13
Quantization Schemes for Euclidean Space

13.1 Ordering Ambiguities

One of the axioms of quantum mechanics states, "To each real-valued function f on the classical phase space there is associated a self-adjoint operator $\hat{f}$ on the quantum Hilbert space." The attentive reader will note that we have not, up to this point, given a general procedure for constructing $\hat{f}$ from f. If we call $\hat{f}$ the *quantization* of f, then we have only discussed the quantizations of a few very special classical observables, such as position, momentum, and energy.

Let us now think about what would go into quantizing a (more-or-less) general observable. Let us consider for simplicity a particle moving in $\mathbb{R}^1$ and let us assume that quantizations of x and p are the usual position and momentum operators X and P. What should the quantization of, say, xp be? Classically, xp and px are the same, but quantum mechanically, XP does not equal PX. Furthermore, neither XP nor PX is self-adjoint, because $(XP)^* = P^*X^* = PX$, and $PX \neq XP$. In this case, then, a reasonable candidate for the quantization would be

$$\widehat{xp} = \frac{1}{2}(XP + PX).$$

The significance of this simple example is that the failure of commutativity among quantum operators creates an ambiguity in the quantization process. It does not make sense to simply "replace x by X and p by P everywhere in the formula," since the ordering of position and momentum makes no difference on the classical side, but it does on the quantum

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side. Up to this point, we have not really had to confront this ambiguity, because of the special form of the observables we have quantized. The Hamiltonian, for example, is typically of the form $H(x,p) = p^2/(2m) + V(x)$. Since each term contains only x or only p, it is natural to quantize H to $\hat{H} = P^2/(2m) + V(X)$, where $V(X)$ may be defined by the functional calculus or simply as multiplication by $V(x)$. In defining the angular momentum operators, we do encounter products of position and momentum, but never of the same component of position and momentum. For a particle in $\mathbb{R}^2$, for example, we have, $J = x_1p_2 - x_2p_1$. On the quantum side, X_1 commutes with P_2 and X_2 with P_2, and thus there is no ambiguity: $X_1P_2 - X_2P_1$ is the same as $P_2X_1 - P_1X_2$.

When we turn to the quantization of a general observable, however, we must confront the ordering ambiguity directly. Groenewold's theorem (Sect. 13.4) suggests that there is no single "perfect" quantization scheme. Nevertheless, there is one that is generally acknowledged as having the best properties, the Weyl quantization, and we spend most of our time with that particular scheme. Other quantization schemes do also play a role in physics, however; Wick-ordered quantization, notably, plays an important role in quantum field theory. (In quantum field theory, the replacement of certain Weyl-quantized operators with their Wick-quantized counterparts is interpreted as a type of renormalization.)

13.2 Some Common Quantization Schemes

In this section, we consider several of the most commonly used quantization schemes. For simplicity, we limit our attention to systems with one degree of freedom and to classical observables that are polynomials in x and p. (We consider the Weyl quantization in greater generality in Sect. 13.3.) Furthermore, we resolve in this section not to worry about domain questions and simply to use $C_c^\infty(\mathbb{R})$ as the domain for all of our operators. Thus, in this section, equality of operators means equality as maps of $C_c^\infty(\mathbb{R})$ to itself. It should be noted that the operators of the sort we will be considering may very well fail to be essentially self-adjoint, even if they are symmetric. Section 9.10 shows, for example, that the operator $P^2 - cX^4$, for $c > 0$, is not essentially self-adjoint on $C_c^\infty(\mathbb{R})$. We follow the terminology of harmonic analysis by referring to a classical symbol f as the *symbol* of its quantization $\hat{f}$. Once we have discussed each quantization scheme briefly, we will formalize the definitions of all the schemes in Definition 13.1.

The simplest approach to quantization is to choose, once and for all, which to put first, the position or the momentum operators. We may, for example, choose to put the momentum operators to the right, acting first, and the position operators to the left, acting second. In this approach, a polynomial in x and p will quantize to a differential operator in "standard form," with all the derivatives acting first, followed by multiplication operators. In harmonic analysis, there is a method for extending this quantization scheme to more-or-less arbitrary symbols, f. For a general (nonpolynomial) symbol f, the resulting operator $\hat{f}$ is known as a *pseudodifferential operator*.

A serious drawback of the pseudodifferential quantization is that even when the symbol f is real-valued, the operator $\hat{f}$ it produces is typically not self-adjoint (or even symmetric). If, for example, $f(x,p) = xp$, then the associated operator is XP, the adjoint of which is PX, which is not equal to XP. The simplest way to fix this problem is to symmetrize the operator by taking half the sum of the operator and its adjoint.

The Weyl quantization, meanwhile, takes more seriously the possibility of different orderings of X and P, by considering *all* possible orderings. Thus, in quantizing, say, x^2p^2, the Weyl quantization will give

$$\frac{1}{6}(X^2P^2 + XPXP + XP^2X + PX^2P + PXPX + P^2X^2).$$

For a general monomial, the Weyl quantization similarly averages all the possible orderings of the position and momentum operators.

For Wick-ordered and anti-Wick-ordered quantization, we no longer regard the position and momentum operators as the "basic" operators, but rather the creation and annihilation operators. Specifically, given any positive real number α, we introduce complex coordinates on the classical phase space by

$$\begin{aligned} z &= x - i\alpha p \\ \bar{z} &= x + i\alpha p. \end{aligned} \tag{13.1}$$

(Although it would seem more natural to define z to be $x + i\alpha p$, this choice would lead to problems later, especially with the Segal–Bargmann transform.) We then consider the corresponding quantum operators, which we call the raising and lowering operators:

$$\begin{aligned} a^* &= X - i\alpha P \\ a &= X + i\alpha P. \end{aligned} \tag{13.2}$$

In comparing these operators to the ones defined in the context of the harmonic oscillator, we should think of α as corresponding to $1/(m\omega)$. Even with this identification, however, the operators in (13.2) differ by a constant from the raising and lowering operators of Chap. 11. [The overall normalization of the raising and lowering operators is not important in this context, provided that we are consistent in the normalization between (13.1) and (13.2).] In particular, the commutator of a and a^* is not I but rather $2\alpha\hbar I$.

In Wick-ordered quantization, we begin by expressing the classical observable f in terms of z and $\bar{z}$ rather than in terms of x and p. When we quantize, we put all the lowering operators (coming from the factors of $\bar{z}$ in f) to the right, acting first, and the raising operators (coming from the factors of z in f) to the left, acting second. This approach to quantization is useful in quantum field theory, where letting the lowering operators act first can cause certain otherwise ill-defined expressions to become well defined. In anti-Wick-ordered quantization, we do the reverse, putting the raising operators to the right, acting first. Although anti-Wick-ordered quantization seems singular in the context of quantum field theory, in systems with finitely many degrees of freedom, it is actually better behaved than Wick-ordered quantization.

Definition 13.1 *Define several different quantization schemes for symbols that are polynomials in x and p as follows. Each scheme is uniquely determined—as a map from polynomials on $\mathbb{R}^2$ into operators on $C_c^\infty(\mathbb{R})$—by the indicated formulas.*

1. ***Pseudodifferential operator quantization:***

$$Q(x^j p^k) = X^j P^k.$$

2. ***Symmetrized pseudodifferential operator quantization:***

$$Q(x^j p^k) = \frac{1}{2}(X^j P^k + P^k X^j).$$

3. ***Weyl quantization:***

$$Q(x^j p^k) = \frac{1}{(j+k)!} \sum_{\sigma \in S_{j+k}} \sigma\left(X, X, \ldots, X, P, P, \ldots, P\right),$$

where for any operators $A_1, A_2, \ldots, A_n$ and any $\sigma \in S_n$, we define

$$\sigma(A_1, A_2, \ldots, A_n) = A_{\sigma(1)} A_{\sigma(2)} \cdots A_{\sigma(n)}. \tag{13.3}$$

4. ***Wick-ordered quantization** with parameter α:*

$$Q((x + i\alpha p)^j (x - i\alpha p)^k) = (X - i\alpha P)^k (X + i\alpha P)^j, \quad \alpha > 0.$$

5. ***Anti-Wick-ordered quantization** with parameter α:*

$$Q((x + i\alpha p)^j (x - i\alpha p)^k) = (X + i\alpha P)^j (X - i\alpha P)^k, \quad \alpha > 0.$$

In applications, the most useful quantization schemes are the Wick-ordered, anti-Wick-ordered, and Weyl schemes. All of the quantization schemes in Definition 13.1 except the pseudodifferential operator quantization have the property of mapping real-valued polynomials to symmetric operators on $C_c^\infty(\mathbb{R})$. (See Exercise 3 in the case of the Wick- and anti-Wick-ordered quantizations.)

In comparing the different quantization schemes, it is important to recognize that two different expressions may describe the same operator. We may calculate, for example, that

$$\begin{aligned}\frac{1}{2}(XP^2 + P^2X) &= \frac{1}{2}(PXP + [X,P]P + PXP - P[X,P]) \\ &= PXP,\end{aligned}$$

since $[X,P]$ is a multiple of the identity and thus commutes with P. As a result, we can eliminate the PXP term in the Weyl quantization of xp^2, with the result that

$$Q_{\mathrm{Weyl}}(xp^2) = \frac{1}{3}(XP^2 + PXP + P^2X) = \frac{1}{2}(XP^2 + P^2X), \tag{13.4}$$

which coincides, in this very special case, with the symmetrized pseudodifferential quantization of xp^2.

Example 13.2 *If $f(x,p) = x^2$, then the Weyl, Wick-ordered and anti-Wick-ordered quantizations of f are as follows:*

$$\begin{aligned}Q_{\mathrm{Weyl}}(x^2) &= X^2 \\ Q_{\mathrm{Wick}}(x^2) &= X^2 - \frac{1}{2}\alpha\hbar I \\ Q_{\mathrm{anti-Wick}}(x^2) &= X^2 + \frac{1}{2}\alpha\hbar I.\end{aligned}$$

Proof. The value for $Q_{\mathrm{Weyl}}(x^2)$ is apparent. To compute the Wick- and anti-Wick-ordered quantizations, we first write x as $(z+\bar{z})/2$, so that

$$x^2 = \frac{(z+\bar{z})^2}{4} = \frac{1}{4}(z^2 + 2z\bar{z} + \bar{z}^2).$$

Thus, we have, for example,

$$Q_{\mathrm{Wick}}(x^2) = \frac{1}{4}\left((X - i\alpha P)^2 + 2(X - i\alpha P)(X + i\alpha P) + (X + i\alpha P)^2\right).$$

When we expand this expression out, the P^2 terms cancel, and the XP and PX terms from $(X - i\alpha P)^2$ will cancel with the XP and PX terms from $(X + i\alpha P)^2$. Thus, we will be left with X^2 terms and the XP and PX terms from the cross-term above:

$$Q_{\mathrm{Wick}}(x^2) = \frac{1}{4}\left(4X^2 + 2i\alpha[X,P]\right).$$

Using the commutation relation between X and P gives the desired result. The calculation of $Q_{\text{antiWick}}(x^2)$ is identical except that the order of the factors in the cross-term is reversed, which gives the opposite sign for the $[X,P]$ term. ■

Proposition 13.3 *The Weyl quantization—viewed as a linear map of the space of polynomials on $\mathbb{R}^2$ into operators on $C_c^\infty(\mathbb{R})$—is uniquely characterized by the following identity:*

$$Q_{\text{Weyl}}((ax+bp)^j) = (aX+bP)^j \tag{13.5}$$

for all non-negative integers j and all $a, b \in \mathbb{C}$.

Proof. The Weyl quantization is easily seen to satisfy the identity

$$\begin{aligned} &Q_{\text{Weyl}}((a_1x+b_1p)\cdots(a_jx+b_jp)) \\ &= \frac{1}{j!}\sum_{\sigma\in S_j}\sigma(a_1X+b_1P,\ldots,a_jX+b_jP), \end{aligned} \tag{13.6}$$

for all sequences $a_1,\ldots,a_j$ and $b_1,\ldots,b_j$ of complex numbers, where the expression $\sigma(\cdot,\cdot,\ldots,\cdot)$ is defined by (13.3). Specializing to the case where all the a_j's are equal to a and all the b_j's are equal to b gives (13.5). Conversely, suppose that Q is any linear map of polynomials into operators on $C_c^\infty(\mathbb{R})$ satisfying $Q((ax+bp)^j) = (aX+bP)^j$ for all a, b, and j. For each j, let V_j denote the space of homogeneous polynomials f of degree j such that $Q(f) = Q_{\text{Weyl}}(f)$. Then V_j contains all polynomials of the form $(ax+bp)^j$, and thus, by Exercise 1, V_j consists of all homogeneous polynomials of degree j, so that $Q = Q_{\text{Weyl}}$. ■

Proposition 13.4 *The Weyl quantization satisfies*

$$Q_{\text{Weyl}}(xg) = Q_{\text{Weyl}}(x)Q_{\text{Weyl}}(g) - \frac{i\hbar}{2}Q_{\text{Weyl}}\left(\frac{\partial g}{\partial p}\right) \tag{13.7}$$

$$= Q_{\text{Weyl}}(g)Q_{\text{Weyl}}(x) + \frac{i\hbar}{2}Q_{\text{Weyl}}\left(\frac{\partial g}{\partial p}\right) \tag{13.8}$$

and

$$Q_{\text{Weyl}}(pg) = Q_{\text{Weyl}}(p)Q_{\text{Weyl}}(g) + \frac{i\hbar}{2}Q_{\text{Weyl}}\left(\frac{\partial g}{\partial x}\right) \tag{13.9}$$

$$= Q_{\text{Weyl}}(g)Q_{\text{Weyl}}(p) - \frac{i\hbar}{2}Q_{\text{Weyl}}\left(\frac{\partial g}{\partial x}\right) \tag{13.10}$$

for all polynomials g in x and p.

It should be noted that the formulas for the Weyl quantization in Proposition 13.4 may not give the same "expression" for $Q_{\text{Weyl}}(f)$ as does Definition 13.1, but it does give the same operator. [Compare (13.4).]

Proof. Suppose $A = (a_1X + b_1P)$ and $B = (a_2X + b_2P)$. Then $[A, B]$ is a multiple of I, from which we can easily verify that

$$AB^j = B^k AB^{j-k} + k[A, B]B^{j-1},$$

for $0 \leq k \leq j$. If we sum this relation over k and divide by $j + 1$, we obtain

$$AB^j = \frac{1}{j+1}\sum_{k=0}^{j} B^k AB^{j-k} + \frac{1}{j+1}\frac{j(j+1)}{2}[A, B]B^{j-1}. \tag{13.11}$$

Now, A is the Weyl quantization of $(a_1X + b_1p)$ and B^j is the Weyl quantization of $(a_2x + b_2p)^j$, and both terms on the right-hand side of (13.11) are easily recognized as Weyl quantizations. Thus, after rearranging the terms and evaluating the commutator, (13.11) becomes,

$$\begin{aligned} &Q_{\mathrm{Weyl}}((a_1x + b_1p)(a_2x + b_2p)^j) \\ &= Q_{\mathrm{Weyl}}(a_1x + b_1p)Q_{\mathrm{Weyl}}((a_2x + b_2p)^j) \\ &- i\hbar\frac{j}{2}(a_1b_2 - a_2b_1)Q_{\mathrm{Weyl}}((a_1x + b_1p)^{j-1}). \end{aligned} \tag{13.12}$$

Meanwhile, if we run the same argument starting with B^jA we obtain a similar result:

$$\begin{aligned} &Q_{\mathrm{Weyl}}((a_1x + b_1p)(a_2x + b_2p)^j) \\ &= Q_{\mathrm{Weyl}}((a_2x + b_2p)^j)Q_{\mathrm{Weyl}}(a_1x + b_1p) \\ &+ i\hbar\frac{j}{2}(a_1b_2 - a_2b_1)Q_{\mathrm{Weyl}}((a_1x + b_1p)^{j-1}). \end{aligned} \tag{13.13}$$

If we specialize to the case $(a_1, b_1) = (1, 0)$ and $(a_2, b_2) = (a, b)$, we get

$$\begin{aligned} Q_{\mathrm{Weyl}}(x(ax + bp)^j) &= Q_{\mathrm{Weyl}}(x)Q_{\mathrm{Weyl}}((ax + bp)^j) \\ &\quad - i\hbar\frac{j}{2}bQ_{\mathrm{Weyl}}((ax + bp)^{j-1}), \end{aligned} \tag{13.14}$$

where the last term on the right-hand side of (13.14) is $-i\hbar/2$ times the Weyl quantization of $\partial(ax+bp)^j/\partial p$. Thus, (13.14) is precisely (13.7) in the case $g(x, p) = (ax + bp)^j$. We can then see from Exercise 1 that (13.7) hold for all polynomials g. The proofs of (13.8), (13.9), and (13.10) are similar. ∎

13.3 The Weyl Quantization for $\mathbb{R}^{2n}$

In this section, we study the Weyl quantization on a much larger class of symbols (i.e., classical observables) than the polynomial symbols considered in the previous section. We also generalize from symbols defined on $\mathbb{R}^2$ to symbols defined on $\mathbb{R}^{2n}$.

13.3.1 Heuristics

It is a straightforward matter to extent the Weyl quantization on polynomials from $\mathbb{R}^2$ to $\mathbb{R}^{2n}$. This extended quantization will satisfy

$$Q_{\mathrm{Weyl}}((\mathbf{a}\cdot\mathbf{p}+\mathbf{b}\cdot\mathbf{p})^j) = (\mathbf{a}\cdot\mathbf{X}+\mathbf{b}\cdot\mathbf{P})^j \tag{13.15}$$

for all $\mathbf{a},\mathbf{b}\in\mathbb{R}^n$ and all non-negative integers j, as in Proposition 13.3 in the $n=1$ case. Suppose we wish to extend Q_{Weyl} to certain nonpolynomial symbols, starting with complex exponentials. If we multiply (13.15) by $(i)^j/j!$ and sum on j, we would expect to have

$$Q_{\mathrm{Weyl}}\left(e^{i(\mathbf{a}\cdot\mathbf{x}+\mathbf{b}\cdot\mathbf{p})}\right) = e^{i(\mathbf{a}\cdot\mathbf{X}+\mathbf{b}\cdot\mathbf{P})}. \tag{13.16}$$

Now, if f is any sufficiently nice function on $\mathbb{R}^{2n}$, we can expand f as an integral involving functions of the form $\exp(i(\mathbf{a}\cdot\mathbf{x}+\mathbf{b}\cdot\mathbf{p}))$, by using the Fourier transform:

$$f(\mathbf{x},\mathbf{p}) = (2\pi)^{-n}\int_{\mathbb{R}^{2n}}\hat{f}(\mathbf{a},\mathbf{b})e^{i(\mathbf{a}\cdot\mathbf{x}+\mathbf{b}\cdot\mathbf{p})}\,d\mathbf{a}\,d\mathbf{b},$$

where $\hat{f}$ is the Fourier transform of f. In light of (13.16), it is then natural to define

$$Q_{\mathrm{Weyl}}(f) = (2\pi)^{-n}\int_{\mathbb{R}^{2n}}\hat{f}(\mathbf{a},\mathbf{b})e^{i(\mathbf{a}\cdot\mathbf{X}+\mathbf{b}\cdot\mathbf{P})}\,d\mathbf{a}\,d\mathbf{b}. \tag{13.17}$$

Before proceeding, let us pause for a moment to compute the operator $\exp(i(\mathbf{a}\cdot\mathbf{X}+\mathbf{b}\cdot\mathbf{P}))$. If A and B are bounded operators that commute with their commutator (i.e., such that $[A,[A,B]]=[B,[A,B]]=0$), then

$$e^{A+B} = e^{-[A,B]/2}e^Ae^B. \tag{13.18}$$

(See Theorem 14.1, which is proved in Sect. 3.1 of [21]. Equation (13.18) is a special case of the Baker–Campbell–Hausdorff Formula.) If we *formally* apply (13.18) with $A=i\mathbf{a}\cdot\mathbf{X}$ and $B=i\mathbf{b}\cdot\mathbf{P}$ (even though these are unbounded operators), we obtain

$$e^{i(\mathbf{a}\cdot\mathbf{X}+\mathbf{b}\cdot\mathbf{P})} = e^{i\hbar(\mathbf{a}\cdot\mathbf{b})/2}e^{i\mathbf{a}\cdot\mathbf{X}}e^{i\mathbf{b}\cdot\mathbf{P}}. \tag{13.19}$$

Meanwhile, by Example 10.16 in Sect. 10.2, we know that

$$(e^{i\mathbf{b}\cdot\mathbf{P}}\psi)(\mathbf{x}) = \psi(\mathbf{x}+\hbar\mathbf{b}).$$

Thus, we may reasonably hope that

$$\left(e^{i(\mathbf{a}\cdot\mathbf{X}+\mathbf{b}\cdot\mathbf{P})}\psi\right)(\mathbf{x}) = e^{i\hbar(\mathbf{a}\cdot\mathbf{b})/2}e^{i\mathbf{a}\cdot\mathbf{x}}\psi\left(\mathbf{x}+\hbar\mathbf{b}\right). \tag{13.20}$$

In general, we get incorrect results if we formally apply results for bounded operators to operators that are unbounded. In this case, however, the result of the formal calculation is correct. The simplest way to prove this is to replace $\mathbf{a}$ and $\mathbf{b}$ by $t\mathbf{a}$ and $t\mathbf{b}$ on the right-hand side of (13.19) and to check that the result is a strongly continuous one-parameter unitary group.

Proposition 13.5 *For all* $\mathbf{a}$ *and* $\mathbf{b}$ *in* $\mathbb{R}^n$, *the operators* $U_{\mathbf{a},\mathbf{b}}(t)$ *on* $L^2(\mathbb{R}^n)$ *given by*

$$(U_{\mathbf{a},\mathbf{b}}(t)\psi)(\mathbf{x}) = e^{it^2\hbar(\mathbf{a}\cdot\mathbf{b})/2}e^{it\mathbf{a}\cdot\mathbf{x}}\psi\left(\mathbf{x}+t\hbar\mathbf{b}\right) \tag{13.21}$$

form a strongly continuous one-parameter unitary group. The infinitesimal generator of this group coincides with $\mathbf{a}\cdot\mathbf{X}+\mathbf{b}\cdot\mathbf{P}$ *on* $C_c^\infty(\mathbb{R}^n)$ *and is essentially self-adjoint on this domain. Thus, if* $\mathbf{a}\cdot\mathbf{X}+\mathbf{b}\cdot\mathbf{P}$ *denotes the unique self-adjoint extension of the infinitesimal generator on* $C_c^\infty(\mathbb{R}^n)$, *it follows from Stone's theorem that*

$$e^{it(\mathbf{a}\cdot\mathbf{X}+\mathbf{b}\cdot\mathbf{P})} = e^{it^2\hbar(\mathbf{a}\cdot\mathbf{b})/2}e^{it\mathbf{a}\cdot\mathbf{X}}e^{it\mathbf{b}\cdot\mathbf{P}}$$

for all $t\in\mathbb{R}$. *In particular, (13.19) and (13.20) hold.*

Proof. It is apparent that $U_{\mathbf{a},\mathbf{b}}$ is unitary for each $\mathbf{a}$ and $\mathbf{b}$, and it is a simple direct computation to show that it is indeed a unitary group. Strong continuity is proved in the usual way using a dense subspace, as in the proof of Example 10.12. When ψ is in $C_c^\infty(\mathbb{R}^n)$, it is easy to differentiate the right-hand side of (13.21) with respect to t at $t=0$ to obtain the formula for the infinitesimal generator. Finally, the essential self-adjointness of $\mathbf{a}\cdot\mathbf{X}+\mathbf{b}\cdot\mathbf{P}$ on $C_c^\infty(\mathbb{R}^n)$ is precisely the content of Proposition 9.40. ■

With the computation of the operator $e^{i(\mathbf{a}\cdot\mathbf{X}+\mathbf{b}\cdot\mathbf{P})}$ in hand, we return to our analysis of the proposed formula (13.17) for the general Weyl quantization. If the Fourier transform of f is in $L^1(\mathbb{R}^{2n})$, we can regard the right-hand side of (13.17) as an absolutely convergent "Bochner" integral with values in the Banach space $\mathcal{B}(\mathbf{H})$. For our purposes, however, it is more convenient to think of operators on $L^2(\mathbb{R}^n)$ as integral operators and to write down a formula for the integral kernel of $Q_{\mathrm{Weyl}}(f)$ in terms of f itself. (But see Exercise 7.)

At a formal level, the operator mapping ψ to $e^{i\hbar(\mathbf{a}\cdot\mathbf{b})/2}e^{i\mathbf{a}\cdot\mathbf{x}}\psi\left(\mathbf{x}+\hbar\mathbf{b}\right)$ may be thought of as an "integral" operator, with integral kernel given by

$$e^{i\hbar(\mathbf{a}\cdot\mathbf{b})/2}e^{i\mathbf{a}\cdot\mathbf{x}}\delta_n(\mathbf{x}+\hbar\mathbf{b}-\mathbf{y}), \tag{13.22}$$

where δ_n is an n-dimensional delta-function (the n-dimensional analog of the distribution in Example A.26). Thus, it should be possible to obtain the integral kernel of $Q_{\mathrm{Weyl}}(f)$ by integrating the preceding expression against $\hat{f}(\mathbf{a},\mathbf{b})$. To evaluate the resulting integral, we make the change of variable $\mathbf{c}=\hbar\mathbf{b}$, in which case we obtain

$$\begin{aligned}
&(2\pi\hbar)^{-n}\int_{\mathbb{R}^n}\int_{\mathbb{R}^n} e^{i(\mathbf{a}\cdot\beta)/2}e^{i\mathbf{a}\cdot\mathbf{x}}\delta_n(\mathbf{x}+\mathbf{c}-\mathbf{y})\hat{f}(\mathbf{a},\mathbf{c}/\hbar)\;d\mathbf{c}\;d\mathbf{a}\\
&=\ (2\pi\hbar)^{-n}\int_{\mathbb{R}^n} e^{i(\mathbf{a}\cdot(\mathbf{y}-\mathbf{x}))/2}e^{i\mathbf{a}\cdot\mathbf{x}}\hat{f}(\mathbf{a},(\mathbf{y}-\mathbf{x})/\hbar)\;d\mathbf{a}\\
&=\ \hbar^{-n}(2\pi)^{-n/2}\left[(2\pi)^{-n/2}\int_{\mathbb{R}^n} e^{i\mathbf{a}\cdot(\mathbf{x}+\mathbf{y})/\mathbf{2}}\hat{f}(\mathbf{a},(\mathbf{y}-\mathbf{x})/\hbar)\;d\mathbf{a}\right].
\end{aligned} \tag{13.23}$$

We may recognize the integral in square brackets in the last line of (13.23) as undoing the Fourier transform of f in the $\mathbf{x}$-variable, leaving us with the partial Fourier transform of f in the $\mathbf{p}$ variable, evaluated at the points $(\mathbf{x}+\mathbf{y})/2$, $(\mathbf{y}-\mathbf{x})/\hbar$. (The partial Fourier transform means the ordinary Fourier transform with respect to one of the variables, with the other variable fixed.) Thus, we expect that $Q_{\mathrm{Weyl}}(f)$ should be the integral operator with integral kernel κ_f given by

$$\kappa_f(\mathbf{x},\mathbf{y}) = (2\pi\hbar)^{-n} \int_{\mathbb{R}^n} f((\mathbf{x}+\mathbf{y})/2,\mathbf{p}) e^{-i(\mathbf{y}-\mathbf{x})\cdot\mathbf{p}/\hbar}\, d\mathbf{p}. \tag{13.24}$$

13.3.2 The L^2 Theory

With the preceding calculations as motivation, we now define $Q_{\mathrm{Weyl}}(f)$ to be the integral operator with kernel κ_f, beginning with the case in which f belongs to $L^2(\mathbb{R}^{2n})$. The resulting operators will turn out to be Hilbert–Schmidt operators on $L^2(\mathbb{R}^n)$.

If $\mathbf{H}$ is a Hilbert space and $A \in \mathcal{B}(\mathbf{H})$ is a non-negative self-adjoint operator on $\mathbf{H}$, then it can be shown that A has a well-defined (but possibly infinite) *trace*. What this means is that the value of

$$\operatorname{trace}(A) := \sum_j \langle e_j, Ae_j\rangle$$

is the same for each orthonormal basis $\{e_j\}$ of $\mathbf{H}$. Note that since A is a non-negative operator, $\langle e_j, Ae_j\rangle$ is a non-negative real number, so that the sum is always defined, but may have the value $+\infty$.

Now, if A is any bounded operator, then A^*A is self-adjoint and non-negative. We say that A is *Hilbert–Schmidt* if

$$\operatorname{trace}(A^*A) < \infty.$$

Given two Hilbert–Schmidt operators A and B, it can be shown that A^*B is a trace-class operator, meaning that the sum

$$\operatorname{trace}(A^*B) := \sum_{j=1}^{\infty} \langle e_j, A^*Be_j\rangle$$

is absolutely convergent and the value of the sum is independent of the choice of orthonormal basis. We define the *Hilbert–Schmidt inner product* of A and B and the associated *Hilbert–Schmidt norm* of A by

$$\langle A, B\rangle_{\mathrm{HS}} := \operatorname{trace}(A^*B)$$
$$\|A\|_{\mathrm{HS}} := \sqrt{\operatorname{trace}(A^*A)}.$$

It can be shown that the space of Hilbert–Schmidt operators on $\mathbf{H}$ forms a Hilbert space with respect to the Hilbert–Schmidt inner product.

(See Sect. 19.2 for more details.) We denote the space of Hilbert–Schmidt operators on $\mathbf{H}$ by $\mathrm{HS}(\mathbf{H})$.

We will make use of the following standard (and elementary) result characterizing Hilbert–Schmidt operators on $L^2(\mathbb{R}^n)$ in terms of integral operators. (See, for example, Theorem VI.23 in Volume I of [34].)

Proposition 13.6 *If κ is in $L^2(\mathbb{R}^n \times \mathbb{R}^n)$ then for every $\psi \in L^2(\mathbb{R}^n)$, the integral*

$$A_\kappa(\psi)(\mathbf{x}) := \int_{\mathbb{R}^n} \kappa(\mathbf{x}, \mathbf{y})\psi(\mathbf{y})\ d\mathbf{y} \tag{13.25}$$

is absolutely convergent for almost every $\mathbf{x} \in \mathbb{R}^n$, and $A_\kappa(\psi)$ also belongs to $L^2(\mathbb{R}^n)$. Furthermore, the operator A_κ is a Hilbert–Schmidt operator on $L^2(\mathbb{R}^n)$ and

$$\|A_\kappa\|_{\mathrm{HS}} = \|\kappa\|_{L^2(\mathbb{R}^n \times \mathbb{R}^n)}\,.$$

Conversely, for any Hilbert–Schmidt operator A on $L^2(\mathbb{R}^n)$, there exists a unique $\kappa \in L^2(\mathbb{R}^n \times \mathbb{R}^n)$ such that $A = A_\kappa$.

We are now ready, using discussion in Sect. 13.3.1 as motivation, to define the Weyl quantization of L^2 symbols.

Definition 13.7 *For all $f \in L^2(\mathbb{R}^{2n})$, define $\kappa_f : \mathbb{R}^{2n} \to \mathbb{C}$ by*

$$\kappa_f(\mathbf{x}, \mathbf{y}) = (2\pi\hbar)^{-n} \int_{\mathbb{R}^n} f((\mathbf{x}+\mathbf{y})/2, \mathbf{p}) e^{-i(\mathbf{y}-\mathbf{x})\cdot\mathbf{p}/\hbar}\ d\mathbf{p}, \tag{13.26}$$

*and define the **Weyl quantization** of f, as an operator on $L^2(\mathbb{R}^n)$, by*

$$Q_{\mathrm{Weyl}}(f) = A_{\kappa_f},$$

where A_{κ_f} is defined by (13.25).

The integral in (13.26) is not necessarily absolutely convergent, and should be understood as computing a partial Fourier transform. Thus, we should, strictly speaking, replace the right-hand side of (13.26) with

$$\lim_{R \to \infty}\ (2\pi\hbar)^{-n} \int_{|\mathbf{p}| \le R} f((\mathbf{x}+\mathbf{y})/2, \mathbf{p}) e^{-i(\mathbf{y}-\mathbf{x})\cdot\mathbf{p}/\hbar}\ d\mathbf{p}, \tag{13.27}$$

where the limit is in the norm topology of $L^2(\mathbb{R}^{2n})$. [The partial Fourier transform maps the Schwartz space $\mathcal{S}(\mathbb{R}^{2n})$ to itself. By Fubini's theorem and the Plancherel formula for $\mathbb{R}^n$, the partial Fourier transform is an L^2-isometry and extends to a unitary map of $L^2(\mathbb{R}^{2n})$ to itself. This unitary map can be computed by the usual formula on functions in $L^1 \cap L^2$ and can be computed by the limiting formula similar to (13.27) in general.]

In words, we may describe the procedure for computing κ_f at a point $(\mathbf{x}^1, \mathbf{x}^2)$ in $\mathbb{R}^{2n}$ as follows. First, compute the partial Fourier transform $\mathcal{F}_{\mathbf{p}}$

of $f(\mathbf{x},\mathbf{p})$ in the $\mathbf{p}$-variable, resulting in the function $(\mathcal{F}_{\mathbf{p}}f)(\mathbf{x},\xi)$. Then evaluate $\mathcal{F}_{\mathbf{p}}f$ at the point $\mathbf{x}=(\mathbf{x}^1+\mathbf{x}^2)/2$, $\xi=(\mathbf{x}^2-\mathbf{x}^1)/\hbar$. Finally, multiply the result by $\hbar^{-n}(2\pi)^{-n/2}$ to get

$$\kappa_f(\mathbf{x}^1,\mathbf{x}^2)=\hbar^{-n}(2\pi)^{-n/2}(\mathcal{F}_{\mathbf{p}}f)((\mathbf{x}^1+\mathbf{x}^2)/2,(\mathbf{x}^2-\mathbf{x}^1)/\hbar). \tag{13.28}$$

Theorem 13.8 *The map Q_{Weyl} is a constant multiple of a unitary map of $L^2(\mathbb{R}^{2n})$ onto $\mathrm{HS}(L^2(\mathbb{R}^n))$. The inverse map $Q_{\mathrm{Weyl}}^{-1}:\mathrm{HS}(L^2(\mathbb{R}^n))\to L^2(\mathbb{R}^{2n})$ is given by*

$$Q_{\mathrm{Weyl}}^{-1}(A)(\mathbf{x},\mathbf{p})=\hbar^n\int_{\mathbb{R}^n}\kappa(\mathbf{x}-\hbar\mathbf{b}/2,\mathbf{x}+\hbar\mathbf{b}/2)e^{i\mathbf{b}\cdot\mathbf{p}}\,d\mathbf{b},$$

where κ is the integral kernel of A as in Proposition 13.6.

Furthermore, for all $f\in L^2(\mathbb{R}^{2n})$, we have $Q_{\mathrm{Weyl}}(\bar{f})=Q_{\mathrm{Weyl}}(f)^*$; in particular, $Q_{\mathrm{Weyl}}(f)$ is self-adjoint if f is real valued.

Properly speaking, the integral in the theorem should be understood as an L^2 limit, as in (13.27). The fact that Q_{Weyl} is unitary (up to a constant) tells us that for an appropriate constant c, the operators $ce^{i(\mathbf{a}\cdot\mathbf{X}+\mathbf{b}\cdot\mathbf{P})}$ form an "orthonormal basis in the continuous sense" for the Hilbert space $\mathrm{HS}(L^2(\mathbb{R}^n))$. (Compare Sect. 6.6.)

It is possible, using the same formulas, to extend the notion of Weyl quantization to symbols belonging the space of tempered distributions, that is, the space of continuous linear functionals on $\mathcal{S}(\mathbb{R}^{2n})$. We will not, however, develop this construction here. See [11] for more information.

Proof. Proposition 13.6 gives a unitary identification of $\mathrm{HS}(L^2(\mathbb{R}^n))$ with $L^2(\mathbb{R}^n\times\mathbb{R}^n)$. Thus, it suffices to show that the map $f\mapsto\kappa_f$ is a multiple of a unitary map. This result holds because the partial Fourier transform is a unitary map of $L^2(\mathbb{R}^{2n})$ to itself and composition with an invertible linear map is a constant multiple of a unitary map. The inverse of the map $f\mapsto\kappa_f$ is obtained by inverting the linear map and undoing the partial Fourier transform. Finally, it is apparent from (13.26) that

$$\kappa_{\bar{f}}(\mathbf{x},\mathbf{y})=\overline{\kappa_f(\mathbf{y},\mathbf{x})}.$$

This, along with Exercise 6, shows that $Q_{\mathrm{Weyl}}(\bar{f})=Q_{\mathrm{Weyl}}(f)^*$. ∎

13.3.3 The Composition Formula

If f and g are L^2 functions on $\mathbb{R}^{2n}$, then $Q_{\mathrm{Weyl}}(f)$ and $Q_{\mathrm{Weyl}}(g)$ are Hilbert–Schmidt operators, in which case their product is again Hilbert–Schmidt. (Indeed, the product of a Hilbert–Schmidt operator and a bounded operator is always Hilbert–Schmidt.) Thus, since Q_{Weyl} is a bijection of $L^2(\mathbb{R}^{2n})$ with $\mathrm{HS}(L^2(\mathbb{R}^n))$, there is a unique L^2 function, which we denote by $f\star g$, such that

$$Q_{\mathrm{Weyl}}(f)Q_{\mathrm{Weyl}}(g)=Q_{\mathrm{Weyl}}(f\star g). \tag{13.29}$$

(Of course, the operator $\star$, like the Weyl quantization itself, depends on $\hbar$, but we suppress this dependence in the notation.)

Proposition 13.9 *The Moyal product $f \star g$ may be characterized in terms of the Fourier transform as*

$$\widehat{(f \star g)}(\mathbf{a}, \mathbf{b}) = (2\pi)^{-n} \iint e^{-i\hbar(\mathbf{a}\cdot\mathbf{b}' - \mathbf{b}\cdot\mathbf{a}')/2} \times \hat{f}(\mathbf{a} - \mathbf{a}', \mathbf{b} - \mathbf{b}')\hat{g}(\mathbf{a}', \mathbf{b}')\ d\mathbf{a}'\ d\mathbf{b}',$$

where both integrals are over $\mathbb{R}^n$.

Note that if we set $\hbar = 0$ in the above formula, $\widehat{f \star g}$ reduces to $(2\pi)^{-n}$ times the convolution of $\hat{f}$ and $\hat{g}$, which is nothing but the Fourier transform of fg. It is thus not difficult to show (Exercise 10) that

$$\lim_{\hbar \to 0^+} f \star g = fg.$$

That is to say, the Moyal product $f \star g$ is a "deformation" of the ordinary pointwise product of functions on $\mathbb{R}^{2n}$. More generally, the Moyal product can be expanded in an asymptotic expansion in powers of $\hbar$, as explained in Sect. 2.3 of [11]. This expansion terminates in the case that f and g are both polynomials.

Proof. It is, of course, possible to obtain this formula using kernel functions. It is, however, easier to work with the (13.17), which can be shown (Exercise 7) to give the same result as Definition 13.7 when f is a Schwartz function. We assume standard properties of the Bochner integral for functions with values in a Banach space [in our case, $\mathcal{B}(\mathbf{H})$], which are similar to those of the Lebesgue integral. (See, for example, Sect. V.5 of [46].)

We have, then,

$$Q_{\text{Weyl}}(f)Q_{\text{Weyl}}(g) = (2\pi)^{-n} \iint \hat{f}(\mathbf{a}, \mathbf{b})e^{i(\mathbf{a}\cdot\mathbf{X} + \mathbf{b}\cdot\mathbf{P})}\ d\mathbf{a}\ d\mathbf{b} \times (2\pi)^{-n} \iint \hat{g}(\mathbf{a}', \mathbf{b}')e^{i(\mathbf{a}'\cdot\mathbf{X} + \mathbf{b}'\cdot\mathbf{P})}\ d\mathbf{a}'\ d\mathbf{b}'. \quad (13.30)$$

Now, it is an easy calculation to verify, using Proposition 13.5, that

$$e^{i(\mathbf{a}\cdot\mathbf{X} + \mathbf{b}\cdot\mathbf{P})} e^{i(\mathbf{a}'\cdot\mathbf{X} + \mathbf{b}'\cdot\mathbf{P})} = e^{-i\hbar(\mathbf{a}\cdot\mathbf{b}' - \mathbf{b}\cdot\mathbf{a}')/2} e^{i((\mathbf{a}+\mathbf{a}')\cdot\mathbf{X} + (\mathbf{b}+\mathbf{b}')\cdot\mathbf{P})}, \quad (13.31)$$

which is what one obtains by formally applying the special case of the Baker–Campbell–Hausdorff formula in (13.18). Thus, we may combine the integrals in (13.30) to obtain

$$Q_{\text{Weyl}}(f)Q_{\text{Weyl}}(g) = (2\pi)^{-2n} \iiiint e^{-i\hbar(\mathbf{a}\cdot\mathbf{b}' - \mathbf{b}\cdot\mathbf{a}')/2} e^{i((\mathbf{a}+\mathbf{a}')\cdot\mathbf{X} + (\mathbf{b}+\mathbf{b}')\cdot\mathbf{P})} \times \hat{f}(\mathbf{a}, \mathbf{b})\hat{g}(\mathbf{a}', \mathbf{b}')\ d\mathbf{a}\ d\mathbf{b}\ d\mathbf{a}'\ d\mathbf{b}'.$$

By introducing new variables $\mathbf{c} = \mathbf{a} + \mathbf{a}'$ and $\mathbf{d} = \mathbf{b} + \mathbf{b}'$ in the $\mathbf{a}$ and $\mathbf{b}$ integrals and reversing the order of integration, we obtain, after simplifying the exponent,

$$\begin{aligned}&Q_{\mathrm{Weyl}}(f)Q_{\mathrm{Weyl}}(g)\\&=(2\pi)^{-n}\iint\left[(2\pi)^{-n}\iint e^{-i\hbar(\mathbf{c}\cdot\mathbf{b}'-\mathbf{d}\cdot\mathbf{a}')/2}\right.\\&\left.\times\hat{f}(\mathbf{c}-\mathbf{a}',\mathbf{d}-\mathbf{b}')\hat{g}(\mathbf{a}',\mathbf{b}')\ d\mathbf{a}'\ d\mathbf{b}'\right]e^{i(\mathbf{c}\cdot\mathbf{X}+\mathbf{d}\cdot\mathbf{P})}\ d\mathbf{c}\ d\mathbf{d}.\end{aligned}$$

From this and (13.17), we see that $Q_{\mathrm{Weyl}}(f)Q_{\mathrm{Weyl}}(g)$ is the Weyl quantization of the function whose Fourier transform is the quantity in square brackets above, which is what we wanted to show. ∎

Proposition 13.10 *The Moyal product $f \star g$ extends to a continuous map of $L^2(\mathbb{R}^{2n}) \times L^2(\mathbb{R}^{2n})$ into $L^2(\mathbb{R}^{2n})$ and the composition formula (13.29) holds for all f and g in $L^2(\mathbb{R}^{2n})$.*

Proof. A standard inequality asserts that for any two Hilbert–Schmidt operators A and B, we have

$$\|AB\|_{\mathrm{HS}} \leq \|A\|_{\mathrm{HS}}\,\|B\|_{\mathrm{HS}}\,.$$

It follows that the product map $(A, B) \mapsto AB$ is a continuous map of $\mathrm{HS}(L^2(\mathbb{R}^n)) \times \mathrm{HS}(L^2(\mathbb{R}^n))$ to $\mathrm{HS}(L^2(\mathbb{R}^n))$. Meanwhile, the Weyl quantization is a constant multiple of a unitary map from $L^2(\mathbb{R}^{2n})$ to $\mathrm{HS}(L^2(\mathbb{R}^n))$. For Schwartz functions f and g, the Moyal product is nothing but

$$f \star g = Q_{\mathrm{Weyl}}^{-1}(Q_{\mathrm{Weyl}}(f)Q_{\mathrm{Weyl}}(g)). \tag{13.32}$$

The right-hand side of (13.32) provides the desired continuous extension of $f \star g$. Clearly, the composition formula (13.29) holds for this extension. ∎

13.3.4 Commutation Relations

In quantum mechanics, the commutator of two operators (divided by $i\hbar$) plays a role similar to that of the Poisson bracket in classical mechanics. Thus, we may naturally ask: To what extent does the Weyl quantization (or any other quantization scheme) map Poisson brackets to commutators? The short answer is: Not always. Indeed, as we will see in Sect. 13.4, no "reasonable" quantization scheme can give an exact correspondence between $\{f, g\}$ on the classical side and $[A, B]/(i\hbar)$ on the quantum side. Nevertheless, such an exact correspondence does hold for various special classes of symbols. If we consider, for example, the class of symbols that depend only on $\mathbf{x}$ and not on $\mathbf{p}$, then on the classical side, all such functions Poisson commute. The Weyl quantization maps such functions $f(\mathbf{x})$ to the operator of multiplication by $f(\mathbf{x})$, and thus the quantizations of any two such functions commute. A more interesting (in particular, noncommutative) example is as follows.

Proposition 13.11 *Suppose f is a polynomial in $\mathbf{x}$ and $\mathbf{p}$* of degree at most 2 *and g is an arbitrary polynomial in $\mathbf{x}$ and $\mathbf{p}$. Then*

$$\frac{1}{i\hbar}\left[Q_{\mathrm{Weyl}}(f), Q_{\mathrm{Weyl}}(g)\right] = Q_{\mathrm{Weyl}}(\{f,g\}), \tag{13.33}$$

where $\{f,g\}$ is the Poisson bracket of f and g.

Here, we define the Weyl quantization by the obvious n-variable extension of Definition 13.1, and we regard all operators as operating simply on $C_c^\infty(\mathbb{R}^n)$. See Exercise 8 for another class of symbols on which (13.33) holds. Although the requirement that g be a polynomial can be relaxed, we will not attempt to obtain the optimal version of the result.

Proof. For notational simplicity, we abbreviate $Q_{\mathrm{Weyl}}(f)$ to $Q(f)$ for the duration of the proof. If f has degree zero, then both sides of the desired equality are zero. Turning to case in which f has degree 1, we use the n-variable extension of Proposition 13.4, the proof of which is essentially the same as the 1-variable result. The result is as follows:

$$\begin{aligned} Q(x_j g) &= Q(x_j)Q(g) - \frac{i\hbar}{2}Q\left(\frac{\partial g}{\partial p_j}\right) \\ &= Q(g)Q(x_j) + \frac{i\hbar}{2}Q\left(\frac{\partial g}{\partial p_j}\right). \end{aligned}$$

By subtracting these two formulas and rearranging, we get

$$\frac{1}{i\hbar}[Q(x_j), Q(g)] = Q\left(\frac{\partial g}{\partial p_j}\right) = Q(\{x_j, g\}).$$

A very similar argument establishes the desired result when $f = p_j$ and thus for all homogeneous polynomials of degree 1.

Suppose now that f_1 and f_2 are homogeneous polynomials of degree 1 in $\mathbf{x}$ and $\mathbf{p}$. Then it follows easily from Proposition 13.4 that for any polynomial h, we have

$$Q(f_j h) = \frac{1}{2}(Q(f_j)Q(h) + Q(h)Q(f_j)), \quad j = 1, 2. \tag{13.34}$$

In particular, we have

$$Q(f_1 f_2) = \frac{1}{2}(Q(f_1)Q(f_2) + Q(f_2)Q(f_1)). \tag{13.35}$$

Using (13.35) and the product rule for commutators (Proposition 3.15), we have

$$\begin{aligned} &\frac{1}{i\hbar}[Q(f_1 f_2), Q(g)] \\ &= \frac{1}{2i\hbar}([Q(f_1), Q(g)]Q(f_2) + Q(f_1)[Q(f_2), Q(g)] \\ &+ [Q(f_2), Q(g)]Q(f_1) + Q(f_2)[Q(f_1), Q(g)]). \end{aligned}$$

Using the degree-1 case of the result we are trying to prove, along with (13.34), we get

$$\begin{aligned}\frac{1}{i\hbar}[Q(f_1 f_2), Q(g)] &= \frac{1}{2}(Q(\{f_1, g\})Q(f_2) + Q(f_1)Q(\{f_2, g\}) \\ &\quad + Q(\{f_2, g\})Q(f_1) + Q(f_2)Q(\{f_1, g\})) \\ &= Q(f_2\{f_1, g\}) + Q(f_1\{f_2, g\}) \\ &= Q(\{f_1 f_2, g\}),\end{aligned} \tag{13.36}$$

where in the last equality we have used the product rule for the Poisson bracket. We have now established the desired result when f is a homogeneous polynomial of degree 0, 1, or 2. ■

At first glance, it appears that one could extend the result to the case where f has degree 3, by considering three homogenous polynomials f_1, f_2, and f_3 of degree 1 and symmetrizing as in (13.35). The argument breaks down, however, because the $Q(f_j)$'s do not commute. The $Q(f_j)$'s will not always occur in the correct order to allow us to pull the f_j's back inside the Weyl quantization, the way we did in (13.36) in the degree-2 case. Indeed, an elementary but tedious calculations shows that

$$\frac{1}{i\hbar}[Q_{\mathrm{Weyl}}(x^2 p), Q_{\mathrm{Weyl}}(xp^2)] = 3X^2P^2 - 6i\hbar XP - \hbar^2 I,$$

whereas

$$Q_{\mathrm{Weyl}}(\{x^2 p, xp^2\}) = 3X^2P^2 - 6i\hbar XP - \frac{3}{2}\hbar^2 I,$$

so that the two expressions differ by $\hbar^2 I/2$.

We conclude this section with a brief glimpse of an important "equivariance" property of the Weyl quantization. Note that the Poisson bracket of two real valued homogeneous polynomials of degree 2 is again real valued and homogeneous of degree 2. The space of real homogeneous polynomials of degree 2 thus forms a Lie algebra (Sect. 16.3) with respect to the Poisson bracket. This Lie algebra is naturally isomorphic to the Lie algebra $\mathsf{sp}(n;\mathbb{R})$ of Lie group $\mathsf{Sp}(n;\mathbb{R})$, the real symplectic group. This group is the group of invertible linear transformations that preserve a skew-symmetric form on $\mathbb{R}^{2n}$. See Chap. 16 for information about Lie groups and their Lie algebras.

If we apply Proposition 13.11 in the case in which both f and g are homogeneous of degree 2, we see that the map $\pi(f) := Q_{\mathrm{Weyl}}(f)$ is a representation of $\mathsf{sp}(n;\mathbb{R})$ in the space of skew-symmetric operators on $L^2(\mathbb{R}^n)$. It can be shown that associated to this representation of $\mathsf{sp}(n;\mathbb{R})$ there is a projective unitary representation Π of the group $\mathsf{Sp}(n;\mathbb{R})$, known as the *metaplectic representation*. (See, again, Chap. 16 for definitions.) Proposition 13.11 is the infinitesimal version of the following equivariance property of the Weyl quantization: For all $A \in \mathsf{Sp}(n;\mathbb{R})$ and all $f \in L^2(\mathbb{R}^{2n})$, we have

$$Q_{\mathrm{Weyl}}(f \circ A^{-1}) = \Pi(A) Q_{\mathrm{Weyl}}(f) \Pi(A)^{-1}.$$

See Theorem 2.15 and Chap. 4 of [11] [where our $\Pi(A)$ corresponds to $\mu((A^*)^{-1})$ in Folland's notation] for this result and much more about the metaplectic representation.

13.4 The "No Go" Theorem of Groenewold

In Sect. 13.3.4, we noted that the Weyl quantization on polynomials satisfies

$$\frac{1}{i\hbar}[Q_{\mathrm{Weyl}}(f), Q_{\mathrm{Weyl}}(g)] = Q_{\mathrm{Weyl}}(\{f, g\}), \tag{13.37}$$

provided that f is a polynomial of degree 2, but not in general. One might think that the failure of (13.37) represents a shortcoming in the definition of the Weyl quantization, which could be remedied by an alternative definition. In this section, however, we will see that no quantization scheme that maps x_j and p_j to the usual position and momentum operators X_j and P_j can satisfy (13.37) for general polynomials in $\mathbf{x}$ and $\mathbf{p}$. This sort of nonexistence result, of a construct satisfying seemingly natural and desirable conditions, is referred to in the physics literature as a "no go" theorem.

In light of this result, one might think that perhaps the position and momentum operators should be defined differently, possibly with an accompanying change in the choice of the quantum Hilbert space. Indeed, there *is* a map Q that satisfies (13.37) for all f and g, namely the prequantization map described in Sect. 23.3. The prequantization map accomplishes this feat by drastically enlarging the quantum Hilbert space, from $L^2(\mathbb{R}^n)$ to $L^2(\mathbb{R}^{2n})$. The Hilbert space $L^2(\mathbb{R}^{2n})$ is considered to be "too big" from a physical standpoint, which explains why the map Q is only "prequantization" rather than "quantization." (The prequantization map has a number of other undesirable features that are described in Sect. 23.3.) If one imposes a natural "smallness" assumption on the quantum Hilbert space (irreducibility under the action of the position and momentum operators), then the Stone–von Neumann theorem will tell us that (modulo certain technical domain assumptions) *any* choice of position and momentum operators satisfying the canonical commutation relations is unitarily equivalent to the usual ones.

The upshot of the discussion in the two preceding paragraphs is that there is no physically reasonable quantization scheme that satisfies (13.37) for all (polynomial) functions f and g.

We turn, now, to Groenewold's "no go" theorem. We need to make domain assumptions, so that it makes sense to compute the commutators of the quantized operators. The simplest approach is to assume that the quantization $Q(f)$ of any polynomial f will be in the algebra generated by the X's and P's, and thus that $Q(f)$ will be a differential operator with polynomial coefficients. There is a variant of this result, known as van

Hove's theorem, that proves a similar "no go" result under a more general assumption about the form of the quantized operators. See [15] for a rigorous proof of van Hove's theorem.

Definition 13.12 *For any $k \geq 0$, let $\mathcal{P}_k$ denote the space of homogeneous polynomials of degree k and let $\mathcal{P}_{\leq k}$ denote the space of all polynomials of degree at most k.*

Theorem 13.13 (Groenewold's Theorem) *Let $\mathcal{D}(\mathbb{R}^n)$ denote the space of differential operators on $\mathbb{R}^n$ with polynomial coefficients. There* does not *exist a linear map $Q : \mathcal{P}_{\leq 4} \to \mathcal{D}(\mathbb{R}^n)$ with the following properties.*

1. *$Q(1) = I$.*
2. *$Q(x_j) = X_j$ and $Q(p_j) = P_j$.*
3. *For all f and g in $\mathcal{P}_{\leq 3}$, we have*

$$Q(\{f, g\}) = \frac{1}{i\hbar}[Q(f), Q(g)]. \tag{13.38}$$

Note that in Property 3 of the theorem, we assume that f and g belong to $\mathcal{P}_{\leq 3}$ rather than $\mathcal{P}_{\leq 4}$. This assumption guarantees that $\{f, g\}$ belongs to $\mathcal{P}_{\leq 4}$, so that the left-hand side of (13.38) is defined.

Our strategy in proving Groenewold's theorem is the following. We know (Proposition 13.11) that the Weyl quantization satisfies (13.38) if f has degree at most 2 and g has degree at most 3. Using this result, we can show that any map Q satisfying the properties in Theorem 13.13 must coincide with the Weyl quantization on $\mathcal{P}_{\leq 3}$. We then identify a polynomial $f \in \mathcal{P}_4$ that can be expressed as a Poisson bracket in two different ways, $f = \{g, h\} = \{g', h'\}$, with g, h, g', and h' in $\mathcal{P}_3$. Upon calculating that $[Q_{\mathrm{Weyl}}(g), Q_{\mathrm{Weyl}}(h)]$ does not coincide with $[Q_{\mathrm{Weyl}}(g'), Q_{\mathrm{Weyl}}(h')]$, we will have a contradiction.

The proof will consist of several lemmas, followed by the *coup de grâce.*

Lemma 13.14 *Consider an element A of $\mathcal{D}(\mathbb{R}^n)$ expressed as*

$$A = \sum_{\mathbf{k}} f_{\mathbf{k}}(\mathbf{x}) \left(\frac{\partial}{\partial \mathbf{x}}\right)^{\mathbf{k}},$$

where $\mathbf{k}$ ranges over multi-indices, where the $f_{\mathbf{k}}$'s are polynomials, and where only finitely many of the $f_{\mathbf{k}}$'s are nonzero. Then A is the zero operator on $C_c^\infty(\mathbb{R}^n)$ only if each of the $f_{\mathbf{k}}$'s is zero.

Proof. For each multi-index $\mathbf{k}$, let $|\mathbf{k}| = k_1 + \cdots + k_n$. Suppose not all the $f_{\mathbf{k}}$'s are zero, let N be the smallest non-negative integer for which $f_{\mathbf{k}}$ is nonzero for some $\mathbf{k}$ with $|\mathbf{k}| = N$, and let $\mathbf{k}_0$ be some multi-index with

$|\mathbf{k}_0| = N$ and $f_{\mathbf{k}_0} \neq 0$. Let us apply A to a function g that is equal, in a neighborhood of the origin, to $\mathbf{x}^{\mathbf{k}_0}$. Then all the terms in Ag other than the $f_{\mathbf{k}_0}$ term will be zero in a neighborhood of the origin, whereas the $f_{\mathbf{k}_0}$ term will be a nonzero constant in a neighborhood of the origin. Thus, A is not the zero operator. ■

Lemma 13.15 *If A belongs to $\mathcal{D}(\mathbb{R}^n)$ and A commutes with X_j and P_j for all $j = 1, \ldots, n$, then $A = cI$ for some $c \in \mathbb{C}$.*

Proof. We may easily prove by induction that

$$\left(\frac{\partial}{\partial x_j}\right)^k (x_j g(\mathbf{x})) = k\left(\frac{\partial}{\partial x_j}\right)^{k-1} g(\mathbf{x}) + x_j \left(\frac{\partial}{\partial x_j}\right)^k g(\mathbf{x})$$

for any polynomial g. Thus, for any multi-index $\mathbf{k}$, we have

$$\left[f(\mathbf{x})\left(\frac{\partial}{\partial \mathbf{x}}\right)^{\mathbf{k}}, X_j\right] = k_j f(\mathbf{x})\left(\frac{\partial}{\partial \mathbf{x}}\right)^{\mathbf{k}-\mathbf{e}_j}. \tag{13.39}$$

Suppose A is a nonzero element of $\mathcal{D}(\mathbb{R}^n)$ that commutes with each X_j. If $\deg(A) = M$, consider a nonzero term in A of degree M:

$$f_{\mathbf{k}_0}(\mathbf{x})\left(\frac{\partial}{\partial \mathbf{x}}\right)^{\mathbf{k}_0}, \quad |\mathbf{k}_0| = M, \; f_{\mathbf{k}_0} \neq 0.$$

If $M > 0$, we can pick some j such that the jth entry of $\mathbf{k}_0$ is nonzero. By (13.39) and our assumption on A, we have

$$0 = [A, X_j] = (\mathbf{k}_0)_j f_{\mathbf{k}_0}(\mathbf{x})\left(\frac{\partial}{\partial \mathbf{x}}\right)^{\mathbf{k}_0-\mathbf{e}_j} + \text{ other terms},$$

where the other terms involve multi-indices of the form $\mathbf{k}-\mathbf{e}_j$, with $\mathbf{k} \neq \mathbf{k}_0$. Thus, by Lemma 13.14, $[A, X_j]$ is not the zero operator.

We see, then, that any $A \in \mathcal{D}(\mathbb{R}^n)$ that commutes with each X_j must be of degree zero; that is, A must simply be multiplication by some polynomial $f(\mathbf{x})$. If, in addition, A commutes with each P_j, then

$$0 = [f(\mathbf{x}), P_j] = i\hbar \frac{\partial f}{\partial x_j}(\mathbf{x}).$$

Thus, actually, f must be constant and A is a multiple of the identity operator. ■

Lemma 13.16 *For any $f \in \mathcal{P}_2$, there exist $g_1, \ldots, g_j$ and $h_1, \ldots, h_j$ in $\mathcal{P}_2$ such that*

$$f = \{g_1, h_1\} + \cdots + \{g_j, h_j\}.$$

Furthermore, for any $f' \in \mathcal{P}_3$, there exist elements $g_1', \ldots, g_k'$ of $\mathcal{P}_3$ and $h_1', \ldots, h_k'$ of $\mathcal{P}_2$ such that

$$f' = \{g_1', h_1'\} + \cdots + \{g_k', h_k'\}.$$

Proof. See Exercise 12. ∎

Lemma 13.17 *If Q satisfies the conditions in Theorem 13.13, then Q coincides with Q_{Weyl} on $\mathcal{P}_{\leq 3}$.*

Proof. Our argument leans heavily on Proposition 13.11. Note that, by assumption, Q coincides with Q_{Weyl} on $\mathcal{P}_{\leq 1}$. For $f \in \mathcal{P}_2$, let us write $Q(f)$ as

$$Q(f) = Q_{\mathrm{Weyl}}(f) + A_f.$$

For any $g \in \mathcal{P}_{\leq 1}$, we have, by (13.38) and Proposition 13.11,

$$\begin{aligned} Q(\{f, g\}) &= \frac{1}{i\hbar}[Q(f), Q(g)] \\ &= \frac{1}{i\hbar}[Q_{\mathrm{Weyl}}(f), Q_{\mathrm{Weyl}}(g)] + \frac{1}{i\hbar}[A_f, Q_{\mathrm{Weyl}}(g)] \\ &= Q_{\mathrm{Weyl}}(\{f, g\}) + \frac{1}{i\hbar}[A_f, Q_{\mathrm{Weyl}}(g)] \\ &= Q(\{f, g\}) + \frac{1}{i\hbar}[A_f, Q_{\mathrm{Weyl}}(g)], \end{aligned} \tag{13.40}$$

since $\{f, g\} \in \mathcal{P}_{\leq 1}$. Thus, $[A_f, Q_{\mathrm{Weyl}}(g)] = 0$ for every $g \in \mathcal{P}_1$, and so, by Lemma 13.15, we must have $A_f = c_f I$ for some constant c_f.

Now, if h is in $\mathcal{P}_2$, we have, by the just-established result and Proposition 13.11,

$$\begin{aligned} Q(\{f, h\}) &= \frac{1}{i\hbar}[Q(f), Q(h)] \\ &= \frac{1}{i\hbar}[Q_{\mathrm{Weyl}}(f) + c_f I, Q_{\mathrm{Weyl}}(h) + c_h I] \\ &= \frac{1}{i\hbar}[Q_{\mathrm{Weyl}}(f), Q_{\mathrm{Weyl}}(h)] \\ &= Q_{\mathrm{Weyl}}(\{f, h\}). \end{aligned} \tag{13.41}$$

That is to say, Q and Q_{Weyl} agree on elements of $\mathcal{P}_2$ of the form $\{f, h\}$, for $f, h \in \mathcal{P}_2$. Thus, by Lemma 13.16, Q and Q_{Weyl} agree on all of $\mathcal{P}_2$, and so on all of $\mathcal{P}_{\leq 2}$.

We now use the $\mathcal{P}_{\leq 2}$ case of the lemma to establish the $\mathcal{P}_3$ case. Given $f \in \mathcal{P}_3$, we write $Q(f) = Q_{\mathrm{Weyl}}(f) + B_f$. Given $g \in \mathcal{P}_{\leq 1}$, we have $\{f, g\} \in \mathcal{P}_{\leq 2}$. Thus, we may argue as in (13.40), applying the just-established $\mathcal{P}_{\leq 2}$ case of the lemma to $\{f, g\}$ in the last step. The conclusion is that $[B_f, Q(g)] = 0$ for all $f \in \mathcal{P}_{\leq 2}$ and thus, by Lemma 13.15, that $B_f = d_f I$ for some constant d_f. Meanwhile, if $h \in \mathcal{P}_2$, we argue as in (13.41), but with c_f replaced by d_f and with c_h now known to be zero. The conclusion is that Q agrees with Q_{Weyl} for all elements of $\mathcal{P}_3$ of the form $\{f, h\}$ with $f \in \mathcal{P}_3$ and $h \in \mathcal{P}_2$, and thus, by Lemma 13.16, for all elements of $\mathcal{P}_3$. ∎

Proof of Theorem 13.13. Assume, toward a contradiction, that a map Q as in the theorem exists. Let f be the polynomial given by

$$f(\mathbf{x},\mathbf{p}) = x_1^2 p_1^2.$$

We observe that f can be written in two different ways as a Poisson bracket:

$$x_1^2 p_1^2 = \frac{1}{9}\{x_1^3, p_1^3\} = \frac{1}{3}\{x_1^2 p_1, x_1 p_1^2\}.$$

Thus, by Lemma 13.17, we must have

$$\begin{aligned}\frac{1}{9}[Q_{\mathrm{Weyl}}(x_1^3), Q_{\mathrm{Weyl}}(p_1^3)] &= i\hbar Q(x_1^2 p_1^2)\\ &= \frac{1}{3}[Q_{\mathrm{Weyl}}(x_1^2 p_1), Q_{\mathrm{Weyl}}(x_1 p_1^2)].\end{aligned}$$

On the other hand, if we apply both commutators to the constant function $\mathbf{1}$ (or to a function equal to 1 in a neighborhood of the origin), we obtain

$$\begin{aligned}\frac{1}{9}[Q_{\mathrm{Weyl}}(x_1^3), Q_{\mathrm{Weyl}}(p_1^3)]\mathbf{1} &= \frac{1}{9}(X_1^3 P_1^3 - P_1^3 X_1^3)\mathbf{1}\\ &= -\frac{1}{9}(-i\hbar)^3 6 \cdot \mathbf{1}.\end{aligned}$$

Meanwhile, if we compute the quantizations as in (13.4) and then drop all terms involving $P_1\mathbf{1}$, we obtain (after a small computation)

$$\begin{aligned}\frac{1}{3}[Q_{\mathrm{Weyl}}(x_1^2 p_1), Q_{\mathrm{Weyl}}(x_1 p_1^2)]\mathbf{1} &= \frac{1}{12}(X_1^2 P_1^3 X_1 + P_1 X_1^2 P_1^2 X_1)\mathbf{1}\\ &\quad - \frac{1}{12}(X_1 P_1^3 X_1^2 + P_1^2 X_1 P_1 X_1^2)\mathbf{1}\\ &= -\frac{1}{12} P_1^2 X_1 P_1 X_1^2 \mathbf{1}\\ &= -\frac{1}{12}(-i\hbar)^3 4 \cdot \mathbf{1}.\end{aligned}$$

Since $6/9$ does not equal $4/12$, we have a contradiction. ■

13.5 Exercises

1. Let $\mathcal{P}_j$ denote the space of complex-valued homogeneous polynomials on $\mathbb{R}^2$ of degree j. Then $\mathcal{P}_j$ is a complex vector space of dimension $j+1$, which we may identify with $\mathbb{C}^{j+1}$ using the obvious basis for $\mathcal{P}_j$. Let V_j denote the complex subspace of $\mathcal{P}_j$ spanned by polynomials of the form $(ax+bp)^j$, with $a, b \in \mathbb{C}$. Show that $V_j = \mathcal{P}_j$.

   Hint: Since every subspace of $\mathbb{C}^{j+1}$ is (topologically) closed, if $\gamma(t)$ is a smooth curve in V_j, the derivative $\gamma'(t)$ will also lie in V_j.

2. Show that symmetrized pseudodifferential operator quantization of x^2p^2 is equal to $Q_{\mathrm{Weyl}}(x^2p^2) - \hbar^2/2$.

3. Show that Wick-ordered and anti-Wick-ordered quantizations map real-valued polynomials to symmetric operators on $C_c^\infty(\mathbb{R})$.

   Hint: Compare the values of each quantization scheme on $z^k\bar{z}^l$ and on $\overline{(z^k\bar{z}^l)}$.

4. Consider a classical harmonic oscillator with Hamiltonian

$$H(x,p) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 = \frac{1}{2}m\omega^2\left(x^2 + \left(\frac{p}{m\omega}\right)^2\right),$$

   where ω is the frequency of the oscillator. Consider the Wick- and anti-Wick-ordered quantizations with parameter $\alpha = 1/(m\omega)$. Show that

$$Q_{\mathrm{Wick}}(H) = Q_{\mathrm{Weyl}}(H) - \frac{1}{2}\hbar\omega$$
$$Q_{\mathrm{anti-Wick}}(H) = Q_{\mathrm{Weyl}}(H) + \frac{1}{2}\hbar\omega.$$

5. Let $U_{\mathbf{a},\mathbf{b}}(t)$ be as in Proposition 13.5. Show by direct calculation that these operators form a one-parameter unitary group.

6. Given $\kappa \in L^2(\mathbb{R}^n \times \mathbb{R}^n)$, let A_κ denote the associated integral operator on $L^2(\mathbb{R}^n)$, as in Proposition 13.6. Show that the adjoint A^* of A is also an integral operator, with integral kernel κ' given by

$$\kappa'(\mathbf{x},\mathbf{y}) = \overline{\kappa(\mathbf{y},\mathbf{x})}.$$

7. Suppose that $f \in L^2(\mathbb{R}^{2n})$ and that $\hat{f} \in L^1(\mathbb{R}^{2n})$. Then the right-hand side of (13.17) may be understood as an absolutely convergent "Bochner" integral with values in the Banach space $\mathcal{B}(L^2(\mathbb{R}^n))$. Show that $Q_{\mathrm{Weyl}}(f)$ as defined by (13.17) coincides with $Q_{\mathrm{Weyl}}(f)$ as defined in Definition 13.7.

   Hint: The Bochner integral commutes with applying a bounded linear functional. Use this result with the linear functional $\Lambda_{\phi,\psi}(A) := \langle \phi, A\psi \rangle$ on $\mathcal{B}(L^2(\mathbb{R}^n))$. Then use the expression in (13.23) for κ_f, which follows from Definition 13.7 by applying a partial Fourier transform.

8. (a) Show that for any polynomial f in one variable, we have

$$Q_{\mathrm{Weyl}}(f(x)p) = f(X)P - \frac{i\hbar}{2}f'(X).$$

(b) Show that for any two polynomials f and g, the Poisson bracket $\{f(x)p, g(x)p\}$ is of the form $h(x)p$ for some polynomial h.

(c) Show that for any two polynomials f and g, we have

$$\frac{1}{i\hbar}\left[Q_{\text{Weyl}}(f(x)p), Q_{\text{Weyl}}(g(x)p)\right] = Q_{\text{Weyl}}(\{f(x)p, g(x)p\}).$$

9. (a) Given ϕ and ψ in $L^2(\mathbb{R}^n)$, let $|\phi\rangle\langle\psi|$ be the operator defined in Notation 3.28. Show that $|\phi\rangle\langle\psi|$ can be expressed as an integral operator as in Proposition 13.6 and determine the associated integral kernel κ.

(b) For $\sigma > 0$, let $\psi_\sigma \in L^2(\mathbb{R}^n)$ be given by the expression

$$\psi_\sigma(\mathbf{x}) = (\pi\sigma)^{-n/4} e^{-|\mathbf{x}|^2/(2\sigma)}.$$

Using Proposition A.22, show that ψ_σ is a unit vector in $L^2(\mathbb{R}^n)$ and that the Weyl symbol of the corresponding one-dimensional projection operator $|\psi_\sigma\rangle\langle\psi_\sigma|$ is given by

$$Q_{\text{Weyl}}^{-1}(|\psi_\sigma\rangle\langle\psi_\sigma|) = 2^n e^{-|\mathbf{x}|^2/\sigma} e^{-\sigma|\mathbf{p}|^2/\hbar^2}.$$

Note: If we give σ the value $\hbar/(m\omega)$, the Gaussian function ψ_α may be thought of as the ground state for an n-dimensional harmonic oscillator. (Compare the functions in Theorem 11.3.) The computation in this exercise plays an important role in the proof of the Stone–von Neumann theorem in Chap. 14.8.

10. If f and g are Schwartz functions on $\mathbb{R}^{2n}$, show that $\widehat{f \star g}$ converges in the L^1 norm to $(2\pi)^{-n}\hat{f} * \hat{g}$, where $*$ denotes convolution. Conclude that $f \star g$ converges uniformly to fg as $\hbar$ tends to zero.

11. Suppose that $f(\mathbf{p}, \mathbf{q})$ is a homogeneous polynomial of degree 2. Show that for each t, the Hamiltonian flow Φ_t associated with f is a linear map of $\mathbb{R}^{2n}$ to itself.

12. Prove Lemma 13.16.

Hint: Let $g_1 \in \mathcal{P}_2$ be given by

$$g_1(\mathbf{x}, \mathbf{p}) = \sum_{j=1}^{n} x_j p_j.$$

Show that for any monomial of the form $\mathbf{x}^{\mathbf{j}}\mathbf{p}^{\mathbf{k}}$, we have $\{g_1, \mathbf{x}^{\mathbf{j}}\mathbf{p}^{\mathbf{k}}\} = (|\mathbf{k}| - |\mathbf{j}|)\mathbf{x}^{\mathbf{j}}\mathbf{p}^{\mathbf{k}}$. Thus, most of the standard basis elements f for $\mathcal{P}_2$ and all of the standard basis elements f for $\mathcal{P}_3$ can be obtained as nonzero multiples of $\{g_1, f\}$.