Hamiltonian is

$$
\begin{aligned}
H_{\mathrm{Int}}(t) &= \lambda\mathrm{e}^{\mathrm{i}tH_0}Q(t)\mathrm{e}^{-\mathrm{i}tH_0} \\
&= \lambda\mathrm{Op}^{a^*,a}\big(q(t,\mathrm{e}^{\mathrm{i}t\varepsilon}a^*,\mathrm{e}^{-\mathrm{i}t\varepsilon}a)\big).
\end{aligned}
$$

Setting $S=\mathrm{Op}^{a^*,a}(s)$, we can write

$$
\begin{aligned}
s(a^*,a) &= \exp\left(\int_{-\infty}^{\infty}\mathrm{d}t_+\int_{-\infty}^{\infty}\mathrm{d}t_-\theta(t_+-t_-)\partial_{a(t_+)}\partial_{a^*(t_-)}\right) \\
&\quad\times\exp\left(-\mathrm{i}\lambda\int_{-\infty}^{\infty}q\left(t,\mathrm{e}^{\mathrm{i}\varepsilon t}a^*(t),\mathrm{e}^{-\mathrm{i}\varepsilon t}a(t)\right)\mathrm{d}t\right)\Bigg|_{\substack{a^*=a^*(t),\\ a=a(t),\ t\in\mathbb{R}}} \\
&= \exp\left(\int_{-\infty}^{\infty}\mathrm{d}t_+\int_{-\infty}^{\infty}\mathrm{d}t_-\mathrm{e}^{\mathrm{i}\varepsilon(t_+-t_-)}\theta(t_+-t_-)\partial_{a(t_+)}\partial_{a^*(t_-)}\right) \\
&\quad\times\exp\left(-\mathrm{i}\lambda\int_{-\infty}^{\infty}q\left(t,a^*(t),a(t)\right)\mathrm{d}t\right)\Bigg|_{\substack{\mathrm{e}^{\mathrm{i}t\varepsilon}a^*=a^*(t),\\ \mathrm{e}^{\mathrm{i}t\varepsilon}a=a(t),\ t\in\mathbb{R}}} \qquad (10.47)\\
&= \frac{\int\mathcal{D}\big(b(\cdot)\big)\exp\Big(\int_{-\infty}^{\infty}\big(\big(b^*(t)-\mathrm{e}^{\mathrm{i}\varepsilon t}a^*\big)(\partial_t+\mathrm{i}\varepsilon)\big(b(t)-\mathrm{e}^{-\mathrm{i}\varepsilon t}a\big)-\mathrm{i}\lambda q\left(t,b^*(t),b(t)\right)\big)\mathrm{d}t\Big)}{\int\mathcal{D}\big(b(\cdot)\big)\exp\int_{-\infty}^{\infty}\Big(\big(b^*(t)-\mathrm{e}^{\mathrm{i}\varepsilon t}a^*\big)(\partial_t+\mathrm{i}\varepsilon)\big(b(t)-\mathrm{e}^{-\mathrm{i}\varepsilon t}a\big)}.
\end{aligned}
$$

In the firtst step we made the substitution

$$a(t) = \mathrm{e}^{-\mathrm{i}t\varepsilon} a_{\mathrm{Int}}(t), \quad a^*(t) = \mathrm{e}^{\mathrm{i}t\varepsilon} a^*_{\mathrm{Int}}(t),$$

subsequently dropping the subscript Int. Then the differential operator was represented as a convolution involving Green's function of the operator $\partial_t + \mathrm{i}\varepsilon$ that has the kernel $\mathrm{e}^{\mathrm{i}\varepsilon(t_+ - t_-)}\theta(t_+ - t_-)$.

11 Diagrammatics

11.1 Friedrichs diagrams

11.1.1 Wick monomials

Monomials in commuting/anticommuting variables $a^*(\xi)$, $a(\xi)$ parametrized by, say, $\xi \in \mathbb{R}^d$, are expressions of the form

$$\begin{aligned} & r(a^*, a) && (11.1)\\ := & \int \cdots \int \mathrm{d}\xi_1^+ \cdots \mathrm{d}\xi_{m^+}^+ \mathrm{d}\xi_{m^-}^- \cdots \mathrm{d}\xi_1^- r(\xi_1^+, \dots, \xi_{m^+}^+, \xi_{m^-}^-, \dots, \xi_1^-) \\ & \times a^*(\xi_{m^+}^+) \cdots a^*(\xi_1^+) a(\xi_1^-) \cdots \hat{a}(\xi_{m^-}^-), && (11.2)\end{aligned}$$

The complex-valued function r, called the *coefficient function* is separately symmetric/antisymmetric in the first m^+ and the last m^- arguments. We call (m^+, m^-) the *degree* of (11.2). A *polynomial* is a sum of monomials.

Consider creation/annihilation operators parametrized by $\xi \in \mathbb{R}^d$:

$$[\hat{a}(\xi), \hat{a}^*(\xi')]_\mp = \delta(\xi - \xi'), \quad (11.3)$$

$$[\hat{a}(\xi), \hat{a}(\xi')]_\mp = [\hat{a}^*(\xi), \hat{a}^*(\xi')]_\mp = 0. \quad (11.4)$$

By a *Wick monomial* we mean an operator on $\Gamma_{\mathrm{s/a}}(L^2(\mathbb{R}^d))$ given formally by

$$\begin{aligned} & r(\hat{a}^*, \hat{a}) && (11.5)\\ := & \int \cdots \int \mathrm{d}\xi_1^+ \cdots \mathrm{d}\xi_{m^+}^+ \mathrm{d}\xi_{m^-}^- \cdots \mathrm{d}\xi_1^- r(\xi_1^+, \dots, \xi_{m^+}^+, \xi_{m^-}^-, \dots, \xi_1^-) \\ & \times \hat{a}^*(\xi_{m^+}^+) \cdots \hat{a}^*(\xi_1^+) \hat{a}(\xi_1^-) \cdots \hat{a}(\xi_{m^-}^-). && (11.6)\end{aligned}$$

A *Wick polynomial* is a sum of Wick monomials.

Thus to each polynomial $q(a^*, a)$ we associate an operator $q(\hat{a}^*, \hat{a})$. $q(\hat{a}^*, \hat{a})$ is called the *Wick quantization of* $q(a^*, a)$. $q(a^*, a)$ is called the *Wick symbol of* $q(\hat{a}^*, \hat{a})$.

m-particle vectors have the form

$$\begin{aligned} & q(\hat{a}^*)\Omega && (11.7)\\ = & \int \cdots \int q(\xi_1, \dots, \xi_m) \hat{a}^*(\xi_m) \cdots \hat{a}^*(\xi_1) \Omega \mathrm{d}\xi_m \cdots \mathrm{d}\xi_1, && (11.8)\end{aligned}$$

where q is a symmetric/antisymmetric function. Clearly,

$$\|q(\hat{a}^*)\Omega\|^2 = m! \int |q(\xi_1, \dots, \xi_m)|^2 \mathrm{d}\xi_m \cdots \mathrm{d}\xi_1. \tag{11.9}$$

Note that if ξ were a discrete variable, then (11.9) would not true in the case of coinciding ξ.

It is convenient to introduce the shorthand

$$|\xi_m, \dots \xi_1) := \hat{a}^*(\xi_m) \cdots \hat{a}^*(\xi_1)\Omega. \tag{11.10}$$

Clearly, (11.10) is not an element of the Fock space, but for many purposes it can be treated as one. It becomes an element of the Fock space after smearing with a L^2 test function, as in (11.8).

If $q(\hat{a}^*, \hat{a})$ is a Wick polynomial, it is convenient to decompose it in a sum of monomials as follows:

$$q(\hat{a}^*, \hat{a}) = \sum_{m^+, m^-} \frac{q_{m^+, m^-}(\hat{a}^*, \hat{a})}{m^+! m^-!}. \tag{11.11}$$

We have then

$$q_{m^+, m^-}\left(\xi^+_{m_+}, \dots, \xi^+_1; \xi^-_{m_-}, \dots, \xi^-_1\right) \tag{11.12}$$

$$= \left(\xi^+_{m_+}, \dots, \xi^+_1 | q(\hat{a}^*, \hat{a}) | \xi^-_{m_-}, \dots, \xi^-_1\right). \tag{11.13}$$

Anticipating the applications to compute the scattering operator, the variables on the right $\xi^-_{m_-}, \dots, \xi^-_1$ will be sometimes called the *incoming particles*, and the variables on the left $\xi^+_{m_+}, \dots, \xi^+_1$ the *outgoing particles*.

11.1.2 Products of Wick monomials

Suppose that $q_n(\hat{a}^*, \hat{a})$,..., $q_1(\hat{a}^*, \hat{a})$ are Wick polynomials. The Wick symbol of their product

$$q(\hat{a}^*, \hat{a}) = q_n(\hat{a}^*, \hat{a}) \cdots q_1(\hat{a}^*, \hat{a}) \tag{11.14}$$

can be computed from the formula

$$q(a^*, a) \tag{11.15}$$

$$= \exp\Big(\sum_{k>j} \partial_{a_k} \partial_{a^*_j}\Big) q_n(a^*_n, a_n) \cdots q_1(a^*_1, a_1) \Big|_{\substack{a = a_n = \cdots = a_1, \\ a^* = a^*_2 = \cdots = a^*_1.}} \tag{11.16}$$

(11.16) leads naturally to a diagrammatic method of computing products of Wick polyomials.

To describe this method assume that r_j are monomials of the degree (m^+_j, m^-_j), $j = 1, \dots, n$. We would like to compute

$$q(\hat{a}^*, \hat{a}) := \frac{r_n(\hat{a}^*, \hat{a})}{m^+_n! m^-_n!} \cdots \frac{r_1(\hat{a}^*, \hat{a})}{m^+_1! m^-_1!}. \tag{11.17}$$

We will describe a diagramatic method for computing $q(a^*, a)$, the Wick symbol of (11.17).

(1) Rules about drawing diagrams.

(i) Suppose that the monomial $r_j(a^*, a)$ has the degree (m_j^+, m_j^-). We associate to it a *vertex* with m_j^- *annihilation legs* on the right and m_j^+ *creation legs* on the left.

(ii) We align the vertices in the ascending order from the right to the left.

(iii) On the right we mark m^- incoming particles. Each corresponds to one of the variables $\xi_{m_-}^-, \dots, \xi_1^-$ and has a single creating legs. On the left m^+ outgoing particles. Each corresponds to on of the variables $\xi_{m_+}^+, \dots, \xi_1^+$ and has a single annihilation leg.

(iv) We connect pairs of legs with lines. All legs have to be connected. A line always goes from a creation vertex on the right to an annihilation vertex on the left.

(2) The product

$$B! := \prod_{j>i} k_{ji}! \prod_j k_j^+! \prod_i k_i^-! \tag{11.18}$$

will be called the *symmetry factor of the diagram.* Here

(i) k_{ji} is the number of lines connecting j and i,

(ii) $k_i^- := m_i^- - \sum_j k_{ji}$ is the number of lines connecting i and incoming particles,

(iii) $k_j^+ := m_j^+ - \sum_i k_{ji}$ is the number of lines connecting j and outgoing particles. We also have

(iv) $m^- := \sum_j k_j^-$, the number of incoming particles, denoted sometimes m_B^-,

(v) $m^+ := \sum_j k_j^+$, the number of outgoing particles, denoted sometimes m_B^+.

(3) Rules about evaluating diagrams.

(i) We put the function $r_j(\dots, \dots)$ for the $j$the vertex. Each leg corresponds to an argument of r_j.

(ii) We put $\int\int \delta(\xi_+ - \xi_-)\mathrm{d}\xi_+ \mathrm{d}\xi_-$ for each line, where ξ_+ is the variable of its creation leg and ξ_- the variable of its annihilation leg.

(iii) For the incoming particle ξ_j^- we put $a(\xi_j^-)$ and for the outgoing particle ξ_j^+ we put $a^*(\xi_j)$.

(iv) In the fermionic case we multiply by $(-1)^q$ where q is the number of crossings of lines.

(v) We multiply all the terms, evaluate the integral, obtaining a polynomial of degree (m_B^+, m_B^-) denoted $q_B(a^*, a)$

(4) We sum the values of diagrams divided by their symmetry factors:

$$q(a^*, a) = \sum_{\text{all diag}} \frac{q_B(a^*, a)}{B!}. \tag{11.19}$$

In particular,

$$\frac{q_{m^+,m^-}(a^*,a)}{m^+!m^-!} = \sum_{B\ :\ (m^+,m^-)=(m_B^+,m_B^-)} \frac{q_B(a^*,a)}{B!}, \tag{11.20}$$

$$\big(\Omega|q(\hat{a}^*,\hat{a})\Omega\big) = q_{0,0} = \sum_{B \text{ has no external lines}} \frac{q_B}{B!} \tag{11.21}$$

Note that $B!$ equals the order of the group of the symmetry of the diagram. More precisely, it is the number of permutations of legs of each vertex which do not change the diagram.

The above method is one of versions of Wick's Theorem. It is proven by moving all annihilation operators to the right and moving all creation operators to the left, until they kill the vacuum. When we commute/anticommute a term with contracted indices is produced, which gives rise to a line.

More elegantly, we can use the formula (11.16). In fact, each diagram B is defined by a collection of integers $\{k_{ji},\ j > i\}$, and we can write

$$\exp\Big(\sum_{j>i} \partial_{a_k}\partial_{a_j^*}\Big) = \sum_B \prod_{j>i} \frac{1}{k_{ji}!}\big(\partial_{a_k}\partial_{a_j^*}\big)^{k_{ij}}. \tag{11.22}$$

This differential operator acts on the function

$$\frac{r_n(a_n^*,a_n)}{m_n^+!m_n^-!}\cdots\frac{r_1(a_1^*,a_1)}{m_1^+!m_1^-!} \tag{11.23}$$

The effect of the component of the differential operator (11.22) corresponding to B is the appropriate contraction of the numerator and the change of the combinatorial factor in the denominator. After identifying all a_j^* and a_i with a^*, a, we obtain

$$\frac{q_B(a^*,a)}{\prod_{j>i} k_{ji}! \prod_j k_j^+! \prod_i k_i^-!}. \tag{11.24}$$

11.1.3 Friedrichs (Wick) diagrams

Consider a Hamiltonian

$$H = H_0 + W(t), \tag{11.25}$$

where

$$H_0 = \int \omega(\xi)\hat{a}^*(\xi)\hat{a}(\xi)\mathrm{d}\xi, \tag{11.26}$$

$$W(t) = \sum_{m^+,m^-} \frac{w_{m^+,m^-}(t,\hat{a}^*,\hat{a})}{m^+!m^-!}. \tag{11.27}$$

Thus the free Hamiltonian is a particle number preserving quadratic Hamiltonian and the perturbation is a Wick polymial. We set as usual

$$H_{\mathrm{Int}}(t) = \mathrm{e}^{\mathrm{i}tH_0} W(t) \mathrm{e}^{-\mathrm{i}tH_0}, \tag{11.28}$$

$$S = \mathrm{Texp}\left(-\mathrm{i} \int_{-\infty}^{\infty} H_{\mathrm{Int}}(t)\mathrm{d}t \right). \tag{11.29}$$

Using

$$\mathrm{e}^{\mathrm{i}tH_0} a^*(\xi) \mathrm{e}^{-\mathrm{i}tH_0} = \mathrm{e}^{\mathrm{i}t\omega(\xi)} a^*(\xi), \tag{11.30}$$

$$\mathrm{e}^{\mathrm{i}tH_0} a(\xi) \mathrm{e}^{-\mathrm{i}tH_0} = \mathrm{e}^{-\mathrm{i}t\omega(\xi)} a(\xi), \tag{11.31}$$

we can write

$$H_{\mathrm{Int}}(t) = \sum \frac{w_{m^+,m^-}(t, \mathrm{e}^{\mathrm{i}t\omega}\hat{a}^*, \mathrm{e}^{-\mathrm{i}t\omega}\hat{a})}{m^+!m^-!}. \tag{11.32}$$

We assume that $w_{m^+,m^-}(t)$ decays sufficiently fast as $|t| \to \infty$. We will describe rules for computing the Wick symbol of the scattering operator

$$S = s(\hat{a}^*, \hat{a}) \tag{11.33}$$

$$= \sum_{m^+,m^-} \frac{s_{m^+,m^-}(\hat{a}^*, \hat{a})}{m^+!m^-!}. \tag{11.34}$$

(1) Rules about drawing diagrams.

  (i) To every monomial $w_{m^+,m^-}(t, a^*, a)$ in the interaction we associate a *vertex* with m^- *annihilation legs* on the right and m^+ *creation legs* on the left.

  (ii) Choose a sequence of vertices $(m_n^+, m_n^-), \dots, (m_1^+, m_1^-)$, and a sequence of corresponding times $t_n > \cdots > t_1$. Align them in the ascending order from the right to the left.

  The remaining rules about drawing the diagrams are the same as in Subsubsect. 11.1.2.

(2) The symmetry factor $B!$, the number of incoming/outgoing particles m_B^- and m_B^+ are defined as in Susbsect. 11.1.2.

(3) Rules about evaluating diagrams

  (i) We put $-\mathrm{i}w_{m_j^+,m_j^-}(t_j, \dots, \dots)$ for the vertex corresponding to t_j. Each argument is associated with a leg.

  (ii) We put $\int\int \mathrm{e}^{-\mathrm{i}(t_{j_+} - t_{j_-})\omega(\xi_+)} \delta(\xi_+ - \xi_-) \mathrm{d}\xi_+ \mathrm{d}\xi_-$ for each line, where ξ_- is the variable associated with its creation leg in the vertex at t_{j_-} and ξ_+ is the variable associated with its annihilation leg in the vertex at t_{j_+}.

  (iii) For an incoming particle ξ_j^- conected to time t_j we put $\mathrm{e}^{\mathrm{i}t_j\omega(\xi_j^-)} a(\xi_j^-)$. To the outgoing particle ξ_j^+ connected to time t_j we put $\mathrm{e}^{-\mathrm{i}t_j\omega(\xi_j^+)} a^*(\xi_j^+)$.

(iv) In the fermionic case we multiply by $(-1)^q$ where q is the number of crossings of lines.

(v) We multiply all terms and evaluate the integral over all ξ, obtaining a polynomial $B(t_n,\dots,t_1,a^*,a)$.

(4) We integrate the diagrams over $t_n>\cdots>t_1$ divided by their symmetry factors:

$$s(a^*,a)=\sum_{n=0}^{\infty}\sum_{\text{all diag.}}\int\cdots\int_{t_n>\cdots>t_1}\frac{B(t_n,\dots,t_1;a^*,a)}{B!}\mathrm{d}t_n\cdots\mathrm{d}t_1. \tag{11.35}$$

In particular,

$$\begin{aligned}
&\frac{s_{m^+,m^-}(a^*,a)}{m^+!m^-!} && (11.36)\\
=&\sum_{n=0}^{\infty}\sum_{B\ :\ (m^+,m^-)=(m_B^+,m_B^-)}\int\cdots\int_{t_n>\cdots>t_1}\frac{B(t_n,\dots,t_1;a^*,a)}{B!}\mathrm{d}t_n\cdots\mathrm{d}t_1, && (11.37)\\
&\big(\Omega|S\Omega\big)=s_{0,0} && (11.38)\\
=&\sum_{n=0}^{\infty}\sum_{B\text{ has no external lines}}\int\cdots\int_{t_n>\cdots>t_1}\frac{B(t_n,\dots,t_1)}{B!}\mathrm{d}t_n\cdots\mathrm{d}t_1.
\end{aligned}$$

The above method apparently was first described by Friedrichs and the corresponding diagrams are sometimes called Friedrichs diagrams. Another natural name, used in lecture notes of Coleman, is Wick diagrams, since it is a graphical expression of Wick's Theorem.

11.1.4 Friedrichs diagrams from path integrals

An elegant even if partly heuristic derivation of Friedrichs diagrams uses path integrals. Let us introduce the relevant formalism.

Let $[0,t]\ni s\mapsto h(s,a^*,a)\in\mathbb{R}$ be a time dependent classical Hamiltonian expressed in terms of the complex coordinates. Set

$$H(t):=\mathrm{Op}^{a^*,a}\big(h(t)\big), \tag{11.39}$$

$$U(t):=\mathrm{Texp}\bigg(-\mathrm{i}\int_0^t H(s)\mathrm{d}s\bigg). \tag{11.40}$$

Now

$$\begin{aligned}
U(t)&=\lim_{n\to\infty}\prod_{j=1}^{n}\mathrm{e}^{-\mathrm{i}\frac{t}{n}h\left(\frac{jt}{n},\hat a^*,\hat a\right)}\\
&=\lim_{n\to\infty}\prod_{j=1}^{n}\mathrm{e}^{-\mathrm{i}\frac{t}{n}h\left(\frac{jt}{n}\right)}(\hat a^*,\hat a).
\end{aligned}$$

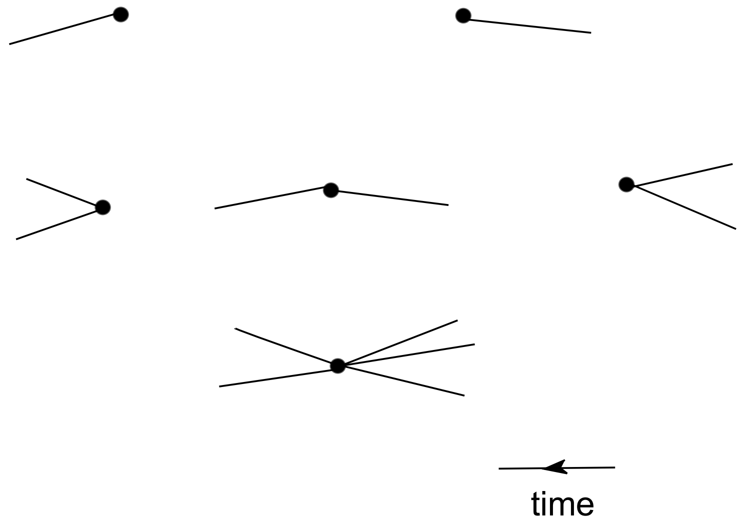

Figure 1: Various Friedrichs vertices

If we set $u(t,\hat{a}^*,\hat{a}) := U(t)$, then

$$u(t,a^*,a) \quad = \quad \lim_{n\to\infty} \exp\Big(\sum_{k>j}\partial_{a_k}\partial_{a_j^*}\Big)\prod_{j=1}^{n}\exp\left(-\tfrac{\mathrm{i}t}{n}h\left(\tfrac{jt}{n},a_j^*,a_j\right)\right)\Big|_{\substack{a=a_n=\cdots=a_1,\\ a^*=a_n^*=\cdots=a_1^*.}} .$$

Heuristically, this can be rewritten as

$$\begin{aligned} u(t,a^*,a) \quad = \quad & \exp\left(\iint\limits_{t>s_+>s_->0} \mathrm{d}s_+\mathrm{d}s_-\partial_{a^*(s_+)}\partial_{a(s_-)}\right) \\ & \times\exp\left(-\mathrm{i}\int_0^t h\left(s,a^*(s),a(s)\right)\mathrm{d}s\right)\Big|_{\substack{a^*=a^*(s),\\ a=a(s),\ t>s>0}} . \qquad (11.41) \end{aligned}$$

Assume now that the Hamiltonian is defined for all times and has the form (11.27). Define the scattering operator S and its Wick symbol s as in (11.29) and (11.33). Using the

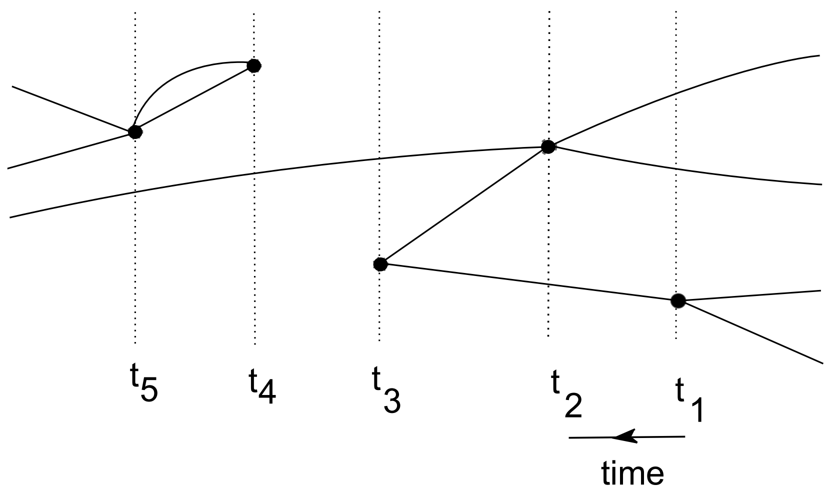

Figure 2: A disconnected Friedrichs diagram

version of (11.41) with $]0,t[$ replaced by $]-\infty,\infty[$, we obtain

$$
\begin{aligned}
s(a^*,a) &= \exp\left(\int\limits_{\infty>t_+>t_->-\infty} \mathrm{d}t_+ \int \mathrm{d}t_-\, \partial_{a(t_+)}\partial_{a^*(t_-)}\right) \\
&\quad \times \exp\left(-\mathrm{i}\lambda\int_{-\infty}^{\infty} w\left(t, \mathrm{e}^{\mathrm{i}\varepsilon t}a^*(t), \mathrm{e}^{-\mathrm{i}\varepsilon t}a(t)\right)\mathrm{d}t\right)\Bigg|_{\substack{a^*=a^*(t),\\ a=a(t),\ t\in\mathbb{R}}} \\
&= \exp\left(\int\limits_{\infty>t_+>t_->-\infty} \mathrm{d}t_+ \int \mathrm{d}t_-\, \mathrm{e}^{\mathrm{i}\varepsilon(t_+-t_-)}\partial_{a(t_+)}\partial_{a^*(t_-)}\right) \\
&\quad \times \exp\left(-\mathrm{i}\lambda\int_{-\infty}^{\infty} w\left(t, a^*(t), a(t)\right)\mathrm{d}t\right)\Bigg|_{\substack{\mathrm{e}^{\mathrm{i}t\varepsilon}a^*=a^*(t),\\ \mathrm{e}^{\mathrm{i}t\varepsilon}a=a(t),\ t\in\mathbb{R}}} .
\end{aligned} \tag{11.42}
$$

In the firtst step we made the substitution

$$a(t) = \mathrm{e}^{-\mathrm{i}t\varepsilon}a_{\mathrm{Int}}(t), \quad a^*(t) = \mathrm{e}^{\mathrm{i}t\varepsilon}a^*_{\mathrm{Int}}(t),$$

subsequently dropping the subscript Int. Then the differential operator was represented as a convolution involving Green's function of the operator $\partial_t + \mathrm{i}\varepsilon$ that has the kernel $\mathrm{e}^{\mathrm{i}\varepsilon(t_+-t_-)}\theta(t_+-t_-)$.

To derive the method of Friedrichs diagrams we can now proceed as in Subsubsect. 11.1.2.

11.1.5 Operator interpretation of Friedrichs diagrams

Denote for shortness the 1-particle space by $\mathcal{V}$. (We usually assume here that $\mathcal{V} = L^2(\mathbb{R}^d)$, but this is not relevant here).

We can interpret $B(t_n, \ldots, t_1; a^*, a)$ as a product of operators. For each line we introduce the Hilbert space isomorphic to $\mathcal{V}$. We have $n+1$ time intervals

$$t > t_n, \ldots, t_{j+1} > t > t_j, \ldots, t_1 > t.$$

For each of these intervals we have a collection of lines that are "open" in this interval. (This should be obvious from the diagram). Within each of these intervals we consider the tensor product of the spaces corresponding to the lines that are open in this interval.

The coefficient function $w_{m^+,m^-}(t)$ of the Wick monomial $w_{m^+,m^-}(t, \hat{a}^*, \hat{a})$ can be interpreted as the integral kernel of an operator from $\otimes^{m^-}\mathcal{V}$ to $\otimes^{m^+}\mathcal{V}$. (We could also interpret it as an operator from $\otimes_{\mathrm{s/a}}^{m^-}\mathcal{V}$ to $\otimes_{\mathrm{s/a}}^{m^+}\mathcal{V}$, but in this subsubsection we prefer the former interpretation). If it is on the jth place in the diagram, this operator will be denoted $W_B^j(t_j)$. $1\!\!1_B^j$ will denote the identity on the tensor product of spaces corresponding to the lines that pass the jth vertex. At the left/right end we put symmetrizators corresponding to external outgoing/incoming lines, denoted Θ_B^+/ Θ_B^-. Between each two consecutive vertices $j+1$ and j we put the free dynamics for time $t_{j+1}-t_j$, which, by the abuse of notation, will be denoted $\mathrm{e}^{-\mathrm{i}(t_{j+1}-t_j)H_0}$, and where H_0 is the sum of ε for each line. For the final/initial interval we put $\mathrm{e}^{\mathrm{i}t_nH_0}$ / $\mathrm{e}^{-\mathrm{i}t_1H_0}$. Thus the evaluation of B is the integral kernel of the operator

$$\begin{aligned} B(t_n, \ldots, t_1) &= (-\mathrm{i})^n \Theta_B^+ \mathrm{e}^{\mathrm{i}t_nH_0} \left(W_B^n(t_n) \otimes 1\!\!1_B^n\right) \mathrm{e}^{-\mathrm{i}(t_n-t_{n-1})H_0} \cdots \\ &\quad \times \mathrm{e}^{-\mathrm{i}(t_2-t_1)H_0} \left(W_B^1(t_1) \otimes 1\!\!1_B^1\right) \mathrm{e}^{-\mathrm{i}t_1H_0} \Theta_B^-. \end{aligned}$$

11.1.6 Linked Cluster Theorem

The *Linked Cluster Theorem* says that instead of the formula (11.35) there is a simpler way of computing the scattering operator, where we need only connected diagrams:

$$\begin{aligned} & s(a^*, a) \\ &= \exp\left(\sum_{n=0}^{\infty} \sum_{\text{con. diag.}} \int_{t_n > \cdots > t_1} \cdots \int \frac{B(t_n, \ldots, t_1; a^*, a)}{B!} \mathrm{d}t_n \cdots \mathrm{d}t_1 \right), \end{aligned} \tag{11.43}$$

$$\begin{aligned} (\Omega|S\Omega) &= s_{0,0} \\ &= \exp\left(\sum_{n=0}^{\infty} \sum_{\substack{\text{con. diag.} \\ \text{no ext. lines}}} \int_{t_n > \cdots > t_1} \cdots \int \frac{B(t_n, \ldots, t_1)}{B!} \mathrm{d}t_n \cdots \mathrm{d}t_1 \right). \end{aligned} \tag{11.44}$$

In (11.43) we sum over all connected diagrams. In (11.44) we sum over all connected diagrams without external lines. Clearly, (11.44) follows from (11.43).

We define the linked scattering operator as

$$S_{\mathrm{link}} := \frac{S}{(\Omega|S\Omega)}. \tag{11.45}$$

If $S_{\mathrm{link}} = s_{\mathrm{link}}(\hat{a}^*, \hat{a})$, then

$$\begin{aligned} s_{\mathrm{link}}(a^*, a) &= \frac{s(a^*, a)}{(\Omega|S\Omega)} \\ &= \sum_{n=0}^{\infty} \sum_{\text{linked diag.}} \int\limits_{t_n > \cdots > t_1} \cdots \int \frac{B(t_n, \dots, t_1; a^*, a)}{B!} \mathrm{d}t_n \cdots \mathrm{d}t_1 \end{aligned} \tag{11.46}$$

$$= \exp\left(\sum_{n=0}^{\infty} \sum_{\substack{\text{con. linked} \\ \text{diag.}}} \int\limits_{t_n > \cdots > t_1} \cdots \int \frac{B(t_n, \dots, t_1; a^*, a)}{B!} \mathrm{d}t_n \cdots \mathrm{d}t_1 \right). \tag{11.47}$$

In (11.46) we sum over all *linked* diagrams, that is, diagrams whose each connected component has at least one external line. In (11.47) we sum over all connected diagrams with at least one external line. Clearly, (11.46) and (11.47) follow from (11.43).

11.1.7 Scattering operator for time-independent perturbations

Let us now assume that the monomials $w_{m^+,m^-}(t) = w_{m^+,m^-}$ do not depend on time.

If the perturbation is time independent, then S often does not exist. In particular, the diagrams with no external legs are either 0 or divergent. If B is a linked diagram, then one can expect that the corresponding contribution

$$\int\limits_{t_n > \cdots > t_1} \cdots \int B(t_n, \dots, t_1) \mathrm{d}t_n \cdots \mathrm{d}t_1 \tag{11.48}$$

is finite. Therefore, we define the *linked scattering operator* as the operator

$$S_{\mathrm{link}} := s_{\mathrm{link}}(\hat{a}^*, \hat{a}) \tag{11.49}$$

with $s_{\mathrm{link}}(a^*, a)$ given by (11.46) or (11.47).

Clearly, S_{link} cannot be defined by the right hand side of (11.45), which does not make sense in the time-independent case.

We can evaluate S_{link} further. For $E \in \mathbb{R}$ we will use the operators

$$\delta(E - H_0), \quad (E - H_0 \pm \mathrm{i}0)^{-1} \tag{11.50}$$

They are not bounded operators in the usual sense, however one can often make sense of them as bounded operators on appropriate weighted spaces. We have partly heuristic identities

$$\int_0^{+\infty} \mathrm{e}^{\mathrm{i}u(H_0-E)}\mathrm{d}u \;=\; -\mathrm{i}\big(E-H_0+\mathrm{i}0\big)^{-1}, \tag{11.51}$$

$$\int_{-\infty}^{0} \mathrm{e}^{\mathrm{i}u(H_0-E)}\mathrm{d}u \;=\; \mathrm{i}\big(E-H_0-\mathrm{i}0\big)^{-1}, \tag{11.52}$$

$$\int \mathrm{e}^{\mathrm{i}t(H_0-E)}\mathrm{d}t \;=\; 2\pi\delta(E-H_0). \tag{11.53}$$

If B is a linked diagram, we introduce its *evaluation for the scattering amplitude at energy* E using the operator interpretation of the diagram B:

$$B_{\mathrm{sc}}(E) := -\,2\pi\mathrm{i}\Theta_B^{+}\delta(E-H_0)W_B^n\otimes 1\!\!1_B^n(E-H_0-\mathrm{i}0)^{-1}\cdots \tag{11.54}$$

$$\times\,(E-H_0-\mathrm{i}0)^{-1}W_B^1\otimes 1\!\!1_B^1\delta(E-H_0)\Theta_B^{-}. \tag{11.55}$$

(11.55) is an operator from $\otimes_{\mathrm{s/a}}\mathcal{V}^{m_B^-}$ to $\otimes_{\mathrm{s/a}}\mathcal{V}^{m_B^+}$. Its integral kernel can be used as the coefficient function of a monomial, denoted $B_{\mathrm{sc}}(E,a^*,a)$.

Theorem 11.1. *For every linked diagram B*

$$\int\cdots\int_{t_n>\cdots>t_1} B(t_n,\dots,t_1)\mathrm{d}t_n\cdots\mathrm{d}t_1 = \int B_{\mathrm{sc}}(E)\mathrm{d}E. \tag{11.56}$$

Proof. We compute the integrand using the operator interpretation of $B(t_n,\dots,t_1)$:

$$\begin{aligned}
B(t_n,\dots,t_1) \;&=\; (-\mathrm{i})^n\Theta_B^{+}\mathrm{e}^{\mathrm{i}t_nH_0}\left(W_B^n\otimes 1\!\!1_B^n\right)\mathrm{e}^{-\mathrm{i}(t_n-t_{n-1})H_0}\cdots\\
&\quad\times\mathrm{e}^{-\mathrm{i}(t_2-t_1)H_0}\left(W_B^1\otimes 1\!\!1_B^1\right)\mathrm{e}^{-\mathrm{i}t_1H_0}\Theta_B^{-}\\
&=\; (-\mathrm{i})^n\int\delta(H_0-E)\mathrm{d}E\,\Theta_B^{+}\left(W_B^n\otimes 1\!\!1_B^n\right)\mathrm{e}^{-\mathrm{i}u_n(H_0-E)}\cdots\\
&\quad\times\mathrm{e}^{-\mathrm{i}u_2(H_0-E)}\left(W_B^1\otimes 1\!\!1_B^1\right)\mathrm{e}^{-\mathrm{i}t_1(H_0-E)}\Theta_B^{-},
\end{aligned}$$

where we substituted

$$u_n := t_n-t_{n-1},\dots,\; u_2 := t_2-t_1.$$

and used

$$1\!\!1 = \int\delta(H_0-E)\mathrm{d}E.$$

Now

$$
\begin{aligned}
& \int_{t_n > \cdots > t_1} \cdots \int B(t_n, \dots, t_1) \mathrm{d}t_n \cdots \mathrm{d}t_1 \\
= \quad & \int \mathrm{d}E \int_0^\infty \mathrm{d}u_n \cdots \int_0^\infty \mathrm{d}u_1 \int_{-\infty}^\infty \mathrm{d}t_1 \delta(H_0 - E) \Theta_B^+ \left(W_n \otimes 1\!\!1_B^n\right) \mathrm{e}^{-\mathrm{i}u_n(H_0 - E)} \cdots \\
& \times \mathrm{e}^{-\mathrm{i}u_2(H_0 - E)} \left(W_1 \otimes 1\!\!1_B^1\right) \mathrm{e}^{-\mathrm{i}t_1(H_0 - E)} \Theta_B^- \\
= \quad & -2\pi \mathrm{i} \int \mathrm{d}E \delta(E - H_0) \Theta_B^+ \left(W_n \otimes 1\!\!1_B^n\right) \big(E - H_0 - \mathrm{i}0)\big)^{-1} \cdots \\
& \times \big(E - H_0 - \mathrm{i}0)\big)^{-1} \left(W_1 \otimes 1\!\!1_B^1\right) \delta(E - H_0) \Theta_B^-,
\end{aligned}
$$

□

By Thm 11.56, (11.47) can be rewritten as

$$
s_{\mathrm{link}}(a^*, a) = \sum_{\text{linked diag.}} \int \frac{B_{\mathrm{sc}}(E, a^*, a)}{B!} \mathrm{d}E.
$$

Note that, at least diagramwise

$$
S_{\mathrm{link}} = \lim_{t \to \infty} \frac{\mathrm{e}^{-\mathrm{i}tH_0} \mathrm{e}^{\mathrm{i}2tH} \mathrm{e}^{-\mathrm{i}tH_0}}{(\Omega | \mathrm{e}^{-\mathrm{i}tH_0} \mathrm{e}^{\mathrm{i}2tH} \mathrm{e}^{-\mathrm{i}tH_0} \Omega)}. \tag{11.57}
$$

We can make (11.57) more general, and possibly somewhat more satisfactory as follows. We introduce a temporal switching function $\mathbb{R} \ni t \mapsto \chi(t)$ that decays fast $t \to \pm\infty$ and $\chi(0) = 1$. We then replace the time independent perturbation W by $W_\epsilon(t) := \chi(t/\epsilon) W$. Let us denote the corresponding scattering operator by S_ϵ. Then the linked scattering operator formally is

$$
S_{\mathrm{link}} = \lim_{\epsilon \searrow 0} \frac{S_\epsilon}{(\Omega | S_\epsilon \Omega)}. \tag{11.58}
$$

One often makes the choice

$$
\chi(t/\epsilon) = \mathrm{e}^{-|t|/\epsilon}, \tag{11.59}
$$

which goes back to Gell-Mann–Low.

Note that S_{link} commutes with H_0. More precisely, each diagram commutes with H_0.

If $H_0 > 0$, then we expect S_{link} to be unitary. Indeed, S_ϵ is a unitary operator. Therefore, by (11.58), we expect that S_{link} is prportional to a unitary operator. $S_{\mathrm{link}}\Omega$ is a linear combination of diagrams with no incoming external lines. Their evaluation is zero because of the conservation of the energy, except for the trivial diagram corresponding to the identity. Therefore, $S_{\mathrm{link}}\Omega = \Omega$. Hence S_{link} is unitary.

11.1.8 Energy shift

We still consider a time independent perturbation. We assume that $H_0 \geq 0$. Let E denote the ground state energy of H, that is $E := \inf \operatorname{sp} H$. E can be called the *energy shift*, since the ground state energy of H_0 is 0. We assume that we can use the heuristic formula for the energy shift

$$E \quad = \quad \lim_{t\to\infty} \frac{\mathrm{i}}{2}\frac{\mathrm{d}}{\mathrm{d}t} \log(\Omega|\mathrm{e}^{\mathrm{i}tH_0}\mathrm{e}^{-\mathrm{i}2tH}\mathrm{e}^{\mathrm{i}tH_0}\Omega), \tag{11.60}$$

To see why we can expect (11.60) to be true, we note that $H_0\Omega = 0$ and assume that Φ is the ground state of H. Hence

$$(\Omega|\mathrm{e}^{\mathrm{i}tH_0}\mathrm{e}^{-\mathrm{i}2tH}\mathrm{e}^{\mathrm{i}tH_0}\Omega) = |(\Omega|\Phi)|^2\mathrm{e}^{-\mathrm{i}2tE} + C(t).$$

If we can argue that for large t the term $C(t)$ does not play a role, we obtain (11.60).

It is convenient to rewrite (11.60) as

$$E \quad = \quad \lim_{t\to\infty} \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t} \log(\Omega|\mathrm{e}^{\mathrm{i}tH_0}\mathrm{e}^{-\mathrm{i}tH}\Omega). \tag{11.61}$$

Let B be a connected diagram with no external lines. Its evaluation is invariant wrt translations in time:

$$B(t_n,\dots,t_1) = B(t_n+s,\dots,t_1+s).$$

Therefore,

$$\begin{aligned} &\underset{t_n>\cdots>t_1}{\int\cdots\int} B(t_n,\dots,t_1)\mathrm{d}t_n\cdots\mathrm{d}t_1 \\ = &\int \mathrm{d}t_1 \underset{u_n>\cdots>u_2>0}{\int\cdots\int} B(u_n,\dots,u_2,0)\mathrm{d}u_n\cdots\mathrm{d}u_2. \end{aligned}$$

This is infinite if nonzero. However, if we do not integrate wrt t_1, we typically obtain a finite expression, which can be used to compute the energy shift.

Theorem 11.2 (Goldstone theorem)**.** *We have*

$$E = \sum_{\substack{\text{con. diag.}\\ \text{no ext. lines}}} \underset{u_n>\cdots>u_2>0}{\int\cdots\int} \frac{B(u_n,\dots,u_2,0)}{B!}\mathrm{d}u_n\cdots\mathrm{d}u_2. \tag{11.62}$$

The terms in (11.62) can be evaluated using the operator interpretation of B:

$$\underset{u_n>\cdots>u_2>0}{\int\cdots\int} B(u_n,\dots,u_2,0)\mathrm{d}u_n\cdots\mathrm{d}u_2 \tag{11.63}$$

$$= (-1)^{n-1}W_B^n\, H_0^{-1}\big(W_B^{n-1}\otimes 1\!\!1_B^{n-1}\big)\dots\big(W_B^2\otimes 1\!\!1_B^2\big)H_0^{-1}\,W_B^1. \tag{11.64}$$

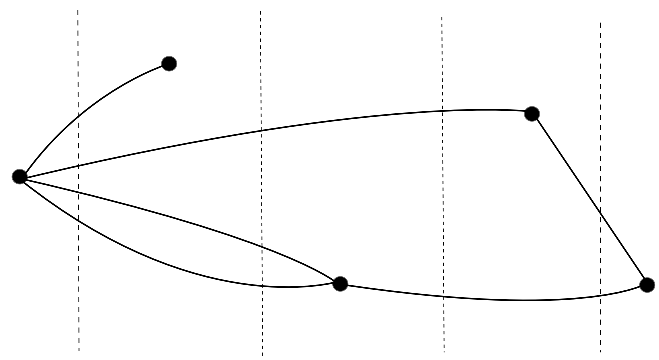

Figure 3: Goldstone diagram

Proof. Applying (11.44), we get

$$\begin{aligned}&\log(\Omega|\mathrm{e}^{\mathrm{i}tH_0}\mathrm{e}^{-\mathrm{i}tH}\Omega)\\ =&\sum_{n=0}^{\infty}\sum_{\substack{\text{con. diag.}\\ \text{no ext. lines}}}(-\mathrm{i}\lambda)^n\int\limits_{t>t_n>\cdots>t_1>0}\cdots\int\frac{B(t_n,\dots,t_1)}{B!}\mathrm{d}t_n\cdots\mathrm{d}t_1.\end{aligned}$$

So

$$\begin{aligned}&\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\log(\Omega|\mathrm{e}^{\mathrm{i}tH_0}\mathrm{e}^{-\mathrm{i}tH}\Omega)\\ =&\sum_{n=0}^{\infty}\sum_{\substack{\text{con. diag.}\\ \text{no ext. lines}}}\mathrm{i}\int\limits_{t>t_{n-1}>\cdots>t_1>0}\cdots\int\frac{B(t,t_{n-1},\dots,t_2,t_1)}{B!}\mathrm{d}t_{n-1}\cdots\mathrm{d}t_1.\end{aligned}$$

Now introduce

$$u_2:=t_2-t_1,\dots,u_{n-1}:=t_{n-1}-t_{n-2},\quad u_n:=t-t_{n-1}.$$

Then $u_2, \dots, u_n \geq 0$, $t \geq u_2 + \cdots + u_n$ and

$$\begin{aligned} B(t, t_{n-1}, \dots, t_2, t_1) &= (-\mathrm{i})^n W_B^n \mathrm{e}^{-\mathrm{i}(t-t_{n-1})H_0} \left(W_B^{n-1} \otimes 1\!\!1_B^{n-1}\right) \cdots \\ &\quad \times \left(W_B^2 \otimes 1\!\!1_B^2\right) \mathrm{e}^{-\mathrm{i}(t_2-t_1)H_0} W_B^1 \\ &= (-\mathrm{i})^n W_B^n \mathrm{e}^{-\mathrm{i}u_n H_0} \left(W_B^{n-1} \otimes 1\!\!1_B^{n-1}\right) \cdots \\ &\quad \times \left(W_B^2 \otimes 1\!\!1_B^2\right) \mathrm{e}^{-\mathrm{i}u_2 H_0} W_B^1. \end{aligned}$$

Then we replace t by $-\infty$ and evaluate the integral using the heuristic relation

$$\int_0^\infty \mathrm{e}^{-\mathrm{i}uH_0} \mathrm{d}u = \frac{-\mathrm{i}}{H_0}. \tag{11.65}$$

□

11.1.9 Example: van Hove Hamiltonian

Consider a time-dependent Van Hove Hamiltonian $H(t) := H_0 + V(t)$ with

$$V(t) = \int v(t,\xi) a^*(\xi) \mathrm{d}\xi + \int \overline{v(t,\xi)} a(\xi) \mathrm{d}\xi.$$

Clearly, the van Hove Hamiltonian in the interaction picture equals

$$H_{\mathrm{Int}}(t) = \int \mathrm{e}^{\mathrm{i}t\omega(\xi)} v(t,\xi) a^*(\xi) \mathrm{d}\xi + \int \mathrm{e}^{-\mathrm{i}t\omega(\xi)} \overline{v(t,\xi)} a(\xi) \mathrm{d}\xi.$$

Theorem 11.3. *The corresponding scattering operator is then given by*

$$\begin{aligned} S &= \mathrm{Texp}\left(-\mathrm{i} \int H_{\mathrm{Int}}(t) \mathrm{d}t\right) \\ &= \exp\left(-\mathrm{i} \int \mathrm{d}\xi \int \mathrm{d}t \mathrm{e}^{\mathrm{i}t\omega(\xi)} v(t,\xi) a^*(\xi)\right) \exp\left(-\mathrm{i} \int \mathrm{d}\xi \int \mathrm{d}t \mathrm{e}^{-\mathrm{i}t\omega(\xi)} \overline{v(t,\xi)} a(\xi)\right) \\ &\quad \times \exp\left(-\frac{1}{2} \int \mathrm{d}\xi \int \mathrm{d}t_1 \int \mathrm{d}t_2 \mathrm{e}^{-\mathrm{i}\omega(\xi)|t_1-t_2|} \overline{v(t_1,\xi)} v(t_2,\xi)\right) \\ &= \exp\left(-\mathrm{i} \int v(\omega(\xi),\xi) a^*(\xi) \mathrm{d}\xi\right) \exp\left(-\mathrm{i} \int \overline{v(\omega(\xi),\xi)} a(\xi) \mathrm{d}\xi\right) \\ &\quad \times \exp\left(\frac{\mathrm{i}}{2\pi} \int \frac{\overline{v(\tau,\xi)} v(\tau,\xi) \omega(\xi)}{\omega(\xi)^2 - \tau^2 - \mathrm{i}0} \mathrm{d}\tau \mathrm{d}\xi\right), \end{aligned}$$

where $v(\tau,\xi) := \int v(t,\xi) \mathrm{e}^{\mathrm{i}t\tau} \mathrm{d}t$.

Proof. Let us derive this using Friedrichs diagrams. We have two kinds of vertices: creation vertex $-\mathrm{i}v(t,\xi)$ and annihilation vertex $-\mathrm{i}\overline{v(t,\xi)}$. For internal lines we put $\theta(t_2 -$

$t_1)\mathrm{e}^{-\mathrm{i}\omega(\xi)(t_2-t_1)}$. For incoming lines we put $\mathrm{e}^{-\mathrm{i}t\omega(\xi)}$ and for outgoing lines we put $\mathrm{e}^{\mathrm{i}t\omega(\xi)}$. There is a single connected diagram without external lines with value

$$\int \mathrm{d}t_2 \int_{t_2 > t_1} \mathrm{d}t_1 (-\mathrm{i})^2 \overline{v(t,\xi)} v(t_1,\xi) \mathrm{e}^{-\mathrm{i}\omega(\xi)(t_2-t_1)} \mathrm{d}\xi \tag{11.66}$$

$$= -\frac{1}{2} \int \mathrm{d}\xi \int \mathrm{d}t_1 \int \mathrm{d}t_2 \mathrm{e}^{-\mathrm{i}\omega(\xi)|t_1-t_2|} \overline{v(t_1,\xi)} v(t_2,\xi) \tag{11.67}$$

$$= \frac{\mathrm{i}}{2\pi} \int \frac{\overline{v(\tau,\xi)} v(\tau,\xi)\omega(\xi)}{\omega(\xi)^2 - \tau^2 - \mathrm{i}0} \mathrm{d}\tau \mathrm{d}\xi. \tag{11.68}$$

Therefore,

$$(\Omega|S\Omega) = \exp\left(\frac{\mathrm{i}}{2\pi} \int \frac{\overline{v(\tau,\xi)} v(\tau,\xi)\omega(\xi)}{\omega(\xi)^2 - \tau^2 - \mathrm{i}0} \mathrm{d}\tau \mathrm{d}\xi \right). \tag{11.69}$$

Next we consider the contributions from the external lines

$$\begin{aligned} &\left(\xi^+_{m_+}, \dots, \xi^+_1 | S | \xi^-_{m_-}, \dots, \xi^-_1\right) \qquad (11.70) \\ = \ & (\Omega|S\Omega) \prod_{j=1}^{m^+} \Big((-\mathrm{i}) v(t_j, \xi_j^+) \mathrm{e}^{\mathrm{i}t_j\omega(\xi_j^+)} \mathrm{d}t_j \Big) \prod_{i=1}^{m^-} \Big((-\mathrm{i}) \overline{v(t_i, \xi_i^-)} \mathrm{e}^{-\mathrm{i}t_i\omega(\xi_i^-)} \mathrm{d}t_i \Big). \end{aligned}$$

□

11.2 Feynman diagrams

11.2.1 Wick powers of the free field

We will use now notation parallel to the notation for a relativistic QFT in $1+3$ dimensions. (Sometimes we replace 3 by d). We restrict ourselves to a bosonic theory.

We will parametrize the creation/annihilation operators by "4-momenta" $k \in \mathbb{R}^{1+3}$, where the energy k^0 is given by a real function $\mathbb{R}^3 \ni \vec{k} \to \varepsilon(\vec{k})$. We would like to put

$$\varepsilon(\vec{k}) = \sqrt{\vec{k}^2 + m^2}, \tag{11.71}$$

but this can be problematic, and therefore we will keep ε an arbitrary function, demanding only

$$\varepsilon(-\vec{k}) = \varepsilon(\vec{k}) \tag{11.72}$$

We use the notation $k = (\varepsilon(\vec{k}), \vec{k}) \in \mathbb{R}^{1+3}$, saying that k is "on shell". We consider $\mathbb{R}^3 \ni \vec{k} \mapsto \hat{a}^*(k), \hat{a}(k)$ satisfying the commutation relations

$$[\hat{a}(k), \hat{a}^*(k')] = \delta(\vec{k} - \vec{k}'), \tag{11.73}$$

$$[\hat{a}(k), \hat{a}(k')] = [\hat{a}^*(k), \hat{a}^*(k')] = 0. \tag{11.74}$$

The free Hamiltonian is

$$H_0 = \int \varepsilon(k) \hat{a}^*(k) \hat{a}(k) \mathrm{d}\vec{k}. \tag{11.75}$$

We will use operators in the free Heisenberg picture (the interaction picture), There exists a distinguished observable, called a *field*

$$\begin{aligned}\hat{\phi}(x) &= \mathrm{e}^{\mathrm{i}tH_0}\hat{\phi}(0,\vec{x})\mathrm{e}^{-\mathrm{i}tH_0} &(11.76)\\ &= \int \mathrm{d}\vec{k}\frac{1}{\sqrt{(2\pi)^3 2\varepsilon(\vec{k})}}\left(\mathrm{e}^{\mathrm{i}kx}\hat{a}(k)+\mathrm{e}^{-\mathrm{i}kx}\hat{a}^*(k)\right). &(11.77)\end{aligned}$$

We sometimes also use the *conjugate field*

$$\hat{\pi}(x) := \dot{\hat{\phi}}(x) = \int \frac{\mathrm{d}\vec{k}\sqrt{\varepsilon(\vec{k})}}{\mathrm{i}\sqrt{(2\pi)^3}\sqrt{2}}\left(\mathrm{e}^{\mathrm{i}kx}\hat{a}(k)-\mathrm{e}^{-\mathrm{i}kx}\hat{a}^*(k)\right). \tag{11.78}$$

Note that $\hat{\phi}$ and $\hat{\pi}$ satisfy the usual equal time commutation relations, independently of the relation (11.71):

$$\begin{aligned}[\hat{\phi}(t,\vec{x}),\hat{\phi}(t,\vec{y})] = [\hat{\pi}(t,\vec{x}),\hat{\pi}(t,\vec{y})] &= 0,\\ [\hat{\phi}(t,\vec{x}),\hat{\pi}(t,\vec{y})] &= \mathrm{i}\delta(\vec{x}-\vec{y}). &(11.79)\end{aligned}$$

For any $x \in \mathbb{R}^{1+3}$, we introduce the *Wick powers of fields*

$$\begin{aligned}&:\hat{\phi}(x)^n: &(11.80)\\ &= \sum_{j=0}^{n}\binom{n}{j}\left(\int \mathrm{d}\vec{k}\frac{\mathrm{e}^{-\mathrm{i}kx}\hat{a}^*(k)}{\sqrt{(2\pi)^3 2\varepsilon(\vec{k})}}\right)^j\left(\int \mathrm{d}\vec{k}\frac{\mathrm{e}^{\mathrm{i}kx}\hat{a}(k)}{\sqrt{(2\pi)^3 2\varepsilon(\vec{k})}}\right)^{n-j}. &(11.81)\end{aligned}$$

Note that, if

$$\int \frac{1}{\varepsilon(\vec{k})}\mathrm{d}\vec{k} < \infty, \tag{11.82}$$

then $\hat{\phi}(x)$ is a well defined (unbounded) operator on the Fock space and

$$:\hat{\phi}(x)^m := \hat{\phi}(x)^n + \sum_{k=1}^{[m/2]} c_k\hat{\phi}(x)^{m-2k}. \tag{11.83}$$

Unfortunately, if (11.71) is satisfied, the constants c_k are divergent, in all dimensions $d = 1, 2, \ldots$. The free Hamiltonian can be rewritten as

$$H_0 = \int \mathrm{d}\vec{x}\int \mathrm{d}\vec{y}:\hat{\phi}(0,\vec{x})\hat{\phi}(0,\vec{y}):g(\vec{x}-\vec{y}) + \int \mathrm{d}\vec{x}:\hat{\pi}(0,\vec{x})^2:, \tag{11.84}$$

where

$$g(x) = \int \mathrm{e}^{\mathrm{i}\vec{k}\vec{x}}\varepsilon(\vec{k})^2\mathrm{d}\vec{k}. \tag{11.85}$$

We also introduce the Feynman propagator

$$D^{\mathrm{c}}(x-y) = \mathrm{i}\Big(\Omega|\mathrm{T}\big(\hat{\phi}(x)\hat{\phi}(y)\big)\Omega\Big) \tag{11.86}$$

We will also use the Feynman propagator in the energy-momentum representation

$$D^{\mathrm{c}}(k) = \int D^{\mathrm{c}}(x)\mathrm{e}^{-\mathrm{i}kx}\mathrm{d}x. \tag{11.87}$$

The Feynman propagator turns out to be one of the inverses of $\varepsilon(\vec{k})^2 - (k^0)^2$:

Theorem 11.4.

$$D^{\mathrm{c}}(k) = \frac{1}{\varepsilon(\vec{k})^2 - (k^0)^2 - \mathrm{i}0}. \tag{11.88}$$

Proof. First we compute in the space-time representation:

$$\begin{aligned} D^{\mathrm{c}}(t,\vec{x}) &= \mathrm{i}\int \left(\mathrm{e}^{-\mathrm{i}\varepsilon(\vec{k})t+\mathrm{i}\vec{k}\vec{x}}\theta(t) + \mathrm{e}^{\mathrm{i}\varepsilon(\vec{k})t-\mathrm{i}\vec{k}\vec{x}}\theta(-t)\right)\frac{\mathrm{d}\vec{k}}{(2\pi)^3 2\varepsilon(\vec{k})} \\ &= \mathrm{i}\int \left(\mathrm{e}^{-\mathrm{i}\varepsilon(\vec{k})t}\theta(t) + \mathrm{e}^{\mathrm{i}\varepsilon(\vec{k})t}\theta(-t)\right)\mathrm{e}^{\mathrm{i}\vec{k}\vec{x}}\frac{\mathrm{d}\vec{k}}{(2\pi)^3 2\varepsilon(\vec{k})}, \end{aligned}$$

where we used the parity of ε (11.72). Next we go to the energy-momentum representation:

$$\begin{aligned} D^{\mathrm{c}}(k^0,\vec{k}) &= \mathrm{i}\int\int D^{\mathrm{c}}(t,\vec{x})\mathrm{e}^{\mathrm{i}k^0t-\mathrm{i}\vec{k}\vec{x}}\mathrm{d}t\mathrm{d}\vec{k} \\ &= \mathrm{i}\int \Big(\mathrm{e}^{-\mathrm{i}\varepsilon(\vec{k})t}\theta(t) + \mathrm{e}^{\mathrm{i}\varepsilon(\vec{k})t}\theta(-t)\Big)\mathrm{e}^{\mathrm{i}k^0t}\frac{\mathrm{d}t}{2\varepsilon(\vec{k})} \\ &= \mathrm{i}\int_0^\infty \Big(\mathrm{e}^{-\mathrm{i}\varepsilon(\vec{k})t+\mathrm{i}k^0t} + \mathrm{e}^{-\mathrm{i}\varepsilon(\vec{k})t-\mathrm{i}k^0t}\frac{\mathrm{d}t}{2\varepsilon(\vec{k})} \\ &= \frac{1}{2\varepsilon(\vec{k})(\varepsilon(\vec{k}) - k^0 - \mathrm{i}0)} + \frac{1}{2\varepsilon(\vec{k})(\varepsilon(\vec{k}) + k^0 - \mathrm{i}0)} \\ &= \frac{1}{\varepsilon(\vec{k})^2 - (k^0)^2 - \mathrm{i}0}. \end{aligned}$$

□

11.2.2 Feynman diagrams for vacuum expectation value of scattering operator

One can argue that a typical quantum field theory should be formally given by a Hamiltonian

$$H = H_0 + W(t), \tag{11.89}$$

where the perturbation (in the Schrödinger picture) is

$$W(t) \quad = \quad \sum_j \int \mathrm{d}\vec{x} f_j\big(t,\vec{x}\big) : \hat{\phi}(0,\vec{x})^j : . \tag{11.90}$$

The Hamiltonian in the interaction picture is therefore

$$H_{\mathrm{Int}}(t) = \sum_j \int \mathrm{d}\vec{x} f_j\big(t,\vec{x}\big) : \hat{\phi}(t,\vec{x})^j : . \tag{11.91}$$

Let S denote the scattering operator for (11.89). We would like to compute

$$(\Omega|S\Omega). \tag{11.92}$$

(1) Rules about drawing diagrams.

  (i) To the term in the interaction of order j we associate a *vertex* with p *legs*.
  (ii) We choose a sequence of vertices $p_n, \ldots, p_1$ and put them without any order.
  (iii) We connect pairs of legs with lines. There are no self-lines.

(2) Consider the group of symmetries of a diagram, where we allow to permute the vertices. We will denote by $[D]!$ the order of this group.

(3) Rule about evaluating diagrams (the space-time approach).

  (i) The jth vertex has its variable x_j. We put $-\mathrm{i}f_{p_j}(x_j)$ for the jth vertex.
  (ii) We put $-\mathrm{i}D^{\mathrm{c}}(x_j - x_i)$ for each line connecting jth and ith vertex.
  (iii) We multiply contributions from all lines, obtaining a number that we denote $D(x_n, \ldots, x_1)$.

(4) We sum up all diagrams divided by symmetry factors and integrate :

$$(\Omega|S\Omega) = \sum_{\substack{\text{all diag.}\\ n \text{ vertices}\\ \text{no ext. lines}}} \int \mathrm{d}x_n \cdots \int \mathrm{d}x_1 \frac{D(x_n, \ldots, x_1)}{[D]!}. \tag{11.93}$$

Instead of (3) we can use

(3)' Rules about evaluating diagrams in the energy-momentum approach

  (i) For the jth vertex with we put

$$-\mathrm{i}f_{p_j}(k_1 + \cdots + k_{p_j}) = -\mathrm{i}\int \mathrm{d}x \mathrm{e}^{-\mathrm{i}(k_1+\cdots+k_{p_j})x} f_{p_j}(x). \tag{11.94}$$

  (ii) We put $-\mathrm{i}\int D^{\mathrm{c}}(k)\frac{\mathrm{d}k}{(2\pi)^4}$ for each internal line.
  (iii) We evaluate the integral over k corresponding to all lines obtaining $\int \mathrm{d}x_n \cdots \int \mathrm{d}x_1 D(x_n, \ldots, x_1)$.

By the Linked Cluster Theorem (11.93) can be rewritten as

$$\log(\Omega|S\Omega) = \sum_{\substack{\text{all con. diag.}\\ n \text{ vertices}\\ \text{no ext. lines}}} \int \mathrm{d}x_n \cdots \int \mathrm{d}x_1 \frac{D(x_n, \ldots, x_1)}{[D]!}.$$

11.2.3 Feynman diagrams for the energy shift

Assume now that $f(t,\vec{x}) = f(\vec{x})$ do not depend on time and $H_0 \geq 0$. We would like to compute the energy shift (or, what is the same, the ground state energy of H).

The rules for drawing Feynman diagrams and symmetry factors are the same as in Subsect. 11.2.2. We use the space-time rules for the evaluation of a diagram D, where we make one change: We do not integrate over one time, for instance over t_1. We obtain

$$E = \sum_{n=0}^{\infty} \sum_{\substack{\text{all con. diag.} \\ n \text{ vertices} \\ \text{no ext. lines}}} \int \mathrm{d}x_n \cdots \int \mathrm{d}x_2 \int \mathrm{d}\vec{x}_1 \frac{D(x_n, \dots, 0, \vec{x}_1)}{[D]!}.$$

11.2.4 Green's functions

Recall that the *N-point Green's function* is defined for $x_N, \dots, x_1$ as follows:

$$\begin{aligned} & \langle \hat{\phi}(x_N) \cdots \hat{\phi}(x_1) \rangle \\ := & \left(\Omega^+ | \mathrm{T}\big(\hat{\phi}(x_N) \cdots \cdots \hat{\phi}(x_1)\big) \Omega^- \right), \end{aligned} \tag{11.95}$$

where

$$\begin{aligned} \Omega^{\pm} &:= \lim_{t \to \pm\infty} \mathrm{Texp} \left(-\mathrm{i} \int_t^0 \hat{H}(s) \mathrm{d}s \right) \Omega \\ &= \mathrm{Texp} \left(-\mathrm{i} \int_{\pm\infty}^0 \hat{H}_{\mathrm{Int}}(s) \mathrm{d}s \right) \Omega. \end{aligned}$$

and the fields $\hat{\phi}(x)$ are in the Heisenberg picture:

$$\hat{\phi}(t, \vec{x}) = \mathrm{Texp}\Big(-\mathrm{i} \int_t^0 \hat{H}(s) \mathrm{d}s \Big) \hat{\phi}(0, \vec{x}) \mathrm{Texp}\Big(-\mathrm{i} \int_0^t \hat{H}(s) \mathrm{d}s \Big). \tag{11.96}$$

One can organize Green's functions in terms of the *generating function*:

$$\begin{aligned} Z(f) &= \sum_{N=0}^{\infty} \int \cdots \int \frac{(-\mathrm{i})^N}{N!} \langle \hat{\phi}(x_N) \cdots \hat{\phi}(x_1) \rangle f(x_N) \cdots f(x_1) \mathrm{d}x_N \cdots \mathrm{d}x_1 \\ &= \left(\Omega^+ \middle| \mathrm{Texp} \left(-\mathrm{i} \int_{-\infty}^{\infty} \left(\hat{H}(t) + \int f(t, \vec{x}) \hat{\phi}(0, \vec{x}) \mathrm{d}\vec{x} \right) \mathrm{d}t \right) \Omega^- \right) \\ &= \left(\Omega \middle| \mathrm{Texp} \left(-\mathrm{i} \int_{-\infty}^{\infty} \hat{H}_{\mathrm{Int}}(t) \mathrm{d}t - \mathrm{i} \int f(x) \hat{\phi}_{\mathrm{fr}}(x) \mathrm{d}x \right) \Omega \right). \end{aligned}$$

Thus $Z(f)$ is the vacuum expectation value of a scattering operator, where the usual interaction Hamiltonian $H_{\mathrm{Int}}(t)$ has been replaced by $H_{\mathrm{Int}}(t) + \int f(t, \vec{x}) \hat{\phi}_{\mathrm{fr}}(t, \vec{x}) \mathrm{d}\vec{x}$. One can retrieve Green's functions from the generating function:

$$\langle \hat{\phi}(x_N) \cdots \hat{\phi}(x_1) \rangle = \mathrm{i}^N \frac{\partial^N}{\partial f(x_N) \cdots \partial f(x_1)} Z(f) \Big|_{f=0}. \tag{11.97}$$

The Fourier transform of Green's function will be denoted as usual by the change of the variables:

$$\begin{aligned}&\langle\hat{\phi}(k_N)\cdots\hat{\phi}(k_1)\rangle\\ :=&\int \mathrm{d}x_n\cdots\int\mathrm{d}x_1\mathrm{e}^{-\mathrm{i}x_nk_n-\cdots-\mathrm{i}x_1k_1}\langle\hat{\phi}(x_N)\cdots\hat{\phi}(x_1)\rangle.\end{aligned}$$

We introduce also *amputated Green's functions*:

$$\begin{aligned}&\langle\hat{\phi}(k_n)\cdots\hat{\phi}(k_1)\rangle_{\mathrm{amp}}\\ =\ &(k_n^2+m^2)\cdots(k_1^2+m^2)\langle\hat{\phi}(k_n)\cdots\hat{\phi}(k_1)\rangle.\end{aligned}\tag{11.98}$$

Amputated Green's functions can be used to compute scattering amplitudes:

$$\begin{aligned}&\Big(k_{m^+}^+,\dots,k_1^+|\,\hat{S}\,|k_{m^-}^-,\dots,k_1^-\Big)\\ =\ &\frac{\langle\hat{\phi}(k_1^+)\cdots\hat{\phi}(k_{m^+}^+)\hat{\phi}(-k_{m^-}^-)\cdots\hat{\phi}(-k_1^-)\rangle_{\mathrm{amp}}}{\sqrt{(2\pi)^{3(m^++m^-)}}\sqrt{2\varepsilon(k_1^+)}\cdots\sqrt{2\varepsilon(k_{m^+}^+)}\sqrt{2\varepsilon(k_{m^-}^-)}\cdots\sqrt{2\varepsilon(k_1^-)}},\end{aligned}\tag{11.99}$$

where all $k_i^\pm$ are on shell, that is $k_i^\pm=\big(\varepsilon(\vec{k}_i^\pm),\vec{k}_i^\pm\big)$.

11.2.5 Feynman diagrams for the scattering operator

We would like to compute the scattering operator, representing it as Wick's polynomial:

$$S=s(\hat{a}^*,\hat{a}).\tag{11.100}$$

The Feynman rules for scattering operator follow from (11.99) and the rules for the vacuum expectation value of the scattering amplitude, if we add additional *insertion vertices*—one-legged vertices corresponding to the term $\int\mathrm{d}xf(x)\hat{\phi}_{\mathrm{fr}}(x)$.

(1) Rules about drawing diagrams.

  (i) To the term in the interaction of order p we associate a *vertex* with p *legs*.
  (ii) We choose a sequence of vertices $p_n,\dots,p_1$ and put them without any order.
  (iii) On the right we put the incoming particles, on the left the outgoing particles, each having a single leg.
  (iv) To the incoming particles we associate the variables $k_{m_-}^-,\dots,k_1^-$. To the outgoing particles we associate the variables $k_{m_+}^+,\dots,k_1^+$.
  (v) We connect pairs of legs with lines. There are no self-lines.

(2) Consider the group of symmetries of a diagram, where we allow to permute the vertices, but not the particles. We will denote by $[D]!$ the order of this group.

(3) Rule about evaluating diagrams (the space-time approach).

  (i) The jth vertex has its variable x_j. We put $-\mathrm{i}f_{p_j}(x_j)$ for the jth vertex.
  (ii) We put $-\mathrm{i}D^{\mathrm{c}}(x_j-x_i)$ for each line connecting jth and ith vertex.

(iii) For the incoming particle k_j^- connected to the vertex at x_j we put $\frac{\mathrm{e}^{\mathrm{i}x_j k_j^-} a(k_j^-)}{\sqrt{(2\pi)^3 2\varepsilon(\vec{k}_j^-)}}$.

(iv) For the outgoing particle k_j^+ connected to the vertex at x_j we put $\frac{\mathrm{e}^{-\mathrm{i}x_j k_j^+} a^*(k_j^+)}{\sqrt{(2\pi)^3 2\varepsilon(\vec{k}_j^+)}}$.

(v) We multiply contributions from all lines, obtaining a polynomial that we denote $D(x_n, \ldots, x_1; a^*, a)$.

(4) We sum up all diagrams divided by symmetry factors:

$$s(a^*, a) = \sum_{n=0}^{\infty} \sum_{\substack{\text{all diag.} \\ n \text{ vertices}}} \int \mathrm{d}x_n \cdots \int \mathrm{d}x_1 \frac{D(x_n, \ldots, x_1; a^*, a)}{[D]!}. \tag{11.101}$$

Instead of (3) we can use

(3)' Rules about evaluating diagrams in the energy-momentum approach

(i) For a vertex with legs $k_1, \ldots, k_p$ we put

$$-\mathrm{i}f(k_1 + \cdots + k_n) = -\mathrm{i} \int \mathrm{d}x \mathrm{e}^{-\mathrm{i}(k_1 + \cdots + k_p)x} f(x). \tag{11.102}$$

(ii) We put $-\mathrm{i} \int D^{\mathrm{c}}(k) \frac{\mathrm{d}k}{(2\pi)^4}$ for each internal line.

(iii) For an incoming line with variable k_j^- we put $\frac{a(k_j^-)}{\sqrt{(2\pi)^3 2\varepsilon(\vec{k}_j^-)}}$.

(iv) For an outgoing line with variable k_j^+ we put $\frac{a^*(k_j^+)}{\sqrt{(2\pi)^3 2\varepsilon(\vec{k}_j^+)}}$.

(v) We evaluate the integral over k_j corresponding to all lines obtaining $\int \mathrm{d}x_n \cdots \int \mathrm{d}x_1 D(x_n, \ldots, x_1; a^*, a)$.

Recall that in (11.45) we defined the linked scattering operator. It can be computed using Feynman diagrams:

$$s_{\mathrm{link}}(a^*, a) \tag{11.103}$$

$$= \sum_{n=0}^{\infty} \sum_{\substack{\text{linked diag.} \\ n \text{ vertices}}} \int \cdots \int \frac{D(x_n, \ldots, x_1; a^*, a)}{[D]!} \mathrm{d}x_n \cdots \mathrm{d}x_1 \tag{11.104}$$

$$= \exp\left(\sum_{n=0}^{\infty} \sum_{\substack{\text{con. linked diag.} \\ n \text{ vertices}}} \int \cdots \int \frac{D(x_n, \ldots, x_1; a^*, a)}{[D]!} \mathrm{d}x_n \cdots \mathrm{d}x_1 \right). \tag{11.105}$$

11.2.6 Feynman diagrams for scattering amplitudes for time-independent perturbations

Assume now that $f(t, \vec{x}) = f(\vec{x})$ do not depend on time. Then the rules for computing the scattering operator slightly change. Let us introduce

$$\begin{aligned} & D_{\rm sc}(E) && (11.106) \\ :=& 2\pi \int \mathrm{d}x_n \cdots \int \mathrm{d}x_2 \int \mathrm{d}\vec{x}_1 \delta(E - H_0) D(x_n, \dots, x_2, 0, \vec{x}_1) \delta(E - H_0), && (11.107) \end{aligned}$$

where we use the operator interpretation of D. Then

$$\begin{aligned} & s_{\rm link}(a^*, a) && (11.108) \\ =& \sum_{\text{linked diag.}} \int \mathrm{d}E \frac{D_{\rm sc}(E; a^*, a)}{[D]!} && (11.109) \\ =& \exp\Bigg(\sum_{\text{con. linked diag.}} \int \mathrm{d}E \frac{D_{\rm sc}(E; a^*, a)}{[D]!} \Bigg). && (11.110) \end{aligned}$$

11.2.7 Quadratic interactions

Suppose that (in the Schrödinger picture)

$$\hat{H}(t) := \int \hat{a}^*(k) \hat{a}(k) \mathrm{d}\vec{k} + \int \frac{1}{2} \kappa(t, \vec{x}) {:}\hat{\phi}^2(0, \vec{x}){:}\Big) \mathrm{d}\vec{x}. \qquad (11.111)$$

There is only one vertex, with the function (in momentum representation) $-\mathrm{i}\kappa(k_1 + k_2)$. Connected diagrams with no external lines are loops with n vertices $n = 2, 3, \dots$. ($n = 1$ is excluded, because there are no self-lines). The value of the nth vertex is

$$\begin{aligned} & (-1)^n \int \mathrm{d}x_n \cdots \int \mathrm{d}x_1 \kappa(x_n) D^{\rm c}(x_n - x_{n-1}) \cdots \kappa(x_1) D^{\rm c}(x_1 - x_n) && (11.112) \\ =& (-1)^n \int \frac{\mathrm{d}k_n}{(2\pi)^4} \cdots \int \frac{\mathrm{d}k_1}{(2\pi)^4} \kappa(k_1 - k_n) D^{\rm c}(k_n) \cdots \kappa(k_2 - k_1) D^{\rm c}(k_1) && (11.113) \\ =& (-1)^n \mathrm{Tr}(\kappa D^{\rm c})^n. && (11.114) \end{aligned}$$

The group of symmetries of the loop with n vertices is the dihedral group D_n, which has $2n$ elements. Therefore,

$$\begin{aligned} \mathcal{E} := \mathrm{i} \log(\Omega | \hat{S} \Omega) &= \mathrm{i} \sum_{n=2}^{\infty} \frac{(-1)^n}{2n} \mathrm{Tr}(\kappa D^{\rm c})^n \\ &= \frac{\mathrm{i}}{2} \mathrm{Tr}\Big(-\log(1 + \kappa D^{\rm c}) + \kappa D^{\rm c} \Big) =: \sum_{n=2}^{\infty} \mathcal{E}_n. \qquad (11.115) \end{aligned}$$

12 Method of characteristics

12.1 Manifolds

Let $\mathcal{X}$ be a manifold and $x \in \mathcal{X}$. $\mathrm{T}_x\mathcal{X}$, resp. $\mathrm{T}_x^{\#}\mathcal{X}$ will denote the tangent, resp. cotangent space at x. $\mathrm{T}\mathcal{X}$, resp. $\mathrm{T}^{\#}\mathcal{X}$ will denote the tangent, resp. cotangent bundle over $\mathcal{X}$.

Suppose that $x = (x^i)$ are coordinates on $\mathcal{X}$. Then we have a natural basis in $\mathrm{T}\mathcal{X}$ denoted ∂_{x^i} and a natural basis in $\mathrm{T}^{\#}\mathcal{X}$, denoted $\mathrm{d}x^i$. Thus every vector field can be written as $v = v(x)\partial_x = v^i(x)\partial_{x^i}$ and every differential 1-form can be written as $\alpha = \alpha(x)\mathrm{d}x = \alpha_i(x)\mathrm{d}x^i$.

We will use the following notation: $\hat{\partial}_x$ is the operator ∂_x that acts on everything on the right. ∂_x acts only on the function immediately to the right. Thus the Leibniz rule can be written as

$$\hat{\partial}_x f(x)g(x) = \partial_x f(x)g(x) + f(x)\partial_x g(x). \tag{12.1}$$

There are situations when we could use both kinds of notation: $\hat{\partial}_x$ and ∂_x, as in the last term of (12.1). In such a case we make a choice based on esthetic reasons.

12.2 1st order differential equations

Let $v(t,x)\partial_x$ be a vector field and $f(t,x)$ a function, both time-dependent. Consider the equation

$$\begin{aligned} \big(\partial_t + v(t,x)\partial_x + f(t,x)\big)\Psi(t,x) &= 0, \\ \Psi(0,x) &= \Psi(x). \end{aligned} \tag{12.2}$$

To solve it one finds first the solution of

$$\left\{ \begin{array}{lcl} \partial_t x(t,y) &=& v(t, x(t,y)) \\ x(0,y) &=& y; \end{array} \right. \tag{12.3}$$

Let $x \mapsto y(t,x)$ be the inverse function.

Proposition 12.1. *Set*

$$F(t,y) := \int_0^t f\big(s, x(s,y)\big)\mathrm{d}s.$$

Then

$$\Psi(t,x) := \mathrm{e}^{-F\left(t,y(t,x)\right)}\Psi\big(y(t,x)\big)$$

is the solution of (12.2).

Proof. Set

$$\Phi(t,y) := \Psi\big(t, x(t,y)\big). \tag{12.4}$$

We have

$$\begin{aligned} \partial_t \Phi(t,y) &= \big(\partial_t + \partial_t x(t,y)\partial_x\big)\Psi\big(t,x(t,y)\big) \\ &= \big(\partial_t + v\big(t,x(t,y)\big)\partial_x\big)\Psi\big(t,x(t,y)\big). \end{aligned}$$

Hence (12.2) can be rewritten as

$$\begin{aligned}\big(\partial_t + f\big(t, x(t,y)\big)\big)\Phi(t,y) &= 0,\\ \Phi(0,y) &= \Psi(y).\end{aligned} \tag{12.5}$$

(12.5) is solved by

$$\Phi(t,y) := \mathrm{e}^{-F(t,y)}\Psi(y).$$

□

Consider now a vector field $v(x)\partial_x$ and a function $f(x)$, both time-independent. Consider the equation

$$\big(v(x)\partial_x + f(x)\big)\Psi(x) = 0. \tag{12.6}$$

Again, first one finds solutions of

$$\partial_t x(t) = v\big(x(t)\big). \tag{12.7}$$

Then we try to find a manifold $\mathcal{Z}$ in $\mathcal{X}$ of codimension 1 that crosses each curve given by a solution of (12.6) exactly once. If the field is everywhere nonzero, this should be possible at least locally. Then we can define a family of solutions of (12.6) denoted $x(t,z)$, $z \in \mathcal{Z}$, satisfying the boundary conditions

$$x(0,z) = z, \quad z \in \mathcal{Z}. \tag{12.8}$$

This gives a local parametrization $\mathbb{R} \times \mathcal{Z} \ni (t,z) \mapsto x(t,z) \in \mathcal{X}$.

Let $x \mapsto \big(t(x), z(x)\big)$ be the inverse function.

Proposition 12.2. *Set*

$$F(t,z) := \int_0^t f\big(x(s,z)\big)\mathrm{d}s.$$

Then

$$\Psi(t,x) := \mathrm{e}^{-F\left(t(x),z(x)\right)}\Psi\big(z(x)\big)$$

is the solution of (12.2).

Proof. Set $\Phi(t,z) := \Psi\big(x(t,z)\big)$. Then

$$\begin{aligned}\partial_t\Phi(t,z) &= \partial_t x(t,z)\partial_x\Psi\big(x(t,z)\big)\\ &= v\big(x(t,z)\big)\partial_x\Psi\big(x(t,z)\big).\end{aligned}$$

Hence we can rewrite (12.6) together with the boundary conditions as

$$\begin{aligned}\big(\partial_t + f\big(x(t,z)\big)\big)\Phi(t,z) &= 0,\\ \Phi(0,z) &= \Psi(z).\end{aligned} \tag{12.9}$$

(12.9) is solved by

$$\Phi(t,z) := \mathrm{e}^{-F(t,z)}\Psi(z).$$

□

12.3 1st order differential equations with a divergence term

Fort a vector field $v(x)\partial_x$ we define

$$\mathrm{div} v(x) = \partial_{x^i} v^i(x).$$

Note that $\mathrm{div} v(x)$ depends on the coordinates.

Consider a time dependent vector field $v(t,x)\partial_x$ and the equation

$$\begin{aligned} \left(\partial_t + v(t,x)\partial_x + \alpha \mathrm{div} v(t,x)\right)\Psi(t,x) &= 0, \\ \Psi(0,x) &= \Psi(x), \end{aligned} \tag{12.10}$$

Proposition 12.3. *(12.10) is solved by*

$$\Psi(t,x) := \big(\det \partial_x y(t,x)\big)^{\alpha} \Psi(y(t,x)). \tag{12.11}$$

Proof. We introduce $\Phi(t,y)$ as in (12.4) and rewrite (12.10) as

$$\begin{aligned} \Big(\partial_t + \alpha \mathrm{div} v\big(t, x(t,y)\big)\Big)\Phi(t,y) &= 0, \\ \Phi(0,y) &= \Psi(y) \end{aligned} \tag{12.12}$$

We have the following identity for the determinant of a matrix valued function $t \mapsto A(t)$:

$$\partial_t \det A(t) = \mathrm{Tr}\left(\partial_t A(t) A(t)^{-1}\right) \det A(t). \tag{12.13}$$

Therefore,

$$\begin{aligned} \partial_t\big(\det \partial_y x(t,y)\big)^{-\alpha} &= -\alpha \mathrm{div} \partial_t x(t,y)\big(\det \partial_y x(t,y)\big)^{-\alpha} \\ &= -\alpha \mathrm{div} v\big(t, x(t,y)\big)\big(\det \partial_y x(t,y)\big)^{-\alpha}. \end{aligned}$$

Therefore, (12.12) is solved by

$$\Phi(t,y) := \big(\det \partial_y x(t,y)\big)^{-\alpha} \Psi(y).$$

□

Consider again a time independent vector field $v(x)\partial_x$ and the equation

$$\left(v(x)\partial_x + \alpha \mathrm{div} v(x)\right)\Psi(x) = 0. \tag{12.14}$$

We introduce the a hypersurface $\mathcal{Z}$ and solutions $x(t,z)$, as described before Prop. 12.2.

Proposition 12.4. *Set*

$$w(x) := \partial_z x\big(t(x), z(x)\big).$$

Then the solution of (12.14) which on $\mathcal{Z}$ equals $\Psi(z)$ is

$$\Psi(x) := \big(\det[v(x), w(x)]\big)^{-\alpha} \Psi\big(z(x)\big). \tag{12.15}$$

Note that if $\mathcal{X}$ is one-dimensional, so that we can locally identify it with $\mathbb{R}$ and v is a number, (12.15) becomes $\Psi(x) = C\big(v(x)\big)^{-\alpha}$.

12.4 α-densities on a vector space

Let $\alpha > 0$. We say that $f : (\mathbb{R}^d)^d \to \mathbb{R}$ is an α-density, if

$$\langle f | av_1, \dots, av_d \rangle = |\det a|^\alpha \langle f | v_1, \dots, v_d \rangle, \tag{12.16}$$

for any linear transformation a on $\mathbb{R}^d$ and $v_1, \dots, v_d \in \mathbb{R}^d$.

If $\mathcal{X}$ is a manifold, then by an α-density we understand a function on $\mathcal{X} \ni x \mapsto \Psi(x)$ where $\Psi(x)$ is an α-density on $\mathrm{T}_x\mathcal{X}$.

Clearly, given coordinates $x = (x^i)$ on $\mathcal{X}$, using the basis ∂_{x_i} in $\mathrm{T}\mathcal{X}$, we can identify an α-density Ψ with the function

$$x \mapsto \langle \Psi | \partial_{x^1}, \dots, \partial_{x^d} \rangle (x), \tag{12.17}$$

which, by abuse of notation will be also denoted $\Psi(x)$. If we use some other coordinates $x' = x'^i$, then we obtain another function $x' \mapsto \Psi'(x')$. We have the transformation property

$$\Psi(x) = |\partial_x x'|^\alpha \, \Psi'(x'). \tag{12.18}$$

A good mnemotechnic way to denote an α-density is to write $\Psi(x)|\mathrm{d}x|^\alpha$. Note that 0-densities are usual functions, 1-densities, or simply densities are measures. $\frac{1}{p}$-densities raised to the pth power give a density, and so one can invariantly define their L^p-norm:

$$\int \left| \Psi(x) |\mathrm{d}x|^{\frac{1}{p}} \right|^p = \int |\Psi(x)|^p \mathrm{d}x = \|\phi\|_p^p. \tag{12.19}$$

Proposition 12.5. *If $v(x)\partial_x$ is a vector field, the operator*

$$v(x)\partial_x + \alpha \mathrm{div} v(x) \tag{12.20}$$

is invariantly defined on α-densities.

Proof. In fact, suppose we consider some other coordinates x'. In the new coordinates the vector field $v(x)\partial_x$ becomes $v'(x')\partial_{x'} = (\partial_x x')v(x(x'))\partial_{x'}$. We will denote $\mathrm{div}'v'$ the divergence in the new coordinates. We need to show that if

$$\Phi = |\det \partial_x x'|^\alpha \Phi', \quad \Psi = |\det \partial_x x'|^\alpha \Psi',$$

then

$$\big(v(x)\partial_x + \alpha \mathrm{div} v(x)\big)\Phi = \Psi$$

is equivalent to

$$\big(v'(x')\partial_{x'} + \alpha \mathrm{div}' v'(x')\big)\Phi' = \Psi'.$$

We have

$$\begin{aligned} \mathrm{div} v' &= \frac{\partial x^j}{\partial x'^i} \frac{\hat{\partial}}{\partial x^j} \frac{\partial x'^i}{\partial x^k} v^k \\ &= \frac{\partial v^j}{\partial x^j} + \frac{\partial x^j}{\partial x'^i} \frac{\partial^2 x'^i}{\partial x^j \partial x^k} v^k \end{aligned}$$

$$v\hat{\partial}_x|\det\partial_x x'|^\alpha \quad = \quad \alpha v^k\frac{\partial^2 x'^i}{\partial x^j\partial x^k}\frac{\partial x^j}{\partial x'^i}|\det\partial_x x'|^\alpha + |\det\partial_x x'|^\alpha v\hat{\partial}_x.$$

Therefore,

$$\begin{aligned} & \big(v(x)\hat{\partial}_x + \alpha \mathrm{div} v(x)\big)|\det\partial_x x'|^\alpha\Phi' \\ = \quad & |\det\partial_x x'|^\alpha\big(v'(x')\hat{\partial}_{x'} + \alpha\mathrm{div}'v'(x')\big)\Phi'. \end{aligned}$$

□

Note that (12.11) can be written as an α-density:

$$\Psi(t,x)|\mathrm{d}x|^\alpha := |\det\partial_x y(t,x)|^\alpha\Psi(y(t,x))|\mathrm{d}x|^\alpha \tag{12.21}$$

Also (12.15) is naturally an α-density.

13 Hamiltonian mechanics

13.1 Symplectic manifolds

Let $\mathcal{Y}$ be a manifold equipped with a 2-form $\omega \in \wedge^2\mathrm{T}^\#\mathcal{Y}$. We say that it is a symplectic manifold iff ω is nondegenerate at every point and $\mathrm{d}\omega = 0$.

Let $(\mathcal{Y}_1,\omega_1),(\mathcal{Y}_2,\omega_2)$ be symplectic manifolds. A diffeomorphism $\rho:\mathcal{Y}_1\to\mathcal{Y}_2$ is called a symplectic transformation if $\rho^\#\omega_2=\omega_1$.

In what follows $(\mathcal{Y},\omega)$ is a symplectic manifold. We will often treat ω as a linear map from $T\mathcal{Y}$ to $T^\#\mathcal{Y}$. Therefore, the action of ω on vector fields u,w will be written in at least two ways

$$\langle\omega|u,w\rangle = \langle u|\omega w\rangle = \omega_{ij}u^iw^j.$$

The inverse of ω as a map $T\mathcal{Y}\to T^\#\mathcal{Y}$ will be denoted ω^{-1}. It can be treated as a section of $\wedge^2 T\mathcal{X}$. The action of ω^{-1} on 1-forms η,ξ can be written in at least two ways

$$\langle\omega^{-1}|\eta,\xi\rangle = \langle\eta|\omega^{-1}\xi\rangle = \omega^{ij}\eta_i\xi_j.$$

If H is a function on $\mathcal{Y}$, then we define its Hamiltonian field $\omega^{-1}\mathrm{d}H$. We will often consider a time dependent Hamiltonian $H(t,y)$ and the corresponding dynamic defined by the *Hamilton equations*

$$\partial_t y(t) = \omega^{-1}\mathrm{d}_y H(t,y(t)). \tag{13.1}$$

Proposition 13.1. *Flows generated by Hamilton equations are symplectic*

If F,G are functions on $\mathcal{Y}$, then we define their Poisson bracket

$$\{F,G\} := \langle\omega^{-1}|\mathrm{d}F,\mathrm{d}G\rangle.$$

Proposition 13.2. $\{\cdot,\cdot\}$ *is a bilinear antisymmetric operation satisfying the Jacobi identity*

$$\{F,\{G,H\}\}+\{H,\{F,G\}\}+\{G,\{H,F\}\}=0 \tag{13.2}$$

and the Leibnitz identity

$$\{F,GH\}=\{F,G\}H+G\{F,H\}. \tag{13.3}$$

Proposition 13.3. *Let $t \mapsto y(t)$ be a trajectory of a Hamiltonian $H(t, y)$. Let $F(t, y)$ be an observable. Then*

$$\frac{\mathrm{d}}{\mathrm{d}t} F\big(t, y(t)\big) = \partial_t F\big(t, y(t)\big) + \{H, F\}\big(t, y(t)\big).$$

In particular,

$$\frac{\mathrm{d}}{\mathrm{d}t} H\big(t, y(t)\big) = \partial_t H\big(t, y(t)\big).$$

13.2 Symplectic vector space

The most obvious example of a symplectic manifold is a symplectic vector space. As we discussed before, it has the form $\mathbb{R}^d \oplus \mathbb{R}^d$ with variables $(x, p) = \big((x^i), (p_j)\big)$ and the symplectic form

$$\omega = \mathrm{d}p_i \wedge \mathrm{d}x^i. \tag{13.4}$$

The Hamilton equations read

$$\begin{aligned} \partial_t x &= \partial_p H(t, x, p), \\ \partial_t p &= -\partial_x H(t, x, p). \end{aligned} \tag{13.5}$$

The Poisson bracket is

$$\{F, G\} = \partial_{x^i} F \partial_{p_i} G - \partial_{p_i} F \partial_{x^i} G. \tag{13.6}$$

Note that Prop 13.1 and 13.2 are easy in a symplectic vector space. To show that ω is invariant under the Hamiltonian flow we compute

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\omega &= \frac{\mathrm{d}}{\mathrm{d}t} \mathrm{d}p(t) \wedge \mathrm{d}x(t) \\ &= -\mathrm{d}\partial_x H\big(x(t), p(t)\big) \wedge \mathrm{d}x(t) + \mathrm{d}p(t) \wedge \mathrm{d}\partial_p H\big(x(t), p(t)\big) \\ &= -\partial_p \partial_x H\big(x(t), p(t)\big) \mathrm{d}p(t) \wedge \mathrm{d}x(t) + \mathrm{d}p(t) \wedge \partial_x \partial_p H\big(x(t), p(t)\big) \mathrm{d}x(t) \;=\; 0 \end{aligned}$$

Proposition 13.4. *The dimension of a symplectic manifold is always even. For any symplectic manifold $\mathcal{Y}$ of dimension $2d$ locally there exists a symplectomorphism onto an open subset of $\mathbb{R}^d \oplus \mathbb{R}^d$.*

Now (13.4) implies Prop. 13.1. Similarly, to see Prop. 13.2 we first check the Jacobi and Leibniz identity for (13.6).

13.3 The cotangent bundle

Let $\mathcal{X}$ be a manifold. We consider the cotangent bundle $\mathrm{T}^{\#}\mathcal{X}$. It is equipped with the canonical projection $\pi : \mathrm{T}^{\#}\mathcal{X} \to \mathcal{X}$.

We can always cover $\mathcal{X}$ with open sets equipped with charts. A chart on $\mathcal{U} \subset \mathcal{X}$ allows us to identify $\mathcal{U}$ with an open subset of $\mathbb{R}^d$ through coordinates $x = (x^i) \in \mathbb{R}^d$. $T^{\#}\mathcal{U}$ can be identified with $\mathcal{U} \times \mathbb{R}^d$, where we use the coordinates $(x, p) = \big((x^i), (p_j)\big)$.

$\mathrm{T}^{\#}\mathcal{X}$ is equipped with the *tautological 1-form*

$$\theta = \sum_i p_i \mathrm{d}x^i, \tag{13.7}$$

(also called *Liouville* or *Poincaré 1-form*), which does not depend on the choice of coordinates. The corresponding symplectic form, called the *canonical symplectic form* is

$$\omega = \mathrm{d}\theta = \sum_i \mathrm{d}p_i \wedge \mathrm{d}x^i. \tag{13.8}$$

Thus locally we can apply the formalism of symplectic vector spaces. In particular, the Hamilton equations have the form (13.5) and the Poisson bracket (13.6).

13.4 Lagrangian manifolds

Let $\mathcal{Y}$ be a symplectic manifold. Let $\mathcal{L}$ be a submanifold of $\mathcal{Y}$ and $i_\mathcal{L} : \mathcal{L} \to \mathcal{Y}$ be its embedding in $\mathcal{Y}$. Then we say that $\mathcal{L}$ is isotropic iff $i_\mathcal{L}^\# \omega = 0$. We say that it is Lagrangian if it is isotropic and of dimension d (which is the maximal possible dimesion for an isotropic manifold). We say that $\mathcal{L}$ is coisotropic if the dimension of the null space of $i_\mathcal{L}^\# \omega$ is maximal possible, that is, $2d - \dim \mathcal{L}$.

Theorem 13.5. *Let $E \in \mathbb{R}$. Let $\mathcal{L}$ be a Lagrangian manifold contained in the level set*

$$H^{-1}(E) := \{y \in \mathcal{Y} \ : \ H(y) = E\}.$$

Then $\omega^{-1}\mathrm{d}H$ is tangent to $\mathcal{L}$.

Proof. Let $y \in \mathcal{Y}$ and $v \in \mathrm{T}_y\mathcal{L}$. Then since $\mathcal{L}$ is contained in a level set of H, we have

$$0 = \langle \mathrm{d}H | v\rangle = -\langle \omega^{-1}\mathrm{d}H | \omega v\rangle. \tag{13.9}$$

By maximality of $\mathrm{T}_y\mathcal{L}$ as an isotropic subspace of $\mathrm{T}_y\mathcal{Y}$, we obtain that $\omega^{-1}\mathrm{d}H \in \mathrm{T}_y\mathcal{L}$. □

Clearly, symplectic transformations map Lagrangian manifolds onto Lagrangian manifolds.

13.5 Lagrangian manifolds in a cotangent bundle

Proposition 13.6. *Let $\mathcal{U}$ be an open subset of $\mathcal{X}$ and consider a function $\mathcal{U} \ni x \mapsto S(x) \in \mathbb{R}$. Then*

$$\big\{ \big(x, \mathrm{d}S(x)\big) \ : \ x \in \mathcal{U} \big\} \tag{13.10}$$

is a Lagrangian submanifold of $T^\#\mathcal{X}$.

Proof. Tangent space of (13.10) at the point $(x^i, \partial_{x^j} S(x)\mathrm{d}x^j)$ is spanned by

$$v_i = \big(\partial_{x^i}, \partial_{x^i}\partial_{x^j} S(x) \partial_{p_j}\big)$$

Now

$$\langle \omega | v_i, v_k\rangle = \sum_{i,j} \partial_{x^i}\partial_{x^j} S(x) - \sum_{k,j} \partial_{x^k}\partial_{x^j} S(x) = 0.$$

□

$\mathcal{U} \ni S(x)$ is called a generating function of the Lagrangian manifold (13.10). If $\mathcal{U}$ is connected, it is uniquely defined up to an additive constant.

Suppose that $\mathcal{L}$ is a connected and simply connected Lagrangian submanifold. Fix $(x_0, p_0) \in \mathcal{L}$. For any $(x,p) \in \mathcal{L}$, let $\gamma_{(x,p)}$ be a path contained in $\mathcal{L}$ joining (x_0, p_0) with (x,p).

$$T\big(x,p\big) \quad := \quad \int_{\gamma_{(x,p)}} \theta.$$

Using that $\mathrm{d}i_{\mathcal{L}}^{\#}\theta = i_{\mathcal{L}}^{\#}\mathrm{d}\theta = i_{\mathcal{L}}^{\#}\omega = 0$ and the Stokes Theorem we see that the integral does not depend on the path. We have

$$\mathrm{d}T = i_{\mathcal{L}}^{\#}\theta. \tag{13.11}$$

If $\pi\Big|_{\mathcal{L}}$ is injective we will say that $\mathcal{L}$ is *projectable on the base*. Then we can use $\mathcal{U} := \pi(\mathcal{L})$ to parametrize $\mathcal{L}$:

$$\mathcal{U} \ni x \mapsto \big(x, p(x)\big) \in \mathcal{L}.$$

We then define

$$S(x) := T\big(x, p(x)\big).$$

We have

$$\partial_{x^i} S(x) \mathrm{d}x^i = \mathrm{d}S(x) = \mathrm{d}T\big(x, p(x)\big) = p_i \mathrm{d}x^i.$$

Hence $x \mapsto S(x)$ is the unique generating functon of $\mathcal{L}$ satisfying $S\big(x(z_0)\big) = 0$.

Both $x \mapsto S(x)$ and $\mathcal{L} \ni (x,p) \mapsto T(x,p)$ will be called *generating functions* of the Lagrangian manifold $\mathcal{L}$. To distinguish between them we may add that the former is *viewed as a function on the base* and the latter is *viewed as a function on* $\mathcal{L}$.

We can generalize the construction of T to more general Lagrangian manifolds. We consider the universal covering $\mathcal{L}^{\mathrm{cov}} \to \mathcal{L}$ with the base point at $\big(x_0, p_0\big)$. Recall that $\mathcal{L}^{\mathrm{cov}}$ is defined as the set of homotopy classes of curves from $(x_0, p_0\big)$ to $\big(x, p\big) \in \mathcal{L}$ contained in $\mathcal{L}$. On $\mathcal{L}^{\mathrm{cov}}$ we define the real function

$$\mathcal{L}^{\mathrm{cov}} \ni [\gamma] \mapsto T([\gamma]) := \int_\gamma \theta. \tag{13.12}$$

Exactly as above we see that (13.12) does not depend on the choice of γ and that (13.11) is true.

13.6 Generating function of a symplectic transformations

Let $(\mathcal{Y}_i, \omega_i)$ be symplectic manifolds. We can than consider the symplectic manifold $\mathcal{Y}_2 \times \mathcal{Y}_1$ with the symplectic form $\omega_1 - \omega_2$. Let $\mathcal{R}$ be the graph of a diffeomorphism ρ, that is

$$\mathcal{R} := (\rho(y), y) \in \mathcal{Y}_2 \times \mathcal{Y}_1. \tag{13.13}$$

Clearly, ρ is symplectic iff $\mathcal{R}$ is a Lagrangian manifold.

Assume that $\mathcal{Y}_i = \mathrm{T}^{\#}\mathcal{X}_i$. We can identify $\mathcal{Y}_2 \times \mathcal{Y}_1$ with $\mathrm{T}^{\#}(\mathcal{X}_2 \times \mathcal{X}_1)$.

Let $\mathrm{T}^{\#}\mathcal{X}_1 \ni (x_1, \xi_1) \mapsto (x_2, \xi_2) \in \mathrm{T}^{\#} X_2$ be a symplectic transformation. A function

$$\mathcal{X}_2 \times \mathcal{X}_1 \ni (x_2, x_1) \mapsto S(x_2, x_1). \tag{13.14}$$

is called a generating function of the transformation ρ if it satisfies

$$\xi_2 = -\nabla_{x_2} S(x_2, x_1), \qquad \xi_1 = \nabla_{x_1} S(x_2, x_1). \tag{13.15}$$

Note that if assume that the graph of ρ is projectable onto $\mathcal{X}_2 \times \mathcal{X}_1$, then we can find a generating function.

13.7 The Legendre transformation

Let $\mathcal{X} = \mathbb{R}^d$ be a vector space. Consider the symplectic vector space $\mathcal{X} \oplus \mathcal{X}^{\#} = \mathbb{R}^d \oplus \mathbb{R}^d$ with the generic variables (v, p). It can be viewed as a cotangent bundle in two ways – we can treat either $\mathcal{X}$ or $\mathcal{X}^{\#}$ as the base. Correspondingly, to describe any Lagrangian manifold $\mathcal{L}$ in $\mathcal{X} \oplus \mathcal{X}^{\#}$ we can try to use a generating function on $\mathcal{X}$ or on $\mathcal{X}^{\#}$. To pass from one description to the other one uses the *Legendre transformation*, which is described in this subsection.

Let $\mathcal{U}$ be a convex set of $\mathcal{X}$. Let

$$\mathcal{U} \ni v \mapsto S(v) \in \mathbb{R} \tag{13.16}$$

be a strictly convex C^2-function. By strict convexity we mean that for distinct $v_1, v_2 \in \mathcal{U}$, $v_1 \neq v_2$, $0 < \tau < 1$,

$$\tau S(v_1) + (1-\tau) S(v_2) > S\big(\tau v_1 + (1-\tau) v_2\big).$$

Then

$$\mathcal{U} \ni v \mapsto p(v) := \partial_v S(v) \in \mathcal{X}^{\#} \tag{13.17}$$

is an injective function. Let $\tilde{\mathcal{U}}$ be the image of (13.17). It is a convex set, because it is the image of a convex set by a convex function. One can define the function

$$\tilde{\mathcal{U}} \ni p \mapsto v(p) \in \mathcal{U}$$

inverse to (13.17). The *Legendre transform* of S is defined as

$$\tilde{S}(p) := p v(p) - S\big(v(p)\big).$$

Theorem 13.7. *(1) $\partial_p \tilde{S}(p) = v(p)$.*

(2) $\partial_p^2 \tilde{S}(p) = \partial_p v(p) = \big(\partial_v^2 S\big(v(p)\big)\big)^{-1}$. Hence $\tilde{S}$ is convex.

(3) $\tilde{\tilde{S}}(v) = S(v)$.

Proof. (1)

$$\partial_p \tilde{S}(p) = v(p) + p\partial_p v(p) - \partial_v S\big(v(p)\big)\partial_p v(p) = v(p).$$

(2)
$$\partial_p^2 \tilde{S}(p) = \partial_p v(p) = \big(\partial_v p\big(v(p)\big)\big)^{-1} = \big(\partial_v^2 S\big(v(p)\big)\big)^{-1}.$$
(3)
$$\tilde{\tilde{S}}(v) = vp(v) - p(v)v\big(p(v)\big) + S\Big(v\big(p(v)\big)\Big) = S(p).$$
□

Thus the same Lagrangian manifold has two descriptions:

$$\big\{\big(v, \mathrm{d}S(v)\big) \ : \ v \in \mathcal{U}\big\} \quad = \quad \big\{\big(\mathrm{d}\tilde{\mathcal{S}}(p), p\big) \ : \ p \in \tilde{\mathcal{U}}\big\}.$$

Examples.

(1) $\mathcal{U} = \mathbb{R}^d$, $S(v) = \frac{1}{2}vmv$,
$\tilde{\mathcal{U}} = \mathbb{R}^d$, $\tilde{S}(p) = \frac{1}{2}pm^{-1}p$,

(2) $\mathcal{U} = \{v \in \mathbb{R}^d \ : \ |v| < 1\}$, $S(v) = -m\sqrt{1-v^2}$.
$\tilde{\mathcal{U}} = \mathbb{R}^d$, $\tilde{S}(p) = \sqrt{p^2 + m^2}$,

(3) $\mathcal{U} = \mathbb{R}$, $S(v) = \mathrm{e}^v$,
$\tilde{\mathcal{U}} =]0, \infty[$, $\tilde{S}(p) = p \log p - p$.

Note that we sometimes apply the Legendre transformation to non-convex functions. For instance, in the first example m can be any nondegenerate matrix.

Proposition 13.8. *Suppose that S depends on an additional parameter α. Then we have the identity*
$$\partial_\alpha S\big(\alpha, v(\alpha, p)\big) = -\partial_\alpha \tilde{S}(\alpha, p). \tag{13.18}$$

Proof. Indeed,

$$\begin{aligned}
\partial_\alpha \tilde{S}(\alpha, p) &= \partial_\alpha\big(pv(\alpha,p) - S\big(\alpha, v(\alpha,p)\big)\big) \\
&= p\partial_\alpha v(\alpha,p) - \partial_\alpha S(\alpha, v(\alpha,p)\big) - \partial_v S(\alpha, v(\alpha,p)\big)\partial_\alpha v(\alpha,p) \\
&= -\partial_\alpha S\big(\alpha, v(\alpha,p)\big).
\end{aligned}$$

□

13.8 The extended symplectic manifold

Let $\mathcal{Y}$ be a symplectic manifold. We introduce the extended symplectic manifold as

$$\mathrm{T}^\# \mathbb{R} \times \mathcal{Y} = \mathbb{R} \times \mathbb{R} \times \mathcal{Y},$$

where its coordinates have generic names (t, τ, y). Here t has the meaning of time, τ of the energy. For the symplectic form we choose

$$\sigma := -\mathrm{d}\tau \wedge \mathrm{d}t + \omega.$$

Let $\mathbb{R}\times\mathcal{Y}\ni(t,y)\mapsto H(t,y)$ be a time dependent function on $\mathcal{Y}$. Let ρ_t be the flow generated by the Hamiltonian $H(t)$, that is

$$\rho_t\big(y(0)\big)=y(t), \tag{13.19}$$

where $y(t)$ solves

$$\partial_t y(t)=\omega^{-1}\mathrm{d}_y H\big(t,y(t)\big). \tag{13.20}$$

Set

$$G(t,\tau,y):=H(t,y)-\tau.$$

It will be convenient to introduce the projection

$$\mathrm{T}^{\#}\mathbb{R}\times\mathcal{Y}\ni(t,\tau,y)\mapsto\kappa(t,\tau,y):=(t,y)\in\mathbb{R}\times\mathcal{Y},$$

that involves forgetting the variable τ. Note that κ restricted to

$$G^{-1}(0):=\{(t,\tau,y)\ :\ G(t,\tau,y)=0\} \tag{13.21}$$

is a bijection onto $\mathbb{R}\times\mathcal{Y}$. Its inverse will be denoted by κ^{-1}, so that

$$\kappa^{-1}(t,y)=\big(t,H(t,y),y\big).$$

Proposition 13.9. *Let $\mathcal{L}$ be a Lagrangian manifold in $\mathcal{Y}$. The set*

$$\mathcal{M}:=\{(t,\tau,y)\ :\ y\in\rho_t(\mathcal{L}),\ \tau=H(t,y),\ t\in\mathbb{R}\} \tag{13.22}$$

satisfies the following properties:

(1) *$\mathcal{M}$ is a Lagrangian manifold in $\mathrm{T}^{\#}\mathbb{R}\times\mathcal{Y}$;*

(2) *$\mathcal{M}$ is contained in $G^{-1}(0)$*

(3) *we have*

$$\kappa(\mathcal{M})\cap\{0\}{\times}\mathcal{Y}=\{0\}\times\mathcal{L}; \tag{13.23}$$

(4) *every point in $\kappa(\mathcal{M})$ is connected to (13.23) by a curve contained in $\kappa(\mathcal{M})$.*

Besides, conditions (1)-(4) determine $\mathcal{M}$ uniquely.

Proof. Let $(t_0,\tau_0,y_0)\in\mathcal{M}$. Let v be tangent to $\rho_{t_0}(\mathcal{L})$ at y_0. Then

$$\langle\mathrm{d}_y H(t_0,y_0)|v\rangle\partial_\tau+v \tag{13.24}$$

is tangent to $\mathcal{M}$. Vectors of the form (13.24) are symplectically orthogonal to one another, because $\rho_{t_0}(\mathcal{L})$ is Lagrangian.

The curve $t\mapsto\big(t,H\big(t,y(t)\big),y(t)\big)$ is contained in $\mathcal{M}$. Hence the following vector is tangent to $\mathcal{M}$:

$$\partial_t+\partial_t H(t_0,y_0)\partial_\tau+\omega^{-1}\mathrm{d}_y H(t_0,y_0). \tag{13.25}$$

The symplectic form applied to (13.24) and (13.25) is

$$-\langle\mathrm{d}_y H(t_0,y_0)|v\rangle+\langle\omega|v,\omega^{-1}\mathrm{d}_y H(t_0,y_0)\rangle=0. \tag{13.26}$$

(13.24) and (13.25) span the tangent space of $\mathcal{M}$. Hence (1) is true ($\mathcal{M}$ is Lagrangian). (2), (3) and (4) are obvious.

Let us show the uniqueness of $\mathcal{M}$ satisfying (1), (2), (3) and (4). Let $\mathcal{M}$ be a Lagrangian submanifold contained in $G^{-1}(0)$ and $(t_0, \tau_0, y_0) \in \mathcal{M}$. By Thm 13.5, the vector

$$\begin{array}{rl} & \sigma^{-1}\mathrm{d}G(t_0, \tau_0, y_0) \\ = & \sigma^{-1}\big(\partial_t H(t_0, y_0)\mathrm{d}t + \mathrm{d}_y H(t_0, y_0) - \mathrm{d}\tau\big) \end{array} \tag{13.27}$$

is tangent to $\mathcal{M}$. But (13.27) coincides with (13.25). Hence

$$\partial_t + \omega^{-1}\mathrm{d}_y H(t_0, y_0). \tag{13.28}$$

is tangent to $\kappa(\mathcal{M})$. This means that $\kappa(\mathcal{M})$ is invariant for the Hamiltonian flow generated by $H(t, y)$. Consequently,

$$\kappa(\mathcal{M}) \supset \bigcup_{t\in\mathbb{R}} \{t\} \times \rho_t(\mathcal{L}). \tag{13.29}$$

$\kappa(\mathcal{M})$ cannot be larger than the rhs of (13.29), because then condition (4) would be violated. $\square$

13.9 Time-dependent Hamilton-Jacobi equations

Let $\mathbb{R} \times \mathrm{T}^{\#}\mathcal{X} \ni (t, x, p) \mapsto H(t, x, p)$ be a time-dependent Hamilonian on $\mathrm{T}^{\#}\mathcal{X}$. Let $\mathcal{X} \supset \mathcal{U} \ni x \mapsto S(x)$ be a given function. The *time-dependent Hamilton-Jacobi equation* equipped with initial conditions reads

$$\begin{array}{rcl} \partial_t S(t, x) - H\big(t, x, \partial_x S(t, x)\big) & = & 0, \\ S(0, x) & = & S(x). \end{array} \tag{13.30}$$

(13.30) can be reinterpreted in more geometric terms as follows: Set

$$G(t, \tau, x, p) := \tau - H(t, x, p).$$

Consider a Lagrangian manifold $\mathcal{L}$ in $\mathcal{Y}$. We want to find a Lagrangian manifold $\mathcal{M}$ in

$$G^{-1}(0) := \{(t, \tau, x, p) \in \mathrm{T}^{\#}\mathbb{R} \times \mathrm{T}^{\#}\mathcal{X} \ : \ \tau - H(t, x, p) = 0\} \tag{13.31}$$

such that

$$\kappa(\mathcal{M}) \cap \{0\}\times\mathrm{T}^{\#}\mathcal{X} = \{0\}\times\mathcal{L}.$$

Here, as in the previous subsection,

$$\kappa(t, \tau, x, p) := (t, x, p).$$

We will also use its inverse

$$\kappa^{-1}(t, x, p) := \big(t, H(t, x, p), x, p\big).$$

The relationship between the two formulations is as follows. Assume that $\mathcal{L}$ is a generating function of $\mathcal{L}$. Then the function $(t,x) \mapsto S(t,x)$ that appears in (13.30) is the generating function of $\mathcal{M}$, which for $t = 0$ coincides with $x \mapsto S(x)$.

Note that the geometic formulation is superior to the traditional one, because it does not have a problem with caustics.

The Hamilton-Jacobi equations can be solved as follows. Let $\mathbb{R} \ni t \mapsto \big(x(t,y), p(t,y)\big) \in \mathrm{T}^{\#}\mathcal{X}$ be the solution of the Hamilton equation with the initial conditions on the Lagrangian manifold $\mathcal{L}$:

$$\big(x(0,y), p(0,y)\big) = \big(y, \partial_y S(y)\big).$$

Then

$$\mathcal{M} = \Big\{\kappa^{-1}\big(t, x(t,y), p(t,y)\big) \ : \ (t,y) \in \mathbb{R} \times \mathcal{U}\Big\}.$$

Let us find the generating function of $\mathcal{M}$. We will use s as an alternate name for the time variable. The tautological 1-form of $\mathrm{T}^{\#}\mathbb{R} \times \mathrm{T}^{\#}\mathcal{X}$ is

$$-\tau \mathrm{d}s + p\mathrm{d}x.$$

Fix a point $y_0 \in \mathcal{U}$. Then the generating function of $\mathcal{M}$ satisfying

$$T\Big(\kappa^{-1}\big(0, y_0, p(0,y_0)\big)\Big) = S(y_0)$$

is given by

$$T\Big(\kappa^{-1}\big(t, x(t,y), p(t,y)\big)\Big) = S(y_0) + \int_\gamma (p\mathrm{d}x - \tau\mathrm{d}s),$$

where γ is a curve in $\mathcal{M}$ joining

$$\kappa^{-1}\big(0, y_0, p(0,y_0)\big) \tag{13.32}$$

$$\text{with} \quad \kappa^{-1}\big(t, x(t,y), p(t,y)\big). \tag{13.33}$$

We can take γ as the union of two disjoint segments: $\gamma = \gamma_1 \cup \gamma_2$. γ_1 is a curve in (13.31) with the time variable equal to zero ending at

$$\kappa^{-1}\big(0, y, p(0,y)\big). \tag{13.34}$$

Clearly, since $\mathrm{d}s = 0$ along γ_1, we have

$$S(y_0) + \int_{\gamma_1} (p\mathrm{d}x - \tau\mathrm{d}s) = S(y_0) + \int_{\gamma_1} p\mathrm{d}x = S(y). \tag{13.35}$$

γ_2 starts at (13.34), ends at (13.33), and is given by the Hamiltonian flow. More precisely, γ_2 is

$$[0,t] \ni s \mapsto \kappa^{-1}\big(s, x(s,y), p(s,y)\big).$$

We have

$$\int_{\gamma_2} (p\mathrm{d}x - \tau\mathrm{d}s) = \int_0^t \Big(p(s,y)\partial_s x(s,y) - H\big(s, x(s,y), p(s,y)\big)\Big)\mathrm{d}s. \tag{13.36}$$

Putting together (13.35) and (13.36) we obtain the formula for the generating function of $\mathcal{M}$ viewed as a function on $\mathcal{M}$:

$$\begin{aligned} T(t,y) &= S(y) \\ &\quad + \int_0^t \Big(p(s,y)\partial_s x(s,y) - H\big(s, x(s,y), p(s,y)\big)\Big) \mathrm{d}s. \end{aligned} \tag{13.37}$$

If we can invert $y \mapsto x(t,y)$ and obtain the function $x \mapsto y(t,x)$, then we have a generating of $\mathcal{M}$ viewed as a function on the base:

$$S(t,x) \quad = \quad T\big(t, y(t,x)\big). \tag{13.38}$$

13.10 The Lagrangian formalism

Given a time-dependent Hamiltonian $H(t,x,p)$ set

$$v := \partial_p H(t,x,p).$$

Suppose that we can express p in terms of t, x, v. We define then the Lagrangian

$$L(t,x,v) := p(t,x,v)v - H\big(t,x,p(t,x,v)\big)$$

naturally defined on $\mathrm{T}\mathcal{X}$. Thus we perform the Legendre transformation wrt p, keeping t, x as parameters. Note that $p = \partial_v L(t,x,v)$ and $\partial_x H(t,x,p) = -\partial_x L(t,x,v)$. The Hamilton equations are equivalent to the Euler-Lagrange equations:

$$\frac{\mathrm{d}}{\mathrm{d}t} x(t) \quad = \quad v(t), \tag{13.39}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \partial_v L\big(t, x(t), v(t)\big) \quad = \quad \partial_x L\big(x(t), v(t)\big). \tag{13.40}$$

Using the Lagrangian, the generating function (13.37) can be rewritten as

$$T(t,y) \quad = \quad S(y) + \int_0^t L\big(s, x(s,y), \dot{x}(s,y)\big) \mathrm{d}s.$$

Lagrangians often have quadratic dependence on velocities:

$$L(x,v) = \frac{1}{2} v g^{-1}(x) v + vA(x) - V(x). \tag{13.41}$$

The momentum and the velocity are related as

$$p = g^{-1}(x)v + A(x), \quad v = g(x)\big(p - A(x)\big). \tag{13.42}$$

The corresponding Hamiltonian depends quadratically on the momenta:

$$H(x,p) = \frac{1}{2}\big(p - A(x)\big) g(x) \big(p - A(x)\big) + V(x). \tag{13.43}$$

13.11 Action integral

In this subsection, which is independent of Subsect. 13.9, we will rederive the formula for the generating function of the Hamiltonian flow constructed (13.37). Unlike in Subsect. 13.9, we will use the Lagrangian formalism.

Let $[0,t] \ni s \mapsto x(s,\alpha), v(s,\alpha) \in \mathrm{T}\mathcal{X}$ be a family of trajectories, parametrized by an auxiliary variable α. We define the action along these trajectories

$$I(t,\alpha) := \int_0^t L(x(s,\alpha), v(s,\alpha))\mathrm{d}s. \tag{13.44}$$

Theorem 13.10.

$$\partial_\alpha I(t,\alpha) = p(x(t,\alpha), v(t,\alpha))\partial_\alpha x(t,\alpha) - p(x(0,\alpha), v(0,\alpha))\partial_\alpha x(0,\alpha). \tag{13.45}$$

Proof.

$$\begin{aligned}
\partial_\alpha I(t,\alpha) &= \int_0^t \partial_x L(x(s,\alpha), \dot{x}(s,\alpha))\partial_\alpha x(s,\alpha)\mathrm{d}s \\
&\quad + \int_0^t \partial_{\dot{x}} L(x(s,\alpha), \dot{x}(s,\alpha))\partial_\alpha \dot{x}(s,\alpha)\mathrm{d}s \\
&= \int_0^t \left(\partial_x L(x(s,\alpha), \dot{x}(s,\alpha)) - \frac{\mathrm{d}}{\mathrm{d}s}\partial_{\dot{x}} L(x(s,\alpha), \dot{x}(s,\alpha))\right)\partial_\alpha x(s,\alpha)\mathrm{d}s \\
&\quad + p(x(s,\alpha), v(s,\alpha))\partial_\alpha x(s,\alpha)\Big|_{s=0}^{s=t}.
\end{aligned}$$

□

Theorem 13.11. *Let $\mathcal{U}$ be an open subset in $\mathcal{X}$. For $y \in \mathcal{U}$ define a family of trajectories $x(t,y), p(t,y)$ solving the Hamilton equation and satisfying the intial conditions*

$$x(0,y) = y, \quad p(0,y) = \partial_y S(y). \tag{13.46}$$

Let $I(t,y)$ be the action along these trajectories defied as in (13.44). We suppose that we can invert the $y \mapsto x(t,y)$ obtaining the function $x \mapsto y(t,x)$. Then

$$S(t,x) := I\big(t, y(t,x)\big) + S(y(t,x)) \tag{13.47}$$

is the solution of (13.30), and

$$\partial_x S(t,x) = p\big(t, y(t,x)\big). \tag{13.48}$$

Proof. We have

$$\begin{aligned}
\partial_y\big(I(t,y) + S(y)\big) &= p(t,y)\partial_y x(t,y) - p(0,y)\partial_y x(0,y) + \partial_y S(y) \\
&= p(t,y)\partial_y x(t,y).
\end{aligned} \tag{13.49}$$

Hence,

$$\partial_x S(t,x) = \partial_x\Big(I\big(t,y(t,x)\big)+S\big(y(t,x)\big)\Big) \tag{13.50}$$
$$= p(t,y)\partial_y x(t,y)\partial_x y(t,x) = p(t,y). \tag{13.51}$$

Now

$$L\big(x(t,y),\dot{x}(t,y)\big) = \partial_t I(t,y) = \partial_t\big(I(t,y)+S(y)\big) \tag{13.52}$$
$$= \partial_t S\big(t,x(t,y)\big) + \partial_x S\big(t,x(t,y)\big)\dot{x}(t,y). \tag{13.53}$$

Therefore,

$$\partial_t S\big(t,x(t,y)\big) = L\big(x(t,y),\dot{x}(t,y)\big) - p(t,y)\dot{x}(t,y) \tag{13.54}$$
$$= -H\big(x(t,y),p(t,y)\big). \tag{13.55}$$

□

13.12 Completely integrable systems

Let $\mathcal{Y}$ be a symplectic manifold of dimension $2d$. We say that functions F_1 and F_2 on $\mathcal{Y}$ are *in involution* if $\{F_1,F_2\}=0$.

Let $F_1,\dots,F_m$ be functions on $\mathcal{Y}$ and $c_1,\dots,c_m\in\mathbb{R}$. Define

$$\mathcal{L} := F_1^{-1}(c_1)\cap\cdots\cap F_m^{-1}(c_m). \tag{13.56}$$

We assume that

$$\mathrm{d}F_1\wedge\cdots\wedge\mathrm{d}F_m \neq 0 \tag{13.57}$$

on $\mathcal{L}$. Then $\mathcal{L}$ is a manifold of dimension $2d-m$.

Proposition 13.12. *Suppose that $F_1,\dots,F_m$ are in involution and satisfy (13.57). Then $m\le d$ and $\mathcal{L}$ is coisotropic. If $m=d$, then $\mathcal{L}$ is Lagrangian.*

Proof. We have

$$\langle \mathrm{d}F_i|\omega^{-1}\mathrm{d}F_j\rangle = \{F_i,F_j\}=0.$$

Hence $\omega^{-1}\mathrm{d}F_j$ is tangent to $\mathcal{L}$.

$$\langle\omega|\omega^{-1}\mathrm{d}F_i,\omega^{-1}\mathrm{d}F_j\rangle = \langle\omega^{-1}\mathrm{d}F_i|\mathrm{d}F_j\rangle = -\{F_i,F_j\}=0.$$

Hence the tangent space of $\mathcal{L}$ contains an m-dimensional subspace on which ω is zero. In the case of a $2d-m$ dimensional manifold this means that $\mathcal{L}$ is coisotropic. □

If H is a single function on $\mathcal{Y}$, we say that it is *completely integrable* if we can find a family of functions in involution $F_1,\dots,F_d$ satisfying (13.57) on $\mathcal{Y}$ such that $H=F_d$.

Note that for completely integrable H it is easy to find Lagrangian manifolds contained in level sets of H – one just takes the sets of the form (13.56).

14 Quantizing symplectic transformations

14.1 Linear symplectic transformations

Let $\rho \in L(\mathbb{R}^d \oplus \mathbb{R}^d)$. Write ρ as a 2×2 matrix and introduce a symplectic form:

$$\rho = \begin{bmatrix} a & b \\ c & d \end{bmatrix}, \quad \omega := \begin{bmatrix} 0 & -1\!\!1 \\ 1\!\!1 & 0 \end{bmatrix}. \tag{14.1}$$

$\rho \in Sp(\mathbb{R}^d \oplus \mathbb{R}^d)$ iff

$$\rho^{\#} \omega \rho = \omega,$$

which means

$$a^{\#} d - c^{\#} b = 1\!\!1, \quad c^{\#} a = a^{\#} c, \quad d^{\#} b = b^{\#} d. \tag{14.2}$$

If

$$\begin{aligned} \hat{x}'^i &= a^i_j \hat{x}^j + b^{ij} \hat{p}_j, \\ \hat{p}'_i &= c_{ij} \hat{x}^j + d^j_i \hat{p}_j, \end{aligned} \tag{14.3}$$

then $\hat{x}'$, $\hat{p}'$ satisfy the same commutation relations as $\hat{x}$, $\hat{p}$. We define $Mp^c(\mathbb{R}^d \oplus \mathbb{R}^d)$ to be the set of $U \in U(L^2(\mathbb{R}^d))$ such that there exists a matrix ρ such that

$$\begin{aligned} U \hat{x}^i U^* &= \hat{x}'^i, \\ U \hat{p}_i U^* &= \hat{p}'_i. \end{aligned}$$

We will say that U implements ρ. Obviously, ρ has to be symplectic, $Mp^c(\mathbb{R}^d \oplus \mathbb{R}^d)$ is a group and the map $U \mapsto \rho$ is a homomorphism.

14.2 Metaplectic group

If χ is a quadratic polynomial on $\mathbb{R}^d \oplus \mathbb{R}^d$, then clearly $\mathrm{e}^{\mathrm{i}t\mathrm{Op}(\chi)} \in Mp^c(\mathbb{R}^d \oplus \mathbb{R}^d)$ and implements the symplectic flow given by the Hamiltonian χ. We will denote the group generated by such maps by $Mp(\mathbb{R}^d \oplus \mathbb{R}^d)$. Every symplectic transformation is implemented by exactly two elements of Mp.

14.3 Generating function of a symplectic transformation

Let ρ be as above with b invertible. We then have the factorization

$$\rho = \begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} 1\!\!1 & 0 \\ e & 1\!\!1 \end{bmatrix} \begin{bmatrix} 0 & b \\ -b^{\#-1} & 0 \end{bmatrix} \begin{bmatrix} 1\!\!1 & 0 \\ f & 1\!\!1 \end{bmatrix}, \tag{14.4}$$

where

$$e = db^{-1} = b^{\#-1} d^{\#},$$

$$f = b^{-1} a = a^{\#} b^{\#-1}.$$

are symmetric. Define

$$\mathcal{X}\times\mathcal{X}\ni(x_1,x_2)\mapsto S(x_1,x_2) \quad := \quad \frac{1}{2}x_1{\cdot}fx_1-x_1{\cdot}b^{-1}x_2+\frac{1}{2}x_2{\cdot}ex_2.$$

Then

$$\begin{bmatrix} a & b\\ c & d\end{bmatrix}\begin{bmatrix} x_1\\ \xi_1\end{bmatrix}=\begin{bmatrix} x_2\\ \xi_2\end{bmatrix} \tag{14.5}$$

iff

$$\nabla_{x_1}S(x_1,x_2)=-\xi_1,\quad \nabla_{x_2}S(x_1,x_2)=\xi_2. \tag{14.6}$$

The function $S(x_1,x_2)$ is called a generating function of the symplectic transformation ρ.

It is easy to check that the operators $\pm U_\rho\in Mp(\mathcal{X}^\#\oplus\mathcal{X})$ implementing ρ have the integral kernel equal to

$$\pm U_\rho(x_1,x_2)=\pm(2\pi\mathrm{i}\hbar)^{-\frac{d}{2}}\sqrt{-\det\nabla_{x_1}\nabla_{x_2}S}\ \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}S(x_1,x_2)}.$$

14.4 Harmonic oscillator

As an example, we cosider the 1-dimensional harmonic oscillator with $\hbar=1$. Let $\chi(x,\xi):=\frac12\xi^2+\frac12x^2$. Then $\mathrm{Op}(\chi)=\frac12D^2+\frac12x^2$. The Weyl-Wigner symbol of $\mathrm{e}^{-t\mathrm{Op}(\chi)}$ equals

$$w(t,x,\xi)=(\mathrm{ch}\tfrac{t}{2})^{-1}\exp(-(x^2+\xi^2)\mathrm{th}\tfrac{t}{2}). \tag{14.7}$$

Its integral kernel is given by

$$W(t,x,y)=\pi^{-\frac12}(\mathrm{sh}t)^{-\frac12}\exp\left(\frac{-(x^2+y^2)\mathrm{ch}t+2xy}{2\mathrm{sh}t}\right).$$

$\mathrm{e}^{-\mathrm{i}t\mathrm{Op}(\chi)}$ has the Weyl-Wigner symbol

$$w(\mathrm{i}t,x,\xi)=(\cos\tfrac{t}{2})^{-1}\exp\left(-\mathrm{i}\,(x^2+\xi^2)\mathrm{tg}\tfrac{t}{2}\right) \tag{14.8}$$

and the integral kernel

$$W(\mathrm{i}t,x,y)=\pi^{-\frac12}|\sin t|^{-\frac12}\mathrm{e}^{-\frac{\mathrm{i}\pi}{4}}\mathrm{e}^{-\frac{\mathrm{i}\pi}{2}[\frac{t}{\pi}]}\exp\left(\frac{-(x^2+y^2)\cos t+2xy}{2\mathrm{i}\sin t}\right).$$

Above, $[c]$ denotes the integral part of c.

We have $W(\mathrm{i}t+2\mathrm{i}\pi,x,y)=-W(\mathrm{i}t,x,y)$. Note the special cases

$$\begin{aligned}
W(0,x,y) &= \delta(x-y),\\
W(\tfrac{\mathrm{i}\pi}{2},x,y) &= (2\pi)^{-\frac12}\mathrm{e}^{-\frac{\mathrm{i}\pi}{4}}\mathrm{e}^{-\mathrm{i}xy},\\
W(\mathrm{i}\pi,x,y) &= \mathrm{e}^{-\frac{\mathrm{i}\pi}{2}}\delta(x+y),\\
W(\tfrac{\mathrm{i}3\pi}{2},x,y) &= (2\pi)^{-\frac12}\mathrm{e}^{-\frac{\mathrm{i}3\pi}{4}}\mathrm{e}^{\mathrm{i}xy}.
\end{aligned}$$

Corollary 14.1. (1) *The operator with kernel* $\pm(2\pi \mathrm{i})^{-\frac{1}{2}}\mathrm{e}^{-\mathrm{i}xy}$ *belongs to the metaplectic group and implements* $\begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$.

(2) *The operator with kernel* $\pm\mathrm{i}\delta(x+y)$ *belongs to the metaplectic group and implements* $\begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}$.

14.5 The stationary phase method

For a quadratic form B, $\mathrm{inert}\, B$ will denote the *inertia of* B, that is $n_+ - n_-$, where $n_\pm$ is the number of positive/negative terms of B in the diagonal form.

Theorem 14.2. *Let a be smooth function on $\mathcal{X}$ and S a function on* $\mathrm{supp} a$*. Let x_0 be a critical point of S, that is it satisfies*

$$\partial_x S(x_0) = 0.$$

(For simplicity we assume that it is the only one on $\mathrm{supp} a$*). Then for small $\hbar$,*

$$\int \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)}a(x)\mathrm{d}x \simeq (2\pi\hbar)^{-\frac{d}{2}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}\mathrm{inert}\,\partial_x^2 S(x_0)}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x_0)}a(x_0) + O(\hbar^{-\frac{d}{2}+1}). \tag{14.9}$$

Proof. The left hand side of (14.2) is approximated by

$$\int \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x_0)+\frac{\mathrm{i}}{2\hbar}(x-x_0)\partial_x^2 S(x_0)(x-x_0)}a(x_0)\mathrm{d}x, \tag{14.10}$$

which equals the right hand side of (14.2). □

14.6 Semiclassical FIO's

Suppose that $\mathcal{X}_2 \times \mathcal{X}_1 \ni (x_2, x_1) \mapsto a(x_2, x_1)$, is a function called an amplitude. Let $\mathrm{supp} a \ni (x_2, x_1) \mapsto S(x_2, x_1)$ be another function, which we calle a phase. We define the Fourier integral operator with amplitude a and phase S to be the operator from $C_\mathrm{c}^\infty(\mathcal{X}_1)$ to $C^\infty(\mathcal{X}_2)$ with the integral kernel

$$\mathrm{FIO}(a, S)(x_2, x_1) = (2\pi\hbar)^{-\frac{d}{2}}\left(\nabla_{x_2}\nabla_{x_1}S(x_2, x_1)\right)^{\frac{1}{2}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x_2,x_1)} \tag{14.11}$$

We treat $\mathrm{FIO}(a, S)$ as a quantization of the symplectic transformation with the generating function S. Suppose that we can solve

$$\nabla_x S(\tilde{x}, x) = p \tag{14.12}$$

obtaining $(x, p) \mapsto \tilde{x}(x, p)$. Then

$$\mathrm{FIO}_\hbar(a_2, S)^* \mathrm{FIO}_\hbar(a_1, S) = \mathrm{Op}_\hbar(b) + O(\hbar), \tag{14.13}$$

where

$$b(x,p) = \overline{a_2(\tilde{x}(x,p),x)}a_1(\tilde{x}(x,p),x). \tag{14.14}$$

In particular, Fourier integral operators with amplitude 1 are asymptotically unitary.

Indeed

$$\begin{aligned}
&\mathrm{FIO}_\hbar(a_2,S)^*\mathrm{FIO}_\hbar(a_1,S)(x_2,x_1)\\
=&\int \mathrm{d}x\sqrt{\partial_x\partial_{x_2}S(x,x_2)}\sqrt{\partial_x\partial_{x_1}S(x,x_1)}\ \overline{a(x_2,x)}a_1(x,x_1)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}S(x,x_2)+\frac{\mathrm{i}}{\hbar}S(x,x_1)}\\
=&\int \mathrm{d}x b(x_2,x,x_1)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p(x_2,x,x_1)(x_2-x_1)}\\
=&\int \mathrm{d}p\partial_p x(x_2,p,x_1)b\big(x_2,x(x_2,p,x_1),x_1\big)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p(x_2-x_1)},
\end{aligned}$$

where

$$\begin{aligned}
b(x_2,x,x_1) &= \sqrt{\partial_x\partial_{x_2}S(x,x_2)}\sqrt{\partial_x\partial_{x_1}S(x,x_1)}\ \overline{a(x_2,x)}a_1(x,x_1),\\
p(x_2,x,x_1) &= \int_0^1 \partial_x S(\tau x_2+(1-\tau)x_1)\mathrm{d}\tau.
\end{aligned}$$

14.7 Composition of FIO's

Suppose that

$$\mathcal{X}\times\mathcal{X}_1 \ni (x,x_1)\mapsto S_1(x,x_1),\quad \mathcal{X}_2\times\mathcal{X}\ni(x_2,x)\mapsto S_2(x_2,x) \tag{14.15}$$

are two functions. Given x_2,x_1, we look for $x(x_2,x_1)$ satisfying

$$\nabla_x S_2(x_2,x(x_2,x_1)) + \nabla_x S_1(x(x_2,x_1),x_1) = 0. \tag{14.16}$$

Suppose such $x(x_2,x_1)$ exists and is unique. Then we define

$$S(x_2,x_1) := S_2(x_2,x(x_2,x_1)) + S_1(x(x_2,x_1),x_1) \tag{14.17}$$

Suppose S_1 is a generating function of a symplectic map $\rho_1 : \mathrm{T}^\#\mathcal{X}_1\to\mathrm{T}^\#\mathcal{X}$ and S_2 is a generating function of a symplectic map $\rho:\mathrm{T}^\#\mathcal{X}\to\mathrm{T}^\#\mathcal{X}_2$. Then S is a generating function of $\rho_2\circ\rho_1$.

Proposition 14.3.

$$\begin{aligned}
\nabla_{x_2}\nabla_{x_1}S(x_2,x_1) &= -\nabla_{x_2}\nabla_x S_2(x_2,x(x_2,x_1))\\
&\quad\times\Big(\nabla_x^{(2)}S_2(x_2,x(x_2,x_1))+\nabla_x^{(2)}S_1(x(x_2,x_1),x_1)\Big)^{-1}\\
&\quad\times\nabla_x\nabla_{x_1}S_1(x(x_2,x_1),x_1).
\end{aligned} \tag{14.18}$$

Proof. Differentiating (14.16) we obtain

$$\begin{aligned}
(\nabla_{x_2}x)(x_1,x_2)\Big(\nabla_x^{(2)}S_2(x_2,x(x_2,x_1))+\nabla_x^{(2)}S_1(x(x_2,x_1),x_1)\Big)&\\
+\nabla_x\nabla_{x_2}S_2(x_2,x(x_2,x_1)) &= 0.
\end{aligned} \tag{14.19}$$

Differentiating (14.17) we obtain

$$\begin{aligned} \nabla_{x_1} S(x_1,x_2) &= \nabla_{x_1} S_1(x(x_1,x_2),x_1), \\ \nabla_{x_2}\nabla_{x_1} S(x_1,x_2) &= (\nabla_{x_2} x)(x_1,x_2)\nabla_x\nabla_{x_1} S_1(x(x_1,x_2),x_1). \end{aligned} \tag{14.20}$$

Then we use (14.19) and (14.20). □

In addition to two phases S_1, S_2, let

$$\mathcal{X}_2\times\mathcal{X}\ni(x_2,x)\mapsto a_2(x_2,x),\qquad \mathcal{X}\times\mathcal{X}_1\ni(x,x_1)\mapsto a_1(x,x_1) \tag{14.21}$$

be two amplitudes. Then we define the composite amplitude as

$$a(x_2,x_1):=a_2(x_2,x(x_2,x_1))a_1(x(x_2,x_1),x_1). \tag{14.22}$$

Theorem 14.4.

$$\mathrm{FIO}_\hbar(a_2,S_2)\mathrm{FIO}_\hbar(a_1,S_1)=\mathrm{FIO}_\hbar(a,S)+O(\hbar). \tag{14.23}$$

15 WKB method

15.1 Lagrangian distributions

Consider a quadratic form

$$\frac{1}{2}xSx:=\frac{1}{2}x^iS_{ij}x^j, \tag{15.1}$$

and a function on $\mathbb{R}^d$

$$\mathrm{e}^{\frac{\mathrm{i}}{2\hbar}xSx}. \tag{15.2}$$

Clearly, we have the identity

$$\big(\hat{p}_i-S_{ij}\hat{x}^j\big)\mathrm{e}^{\frac{\mathrm{i}}{2\hbar}xSx}=0,\quad i=1,\dots,d.$$

One can say that the phase space support of (15.2) is concentrated on

$$\{(x,p)\ :\ p_i-S_{ij}x^j=0,\ i=1,\dots,d\}, \tag{15.3}$$

which is a Lagrangian subspace of $\mathbb{R}^d\oplus\mathbb{R}^d$.

Let us generalize (15.2). Let $\mathcal{L}$ be an arbitrary Lagrangian subspace of $\mathbb{R}^d\oplus\mathbb{R}^d$. Let $\mathcal{L}^{\mathrm{an}}$ be the set of linear functionals on $\mathbb{R}^d\oplus\mathbb{R}^d$ such that

$$\mathcal{L}=\underset{\phi\in\mathcal{L}^{\mathrm{an}}}{\cap}\mathrm{Ker}\phi.$$

Every functional in $\mathcal{L}^{\mathrm{an}}$ has the form

$$\phi(\xi,\eta)=\xi_jx^j+\eta^jp_j.$$

The corresponding operator on $L^2(\mathbb{R}^d)$ will be decorated by a hat:

$$\hat{\phi}(\xi, \eta) = \xi_{ij}\hat{x}^j + \eta_i^j \hat{p}_j.$$

We say that $f \in \mathcal{S}'(\mathbb{R}^d)$ is a Lagrangian distribution associated with the subspace $\mathcal{L}$ iff

$$\hat{\phi}(\xi, \eta) f = 0, \quad \phi(\xi, \eta) \in \mathcal{L}^{\mathrm{an}}.$$

In the generic case, the intersection of $\mathcal{L}$ and $0 \oplus \mathbb{R}^d$ is $(0, 0)$. We then say that the Lagrangian subspace is projectable onto the configuration space. Then one can find a generating function of the distribution $\mathcal{L}$ of the form (15.1). Lagrangian distributions associated with $\mathcal{L}$ are then multiples of (15.2).

The opposite case is $\mathcal{L} = 0 \oplus \mathbb{R}^d$. $\mathcal{L}^{\mathrm{an}}$ is then spanned by x^i, $i = 1, \ldots, d$. The corresponding Lagrangian distributions are multiples of $\delta(x)$

15.2 Semiclassical Fourier transform of Lagrangian distributions

Consider now the *semiclassical Fourier transformation*, which is an operator $\mathcal{F}_\hbar$ on $L^2(\mathbb{R}^d)$ given by the kernel

$$\mathcal{F}_\hbar(p, x) := \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}xp}. \tag{15.4}$$

Note that for all $\hbar$, $(2\pi\hbar)^{-d/2}\mathcal{F}_\hbar$ is unitary – it will be called the *unitary semiclassical Fourier transformation.* Multiplied by $\pm\mathrm{i}^d$ it is an element of the metaplectic group.

Consider the Lagrangian distribution

$$\mathrm{e}^{\frac{\mathrm{i}}{2\hbar}xSx}, \tag{15.5}$$

with an invertible S. Then its is easy to see that the image of (15.5) under $(2\pi\hbar)^{-d/2}\mathcal{F}_\hbar$ is

$$\mathrm{i}^{d/2}(\det S^{-1})^{1/2}\mathrm{e}^{-\frac{\mathrm{i}}{2\hbar}pS^{-1}p}.$$

More generally, we can check that the semiclassical Fourier transformation in all or only a part of the variables preserves the set of Lagrangian distributions.

15.3 The time dependent WKB approximation for Hamiltonians

In this subsection we describe the WKB approximation for the time-dependent Schrödinger equation and Hamiltonians quadratic in the momenta. For simplicity we will restrict ourselves to stationary Hamiltonians – one could generalize this subsection to time-dependent Hamiltonians.

Consider the classical Hamiltonian

$$H(x, p) = \frac{1}{2}(p - A(x))g(x)(p - A(x)) + V(x) \tag{15.6}$$

with the corresponding Lagrangian

$$L(x, v) = \frac{1}{2}vg^{-1}(x)v + vA(x) - V(x). \tag{15.7}$$

We quantize the Hamiltonian in the naive way:

$$H_\hbar := \frac{1}{2}(-\mathrm{i}\hbar\hat{\partial} - A(x))g(x)(-\mathrm{i}\hbar\hat{\partial} - A(x)) + V(x). \tag{15.8}$$

We look for solutions of

$$\mathrm{i}\hbar\partial_t\Psi_\hbar(t,x) \quad = \quad H_\hbar\Psi_\hbar(t,x). \tag{15.9}$$

We make an ansatz

$$\begin{aligned}\Psi_\hbar(t,x) &= \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(t,x)}a_\hbar(t,x), &(15.10)\\ \Psi_\hbar(0,x) &= \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)}a(x). &(15.11)\end{aligned}$$

where $a(x), S(x)$ are given functions. We multiply the Schrödinger equation by $\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}S(t,x)}$ obtaining

$$\begin{aligned}&\left(\mathrm{i}\hbar\hat{\partial}_t - \partial_t S(t,x)\right) a_\hbar(t,x) &(15.12)\\ =\; &\left(\frac{1}{2}(\mathrm{i}^{-1}\hbar\hat{\partial}_x + \partial_x S(t,x) - A(x))g(x)(\mathrm{i}^{-1}\hbar\hat{\partial}_x + \partial_x S(t,x) - A(x)) + V(x)\right) a_\hbar(t,x).\end{aligned}$$

To make the zeroth order in $\hbar$ part of (15.12) vanish we demand that

$$-\partial_t S(t,x) \quad = \quad \frac{1}{2}(\partial_x S(t,x) - A(x))g(x)(\partial_x S(t,x) - A(x)) + V(x). \tag{15.13}$$

This is the Hamilton-Jacobi equation for the Hamiltonian H. Together with the initial conditions (15.13) can be rewritten as

$$\begin{aligned}-\partial_t S(t,x) &= H\big(x, \partial_x S(x)\big), &(15.14)\\ S(0,x) &= S(x),\end{aligned}$$

Recall that (15.14) is solved as follows. First we need to solve the equations of motion:

$$\begin{aligned}\dot{x}(t,y) &= \partial_p H\big(x(t,y), p(t,y)\big),\\ \dot{p}(t,y) &= -\partial_x H\big(x(t,y), p(t,y)\big),\\ x(0,y) &= y,\\ p(0,y) &= \partial_y S(y).\end{aligned}$$

We can do it in the Lagrangian formalism. We replace the variable p by v:

$$v(t,x) = \partial_p H\big(x, \partial_x S(t,x)\big).$$

Then

$$\begin{aligned}\dot{x}(t,y) &= v(t,y),\\ \dot{v}(t,y) &= \partial_x L\big(x(t,y), v(t,y)\big),\\ x(0,y) &= y,\\ v(0,y) &= \partial_p H\big(y, \partial_y S(y)\big).\end{aligned}$$

Then

$$S\big(t, x(t, y)\big) = S(y) + \int_0^t L\big(x(s, y), v(s, y)\big)\mathrm{d}s$$

defines the solution of (15.14) with the initial condition (15.11), provided that we can invert $y \mapsto x(t, y)$.

We have also the equation for the amplitude:

$$\left(\hat{\partial}_t + \frac{1}{2}(v(t, x)\hat{\partial}_x + \hat{\partial}_x v(t, x))\right) a_\hbar(t, x) = \frac{\mathrm{i}\hbar}{2}\hat{\partial}_x g(x)\hat{\partial}_x a_\hbar(t, x). \tag{15.15}$$

Note that for any function b

$$\left(\hat{\partial}_t + \frac{1}{2}(v(t, x)\hat{\partial}_x + \hat{\partial}_x v(t, x))\right) (\det \partial_x y(t, x))^{\frac{1}{2}}\, b(y(t, x)) = 0 \tag{15.16}$$

Thus setting

$$\Psi_{\mathrm{cl}}(t, x) := (\det \partial_x y(t, x))^{\frac{1}{2}}\, a\big(y(t, x)\big)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(t,x)}. \tag{15.17}$$

We solve the Schrödinger equation modulo $O(\hbar)$, taking into account the initial condition:

$$\begin{array}{rcl} \mathrm{i}\hbar\partial_t\Psi_{\mathrm{cl}}(t, x) & = & H_\hbar\Psi_{\mathrm{cl}}(t, x) + O(\hbar^2), \\ \Psi_{\mathrm{cl}}(0, x) & = & \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)}a(x) \end{array}$$

We can improve on Ψ_{cl} by setting

$$\Psi_\hbar(t, x) := (\det \partial_x y(t, x))^{\frac{1}{2}} \sum_{n=0}^{\infty} \hbar^n b_n(t, y(t, x))\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(t,x)}, \tag{15.18}$$

where

$$\begin{array}{rcl} b_0(y) & = & a(y), \\ \partial_t b_{n+1}\big(t, y(t, x)\big) & = & \mathrm{i}\hbar\,(\det \partial_x y(t, x))^{-\frac{1}{2}}\, \hat{\partial}_x g(x)\hat{\partial}_x\, (\det \partial_x y(t, x))^{\frac{1}{2}}\, b_n\big(t, y(t, x)\big). \end{array}$$

(The 0th order yields $\Psi_{\mathrm{cl}}(t, x)$). If caustics develop after some time we can use the prescription of Subsection 15.11 to pass them.

15.4 Stationary WKB metod

The WKB method can be used to compute eigenfunctions of Hamiltonians. Let H and $H_\hbar$ be as in (15.6) and (15.8). We would like to solve

$$H_\hbar\Psi_\hbar = E\Psi_\hbar.$$

We make the ansatz

$$\Psi_\hbar(x) := \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)}a_\hbar(x).$$

We multiply the Schrödinger equation by $\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}S(x)}$ obtaining

$$\begin{aligned} &Ea_\hbar(x) \\ =\ &\left(\frac{1}{2}(\mathrm{i}^{-1}\hbar\hat{\partial}_x + \partial_x S(x) - A(x))g(x)(\mathrm{i}^{-1}\hbar\hat{\partial}_x + \partial_x S(x) - A(x)) + V(x)\right)a_\hbar(x). \end{aligned} \tag{15.19}$$

To make the zeroth order in $\hbar$ part of (15.19) vanish we demand that

$$E = \frac{1}{2}(\partial_x S(x) - A(x))g(x)(\partial_x S(x) - A(x)) + V(x),$$

which is the stationary version of the Hamilton-Jacobi equation, called sometimes the *eikonal equation.* Set $v(x) = \partial_p H\big(x, \partial_x S(x)\big)$. We have the equation for the amplitude

$$\frac{1}{2}\Big(v(x)\hat{\partial}_x + \hat{\partial}_x v(x)\Big)a_\hbar(x) = \frac{\mathrm{i}\hbar}{2}\hat{\partial}_x g(x)\hat{\partial}_x a_\hbar(x). \tag{15.20}$$

We set

$$a_\hbar(x) := \sum_{n=0}^{\infty}\hbar^n a_n(x). \tag{15.21}$$

Now (15.20) can be rewritten as

$$\begin{aligned} \frac{1}{2}\Big(v(x)\hat{\partial}_x + \hat{\partial}_x v(x)\Big)a_0(x) &= 0, \\ \frac{1}{2}\Big(v(x)\hat{\partial}_x + \hat{\partial}_x v(x)\Big)a_{n+1}(x) &= \mathrm{i}\hbar\hat{\partial}_x g(x)\hat{\partial}_x a_n(x). \end{aligned} \tag{15.22}$$

In dimension 1 we can solve (15.22) obtaining

$$a_0(x) = |v(x)|^{-\frac{1}{2}}.$$

This leads to an improved ansatz

$$\Psi_\hbar(x) = |v(x)|^{-\frac{1}{2}}\sum_{n=0}^{\infty}\hbar^n b_n(x)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)}$$

We obtain the chain of equations

$$\begin{aligned} b_0(x) &= 1, \\ \partial_t b_{n+1}\big(x\big) &= \mathrm{i}\hbar|v(x)|^{\frac{1}{2}}\hat{\partial}_x g(x)\hat{\partial}_x|v(x)|^{-\frac{1}{2}}b_n\big(x\big). \end{aligned}$$

Thus the leading approximation is

$$\Psi_0(x) := |v(x)|^{-\frac{1}{2}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)}. \tag{15.23}$$

In the case of quadratic Hamiltonians we can solve for $v(x)$ and $S(x)$:

$$\begin{aligned} v(x) &= g(x)^{-1}\sqrt{2\big(E - V(x)\big)}, \\ \partial_x S(x) &= g(x)^{-1}\sqrt{2\big(E - V(x)\big)} + A(x). \end{aligned}$$

15.5 Three-variable symbols

Sometimes the following technical result is useful:

Theorem 15.1. *Let*

$$|\partial_x^\alpha \partial_p^\beta \partial_y^\gamma c| \leq C_{\alpha,\beta,\gamma}, \quad \alpha, \beta, \gamma.$$

Then the operator B with the kernel

$$B(x,y) = (2\pi\hbar)^{-d} \int c(x,p,y) \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(x-y)p} \mathrm{d}p$$

belongs to Ψ_{00}^0 and equals $\mathrm{Op}(b)$, where

$$b(x,p) = \mathrm{e}^{\frac{\mathrm{i}\hbar}{2} D_p(-D_x + D_y)} c(x,p,y)\Big|_{x=y}.$$

Consequently,

$$b(x,p) = c(x,p,x) + \frac{\mathrm{i}\hbar}{2}\big(\partial_x c(x,p,y) - \partial_y c(x,p,y)\big)\Big|_{x=y} + O(\hbar^2). \tag{15.24}$$

Proof. We compute:

$$b(x,p) = (2\pi\hbar)^{-d} \int \mathrm{e}^{\frac{\mathrm{i}}{\hbar} z(w-p)} c\big(x + \frac{z}{2}, w, x - \frac{z}{2}\big) \mathrm{d}z \mathrm{d}w,$$

then we apply (**??**). $\square$

15.6 Conjugating quantization with a WKB phase

Lemma 15.2. *The operator $B_\hbar$ with the kernel*

$$(2\pi\hbar)^{-\frac{d}{2}} \int b(x,y) p \exp\Big(\frac{\mathrm{i}}{\hbar}(x-y)p\Big) \mathrm{d}p \tag{15.25}$$

equals

$$\frac{\hbar}{2\mathrm{i}}\Big(\hat{\partial}_x b(x,x) + b(x,x)\hat{\partial}_x\Big) + \mathrm{i}\hbar\left(\partial_x b(x,y) - \partial_y b(x,y)\right)\Big|_{y=x}. \tag{15.26}$$

Proof. We apply Theorem 15.1. $\square$

Theorem 15.3. *Let S, h be smooth functions. Then*

$$\begin{aligned} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}S(x)} \mathrm{Op}_\hbar(G) \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)} &= G(x, \partial_x S(x)) \\ &\quad + \frac{\hbar}{2\mathrm{i}}\Big(\hat{\partial}_x \partial_p G\big(x, \partial_x S(x)\big) + \partial_p G\big(x, \partial_x S(x)\big)\hat{\partial}_x\Big) + O(\hbar^2). \end{aligned} \tag{15.27}$$

Proof. The integral kernel of the left-hand side equals

$$
\begin{aligned}
& (2\pi\hbar)^{-\frac{d}{2}} \int G\Big(\frac{x+y}{2}, p\Big) \exp\Big(\frac{\mathrm{i}}{\hbar}\big(-S(x)+S(y)+(x-y)p\big)\Big) \mathrm{d}p \\
= \;& (2\pi\hbar)^{-\frac{d}{2}} \int G\Big(\frac{x+y}{2}, p\Big) \exp \frac{\mathrm{i}}{\hbar}(x-y)\Big(-\int_0^1 \partial S\big(\tau x+(1-\tau)y\big)\mathrm{d}\tau + p\Big) \mathrm{d}p \\
= \;& (2\pi\hbar)^{-\frac{d}{2}} \int G\Big(\frac{x+y}{2}, p + \int_0^1 \partial S\big(\tau x+(1-\tau)y\big)\mathrm{d}\tau\Big) \exp\Big(\frac{\mathrm{i}}{\hbar}(x-y)p\Big) \mathrm{d}p \\
= \;& (2\pi\hbar)^{-\frac{d}{2}} \int G\Big(\frac{x+y}{2}, \int_0^1 \partial S\big(\tau x+(1-\tau)y\big)\mathrm{d}\tau\Big) \exp\Big(\frac{\mathrm{i}}{\hbar}(x-y)p\Big) \mathrm{d}p \qquad (15.28) \\
+ \;& (2\pi\hbar)^{-\frac{d}{2}} \int p\partial_p G\left(\frac{x+y}{2}, \int_0^1 \partial S(\tau x+(1-\tau)y)\mathrm{d}\tau\right) \exp\Big(\frac{\mathrm{i}}{\hbar}(x-y)p\Big) \mathrm{d}p \qquad (15.29) \\
+ \;& (2\pi\hbar)^{-\frac{d}{2}} \int \int_0^1 \mathrm{d}\sigma(1-\sigma)pp \\
& \times \partial_p\partial_p G\left(\frac{x+y}{2}, \sigma p + \int_0^1 \partial S(\tau x+(1-\tau)y)\mathrm{d}\tau\right) \exp\Big(\frac{\mathrm{i}}{\hbar}(x-y)p\Big) \mathrm{d}p. \qquad (15.30)
\end{aligned}
$$

We have

$$
\begin{aligned}
(15.28) &= G(x, \partial_x S(x)), \\
(15.29) &= \frac{\hbar}{2\mathrm{i}}\left(\hat{\partial}_x \partial_p G(x, \partial_x S(x)) + \partial_p G(x, \partial_x S(x))\hat{\partial}_x\right), \\
(15.28) &= O(\hbar^2),
\end{aligned}
$$

where we used Lemma 15.2 to compute the second term. □

15.7 WKB approximation for general Hamiltonians

The WKB approximation is not restricted to quadratic Hamiltonians. Using Theorem 15.3 we easily see that the WKB method works for general Hamiltonians.

One can actually unify the time-dependent and stationary WKB method into one setup. Consider a function H on $\mathbb{R}^d \oplus \mathbb{R}^d$ having the interpretation of the Hamiltonian. We are interested in the two basic equations of quantum mechanics:

(1) The time-dependent Schrödinger equation:

$$(\mathrm{i}\hbar\partial_t - \mathrm{Op}_\hbar(H))\, \Phi_\hbar(t,x) = 0. \qquad (15.31)$$

(2) The stationary Schrödinger equation:

$$(\mathrm{Op}_\hbar(H) - E)\, \Phi_\hbar(x) = 0 \qquad (15.32)$$

They can be written as

$$\mathrm{Op}_\hbar(G)\Phi_\hbar(x) = 0, \tag{15.33}$$

where

(1) for (15.31), instead of the variable x actually we have $t, x \in \mathbb{R}\times\mathbb{R}^d$, instead of p we have $\tau, p \in \mathbb{R}\times\mathbb{R}^d$ and

$$G(x,t,p,\tau) = \tau - H(x,p).$$

(2) for (15.31),

$$G(x,p) = H(x,p) - E.$$

In order to solve (15.33) modulo $O(\hbar)$ we make an ansatz

$$\Phi_\hbar(x) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)}a_\hbar(x).$$

We insert $\Phi_\hbar$ into (15.33), we multiply by $\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}S(x)}$, we set

$$v(x) := \partial_p G(x,p),$$

and by (15.27) we obtain

$$\begin{aligned}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}S(x)}\mathrm{Op}_\hbar(G)\Phi_\hbar &= G\big(x,\partial_x S(x)\big)a_\hbar(x)\\ &\quad+\frac{\hbar}{2\mathrm{i}}\left(\hat\partial_x v(x) + v(x)\hat\partial_x\right)a_\hbar(x)\\ &\quad+O(\hbar^2).\end{aligned}$$

Thus we obtain the Hamilton-Jacobi equation

$$G(x,\partial_x S(x)) = 0$$

and the transport equation

$$\frac{1}{2}\left(\hat\partial_x v(x) + v(x)\hat\partial_x\right)a_\hbar(x) = O(\hbar).$$

If we choose any solution of

$$\frac{1}{2}\left(\hat\partial_x v(x) + v(x)\hat\partial_x\right)a_0 = 0$$

and set

$$\Phi_{\mathrm{cl}}(x) := \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)}a_0(x)$$

then we obtain an approximate solution:

$$\mathrm{Op}_\hbar(G)\Phi_{\mathrm{cl}}(x) = O(\hbar).$$

15.8 WKB functions. The naive approach

Distributions associated with a Lagrangian subspaces have a natural generalization to Lagrangian manifolds in a cotangent bundle.

Let $\mathcal{X}$ be a manifold and $\mathcal{L}$ a Lagrangian manifold in $\mathrm{T}^{\#}\mathcal{X}$. First assume that $\mathcal{L}$ is projectable onto $\mathcal{U} \subset \mathcal{X}$ and $\mathcal{U} \ni x \mapsto S(x)$ is a generating function of $\mathcal{L}$. Then

$$\mathcal{U} \ni x \mapsto a(x)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)} \tag{15.34}$$

is a function that semiclassically is concentrated in $\mathcal{L}$.

Suppose now that $\mathcal{L}$ is not necessarily projectable. Then we can consider its covering $\mathcal{L}^{\mathrm{cov}}$ parametrized by $z \mapsto \big(x(z), p(z)\big) \in \mathcal{L}^{\mathrm{cov}}$. Let T be a generating function of $\mathcal{L}$ viewed as a function on $\mathcal{L}^{\mathrm{cov}}$. We would like to think of (15.34) as derived from a half-density on the Lagrangian manifold

$$z \mapsto b\big(x(z), p(z)\big)|\mathrm{d}z|^{1/2}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}T(x(z),p(z))}. \tag{15.35}$$

where b is a nice function on $\mathcal{L}^{\mathrm{cov}}$.

If a piece of $\mathcal{L}^{\mathrm{cov}}$ is projectable over $\mathcal{U} \subset \mathcal{X}$, then we can express (15.35) in terms of x:

$$\mathcal{U} \ni x \mapsto b\big(x, p(z(x))\big)\big|\det \partial_x z(x)\big|^{1/2}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}T\left(x,p(z(x))\right)}|\mathrm{d}x|^{1/2}. \tag{15.36}$$

(15.36) is actually not quite correct – there is a problem along the caustics, which should be corrected by the so-called Maslov index.

15.9 Semiclassical Fourier transform of WKB functions

Let us apply $(2\pi\hbar)^{-d/2}\mathcal{F}_\hbar$ to a function given by the WKB ansatz:

$$\Psi_\hbar(x) := a(x)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)}. \tag{15.37}$$

Thus we consider

$$(2\pi\hbar)^{-d/2}\int a(x)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\left(S(x)-xp\right)}\mathrm{d}x.$$

We apply the stationary phase method. Given p we define $x(p)$ by

$$\partial_x(S(x(p)) - x(p)p) = \partial_x S(x(p)) - p = 0.$$

We assume that we can invert this function obtaining $p \mapsto x(p)$. Note that

$$\partial_p x(p) = \big(\partial_x^2 S\big(x(p)\big)\big)^{-1},$$

so locally it is possible if $\partial_x^2 S$ is invertible. Let $p \mapsto \tilde{S}(p)$ denote the Legendre transform of $x \mapsto S(x)$, that is

$$\tilde{S}(p) = px(p) - S\big(x(p)\big).$$

Then by the stationary phase method

$$\begin{aligned}(2\pi\hbar)^{-d/2}\mathcal{F}_\hbar\Psi_\hbar(p) &= \mathrm{e}^{\frac{\mathrm{i}\pi\,\mathrm{inert}\,\partial_x^2 S(x(p))}{4}}|\partial_x^2 S\big(x(p)\big)|^{-1/2}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\tilde{S}(p)}a(x(p)) + O(\hbar)\\ &= \mathrm{e}^{\frac{\mathrm{i}\pi\,\mathrm{inert}\,\partial_p^2\tilde{S}(p)}{4}}|\partial_p^2\tilde{S}(p)|^{1/2}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\tilde{S}(p)}a(x(p)) + O(\hbar).\end{aligned}$$

One can make this formula more symmetric by replacing $\Psi_\hbar$ with

$$\Phi_\hbar(x) := |\partial_x^2 S(x)|^{1/4}a(x)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)}. \tag{15.38}$$

Then

$$(2\pi\hbar)^{-d/2}\mathcal{F}_\hbar\Phi_\hbar(p) = \mathrm{e}^{\frac{\mathrm{i}\pi\,\mathrm{inert}\,\partial_p^2\tilde{S}(p)}{4}}|\partial_p^2\tilde{S}(p)|^{1/4}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\tilde{S}(p)}a(x(p)) + O(\hbar).$$

15.10 WKB functions in a neighborhood of a fold

Let us consider $\mathbb{R}\times\mathbb{R}$ and the Lagrangian manifold given by $x = -p^2$. Note that it is not projectable in the x coordinates. It is however projectable in the p coordinates. Its generating function in the p coordinates is $p \mapsto \frac{p^3}{3}$.

We consider a function given in the p variables by the WKB ansatz

$$(2\pi\hbar)^{-\frac{1}{2}}\mathcal{F}_\hbar\Psi_\hbar(p) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\frac{p^3}{3}}b(p). \tag{15.39}$$

Then

$$\Psi_\hbar(x) = (2\pi\hbar)^{-\frac{1}{2}}\int \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\frac{p^3}{3}+xp)}b(p)\mathrm{d}p. \tag{15.40}$$

The stationary phase method gives for $x<0$, $p(x) = \pm\sqrt{-x}$. Thus, for $x<0$,

$$\begin{aligned}\Psi_\hbar(x) \simeq\ & \mathrm{e}^{\frac{\mathrm{i}\pi}{4}-\frac{\mathrm{i}2}{\hbar 3}(-x)^{\frac{3}{2}}}(-x)^{-\frac{1}{4}}b(-\sqrt{-x})\\ &+\mathrm{e}^{-\frac{\mathrm{i}\pi}{4}+\frac{\mathrm{i}2}{\hbar 3}(-x)^{\frac{3}{2}}}(-x)^{-\frac{1}{4}}b(\sqrt{-x}).\end{aligned} \tag{15.41}$$

Thus we see that the phase jumps by $\mathrm{e}^{\frac{\mathrm{i}\pi}{2}}$.

For $x>0$ the non-stationary method gives $\Psi_\hbar(x) \simeq O(\hbar^\infty)$. If b is analytic, we can apply the steepest descent method to obtain

$$\Psi_\hbar(x) \simeq \mathrm{e}^{-\frac{2}{\hbar 3}x^{\frac{3}{2}}}x^{-\frac{1}{4}}b(\mathrm{i}\sqrt{x}) \tag{15.42}$$

Note that the stationary phase and steepest descent method are poor in a close vicinity of the fold – they give a singular behavior, even though in reality the function is continuous. It can be approximated by replacing $b(p)$ with $b(0)$ in terms of the *Airy function*

$$\mathrm{Ai}(x) := \frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{e}^{\frac{\mathrm{i}}{3}p^2+\mathrm{i}px}\mathrm{d}p.$$

In fact,

$$\Psi_\hbar(x) \approx b(0)(2\pi)^{1/2}\hbar^{-1/6}\mathrm{Ai}(\hbar^{-2/3}x).$$

15.11 Caustics and the Maslov correction

Let us go back to the construction described in Subsection 15.8. Recall that we had problems with the WKB approximation near a point where the Lagrangian manifold is not projectable. There can be various behaviors of $\mathcal{L}$ near such point, but it is enough to assume that we have a simple fold. We can then represent locally the manifold as $\mathcal{X} = \mathbb{R} \times \mathcal{X}_\perp$ with coordinates $(x_1, x_\perp)$. The corresponding coordinates on the cotangent bundle $\mathrm{T}^\# \mathcal{X} = \mathbb{R} \times \mathbb{R} \times \mathrm{T}^\# \mathcal{X}_\perp$ are $(x_1, p_1, x_\perp, p_\perp)$.

Suppose that we have a Lagrangian manifold that locally can be parametrized by $(p_1, x_\perp)$ with a generating function $(p_1, x_\perp) \mapsto T(p_1, x_\perp)$, but is not projectable on $\mathcal{X}$. More precisely, we assume that it projects to the left of $x_1 = 0$, where it has a fold. Thus it has two sheets given by

$$\{x = (x_1, x_\perp) \ : \ x_1 \leq 0\} \ni x \mapsto p^\pm(x).$$

By applying the Legendre transformation in x_1 we obtain two generating functions

$$\{(x_1, x_\perp) \ : \ x_1 \leq 0\} \ni x \mapsto S^\pm(x).$$

Suppose that we start from a function given by

$$\Phi_\hbar(p_1, x_\perp) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar} T(p_1, x_\perp) + \mathrm{i}\alpha} b(p_1, x_\perp),$$

where α is a certain phase. If we apply the unitary semiclassical Fourier transformation wrt the variable p_1 we obtain

$$\begin{aligned} \Psi_\hbar(x) \quad = \quad & \mathrm{e}^{\frac{\mathrm{i}}{\hbar} S^-(x_1, x_\perp) + \mathrm{i}\alpha - \mathrm{i}\frac{\pi}{4}} b\big(p_1^-(x), x_\perp\big) \big| \det \partial_{x_1} p_1^-(x) \big|^{\frac{1}{2}} & (15.43) \\ & + \mathrm{e}^{\frac{\mathrm{i}}{\hbar} S^+(x_1, x_\perp) + \mathrm{i}\alpha + \mathrm{i}\frac{\pi}{4}} b\big(p_1^+(x), x_\perp\big) \big| \det \partial_{x_1} p_1^+(x) \big|^{\frac{1}{2}} + O(\hbar). & (15.44) \end{aligned}$$

Thus the naive ansatz is corrected by the factor of $\mathrm{e}^{\mathrm{i}\frac{\pi}{2}}$.

In the case of a general Lagrangian manifold, we can slightly deform it so that we can reach each point by passing caustics only through simple folds.

15.12 Global problems of the WKB method

Let us return to the setup of Subsection 15.7. Note that the WKB method gives only a local solution. To find a global solution we need to look for a Lagrangian manifold $\mathcal{L}$ in $G^{-1}(0)$. Suppose we found such a manifold. We divide it into projectable patches $\mathcal{L}_i$ such that $\pi(\mathcal{L}_i) = \mathcal{U}_i$. For each of these patches on $\mathcal{U}_i$ we can write the WKB ansatz

$$\mathrm{e}^{\frac{\mathrm{i}}{\hbar} S(x)} a(x).$$

Then we try to sew them together using the Maslov conditon.

This might work in the time dependent case. In fact, we can choose a WKB ansatz corresponding to a projectable Lagrangian manifold at time $t = 0$, with a well defined generating function. For small times typically the evolved Lagrangian manifold will stay projectable and the WKB method will work well. Then caustics may form – we can then consider the generating function viewed as a (univalued) function on the Lagrangian manifold and use the Maslov prescription.

When we apply the WKB method in more than 1 dimension for the stationary Schrödinger equation, problems are more serious. First, it is not obvious that we will find a Lagrangian manifold. Even if we find it, it is typically not simply connected. In principle we should use its universal covering. Thus above a single x we can have contributions from various sheets of $\mathcal{L}^{\mathrm{cov}}$ – typically, infinitely many of them. They may cause "destructive interference".

15.13 Bohr–Sommerfeld conditions

The stationary WKB method works well in the special case of $X = \mathbb{R}$. Typically, a Lagrangian manifold coincides in this case with a connected component of the level set $\{(x, p) \in \mathbb{R} \times \mathbb{R} \ : \ H(x, p) = E\}$. The transport equation has a univalued solution. $\mathcal{L}$ is topologically a circle, and it is the boundary of a region $\mathcal{D}$, which is topologically a disc. (This equips $\mathcal{L}$ with an orientation). The function T after going around $\mathcal{L}$ increases by $\int_{\mathcal{L}} \theta = \int_{\mathcal{D}} \omega$. Suppose that $\mathcal{L}$ crosses caustics only at simple folds, n_+ of them in the "positive" direction and n_- in the "negative" direction. Clearly, $n_+ - n_- = 2$. (In fact, in a typical case, such as that of a circle, we have $n_+ = 2$, $n_- = 0$). Then when we come back to the initial point the WKB solution changes by

$$\mathrm{e}^{\frac{\mathrm{i}}{\hbar} \int_{\mathcal{D}} \omega - \mathrm{i}\pi}. \tag{15.45}$$

If (15.45) is different from 1, then going around we obtain contributions to WKB that intefere destructively. Thus (15.45) has to be 1. This leads to the condition

$$\frac{1}{\hbar} \int_{\mathcal{D}} \omega - \pi = 2\pi n, \quad n \in \mathbb{Z}, \tag{15.46}$$

or

$$\frac{1}{2\pi} \int_{\mathcal{D}} \omega = \hbar \left(n + \frac{1}{2} \right), \tag{15.47}$$

which is the famous Bohr-Sommerfeld condition.

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