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Introduction to Wigner-Weyl calculus

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These notes are based on two lectures (3 hrs in total) given at the end of an analytical mechanics course (based on [1]). The aim is to point out the – maybe not immediately obvious – similarity between quantum and classical mechanics and discuss the quantum to classical correspondence. To this end quantum mechanics is formulated on phase space. In particular we show that the fact that one finds the same relations for commutators of quantum observables as one obtains for Poisson brackets of the corresponding classical observables in not a mere coincidence… We also discuss how this correspondence can be exploited in order to control quantum time evolution in terms of classical dynamics.

We won't put too much emphasis on mathematical rigorousity especially when it comes to precise statements of domains of operators, conditions for boundedness etc. (i.e. *all statements hold whenever they make sense* ;-). More elaborate texts on this subject in a similar (physics) style are e.g. [2, 3]. Notice, however, that everything presented here can be done in a mathematically rigorous fashion and that the formalism developed is actively used for proving theorems in mathematical physics. An introductory mathematical text accessible for physicists is [4]. Further reading includes [5, 6, 7, 8]. (This is a very incomplete list!)

Contents

1 Recap: Hamiltonian Mechanics

So far we have seen various formulations of classical mechanics. The Hamiltonian version explictly lives on phase space, a symplectic manifold – for definiteness in the following this will always be $\mathbb{R}^d \times \mathbb{R}^d \cong \mathbb{R}^{2d}$ – where we can choose coordinates (p, x), canonically conjugate momenta and positions. Observables are given by functions on phase space, $A : \mathbb{R}^{2d} \to \mathbb{R}$.

A special role is played by the Hamiltonian $H(p, x)$ (which for simplicity shall be time-independent) determining the time evolution through Hamilton's equations of motion,

$$\dot{x} = \nabla_p H(p, x)\,, \quad \dot{p} = -\nabla_x H(p, x)\,. \tag{1.1}$$

Defining the Poisson bracket of two observables by

$$\{A, B\} := (\nabla_p A)(\nabla_x B) - (\nabla_x A)(\nabla_p B) \tag{1.2}$$

Hamilton's equations of motion can be written in an even more symmetric way,

$$\boxed{\dot{x} = \{H, x\}\,, \quad \dot{p} = \{H, p\}\,.} \tag{1.3}$$

In fact the time evolution of any observable A is governed by the differential equation

$$\dot{A} = \{H, A\}\,. \tag{1.4}$$

Notation: If $(p(t), x(t))$ denotes the solution of (1.3) with initial conditions $(p(0), x(0)) = (p_0, x_0)$ then we also write

$$\phi^t(p_0, x_0) := (p(t), x(t))\,, \tag{1.5}$$

where $\phi^t : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ denotes the Hamiltonian flow with the obvious properties

$$\phi^0 = \mathrm{id} \quad \text{and} \quad \phi^t \circ \phi^{t'} = \phi^{t+t'}\,. \tag{1.6}$$

2 Brief Introduction to Quantum Mechanics

Im quantum mechanics (in the Schrödinger representation) the state of the system is represented by a wave function $\psi \in L^2(\mathbb{R}^d)$.

The interpretation of ψ is that $|\psi(x)|^2$ (suitably normalised) yields the probability density for finding the particle at position x. Then the expectation value for, say, x^n is given by

$$\int x^n\, |\psi(x)|^2 \mathrm{d}x\,. \tag{2.1}$$

In general observables are represented by self-adjoint operators $\hat{A}$ and physically meaningful quantities are, e.g., expectation values

$$\langle\psi, \hat{A}\psi\rangle = \int_{\mathbb{R}^d} \overline{\psi}(x)\,(\hat{A}\psi)(x)\,\mathrm{d}^d x \tag{2.2}$$

(the wave functions are assumed to be normalised, i.e. $\langle\psi,\psi\rangle = 1$).

In the Schrödinger picture time evolution is governed by the Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t}(x,t) = \hat{H}\,\psi(x,t)\,, \tag{2.3}$$

where the (quantum) Hamiltonian $\hat{H}$ is the quantisation of the (classical) Hamiltonian $H(p,x)$ (see below). Thus,

$$\psi(x,t) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}\,\psi(x,0)\,, \tag{2.4}$$

and the information of time evolution is carried by the wave function whereas the operators are time independent.

Conversely, in the Heisenberg picture the wave function is time independent and operators evolve according to

$$\hat{A}(t) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}t}\hat{A}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}\,, \tag{2.5}$$

and one easily verifies that $\hat{A}(t)$ solves

$$\dot{\hat{A}}(t) = -\frac{\mathrm{i}}{\hbar}[\hat{H},\hat{A}(t)]\,. \tag{2.6}$$

Notice that in both pictures expectation values (and their time dependence) are the same, as they have to be!

Also notice that (2.6) looks a lot like (1.4) if only we were able to relate the classical Poisson bracket and the quantum mechanical commutator. We will return to this problem and make precise statements about it in sections 3.2 and 4.

The basic classical observables are "translated" to quantum mechanics ("quantised") by the rules,

phase space variable	$\longrightarrow$	operator ...		in Schrödinger representation
x	$\longrightarrow$	$\hat{x}$	$=$	x
p	$\longrightarrow$	$\hat{p}$	$=$	$\frac{\hbar}{\mathrm{i}}\nabla$

which imply the canonical commutation relations

$$[\hat{p}_j, \hat{x}_k] = \frac{\hbar}{\mathrm{i}}\,\delta_{jk}\,. \tag{2.7}$$

For more general observables $A \longrightarrow \hat{A} =$ "$A(\hat{p},\hat{x})$" may lead to an ordering problem.

A possible (good) choice is to take symmetrised products of p and x, i.e. (for one degree of freedom)

$$xp \quad \longrightarrow \quad \frac{1}{2}(\hat{x}\hat{p}+\hat{p}\hat{x})\,, \tag{2.8}$$

which is called Weyl ordering.

2.1 The Fourier Transform

Since we will make heavy use of Fourier transforms in the following, let us fix some conventions and notation and list some (only a few!) properties which we will use later.

For a function $f \in L^1(\mathbb{R}^d)$ we define its Fourier transform by

$$\tilde{f}(p) = \frac{1}{(2\pi\hbar)^d}\int_{\mathbb{R}^d} f(x)\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}px}\,\mathrm{d}^d x =: \mathcal{F}[f](p) \tag{2.9}$$

The inverse transform then reads

$$f(x) = \int_{\mathbb{R}^d} \tilde{f}(p)\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}px}\,\mathrm{d}^d p =: \mathcal{F}^{-1}[\tilde{f}](x)\,. \tag{2.10}$$

The following two properties/consequences will be used later on:

- The Fourier transform of a derivative yields the Fourier transform of the function itself multiplied by (powers of) the Fourier variable:

$$\begin{aligned}\mathcal{F}\left[\frac{\partial^n f}{\partial x_j\cdots\partial x_k}\right](p) &= \frac{1}{(2\pi\hbar)^d}\int_{\mathbb{R}^d}\frac{\partial^n f}{\partial x_j\cdots\partial x_k}(x)\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}px}\,\mathrm{d}^d x\\ &\quad n\text{-fold partial integration}\\ &= \left(\frac{\mathrm{i}}{\hbar}\right)^n p_j\cdots p_k\,\tilde{f}(p)\,.\end{aligned} \tag{2.11}$$

- By subsequently applying Fourier transform and inverse Fourier transform,

$$f(x) = \int_{\mathbb{R}^d}\tilde{f}(p)\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}px}\,\mathrm{d}^d p = \frac{1}{(2\pi\hbar)^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} f(y)\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(px-py)}\,\mathrm{d}^d y\,\mathrm{d}^d p \tag{2.12}$$

  we can read off the Fourier representation of the δ-function (which is actually a distribution),

$$\delta(x) = \frac{1}{(2\pi\hbar)^d}\int_{\mathbb{R}^d}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}px}\,\mathrm{d}^d p\,, \tag{2.13}$$

  with properties (evaluated on suitable test functions $f \in \mathcal{S}(\mathbb{R}^d)$)

$$\int_{\mathbb{R}^d} f(x)\,\delta(x-y)\,\mathrm{d}^d x = f(y) \tag{2.14}$$

and

$$f(x)\,\frac{\partial}{\partial x_j}\delta(x) = -\delta(x)\,\frac{\partial}{\partial x_j}f(x)\,. \tag{2.15}$$

The latter can be verified by partial integration.

3 Weyl Quantisation

Let us try to rewrite and formalise the quantisation rules of section 2 a bit.

Consider a classical observable $A(x)$ which depends only on x. According to our rules we quantise it as

$$A(x) \quad \longrightarrow \quad \hat{A} = A(\hat{x})\,. \tag{3.1}$$

Using the δ-function this can be written as

$$\hat{A} = \int_{\mathbb{R}^d} A(x)\,\delta(x-\hat{x})\,\mathrm{d}^d x\,. \tag{3.2}$$

In order to define the δ-function of an operator we use the Fourier representation (2.13) and obtain

$$\hat{A} = \frac{1}{(2\pi\hbar)^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} A(x)\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\xi(x-\hat{x})}\,\mathrm{d}^d\xi\,\mathrm{d}^d x\,. \tag{3.3}$$

Notice that ξ has the dimension of a momentum, i.e. the integral extends over phase space. Obviously we can write down an analogous expression for an observable which depends only on p but nor on x.

For a general observable $A(p,x)$ we would now like to write something like

$$\hat{A} = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} A(p,x)\,\text{“}\delta(x-\hat{x})\,\delta(p-\hat{p})\text{”}\,\mathrm{d}^d p\,\mathrm{d}^d x\,. \tag{3.4}$$

where the quotes indicate the ordering problem. As a possible choice we try a symmetric Fourier-like representation of the product of the two δ-functions, i.e.

$$\text{“}\ldots\text{”} = \frac{1}{(2\pi\hbar)^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}[\xi(x-\hat{x})+y(p-\hat{p})]}\mathrm{d}^d\xi\,\mathrm{d}^d y\,. \tag{3.5}$$

In order see whether this is equivalent to Weyl ordering of products we calculate the quantisation of xp, i.e. we compare with (2.8) Let us also introduce the following NOTATION: $\mathrm{Op}[A] = \hat{A}$. Then

$$\mathrm{Op}[px] = \frac{1}{(2\pi\hbar)^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} px\;\underbrace{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}[\xi(x-\hat{x})+y(p-\hat{p})]}}_{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}[\xi x+yp]}\;\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}[\xi\hat{x}+y\hat{p}]}}\;\mathrm{d}\xi\,\mathrm{d}y\,\mathrm{d}p\,\mathrm{d}x\,. \tag{3.6}$$

Using the Baker-Campbell-Hausdorff rule we can split the exponential according to

$$\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}[\xi\hat{x}+y\hat{p}]} = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\xi\hat{x}}\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}y\hat{p}}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\frac{\xi y}{2}}\,. \tag{3.7}$$

By further changing variables from x to $x' = x + \frac{y}{2}$ we obtain

$$\begin{aligned}
\mathrm{Op}[px] &= \frac{1}{(2\pi\hbar)^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} p(x'-\frac{y}{2})\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\xi(x'-\hat{x})}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}y(p-\hat{p})}\,\mathrm{d}\xi\mathrm{d}y\mathrm{d}p\mathrm{d}x' \\
&= \hat{x}\hat{p} - \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} p\,\underbrace{\frac{y}{2}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}y(p-\hat{p})}}_{\frac{\hbar}{2\mathrm{i}}\frac{\partial}{\partial p}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}y(p-\hat{p})}}\,\mathrm{d}y\mathrm{d}p \\
&= \hat{x}\hat{p} - \int_{-\infty}^{\infty} p\frac{\hbar}{2\mathrm{i}}\,\delta'(p-\hat{p})\,\mathrm{d}p \\
&\qquad\qquad\qquad f(x)\,\delta'(x) = -f'(x)\,\delta(x) \\
&= \hat{x}\hat{p} + \frac{\hbar}{2\mathrm{i}}\,.
\end{aligned} \tag{3.8}$$

This should be compared to

$$\frac{1}{2}(\hat{x}\hat{p}+\hat{p}\hat{x}) = \frac{1}{2}(\hat{x}\hat{p}+\hat{x}\hat{p}-[\hat{x},\hat{p}]) = \hat{x}\hat{p} + \frac{\hbar}{2\mathrm{i}}\,. \tag{3.9}$$

Thus, we conclude that

$$\boxed{\hat{A} \equiv \mathrm{Op}[A] = \frac{1}{(2\pi\hbar)^{2d}}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} A(p,x)\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}[\xi(x-\hat{x})+y(p-\hat{p})]}\,\mathrm{d}^d\xi\,\mathrm{d}^d y\,\mathrm{d}^d p\,\mathrm{d}^d x} \tag{3.10}$$

is a good definition! – called Weyl quantisation.

REMARKS:

- $A(p,x)$ is called the (Weyl-)symbol of $\hat{A}$
  NOTATION: $\mathrm{symb}[\hat{A}](p,x) = A(p,x)$
- If the symbol $A(p,x)$ satisfies certain conditions then $\hat{A}$ is a Pseudo-Differential-Operator (ψDO) of a certain type.

Now we would like to have a more explicit formula (without formal operators in the exponent), i.e. let's calculate $(\hat{A}\psi)(z)$ in the Schrödinger representation. Notice that

$$\begin{aligned}
\left(\mathrm{e}^{-\frac{\hbar}{\mathrm{i}}\xi\hat{x}}\psi\right)(z) &= \mathrm{e}^{-\frac{\hbar}{\mathrm{i}}\xi z}\psi(z) \quad \text{and} \\
\left(\mathrm{e}^{-\frac{\hbar}{\mathrm{i}}y\hat{p}}\psi\right)(z) &= \psi(z-y)
\end{aligned} \tag{3.11}$$

(for the latter expand the exponential, use $\hat{p} = \frac{\hbar}{\mathrm{i}}\nabla$ and you find the Taylor expansion of ψ).

Using these relations along with (3.7) we find

$$(\hat{A}\psi)(z) = \frac{1}{(2\pi\hbar)^{2d}} \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} A(p,x)\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\xi x + yp + \frac{\xi y}{2})}\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\xi z}\,\psi(z-y)\,\mathrm{d}^d\xi\,\mathrm{d}^d y\,\mathrm{d}^d p\,\mathrm{d}^d x\,. \tag{3.12}$$

The ξ-integral yields $\delta(x + \frac{y}{2} - z)$, which we use in order to perform the x-integral,

$$(\hat{A}\psi)(z) = \frac{1}{(2\pi\hbar)^{d}} \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} A(p, z - \tfrac{y}{2})\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}py}\,\psi(z-y)\,\mathrm{d}^d p\,\mathrm{d}^d y \tag{3.13}$$

and changing variables from y to $x = z - y$ we obtain

$$\boxed{(\hat{A}\psi)(z) = \frac{1}{(2\pi\hbar)^{d}} \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} A\left(p, \frac{z+x}{2}\right)\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p(z-x)}\,\psi(x)\,\mathrm{d}^d p\,\mathrm{d}^d y}\,, \tag{3.14}$$

which is usually referred to as the definition of Weyl quantisation.

Now assume that $\hat{A}$ has a representation with integral kernel $K_{\hat{A}}(x,y)$, i.e.

$$(\hat{A}\psi)(x) = \int_{\mathbb{R}^d} K_{\hat{A}}(x,y)\,\psi(y)\,\mathrm{d}^d y\,. \tag{3.15}$$

By comparing with (3.14) we can read off the identity

$$\boxed{K_{\hat{A}}(x,y) = \frac{1}{(2\pi\hbar)^{d}} \int_{\mathbb{R}^d} A\left(p, \frac{y+x}{2}\right)\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p(x-y)}\mathrm{d}^d p}\,. \tag{3.16}$$

In order to obtain the inverse relation, introduce the variables $X = \frac{x+y}{2}$ and $z = x - y$,

$$K_{\hat{A}}(X + \tfrac{z}{2}, X - \tfrac{z}{2}) = \frac{1}{(2\pi\hbar)^{d}} \int_{\mathbb{R}^d} A\left(p, X\right)\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}pz}\mathrm{d}^d p \tag{3.17}$$

and invert the Fourier transform,

$$\boxed{\mathrm{symb}[\hat{A}] \equiv A(P,X) = \int_{\mathbb{R}^d} K_{\hat{A}}(X + \tfrac{z}{2}, X - \tfrac{z}{2})\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Pz}\,\mathrm{d}^d z} \tag{3.18}$$

Now we can go back and forth between operators (kernels) and symbols (which live on phase space) and with equations (3.14), (3.16) and (3.18) we have rigorous and convenient definitions at hand.

3.1 The Wigner Function

Now that we have a phase space representation for quantum observables let us see if can also represent the wave function on phase space. To this end consider the operator $\hat{P}_\psi$ which projects onto the state ψ,

$$(\hat{P}_\psi \phi)(x) := \psi(x) \int_{\mathbb{R}^d} \overline{\psi(y)}\, \phi(y)\, \mathrm{d}^d y \tag{3.19}$$

(or $\hat{P}_\psi = |\psi\rangle\langle\psi|$ in Dirac bracket notation). Its integral kernel is obviously given by $\psi(x)\overline{\psi(y)}$, and its symbol is called Wigner function,

$$\begin{aligned} W[\psi](p,x) : &= \mathrm{symb}[\hat{P}_\psi](p,x) \\ &= \int_{\mathbb{R}^d} \psi(x + \tfrac{z}{2})\, \overline{\psi(x - \tfrac{z}{2})}\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} pz}\, \mathrm{d}^d z\,. \end{aligned} \tag{3.20}$$

The Winger function is often referred to as a quasi-probability density (it's not a probability density because it can take negative or even complex values) since it's marginals (divided by $(2\pi\hbar)^d$),

$$\frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^d} W[\psi](p,x)\, \mathrm{d}^d p = |\psi(x)|^2 \tag{3.21}$$

and

$$\frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^d} W[\psi](p,x)\, \mathrm{d}^d x = |g(p)|^2\,, \tag{3.22}$$

are probability densities for position and momentum. (Here $g(p)$ denotes the normalised Fourier transform of ψ, $g(p) := (2\pi\hbar)^{-d/2}\, \tilde{\psi}(p)$.)

Remark: In the same way one can also define the Wigner function for an arbitrary density operator $\hat{D} = \sum_n p_n |\psi_n\rangle\langle\psi_n|$ and the Wigner transform of two states, say ψ and ϕ, i.e. the Weyl symbol of the kernel $\psi(x)\overline{\phi(y)}$.

It turns out that we can calculate expectation values using Wigner function and Weyl symbol as follows,

$$\boxed{\langle\psi, \hat{A}\psi\rangle = \frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} W[\psi](p,x)\, A(p,x)\, \mathrm{d}^d p\, \mathrm{d}^d x}\,. \tag{3.23}$$

PROOF:

$$\text{r.h.s} = \frac{1}{(2\pi\hbar)^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\psi(x+\tfrac{z}{2})\,\overline{\psi(x-\tfrac{z}{2})}\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}zp}\,\mathrm{d}^d z\int_{\mathbb{R}^d}K_{\hat{A}}(x+\tfrac{z'}{2},x-\tfrac{z'}{2})\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}z'p}\,\mathrm{d}^d z'\,\mathrm{d}^d p\,\mathrm{d}^d x$$

p-integral yields $\delta(z+z')$, perform z'-integral

$$= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\psi(x+\tfrac{z}{2})\,\overline{\psi(x-\tfrac{z}{2})}\,K_{\hat{A}}(x-\tfrac{z}{2},x+\tfrac{z}{2})\,\mathrm{d}^d x\,\mathrm{d}^d z$$

change variables to $y = x-\frac{z}{2}$, $y' = x+\frac{z}{2}$

$$= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\overline{\psi(y)}\,K_{\hat{A}}(y,y')\,\psi(y')\,\mathrm{d}^d y\,\mathrm{d}^d y'$$

$$= \int_{\mathbb{R}^d}\overline{\psi(y)}\,(\hat{A}\psi)(y)\,\mathrm{d}^d y = \langle\psi,\hat{A}\psi\rangle \qquad \square \tag{3.24}$$

Altogether everything looks like classical mechanics now (we have a phase space "density" describing the state of the system and a phase space function describing an observable) – so where's quantum mechanics?

CAVE: Symbols can depend on $\hbar$!

Recall: $\mathrm{Op}[xp] = \hat{x}\hat{p} + \frac{\hbar}{2\mathrm{i}}$

$\Rightarrow \quad xp = \mathrm{symb}[\hat{x}\hat{p} + \frac{\hbar}{2\mathrm{i}}] = \mathrm{symb}[\hat{x}\hat{p}] + \frac{\hbar}{2\mathrm{i}}$

$\Rightarrow \quad \mathrm{symb}[\hat{x}\hat{p}] = xp - \frac{\hbar}{2\mathrm{i}}$

In the limit $\hbar \to 0$ we obtain what we may have expected. This leads us to the following definition.

DEFINITION: We say that $\hat{A} = \mathrm{Op}[A]$ is a semiclassical ψDO (with classical symbol) if it has an asymptotic expansion of the form

$$A(p,x) \sim \hbar^a \sum_{n\geq 0} A_n(p,x)\,\hbar^n\,, \quad \hbar \to 0 \tag{3.25}$$

with $a \in \mathbb{R}$ and where the $A_n(p,x)$ do not depend on $\hbar$.

$A_0(p,x)$ is called the principal symbol of $\hat{A}$.
($A_1(p,x)$ is called the sub-principal symbol of $\hat{A}$.)

The principal symbol $A_0(p,x)$ is the classical observable corresponding to the quantum observable $\hat{A}$.

3.2 The Moyal Product

We know how to multiply classical and quantum observables (operators). In the first case multiplication is commutative whereas in the latter case in general it is not. Thus it is interesting to see how the symbol of $\hat{A}\hat{B}$ relates to the symbols of $\hat{A}$ and $\hat{B}$.

For convenience introduce also the Fourier transform $\tilde{A}$ of $A = \mathrm{symb}[\hat{A}]$ by

$$A(p,x) = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \tilde{A}(\alpha,\beta)\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(p\alpha+x\beta)}\, \mathrm{d}^d\alpha\, \mathrm{d}^d\beta\,. \tag{3.26}$$

Inserting into (3.16) we obtain

$$K_{\hat{A}}(x,y) = \frac{1}{(2\pi\hbar)^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \tilde{A}(\alpha,\beta)\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}[p(x-y+\alpha)+\frac{x+y}{2}\beta]}\, \mathrm{d}^d p\, \mathrm{d}^d\alpha\, \mathrm{d}^d\beta\,, \tag{3.27}$$

where the p-integral yields $\delta(x-y+\alpha)$, which we use in order to perform the α-integral. Then

$$\boxed{K_{\hat{A}}(x,y) = \int_{\mathbb{R}^d} \tilde{A}(y-x,\beta)\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\frac{x+y}{2}\beta} \mathrm{d}^d\beta} \tag{3.28}$$

is yet another way to express the relation between operators (kernels) and symbols.

Now

$$K_{\hat{A}\hat{B}}(x,y) = \int_{\mathbb{R}^d} K_{\hat{A}}(x,z)\, K_{\hat{B}}(z,y)\, \mathrm{d}^d z \tag{3.29}$$

$$\begin{aligned}
\mathrm{symb}[\hat{A}\hat{B}](p,x) &= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} K_{\hat{A}}(x+\tfrac{z}{2},y)\, K_{\hat{B}}(y,x-\tfrac{z}{2})\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}pz}\, \mathrm{d}^d y\, \mathrm{d}^d z \\
&= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \tilde{A}(y-x-\tfrac{z}{2},\alpha)\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\alpha\frac{x+y+z/2}{2}} \\
&\qquad\qquad \tilde{B}(-y+x-\tfrac{z}{2},\beta)\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\beta\frac{x+y-z/2}{2}}\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}pz}\, \mathrm{d}^d y\, \mathrm{d}^d z\, \mathrm{d}^d\alpha\, \mathrm{d}^d\beta
\end{aligned}$$

change variables from y,z to $X = y-x+\frac{z}{2}$ and $Y = -y+x-\frac{z}{2}$,

i.e. $z = -(X+Y)$, $y = \dfrac{X-Y}{2} + x$

$$= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \tilde{A}(X,\alpha)\, \tilde{B}(Y,\beta)\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\alpha\frac{2x-Y}{2}}\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\beta\frac{2x+Y}{2}}\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}p(X+Y)}\, \mathrm{d}^d X\, \mathrm{d}^d Y\, \mathrm{d}^d\alpha\, \mathrm{d}^d\beta\,. \tag{3.30}$$

The total argument of the exponentials in the last expression is

$$\frac{\mathrm{i}}{\hbar}\Big[\underbrace{x(\alpha+\beta)+p(X+Y)}_{\text{(i)}}\underbrace{-\tfrac{1}{2}\alpha Y+\tfrac{1}{2}\beta X}_{\text{(ii)}}\Big] \tag{3.31}$$

- The terms (i) will give us Fourier transforms (recall that we integrate over α, β, X and Y) replacing $\tilde{A}(X,\alpha)$ and $\tilde{B}(Y,\beta)$ by $A(p,x)$ and $B(p,x)$ (same arguments!).

- But we also have the terms (ii). For those we expand the exponential and then each multiplication with α, β (or X, Y) will give rise to a derivative in the corresponding Fourier variable, x (or p), cf. (2.11).

Hence,

$$\begin{aligned}\mathrm{symb}[\hat{A}\hat{B}](p,x) &= \sum_{n=0}^{\infty}\frac{1}{n!}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}[x(\alpha+\beta)+p(X+Y)]}\\ &\qquad\qquad \tilde{A}(X,\alpha)\left[\frac{\mathrm{i}}{2\hbar}(X\beta-\alpha Y)\right]^n\tilde{B}(Y,\beta)\,\mathrm{d}^dX\,\mathrm{d}^dY\,\mathrm{d}^d\alpha\,\mathrm{d}^d\beta\\ &= \sum_{n=0}^{\infty}\frac{1}{n!}A(p,x)\left[\frac{\mathrm{i}}{2\hbar}\left(\frac{\hbar}{\mathrm{i}}\overleftarrow{\nabla}_p\frac{\hbar}{\mathrm{i}}\overrightarrow{\nabla}_x-\frac{\hbar}{\mathrm{i}}\overleftarrow{\nabla}_x\frac{\hbar}{\mathrm{i}}\overrightarrow{\nabla}_p\right)\right]^n B(p,x)\end{aligned} \tag{3.32}$$

where the arrows indicate that the derivatives act only on functions standing to the left or right, respectively, of the corresponding differential operator. (Multiplication with, say, X will only give rise to differentiation of A with respect to p but not of B, since $\tilde{B}$ did not contain any X.)

Finally, we have obtained the following asymptotic expansion of the symbol of the $\hat{A}\hat{B}$:

$$\begin{aligned}\mathrm{symb}[\hat{A}\hat{B}](p,x) &= \sum_{n=0}^{\infty}\frac{1}{n!}A(p,x)\left[\frac{\hbar}{2\mathrm{i}}\left(\overleftarrow{\nabla}_p\overrightarrow{\nabla}_x-\overleftarrow{\nabla}_x\overrightarrow{\nabla}_p\right)\right]^n B(p,x)\\ &= A(p,x)\,B(p,x)+\frac{\hbar}{2\mathrm{i}}\underbrace{\left(\nabla_pA\,\nabla_xB-\nabla_xA\,\nabla_pB\right)}_{\{A,B\}}(p,x)+\mathcal{O}(\hbar^2)\,,\end{aligned} \tag{3.33}$$

i.e. the leading order term is just the product of the two symbols as expected, but there are $\hbar$-corrections. In particular the Poisson bracket shows up in next-to-leading order. Equation (3.33) (first line) is known as the Moyal product. For the symbol of the commutator this implies

$$\boxed{\mathrm{symb}\big[[\hat{A},\hat{B}]\big]=\frac{\hbar}{\mathrm{i}}\{A,B\}+\mathcal{O}(\hbar^2)}\,, \tag{3.34}$$

or, even more meaningful,

$$\mathrm{symb}\big[[\hat{A},\hat{B}]\big]=\frac{\hbar}{\mathrm{i}}\{A_0,B_0\}+\mathcal{O}(\hbar^2) \tag{3.35}$$

(for $A=A_0+\mathcal{O}(\hbar)$ and B analogous).

$\Rightarrow$ The principal symbol of the commutator is the Poisson bracket of the principal symbols.

4 Time Evolution

4.1 Egorov's Theorem

In the Heisenberg picture operators are time-dependent and obey (cf. section 2)

$$\dot{\hat{A}}(t) = -\frac{\mathrm{i}}{\hbar}[\hat{H}, \hat{A}(t)] \,. \tag{2.6'}$$

We denote the symbol of $\hat{A}(t)$ by $A(p,x,t)$, i.e.

$$A(p,x,t) = \mathrm{symb}[\hat{A}(t)](p,x) \,, \tag{4.1}$$

which is related to the previous notation by $A(p,x) = \mathrm{symb}[\hat{A}](p,x) = A(p,x,0)$. One can show that if $\hat{A}$ is a semiclassical ψDO then $\hat{A}(t)$ also has a classical symbol, i.e

$$A(p,x,t) \sim \hbar^a \left(A_0(p,x,t) + \hbar A_1(p,x,t) + \mathcal{O}(\hbar^2) \right) \,. \tag{4.2}$$

Let us determine the time evolution of symbols by calculating the symbol of both sides of equation (2.6):

$$\text{l.h.s} = \mathrm{symb}\left[\dot{\hat{A}}(t) \right](p,x) = \frac{\partial}{\partial t} \mathrm{symb}[\hat{A}(t)](p,x) \sim \hbar^a \, \frac{\partial A_0}{\partial t}(p,x,t) \left(1 + \mathcal{O}(\hbar) \right) , \tag{4.3}$$

$$\text{r.h.s} = \mathrm{symb}\left[\frac{\mathrm{i}}{\hbar}[\hat{H}, \hat{A}(t)] \right](p,x) = \hbar^a \{H_0, A_0\}(p,x,t) \left(1 + \mathcal{O}(\hbar) \right) . \tag{4.4}$$

Solving the equation order by order in $\hbar$, in leading order we find

$$\frac{\partial A_0}{\partial t}(p,x,t) = \{H_0, A_0\}(p,x,t) \,, \tag{4.5}$$

which is the classical equation of motion (1.4). Thus, we conclude that the principal symbol of the time evolved operator is given by the classical time evolution of the principal symbol of the operator at time zero, i.e

$$A_0(p,x,t) = A_0(\phi^t(p,x)) \equiv A_0(\phi^t(p,x), 0) \,, \tag{4.6}$$

or, equivalently,

$$\boxed{A(p,x,t) = \hbar^a \, A_0(\phi^t(p,x)) \left(1 + \mathcal{O}(\hbar) \right)} \,, \tag{4.7}$$

This statement is known as Egorov's theorem.

4.2 The Ehrenfest Time

Egorov's theorem (4.7) holds for fixed time t in the formal limit $\hbar \to 0$. If one wants to control time evolution for fixed $\hbar$ and t one needs to know the time dependence of the

$\mathcal{O}(\hbar)$-term in (4.7), i.e. one has to investigate the simultaneous limits $\hbar \to 0$ and $t \to \infty$. Precisely one would like to know how fast t may go to infinity (as a function of $\hbar$) such that a statement like (4.7) is still true.

We will not derive this relation here but only do a little calculation for getting an impression and state the result.

Consider the symbol of the time evolved observable $\hat{A}(t)$ at phase space point (p', x'). Egorov's theorem tells us that

$$A(p', x', t) = \hbar^a A_0(\phi^t(p', x')) \left(1 + \mathcal{O}(\hbar)\right). \tag{4.8}$$

If we choose (p', x') to be very close to (p, x), more precisely $||(p', x') - (p, x)|| = \mathcal{O}(\hbar)$ then we can expand the symbol $A(p', x')$ about $(p', x') = (p, x)$ and absorb everything but the leading term into the sub-principal symbol (which doesn't show up in Egorov's theorem!). Applying Egorov once more then yields

$$A(p', x', t) = \hbar^a A_0(\phi^t(p, x)) \left(1 + \mathcal{O}(\hbar)\right). \tag{4.9}$$

The difference between (4.8) and (4.9) is in the $\mathcal{O}(\hbar)$-term, since we chose $||(p', x') - (p, x)|| = \mathcal{O}(\hbar)$, but as a function of time has to grow like the difference $||\phi^t(p', x') - \phi^t(p, x)||$. For integrable (regular) systems the distance between neighbouring trajectories grows at most polynomially with time. If the dynamics, however, are chaotic (hyperbolic) then this distance can grow exponentially in time, i.e.

$$||\phi^t(p', x') - \phi^t(p, x)|| \sim ||(p', x') - (p, x)|| \mathrm{e}^{\lambda t} \tag{4.10}$$

("sensitive dependence on initial conditions" – "butterfly effect") where λ is called Lyapunov exponent.

Thus, for chaotic systems we have found an $\mathcal{O}(\hbar)$-correction which blows up exponentially in time and thus – if we want the error to remain small – t may at most grow logarithmically in $1/\hbar$. This time up to which Egorov's theorem holds is known as the Ehrenfest time,

$$\boxed{t_{\mathrm{E}} := \frac{1}{\lambda} \log \frac{1}{\hbar}}, \tag{4.11}$$

or "log-breaking-time".

In the physics literature the observation that semiclassical time evolution (for observables as discussed here or, more common, similar statements for wave packet dynamics or expectation values) can hold only up to the Ehrenfest time t_E was made already in the late 1970s [9, 10]. Rigorous proofs were only given about twenty years later, see e.g. [11, 12], and (semiclassical) estimates for the time evolution on larger time scales than t_E are an active area of research, see e.g. [13, 14] for some recent developments.

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