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*

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

(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:

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

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,

$$\hbar\frac{\mathrm{d}A(t)}{\mathrm{d}t} = \mathrm{i}[H,A(t)], \quad A(t_0)=A,$$

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:

$$\mathrm{e}^{\frac{\mathrm{i}t}{\hbar}H}AB\mathrm{e}^{-\frac{\mathrm{i}t}{\hbar}H} = \mathrm{e}^{\frac{\mathrm{i}t}{\hbar}H}A\mathrm{e}^{-\frac{\mathrm{i}t}{\hbar}H}\mathrm{e}^{\frac{\mathrm{i}t}{\hbar}H}B\mathrm{e}^{-\frac{\mathrm{i}t}{\hbar}H}.$$

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

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

1.3 Concept of quantization

Quantization usually means a linear transformation with good properties, 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 $L^2(\mathbb{R}^d)$. (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 $\mathrm{Op}^\bullet(b)$ – x, p play the role of coordinate functions on the phase space and not its 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) $[\big(\mathrm{Op}^\bullet(b),\mathrm{Op}^\bullet(c)]\approx \mathrm{i}\hbar\mathrm{Op}^\bullet(\{b,c\})$.

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

The function b will be called the *symbol* (or *dequantization*) of the operator B.

Note that (1) implies that (3) and (4) is true at least if b is a 1st order 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. The momentum is scaled. 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 equal footing. This approach is typical when we consider coherent states.

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

2.1 Fourier tranformation

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

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

Hence

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

Proposition 2.1. *The Fourier transform of* $\mathrm{e}^{-\mathrm{i}tpx}$ *is* $(2\pi)^{-d}t^{-d}\mathrm{e}^{\frac{\mathrm{i}\eta\xi}{t}}$.

Proof.

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

□

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

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

Clearly,

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

2.2 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

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

Proposition 2.2. *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.

$$\begin{aligned} \big(\mathcal{F}_\hbar^{-1}\hat{x}\mathcal{F}_\hbar\Psi\big)(p) &= \frac{1}{(2\pi\hbar)^d}\int \mathrm{d}x \int \mathrm{d}k \mathrm{e}^{\frac{\mathrm{i}}{\hbar}px} x \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}kx}\Psi(k) && (2.3)\\ &= \frac{1}{(2\pi\hbar)^d}\int \mathrm{d}x \int \mathrm{d}k \hbar\mathrm{i}\partial_k \mathrm{e}^{\frac{\mathrm{i}}{\hbar}px}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}kx}\Psi(k) && (2.4)\\ &= -\frac{1}{(2\pi\hbar)^d}\int \mathrm{d}x \int \mathrm{d}k \mathrm{e}^{\frac{\mathrm{i}}{\hbar}px}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}kx}\hbar\mathrm{i}\partial_k\Psi(k) \quad = \quad \hat{p}\Psi(p). && (2.5) \end{aligned}$$

$$\begin{aligned} \big(\mathcal{F}_\hbar^{-1}\hat{p}\mathcal{F}_\hbar\Psi\big)(x) &= \frac{1}{(2\pi\hbar)^d}\int \mathrm{d}x \int \mathrm{d}k \mathrm{e}^{\frac{\mathrm{i}}{\hbar}px}\frac{\hbar}{\mathrm{i}}\partial_p \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}py}\Psi(y) && (2.6)\\ &= -\frac{1}{(2\pi\hbar)^d}\int \mathrm{d}x \int \mathrm{d}k \mathrm{e}^{\frac{\mathrm{i}}{\hbar}px} y \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}py}\Psi(y) \quad = \quad -\hat{x}\Psi(x). && (2.7) \end{aligned}$$

□Hence, for Borel functions

$$\begin{aligned} \mathcal{F}_\hbar^{-1} f(\hat{x})\mathcal{F}_\hbar &= f(\hat{p}), && (2.8)\\ \mathcal{F}_\hbar^{-1} g(\hat{p})\mathcal{F}_\hbar &= g(-\hat{x}). && (2.9) \end{aligned}$$

(2.9) can be rewritten as

$$\begin{aligned} \big(g(\hat{p})\Psi\big)(x) &= \frac{1}{(2\pi\hbar)^d}\int\int \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(x-y)p} g(p)\Psi(y)\mathrm{d}y\mathrm{d}p && (2.10)\\ &= \frac{1}{(2\pi\hbar)^d}\int \hat{g}\Big(\frac{y-x}{\hbar}\Big)\Psi(y)\mathrm{d}y. && (2.11) \end{aligned}$$

2.3 Gaussian integrals

Suppose that ν is positive definite. Then

$$\int \mathrm{e}^{-\frac{1}{2}x\cdot\nu x+\eta\cdot x}\mathrm{d}x = (2\pi)^{\frac{d}{2}}(\det\nu)^{-\frac{1}{2}}\mathrm{e}^{\frac{1}{2}\eta\cdot\nu^{-1}\eta}. \tag{2.12}$$

In particular, if $f(x) = \mathrm{e}^{-\frac{1}{2}x\cdot\nu x}$, its Fourier transform is

$$\hat{f}(\xi) = (2\pi)^{\frac{d}{2}}(\det\nu)^{-\frac{1}{2}}\mathrm{e}^{-\frac{1}{2}\xi\cdot\nu^{-1}\xi}. \tag{2.13}$$

Consequently,

$$\begin{aligned}
\mathrm{e}^{\frac{1}{2}\partial_x\cdot\nu\partial_x}\Psi(x) &= \mathrm{e}^{-\frac{1}{2}\hat{p}\cdot\nu\hat{p}}\Psi(x) &(2.14)\\
&= (2\pi)^{-\frac{d}{2}}(\det\nu)^{-\frac{1}{2}}\int \mathrm{e}^{-\frac{1}{2}y\cdot\nu^{-1}y}\Psi(x+y)\mathrm{d}y &(2.15)\\
&= \frac{\int \mathrm{e}^{-\frac{1}{2}y\cdot\nu^{-1}y}\Psi(x+y)\mathrm{d}y}{\int \mathrm{e}^{-\frac{1}{2}y\cdot\nu^{-1}y}\mathrm{d}y}.
\end{aligned}$$

As a consequence, we obtain the following identity

$$\begin{aligned}
\mathrm{e}^{\frac{1}{2}\partial_x\cdot\nu\partial_x}\Psi(0) &= (\det 2\pi\nu)^{-\frac{1}{2}}\int \Psi(x)\mathrm{e}^{-\frac{1}{2}x\cdot\nu^{-1}x}\mathrm{d}x &(2.16)\\
&= \frac{\int \Psi(x)\mathrm{e}^{-\frac{1}{2}x\cdot\nu^{-1}x}\mathrm{d}x}{\int \mathrm{e}^{-\frac{1}{2}x\cdot\nu^{-1}x}\mathrm{d}x}.
\end{aligned}$$

For example,

$$\mathrm{e}^{\mathrm{i}\hbar\partial_x\partial_p}\Phi(x,p) = (2\pi\hbar)^{-d}\int \mathrm{e}^{\frac{\mathrm{i}}{\hbar}yw}\Phi(x+y,p+w)\mathrm{d}y\mathrm{d}w. \tag{2.17}$$

As an exercise let us check (2.14) for polynomial Ψ. By diagonalizing ν and then changing the variables, we can reduce ourselves to 1 dimension. Now

$$\begin{aligned}
\mathrm{e}^{\frac{1}{2}\partial_x^2}x^n &= \sum_{k=0}^{\infty}\frac{n!}{2^k(n-2k)!k!}x^{n-2k}; &(2.18)\\
(2\pi)^{-\frac{1}{2}}\int \mathrm{e}^{-\frac{1}{2}y^2}(y+x)^n\mathrm{d}y &= \sum_{m=0}^{\infty}x^{n-m}(2\pi)^{-\frac{1}{2}}\frac{n!}{(n-m)!m!}\int \mathrm{e}^{-\frac{1}{2}y^2}y^m\mathrm{d}y.
\end{aligned}$$

Now

$$\begin{aligned}
(2\pi)^{-\frac{1}{2}}\int \mathrm{e}^{-\frac{1}{2}y^2}y^{2k+1}\mathrm{d}y &= 0,\\
(2\pi)^{-\frac{1}{2}}\int \mathrm{e}^{-\frac{1}{2}y^2}y^{2k}\mathrm{d}y &= \frac{(2k)!}{2^k k!}. &(2.19)
\end{aligned}$$

Indeed, the lhs of (2.19) is

$$\pi^{-\frac{1}{2}}2^k\int_0^\infty \mathrm{e}^{-\frac{1}{2}y^2}\Big(\frac{1}{2}y^2\Big)^{k-\frac{1}{2}}\mathrm{d}\Big(\frac{1}{2}y^2\Big) = \pi^{-\frac{1}{2}}2^k\Gamma\Big(k+\frac{1}{2}\Big),$$

which using

$$\Gamma\Big(k+\frac{1}{2}\Big) = \pi^{\frac{1}{2}}\frac{(2k)!}{2^{2k}k!}$$

equals the rhs of (2.19).

Therefore, (2.18)=(2.19).

2.4 Gaussian integrals in complex variables

Consider the space $\mathbb{R}^d \oplus \mathbb{R}^d$ with the generic variables x, p. It is often natural to identify it with the complex space $\mathbb{C}^d$ by introducing the variables

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

so that

$$x_i = 2^{-1/2}(a + a^*), \quad p_i = -\mathrm{i}2^{-1/2}(a - a^*). \tag{2.20}$$

The Lebesgue measure $\mathrm{d}x\mathrm{d}p$ will be denoted $\mathrm{i}^{-d}\mathrm{d}a^*\mathrm{d}a$. To justify this notation note that

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

Let β be a Hermitian positive quadratic form. We then have

$$\int \mathrm{e}^{-a^*\cdot\beta a + w_1\cdot a^* + \overline{w}_2\cdot a}\mathrm{d}a^*\mathrm{d}a = (2\pi\mathrm{i})^d(\det\beta)^{-1}\mathrm{e}^{w_1\cdot\beta^{-1}\overline{w}_2}, \tag{2.21}$$

$$\begin{aligned} \mathrm{e}^{\partial_{a^*}\cdot\beta\partial_a}\Phi(a^*, a) &= (2\pi\mathrm{i})^{-d}(\det\beta)^{-1}\int \mathrm{e}^{-b^*\cdot\beta^{-1}b}\Phi(a^* + b^*, a + b)\mathrm{d}b^*\mathrm{d}b && (2.22) \\ &= \frac{\int \mathrm{e}^{-b^*\cdot\beta^{-1}b}\Phi(a^* + b^*, a + b)\mathrm{d}b^*\mathrm{d}b}{\int \mathrm{e}^{-b^*\cdot\beta^{-1}b}\mathrm{d}b^*\mathrm{d}b}. && (2.23) \end{aligned}$$

As a consequence, we obtain the following identity

$$\begin{aligned} \mathrm{e}^{\partial_{a^*}\cdot\beta\partial_a}\Phi(0, 0) &= (2\pi\mathrm{i})^{-d}(\det\beta)^{-1}\int \Phi(a^*, a)\mathrm{e}^{-a\cdot\beta^{-1}a^*}\mathrm{d}a^*\mathrm{d}a \\ &= \frac{\int \Phi(a^*, a)\mathrm{e}^{-a\cdot\beta^{-1}a^*}\mathrm{d}a^*\mathrm{d}a}{\int \mathrm{e}^{-a\cdot\beta^{-1}a^*}\mathrm{d}a^*\mathrm{d}a}. && (2.24) \end{aligned}$$

In practice, it is convenient to view the pair a_i, a_i^* not necessarily as a pair of conjugate complex variables, but as independent complex variables. If the integrand is separately holomorphic in a_i and a_i^*, then all the formulas remain valid by analytic continuation.

As an exercise let us check (2.23) for polynomial Φ. By diagonalizing β and then changing the variables, we can reduce ourselves to 1 (complex) dimension. Now

$$\begin{aligned} \mathrm{e}^{\partial_{a^*}\partial_a}a^{*n}a^m &= \sum_{k=0}^{\infty}\frac{n!m!}{(n-k)!(m-k)!k!}a^{*(n-k)}a^{m-k}; && (2.25) \\ & (2\pi\mathrm{i})^{-1}\int \mathrm{e}^{-b^*b}(a^* + b^*)^n(a + b)^m\mathrm{d}b^*\mathrm{d}b && (2.26) \\ &= \sum_{k,l=0}^{\infty}a^{*(n-k)}a^{(m-l)}\frac{n!m!}{k!(n-k)!l!(m-l)!}\int \mathrm{e}^{-b^*b}b^{*k}b^l\mathrm{d}b^*\mathrm{d}b. \end{aligned}$$

Now

$$(2\pi\mathrm{i})^{-1}\int \mathrm{e}^{-b^*b}b^{*k}b^l\mathrm{d}b^*\mathrm{d}b \quad = \quad k!\delta_{kl}. \tag{2.27}$$

Indeed, if we use the polar coordinates with $b^*b = \frac{1}{2}r^2$, the lhs of (2.27) becomes

$$\begin{aligned} & (2\pi)^{-1}\int_0^\infty \mathrm{e}^{-\frac{1}{2}r^2}\Big(\frac{1}{2}r^2\Big)^{\frac{1}{2}(k+l)}\mathrm{e}^{\mathrm{i}(n-m)\phi}r\mathrm{d}r\mathrm{d}\phi \\ = \quad & \delta_{kl}\int_0^\infty \mathrm{e}^{-\frac{1}{2}r^2}\Big(\frac{1}{2}r^2\Big)^k\mathrm{d}\Big(\frac{1}{2}r^2\Big) \end{aligned}$$

which equals the rhs of (2.27).

Therefore, (2.25)=(2.26).

Here is a useful generalization of (2.21). (We assume that γ_1, γ_2 are symmetric matrices).

$$\begin{aligned} & \int \mathrm{e}^{-a^*\cdot\beta a-\frac{1}{2}a^*\gamma_1 a^*-\frac{1}{2}a^*\overline{\gamma}_2 a^*+w_1\cdot a^*+\overline{w}_2\cdot a}\mathrm{d}a^*\mathrm{d}a \\ = & (2\pi\mathrm{i})^d\Big(\det\begin{bmatrix}\beta & \gamma_1\\ \overline{\gamma}_2 & \beta^{\#}\end{bmatrix}\Big)^{-\frac{1}{2}}\exp\Big(\frac{1}{2}[w_1,\overline{w}_2]\begin{bmatrix}\beta & \gamma_1\\ \overline{\gamma}_2 & \beta^{\#}\end{bmatrix}^{-1}\begin{bmatrix}\overline{w}_2\\ w_1\end{bmatrix}\Big). \end{aligned} \tag{2.28}$$

2.5 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

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

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

2.6 Tempered distributions

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

$$\mathcal{S}(\mathbb{R}^n) := \big\{\Psi \in C^\infty(\mathbb{R}^n) \ : \ \int |x^\alpha\nabla_x^\beta\Psi(x)|^2\mathrm{d}x < \infty, \quad \alpha,\beta\in\mathbb{N}^n\big\}. \tag{2.29}$$

Remark 2.3. *The definition (2.29) is equivalent to*

$$\mathcal{S}(\mathbb{R}^n) = \big\{ \Psi \in C^\infty(\mathbb{R}^n) \ : \ |x^\alpha \nabla_x^\beta \Psi(x)| \leq c_{\alpha,\beta}, \qquad \alpha, \beta \in \mathbb{N}^n \big\}. \tag{2.30}$$

$\mathcal{S}'(\mathbb{R}^n)$ 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

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

We will use the integral notation

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

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

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

Here are some examples of elements of $\mathcal{S}'(\mathbb{R})$:

$$\begin{aligned} \int \delta(t)\Phi(t)\mathrm{d}t &:= \Phi(0), \\ \int (t \pm \mathrm{i}0)^\lambda \Phi(t)\mathrm{d}t &:= \lim_{\epsilon \searrow 0} \int (t \pm \mathrm{i}\epsilon)^\lambda \Phi(t)\mathrm{d}t. \end{aligned}$$

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*

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

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. .

2.7 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 2.5. *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

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

2.8 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:

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

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

$$\mathrm{Tr} BC = \int B(y,x) C(x,y) \mathrm{d}x \mathrm{d}y. \tag{2.31}$$

In particular by setting $B = \mathbb{1}$, 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

$$\big(f(\hat{x})g(\hat{p})\big)\Psi(x) = (2\pi\hbar)^{-d}\int \mathrm{d}p \int \mathrm{d}y f(x)g(p)\mathrm{e}^{\frac{\mathrm{i}(x-y)p}{\hbar}}\Psi(y). \tag{3.32}$$

Hence we can generalize (3.32) for a general function on the phase space b

$$\big(\mathrm{Op}^{x,p}(b)\Psi\big)(x) = (2\pi\hbar)^{-d}\int \mathrm{d}p \int \mathrm{d}y b(x,p)\mathrm{e}^{\frac{\mathrm{i}(x-y)p}{\hbar}}\Psi(y). \tag{3.33}$$

In the PDE-community one writes

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

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

$$\big(\mathrm{Op}^{p,x}(b)\Psi\big)(x) = (2\pi\hbar)^{-d}\int \mathrm{d}p \int \mathrm{d}y b(y,p)\mathrm{e}^{\frac{\mathrm{i}(x-y)p}{\hbar}}\Psi(y). \tag{3.34}$$

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

$$\mathrm{Op}^{x,p}(b_{x,p}) = B, \quad B(x,y) = (2\pi\hbar)^{-d}\int \mathrm{d}p b_{x,p}(x,p)\mathrm{e}^{\frac{\mathrm{i}(x-y)p}{\hbar}}, \tag{3.35}$$

$$\mathrm{Op}^{p,x}(b_{p,x}) = B, \quad B(x,y) = (2\pi\hbar)^{-d}\int \mathrm{d}p b_{p,x}(y,p)\mathrm{e}^{\frac{\mathrm{i}(x-y)p}{\hbar}}. \tag{3.36}$$

Proposition 3.1. *We can compute the symbol from the kernel: If (3.35), then*

$$b_{x,p}(x,p) = \int B(x,x-z)\mathrm{e}^{-\frac{\mathrm{i}zp}{\hbar}}\mathrm{d}z. \tag{3.37}$$

Proof.

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

We apply the Fourier transform. □

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 (3.35) and (3.36) hold, then*

$$\mathrm{e}^{-\mathrm{i}\hbar D_x D_p} b_{x,p}(x,p) = b_{p,x}(x,p). \tag{3.38}$$

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,

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

Proposition 3.4. *We have the following formula for the symbol of the product: If*

$$\mathrm{Op}^{x,p}(b)\mathrm{Op}^{x,p}(c) = \mathrm{Op}^{x,p}(d), \tag{3.39}$$

then

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

Proof.

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

□

Besides d given by (3.39), let

$$\mathrm{Op}^{x,p}(c)\mathrm{Op}^{x,p}(b) = \mathrm{Op}^{x,p}(d_1), \tag{3.40}$$

Note that formally

$$\begin{aligned} d(x,p) &= b(x,p)c(x,p) - \mathrm{i}\hbar\partial_p b(x,p)\partial_x c(x,p) + O(\hbar^2), \\ d_1(x,p) &= b(x,p)c(x,p) - \mathrm{i}\hbar\partial_x b(x,p)\partial_p c(x,p) + O(\hbar^2). \end{aligned}$$

Therefore,

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

Obviously,

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

3.2 Weyl-Wigner quantization

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

$$\big(\mathrm{Op}(b)\Psi\big)(x) = (2\pi\hbar)^{-d}\int \mathrm{d}p \int \mathrm{d}y b\Big(\frac{x+y}{2}, p\Big)\mathrm{e}^{\frac{\mathrm{i}(x-y)p}{\hbar}}\Psi(y). \tag{3.41}$$

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:

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

Proposition 3.5. *We can compute the symbol from the kernel:*

$$b(x,p) = \int B\Big(x + \frac{z}{2}, x - \frac{z}{2}\Big)\mathrm{e}^{-\frac{\mathrm{i}zp}{\hbar}}\mathrm{d}z. \tag{3.42}$$

Proof.

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

We apply the Fourier transform. □

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

Let P_0 be the orthogonal projection onto the normalized vector $\pi^{-\frac{d}{4}}\mathrm{e}^{-\frac{1}{2}x^2}$. The integral kernel of P_0 equals

$$P_0(x,y) = \pi^{-\frac{d}{2}}\mathrm{e}^{-\frac{1}{2}x^2 - \frac{1}{2}y^2}.$$

Its various symbols equal

$$\begin{aligned}
x,p\text{-symbol:} &\quad 2^{\frac{d}{2}}\mathrm{e}^{-\frac{1}{2}x^2 - \frac{1}{2}p^2 - \mathrm{i}x\cdot p}, \\
p,x\text{-symbol:} &\quad 2^{\frac{d}{2}}\mathrm{e}^{-\frac{1}{2}x^2 - \frac{1}{2}p^2 + \mathrm{i}x\cdot p}, \\
\text{Weyl-Wigner symbol:} &\quad 2^{\frac{d}{2}}\mathrm{e}^{-\frac{1}{2}x^2 - \frac{1}{2}p^2}.
\end{aligned}$$

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

$$\text{if} \quad \mathrm{Op}^{x,p}(b_{x,p}) = \mathrm{Op}(b), \quad \text{then}$$
$$\mathrm{e}^{\frac{\mathrm{i}}{2}\hbar D_x D_p} b(x,p) = b_{x,p}(x,p). \tag{3.43}$$

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

3.3 Star product

Proposition 3.7. *We have the following formula for the symbol of the product:*

$$\text{if} \quad \mathrm{Op}(b)\mathrm{Op}(c) = \mathrm{Op}(d), \quad \text{then} \tag{3.44}$$
$$d(x,p) = \mathrm{e}^{\frac{\mathrm{i}}{2}\hbar(D_{p_1}D_{x_2} - D_{x_1}D_{p_2})} b(x_1,p_1)c(x_2,p_2)\Big|_{\substack{x := x_1 = x_2, \\ p := p_1 = p_2.}} .$$

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
$$z_1 = \frac{x+2^{-1}u+y}{2}, \quad z_2 = \frac{x-2^{-1}u+y}{2}, \tag{3.45}$$
□

As a consequence,
$$\begin{aligned} \frac{1}{2}\big(\mathrm{Op}(b)\mathrm{Op}(c) + \mathrm{Op}(c)\mathrm{Op}(b)\big) &= \mathrm{Op}(bc) + O(\hbar^2), & (3.46) \\ [\mathrm{Op}(b), \mathrm{Op}(c)] &= \mathrm{i}\hbar\mathrm{Op}(\{b,c\}) + O(\hbar^3), & (3.47) \\ \text{if} \ \ \mathrm{supp} b \cap \mathrm{supp} c = \emptyset, \quad \text{then} \quad \mathrm{Op}(b)\mathrm{Op}(c) &= O(\hbar^\infty). & (3.48) \end{aligned}$$

Often one denotes d in (3.44) by $b * c$ and calls the *star product* or the *Moyal product* of b and c.

Proposition 3.8. *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 3.9. *Let h be a polynomial of degree ≤ 2. Then*

(1)
$$[\mathrm{Op}(h),\mathrm{Op}(b)] = \mathrm{i}\hbar\mathrm{Op}(\{h,b\}). \tag{3.49}$$

(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

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

Proof.

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

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

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

$\square$

3.4 Weyl operators

Proposition 3.10 (Baker-Campbell-Hausdorff formula)**.** *Suppose that*

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

Then

$$\mathrm{e}^{A+B} = \mathrm{e}^{A}\mathrm{e}^{B}\mathrm{e}^{-\frac{1}{2}[A,B]}.$$

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

$$\mathrm{e}^{t(A+B)} = \mathrm{e}^{tA}\mathrm{e}^{tB}\mathrm{e}^{-\frac{1}{2}t^2[A,B]}. \tag{3.50}$$

First, using the Lie formula, we obtain

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

Now

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{tA}\mathrm{e}^{tB}\mathrm{e}^{-\frac{1}{2}t^2[A,B]} &= A\mathrm{e}^{tA}\mathrm{e}^{tB}\mathrm{e}^{-\frac{1}{2}t^2[A,B]}\\ &\quad +\mathrm{e}^{tA}B\mathrm{e}^{tB}\mathrm{e}^{-\frac{1}{2}t^2[A,B]}\\ &\quad -\mathrm{e}^{tA}\mathrm{e}^{tB}t[A,B]\mathrm{e}^{-\frac{1}{2}t^2[A,B]}\\ &= (A+B)\mathrm{e}^{tA}\mathrm{e}^{tB}\mathrm{e}^{-\frac{1}{2}t^2[A,B]}.\end{aligned}$$

Besides, (3.50) is true for $t=0$. $\square$

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,

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

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

$$e^{i(\xi_i\hat{x}_i+\eta_i\hat{p}_i)}e^{i(\xi_i'\hat{x}_i+\eta_i'\hat{p}_i)} = e^{-\frac{i\hbar}{2}(\xi_i\eta_i'-\eta_i\xi_i')}e^{i\left((\xi_i+\xi_i')\hat{x}_i+(\eta_i+\eta_i')\hat{p}_i\right)} \tag{3.51}$$

They translate the position and momentum:

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

3.5 Weyl-Wigner quantization in terms of Weyl operators

Note that

$$e^{i(\xi_i\hat{x}_i+\eta_i\hat{p}_i)} = e^{\frac{i}{2}\xi_i\hat{x}_i}e^{i\eta_i\hat{p}_i}e^{\frac{i}{2}\xi_i\hat{x}_i}. \tag{3.52}$$

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

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

Therefore,

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

More generally, if f is a function on $\mathbb{R}$, then

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

Therefore,

$$\mathrm{Op}\big(f(\xi_i x_i+\eta_i p_i)\big) = f(\xi_i\hat{x}_i+\eta_i\hat{p}_i). \tag{3.53}$$

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

$$b(x,p) = (2\pi)^{-2d}\int\int\int\int e^{i(x_i-y_i)\xi_i+i(p_i-w_i)\eta_i}b(y,w)dydwd\xi d\eta. \tag{3.54}$$

This leads to

$$\mathrm{Op}(b) = (2\pi)^{-2d}\int\int\int\int e^{i(\hat{x}_i-y_i)\xi_i+i(\hat{p}_i-w_i)\eta_i}b(y,w)dydwd\xi d\eta, \tag{3.55}$$

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

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, $j = 1, \ldots, 2d$ 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 $[\omega_{ij}]$.

With every symplectic space we have a classical system. Indeed, we can define the Poisson bracket for functions b, c on $\mathbb{R}^{2d}$:

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

Proposition 3.11. *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*

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

We also have a quantum system with operators $\hat{\phi}^j$, $j = 1, \ldots, 2d$ satisfying

$$[\hat{\phi}^j, \hat{\phi}^k] = \mathrm{i}\omega^{jk}\mathbb{1}. \tag{3.56}$$

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.

Proposition 3.12. *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 (3.56). 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

$$\mathrm{Op}\big(\mathrm{e}^{\mathrm{i}\phi\cdot\zeta}\big) = \mathrm{e}^{\mathrm{i}\hat{\phi}\cdot\zeta}. \tag{3.57}$$

More generally, for any Borel function f

$$\mathrm{Op}\big(f(\phi\cdot\zeta)\big) = f(\hat{\phi}\cdot\zeta). \tag{3.58}$$

Proposition 3.13.

$$\mathrm{Op}\big(\phi\zeta_1 \cdots \phi\zeta_n\big) = \frac{1}{n!} \sum_{\sigma\in S_n} \hat{\phi}\zeta_{\sigma(i)} \cdots \hat{\phi}\zeta_{\sigma(n)}. \tag{3.59}$$

Proof. We have

$$\mathrm{Op}\big((\phi\zeta)^n\big) = (\hat{\phi}\zeta)^n. \tag{3.60}$$

This is a special case of (3.59), it is also seen directly from (3.57) by expanding into a power series. Let $t_1, \dots, t_n \in \mathbb{R}$. By (3.60),

$$\mathrm{Op}\big((t_1\phi\cdot\zeta_1 + \cdots + t_n\phi\cdot\zeta_n)^n\big) = (t_1\hat{\phi}\cdot\zeta_1 + \cdots + t_n\hat{\phi}\cdot\zeta_n)^n. \tag{3.61}$$

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,

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

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

$$\mathrm{Op}(x^2 + p^2 - \hbar) \geq 0, \tag{3.62}$$

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

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

Hence

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

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

3.9 Parity operator

Define the parity operator

$$I\Psi(x) = \Psi(-x). \tag{3.63}$$

More generally, set

$$I_{(y,w)} := \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(-y\hat{p} + w\hat{x})} I \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(y\hat{p} - w\hat{x})}. \tag{3.64}$$

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 3.14.

$$\mathrm{Op}\big((\pi\hbar)^d\delta_{(0,0)}\big) = I. \tag{3.65}$$

More generally,

$$\mathrm{Op}\big((\pi\hbar)^d\delta_{(y,w)}\big) = I_{(y,w)}. \tag{3.66}$$

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:

$$\int\delta\Big(\frac{x+y}{2}\Big)\Phi(y)\mathrm{d}y = \int\delta\Big(\frac{x}{2}+\tilde{y}\Big)\Phi(2\tilde{y})2^d\mathrm{d}\tilde{y} = 2^d\Phi(-x). \tag{3.67}$$

□

Theorem 3.15. *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*

$$B = (\pi\hbar)^{-d}\int I_{(x,p)}b(x,p)\mathrm{d}x\mathrm{d}p. \tag{3.68}$$

Hence,

$$\|B\| \leq (\pi\hbar)^{-d}\|b\|_1. \tag{3.69}$$

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

$$b(x,p) = 2^d\mathrm{Tr}I_{(x,p)}B. \tag{3.70}$$

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 3.16. *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 () involve only partial Fourier transforms and some constant coefficients. □

Proposition 3.17. *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

$$\mathrm{Tr}\mathrm{Op}^{x,p}(b)^*\mathrm{Op}^{x,p}(c) = \mathrm{Tr}\mathrm{Op}(b)^*\mathrm{Op}(c) = (2\pi\hbar)^{-d}\int \overline{b(x,p)}c(x,p)\mathrm{d}x\mathrm{d}p. \tag{3.71}$$

One often uses (3.71) when $B = \mathrm{Op}(b)$ is, say, bounded and describes an observable, and $C = \mathrm{Op}(c)$ is trace class, and describes a density matrix. Setting $b(x,p) = 1$ we formally obtain

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

With the x,p-quantization we can compute the so-called marginals involving the position and momentum:

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

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

With the Weyl-Wigner quantization we have much more possibilities: eg. for any α

$$\mathrm{Tr} f(\cos\alpha\hat{x} + \sin\alpha\hat{p})\mathrm{Op}(c) = (2\pi\hbar)^{-d}\int f(\cos\alpha x + \sin\alpha p)c(x,p)\mathrm{d}x\mathrm{d}p.$$

4 Coherent states

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.

$$(2\pi\hbar)^{-d}\int P_{(y,w)}\mathrm{d}y\mathrm{d}w = \mathbb{1}. \tag{4.72}$$

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

$$\mathrm{Op}^{\mathrm{ct}}(b) := (2\pi\hbar)^{-d}\int P_{(x,p)}b(x,p)\mathrm{d}x\mathrm{d}p. \tag{4.73}$$

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

We have

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

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

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

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

(5) Let $b \geq 0$. Then $\mathrm{Op}^{\mathrm{ct}}(b) \geq 0$.

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

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

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

(4) Let $\mathrm{Op}^{\mathrm{cv}}(b) \geq 0$. Then $b^{\mathrm{cv}} \geq 0$.

(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.

Let

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

Then

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

We have

$$\mathrm{Tr}\mathrm{Op}^{\mathrm{cv}}(a)\mathrm{Op}^{\mathrm{ct}}(b) = (2\pi\hbar)^{-d}\int \overline{a(x,p)}b(x,p)\mathrm{d}x\mathrm{d}p. \tag{4.74}$$

Indeed, let $A = \mathrm{Op}^{\mathrm{cv}}(a)$. Then the lhs of (4.74) is

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

which is the rhs of (4.74).

4.5 Gaussian coherent vectors

Consider the normalized gaussian vector scaled appropriately with the Planck constant

$$\Omega(x) = (\pi\hbar)^{-\frac{d}{4}}\mathrm{e}^{-\frac{1}{2\hbar}x^2}. \tag{4.75}$$

The corresponding coherent vectors are equal to

$$\Omega_{(y,w)}(x) = (\pi\hbar)^{-\frac{d}{4}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}w\cdot x - \frac{\mathrm{i}}{2\hbar}y\cdot w - \frac{1}{2\hbar}(x-y)^2}. \tag{4.76}$$

In the literature, when one speaks about coherent states, one has usually in mind (4.76). They are also called *Gaussian or Glauber's coherent states.*

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

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) anti-Wick symbol,
- (ii) Glauber-Sudarshan function,
- (iii) P-function;

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

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

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

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

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

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

$$x_i = \frac{\hbar^{1/2}}{2^{1/2}}(a_i + a_i^*), \quad p_i = \frac{\hbar^{1/2}}{\mathrm{i}2^{1/2}}(a_i - a_i^*). \tag{4.77}$$

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:

$$\frac{\hbar^d}{\mathrm{i}^d}\mathrm{d}a^*\mathrm{d}a = \mathrm{d}x\mathrm{d}p. \tag{4.78}$$

To justify the notation (4.78) 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

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

We have

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

$$\hat{x}_i = \frac{\hbar^{1/2}}{2^{1/2}}(\hat{a}_i + \hat{a}_i^*), \quad \hat{p}_i = \frac{\hbar^{1/2}}{\mathrm{i}2^{1/2}}(\hat{a}_i - \hat{a}_i^*). \tag{4.79}$$

Let b, b^* be classical variables obtained from y, w, as above. Note that

$$\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(-y\hat{p}+w\hat{x})} = \mathrm{e}^{(-b^*\hat{a}+b\hat{a}^*)}. \tag{4.80}$$

We have

$$\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(-y\hat{p}+w\hat{x})}\hat{x} = (\hat{x}+y)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(-y\hat{p}+w\hat{x})}, \qquad \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(-y\hat{p}+w\hat{x})}\hat{p} = (\hat{p}+w)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(-y\hat{p}+w\hat{x})}, \tag{4.81}$$

$$\mathrm{e}^{(-b^*\hat{a}+b\hat{a}^*)}\hat{a}^* = (\hat{a}^*+b^*)\mathrm{e}^{(-b^*\hat{a}+b\hat{a}^*)}, \qquad \mathrm{e}^{(-b^*\hat{a}+b\hat{a}^*)}\hat{a} = (\hat{a}+b)\mathrm{e}^{(-b^*\hat{a}+b\hat{a}^*)}. \tag{4.82}$$

Recall that in the real notation we had coherent vectors

$$\Omega_{y,w} := \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(-y\hat{p}+w\hat{x})}\Omega. \tag{4.83}$$

In the complex notation they become

$$\Omega_b := \mathrm{e}^{(-b^*\hat{a}+b\hat{a}^*)}\Omega. \tag{4.84}$$

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 (4.82),

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

Note that the identity (4.72) can be rewritten as

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

4.7 Quantization by an ordering prescription

Consider a polynomial function on the phase space:

$$w(x,p) = \sum_{\alpha,\beta} w_{\alpha,\beta}x^\alpha p^\beta. \tag{4.85}$$

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 (3.59).

We can also rewrite the polynomial (4.85) in terms of a_i, a_i^* by inserting (4.77). Thus we obtain

$$w(x,p)=\sum_{\gamma,\delta}\tilde{w}_{\gamma,\delta}a^{*\gamma}a^{\delta}=:\tilde{w}(a^*,a). \tag{4.86}$$

Then we can introduce the *Wick quantization*

$$\mathrm{Op}^{a^*,a}(w)=\sum_{\gamma,\delta}\tilde{w}_{\gamma,\delta}\hat{a}^{*\gamma}\hat{a}^{\delta} \tag{4.87}$$

and the *anti-Wick quantization*

$$\mathrm{Op}^{a,a^*}(w)=\sum_{\gamma,\delta}\tilde{w}_{\gamma,\delta}\hat{a}^{\delta}\hat{a}^{*\gamma}. \tag{4.88}$$

Theorem 4.2. (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

$$\big(\Omega|\mathrm{Op}^{a^*,a}(w)\Omega)=\tilde{w}(0,0). \tag{4.89}$$

4.8 Connection between the Wick and anti-Wick quantization

As described in equation (4.85), 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

$$\begin{aligned} w^{a^*,a}(x,p) &= \mathrm{e}^{\frac{\hbar}{2}(\partial_x^2+\partial_p^2)} w^{a,a^*}(x,p) \\ &= (2\pi\hbar)^{-d} \int\int \mathrm{e}^{-\frac{1}{2\hbar}\left((x-y)^2+(p-w)^2\right)} w^{a,a^*}(y,w)\mathrm{d}y\mathrm{d}w, \qquad (4.90) \\ \tilde{w}^{a^*,a}(a^*,a) &= \mathrm{e}^{\partial_{a^*}\partial_a} \tilde{w}^{a,a^*}(a^*,a) \\ &= (2\pi\mathrm{i})^{-d} \int\int \mathrm{e}^{-(a^*-b^*)(a-b)} \tilde{w}^{a,a^*}(b^*,b)\mathrm{d}b^*\mathrm{d}b.. \qquad (4.91) \end{aligned}$$

(4.90) was proven before. To see that (4.91) and (4.90) 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 (4.91) 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

Suppose that

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

Then

$$\tilde{w}(a^*,a) = \mathrm{e}^{\partial_{a_2}\partial_{a_1^*}} \tilde{w}_2(a_2^*, a_2)\tilde{w}_1(a_1^*, a_1)\Big|_{a = a_2 = a_1}. \qquad (4.92)$$

(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 (4.91). Using (2.22), one can rewrite (4.92) as an integral:

$$\tilde{w}(a^*, a) = \int\int \mathrm{e}^{-b^* b} \tilde{w}_2(a^*, a+b)\tilde{w}_1(a^* + b^*, a) \frac{\mathrm{d}b^* \mathrm{d}b}{(2\pi \mathrm{i})^d}. \tag{4.93}$$

Note that in (4.93) 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.

We also have a version of (4.92) for an arbitrary number of factors. Let

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

Then

$$\tilde{w}(a^*, a) = \exp\Big(\sum_{k>j} \partial_{a_k} \partial_{a_j^*}\Big) \tilde{w}_n(a_n^*, a_n) \cdots \tilde{w}_1(a_1^*, a_1)\Big|_{\ a = a_n = \cdots = a_1.} \tag{4.94}$$

Consequenly,

$$\begin{aligned} & \big(\Omega|\mathrm{Op}^{a^*,a}(w_n) \cdots \mathrm{Op}^{a^*,a}(w_1)\Omega\big) \\ = \ & \exp\Big(\sum_{k>j} \partial_{a_k} \partial_{a_j^*}\Big) \tilde{w}_n(a_n^*, a_n) \cdots \tilde{w}_1(a_1^*, a_1)\Big|_{\ 0 = a_n = \cdots = a_1.} \end{aligned}$$

We can rewrite (4.94) as an integral:

$$\begin{aligned} & \tilde{w}(a^*, a) \qquad\qquad (4.95) \\ = & \int \cdots \int \exp\Big(\sum_{j=1}^{n} (b_{j+1} - b_j) b_j^*\Big) \tilde{w}_n(a^* + b_n^*, a + b_n,) \cdots \tilde{w}_1(a^* + b_1^*, a + b_1) \prod_{j=1}^{n-1} \frac{\mathrm{d}b_{j+1} \mathrm{d}b_j^*}{(2\pi \mathrm{i})^d} \\ = & \int \cdots \int \exp\Big(\sum_{j=1}^{n} b_j(-b_j^* + b_{j-1}^*)\Big) \tilde{w}_n(a^* + b_n^*, a + b_n,) \cdots \tilde{w}_1(a^* + b_1^*, a + b_1) \prod_{j=1}^{n-1} \frac{\mathrm{d}b_{j+1} \mathrm{d}b_j^*}{(2\pi \mathrm{i})^d} \end{aligned}$$

where we set $b_1 = 0$, $b_n^* = 0$.

Indeed, introduce new variables

$$d_n := a_n - a_{n-1}, \quad d_{n-1} := a_{n-1} - a_{n-2}, \quad \ldots, \quad d_2 := a_2 - a.$$

Then

$$a_n = d_n + \cdots + d_2 + a, \quad a_{n-1} = d_{n-1} + \cdots + d_2 + a, \quad \ldots, \quad a_2 = d_2 + a.$$

Therefore,

$$\partial_{d_n} = \partial_{a_n}, \quad \partial_{d_{n-1}} = \partial_{a_n} + \partial_{a_{n-1}}, \ldots, \quad \partial_{d_2} = \partial_{a_n} + \cdots + \partial_{a_2}.$$

Therefore,

$$
\begin{aligned}
&\exp\Big(\sum_{k>j}\partial_{a_k}\partial_{a_j^*}\Big)\Psi(a^*,a_n,\dots,a_1^*,a) && (4.96)\\
&=\exp\Big(\sum_{j=1}^{n-1}\partial_{d_{j+1}}\partial_{a_j^*}\Big)\Psi(a^*,a_n,\dots,a_1^*,a)\\
&=\int\cdots\int\exp\Big(-\sum_{j=1}^{n-1}c_{j+1}b_j^*\Big)\prod_{j=1}^{n-1}\frac{\mathrm{d}c_{j+1}\mathrm{d}b_j^*}{(2\pi\mathrm{i})^d}\\
&\quad\times\Psi(a^*,a+c_2+\cdots+c_n,a^*+b_{n-1}^*,a+c_2+\cdots+c_{n-1},\dots,a^*+b_1^*,a)\\
&=\int\cdots\int\exp\Big(-\sum_{j=1}^{n-1}\big(b_{j+1}-b_j\big)b_j^*\Big)\prod_{j=1}^{n-1}\frac{\mathrm{d}b_{j+1}\mathrm{d}b_j^*}{(2\pi\mathrm{i})^d} && (4.97)\\
&\quad\times\Psi(a^*,a+b_n,a^*+b_{n-1}^*,a+b_{n-1},\dots,a^*+b_1^*,a).
\end{aligned}
$$

5 Pseudodifferential calculus with uniform symbol classes

5.1 Gaussian dynamics on uniform symbol classes

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

$$|\partial_x^\alpha b|\le C_\alpha.$$

Note that $S(\mathbb{R}^n)$ has the structure of a Frechet space.

Theorem 5.1. *Let ν be a quadratic form. Then $\mathrm{e}^{\frac{\mathrm{i}}{2}D\nu D}$ is bounded on $S(\mathbb{R}^n)$. Then, for ν in a bounded set of quadratic forms, there exist C and m such that*

$$\sup|\mathrm{e}^{\frac{\mathrm{i}}{2}D\nu D}b(x)|\le C\sup_{|\beta|\le m}|\partial_\beta b(x)|. \tag{5.98}$$

Consequently, $\mathrm{e}^{\frac{\mathrm{i}}{2}D\nu D}$ is bounded on $S(\mathbb{R}^n)$.

5.2 The boundedness of quantized uniform symbols

Let us set $\hbar=1$.

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

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

Theorem 5.2 (The Calderon-Vaillancourt Theorem)**.** *If $b\in S(\mathbb{R}^d\oplus\mathbb{R}^d)$, then $\mathrm{Op}^{x,p}(b)$ is bounded and*

$$\|\mathrm{Op}^{x,p}(b)\|\le C(n)\sum_{|\alpha|+|\beta|\le N(n)}\sup|\partial_x^\alpha\partial_p^\beta b(x,p)|.$$

There exists also a version of the Calderon-Vaillancourt Theorem with the Weyl quantization replacing the x,p-quantization.

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

Theorem 5.3. *The following conditions are equivalent:*

(1)
$$\mathrm{ad}_{\hat{x}}^{\alpha}\mathrm{ad}_{\hat{p}}^{\beta} B \in B(L^2(\mathbb{R}^d)), \quad \alpha, \beta.$$

(2) $B = \mathrm{Op}^{x,p}(b), \quad b \in S(\mathbb{R}^d \oplus \mathbb{R}^d)$,

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

The implication (1)⇒(2) is called the *Beals Criterion*. The Calderon-Vaillancourt Theorem implies (1)⇐(2). Let us denote by Ψ the set of operators described in Theorem 5.3.

Theorem 5.4. (1) *Ψ is an algebra.*

(2) *Let $B \in \Psi$ be boundedly invertible. Then $B^{-1} \in \Psi$.*

(3) *Let f be a function holomorphic on $\mathrm{sp}\, B$, where $B \in \Psi$. Then $f(B) \in \Psi$.*

(4) *Let f be a function smooth on $\mathrm{sp}\, B$, where $B = B^* \in \Psi$. Then $f(B) \in \Psi$.*

5.3 Semiclassical calculus

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

Theorem 5.5. *Let $a, b \in S(\mathbb{R}^d \oplus \mathbb{R}^d)$. Then there exist $c_0, \dots, c_n \in S$ and $\hbar \mapsto r_\hbar \in S(\mathbb{R}^d \oplus \mathbb{R}^d)$ such that*

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

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

Besides,

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

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

For a complex function b let $\mathrm{ran}(b)$ denote the closure of the image of b.

Theorem 5.6. *Let $b \in S$ and $0 \notin \mathrm{ran}(b)$. 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*

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

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

Besides,

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

As a corollary of the above theorem, for any neighborhood of $\mathrm{ran}(b)$ 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 5.7. *Let $b \in S$ 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 $\mathrm{sp}\big(\mathrm{Op}_\hbar(b)\big)$ and there exist $c_0, c_2, \dots, c_{2n} \in S$ and $\hbar \mapsto r_\hbar \in S$ such that*

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

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

Besides,

$$c_0 = f \circ b.$$

If b is real and smooth, then the same conclusion holds.

Theorem 5.8. *Let $c \in S(\mathbb{R}^d \oplus \mathbb{R}^d \oplus \mathbb{R}^d)$. 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 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,

$$b(x,p) = c(x,p,x) + \frac{\mathrm{i}\hbar}{2}\big(\partial_x c(x,p,y) - \partial_y c(x,p,y)\big)\Big|_{x=y} + O(\hbar^2). \tag{5.99}$$

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 (2.17). □

5.4 Inequalities

Theorem 5.9. (1) *Let $b \in S$ and $\mathrm{Op}(b) = \mathrm{Op}^{a^*,a}(b^{a^*,a})$. Then $b^{a^*,a} \in S$ and $b - b^{a^*,a} = O(\hbar)$ in S*

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

Proof. We use

$$b^{a^*,a} = \mathrm{e}^{\frac{\hbar}{4}(\partial_x^2+\partial_p^2)}b, \tag{5.100}$$

$$b = \mathrm{e}^{\frac{\hbar}{4}(\partial_x^2+\partial_p^2)}b^{a,a^*}, \tag{5.101}$$

and the obvious mapping properties of $\mathrm{e}^{\frac{\hbar}{4}(\partial_x^2+\partial_p^2)}$. □

Theorem 5.10 (Sharp Gaarding Inequality)**.** *Let $b \in S$ be positive. Then*

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

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

$$\mathrm{Op}^{a,a^*}(b_0) = \mathrm{Op}(b). \tag{5.102}$$

Then, by Thm 5.9 (1), we have $b_0 \in S$ and $b_0 - b = O(\hbar)$ in S. Besides,

$$\mathrm{Op}(b_0) = \mathrm{Op}^{a^*,a}(b). \tag{5.103}$$

Now

$$\mathrm{Op}(b) = \mathrm{Op}(b_0) + \mathrm{Op}(b - b_0) = \mathrm{Op}^{a^*,a}(b) + O(\hbar). \tag{5.104}$$

The first term on the right of (5.104) is positive, because it is the anti-Wick quantization of a positive symbol. □

Theorem 5.11 (Fefferman-Phong Inequality)**.** *Let $b \in S$ 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 $c_j \in S$. 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.

5.5 Semiclassical asymptotics of the dynamics

Theorem 5.12 (Egorov Theorem)**.** *Let h be the sum of a polynomial of second order and a $S(\mathbb{R}^d \oplus \mathbb{R}^d)$ 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 $S(\mathbb{R}^d \oplus \mathbb{R}^d)$.

(2) *Let* $b \in S(\mathbb{R}^d \oplus \mathbb{R}^d)$. *Then there exist* $b_{t,2j} \in S(\mathbb{R}^d \oplus \mathbb{R}^d)$, $j = 0, 1, \dots$, *such that for* $|t| \le t_0$

$$\mathrm{e}^{\frac{\mathrm{i}t}{\hbar}\mathrm{Op}(h)}\mathrm{Op}(b)\mathrm{e}^{-\frac{\mathrm{i}t}{\hbar}\mathrm{Op}(h)} - \sum_{j=0}^{n} \mathrm{Op}\big(\hbar^{2j} b_{t,2j}\big) = O(\hbar^{2n+2}). \tag{5.105}$$

Moreover,

$$b_{t,0}(x,p) = b\big(\gamma_t^{-1}(x,p)\big) \tag{5.106}$$

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

Proof. We have

$$\sum_{j=0}^{n} \hbar^{2j} \frac{\mathrm{d}}{\mathrm{d}t} \mathrm{e}^{-\frac{\mathrm{i}t}{\hbar}\mathrm{Op}(h)}\mathrm{Op}\big(b_{t,2j}\big)\mathrm{e}^{\frac{\mathrm{i}t}{\hbar}\mathrm{Op}(h)} \tag{5.107}$$

$$= \sum_{j=0}^{n} \hbar^{2j} \mathrm{e}^{\frac{-\mathrm{i}t}{\hbar}\mathrm{Op}(h)}\Big(-\frac{\mathrm{i}}{\hbar}\big[\mathrm{Op}(h), \mathrm{Op}\big(b_{t,2j}\big)\big] + \mathrm{Op}\big(\frac{\mathrm{d}}{\mathrm{d}t} b_{t,2j}\big)\Big)\mathrm{e}^{\frac{\mathrm{i}t}{\hbar}\mathrm{Op}(h)} \tag{5.108}$$

This gives us a sequence of equations for $b_{t,2j}$ of the form

$$\frac{\mathrm{d}}{\mathrm{d}t} b_{t,0} = \{b_{t,0}, h\}, \tag{5.109}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} b_{t,2} = \{b_{t,2}, h\} + r_{t,2}, \tag{5.110}$$

$$\dots\dots \tag{5.111}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} b_{t,2j} = \{b_{t,2j}, h\} + r_{t,2j}, \tag{5.112}$$

where $r_{t,2j}$ involve $b_{t,0}, \dots, b_{t,2j-2}$. The initial conditions are

$$b_{t,0} = b, \tag{5.113}$$

$$b_{t,2} = 0, \tag{5.114}$$

$$\dots\dots \tag{5.115}$$

$$b_{t,2j} = 0. \tag{5.116}$$

(5.109) is solved by (5.106). (5.112) is solved by

$$b_{t,2j}(x,p) = \int_0^t r_{t-s,2j}\big(\gamma_s^{-1}(x,p)\big)\mathrm{d}s. \tag{5.117}$$

The error term in (5.108) is $O(\hbar^{2n+2})$. Integrating (5.108) from 0 to t we obtain the estimate (5.105). □

5.6 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 5.13. *The following conditions are equivlent:*

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

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

(2) *There exists a neighborhood $\mathcal{U}$ of (x_0, p_0) such that for all $c \in C_\mathrm{c}^\infty(\mathcal{U})$*

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

The set of points in $\mathbb{R}^d \oplus \mathbb{R}^d$ that do not satisfy the conditions of Theorem 5.13 is called the frequency set of $\hbar \mapsto \psi_\hbar$ and denoted $FS(\psi_\hbar)$.

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

5.7 Properties of the frequency set

Theorem 5.14. *Let $a \in S$. Then*

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

Theorem 5.15. *Let $h \in S + \mathrm{Pol}^{\leq 2}$ be real. Let $t \mapsto \gamma_t$ be the Hamiltonian flow generated by h. Then*

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

Theorem 5.16. *Let*

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

Then

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

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

$$\left((2\pi\hbar)^{-\frac{d}{2}}\mathcal{F}_\hbar \mathrm{Op}_\hbar^{p,x}(b)\psi_\hbar\right)(p) \quad = \quad (2\pi\hbar)^{-\frac{d}{2}}\int \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}xp} b(p,x)a(x)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)}\mathrm{d}x. \tag{5.118}$$

Let

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

Let

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

be the transpose of T. Clearly,

$$-\mathrm{i}\hbar T \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(S(x) - xp)} = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(S(x) - xp)}. \tag{5.119}$$

Therefore, (5.118) equals

$$
\begin{aligned}
& (-\mathrm{i}\hbar)^n (2\pi\hbar)^{-\frac{d}{2}} \int b(p,x) a(x) T^n \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(S(x)-xp)} \mathrm{d}x && (5.120)\\
= \quad & (-\mathrm{i}\hbar)^n (2\pi\hbar)^{-\frac{d}{2}} \int \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(S(x)-xp)} T^{\#n} b(p,x) a(x) \mathrm{d}x = O(\hbar^{n-\frac{d}{2}}). && (5.121)
\end{aligned}
$$

□

5.8 Algebras with a filtration/gradation

Let S be an algebra.

We say that it is an algebra with filtration $\{S^m \ : \ m \in \mathbb{Z}_-\}$ iff S^m are linear subspaces of S such that $S = S^0$, $S^m \subset S^{m'}$, $m \leq m'$ and $S^m \cdot S^{m'} \subset S^{m+m'}$. We write $S^{-\infty} := \bigcap\limits_m S^m$. Clearly, $S^{-\infty}$ is an ideal and so are S^m.

We say that S is an algebra with a gradation if $S = \underset{m\in\mathbb{Z}_-}{\oplus} S^{(m)}$ such that $S^{(m)} \cdot S^{(m')} \subset S^{(m+m')}$. Clearly, a gradation induces a filtration by taking $S^m := \sum\limits_{m'\leq m} S^{(m')}$.

Instead of $\mathbb{Z}_+$ we can take any ordered group, eg. $\mathbb{Z}$ or $\mathbb{R}$, then the definition slightly changes: the full algebra is denoted S^∞ and satisfies $S^\infty = \sum\limits_m S^m$. $S^{-\infty}$ is an ideal in S^∞. S^m for $m \geq 0$ are ideals in the algebra S^0.

5.9 Algebra of semiclassical operators

We say that $\hbar \mapsto b_\hbar$ is a admissible semiclassical symbol if for any n there exist $b_0, \dots, b_n \in S$ and $\hbar \mapsto r_\hbar \in S$ such that for any n

$$
b = \sum_{j=0}^{n} \hbar^j b_j + \hbar^{n+1} r_\hbar
$$

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

Note that the sequence $b_0, b_1, \dots$ is uniquely defined (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 $b_0, b_1, \dots = 0$ outside Θ.

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

Clearly, Ψ_{sc} is an algebra with gradation given by $\Psi_{\mathrm{sc}}^{-m} := \hbar^m \Psi_{\mathrm{sc}}$. It is closed wrt operations described in Theorems. $\Psi_{\mathrm{sc}}(\Theta)$ are ideals in Ψ_{sc}.

5.10 Principal and subprincipal symbols

Recall that by $\mathrm{s}(A_\hbar) = a_\hbar(x,\xi)$ we denote the symbol of $A_\hbar$. We have $a_\hbar \simeq \sum_{m=0}^{\infty} \hbar^j a_{-j}$. We call a_0 the principal and a_{-1} the subprincipal symbol. Let us introduce the extended principal sumbol:

$$\mathrm{s}_{\mathrm{ep}}(A) := a_0 + \hbar a_{-1}.$$

If $A = \mathrm{Op}^{x,p}(b)$ and $b \simeq \sum_{k=0}^{\infty} \hbar^k b_{-k}$, then the principal symbol is b_0 and the subprincipal symbol is $b_{-1} + \frac{\mathrm{i}\hbar}{2}\partial_x\partial_\xi b_0$.

Theorem 5.17. *Let $A \in \Psi_{\mathrm{sc}}$ and $A' \in \Psi_{\mathrm{sc}}$. Then*

$$
\begin{aligned}
A_\hbar A'_\hbar \in \Psi_{\mathrm{sc}} \quad & \textit{and} && (5.122)\\
\mathrm{s}_{\mathrm{ep}}\left(\frac{1}{2}[A_\hbar, A'_\hbar]_+\right) \quad & = \quad \mathrm{s}_{\mathrm{ep}}(A_\hbar)\mathrm{s}_{\mathrm{ep}}(A'_\hbar) \ (\mathrm{mod}\ \ \hbar^2), && (5.123)\\
[A_\hbar, A'_\hbar] \in \hbar\Psi_{\mathrm{sc}} \quad & \textit{and} && (5.124)\\
\mathrm{s}_{\mathrm{ep}}\left(\hbar^{-1}[A_\hbar, A'_\hbar]\right) \quad & = \quad \{\mathrm{s}_{\mathrm{ep}}(A_\hbar), \mathrm{s}_{\mathrm{ep}}(A'_\hbar)\} \ (\mathrm{mod}\ \ \hbar^2). && (5.125)
\end{aligned}
$$

5.11 Algebra of formal semiclassical operators

We also have the space of formal semiclassical symbols, which are formal power series

$$b = \sum_{j=0}^{n} \hbar^j b_j$$

with coefficients, say, in S. We denote this space by $S_{\mathrm{sc}}^{\mathrm{f}}$ and their quantizations by $\Psi_{\mathrm{sc}}^{\mathrm{f}}$.

Theorem 5.18. *We have the isomorphism*

$$\Psi_{\mathrm{sc}}/\Psi_{\mathrm{sc}}^{-\infty} = \Psi_{\mathrm{sc}}^{\mathrm{f}}.$$

5.12 More about star product

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

$$
\begin{aligned}
b * c(x,p) \quad & = \quad b\Big(x - \frac{\hbar}{2}D_p, p + \frac{\hbar}{2}D_x\Big)c(x,p) && (5.126)\\
& = \quad b\Big(x - \frac{\hbar}{2}D_p, p + \frac{\hbar}{2}D_x\Big)c(x,p). && (5.127)
\end{aligned}
$$

Note that the operators $x - \frac{\hbar}{2}D_p$ and $p + \frac{\hbar}{2}D_x$ commute. Thus we can understand the rhs of(5.126) as a function of two commuting operators. Alternatively, we can understand it as the PDE notation for the x,p quantization. Alternatively, (5.127) gives us an interpretation in terms of the Weyl quantization.

To see this we start from

$$b * c(x,p) = \mathrm{e}^{\frac{\mathrm{i}}{2}\hbar(D_{p_1}D_{x_2} - D_{x_1}D_{p_2})} b(x_1,p_1)c(x_2,p_2)\Big|_{\substack{x := x_1 = x_2, \\ p := p_1 = p_2.}} . \qquad (5.128)$$

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 LHS of (5.128).

Note the following consequences:

$$\begin{aligned}
&f\big(\mathrm{Op}(h)\big)\mathrm{Op}(b)\\
=\ &\mathrm{Op}\left(f\left(h\Big(x-\frac{\hbar}{2}D_p,p+\frac{\hbar}{2}D_x\Big)\right)b\right),\\
&f\big(\mathrm{Op}(h)\big)\\
=\ &\mathrm{Op}\left(f\left(\frac{1}{2}h\Big(x-\frac{\hbar}{2}D_p,p+\frac{\hbar}{2}D_x\Big)+\frac{1}{2}h\Big(x+\frac{\hbar}{2}D_p,p-\frac{\hbar}{2}D_x\Big)\right)1\right),\\
&\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\mathrm{Op}(h)}\mathrm{Op}(b)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\mathrm{Op}(h)}\\
=\ &\mathrm{Op}\left(\exp\frac{\mathrm{i}}{\hbar}\left(h\Big(x-\frac{\hbar}{2}D_p,p+\frac{\hbar}{2}D_x\Big)-h\Big(x+\frac{\hbar}{2}D_p,p-\frac{\hbar}{2}D_x\Big)\right)b\right).
\end{aligned}$$

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

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

Then

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

6 Spectral asymptotics

6.1 Functional calculus and Weyl asymptotics

It follows from (3.46) that

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

Hence for polynomial functions

$$f\big(\mathrm{Op}(b)\big)=\mathrm{Op}(f\circ b)+O(\hbar^2). \tag{6.129}$$

One can expect (6.129) to be true for a larger class of nice functions. Consequently,

$$\begin{aligned}
\mathrm{Tr}f\big(\mathrm{Op}(b)\big)&=\mathrm{Tr}\Big(\mathrm{Op}(f\circ b)+O(\hbar^2)\Big)\\
&=(2\pi\hbar)^{-d}\int f\big(b(x,p)\big)\mathrm{d}x\mathrm{d}p+O(\hbar^{-d+2}).
\end{aligned} \tag{6.130}$$

In particular, we can try to use $f = 1\!\!1_{]-\infty,\mu]}$. It is too optimistic to expect

$$1\!\!1_{]-\infty,\mu]}(\mathrm{Op}(h)) = \mathrm{Op}\big(1\!\!1_{]-\infty,\mu]}(h)\big) + O(\hbar^2). \tag{6.131}$$

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 for some weaker error term instead of $O(\hbar^2)$.

6.2 Weyl asymptotics

For a bounded from below self-adjoint operator H set

$$\begin{aligned} N_\mu(H) &:= \#\{\text{eigenvalues of } H \text{ counted with multiplicity } \leq \mu\} && (6.132)\\ &= \mathrm{Tr} 1\!\!1_{]-\infty,\mu]}(H). && (6.133)\end{aligned}$$

If (6.131) were true, then we would have

$$N_\mu\big(\mathrm{Op}(h)\big) \quad = \quad (2\pi\hbar)^{-d} \int_{h(x,p)\leq\mu} \mathrm{d}x\mathrm{d}p + O(\hbar^{-d+2}). \tag{6.134}$$

Asymptotics of the form (6.134) are called the *Weyl asymptotics*. In practice the error term $O(\hbar^{-d+2})$ may be too optimistic and one gets something worse (but hopefully at least $o(\hbar^{-d})$).

We will show that if V is continuous potential with $V - \mu > 0$ outside a compact set then

$$N_\mu(-\hbar^2\Delta + V(x)) \simeq (2\pi\hbar)^{-d} c_d \int_{V(x)\leq\mu} |V(x) - \mu|_-^{\frac{d}{2}} \mathrm{d}x + o(\hbar^{-d}). \tag{6.135}$$

This is (6.134) for $H = p^2 + V(x)$ with a rather weak error estimate.

We will prove this without using the Weyl calculus. Here are the tools that we will use:

$$A \leq B \;\Rightarrow\; N_\mu(A) \geq N_\mu(B),$$

$$N_\mu(A \oplus B) = N_\mu(A) + N_\mu(B).$$

To simplify we will assume that $d = 1$.

Lemma 6.1. *Let $\Delta_{[0,L],D}$, resp. $\Delta_{[0,L],N}$ denote the Dirichlet, resp. Neumann Laplacian on $[0, L]$. For $\alpha \in \mathbb{R}$ let $[\alpha]$ denote the largest integer $\leq \alpha$, $\theta(\alpha)$ the Heavyside function and $|\mu|_+ := \mu\theta(\mu)$. Then*

$$\begin{aligned} N_\mu\big(-\hbar^2\Delta_{[0,L],D}\big) &= [L(\pi\hbar)^{-1}|\mu|_+^{1/2}],\\ N_\mu\big(-\hbar^2\Delta_{[0,L],N}\big) &= [L(\pi\hbar)^{-1}|\mu|_+^{1/2}] + \theta(\mu).\end{aligned}$$

Proof. The eigenfunctions and the spectrum of $\Delta_{[0,L],D}$, resp. $\Delta_{[0,L],N}$ are

$$\begin{aligned} &\sin\frac{\pi n x}{L}, \qquad \frac{\hbar^2\pi^2 n^2}{L^2}, \quad n = 1, 2, \dots;\\ &\cos\frac{\pi n x}{L}, \qquad \frac{\hbar^2\pi^2 n^2}{L^2}, \quad n = 0, 1, 2, \dots.\end{aligned}$$

Thus the last eigenvalue has the number $n = [L(\hbar\pi)^{-1}|\mu|_+^{1/2}]$. $\Box$

Divide $\mathbb{R}$ into intervals

$$I_{N,j} := \Big[(j-1/2)N^{-1}, (j+1/2)N^{-1}\Big].$$

Put at the borders of the intervals Neumann/Dirichlet boundary conditions. The Neumann conditions lower the expectation value and the Dirichlet conditions increase them. Set

$$\begin{aligned}\overline{V}_{N,j} &= \sup\{V(x) \ : \ x \in I_{N,j}\},\\ \underline{V}_{N,j} &= \inf\{V(x) \ : \ x \in I_{N,j}\}.\end{aligned}$$

We have

$$\begin{aligned}&\mathop{\oplus}_{j\in\mathbb{Z}}\Big(-\hbar^2\Delta_{I_{N,j},N} + \underline{V}_{N,j}\Big)\\ \leq\ -\hbar^2\Delta + V(x) \quad \leq \quad &\mathop{\oplus}_{j\in\mathbb{Z}}\Big(-\hbar^2\Delta_{I_{N,j},D} + \overline{V}_{N,j}\Big).\end{aligned}$$

Hence,

$$\begin{aligned}&\sum_{j\in\mathbb{Z}} N_\mu\Big(-\hbar^2\Delta_{I_{N,j},N} + \underline{V}_{N,j}\Big)\\ \geq\ N_\mu\Big(-\hbar^2\Delta + V(x)\Big) \quad \geq \quad &\sum_{j\in\mathbb{Z}} N_\mu\Big(-\hbar^2\Delta_{I_{N,j},D} + \overline{V}_{N,j}\Big).\end{aligned}$$

Therefore,

$$\begin{aligned}&\sum_{j\in\mathbb{Z}} N^{-1}(\hbar\pi)^{-1}|\underline{V}_{N,j} - \mu|_-^{1/2} + \sum_{j\in\mathbb{Z}}\theta\big(\mu - \underline{V}_{N,j}\big)\\ \geq\ N_\mu\Big(-\hbar^2\Delta + V(x)\Big) \quad \geq \quad &\sum_{j\in\mathbb{Z}} N^{-1}(\hbar\pi)^{-1}|\overline{V}_{N,j} - \mu|_-^{1/2}.\end{aligned}$$

Using the fact that $|V-\mu|_-$ has a compact support, we can estimate

$$\sum_{j\in\mathbb{Z}}\theta\big(\mu - \underline{V}_{N,j}\big) \quad \leq \quad NC.$$

By properties of Riemann sums we can find N_ϵ such that for $N \geq N_\epsilon$

$$\Big|\sum_{j\in\mathbb{Z}} N^{-1}|\underline{V}_{N,j} - \mu|_-^{1/2} - \int|V(x) - \mu|_-^{1/2}\mathrm{d}x\Big| \quad < \quad \epsilon/3, \tag{6.136}$$

$$\Big|\sum_{j\in\mathbb{Z}} N^{-1}|\overline{V}_{N,j} - \mu|_-^{1/2} - \int|V(x) - \mu|_-^{1/2}\mathrm{d}x\Big| \quad < \quad \epsilon/3. \tag{6.137}$$

Therefore,

$$\Big|N_\mu\Big(-\hbar^2\Delta + V(x)\Big) - \frac{1}{\hbar\pi}\int|V(x) - \mu|_-^{1/2}\mathrm{d}x\Big| \quad < \quad \frac{2\epsilon}{\hbar\pi 3} + \frac{CN_\epsilon}{\pi}. \tag{6.138}$$

Hence the right hand side of (6.138) is $o(\hbar^{-1})$. This proves (6.135)

If we assume that V is differentiable, then N_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 $O(\hbar^{-1/2})$.

6.3 Energy of many fermion systems

Consider fermions with the 1-particle space is spanned by an orthonormal basis $\Phi_1, \Phi_2, \dots$. The n-particle fermionic space 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 will be denoted by $\mathrm{d}\Gamma^n(H)$.

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

$$\Psi := \frac{1}{\sqrt{n!}} \Phi_1 \wedge \cdots \wedge \Phi_n. \tag{6.139}$$

The ground state energy is $E_1 + \cdots + E_n$.

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 the 1-particle density matrix of the ground state is given by $\mathbb{1}_{]-\infty,\mu]}(H)$, where we find μ from the relation

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

If B is a 1-particle observable, then its expectation value in an 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 $0 \leq \gamma_\Psi \leq \mathbb{1}$ and $\mathrm{Tr}\gamma_\Psi = n$. The reduced 1-particle density matrix of the Slater determinant (6.139) Ψ is the projection onto the space spanned by $\Phi_1, \dots, \Phi_n$.

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,

$$\gamma_\Psi(x, y) = \int \mathrm{d}x_2 \cdots \int \mathrm{d}x_n \overline{\Psi(x, x_2, \cdots, x_n)}\Psi(y, x_2, \cdots, x_n). \tag{6.140}$$

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

$$\int \rho_\Psi(x)\mathrm{d}x = n. \tag{6.141}$$

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

$$1\!\!1_{]-\infty,\mu]}\big(h(x,p)\big).$$

Hence, the reduced 1-particle density matrix of the ground state is $\gamma = 1\!\!1_{]-\infty,\mu]}(H)$. 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

$$\begin{aligned}
\rho(x) &\approx (2\pi\hbar)^{-d}\int\limits_{p^2+v(x)\leq\mu}\mathrm{d}p \\
&= (2\pi\hbar)^{-d}c_d|v(x)-\mu|_-^{\frac{d}{2}}.
\end{aligned}$$

Let us compute the kinetic energy

$$\begin{aligned}
\mathrm{Tr}\hat{p}^2 1\!\!1_{]-\infty,\mu]}(H) &\approx (2\pi\hbar)^{-d}\iint\limits_{p^2+v(x)<\mu} p^2\mathrm{d}x\mathrm{d}p \\
&= (2\pi\hbar)^{-d}\int\mathrm{d}x\int\limits_{|p|<|v(x)-\mu|_-^{\frac{1}{2}}} dc_d|p|^{d+1}\mathrm{d}|p| \\
&= (2\pi\hbar)^{-d}\int\mathrm{d}x\frac{dc_d}{d+2}|v(x)-\mu|_-^{\frac{d+2}{2}} \\
&\approx (2\pi\hbar)^{-d}\frac{d}{d+2}c_d^{-2/d}\int\rho^{\frac{d+2}{d}}(x)\mathrm{d}x.
\end{aligned}$$

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

$$E_{\mathrm{kin}}(\rho) := (2\pi\hbar)^{-d}\frac{d}{d+2}c_d^{-2/d}\int\rho^{\frac{d+2}{d}}(x)\mathrm{d}x. \tag{6.142}$$

Clearly, the potential energy of a state with density ρ in the potential V is given by

$$E_{\mathrm{pot}}(\rho) := \int V(x)\rho(x)\mathrm{d}x. \tag{6.143}$$

Suppose in addition that the fermions interact with the potential W. That is, we consider the Hamiltonian

$$\sum_{i=1}^{N}\left(p_i^2 + V(x_i)\right) + \sum_{1\leq i<j\leq N} W(x_i - x_j) \tag{6.144}$$

on the N-particle antisymmetric space $\wedge^N L^2(\mathbb{R}^d)$.

Then we can expect by classical arguments that for a state Ψ

$$\Big(\Psi|\sum_{1\leq i<j\leq N} W(x_i - x_j)\Psi\Big) \simeq \int\int W(x-y)\rho_\Psi(x)\rho_\Psi(y)\mathrm{d}x\mathrm{d}y.$$

This suggests to introduce the interaction functiona

$$E_{\mathrm{int}}(\rho) := \int\int W(x-y)\rho(x)\rho(y)\mathrm{d}x\mathrm{d}y. \tag{6.145}$$

The Thomas-Fermi functional is given by the sum of (6.142), (6.143) and ((6.145):

$$\begin{aligned} E_{\mathrm{TF}}(\rho) &:= E_{\mathrm{kin}}(\rho) + E_{\mathrm{pot}}(\rho) + E_{\mathrm{int}}(\rho) && (6.146)\\ &= (2\pi\hbar)^{-d}\frac{d}{d+2}c_d^{-2/d}\int \rho^{\frac{d+2}{d}}(x)\mathrm{d}x \\ &\quad + \int V(x)\rho(x)\mathrm{d}x + \int\int W(x-y)\rho(x)\rho(y)\mathrm{d}x\mathrm{d}y. && (6.147)\end{aligned}$$

We expect that

$$\inf\Big\{E_{\mathrm{TF}}(\rho) \mid \rho\geq 0, \quad \int\rho(x)\mathrm{d}x = n\Big\} \tag{6.148}$$

approximates the ground state energy of (6.144).

7 Standard pseudodifferential calculus on $\mathbb{R}^d$

7.1 Classes of symbols

We will often write $\mathcal{X} = \mathbb{R}^d$.

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

$$a(x,\xi) = \sum_{|\beta|\leq m} a_\beta(x)\xi^\beta, \tag{7.149}$$

where

$$|\partial_x^\alpha a_\beta| \leq c_{\alpha,\beta}. \tag{7.150}$$

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

$$|\partial_x^\alpha \partial_\xi^\beta a(x,\xi)| \leq c_{\alpha,\beta} \langle \xi \rangle^{m-|\beta|}. \tag{7.151}$$

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 of degree $m-k$ such that

$$\begin{array}{rcl} |\partial_x^\alpha \partial_\xi^\beta a_{m-k}(x,\xi)| & \leq & c_{\alpha,\beta} |\xi|^{m-k-|\beta|}, \ |\xi| > 1, \\ \left| \partial_x^\alpha \partial_\xi^\beta \Big(a(x,\xi) - \sum\limits_{k=0}^{n} a_{m-k}(x,\xi) \Big) \right| & \leq & c_{\alpha,\beta,n} |\xi|^{m-k-n-1}. \ |\xi| > 1. \end{array}$$

We then write $a \simeq \sum_{k=0}^\infty a_{m-k}$, where a_{m-k} are uniquely determined.

We introduce also

$$S^{-\infty} := \mathop{\cap}_m S^m = \mathop{\cap}_m S^m_{\mathrm{ph}},$$

$$S^\infty := \mathop{\cup}_m S^m, \quad S^\infty_{\mathrm{ph}} := \mathop{\cup}_m S^m_{\mathrm{ph}}, \quad S^\infty_{\mathrm{pol}} := \mathop{\cup}_m S^m_{\mathrm{pol}}.$$

Clearly, for $m \in \mathbb{N}$, $S^m_{\mathrm{pol}} \subset S^m_{\mathrm{ph}}$. For any $m \in \mathbb{R}$, $S^m_{\mathrm{ph}} \subset S^m$.

7.2 Classes of pseudodifferential operators

Let A be an operator from $\mathcal{S}(\mathbb{R}^d)$ to $\mathcal{S}'(\mathbb{R}^d)$. We will say that $A \in \Psi^m, \Psi^m_{\mathrm{ph}}, \Psi^m_{\mathrm{pol}}$ iff

$$A = \mathrm{Op}(a)$$

for $a \in S^m, S^m_{\mathrm{ph}}, S^m_{\mathrm{pol}}$. (Note, that instead of the Weyl quantization we could use the Kohn-Nirenberg quantization as well, obtaining the same class of operators).

For $k \in \mathbb{R}$, the kth Sobolev space is defined as

$$L^{2,k}(\mathbb{R}^d) := (1-\Delta)^{-k/2} L^2(\mathbb{R}^d).$$

We also write

$$L^{2,\infty} := \mathop{\cap}_k L^{2,k}(\mathbb{R}^d), \quad L^{2,-\infty} := \mathop{\cup}_k L^{2,k}(\mathbb{R}^d).$$

The Calderon-Vaillancourt Theorem implies immediately the following theorem:

Theorem 7.1. *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 $L^{2,-\infty}$. $A \in \Psi^{-\infty}$ maps $L^{2,-\infty}$ to $L^{2,\infty}$.

7.3 Extended principal symbol

We will write $s_{\rm ep}(A)$ for $s(A)\,({\rm mod} S^{(m-2)})$ and call it the *extended principal symbol* of a.

If $A = \mathrm{Op}(a)$ and $a \simeq \sum_{k=0}^{\infty} a_{m-k}$, then a_m is called the *principal symbol* and a_{m-1} the *subprincipal symbol* of a. We can then identify $a_{\rm ep}$ with $a_m + a_{m-1}$.

If $A = \mathrm{Op}^{x,p}(b)$ and $b \simeq \sum_{k=0}^{\infty} b_{m-k}$, then the principal symbol is b_m and the subprincipal symbol is $b_{m-1} + \frac{\mathrm{i}}{2}\partial_x\partial_\xi b_m$.

Theorem 7.2. *Let $A \in \Psi^m$ and $A' \in \Psi^{m'}$. Then*

$$AA' \in \Psi^{m+m'} \quad \textit{and} \tag{7.152}$$

$$\mathrm{s}_{\rm ep}\Big(\frac{1}{2}[A, A']_+\Big) = \mathrm{s}_{\rm ep}(A)\mathrm{s}_{\rm ep}(A')(\mathrm{mod} \quad S^{m+m'-2}) \tag{7.153}$$

$$[A, A'] \in \Psi^{m+m'-1} \quad \textit{and} \tag{7.154}$$

$$\mathrm{s}_{\rm ep}\left([A, A']\right) = \{\mathrm{s}_{\rm ep}(A), \mathrm{s}_{\rm ep}(A')\}(\mathrm{mod} \quad S^{m+m'-3}). \tag{7.155}$$

7.4 Diffeomorphism invariance

Let $F : \mathbb{R}^d \to \mathbb{R}^d$ be a diffeomorphism that moves only a bounded part of $\mathbb{R}^d$. We can define its prolongation to the cotangent bundle $\mathrm{T}^\#\mathbb{R}^d$, denoted $\mathrm{T}^\# F$ and the corresponding acttion on $\mathcal{S}(\mathbb{R}^d)$, denoted $F_\#$.

Theorem 7.3. *The spaces $S^m_{\rm pol}(\mathrm{T}^\#\mathbb{R}^d)$, $S^m_{\rm ph}(\mathrm{T}^\#\mathbb{R}^d)$, $S^m(\mathrm{T}^\#\mathbb{R}^d)$ are invariant wrt $\mathrm{T}^\# F$.*

The operators $F_\#$ are bounded invertible on spaces $L^{2,m}$.

The algebras $\Psi_{\rm pol}(\mathbb{R}^d)$, $\Psi_{\rm ph}(\mathbb{R}^d)$ and $\Psi(\mathbb{R}^d)$ are invariant wrt $F_\#$.

7.5 Ellipticity

Let $m \geq 0$. We say that $b \in S^m(\mathbb{R}^d)$ is elliptic if b is real and for some r, $c_0 > 0$

$$b(x, \xi) \geq c_0|\xi|^m, \quad |\xi| > r.$$

Theorem 7.4. *Let $p \in \mathbb{R}$. Let $b \in S^m(\mathbb{R}^d)$ be elliptic and $z - b(x, \xi)$ invertible.*

(1) *$(-z + b(x, \xi))^p$ is well defined and belongs to $S^{mp}(T^\#\mathbb{R}^d)$.*

(2) *$\mathrm{Op}(b)$ is essentially selfadjoint and there exists c such that for $z \in \mathbb{C}\backslash[c, \infty[$*

$$z \notin \mathrm{sp}\,\mathrm{Op}(b), \quad (z - \mathrm{Op}(b))^m \in \Psi^{mp}(\mathbb{R}^d).$$

7.6 Asymptotics of the dynamics

Theorem 7.5 (Egorov Theorem)**.** *Let $h \in S^1_{\rm ph}$ be real and elliptic.*

(1) *Let $x(t), \xi(t)$ solve the Hamilton equations with the Hamiltonian h 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 $b \in S^m_{\mathrm{ph}}$. Then there exist $b_{t,m-2j} \in S^{m-2j}$, $j = 0, 1, \dots,$ and $R_{t,m-2n-2}$ uniformly in $B(L^{2,k}, L^{2,k-2n-2}))$. such that for $|t| \le t_0$*

$$\mathrm{e}^{\mathrm{i}t\mathrm{Op}(h)}\mathrm{Op}(b)\mathrm{e}^{-\mathrm{i}t\mathrm{Op}(h)} = \sum_{j=0}^{n} \mathrm{Op}\big(b_{t,m-2j}\big) + R_{t,m-2n-2}. \tag{7.156}$$

Moreover,

$$b_{t,m}(x,\xi) = b\big(\gamma_t(x,\xi)\big) \tag{7.157}$$

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

We will say that $a \in S^m$ has a homogeneous principal symbol if there exists $a_m \in S^m$ homogeneous of degree m in ξ and $m_1 < m$ such that $a - a_m \in S^{m_1}$ for $|\xi| > 1$.

7.7 Singular support

Let $f \in \mathcal{D}'_{\mathrm{c}}(\mathbb{R}^d)$. It belongs to $C^\infty_{\mathrm{c}}(\mathbb{R}^d)$ iff

$$|\hat{f}(\xi)| \le c_n \langle\xi\rangle^{-n}, \quad n \in \mathbb{N}. \tag{7.158}$$

Let $f \in \mathcal{D}'(\mathbb{R}^d)$ and $x_0 \in \mathbb{R}^d$. Clearly, f is C^∞ in a neighborhood of x_0 iff

$$\exists_{\chi \in C^\infty_{\mathrm{c}}(\mathbb{R}^d)}\ \chi(x_0) \neq 0, \quad |\widehat{\chi f}(\xi)| \le c_n \langle\xi\rangle^{-n}, \quad n \in \mathbb{N}.. \tag{7.159}$$

This is equivalent to saying that

$$\exists_{\mathcal{U} \text{ a neighborhood of } x_0} \forall_{\chi \in C^\infty_{\mathrm{c}}(\mathcal{U})}\ |\widehat{\chi f}(\xi)| \le c_n \langle\xi\rangle^{-n}, \quad n \in \mathbb{N}. \tag{7.160}$$

The complement of points where f is C^∞ is called the singular support of f.

7.8 Preservation of the singular support

Theorem 7.6. *Let $f \in L^{2,-\infty}$ and $A \in \Psi^\infty$. Then Af is C^∞ away from* $\mathrm{supp} f$.

Proof. Let $f \in L^{2,k}$ and $A \in \Psi^m$. Let $\chi, \chi_1, \in C^\infty$ have all bounded derivatives. Let $\chi = 1$ on $\mathrm{supp} f$ and $\chi_1 = 0$ on $\mathrm{supp}\chi$. Let

$$\chi_1(x)Af = \chi_1(x)A\chi(x)^n f = \chi_1(x)\mathrm{ad}^n_\chi(A) \tag{7.161}$$

But $\mathrm{ad}^n_\chi(A) \in \Psi^{m-n}$. Thus (7.161) belongs to $L^{2,k-m+n}$. □

7.9 Wave front

We equip $\mathcal{X} \oplus (\mathcal{X}^\# \backslash \{0\})$ with an action of $\mathbb{R}_+$ as follows:

$$(x,\xi) \mapsto (x, t\xi). \tag{7.162}$$

We say that a subset of $\mathcal{X} \oplus (\mathcal{X}^\# \backslash \{0\})$ is conical iff it is invariant with respect to this action. Conical subsets can be identified with $\mathcal{X} \oplus (\mathcal{X}^\# \backslash \{0\})/\mathbb{R}_+$.

Let $(x_0, \xi_0 \in \mathcal{X} \oplus \mathcal{X}^\# \backslash \{0\}$. We say that f is smooth in a conical neighborhood of (x_0, ξ_0) iff there exists $\chi \in C_\mathrm{c}^\infty(\mathcal{X})$ and a conical neighborhood $\mathcal{U}$ of $\xi \in \mathcal{U}$ such that

$$|\hat{\chi f}(\xi)| \leq c_n \langle \xi \rangle^{-n}, \quad n \in \mathbb{N}. \tag{7.163}$$

The complement in $\mathcal{X} \oplus (\mathcal{X}^\# \backslash \{0\})/\mathbb{R}_+$. of points where f is smooth is called the wave front set of f and denoted $WF(f)$.

We will write $S_\mathrm{ph}^m(\Theta)$ for the set of $a \in S_\mathrm{ph}^m$ with $a \simeq \sum\limits_{k=0}^{\infty} a_{m-k}$ such that $\mathrm{supp} a_{m-k} \subset \Theta$.

The following theorem gives two possible alternative definitions of the wave front set.

Theorem 7.7. *Let $u \in L^{-\infty}$. The following conditions are equivalent:*

(1) *There exists $b \in S_\mathrm{ph}^m$ such that $b_m(x_0, \xi_0) \neq 0$ and*

$$\mathrm{Op}(b)u \in L^{2,\infty}.$$

(2) *There exists a conical neighborhood $\mathcal{U}$ of (x_0, ξ_0) such that for all $c \in S_\mathrm{ph}^m(\mathcal{U})$*

$$\mathrm{Op}(c)u \in L^{2,\infty}.$$

7.10 Properties of the wave front set

Example 7.8. *Let $\mathcal{Y}$ be a k-dimensional submanifold 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 $\mathcal{Y}$:

$$WF(F) \subset \mathcal{N}^\# \mathcal{Y} := \{(x, \xi) \ : \ x \in \mathcal{Y}, \langle \xi | v \rangle = 0, \ v \in \mathrm{T}\mathcal{Y}\}.$$

Example 7.9. *For $\mathcal{X} = \mathbb{R}$,*

$$WF((x + \mathrm{i}0)^{-1}) = \{(0, \xi) \ : \ \xi > 0\}.$$

Example 7.10. *Let H be a homogeneous function of degree 1 smooth away from the origin and $v \in C^\infty$,*

$$|\partial_\xi^\beta v(\xi)| \leq c_\beta \langle \xi \rangle^{m - |\beta|}$$

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 7.11. *Let $u \in L^{2,-\infty}$ and $a \simeq \sum\limits_{k=0}^{\infty} a_{m-k} \in S_{\mathrm{ph}}^{m}$. Then*

$$WF(\mathrm{Op}(a)u) = WF(u) \cap \bigcap_{k=0}^{\infty} \mathrm{supp} a_{m-k}.$$

Theorem 7.12 (Theorem about propagation of singularities)**.** *Let $h \in S_{\mathrm{ph}}^{1}$ be real and elliptic. Then*

$$WF(\mathrm{e}^{\mathrm{i}t\mathrm{Op}(h)}u) = \gamma_t\left(WF(u)\right).$$

8 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.

8.1 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

$$U(t_+,t_-) = \sum_{n=0}^{\infty} \int_{t_+>t_n>\cdots>t_1>t_-}\!\!\cdots\int B(t_n)\cdots B(t_1)\mathrm{d}t_n\cdots\mathrm{d}t_1.$$

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

$$U(t) := \mathrm{Texp}\left(\int_0^t B(s)\mathrm{d}s\right). \tag{8.164}$$

Note that the whole evolution can be retrieved from (8.164) by

$$U(t_+,t_-)=U(t_+)U(t_-)^{-1}.$$

We have

$$U(t)=\lim_{n\to\infty}\prod_{j=1}^{n}\mathrm{e}^{\frac{t}{n}B(\frac{jt}{n})}. \tag{8.165}$$

(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

$$U(t)=\lim_{n\to\infty}\prod_{j=1}^{n}F\Big(\frac{jt}{n},\frac{t}{n}\Big). \tag{8.166}$$

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 8.1. (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*

$$U(t) = \lim_{n\to\infty} \prod_{j=1}^{n} \mathrm{e}^{\frac{t}{n}A(\frac{jt}{n})}\mathrm{e}^{\frac{t}{n}C(\frac{jt}{n})}. \tag{8.167}$$

In particular, we obtain the Lie-Trotter formula

$$\mathrm{e}^{t(A+C)} = \lim_{n\to\infty} \left(\mathrm{e}^{\frac{t}{n}A}\mathrm{e}^{\frac{t}{n}C}\right)^n.$$

8.2 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,

$$\begin{aligned}
S(t_+,t_-) &= \mathrm{Texp}\Big(-\mathrm{i}\int_{t_-}^{t_+} H_{\mathrm{Int}}(t)\mathrm{d}t\Big),\\
S &= \mathrm{Texp}\Big(-\mathrm{i}\int_{-\infty}^{\infty} H_{\mathrm{Int}}(t)\mathrm{d}t\Big)
\end{aligned}$$

8.3 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:

$$E - E_0 \quad = \quad \lim_{t\to\pm\infty} (2\mathrm{i})^{-1} \frac{\mathrm{d}}{\mathrm{d}t} \log(\Phi_0 | \mathrm{e}^{-\mathrm{i}tH_0} \mathrm{e}^{\mathrm{i}2tH} \mathrm{e}^{-\mathrm{i}tH_0} \Phi_0). \tag{8.168}$$

To see why we can expect (8.168) 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 (8.168).

8.4 Path integrals for Schrödinger operators

We consider

$$\begin{aligned} h(t,x,p) \quad &:= \quad \frac{1}{2}p^2 + V(t,x), \\ H(t) := \mathrm{Op}(h(t)) \quad &= \quad -\frac{1}{2}\Delta + V(t,x), \\ U(t) \quad &:= \quad \mathrm{Texp}\left(-\mathrm{i}\int_0^t H(s)\mathrm{d}s\right). \end{aligned} \tag{8.169}$$

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

$$\begin{aligned} U(t,x,y) \quad &= \quad \lim_{n\to\infty} \int \mathrm{d}x_{n-1} \cdots \int \mathrm{d}x_1 \prod_{j=1}^{n} \Big(\frac{2\pi \mathrm{i}t}{n}\Big)^{-\frac{d}{2}} \mathrm{e}^{\frac{\mathrm{i}n(x_{j-1}-x_j)^2}{2t} - \mathrm{i}\frac{t}{n}V(\frac{jt}{n},x_j)} \Big|_{\substack{y = x_0,\\ x = x_n.}} \\ &= \quad \lim_{n\to\infty} \Big(\frac{2\pi \mathrm{i}t}{n}\Big)^{-\frac{dn}{2}} \int \mathrm{d}x_{n-1} \cdots \int \mathrm{d}x_1 \\ &\quad \times \exp\left(\frac{\mathrm{i}t}{n}\sum_{j=1}^{n}\Big(\frac{n^2(x_{j-1}-x_j)^2}{2t^2} - V\Big(\frac{jt}{n},x_j\Big)\Big)\right)\Big|_{\substack{y = x_0,\\ x = x_n.}} . \end{aligned}$$

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

$$\mathcal{D}_{x,y}\big(x(\cdot)\big) := \lim_{n\to\infty}\Big(\frac{2\pi\mathrm{i}t}{n}\Big)^{-\frac{dn}{2}}\mathrm{d}x\Big(\frac{(n-1)t}{n}\Big)\cdots\mathrm{d}x\Big(\frac{t}{n}\Big) \tag{8.170}$$

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 $x(t)=x$.

8.5 Example–the harmonic oscillator

Let

$$H = \frac{1}{2}p^2 + \frac{1}{2}x^2.$$

It is well-known that for $t\in]0,\pi[$,

$$\mathrm{e}^{-\mathrm{i}tH}(x,y) = (2\pi\mathrm{i}\sin t)^{-\frac{1}{2}}\exp\Big(\frac{-(x^2+y^2)\cos t + 2xy}{2\mathrm{i}\sin t}\Big). \tag{8.171}$$

(8.171) is called the Mehler formula.

We will derive (8.171) from the path integral formalism. We will use the explicit formula for the free dynamics with $H_0 = \frac{1}{2}p^2$:

$$\mathrm{e}^{-\mathrm{i}tH_0}(x,y) = (2\pi\mathrm{i}t)^{-\frac{1}{2}}\exp\Big(\frac{-(x-y)^2}{2\mathrm{i}t}\Big). \tag{8.172}$$

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:

$$x_{\mathrm{cl}}(s) = \frac{\cos(s-\frac{t}{2})}{\cos\frac{t}{2}}(x+y) + \frac{\sin(s-\frac{t}{2})}{\sin\frac{t}{2}}(x-y), \tag{8.173}$$

$$x_{0,\mathrm{cl}}(s) = x\frac{s}{t} + y\frac{(t-s)}{t}. \tag{8.174}$$

Now we set $x(s) = x_{\mathrm{cl}}(s) + z(s)$ and obtain

$$\int_0^t L\big(x(s),\dot{x}(s)\big)\mathrm{d}s = \int_0^t \frac{1}{2}\big(\dot{x}^2(s) - x^2(s)\big)\mathrm{d}s \tag{8.175}$$

$$= \int_0^t L\big(x_{\mathrm{cl}}(s),\dot{x}_{\mathrm{cl}}(s)\big)\mathrm{d}s + \int_0^t L\big(z(s),\dot{z}(s)\big)\mathrm{d}s \tag{8.176}$$

$$= \frac{(x^2+y^2)\cos t - 2xy}{2\sin t} + \int_0^t \frac{1}{2}\big(\dot{z}^2(s) - z^2(s)\big)\mathrm{d}s. \tag{8.177}$$

Similarly, setting $x(s)=x_{0,\mathrm{cl}}(s)+z(s)$ we obtain

$$\int_0^t L_0\big(x(s),\dot{x}(s)\big)\mathrm{d}s = \int_0^t \frac{1}{2}\dot{x}^2(s)\mathrm{d}s \tag{8.178}$$

$$\tag{8.179}$$

$$= \frac{(x-y)^2}{2t} + \int_0^t \frac{1}{2}\dot{z}^2(s)\mathrm{d}s. \tag{8.180}$$

Therefore,

$$\frac{\mathrm{e}^{-\mathrm{i}tH}(x,y)}{\mathrm{e}^{-\mathrm{i}tH_0}(x,y)} = \frac{\int \exp\Big(\mathrm{i}\int_0^t L\big(x(s),\dot{x}(s)\big)\mathrm{d}s\Big)\mathcal{D}_{x,y}\big(x(\cdot)\big)}{\int \exp\Big(\mathrm{i}\int_0^t L_0\big(x(s),\dot{x}(s)\big)\mathrm{d}s\Big)\mathcal{D}_{x,y}\big(x(\cdot)\big)} \tag{8.181}$$

$$= \frac{\int \exp\Big(\mathrm{i}\frac{(x^2+y^2)\cos t-2xy}{2\sin t} + \mathrm{i}\int_0^t \frac{1}{2}\big(\dot{z}^2(s)-z^2(s)\big)\mathrm{d}s\Big)\mathcal{D}_{0,0}\big(z(\cdot)\big)}{\int \exp\Big(\mathrm{i}\frac{(x-y)^2}{2t} + \mathrm{i}\int_0^t \frac{1}{2}\dot{z}^2(s)\mathrm{d}s\Big)\mathcal{D}_{0,0}\big(z(\cdot)\big)} \tag{8.182}$$

$$= \det\left(\frac{\frac{\mathrm{i}}{2}(-\Delta)}{\frac{\mathrm{i}}{2}(-\Delta-1)}\right)^{\frac{1}{2}} \frac{\exp\Big(\mathrm{i}\frac{(x^2+y^2)\cos t-2xy}{2\sin t}\Big)}{\exp\Big(\mathrm{i}\frac{(x-y)^2}{2t}\Big)} \tag{8.183}$$

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,

$$\det\left(\frac{\frac{\mathrm{i}}{2}(-\Delta)}{\frac{\mathrm{i}}{2}(-\Delta-1)}\right) = \frac{1}{\det\Big(\mathbb{1}+\Delta^{-1}\Big)} \tag{8.184}$$

$$= \prod_{k=1}^{\infty}\Big(1-\frac{t^2}{\pi^2k^2}\Big) = \frac{t}{\sin t}. \tag{8.185}$$

Now (8.172) implies (8.171).

8.6 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":

$$U^{\mathrm{E}}(t) := \mathrm{Texp}\Big(-\int_0^t H(s)\mathrm{d}s\Big) \quad = \quad \lim_{n\to\infty}\prod_{j=1}^{n} \mathrm{e}^{-\frac{t}{n}V(\frac{jt}{n},x)}\mathrm{e}^{\frac{t}{n}\Delta}.$$

Using
$$\mathrm{e}^{\frac{1}{2}t\Delta}(x,y)=(2\pi t)^{-d/2}\mathrm{e}^{-\frac{1}{2t}(x-y)^2}.$$
we obtain
$$\begin{aligned}U^{\mathrm{E}}(t,x,y) &= \lim_{n\to\infty}\Big(\frac{2\pi t}{n}\Big)^{-\frac{dn}{2}}\int\mathrm{d}x_{n-1}\cdots\int\mathrm{d}x_1\\ &\quad\times\exp\left(\frac{t}{n}\sum_{j=1}^{n}\Big(\frac{-n^2(x_j-x_{j-1})^2}{2t^2}-V\Big(\frac{jt}{n},x_j\Big)\Big)\right)\Big|_{\substack{y=x_0,\\ x=x_n.}}\end{aligned}.$$
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
$$L^{\mathrm{E}}(s,x,\dot{x}):=\frac{1}{2}\dot{x}^2+V(s,x)$$
is the "Euclidean Lagrangian" and
$$\mathcal{D}^{\mathrm{E}}_{x,y}(x(\cdot)\big):=\lim_{n\to\infty}\Big(\frac{2\pi t}{n}\Big)^{-\frac{dn}{2}}\mathrm{d}x\Big(\frac{(n-1)t}{n}\Big)\cdots\mathrm{d}x\Big(\frac{t}{n}\Big)$$
is similar to (8.170).

8.7 Wiener measure

$$\mathrm{d}W_y\big(x(\cdot)\big)=\exp\Big(-\int_0^t\frac{1}{2}\dot{x}^2(s)\Big)\mathrm{d}s\mathcal{D}^{\mathrm{E}}_{x(t),y}\big(x(\cdot)\big)\mathrm{d}x(t)$$
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
$$\begin{aligned}&\int\mathrm{d}W_y\big(x(\cdot)\big)F\big(x(\cdot)\big) \qquad (8.186)\\ &=\int F_{t_n,\dots,t_1}(x_n,\dots,x_1)\frac{\mathrm{e}^{-\frac{(x_n-x_{n-1})^2}{2(t_n-t_{n-1})}}}{\big(2\pi(t_n-t_{n-1})\big)^{\frac{d}{2}}}\mathrm{d}x_n\cdots\frac{\mathrm{e}^{-\frac{(x_2-x_1)^2}{2(t_2-t_1)}}}{\big(2\pi(t_2-t_1)\big)^{\frac{d}{2}}}\mathrm{d}x_2\frac{\mathrm{e}^{-\frac{(x_1-y)^2}{2t_1}}}{\big(2\pi t_1\big)^{\frac{d}{2}}}\mathrm{d}x_1.\end{aligned}$$
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

$$
\begin{aligned}
&(\Phi|U^{\mathrm{E}}(t)\Psi) \qquad (8.187)\\
&= \int \mathrm{d}x(0) \int \mathrm{d}W_{x(0)}\big(x(\cdot)\big)\overline{\Phi\big(x(t)\big)}\Psi\big(x(0)\big)\exp\Big(-\int_0^t V(s,x(s))\mathrm{d}s\Big).
\end{aligned}
$$

Theorem 8.2. *Let $t, t_1, t_2 > 0$. Then*

$$
\int x(t)\mathrm{d}W_0\big(x(\cdot)\big) = 0, \qquad (8.188)
$$

$$
\int x_i(t_2)x_j(t_1)\mathrm{d}W_0\big(x(\cdot)\big) = \delta_{ij}\min(t_2,t_1), \qquad (8.189)
$$

$$
\int \big(x(t_2)-x(t_1)\big)^2\mathrm{d}W_0\big(x(\cdot)\big) = d|t_2-t_1|. \qquad (8.190)
$$

Proof. Let us prove (8.189). Let $t_2 > t_1$. Then

$$
\begin{aligned}
\int x(t_2)x(t_1)\mathrm{d}W_0\big(x(\cdot)\big) &= \int\int x_2\frac{\mathrm{e}^{-\frac{(x_2-x_1)^2}{2(t_2-t_1)}}}{(2\pi(t_2-t_1))^{\frac{d}{2}}}x_1\frac{\mathrm{e}^{-\frac{x_1^2}{2t_1}}}{(2\pi t_1)^{\frac{d}{2}}}\mathrm{d}x_1\mathrm{d}x_2 \qquad (8.191)\\
&= \int x_1^2\frac{\mathrm{e}^{-\frac{x_1^2}{2t_1}}}{(2\pi t_1)^{\frac{d}{2}}}\mathrm{d}x_1 \quad = \quad t_1. \qquad (8.192)
\end{aligned}
$$

□

Recall the formula (2.16)

$$
\mathrm{e}^{\frac{1}{2}\partial_x\cdot\nu\partial_x}\Psi(0) \quad = \quad (\det 2\pi\nu)^{-\frac{1}{2}}\int\Psi(x)\mathrm{e}^{-\frac{1}{2}x\cdot\nu^{-1}x}\mathrm{d}x, \qquad (8.193)
$$

which says that for Gaussian measures you can "integrate by differentiating". The Wiener measure is Gaussian, and in this case (8.193) has the form

$$
\int \mathrm{d}W_0\big(x(\cdot)\big)F\big(x(\cdot)\big) = \exp\Big(\frac{1}{2}\partial_{x(s_2)}\min(s_2,s_1)\partial_{x(s_1)}\Big)F\big(x(\cdot)\big). \qquad (8.194)
$$

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.

8.8 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 (8.169).

Lemma 8.3.

$$\mathrm{e}^{-\mathrm{i}u\mathrm{Op}\big(h(s)\big)} - \mathrm{Op}\big(\mathrm{e}^{-\mathrm{i}uh(s)}\big) = O(u^3). \tag{8.195}$$

Proof. Let us drop the reference to s in $h(s)$. We have

$$\frac{\mathrm{d}}{\mathrm{d}u}\mathrm{e}^{\mathrm{i}u\mathrm{Op}(h)}\mathrm{Op}\big(\mathrm{e}^{-\mathrm{i}uh}\big) \quad = \quad \mathrm{i}\mathrm{e}^{\mathrm{i}u\mathrm{Op}(h)}\Big(\mathrm{Op}(h)\mathrm{Op}\big(\mathrm{e}^{-\mathrm{i}uh}\big) - \mathrm{Op}\big(h\mathrm{e}^{-\mathrm{i}uh}\big)\Big). \tag{8.196}$$

Now

$$\mathrm{Op}(h)\mathrm{Op}(\mathrm{e}^{-\mathrm{i}uh}) = \mathrm{Op}\big(h\mathrm{e}^{-\mathrm{i}uh}\big) + \frac{\mathrm{i}}{2}\mathrm{Op}\big(\{h, \mathrm{e}^{-\mathrm{i}uh}\}\big) + O(u^2). \tag{8.197}$$

The second term on the right of (8.197) is zero. Therefore, (8.196) is $O(u^2)$. Clearly, $\mathrm{e}^{\mathrm{i}u\mathrm{Op}(h)}\mathrm{Op}\big(\mathrm{e}^{-\mathrm{i}uh}\big)\big|_{u=0} = \mathbb{1}$. 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 (8.166), so that

$$U(t) \quad = \quad \lim_{n\to\infty}\prod_{j=1}^{n}\mathrm{Op}\big(\mathrm{e}^{-\mathrm{i}\frac{t}{n}h\left(\frac{jt}{n}\right)}\big)$$

Thus

$$\begin{aligned} U(t,x,y) \quad &= \quad \lim_{n\to\infty}\int\cdots\int\prod_{j=1}^{n}\exp\left(-\tfrac{\mathrm{i}t}{n}h\left(\tfrac{jt}{n},\tfrac{x_j+x_{j-1}}{2},p_j\right)+\mathrm{i}(x_j-x_{j-1})p_j\right) \\ &\quad\times\prod_{j=1}^{n-1}\mathrm{d}x_j\prod_{j=1}^{n}\frac{\mathrm{d}p_j}{(2\pi)^d}\Big|_{\substack{y=x_0,\\ x=x_n.}} \end{aligned} \tag{8.198}$$

$$\begin{aligned} \quad &= \quad \lim_{n\to\infty}\int\cdots\int\exp\left(\tfrac{\mathrm{i}t}{n}\sum_{j=0}^{n}\left(\tfrac{(x_j-x_{j-1})p_j}{\frac{t}{n}}-h\left(\tfrac{jt}{n},\tfrac{x_j+x_{j-1}}{2},p_j\right)\right)\right) \\ &\quad\times\prod_{j=1}^{n-1}\mathrm{d}x_j\prod_{j=1}^{n}\frac{\mathrm{d}p_j}{(2\pi)^d}\Big|_{\substack{y=x_0,\\ x=x_n.}}\quad . \end{aligned} \tag{8.199}$$

Heuristically, this is written as follows:

$$U(t,x,y) \quad = \quad \int\mathrm{D}_{x,y}\left(x(\cdot)\right)\mathrm{D}\left(p(\cdot)\right)\exp\left(\mathrm{i}\int_0^t\left(\dot{x}(s)p(s)-h(s,x(s),p(s))\,\mathrm{d}s\right)\right),$$

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

$$\mathrm{D}_{x,y}\left(x(\cdot)\right) = \lim_{n\to\infty}\prod_{j=1}^{n-1}\mathrm{d}x\Big(\frac{jt}{n}\Big), \quad \mathrm{D}\big(p(\cdot)\big) = \prod_{j=1}^{n}\frac{\mathrm{d}p\Big((j-\frac{1}{2})\frac{t}{n}\Big)}{(2\pi)^d}.$$

8.9 Hamiltonians quadratic in momenta I

Assume in addition that

$$h(t,x,p) = \frac{1}{2}(p - A(t,x))^2 + V(t,x). \tag{8.200}$$

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 (8.200) is

$$L(t,x,v) = \frac{1}{2}v^2 + vA(t,x) - V(t,x).$$

Consider the phase space path integral (8.199). 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:

$$\begin{aligned}
U(t,x,y) \quad &= \quad \lim_{n\to\infty} \int \cdots \int \exp\Bigg(\tfrac{\mathrm{i}t}{n} \sum_{j=1}^{n} \Big(\tfrac{(x_j - x_{j-1})}{\frac{t}{n}} \big(v_j + A(\tfrac{jt}{n}, \tfrac{x_j + x_{j-1}}{2})\big) \\
&\qquad -\frac{1}{2}v_j^2 - V\big(\tfrac{jt}{n}, \tfrac{x_j+x_{j-1}}{2}\big)\Big)\Bigg) \prod_{j=1}^{n-1} \mathrm{d}x_j \prod_{j=1}^{n} \frac{\mathrm{d}v_j}{(2\pi)^d} \Bigg|_{\substack{y = x_0,\\ x = x_n}} \\
&= \quad \lim_{n\to\infty} \int \cdots \int \exp\left(\tfrac{\mathrm{i}t}{n} \sum_{j=1}^{n} L\left(\frac{jt}{n}, \frac{x_j + x_{j-1}}{2}, \frac{(x_j - x_{j-1})}{\frac{t}{n}}\right)\right) \\
&\qquad \times (2\pi \tfrac{\mathrm{i}t}{n})^{-n\frac{d}{2}} \prod_{j=1}^{n-1} \mathrm{d}x_j \Bigg|_{\substack{y = x_0,\\ x = x_n}} .
\end{aligned} \tag{8.201}$$

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 (8.170)

8.10 Hamiltonians quadratic in momenta II

Suppose, more generally, that

$$h(t,x,p)=\frac{1}{2}(p_i-A_i(t,x))g^{ij}(t,x)(p_j-A_j(t,x))+V(t,x). \tag{8.202}$$

Then

$$\begin{aligned}\mathrm{Op}\big(h(t)\big) &= \frac{1}{2}(p_i-A_i(t,x))g^{ij}(t,x)(p_j-A_j(t,x))+V(t,x)\\ &\quad -\frac{1}{4}\sum_{ij}\partial_{x^i}\partial_{x^j}g^{ij}(t,x).\end{aligned}$$

(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 (8.202) is

$$L(t,x,v)=\frac{1}{2}v^ig_{ij}(t,x)v^j+v^jA_j(t,x)-V(t,x).$$

Consider the phase space path integral (8.199). 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 $p(\cdot)$:

$$\begin{aligned}U(t,x,y) &= \int \mathrm{D}_{x,y}\big(x(\cdot)\big)\mathrm{D}\big(p(\cdot)\big)\exp\Bigg(\mathrm{i}\int_0^t\Big(\dot{x}(s)p(s)\\ &\quad -\frac{1}{2}\big(p(s)-A(s,x(s)\big)g^{-1}\big(s,x(s)\big)\big(p(s)-A\big(s,x(s)\big)-V\big(s,x(s)\big)\Big)\mathrm{d}s\Bigg)\\ &= \int \mathcal{D}_{x,y}\big(x(\cdot)\big)\exp\Bigg(\mathrm{i}\int_0^t\Big(\frac{1}{2}\dot{x}(s)g\big(s,x(s)\big)\dot{x}(s)+\dot{x}(s)A\big(s,x(s)\big)-V\big(s,x(s)\big)\Big)\mathrm{d}s\\ &\quad +\frac{1}{2}\int_0^t\mathrm{Tr}g\big(s,x(s)\big)\mathrm{d}s\Bigg)\\ &= \int \mathcal{D}_{x,y}\left(x(\cdot)\right)\exp\left(\int_0^t\Big(\mathrm{i}L(s,x(s),\dot{x}(s))+\frac{1}{2}\mathrm{Tr}g\big(s,x(s)\big)\Big)\mathrm{d}s\right).\end{aligned} \tag{8.203}$$

8.11 Semiclassical path integration

Let us repeat the most important formulas in the presence of a Planck constant $\hbar$.

$$U(t) \;:=\; \mathrm{Texp}\left(-\frac{\mathrm{i}}{\hbar}\int_0^t H(s)\mathrm{d}s\right). \tag{8.204}$$

$$U(t,x,y) \quad = \quad \int \mathrm{D}_{x,y}\left(x(\cdot)\right)\mathrm{D}\left(\hbar^{-1}p(\cdot)\right)\exp\left(\frac{\mathrm{i}}{\hbar}\int_0^t \left(\dot{x}(s)p(s) - h(s,x(s),p(s))\right)\mathrm{d}s\right),$$

We assume in addition that the Hamiltonian has the form (8.202), 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 $x_{\mathrm{cl}}(t) = x$.

$$\begin{aligned}
U(t,x,y) \quad &= \quad \hbar^{-\frac{d}{2}}\int \mathcal{D}_{x,y}\left(\hbar^{-\frac{1}{2}}x(\cdot)\right)\exp\left(\frac{\mathrm{i}}{\hbar}\int_0^t L(s,x(s),\dot{x}(s))\mathrm{d}s\right)\\
&= \quad \hbar^{-\frac{d}{2}}\exp\left(\frac{\mathrm{i}}{\hbar}\int_0^t L(s,x_{\mathrm{cl}}(s),\dot{x}_{\mathrm{cl}}(s))\mathrm{d}s\right)\\
&\quad\times\int \mathcal{D}_{0,0}\left(z(\cdot)\right)\exp\Bigg(\frac{\mathrm{i}}{2}\int_0^t \Big(\partial_{x(s)}^2 L\big(s,x_{\mathrm{cl}}(s),x_{\mathrm{cl}}(s)\big)z(s)z(s)\\
&\quad+2\partial_{x(s)}\partial_{\dot{x}(s)}L\big(s,x_{\mathrm{cl}}(s),x_{\mathrm{cl}}(s)\big)z(s)\dot{z}(s)\\
&\quad+\partial_{\dot{x}(s)}^2 L\big(s,x_{\mathrm{cl}}(s),x_{\mathrm{cl}}(s)\big)\dot{z}(s)\dot{z}(s) + O(\sqrt{\hbar})\Big)\mathrm{d}s\Bigg)\\
&= \hbar^{-\frac{d}{2}}\det\left(\frac{1}{2\pi}\begin{bmatrix}\int_0^t \partial_{x(s)}^2 L\big(s,x_{\mathrm{cl}}(s),x_{\mathrm{cl}}(s)\big) & \int_0^t \partial_{x(s)}\partial_{\dot{x}(s)}L\big(s,x_{\mathrm{cl}}(s),x_{\mathrm{cl}}(s)\big)\\ \int_0^t \partial_{x(s)}\partial_{\dot{x}(s)}L\big(s,x_{\mathrm{cl}}(s),x_{\mathrm{cl}}(s)\big) & \int_0^t \partial_{\dot{x}(s)}^2 L\big(s,x_{\mathrm{cl}}(s),x_{\mathrm{cl}}(s)\big)\end{bmatrix}\right)^{-\frac{1}{2}}\\
&\quad\times\exp\left(\frac{\mathrm{i}}{\hbar}\int_0^t L(s,x_{\mathrm{cl}}(s),\dot{x}_{\mathrm{cl}}(s))\mathrm{d}s\right)\big(1+O(\sqrt{\hbar})\big).
\end{aligned}$$

8.12 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 (8.204). (We drop the tilde from $\tilde{h}$ and $\tilde{u}$, as compared with the notation of (4.85).)

Following Lemma 8.3 we prove that

$$\mathrm{e}^{-\mathrm{i}u\mathrm{Op}^{a^*,a}\left(h(s)\right)} - \mathrm{Op}^{a^*,a}\big(\mathrm{e}^{-\mathrm{i}uh(s)}\big) = O(u^2). \tag{8.205}$$

Thus we can use $F(s,u) := \mathrm{Op}^{a^*,a}\big(\mathrm{e}^{-\mathrm{i}uh(s)}\big)$ in (8.166), so that

$$\mathrm{Op}^{a^*,a}\big(u(t)\big) \ := \ U(t) \quad = \quad \lim_{n\to\infty}\prod_{j=1}^{n}\mathrm{Op}^{a^*,a}\big(\mathrm{e}^{-\mathrm{i}\frac{t}{n}h\left(\frac{jt}{n}\right)}\big).$$

Thus, by (4.94),

$$u(t,a^*,a) \quad = \quad \lim_{n\to\infty} \exp\Big(\sum_{k>j} \partial_{a_k}\partial_{a_j^*}\Big) \prod_{j=1}^{n} \exp\left(-\tfrac{\mathrm{i}t}{n} h\left(\tfrac{jt}{n}, a_j^*, a_j\right)\right)\Big| \quad a = a_n = \cdots = a_1. \quad .$$

Heuristically, this can be rewritten as

$$\begin{aligned} u(t,a^*,a) \quad &= \quad \exp\left(\int_0^t \mathrm{d}s_+ \int_0^t \mathrm{d}s_- \theta(s_+ - s_-)\partial_{a^*(s_+)}\partial_{a(s_-)}\right) \\ &\quad \times \exp\left(-\mathrm{i}\int_0^t h\left(s, a^*(s), a(s)\right)\mathrm{d}s\right)\Big|_{a=a(s), t>s>0}. \end{aligned} \tag{8.206}$$

Alternatively, we can use the integral formula (4.95), and rewrite (8.206) as

$$\begin{aligned} u(t,a^*,a) = \int\cdots\int \exp\Big(\sum_{j=1}^{n-1}\Big(-\frac{(b_{j+1}-b_j)b_j^*}{2} + \frac{b_{j+1}(b_{j+1}^* - b_j^*)}{2}\Big) \\ \times \prod_{j=1}^{n} \exp\left(-\tfrac{\mathrm{i}t}{n} h\left(\tfrac{jt}{n}, a^* + b_j^*, a + b_j\right)\right) \prod_{j=1}^{n-1} \frac{\mathrm{d}b_{j+1}\mathrm{d}b_j^*}{(2\pi\mathrm{i})^d}\Big|_{b_n^*=0,\, b_1=0}. \end{aligned} \tag{8.207}$$

Heuristically, it can be rewritten as

$$\begin{aligned} &u(t,a^*,a) \\ = \quad &\frac{\int \mathcal{D}\big(b^*(\cdot),b(\cdot)\big)\exp\Big(\int_0^t\Big(-\frac{b^*(s)\partial_s b(s)}{2} + \frac{\partial_s b^*(s) b(s)}{2} - \mathrm{i}h\left(s, a^* + b^*(s), a + b(s)\right)\Big)\mathrm{d}s\Big)}{\int \mathcal{D}\big(b^*(\cdot),b(\cdot)\big)\exp\Big(\int_0^t\big(-\frac{b^*(s)\partial_s b(s)}{2} + \frac{\partial_s b^*(s) b(s)}{2}\big)\mathrm{d}s\Big)}. \end{aligned} \tag{8.208}$$

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 (8.208), which starts from (8.206). 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 (2.23), (8.206) can be rewritten formally as (8.208).

8.13 Vacuum expectation value

In particular, we have the following expression for the vacuum expectation value:

$$\begin{aligned}&\big(\Omega|U(t)\Omega\big)\\ =\quad&\frac{\int\mathcal{D}\big(a(\cdot)\big)\exp\Big(\int_0^t\left(a^*(s)\partial_s a(s)-\mathrm{i}h\left(s,a^*(s),a(s)\right)\right)\mathrm{d}s\Big)}{\int\mathcal{D}\big(a(\cdot)\big)\exp\big(\int_0^t a^*(s)\partial_s a(s)\mathrm{d}s\big)}.\end{aligned}\tag{8.209}$$

For $f,g\in\mathbb{C}^d$ we will write

$$a^*(f)=a_i f_i,\quad a(g)=a_i\overline{g}_i.$$

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

$$\begin{aligned}Z(sF,u\overline{G})&=\lim_{\epsilon\to0}\Big(\Omega|\mathrm{e}^{-\mathrm{i}s\frac{\epsilon}{\epsilon}a(f)}U(t)\mathrm{e}^{-\mathrm{i}u\frac{\epsilon}{\epsilon}a^*(g)}\Omega\Big)\\ &=\Big(\mathrm{e}^{\mathrm{i}sa^*(f)}\Omega|U(t)\mathrm{e}^{-\mathrm{i}ua^*(g)}\Omega\Big).\end{aligned}$$

Now

$$
\begin{aligned}
& F_1 \cdots F_1 \overline{G}_1 \cdots \overline{G}_1 \partial_F^n \partial_{\overline{G}}^m Z(F, \overline{G})\Big|_{F=0, \overline{G}=0} \\
= \; & \partial_s^n \partial_u^m \Big(\mathrm{e}^{\mathrm{i}sa^*(f)} \Omega | U(t) \mathrm{e}^{-\mathrm{i}ua^*(g)} \Omega \Big)\Big|_{s=0,\ u=0} \\
= \; & \mathrm{i}^{n-m} \Big(a^*(f_1)^n \Omega | U(t) a^*(g_1)^m \Omega \Big).
\end{aligned}
$$

8.14 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

$$
\begin{aligned}
s(a^*, a) &= \exp\Big(\int_{-\infty}^{\infty} \mathrm{d}t_+ \int_{-\infty}^{\infty} \mathrm{d}t_- \theta(t_+ - t_-) \partial_{a(t_+)} \partial_{a^*(t_-)} \Big) \\
&\quad \times \exp\Big(-\mathrm{i}\lambda \int_{-\infty}^{\infty} q\left(t, \mathrm{e}^{\mathrm{i}\varepsilon t} a^*(t), \mathrm{e}^{-\mathrm{i}\varepsilon t} a(t)\right) \mathrm{d}t \Big) \Big|_{\substack{a^* = a^*(t), \\ a = a(t),\ t \in \mathbb{R}}} \\
&= \exp\Big(\int_{-\infty}^{\infty} \mathrm{d}t_+ \int_{-\infty}^{\infty} \mathrm{d}t_- \mathrm{e}^{\mathrm{i}\varepsilon(t_+ - t_-)} \theta(t_+ - t_-) \partial_{a(t_+)} \partial_{a^*(t_-)} \Big) \\
&\quad \times \exp\Big(-\mathrm{i}\lambda \int_{-\infty}^{\infty} q\left(t, a^*(t), a(t)\right) \mathrm{d}t \Big) \Big|_{\substack{\mathrm{e}^{\mathrm{i}t\varepsilon} a^* = a^*(t), \\ \mathrm{e}^{\mathrm{i}t\varepsilon} a = a(t),\ t \in \mathbb{R}}} \\
&= \frac{\int \mathcal{D}\big(b(\cdot)\big) \exp\Big(\int_{-\infty}^{\infty} \Big(\big(b^*(t) - \mathrm{e}^{\mathrm{i}\varepsilon t} a^*\big)(\partial_t + \mathrm{i}\varepsilon)\big(b(t) - \mathrm{e}^{-\mathrm{i}\varepsilon t} a\big) - \mathrm{i}\lambda q\left(t, b^*(t), b(t)\right) \Big) \mathrm{d}t \Big)}{\int \mathcal{D}\big(b(\cdot)\big) \exp \int_{-\infty}^{\infty} \Big(\big(b^*(t) - \mathrm{e}^{\mathrm{i}\varepsilon t} a^*\big)(\partial_t + \mathrm{i}\varepsilon)\big(b(t) - \mathrm{e}^{-\mathrm{i}\varepsilon t} a\big)}.
\end{aligned}
\tag{8.210}
$$

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 $\mathrm{e}^{\mathrm{i}\varepsilon(t_+ - t_-)}\theta(t_+ - t_-)$.

9 Diagrammatics

9.1 Friedrichs diagrams

9.1.1 Wick monomials

Monomials in commuting/anticommuting variables $a^*(\xi)$, $a(\xi)$ parametrized by, say, $\xi \in \mathbb{R}^d$, are expressions of the form

$$\begin{aligned} & r(a^*, a) && (9.211) \\ := & \int\cdots\int \mathrm{d}\xi_1^+ \cdots \mathrm{d}\xi_{m^+}^+ \mathrm{d}\xi_{m^-}^- \cdots \mathrm{d}\xi_1^- r(\xi_1^+, \dots, \xi_{m^+}^+, \xi_{m^-}^-, \dots, \xi_1^-) \\ & \times a^*(\xi_{m^+}^+) \cdots a^*(\xi_1^+) a(\xi_1^-) \cdots \hat{a}(\xi_{m^-}^-), && (9.212) \end{aligned}$$

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 (9.212). A *polynomial* is a sum of monomials.

Consider creation/annihilation operators parametrized by $\xi \in \mathbb{R}^d$:

$$[\hat{a}(\xi), \hat{a}^*(\xi')]_\mp = \delta(\xi - \xi'), \qquad (9.213)$$

$$[\hat{a}(\xi), \hat{a}(\xi')]_\mp = [\hat{a}^*(\xi), \hat{a}^*(\xi')]_\mp = 0. \qquad (9.214)$$

By a *Wick monomial* we mean an operator on $\Gamma_{\mathrm{s/a}}(L^2(\mathbb{R}^d))$ given formally by

$$\begin{aligned} & r(\hat{a}^*, \hat{a}) && (9.215) \\ := & \int\cdots\int \mathrm{d}\xi_1^+ \cdots \mathrm{d}\xi_{m^+}^+ \mathrm{d}\xi_{m^-}^- \cdots \mathrm{d}\xi_1^- r(\xi_1^+, \dots, \xi_{m^+}^+, \xi_{m^-}^-, \dots, \xi_1^-) \\ & \times \hat{a}^*(\xi_{m^+}^+) \cdots \hat{a}^*(\xi_1^+) \hat{a}(\xi_1^-) \cdots \hat{a}(\xi_{m^-}^-). && (9.216) \end{aligned}$$

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

$$\begin{aligned} & q(\hat{a}^*)\Omega && (9.217) \\ = & \int\cdots\int q(\xi_1, \dots, \xi_m) \hat{a}^*(\xi_m) \cdots \hat{a}^*(\xi_1) \Omega \mathrm{d}\xi_m \cdots \mathrm{d}\xi_1, && (9.218) \end{aligned}$$

where q is a symmetric/antisymmetric function. Clearly,

$$\|q(\hat{a}^*)\Omega\|^2 = m! \int |q(\xi_1, \dots, \xi_m)|^2 \mathrm{d}\xi_m \cdots \mathrm{d}\xi_1. \tag{9.219}$$

Note that if ξ were a discrete variable, then (9.219) would not true in the case of coinciding ξ.

It is convenient to introduce the shorthand

$$|\xi_m, \dots \xi_1) := \hat{a}^*(\xi_m) \cdots \hat{a}^*(\xi_1)\Omega. \tag{9.220}$$

Clearly, (9.220) 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 (9.218).

If $q(\hat{a}^*, \hat{a})$ is a Wick polynomial, it is convenient to decompose it in a sum of monomials as follows:

$$q(\hat{a}^*, \hat{a}) = \sum_{m^+, m^-} \frac{q_{m^+, m^-}(\hat{a}^*, \hat{a})}{m^+! m^-!}. \tag{9.221}$$

We have then

$$q_{m^+, m^-}\big(\xi^+_{m_+}, \dots, \xi^+_1; \xi^-_{m_-}, \dots, \xi^-_1\big) \tag{9.222}$$

$$= \big(\xi^+_{m_+}, \dots, \xi^+_1 | q(\hat{a}^*, \hat{a}) | \xi^-_{m_-}, \dots, \xi^-_1\big). \tag{9.223}$$

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*.

9.1.2 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

$$q(\hat{a}^*, \hat{a}) = q_n(\hat{a}^*, \hat{a}) \cdots q_1(\hat{a}^*, \hat{a}) \tag{9.224}$$

can be computed from the formula

$$q(a^*, a) \tag{9.225}$$

$$= \exp\Big(\sum_{k>j} \partial_{a_k} \partial_{a^*_j}\Big) q_n(a^*_n, a_n) \cdots q_1(a^*_1, a_1)\Big|_{\substack{a = a_n = \cdots = a_1, \\ a^* = a^*_2 = \cdots = a^*_1.}} \tag{9.226}$$

(9.226) 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

$$q(\hat{a}^*, \hat{a}) := \frac{r_n(\hat{a}^*, \hat{a})}{m^+_n! m^-_n!} \cdots \frac{r_1(\hat{a}^*, \hat{a})}{m^+_1! m^-_1!}. \tag{9.227}$$

We will describe a diagramatic method for computing $q(a^*, a)$, the Wick symbol of (9.227).

(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

$$B! := \prod_{j>i} k_{ji}! \prod_j k_j^+! \prod_i k_i^-! \tag{9.228}$$

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:

$$q(a^*, a) = \sum_{\text{all diag}} \frac{q_B(a^*, a)}{B!}. \tag{9.229}$$

In particular,

$$\frac{q_{m^+,m^-}(a^*,a)}{m^+!m^-!} = \sum_{B\ :\ (m^+,m^-)=(m_B^+,m_B^-)} \frac{q_B(a^*,a)}{B!}, \tag{9.230}$$

$$\big(\Omega|q(\hat{a}^*,\hat{a})\Omega\big) = q_{0,0} = \sum_{B \text{ has no external lines}} \frac{q_B}{B!} \tag{9.231}$$

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 (9.226). In fact, each diagram B is defined by a collection of integers $\{k_{ji},\ j>i\}$, and we can write

$$\exp\Big(\sum_{j>i}\partial_{a_k}\partial_{a_j^*}\Big) = \sum_B \prod_{j>i} \frac{1}{k_{ji}!}\big(\partial_{a_k}\partial_{a_j^*}\big)^{k_{ij}}. \tag{9.232}$$

This differential operator acts on the function

$$\frac{r_n(a_n^*,a_n)}{m_n^+!m_n^-!}\cdots\frac{r_1(a_1^*,a_1)}{m_1^+!m_1^-!} \tag{9.233}$$

The effect of the component of the differential operator (9.232) 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

$$\frac{q_B(a^*,a)}{\prod_{j>i}k_{ji}!\prod_j k_j^+!\prod_i k_i^-!}. \tag{9.234}$$

9.1.3 Friedrichs (Wick) diagrams

Consider a Hamiltonian

$$H = H_0 + W(t), \tag{9.235}$$

where

$$H_0 = \int \omega(\xi)\hat{a}^*(\xi)\hat{a}(\xi)\mathrm{d}\xi, \tag{9.236}$$

$$W(t) = \sum_{m^+,m^-} \frac{w_{m^+,m^-}(t,\hat{a}^*,\hat{a})}{m^+!m^-!}. \tag{9.237}$$

Thus the free Hamiltonian is a particle number preserving quadratic Hamiltonian and the perturbation is a Wick polymial. We set as usual

$$H_{\rm Int}(t) = \mathrm{e}^{\mathrm{i}tH_0} W(t) \mathrm{e}^{-\mathrm{i}tH_0}, \tag{9.238}$$

$$S = \mathrm{Texp}\Big(-\mathrm{i} \int_{-\infty}^{\infty} H_{\rm Int}(t)\mathrm{d}t \Big). \tag{9.239}$$

Using

$$\mathrm{e}^{\mathrm{i}tH_0} a^*(\xi) \mathrm{e}^{-\mathrm{i}tH_0} = \mathrm{e}^{\mathrm{i}t\omega(\xi)} a^*(\xi), \tag{9.240}$$

$$\mathrm{e}^{\mathrm{i}tH_0} a(\xi) \mathrm{e}^{-\mathrm{i}tH_0} = \mathrm{e}^{-\mathrm{i}t\omega(\xi)} a(\xi), \tag{9.241}$$

we can write

$$H_{\rm Int}(t) = \sum \frac{w_{m^+,m^-}(t, \mathrm{e}^{\mathrm{i}t\omega}\hat{a}^*, \mathrm{e}^{-\mathrm{i}t\omega}\hat{a})}{m^+! m^-!}. \tag{9.242}$$

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

$$S = s(\hat{a}^*, \hat{a}) \tag{9.243}$$

$$= \sum_{m^+,m^-} \frac{s_{m^+,m^-}(\hat{a}^*, \hat{a})}{m^+! m^-!}. \tag{9.244}$$

(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. 9.1.2.

(2) The symmetry factor $B!$, the number of incoming/outgoing particles m_B^- and m_B^+ are defined as in Susbsect. 9.1.2.

(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:

$$s(a^*, a) = \sum_{n=0}^{\infty} \sum_{\text{all diag.}} \int_{t_n > \cdots > t_1} \cdots \int \frac{B(t_n, \dots, t_1; a^*, a)}{B!} \mathrm{d}t_n \cdots \mathrm{d}t_1. \tag{9.245}$$

In particular,

$$\begin{aligned} &\frac{s_{m^+, m^-}(a^*, a)}{m^+! m^-!} &(9.246)\\ &= \sum_{n=0}^{\infty} \sum_{B\ :\ (m^+, m^-) = (m_B^+, m_B^-)} \int_{t_n > \cdots > t_1} \cdots \int \frac{B(t_n, \dots, t_1; a^*, a)}{B!} \mathrm{d}t_n \cdots \mathrm{d}t_1, &(9.247)\\ &\big(\Omega | S \Omega\big) = s_{0,0} &(9.248)\\ &= \sum_{n=0}^{\infty} \sum_{B \text{ has no external lines}} \int_{t_n > \cdots > t_1} \cdots \int \frac{B(t_n, \dots, t_1)}{B!} \mathrm{d}t_n \cdots \mathrm{d}t_1. \end{aligned}$$

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.

9.1.4 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

$$H(t) := \mathrm{Op}^{a^*, a}\big(h(t)\big), \tag{9.249}$$

$$U(t) := \mathrm{Texp}\bigg(-\mathrm{i} \int_0^t H(s) \mathrm{d}s\bigg). \tag{9.250}$$

Now

$$\begin{aligned} U(t) &= \lim_{n \to \infty} \prod_{j=1}^{n} \mathrm{e}^{-\mathrm{i} \frac{t}{n} h\left(\frac{jt}{n}, \hat{a}^*, \hat{a}\right)} \\ &= \lim_{n \to \infty} \prod_{j=1}^{n} \mathrm{e}^{-\mathrm{i} \frac{t}{n} h\left(\frac{jt}{n}\right)} (\hat{a}^*, \hat{a}). \end{aligned}$$

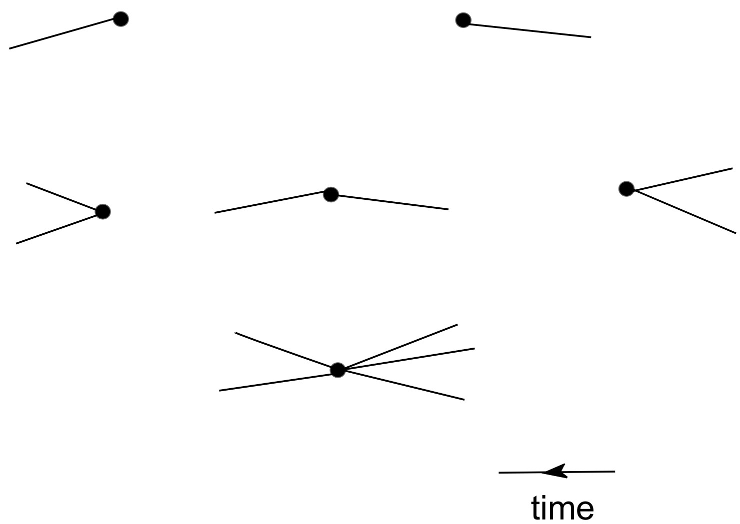

Figure 1: Various Friedrichs vertices

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

$$\begin{aligned} u(t,a^*,a) \quad &= \quad \exp\left(\int\!\!\int_{t>s_+>s_->0} \mathrm{d}s_+\mathrm{d}s_-\partial_{a^*(s_+)}\partial_{a(s_-)}\right) \\ &\quad \times \exp\left(-\mathrm{i}\int_0^t h\left(s,a^*(s),a(s)\right)\mathrm{d}s\right)\Big|_{\substack{a^*=a^*(s),\\ a=a(s),\ t>s>0}} . \end{aligned} \tag{9.251}$$

Assume now that the Hamiltonian is defined for all times and has the form (9.237). Define the scattering operator S and its Wick symbol s as in (9.239) and (9.243). Using the

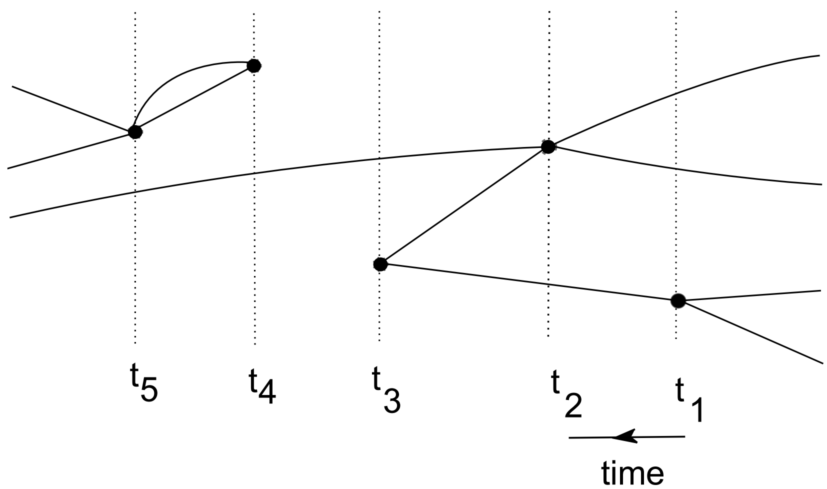

Figure 2: A disconnected Friedrichs diagram

version of (9.251) with $]0,t[$ replaced by $]-\infty,\infty[$, we obtain

$$
\begin{aligned}
s(a^*,a) &= \exp\left(\int\limits_{\infty>t_+>t_->-\infty}\mathrm{d}t_+\int\mathrm{d}t_-\,\partial_{a(t_+)}\partial_{a^*(t_-)}\right) \\
&\quad\times\exp\left(-\mathrm{i}\lambda\int_{-\infty}^{\infty}w\left(t,\mathrm{e}^{\mathrm{i}\varepsilon t}a^*(t),\mathrm{e}^{-\mathrm{i}\varepsilon t}a(t)\right)\mathrm{d}t\right)\Bigg|_{\substack{a^*=a^*(t),\\ a=a(t),\ t\in\mathbb{R}}} \\
&= \exp\left(\int\limits_{\infty>t_+>t_->-\infty}\mathrm{d}t_+\int\mathrm{d}t_-\,\mathrm{e}^{\mathrm{i}\varepsilon(t_+-t_-)}\partial_{a(t_+)}\partial_{a^*(t_-)}\right) \\
&\quad\times\exp\left(-\mathrm{i}\lambda\int_{-\infty}^{\infty}w\left(t,a^*(t),a(t)\right)\mathrm{d}t\right)\Bigg|_{\substack{\mathrm{e}^{\mathrm{i}t\varepsilon}a^*=a^*(t),\\ \mathrm{e}^{\mathrm{i}t\varepsilon}a=a(t),\ t\in\mathbb{R}}}\ . \qquad (9.252)
\end{aligned}
$$

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 $\mathrm{e}^{\mathrm{i}\varepsilon(t_+-t_-)}\theta(t_+-t_-)$.

To derive the method of Friedrichs diagrams we can now proceed as in Subsubsect. 9.1.2.

9.1.5 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 $B(t_n, \dots, t_1; a^*, a)$ as a product of operators. For each line we introduce the Hilbert space isomorphic to $\mathcal{V}$. We have $n+1$ time intervals

$$t > t_n, \dots, t_{j+1} > t > t_j, \dots, t_1 > t.$$

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 $W_B^j(t_j)$. $\mathbb{1}_B^j$ 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

$$\begin{aligned} B(t_n, \dots, t_1) &= (-\mathrm{i})^n \Theta_B^+ \mathrm{e}^{\mathrm{i}t_nH_0} \left(W_B^n(t_n) \otimes \mathbb{1}_B^n\right) \mathrm{e}^{-\mathrm{i}(t_n-t_{n-1})H_0} \cdots \\ &\quad \times \mathrm{e}^{-\mathrm{i}(t_2-t_1)H_0} \left(W_B^1(t_1) \otimes \mathbb{1}_B^1\right) \mathrm{e}^{-\mathrm{i}t_1H_0} \Theta_B^-. \end{aligned}$$

9.1.6 Linked Cluster Theorem

The *Linked Cluster Theorem* says that instead of the formula (9.245) there is a simpler way of computing the scattering operator, where we need only connected diagrams:

$$\begin{aligned} &s(a^*, a) \\ &= \exp\left(\sum_{n=0}^{\infty} \sum_{\text{con. diag.}} \int\cdots\int_{t_n>\cdots>t_1} \frac{B(t_n, \dots, t_1; a^*, a)}{B!} \mathrm{d}t_n \cdots \mathrm{d}t_1\right), \end{aligned} \tag{9.253}$$

$$\begin{aligned} (\Omega|S\Omega) &= s_{0,0} \\ &= \exp\left(\sum_{n=0}^{\infty} \sum_{\substack{\text{con. diag.} \\ \text{no ext. lines}}} \int\cdots\int_{t_n>\cdots>t_1} \frac{B(t_n, \dots, t_1)}{B!} \mathrm{d}t_n \cdots \mathrm{d}t_1\right). \end{aligned} \tag{9.254}$$

In (9.253) we sum over all connected diagrams. In (9.254) we sum over all connected diagrams without external lines. Clearly, (9.254) follows from (9.253).

We define the linked scattering operator as

$$S_{\mathrm{link}} := \frac{S}{(\Omega|S\Omega)}. \tag{9.255}$$

If $S_{\mathrm{link}} = s_{\mathrm{link}}(\hat{a}^*, \hat{a})$, then

$$\begin{aligned} s_{\mathrm{link}}(a^*, a) &= \frac{s(a^*, a)}{(\Omega|S\Omega)} \\ &= \sum_{n=0}^{\infty} \sum_{\text{linked diag.}} \int_{t_n > \cdots > t_1} \cdots \int \frac{B(t_n, \ldots, t_1; a^*, a)}{B!} \mathrm{d}t_n \cdots \mathrm{d}t_1 \end{aligned} \tag{9.256}$$

$$= \exp\left(\sum_{n=0}^{\infty} \sum_{\substack{\text{con. linked} \\ \text{diag.}}} \int_{t_n > \cdots > t_1} \cdots \int \frac{B(t_n, \ldots, t_1; a^*, a)}{B!} \mathrm{d}t_n \cdots \mathrm{d}t_1 \right). \tag{9.257}$$

In (9.256) we sum over all *linked* diagrams, that is, diagrams whose each connected component has at least one external line. In (9.257) we sum over all connected diagrams with at least one external line. Clearly, (9.256) and (9.257) follow from (9.253).

9.1.7 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

$$\int_{t_n > \cdots > t_1} \cdots \int B(t_n, \ldots, t_1) \mathrm{d}t_n \cdots \mathrm{d}t_1 \tag{9.258}$$

is finite. Therefore, we define the *linked scattering operator* as the operator

$$S_{\mathrm{link}} := s_{\mathrm{link}}(\hat{a}^*, \hat{a}) \tag{9.259}$$

with $s_{\mathrm{link}}(a^*, a)$ given by (9.256) or (9.257).

Clearly, S_{link} cannot be defined by the right hand side of (9.255), 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

$$\delta(E - H_0), \quad (E - H_0 \pm \mathrm{i}0)^{-1} \tag{9.260}$$

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

$$\int_0^{+\infty} \mathrm{e}^{\mathrm{i}u(H_0-E)}\mathrm{d}u = -\mathrm{i}\big(E - H_0 + \mathrm{i}0\big)^{-1}, \tag{9.261}$$

$$\int_{-\infty}^{0} \mathrm{e}^{\mathrm{i}u(H_0-E)}\mathrm{d}u = \mathrm{i}\big(E - H_0 - \mathrm{i}0\big)^{-1}, \tag{9.262}$$

$$\int \mathrm{e}^{\mathrm{i}t(H_0-E)}\mathrm{d}t = 2\pi\delta(E - H_0). \tag{9.263}$$

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:

$$B_{\mathrm{sc}}(E) := -2\pi\mathrm{i}\Theta_B^+\delta(E-H_0)W_B^n\otimes 1\!\!1_B^n(E-H_0-\mathrm{i}0)^{-1}\cdots \tag{9.264}$$

$$\times (E-H_0-\mathrm{i}0)^{-1}W_B^1\otimes 1\!\!1_B^1\delta(E-H_0)\Theta_B^-. \tag{9.265}$$

(9.265) 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 9.1. *For every linked diagram B*

$$\underset{t_n>\cdots>t_1}{\int\cdots\int} B(t_n,\dots,t_1)\mathrm{d}t_n\cdots\mathrm{d}t_1 = \int B_{\mathrm{sc}}(E)\mathrm{d}E. \tag{9.266}$$

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

$$\begin{aligned}
&\int\cdots\int_{t_n>\cdots>t_1} B(t_n,\dots,t_1)\mathrm{d}t_n\cdots\mathrm{d}t_1\\
=\ &\int \mathrm{d}E\int_0^\infty \mathrm{d}u_n\cdots\int_0^\infty \mathrm{d}u_1\int_{-\infty}^\infty \mathrm{d}t_1\delta(H_0-E)\Theta_B^+\left(W_n\otimes 1\!\!1_B^n\right)\mathrm{e}^{-\mathrm{i}u_n(H_0-E)}\cdots\\
&\times\mathrm{e}^{-\mathrm{i}u_2(H_0-E)}\left(W_1\otimes 1\!\!1_B^1\right)\mathrm{e}^{-\mathrm{i}t_1(H_0-E)}\Theta_B^-\\
=\ &-2\pi\mathrm{i}\int \mathrm{d}E\delta(E-H_0)\Theta_B^+\left(W_n\otimes 1\!\!1_B^n\right)\big(E-H_0-\mathrm{i}0)\big)^{-1}\cdots\\
&\times\big(E-H_0-\mathrm{i}0)\big)^{-1}\left(W_1\otimes 1\!\!1_B^1\right)\delta(E-H_0)\Theta_B^-,
\end{aligned}$$

□

By Thm 9.266, (9.257) 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

$$S_{\mathrm{link}}=\lim_{t\to\infty}\frac{\mathrm{e}^{-\mathrm{i}tH_0}\mathrm{e}^{\mathrm{i}2tH}\mathrm{e}^{-\mathrm{i}tH_0}}{(\Omega|\mathrm{e}^{-\mathrm{i}tH_0}\mathrm{e}^{\mathrm{i}2tH}\mathrm{e}^{-\mathrm{i}tH_0}\Omega)}. \tag{9.267}$$

We can make (9.267) 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

$$S_{\mathrm{link}}=\lim_{\epsilon\searrow 0}\frac{S_\epsilon}{(\Omega|S_\epsilon\Omega)}. \tag{9.268}$$

One often makes the choice

$$\chi(t/\epsilon)=\mathrm{e}^{-|t|/\epsilon}, \tag{9.269}$$

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 (9.268), 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.

9.1.8 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 $E := \inf \mathrm{sp}\, H$. 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

$$E \quad = \quad \lim_{t\to\infty} \frac{\mathrm{i}}{2}\frac{\mathrm{d}}{\mathrm{d}t} \log(\Omega|\mathrm{e}^{\mathrm{i}tH_0}\mathrm{e}^{-\mathrm{i}2tH}\mathrm{e}^{\mathrm{i}tH_0}\Omega), \tag{9.270}$$

To see why we can expect (9.270) 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 (9.270).

It is convenient to rewrite (9.270) as

$$E \quad = \quad \lim_{t\to\infty} \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t} \log(\Omega|\mathrm{e}^{\mathrm{i}tH_0}\mathrm{e}^{-\mathrm{i}tH}\Omega). \tag{9.271}$$

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,

$$\begin{aligned}
&\int\cdots\int_{t_n>\cdots>t_1} B(t_n,\dots,t_1)\mathrm{d}t_n\cdots\mathrm{d}t_1 \\
= &\int \mathrm{d}t_1 \int\cdots\int_{u_n>\cdots>u_2>0} B(u_n,\dots,u_2,0)\mathrm{d}u_n\cdots\mathrm{d}u_2.
\end{aligned}$$

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 9.2 (Goldstone theorem)**.** *We have*

$$E = \sum_{\substack{\text{con. diag.}\\ \text{no ext. lines}}} \int\cdots\int_{u_n>\cdots>u_2>0} \frac{B(u_n,\dots,u_2,0)}{B!}\mathrm{d}u_n\cdots\mathrm{d}u_2. \tag{9.272}$$

The terms in (9.272) can be evaluated using the operator interpretation of B:

$$\int\cdots\int_{u_n>\cdots>u_2>0} B(u_n,\dots,u_2,0)\mathrm{d}u_n\cdots\mathrm{d}u_2 \tag{9.273}$$

$$= (-1)^{n-1}W_B^n\, H_0^{-1}\big(W_B^{n-1}\otimes 1\!\!1_B^{n-1}\big)\dots\big(W_B^2\otimes 1\!\!1_B^2\big)H_0^{-1}\, W_B^1. \tag{9.274}$$

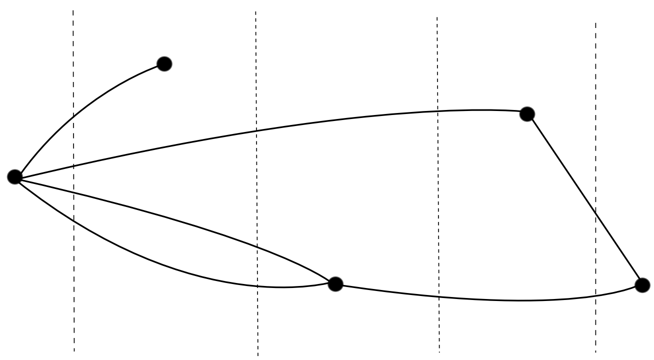

Figure 3: Goldstone diagram

Proof. Applying (9.254), 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

$$\int_0^\infty \mathrm{e}^{-\mathrm{i}uH_0} \mathrm{d}u = \frac{-\mathrm{i}}{H_0}. \tag{9.275}$$

□

9.1.9 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 9.3. *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

$$\begin{aligned}
& \int \mathrm{d}t_2 \int_{t_2 > t_1} \mathrm{d}t_1 (-\mathrm{i})^2 \overline{v(t,\xi)} v(t_1,\xi) \mathrm{e}^{-\mathrm{i}\omega(\xi)(t_2-t_1)} \mathrm{d}\xi && (9.276) \\
= \; & -\frac{1}{2}\int \mathrm{d}\xi \int \mathrm{d}t_1 \int \mathrm{d}t_2 \mathrm{e}^{-\mathrm{i}\omega(\xi)|t_1-t_2|} \overline{v(t_1,\xi)} v(t_2,\xi) && (9.277) \\
= \; & \frac{\mathrm{i}}{2\pi}\int \frac{\overline{v(\tau,\xi)} v(\tau,\xi)\omega(\xi)}{\omega(\xi)^2-\tau^2-\mathrm{i}0} \mathrm{d}\tau \mathrm{d}\xi. && (9.278)
\end{aligned}$$

Therefore,

$$(\Omega|S\Omega) = \exp\left(\frac{\mathrm{i}}{2\pi}\int \frac{\overline{v(\tau,\xi)} v(\tau,\xi)\omega(\xi)}{\omega(\xi)^2-\tau^2-\mathrm{i}0} \mathrm{d}\tau \mathrm{d}\xi\right). \tag{9.279}$$

Next we consider the contributions from the external lines

$$\begin{aligned}
& \left(\xi^+_{m_+},\dots,\xi^+_1|S|\xi^-_{m_-},\dots,\xi^-_1\right) && (9.280) \\
= \; & (\Omega|S\Omega)\prod_{j=1}^{m^+}\Big((-\mathrm{i})v(t_j,\xi_j^+)\mathrm{e}^{\mathrm{i}t_j\omega(\xi_j^+)}\mathrm{d}t_j\Big)\prod_{i=1}^{m^-}\Big((-\mathrm{i})\overline{v(t_i,\xi_i^-)}\mathrm{e}^{-\mathrm{i}t_i\omega(\xi_i^-)}\mathrm{d}t_i\Big).
\end{aligned}$$

□

9.2 Feynman diagrams

9.2.1 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

$$\varepsilon(\vec{k}) = \sqrt{\vec{k}^2+m^2}, \tag{9.281}$$

but this can be problematic, and therefore we will keep ε an arbitrary function, demanding only

$$\varepsilon(-\vec{k}) = \varepsilon(\vec{k}) \tag{9.282}$$

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

$$\begin{aligned}
[\hat{a}(k),\hat{a}^*(k')] &= \delta(\vec{k}-\vec{k}'), && (9.283) \\
[\hat{a}(k),\hat{a}(k')] = [\hat{a}^*(k),\hat{a}^*(k')] &= 0. && (9.284)
\end{aligned}$$

The free Hamiltonian is

$$H_0 = \int \varepsilon(k)\hat{a}^*(k)\hat{a}(k)\mathrm{d}\vec{k}. \tag{9.285}$$

We will use operators in the free Heisenberg picture (the interaction picture), There exists a distinguished observable, called a *field*

$$\begin{aligned}\hat\phi(x) &= \mathrm{e}^{\mathrm{i}tH_0}\hat\phi(0,\vec x)\mathrm{e}^{-\mathrm{i}tH_0} &(9.286)\\ &= \int \mathrm{d}\vec k \frac{1}{\sqrt{(2\pi)^3 2\varepsilon(\vec k)}}\left(\mathrm{e}^{\mathrm{i}kx}\hat a(k)+\mathrm{e}^{-\mathrm{i}kx}\hat a^*(k)\right). &(9.287)\end{aligned}$$

We sometimes also use the *conjugate field*

$$\hat\pi(x) := \dot{\hat\phi}(x) = \int \frac{\mathrm{d}\vec k\sqrt{\varepsilon(\vec k)}}{\mathrm{i}\sqrt{(2\pi)^3}\sqrt2}\left(\mathrm{e}^{\mathrm{i}kx}\hat a(k)-\mathrm{e}^{-\mathrm{i}kx}\hat a^*(k)\right). \tag{9.288}$$

Note that $\hat\phi$ and $\hat\pi$ satisfy the usual equal time commutation relations, independently of the relation (9.281):

$$\begin{aligned}[\hat\phi(t,\vec x),\hat\phi(t,\vec y)]=[\hat\pi(t,\vec x),\hat\pi(t,\vec y)] &= 0,\\ [\hat\phi(t,\vec x),\hat\pi(t,\vec y)] &= \mathrm{i}\delta(\vec x-\vec y). &(9.289)\end{aligned}$$

For any $x\in\mathbb{R}^{1+3}$, we introduce the *Wick powers of fields*

$$\begin{aligned}&:\hat\phi(x)^n: &(9.290)\\ &=\sum_{j=0}^n\binom{n}{j}\left(\int \mathrm{d}\vec k\frac{\mathrm{e}^{-\mathrm{i}kx}\hat a^*(k)}{\sqrt{(2\pi)^3 2\varepsilon(\vec k)}}\right)^j\left(\int \mathrm{d}\vec k\frac{\mathrm{e}^{\mathrm{i}kx}\hat a(k)}{\sqrt{(2\pi)^3 2\varepsilon(\vec k)}}\right)^{n-j}. &(9.291)\end{aligned}$$

Note that, if

$$\int \frac{1}{\varepsilon(\vec k)}\mathrm{d}\vec k<\infty, \tag{9.292}$$

then $\hat\phi(x)$ is a well defined (unbounded) operator on the Fock space and

$$:\hat\phi(x)^m := \hat\phi(x)^n+\sum_{k=1}^{[m/2]}c_k\hat\phi(x)^{m-2k}. \tag{9.293}$$

Unfortunately, if (9.281) is satisfied, the constants c_k are divergent, in all dimensions $d=1,2,\dots$. The free Hamiltonian can be rewritten as

$$H_0=\int\mathrm{d}\vec x\int\mathrm{d}\vec y :\hat\phi(0,\vec x)\hat\phi(0,\vec y): g(\vec x-\vec y)+\int\mathrm{d}\vec x :\hat\pi(0,\vec x)^2:, \tag{9.294}$$

where

$$g(x)=\int \mathrm{e}^{\mathrm{i}\vec k\vec x}\varepsilon(\vec k)^2\mathrm{d}\vec k. \tag{9.295}$$

We also introduce the Feynman propagator

$$D^{\mathrm{c}}(x-y)=\mathrm{i}\Big(\Omega|\mathrm{T}\big(\hat\phi(x)\hat\phi(y)\big)\Omega\Big) \tag{9.296}$$

We will also use the Feynman propagator in the energy-momentum representation

$$D^{\rm c}(k)=\int D^{\rm c}(x){\rm e}^{-{\rm i}kx}{\rm d}x. \tag{9.297}$$

The Feynman propagator turns out to be one of the inverses of $\varepsilon(\vec{k})^2-(k^0)^2$:

Theorem 9.4.

$$D^{\rm c}(k)=\frac{1}{\varepsilon(\vec{k})^2-(k^0)^2-{\rm i}0}. \tag{9.298}$$

Proof. First we compute in the space-time representation:

$$\begin{aligned}
D^{\rm c}(t,\vec{x}) &= {\rm i}\int\left({\rm e}^{-{\rm i}\varepsilon(\vec{k})t+{\rm i}\vec{k}\vec{x}}\theta(t)+{\rm e}^{{\rm i}\varepsilon(\vec{k})t-{\rm i}\vec{k}\vec{x}}\theta(-t)\right)\frac{{\rm d}\vec{k}}{(2\pi)^3 2\varepsilon(\vec{k})}\\
&= {\rm i}\int\left({\rm e}^{-{\rm i}\varepsilon(\vec{k})t}\theta(t)+{\rm e}^{{\rm i}\varepsilon(\vec{k})t}\theta(-t)\right){\rm e}^{{\rm i}\vec{k}\vec{x}}\frac{{\rm d}\vec{k}}{(2\pi)^3 2\varepsilon(\vec{k})},
\end{aligned}$$

where we used the parity of ε (9.282). Next we go to the energy-momentum representation:

$$\begin{aligned}
D^{\rm c}(k^0,\vec{k}) &= {\rm i}\int\int D^{\rm c}(t,\vec{x}){\rm e}^{{\rm i}k^0t-{\rm i}\vec{k}\vec{x}}{\rm d}t{\rm d}\vec{k}\\
&= {\rm i}\int\Big({\rm e}^{-{\rm i}\varepsilon(\vec{k})t}\theta(t)+{\rm e}^{{\rm i}\varepsilon(\vec{k})t}\theta(-t)\Big){\rm e}^{{\rm i}k^0t}\frac{{\rm d}t}{2\varepsilon(\vec{k})}\\
&= {\rm i}\int_0^\infty\Big({\rm e}^{-{\rm i}\varepsilon(\vec{k})t+{\rm i}k^0t}+{\rm e}^{-{\rm i}\varepsilon(\vec{k})t-{\rm i}k^0t}\frac{{\rm d}t}{2\varepsilon(\vec{k})}\\
&= \frac{1}{2\varepsilon(\vec{k})(\varepsilon(\vec{k})-k^0-{\rm i}0)}+\frac{1}{2\varepsilon(\vec{k})(\varepsilon(\vec{k})+k^0-{\rm i}0)}\\
&= \frac{1}{\varepsilon(\vec{k})^2-(k^0)^2-{\rm i}0}.
\end{aligned}$$

□

9.2.2 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

$$H=H_0+W(t), \tag{9.299}$$

where the perturbation (in the Schrödinger picture) is

$$W(t) = \sum_j\int{\rm d}\vec{x}f_j\big(t,\vec{x}\big):\hat{\phi}(0,\vec{x})^j:. \tag{9.300}$$

The Hamiltonian in the interaction picture is therefore

$$H_{\rm Int}(t)=\sum_j\int{\rm d}\vec{x}f_j\big(t,\vec{x}\big):\hat{\phi}(t,\vec{x})^j:. \tag{9.301}$$

Let S denote the scattering operator for (9.299). We would like to compute

$$(\Omega|S\Omega). \tag{9.302}$$

(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 $p_n, \dots, p_1$ 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 $D(x_n, \dots, x_1)$.

(4) We sum up all diagrams divided by symmetry factors and integrate :

$$\big(\Omega|S\Omega\big) = \sum_{\substack{\text{all diag.} \\ n \text{ vertices} \\ \text{no ext. lines}}} \int \mathrm{d}x_n \dots \int \mathrm{d}x_1 \frac{D(x_n, \dots, x_1)}{[D]!}. \tag{9.303}$$

Instead of (3) we can use

(3)' Rules about evaluating diagrams in the energy-momentum approach

- (i) For the jth vertex with we put

$$-\mathrm{i}f_{p_j}(k_1 + \dots + k_{p_j}) = -\mathrm{i} \int \mathrm{d}x \mathrm{e}^{-\mathrm{i}(k_1 + \dots + k_{p_j})x} f_{p_j}(x). \tag{9.304}$$

- (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 $\int \mathrm{d}x_n \dots \int \mathrm{d}x_1 D(x_n, \dots, x_1)$.

By the Linked Cluster Theorem (9.303) can be rewritten as

$$\log \big(\Omega|S\Omega\big) = \sum_{\substack{\text{all con. diag.} \\ n \text{ vertices} \\ \text{no ext. lines}}} \int \mathrm{d}x_n \dots \int \mathrm{d}x_1 \frac{D(x_n, \dots, x_1)}{[D]!}.$$

9.2.3 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. 9.2.2. 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

$$E = \sum_{n=0}^{\infty} \sum_{\substack{\text{all con. diag.} \\ n \text{ vertices} \\ \text{no ext. lines}}} \int \mathrm{d}x_n \cdots \int \mathrm{d}x_2 \int \mathrm{d}\vec{x}_1 \frac{D(x_n,\dots,0,\vec{x}_1)}{[D]!}.$$

9.2.4 Green's functions

Recall that the *N-point Green's function* is defined for $x_N,\dots,x_1$ as follows:

$$\begin{aligned} & \langle \hat{\phi}(x_N)\cdots\hat{\phi}(x_1)\rangle \\ := & \Big(\Omega^+ | \mathrm{T}\big(\hat{\phi}(x_N)\cdots\cdots\hat{\phi}(x_1)\big)\Omega^-\Big), \end{aligned} \tag{9.305}$$

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:

$$\hat{\phi}(t,\vec{x}) = \mathrm{Texp}\Big(-\mathrm{i}\int_t^0 \hat{H}(s)\mathrm{d}s\Big)\hat{\phi}(0,\vec{x})\mathrm{Texp}\Big(-\mathrm{i}\int_0^t \hat{H}(s)\mathrm{d}s\Big). \tag{9.306}$$

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:

$$\langle\hat{\phi}(x_N)\cdots\hat{\phi}(x_1)\rangle = \mathrm{i}^N \frac{\partial^N}{\partial f(x_N)\cdots\partial f(x_1)} Z(f)\Big|_{f=0}. \tag{9.307}$$

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*:

$$\begin{aligned}&\langle\hat{\phi}(k_n)\cdots\hat{\phi}(k_1)\rangle_{\mathrm{amp}}\\ =&\ (k_n^2+m^2)\cdots(k_1^2+m^2)\langle\hat{\phi}(k_n)\cdots\hat{\phi}(k_1)\rangle.\end{aligned}\tag{9.308}$$

Amputated Green's functions can be used to compute scattering amplitudes:

$$\begin{aligned}&\Big(k_{m^+}^+,\dots,k_1^+|\,\hat{S}\,|k_{m^-}^-,\dots,k_1^-\Big)\\ =&\ \frac{\langle\hat{\phi}(k_1^+)\cdots\hat{\phi}(k_{m^+}^+)\hat{\phi}(-k_{m^-}^-)\cdots\hat{\phi}(-k_1^-)\rangle_{\mathrm{amp}}}{\sqrt{(2\pi)^{3(m^++m^-)}}\sqrt{2\varepsilon(k_1^+)}\cdots\sqrt{2\varepsilon(k_{m^+}^+)}\sqrt{2\varepsilon(k_{m^-}^-)}\cdots\sqrt{2\varepsilon(k_1^-)}},\end{aligned}\tag{9.309}$$

where all $k_i^\pm$ are on shell, that is $k_i^\pm=\big(\varepsilon(\vec{k}_i^\pm),\vec{k}_i^\pm\big)$.

9.2.5 Feynman diagrams for the scattering operator

We would like to compute the scattering operator, representing it as Wick's polynomial:

$$S=s(\hat{a}^*,\hat{a}).\tag{9.310}$$

The Feynman rules for scattering operator follow from (9.309) 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 $\int \mathrm{d}x f(x)\hat{\phi}_{\mathrm{fr}}(x)$.

(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 $D(x_n, \dots, x_1; a^*, a)$.

(4) We sum up all diagrams divided by symmetry factors:

$$s(a^*, a) = \sum_{n=0}^{\infty} \sum_{\substack{\text{all diag.} \\ n \text{ vertices}}} \int \mathrm{d}x_n \cdots \int \mathrm{d}x_1 \frac{D(x_n, \dots, x_1; a^*, a)}{[D]!}. \tag{9.311}$$

Instead of (3) we can use

(3)' Rules about evaluating diagrams in the energy-momentum approach

(i) For a vertex with legs $k_1, \dots, k_p$ we put

$$-\mathrm{i}f(k_1 + \cdots + k_n) = -\mathrm{i} \int \mathrm{d}x \mathrm{e}^{-\mathrm{i}(k_1 + \cdots + k_p)x} f(x). \tag{9.312}$$

(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 $\int \mathrm{d}x_n \cdots \int \mathrm{d}x_1 D(x_n, \dots, x_1; a^*, a)$.

Recall that in (9.255) we defined the linked scattering operator. It can be computed using Feynman diagrams:

$$s_{\mathrm{link}}(a^*, a) \tag{9.313}$$

$$= \sum_{n=0}^{\infty} \sum_{\substack{\text{linked diag.} \\ n \text{ vertices}}} \int \cdots \int \frac{D(x_n, \dots, x_1; a^*, a)}{[D]!} \mathrm{d}x_n \cdots \mathrm{d}x_1 \tag{9.314}$$

$$= \exp\left(\sum_{n=0}^{\infty} \sum_{\substack{\text{con. linked diag.} \\ n \text{ vertices}}} \int \cdots \int \frac{D(x_n, \dots, x_1; a^*, a)}{[D]!} \mathrm{d}x_n \cdots \mathrm{d}x_1 \right). \tag{9.315}$$

9.2.6 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

$$D_{\mathrm{sc}}(E) \tag{9.316}$$

$$:=2\pi \int \mathrm{d}x_n \cdots \int \mathrm{d}x_2 \int \mathrm{d}\vec{x}_1 \delta(E - H_0) D(x_n, \dots, x_2, 0, \vec{x}_1) \delta(E - H_0), \tag{9.317}$$

where we use the operator interpretation of D. Then

$$s_{\mathrm{link}}(a^*, a) \tag{9.318}$$

$$= \sum_{\text{linked diag.}} \int \mathrm{d}E \frac{D_{\mathrm{sc}}(E; a^*, a)}{[D]!} \tag{9.319}$$

$$= \exp\Big(\sum_{\text{con. linked diag.}} \int \mathrm{d}E \frac{D_{\mathrm{sc}}(E; a^*, a)}{[D]!} \Big). \tag{9.320}$$

9.2.7 Quadratic interactions

Suppose that (in the Schrödinger picture)

$$\hat{H}(t) := \int \hat{a}^*(k)\hat{a}(k)\mathrm{d}\vec{k} + \int \frac{1}{2}\kappa(t,\vec{x}){:}\hat{\phi}^2(0,\vec{x}){:}\Big)\mathrm{d}\vec{x}. \tag{9.321}$$

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

$$(-1)^n \int \mathrm{d}x_n \cdots \int \mathrm{d}x_1 \kappa(x_n) D^{\mathrm{c}}(x_n - x_{n-1}) \cdots \kappa(x_1) D^{\mathrm{c}}(x_1 - x_n) \tag{9.322}$$

$$=(-1)^n \int \frac{\mathrm{d}k_n}{(2\pi)^4} \cdots \int \frac{\mathrm{d}k_1}{(2\pi)^4} \kappa(k_1 - k_n) D^{\mathrm{c}}(k_n) \cdots \kappa(k_2 - k_1) D^{\mathrm{c}}(k_1) \tag{9.323}$$

$$=(-1)^n \mathrm{Tr}(\kappa D^{\mathrm{c}})^n. \tag{9.324}$$

The group of symmetries of the loop with n vertices is the dihedral group D_n, which has $2n$ elements. Therefore,

$$\begin{aligned}\mathcal{E} &:= \mathrm{i}\log(\Omega|\hat{S}\Omega) = \mathrm{i}\sum_{n=2}^{\infty} \frac{(-1)^n}{2n} \mathrm{Tr}(\kappa D^{\mathrm{c}})^n \\ &= \frac{\mathrm{i}}{2}\mathrm{Tr}\Big(-\log(1 + \kappa D^{\mathrm{c}}) + \kappa D^{\mathrm{c}}\Big) =: \sum_{n=2}^{\infty} \mathcal{E}_n.\end{aligned} \tag{9.325}$$

10 Method of characteristics

10.1 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

$$\hat{\partial}_x f(x)g(x) = \partial_x f(x)g(x) + f(x)\partial_x g(x). \tag{10.326}$$

There are situations when we could use both kinds of notation: $\hat{\partial}_x$ and ∂_x, as in the last term of (10.326). In such a case we make a choice based on esthetic reasons.

10.2 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

$$\begin{aligned} \big(\partial_t + v(t,x)\partial_x + f(t,x)\big)\Psi(t,x) &= 0, \\ \Psi(0,x) &= \Psi(x). \end{aligned} \tag{10.327}$$

To solve it one finds first the solution of

$$\left\{ \begin{array}{lll} \partial_t x(t,y) &=& v(t,x(t,y)) \\ x(0,y) &=& y; \end{array} \right. \tag{10.328}$$

Let $x \mapsto y(t,x)$ be the inverse function.

Proposition 10.1. *Set*

$$F(t,y) := \int_0^t f\big(s, x(s,y)\big)\mathrm{d}s.$$

Then

$$\Psi(t,x) := \mathrm{e}^{-F\big(t,y(t,x)\big)}\Psi\big(y(t,x)\big)$$

is the solution of (10.327).

Proof. Set

$$\Phi(t,y) := \Psi\big(t, x(t,y)\big). \tag{10.329}$$

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 (10.327) can be rewritten as

$$\begin{aligned}\big(\partial_t + f\big(t, x(t,y)\big)\big)\Phi(t,y) &= 0,\\ \Phi(0,y) &= \Psi(y).\end{aligned} \tag{10.330}$$

(10.330) 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

$$\big(v(x)\partial_x + f(x)\big)\Psi(x) = 0. \tag{10.331}$$

Again, first one finds solutions of

$$\partial_t x(t) = v\big(x(t)\big). \tag{10.332}$$

Then we try to find a manifold $\mathcal{Z}$ in $\mathcal{X}$ of codimension 1 that crosses each curve given by a solution of (10.331) exactly once. If the field is everywhere nonzero, this should be possible at least locally. Then we can define a family of solutions of (10.331) denoted $x(t,z)$, $z \in \mathcal{Z}$, satisfying the boundary conditions

$$x(0,z) = z, \quad z \in \mathcal{Z}. \tag{10.333}$$

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 10.2. *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 (10.327).

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 (10.331) together with the boundary conditions as

$$\begin{aligned}\big(\partial_t + f\big(x(t,z)\big)\big)\Phi(t,z) &= 0,\\ \Phi(0,z) &= \Psi(z).\end{aligned} \tag{10.334}$$

(10.334) is solved by

$$\Phi(t,z) := \mathrm{e}^{-F(t,z)}\Psi(z).$$

□

10.3 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

$$\begin{aligned} \left(\partial_t + v(t,x)\partial_x + \alpha \mathrm{div}v(t,x)\right)\Psi(t,x) &= 0, \\ \Psi(0,x) &= \Psi(x), \end{aligned} \tag{10.335}$$

Proposition 10.3. *(10.335) is solved by*

$$\Psi(t,x) := \big(\det \partial_x y(t,x)\big)^{\alpha} \Psi(y(t,x)). \tag{10.336}$$

Proof. We introduce $\Phi(t,y)$ as in (10.329) and rewrite (10.335) as

$$\begin{aligned} \big(\partial_t + \alpha \mathrm{div}v\big(t, x(t,y)\big)\big)\Phi(t,y) &= 0, \\ \Phi(0,y) &= \Psi(y) \end{aligned} \tag{10.337}$$

We have the following identity for the determinant of a matrix valued function $t \mapsto A(t)$:

$$\partial_t \det A(t) = \mathrm{Tr}\left(\partial_t A(t) A(t)^{-1}\right) \det A(t). \tag{10.338}$$

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, (10.337) 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

$$\left(v(x)\partial_x + \alpha \mathrm{div}v(x)\right)\Psi(x) = 0. \tag{10.339}$$

We introduce the a hypersurface $\mathcal{Z}$ and solutions $x(t,z)$, as described before Prop. 10.2.

Proposition 10.4. *Set*

$$w(x) := \partial_z x\big(t(x), z(x)\big).$$

Then the solution of (10.339) which on $\mathcal{Z}$ equals $\Psi(z)$ is

$$\Psi(x) := \big(\det[v(x), w(x)]\big)^{-\alpha} \Psi\big(z(x)\big). \tag{10.340}$$

Note that if $\mathcal{X}$ is one-dimensional, so that we can locally identify it with $\mathbb{R}$ and v is a number, (10.340) becomes $\Psi(x) = C\big(v(x)\big)^{-\alpha}$.

10.4 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

$$\langle f | av_1, \dots, av_d \rangle = |\det a|^\alpha \langle f | v_1, \dots, v_d \rangle, \tag{10.341}$$

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

$$x \mapsto \langle \Psi | \partial_{x^1}, \dots, \partial_{x^d} \rangle(x), \tag{10.342}$$

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

$$\Psi(x) = |\partial_x x'|^\alpha \, \Psi'(x'). \tag{10.343}$$

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:

$$\int \left| \Psi(x) |\mathrm{d}x|^{\frac{1}{p}} \right|^p = \int |\Psi(x)|^p \mathrm{d}x = \|\phi\|_p^p. \tag{10.344}$$

Proposition 10.5. *If $v(x)\partial_x$ is a vector field, the operator*

$$v(x)\partial_x + \alpha \mathrm{div} v(x) \tag{10.345}$$

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 (10.336) can be written as an α-density:

$$
\Psi(t,x)|\mathrm{d}x|^\alpha := |\det\partial_x y(t,x)|^\alpha\Psi(y(t,x))|\mathrm{d}x|^\alpha \tag{10.346}
$$

Also (10.340) is naturally an α-density.

11 Hamiltonian mechanics

11.1 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 $\wedge^2T\mathcal{X}$. 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*

$$
\partial_t y(t) = \omega^{-1}\mathrm{d}_yH(t,y(t)). \tag{11.347}
$$

Proposition 11.1. *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 11.2. $\{\cdot,\cdot\}$ *is a bilinear antisymmetric operation satisfying the Jacobi identity*

$$
\{F,\{G,H\}\}+\{H,\{F,G\}\}+\{G,\{H,F\}\}=0 \tag{11.348}
$$

and the Leibnitz identity

$$
\{F,GH\}=\{F,G\}H+G\{F,H\}. \tag{11.349}
$$

Proposition 11.3. *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,

$$\frac{\mathrm{d}}{\mathrm{d}t}H\big(t,y(t)\big) = \partial_t H\big(t,y(t)\big).$$

11.2 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

$$\omega = \mathrm{d}p_i \wedge \mathrm{d}x^i. \tag{11.350}$$

The Hamilton equations read

$$\begin{aligned} \partial_t x &= \partial_p H(t,x,p), \\ \partial_t p &= -\partial_x H(t,x,p). \end{aligned} \tag{11.351}$$

The Poisson bracket is

$$\{F,G\} = \partial_{x^i} F \partial_{p_i} G - \partial_{p_i} F \partial_{x^i} G. \tag{11.352}$$

Note that Prop 11.1 and 11.2 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 11.4. *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 (11.4) implies Prop. 11.1. Similarly, to see Prop. 11.2 we first check the Jacobi and Leibniz identity for (11.352).

11.3 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*

$$\theta = \sum_i p_i \mathrm{d}x^i, \tag{11.353}$$

(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

$$\omega = \mathrm{d}\theta = \sum_i \mathrm{d}p_i \wedge \mathrm{d}x^i. \tag{11.354}$$

Thus locally we can apply the formalism of symplectic vector spaces. In particular, the Hamilton equations have the form (11.351) and the Poisson bracket (11.352).

11.4 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 11.5. *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

$$0 = \langle \mathrm{d}H | v \rangle = -\langle \omega^{-1}\mathrm{d}H | \omega v \rangle. \tag{11.355}$$

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.

11.5 Lagrangian manifolds in a cotangent bundle

Proposition 11.6. *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*

$$\big\{\big(x, \mathrm{d}S(x)\big) \ : \ x \in \mathcal{U}\big\} \tag{11.356}$$

is a Lagrangian submanifold of $T^{\#}\mathcal{X}$.

Proof. Tangent space of (11.356) 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 (11.356). 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

$$\mathrm{d}T = i_{\mathcal{L}}^{\#}\theta. \tag{11.357}$$

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

$$\mathcal{L}^{\mathrm{cov}} \ni [\gamma] \mapsto T([\gamma]) := \int_\gamma \theta. \tag{11.358}$$

Exactly as above we see that (11.358) does not depend on the choice of γ and that (11.357) is true.

11.6 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

$$\mathcal{R} := (\rho(y), y) \in \mathcal{Y}_2 \times \mathcal{Y}_1. \tag{11.359}$$

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

$$\mathcal{X}_2 \times \mathcal{X}_1 \ni (x_2, x_1) \mapsto S(x_2, x_1). \tag{11.360}$$

is called a generating function of the transformation ρ if it satisfies

$$\xi_2 = -\nabla_{x_2} S(x_2, x_1), \qquad \xi_1 = \nabla_{x_1} S(x_2, x_1). \tag{11.361}$$

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.

11.7 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

$$\mathcal{U} \ni v \mapsto S(v) \in \mathbb{R} \tag{11.362}$$

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

$$\mathcal{U} \ni v \mapsto p(v) := \partial_v S(v) \in \mathcal{X}^{\#} \tag{11.363}$$

is an injective function. Let $\tilde{\mathcal{U}}$ be the image of (11.363). 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 (11.363). The *Legendre transform* of S is defined as

$$\tilde{S}(p) := pv(p) - S\big(v(p)\big).$$

Theorem 11.7. (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 11.8. *Suppose that S depends on an additional parameter α. Then we have the identity*
$$\partial_\alpha S\big(\alpha,v(\alpha,p)\big)=-\partial_\alpha\tilde{S}(\alpha,p).\tag{11.364}$$

Proof. Indeed,
$$\begin{aligned}\partial_\alpha\tilde{S}(\alpha,p)&=\partial_\alpha\big(pv(\alpha,p)-S\big(\alpha,v(\alpha,p)\big)\\&=p\partial_\alpha v(\alpha,p)-\partial_\alpha S(\alpha,v(\alpha,p)\big)-\partial_v S(\alpha,v(\alpha,p)\big)\partial_\alpha v(\alpha,p)\\&=-\partial_\alpha S\big(\alpha,v(\alpha,p)\big).\end{aligned}$$
□

11.8 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

$$\rho_t\big(y(0)\big) = y(t), \tag{11.365}$$

where $y(t)$ solves

$$\partial_t y(t) = \omega^{-1} \mathrm{d}_y H\big(t, y(t)\big). \tag{11.366}$$

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

$$G^{-1}(0) := \{(t, \tau, y) \ : \ G(t, \tau, y) = 0\} \tag{11.367}$$

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 11.9. *Let $\mathcal{L}$ be a Lagrangian manifold in $\mathcal{Y}$. The set*

$$\mathcal{M} := \{(t, \tau, y) \ : \ y \in \rho_t(\mathcal{L}), \ \tau = H(t, y), \ t \in \mathbb{R}\} \tag{11.368}$$

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*

$$\kappa(\mathcal{M}) \cap \{0\} \times \mathcal{Y} = \{0\} \times \mathcal{L}; \tag{11.369}$$

(4) *every point in $\kappa(\mathcal{M})$ is connected to (11.369) 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

$$\langle \mathrm{d}_y H(t_0, y_0) | v \rangle \partial_\tau + v \tag{11.370}$$

is tangent to $\mathcal{M}$. Vectors of the form (11.370) 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 $\mathcal{M}$:

$$\partial_t + \partial_t H(t_0, y_0) \partial_\tau + \omega^{-1} \mathrm{d}_y H(t_0, y_0). \tag{11.371}$$

The symplectic form applied to (11.370) and (11.371) is

$$-\langle \mathrm{d}_y H(t_0, y_0) | v \rangle + \langle \omega | v, \omega^{-1} \mathrm{d}_y H(t_0, y_0) \rangle = 0. \tag{11.372}$$

(11.370) and (11.371) 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 11.5, the vector

$$\begin{aligned} & \sigma^{-1}\mathrm{d}G(t_0, \tau_0, y_0) \\ = \; & \sigma^{-1}\big(\partial_t H(t_0, y_0)\mathrm{d}t + \mathrm{d}_y H(t_0, y_0) - \mathrm{d}\tau\big) \end{aligned} \tag{11.373}$$

is tangent to $\mathcal{M}$. But (11.373) coincides with (11.371). Hence

$$\partial_t + \omega^{-1}\mathrm{d}_y H(t_0, y_0). \tag{11.374}$$

is tangent to $\kappa(\mathcal{M})$. This means that $\kappa(\mathcal{M})$ is invariant for the Hamiltonian flow generated by $H(t, y)$. Consequently,

$$\kappa(\mathcal{M}) \supset \bigcup_{t\in\mathbb{R}} \{t\} \times \rho_t(\mathcal{L}). \tag{11.375}$$

$\kappa(\mathcal{M})$ cannot be larger than the rhs of (11.375), because then condition (4) would be violated. □

11.9 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

$$\begin{aligned} \partial_t S(t, x) - H\big(t, x, \partial_x S(t, x)\big) &= 0, \\ S(0, x) &= S(x). \end{aligned} \tag{11.376}$$

(11.376) 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

$$G^{-1}(0) := \{(t, \tau, x, p) \in \mathrm{T}^{\#}\mathbb{R} \times \mathrm{T}^{\#}\mathcal{X} \ : \ \tau - H(t, x, p) = 0\} \tag{11.377}$$

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 (11.376) 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

$$\kappa^{-1}\big(0, y_0, p(0,y_0)\big) \tag{11.378}$$

$$\text{with} \quad \kappa^{-1}\big(t, x(t,y), p(t,y)\big). \tag{11.379}$$

We can take γ as the union of two disjoint segments: $\gamma = \gamma_1 \cup \gamma_2$. γ_1 is a curve in (11.377) with the time variable equal to zero ending at

$$\kappa^{-1}\big(0, y, p(0,y)\big). \tag{11.380}$$

Clearly, since $\mathrm{d}s = 0$ along γ_1, we have

$$S(y_0) + \int_{\gamma_1} (p\mathrm{d}x - \tau\mathrm{d}s) = S(y_0) + \int_{\gamma_1} p\mathrm{d}x = S(y). \tag{11.381}$$

γ_2 starts at (11.380), ends at (11.379), 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

$$\int_{\gamma_2} (p\mathrm{d}x - \tau\mathrm{d}s) = \int_0^t \Big(p(s,y)\partial_s x(s,y) - H\big(s, x(s,y), p(s,y)\big)\Big)\mathrm{d}s. \tag{11.382}$$

Putting together (11.381) and (11.382) we obtain the formula for the generating function of $\mathcal{M}$ viewed as a function on $\mathcal{M}$:

$$\begin{aligned} T(t,y) &= S(y) \\ &\quad + \int_0^t \Big(p(s,y)\partial_s x(s,y) - H\big(s, x(s,y), p(s,y)\big)\Big)\mathrm{d}s. \end{aligned} \tag{11.383}$$

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:

$$S(t,x) = T\big(t, y(t,x)\big). \tag{11.384}$$

11.10 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:

$$\frac{\mathrm{d}}{\mathrm{d}t}x(t) = v(t), \tag{11.385}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\partial_v L\big(t, x(t), v(t)\big) = \partial_x L\big(x(t), v(t)\big). \tag{11.386}$$

Using the Lagrangian, the generating function (11.383) can be rewritten as

$$T(t,y) = S(y) + \int_0^t L\big(s, x(s,y), \dot{x}(s,y)\big)\mathrm{d}s.$$

Lagrangians often have quadratic dependence on velocities:

$$L(x,v) = \frac{1}{2}vg^{-1}(x)v + vA(x) - V(x). \tag{11.387}$$

The momentum and the velocity are related as

$$p = g^{-1}(x)v + A(x), \quad v = g(x)\big(p - A(x)\big). \tag{11.388}$$

The corresponding Hamiltonian depends quadratically on the momenta:

$$H(x,p) = \frac{1}{2}\big(p - A(x)\big)g(x)\big(p - A(x)\big) + V(x). \tag{11.389}$$

11.11 Action integral

In this subsection, which is independent of Subsect. 11.9, we will rederive the formula for the generating function of the Hamiltonian flow constructed (11.383). Unlike in Subsect. 11.9, 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

$$I(t,\alpha) := \int_0^t L(x(s,\alpha), v(s,\alpha))\mathrm{d}s. \tag{11.390}$$

Theorem 11.10.

$$\partial_\alpha I(t,\alpha) = p(x(t,\alpha), v(t,\alpha))\partial_\alpha x(t,\alpha) - p(x(0,\alpha), v(0,\alpha))\partial_\alpha x(0,\alpha). \tag{11.391}$$

Proof.

$$\begin{aligned}
\partial_\alpha I(t,\alpha) &= \int_0^t \partial_x L(x(s,\alpha), \dot{x}(s,\alpha))\partial_\alpha x(s,\alpha)\mathrm{d}s \\
&\quad + \int_0^t \partial_{\dot{x}} L(x(s,\alpha), \dot{x}(s,\alpha))\partial_\alpha \dot{x}(s,\alpha)\mathrm{d}s \\
&= \int_0^t \Big(\partial_x L(x(s,\alpha), \dot{x}(s,\alpha)) - \frac{\mathrm{d}}{\mathrm{d}s}\partial_{\dot{x}} L(x(s,\alpha), \dot{x}(s,\alpha)) \Big) \partial_\alpha x(s,\alpha)\mathrm{d}s \\
&\quad + p(x(s,\alpha), v(s,\alpha))\partial_\alpha x(s,\alpha)\Big|_{s=0}^{s=t}.
\end{aligned}$$

□

Theorem 11.11. *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*

$$x(0,y) = y, \quad p(0,y) = \partial_y S(y). \tag{11.392}$$

Let $I(t,y)$ be the action along these trajectories defied as in (11.390). We suppose that we can invert the $y \mapsto x(t,y)$ obtaining the function $x \mapsto y(t,x)$. Then

$$S(t,x) := I\big(t, y(t,x)\big) + S(y(t,x)) \tag{11.393}$$

is the solution of (11.376), and

$$\partial_x S(t,x) = p\big(t, y(t,x)\big). \tag{11.394}$$

Proof. We have

$$\begin{aligned}
\partial_y \big(I(t,y) + S(y)\big) &= p(t,y)\partial_y x(t,y) - p(0,y)\partial_y x(0,y) + \partial_y S(y) \\
&= p(t,y)\partial_y x(t,y).
\end{aligned} \tag{11.395}$$

Hence,

$$\partial_x S(t,x) = \partial_x\Big(I\big(t,y(t,x)\big)+S\big(y(t,x)\big)\Big) \tag{11.396}$$
$$= p(t,y)\partial_y x(t,y)\partial_x y(t,x) = p(t,y). \tag{11.397}$$

Now

$$L\big(x(t,y),\dot{x}(t,y)\big) = \partial_t I(t,y) = \partial_t\big(I(t,y)+S(y)\big) \tag{11.398}$$
$$= \partial_t S\big(t,x(t,y)\big)+\partial_x S\big(t,x(t,y)\big)\dot{x}(t,y). \tag{11.399}$$

Therefore,

$$\partial_t S\big(t,x(t,y)\big) = L\big(x(t,y),\dot{x}(t,y)\big)-p(t,y)\dot{x}(t,y) \tag{11.400}$$
$$= -H\big(x(t,y),p(t,y)\big). \tag{11.401}$$

□

11.12 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

$$\mathcal{L} := F_1^{-1}(c_1)\cap\cdots\cap F_m^{-1}(c_m). \tag{11.402}$$

We assume that

$$\mathrm{d}F_1\wedge\cdots\wedge\mathrm{d}F_m\neq 0 \tag{11.403}$$

on $\mathcal{L}$. Then $\mathcal{L}$ is a manifold of dimension $2d-m$.

Proposition 11.12. *Suppose that $F_1,\dots,F_m$ are in involution and satisfy (11.403). Then $m\leq d$ 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 (11.403) 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 (11.402).

12 Quantizing symplectic transformations

12.1 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:

$$\rho = \begin{bmatrix} a & b \\ c & d \end{bmatrix}, \quad \omega := \begin{bmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{bmatrix}. \tag{12.404}$$

$\rho \in Sp(\mathbb{R}^d \oplus \mathbb{R}^d)$ iff

$$\rho^{\#}\omega\rho = \omega,$$

which means

$$a^{\#}d - c^{\#}b = \mathbb{1}, \quad c^{\#}a = a^{\#}c, \quad d^{\#}b = b^{\#}d. \tag{12.405}$$

If

$$\begin{aligned} \hat{x}'^i &= a^i_j \hat{x}^j + b^{ij}\hat{p}_j, \\ \hat{p}'_i &= c_{ij}\hat{x}^j + d^j_i \hat{p}_j, \end{aligned} \tag{12.406}$$

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.

12.2 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.

12.3 Generating function of a symplectic transformation

Let ρ be as above with b invertible. We then have the factorization

$$\rho = \begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} \mathbb{1} & 0 \\ e & \mathbb{1} \end{bmatrix} \begin{bmatrix} 0 & b \\ -b^{\#-1} & 0 \end{bmatrix} \begin{bmatrix} \mathbb{1} & 0 \\ f & \mathbb{1} \end{bmatrix}, \tag{12.407}$$

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

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}\begin{bmatrix} x_1 \\ \xi_1 \end{bmatrix} = \begin{bmatrix} x_2 \\ \xi_2 \end{bmatrix} \tag{12.408}$$

iff

$$\nabla_{x_1}S(x_1,x_2) = -\xi_1, \quad \nabla_{x_2}S(x_1,x_2) = \xi_2. \tag{12.409}$$

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

$$\pm U_\rho(x_1,x_2) = \pm(2\pi\mathrm{i}\hbar)^{-\frac{d}{2}}\sqrt{-\det\nabla_{x_1}\nabla_{x_2}S}\ \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}S(x_1,x_2)}.$$

12.4 Harmonic oscillator

As an example, we cosider the 1-dimensional harmonic oscillator with $\hbar = 1$. Let $\chi(x,\xi) := \frac{1}{2}\xi^2 + \frac{1}{2}x^2$. Then $\mathrm{Op}(\chi) = \frac{1}{2}D^2 + \frac{1}{2}x^2$. The Weyl-Wigner symbol of $\mathrm{e}^{-t\mathrm{Op}(\chi)}$ equals

$$w(t,x,\xi) = (\mathrm{ch}\tfrac{t}{2})^{-1}\exp(-(x^2+\xi^2)\mathrm{th}\tfrac{t}{2}). \tag{12.410}$$

Its integral kernel is given by

$$W(t,x,y) = \pi^{-\frac{1}{2}}(\mathrm{sh}t)^{-\frac{1}{2}}\exp\left(\frac{-(x^2+y^2)\mathrm{ch}t + 2xy}{2\mathrm{sh}t}\right).$$

$\mathrm{e}^{-\mathrm{i}t\mathrm{Op}(\chi)}$ has the Weyl-Wigner symbol

$$w(\mathrm{i}t,x,\xi) = (\cos\tfrac{t}{2})^{-1}\exp\left(-\mathrm{i}\,(x^2+\xi^2)\mathrm{tg}\tfrac{t}{2}\right) \tag{12.411}$$

and the integral kernel

$$W(\mathrm{i}t,x,y) = \pi^{-\frac{1}{2}}|\sin t|^{-\frac{1}{2}}\mathrm{e}^{-\frac{\mathrm{i}\pi}{4}}\mathrm{e}^{-\frac{\mathrm{i}\pi}{2}[\frac{t}{\pi}]}\exp\left(\frac{-(x^2+y^2)\cos t + 2xy}{2\mathrm{i}\sin t}\right).$$

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

$$\begin{aligned} W(0,x,y) &= \delta(x-y), \\ W(\tfrac{\mathrm{i}\pi}{2},x,y) &= (2\pi)^{-\frac{1}{2}}\mathrm{e}^{-\frac{\mathrm{i}\pi}{4}}\mathrm{e}^{-\mathrm{i}xy}, \\ W(\mathrm{i}\pi,x,y) &= \mathrm{e}^{-\frac{\mathrm{i}\pi}{2}}\delta(x+y), \\ W(\tfrac{\mathrm{i}3\pi}{2},x,y) &= (2\pi)^{-\frac{1}{2}}\mathrm{e}^{-\frac{\mathrm{i}3\pi}{4}}\mathrm{e}^{\mathrm{i}xy}. \end{aligned}$$

Corollary 12.1. (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* $\begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}$.

12.5 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 12.2. *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 $\hbar$,*

$$\int \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)}a(x)\mathrm{d}x \simeq (2\pi\hbar)^{-\frac{d}{2}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}\mathrm{inert}\,\partial_x^2 S(x_0)}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x_0)}a(x_0) + O(\hbar^{-\frac{d}{2}+1}). \tag{12.412}$$

Proof. The left hand side of (12.2) is approximated by

$$\int \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x_0)+\frac{\mathrm{i}}{2\hbar}(x-x_0)\partial_x^2 S(x_0)(x-x_0)}a(x_0)\mathrm{d}x, \tag{12.413}$$

which equals the right hand side of (12.2). □

12.6 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

$$\mathrm{FIO}(a,S)(x_2,x_1) = (2\pi\hbar)^{-\frac{d}{2}}\left(\nabla_{x_2}\nabla_{x_1}S(x_2,x_1)\right)^{\frac{1}{2}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x_2,x_1)} \tag{12.414}$$

We treat $\mathrm{FIO}(a,S)$ as a quantization of the symplectic transformation with the generating function S. Suppose that we can solve

$$\nabla_x S(\tilde{x}, x) = p \tag{12.415}$$

obtaining $(x,p) \mapsto \tilde{x}(x,p)$. Then

$$\mathrm{FIO}_\hbar(a_2,S)^*\mathrm{FIO}_\hbar(a_1,S) = \mathrm{Op}_\hbar(b) + O(\hbar), \tag{12.416}$$

where

$$b(x,p) = \overline{a_2(\tilde{x}(x,p),x)}a_1(\tilde{x}(x,p),x). \tag{12.417}$$

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

$$\begin{aligned}
b(x_2,x,x_1) &= \sqrt{\partial_x\partial_{x_2}S(x,x_2)}\sqrt{\partial_x\partial_{x_1}S(x,x_1)}\ \overline{a(x_2,x)}a_1(x,x_1),\\
p(x_2,x,x_1) &= \int_0^1 \partial_x S(\tau x_2+(1-\tau)x_1)\mathrm{d}\tau.
\end{aligned}$$

12.7 Composition of FIO's

Suppose that

$$\mathcal{X}\times\mathcal{X}_1 \ni (x,x_1)\mapsto S_1(x,x_1),\quad \mathcal{X}_2\times\mathcal{X}\ni(x_2,x)\mapsto S_2(x_2,x) \tag{12.418}$$

are two functions. Given x_2,x_1, we look for $x(x_2,x_1)$ satisfying

$$\nabla_x S_2(x_2,x(x_2,x_1))+\nabla_x S_1(x(x_2,x_1),x_1)=0. \tag{12.419}$$

Suppose such $x(x_2,x_1)$ exists and is unique. Then we define

$$S(x_2,x_1):=S_2(x_2,x(x_2,x_1))+S_1(x(x_2,x_1),x_1) \tag{12.420}$$

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 12.3.

$$\begin{aligned}
\nabla_{x_2}\nabla_{x_1}S(x_2,x_1) &= -\nabla_{x_2}\nabla_x S_2(x_2,x(x_2,x_1))\\
&\quad\times\left(\nabla_x^{(2)}S_2(x_2,x(x_2,x_1))+\nabla_x^{(2)}S_1(x(x_2,x_1),x_1)\right)^{-1}\\
&\quad\times\nabla_x\nabla_{x_1}S_1(x(x_2,x_1),x_1).
\end{aligned} \tag{12.421}$$

Proof. Differentiating (12.419) we obtain

$$\begin{aligned}
(\nabla_{x_2}x)(x_1,x_2)&\left(\nabla_x^{(2)}S_2(x_2,x(x_2,x_1))+\nabla_x^{(2)}S_1(x(x_2,x_1),x_1)\right)\\
&+\nabla_x\nabla_{x_2}S_2(x_2,x(x_2,x_1)) = 0.
\end{aligned} \tag{12.422}$$

Differentiating (12.420) we obtain

$$\begin{aligned}\nabla_{x_1} S(x_1,x_2) &= \nabla_{x_1} S_1(x(x_1,x_2),x_1),\\ \nabla_{x_2}\nabla_{x_1} S(x_1,x_2) &= (\nabla_{x_2} x)(x_1,x_2)\nabla_x\nabla_{x_1} S_1(x(x_1,x_2),x_1).\end{aligned}\tag{12.423}$$

Then we use (12.422) and (12.423). □

In addition to two phases S_1, S_2, let

$$\mathcal{X}_2\times\mathcal{X}\ni(x_2,x)\mapsto a_2(x_2,x),\qquad \mathcal{X}\times\mathcal{X}_1\ni(x,x_1)\mapsto a_1(x,x_1)\tag{12.424}$$

be two amplitudes. Then we define the composite amplitude as

$$a(x_2,x_1):=a_2(x_2,x(x_2,x_1))a_1(x(x_2,x_1),x_1).\tag{12.425}$$

Theorem 12.4.

$$\mathrm{FIO}_\hbar(a_2,S_2)\mathrm{FIO}_\hbar(a_1,S_1)=\mathrm{FIO}_\hbar(a,S)+O(\hbar).\tag{12.426}$$

13 WKB method

13.1 Lagrangian distributions

Consider a quadratic form

$$\frac12 xSx:=\frac12 x^iS_{ij}x^j,\tag{13.427}$$

and a function on $\mathbb{R}^d$

$$\mathrm{e}^{\frac{\mathrm{i}}{2\hbar}xSx}.\tag{13.428}$$

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 (13.428) is concentrated on

$$\{(x,p)\ :\ p_i-S_{ij}x^j=0,\ i=1,\dots,d\},\tag{13.429}$$

which is a Lagrangian subspace of $\mathbb{R}^d\oplus\mathbb{R}^d$.

Let us generalize (13.428). 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 (13.427). Lagrangian distributions associated with $\mathcal{L}$ are then multiples of (13.428).

The opposite case is $\mathcal{L} = 0 \oplus \mathbb{R}^d$. $\mathcal{L}^{\mathrm{an}}$ is then spanned by x^i, $i = 1, \dots, d$. The corresponding Lagrangian distributions are multiples of $\delta(x)$

13.2 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

$$\mathcal{F}_\hbar(p,x) := \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}xp}. \tag{13.430}$$

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

$$\mathrm{e}^{\frac{\mathrm{i}}{2\hbar}xSx}, \tag{13.431}$$

with an invertible S. Then its is easy to see that the image of (13.431) 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.

13.3 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

$$H(x,p) = \frac{1}{2}(p - A(x))g(x)(p - A(x)) + V(x) \tag{13.432}$$

with the corresponding Lagrangian

$$L(x,v) = \frac{1}{2}vg^{-1}(x)v + vA(x) - V(x). \tag{13.433}$$

We quantize the Hamiltonian in the naive way:

$$H_\hbar := \frac{1}{2}(-\mathrm{i}\hbar\hat{\partial} - A(x))g(x)(-\mathrm{i}\hbar\hat{\partial} - A(x)) + V(x). \tag{13.434}$$

We look for solutions of

$$\mathrm{i}\hbar\partial_t\Psi_\hbar(t,x) \quad = \quad H_\hbar\Psi_\hbar(t,x). \tag{13.435}$$

We make an ansatz

$$\begin{aligned}
\Psi_\hbar(t,x) &= \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(t,x)}a_\hbar(t,x), && (13.436)\\
\Psi_\hbar(0,x) &= \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)}a(x). && (13.437)
\end{aligned}$$

where $a(x), S(x)$ are given functions. We multiply the Schrödinger equation by $\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}S(t,x)}$ obtaining

$$\begin{aligned}
&\left(\mathrm{i}\hbar\hat{\partial}_t - \partial_t S(t,x)\right)a_\hbar(t,x) && (13.438)\\
= &\left(\frac{1}{2}(\mathrm{i}^{-1}\hbar\hat{\partial}_x + \partial_x S(t,x) - A(x))g(x)(\mathrm{i}^{-1}\hbar\hat{\partial}_x + \partial_x S(t,x) - A(x)) + V(x)\right)a_\hbar(t,x).
\end{aligned}$$

To make the zeroth order in $\hbar$ part of (13.438) vanish we demand that

$$-\partial_t S(t,x) \quad = \quad \frac{1}{2}(\partial_x S(t,x) - A(x))g(x)(\partial_x S(t,x) - A(x)) + V(x). \tag{13.439}$$

This is the Hamilton-Jacobi equation for the Hamiltonian H. Together with the initial conditions (13.439) can be rewritten as

$$\begin{aligned}
-\partial_t S(t,x) &= H\big(x, \partial_x S(x)\big), && (13.440)\\
S(0,x) &= S(x),
\end{aligned}$$

Recall that (13.440) 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 (13.440) with the initial condition (13.437), provided that we can invert $y\mapsto x(t,y)$.

We have also the equation for the amplitude:

$$\left(\hat\partial_t+\frac{1}{2}(v(t,x)\hat\partial_x+\hat\partial_x v(t,x))\right)a_\hbar(t,x)=\frac{\mathrm{i}\hbar}{2}\hat\partial_x g(x)\hat\partial_x a_\hbar(t,x). \tag{13.441}$$

Note that for any function b

$$\left(\hat\partial_t+\frac{1}{2}(v(t,x)\hat\partial_x+\hat\partial_x v(t,x))\right)(\det\partial_x y(t,x))^{\frac{1}{2}}\,b(y(t,x))=0 \tag{13.442}$$

Thus setting

$$\Psi_{\mathrm{cl}}(t,x):=(\det\partial_x y(t,x))^{\frac{1}{2}}\,a\big(y(t,x)\big)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(t,x)}. \tag{13.443}$$

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

$$\Psi_\hbar(t,x):=(\det\partial_x y(t,x))^{\frac{1}{2}}\sum_{n=0}^\infty\hbar^n b_n(t,y(t,x))\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(t,x)}, \tag{13.444}$$

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 13.10 to pass them.

13.4 Stationary WKB metod

The WKB method can be used to compute eigenfunctions of Hamiltonians. Let H and $H_\hbar$ be as in (13.432) and (13.434). 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

$$\begin{aligned} & Ea_\hbar(x) \\ = & \left(\frac{1}{2}(\mathrm{i}^{-1}\hbar\hat{\partial}_x + \partial_x S(x) - A(x))g(x)(\mathrm{i}^{-1}\hbar\hat{\partial}_x + \partial_x S(x) - A(x)) + V(x)\right) a_\hbar(x). \end{aligned} \tag{13.445}$$

To make the zeroth order in $\hbar$ part of (13.445) 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

$$\frac{1}{2}\Big(v(x)\hat{\partial}_x + \hat{\partial}_x v(x)\Big)a_\hbar(x) = \frac{\mathrm{i}\hbar}{2}\hat{\partial}_x g(x)\hat{\partial}_x a_\hbar(x). \tag{13.446}$$

We set

$$a_\hbar(x) := \sum_{n=0}^{\infty} \hbar^n a_n(x). \tag{13.447}$$

Now (13.446) can be rewritten as

$$\begin{aligned} \frac{1}{2}\Big(v(x)\hat{\partial}_x + \hat{\partial}_x v(x)\Big)a_0(x) &= 0, \\ \frac{1}{2}\Big(v(x)\hat{\partial}_x + \hat{\partial}_x v(x)\Big)a_{n+1}(x) &= \mathrm{i}\hbar\hat{\partial}_x g(x)\hat{\partial}_x a_n(x). \end{aligned} \tag{13.448}$$

In dimension 1 we can solve (13.448) 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

$$\Psi_0(x) := |v(x)|^{-\frac{1}{2}} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)}. \tag{13.449}$$

In the case of quadratic Hamiltonians we can solve for $v(x)$ and $S(x)$:

$$\begin{aligned} v(x) &= g(x)^{-1}\sqrt{2\big(E - V(x)\big)}, \\ \partial_x S(x) &= g(x)^{-1}\sqrt{2\big(E - V(x)\big)} + A(x). \end{aligned}$$

13.5 Conjugating quantization with a WKB phase

Lemma 13.1. *The operator $B_\hbar$ with the kernel*

$$(2\pi\hbar)^{-\frac{d}{2}}\int b(x,y)p\exp\Big(\frac{\mathrm{i}}{\hbar}(x-y)p\Big)\mathrm{d}p \tag{13.450}$$

equals

$$\frac{\hbar}{2\mathrm{i}}\Big(\hat{\partial}_x b(x,x)+b(x,x)\hat{\partial}_x\Big)+\mathrm{i}\hbar\left(\partial_x b(x,y)-\partial_y b(x,y)\right)\Big|_{y=x}. \tag{13.451}$$

Proof. We apply Theorem 5.8. □

Theorem 13.2. *Let S,h be smooth functions. Then*

$$\begin{aligned}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}S(x)}\mathrm{Op}_\hbar(G)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)} &= G(x,\partial_x S(x)) &(13.452)\\ &+\frac{\hbar}{2\mathrm{i}}\Big(\hat{\partial}_x\partial_p G\big(x,\partial_x S(x)\big)+\partial_p G\big(x,\partial_x S(x)\big)\hat{\partial}_x\Big)+O(\hbar^2).\end{aligned}$$

Proof. The integral kernel of the left-hand side equals

$$\begin{aligned}
&(2\pi\hbar)^{-\frac{d}{2}}\int G\Big(\frac{x+y}{2},p\Big)\exp\Big(\frac{\mathrm{i}}{\hbar}\big(-S(x)+S(y)+(x-y)p\big)\Big)\mathrm{d}p\\
=\ &(2\pi\hbar)^{-\frac{d}{2}}\int G\Big(\frac{x+y}{2},p\Big)\exp\frac{\mathrm{i}}{\hbar}(x-y)\Big(-\int_0^1\partial S\big(\tau x+(1-\tau)y\big)\mathrm{d}\tau+p\Big)\mathrm{d}p\\
=\ &(2\pi\hbar)^{-\frac{d}{2}}\int G\Big(\frac{x+y}{2},p+\int_0^1\partial S\big(\tau x+(1-\tau)y\big)\mathrm{d}\tau\Big)\exp\Big(\frac{\mathrm{i}}{\hbar}(x-y)p\Big)\mathrm{d}p\\
=\ &(2\pi\hbar)^{-\frac{d}{2}}\int G\Big(\frac{x+y}{2},\int_0^1\partial S\big(\tau x+(1-\tau)y\big)\mathrm{d}\tau\Big)\exp\Big(\frac{\mathrm{i}}{\hbar}(x-y)p\Big)\mathrm{d}p &(13.453)\\
+\ &(2\pi\hbar)^{-\frac{d}{2}}\int p\partial_p G\left(\frac{x+y}{2},\int_0^1\partial S(\tau x+(1-\tau)y)\mathrm{d}\tau\right)\exp\Big(\frac{\mathrm{i}}{\hbar}(x-y)p\Big)\mathrm{d}p &(13.454)\\
+\ &(2\pi\hbar)^{-\frac{d}{2}}\int\int_0^1\mathrm{d}\sigma(1-\sigma)pp\\
&\times\partial_p\partial_p G\left(\frac{x+y}{2},\sigma p+\int_0^1\partial S(\tau x+(1-\tau)y)\mathrm{d}\tau\right)\exp\Big(\frac{\mathrm{i}}{\hbar}(x-y)p\Big)\mathrm{d}p. &(13.455)
\end{aligned}$$

We have

$$\begin{aligned}
(13.453) &= G(x,\partial_x S(x)),\\
(13.454) &= \frac{\hbar}{2\mathrm{i}}\Big(\hat{\partial}_x\partial_p G(x,\partial_x S(x))+\partial_p G(x,\partial_x S(x))\hat{\partial}_x\Big),\\
(13.453) &= O(\hbar^2),
\end{aligned}$$

where we used Lemma 13.1 to compute the second term. □

13.6 WKB approximation for general Hamiltonians

The WKB approximation is not restricted to quadratic Hamiltonians. Using Theorem 13.2 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:

$$(\mathrm{i}\hbar\partial_t - \mathrm{Op}_\hbar(H))\,\Phi_\hbar(t,x) = 0. \tag{13.456}$$

(2) The stationary Schrödinger equation:

$$(\mathrm{Op}_\hbar(H) - E)\,\Phi_\hbar(x) = 0 \tag{13.457}$$

They can be written as

$$\mathrm{Op}_\hbar(G)\Phi_\hbar(x) = 0, \tag{13.458}$$

where

(1) for (13.456), 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 (13.456),

$$G(x,p) = H(x,p) - E.$$

In order to solve (13.458) 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 (13.458), we multiply by $\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}S(x)}$, we set

$$v(x) := \partial_p G(x,p),$$

and by (13.452) we obtain

$$\begin{aligned}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}S(x)}\mathrm{Op}_\hbar(G)\Phi_\hbar &= G\big(x,\partial_x S(x)\big)a_\hbar(x)\\ &+\frac{\hbar}{2\mathrm{i}}\left(\hat{\partial}_x v(x) + v(x)\hat{\partial}_x\right)a_\hbar(x)\\ &+O(\hbar^2).\end{aligned}$$

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:

$$\mathrm{Op}_\hbar(G)\Phi_{\mathrm{cl}}(x) = O(\hbar).$$

13.7 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

$$\mathcal{U} \ni x \mapsto a(x)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)} \tag{13.459}$$

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 (13.459) as derived from a half-density on the Lagrangian manifold

$$z \mapsto b\big(x(z), p(z)\big)|\mathrm{d}z|^{1/2}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}T(x(z),p(z))}. \tag{13.460}$$

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 (13.460) in terms of x:

$$\mathcal{U} \ni x \mapsto b\big(x, p(z(x))\big)\big|\det \partial_x z(x)\big|^{1/2}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}T\big(x,p(z(x))\big)}|\mathrm{d}x|^{1/2}. \tag{13.461}$$

(13.461) is actually not quite correct – there is a problem along the caustics, which should be corrected by the so-called Maslov index.

13.8 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:

$$\Psi_\hbar(x) := a(x)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)}. \tag{13.462}$$

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

$$\partial_p x(p)=\left(\partial_x^2 S\big(x(p)\big)\right)^{-1},$$

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

$$\Phi_\hbar(x):=|\partial_x^2 S(x)|^{1/4}a(x)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x)}. \tag{13.463}$$

Then

$$(2\pi\hbar)^{-d/2}\mathcal{F}_\hbar\Phi_\hbar(p) = \mathrm{e}^{\frac{\mathrm{i}\pi\,\mathrm{inert}\,\partial_p^2\tilde{S}(p)}{4}}|\partial_p^2\tilde{S}(p)|^{1/4}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\tilde{S}(p)}a(x(p))+O(\hbar).$$

13.9 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

$$(2\pi\hbar)^{-\frac{1}{2}}\mathcal{F}_\hbar\Psi_\hbar(p)=\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\frac{p^3}{3}}b(p). \tag{13.464}$$

Then

$$\Psi_\hbar(x)=(2\pi\hbar)^{-\frac{1}{2}}\int \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\frac{p^3}{3}+xp)}b(p)\mathrm{d}p. \tag{13.465}$$

The stationary phase method gives for $x<0$, $p(x)=\pm\sqrt{-x}$. Thus, for $x<0$,

$$\begin{aligned}\Psi_\hbar(x) \simeq\ & \mathrm{e}^{\frac{\mathrm{i}\pi}{4}-\frac{\mathrm{i}2}{\hbar 3}(-x)^{\frac{3}{2}}}(-x)^{-\frac{1}{4}}b(-\sqrt{-x})\\ &+\mathrm{e}^{-\frac{\mathrm{i}\pi}{4}+\frac{\mathrm{i}2}{\hbar 3}(-x)^{\frac{3}{2}}}(-x)^{-\frac{1}{4}}b(\sqrt{-x}).\end{aligned} \tag{13.466}$$

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

$$\Psi_\hbar(x) \quad \simeq \quad \mathrm{e}^{-\frac{2}{\hbar 3}x^{\frac{3}{2}}} x^{-\frac{1}{4}} b(\mathrm{i}\sqrt{x}) \tag{13.467}$$

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,

$$\Psi_\hbar(x) \quad \approx \quad b(0)(2\pi)^{1/2}\hbar^{-1/6}\mathrm{Ai}(\hbar^{-2/3}x).$$

13.10 Caustics and the Maslov correction

Let us go back to the construction described in Subsection 13.7. 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

$$\Psi_\hbar(x) \quad = \quad \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S^-(x_1, x_\perp) + \mathrm{i}\alpha - \mathrm{i}\frac{\pi}{4}} b\big(p_1^-(x), x_\perp\big)\big|\det \partial_{x_1} p_1^-(x)\big|^{\frac{1}{2}} \tag{13.468}$$

$$+\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S^+(x_1, x_\perp) + \mathrm{i}\alpha + \mathrm{i}\frac{\pi}{4}} b\big(p_1^+(x), x_\perp\big)\big|\det \partial_{x_1} p_1^+(x)\big|^{\frac{1}{2}} + O(\hbar). \tag{13.469}$$

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.

13.11 Global problems of the WKB method

Let us return to the setup of Subsection 13.6. 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".

13.12 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

$$\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\int_{\mathcal{D}}\omega - \mathrm{i}\pi}. \tag{13.470}$$

If (13.470) is different from 1, then going around we obtain contributions to WKB that intefere destructively. Thus (13.470) has to be 1. This leads to the condition

$$\frac{1}{\hbar}\int_{\mathcal{D}} \omega - \pi = 2\pi n, \quad n \in \mathbb{Z}, \tag{13.471}$$

or

$$\frac{1}{2\pi}\int_{\mathcal{D}} \omega = \hbar\left(n + \frac{1}{2}\right), \tag{13.472}$$

which is the famous Bohr-Sommerfeld condition.

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