

**The symbol of a function of a pseudodifferential operator**

by

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## Abstract

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Let  $\widehat{A}$  be an pseudodifferential operator in  $L^2(\mathbb{R}^N)$  with Weyl -symbol  $A$  and let  $f$  be a smooth function. Then  $\widehat{B} := f(\widehat{A})$  is another operator, with symbol  $B$ . What is  $B$  in terms of  $A$  and  $f$ ? In this thesis, we provide an answer to this question in the form of a formula “à la Feynman”. We express  $B$  as a power series in  $\hbar$  whose terms are labeled by diagrams. The contribution of each term is a combinatorial calculation which can be explicitly computed.

We then consider generalizations of this result to other quantizations and to functions of various variables. We finally derive various applications to quantum mechanics, including Bohr–Sommerfeld quantization rules at all orders in  $\hbar$ .

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Professor Alan Weinstein  
Dissertation Committee Chair

## DEDICATION

A mi madre, por su coraje.

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# Introduction

The main goal of this thesis is to provide a realistically computable formula for the symbol of a function of an operator. Here is our main problem:

**Statement of the problem:** *Let  $\widehat{A}$  be a pseudo-differential operator in  $L^2(\mathbb{R}^N)$  which admits a self-adjoint extension. Let  $A \in \mathcal{C}^\infty(T^*\mathbb{R}^N)$  be the symbol of  $\widehat{A}$ . Let  $f : \mathbb{R} \rightarrow \mathbb{R}$  be a smooth function and let  $\widehat{B} = f(\widehat{A})$  be an operator with symbol  $B$ . What is  $B$  in terms of  $A$  and  $f$ ?* ✠

We need to give some background to understand ✠. Consider the case of a particle in  $N$  dimensions. The observables are the physical quantities that we want to study (e.g. the energy). In classical mechanics, the observables, which we call symbols, are real-valued smooth functions on the manifold  $T^*(\mathbb{R}^N)$  and depending on a formal parameter  $\hbar$ . In quantum mechanics, the observables are essentially self-adjoint operators on the Hilbert space  $L^2(\mathbb{R}^N)$ , also depending on the formal parameter  $\hbar$ . Weyl quantization provides a correspondence between classical and quantum observables, i.e.

between symbols and operators:

$$A \in \mathcal{C}^\infty(T^*\mathbb{R}^N)[[\hbar]] \quad \mapsto \quad \widehat{A} \in \text{Op}(L^2(\mathbb{R}^N))[[\hbar]].$$

This correspondence is a bijection when we restrict the domain and the range, so we can talk about the symbol of an operator, and the question  $\spadesuit$  makes sense.

Our interest in this problem comes from Bohr–Sommerfeld quantization rules, which are an algorithm to calculate asymptotically the eigenvalues of an operator as a formal power series in  $\hbar$ . Colin de Verdière [7] (inspired by Voros [28]) obtained the following results:

- Let  $\widehat{H}$  be a pseudodifferential operator in  $L^2(\mathbb{R})$  with symbol  $H$ . Then, under certain hypotheses, there exist a function

$$S: \mathbb{R} \mapsto \mathbb{R}[[\hbar]],$$

called the semiclassical action, such that

$$E \text{ is an eigenvalue of } \widehat{H} \quad \iff \quad \frac{S(E)}{2\pi\hbar} \in \mathbb{N}.$$

- The semiclassical action for an operator  $\widehat{H}$  can be entirely calculated from the symbol  $H$ , provided we have an answer to  $\spadesuit$ .

Colin de Verdière proves the existence of a universal formula to answer  $\spadesuit$  (like our Equation (0.1) below), and explains how to calculate  $S(E)$  from it. It does not, however, give an explicit solution to  $\spadesuit$ . Instead, [7, 28] give an algorithm which theoretically allows us to calculate the symbol of a function of an operator at any given order in  $\hbar$ ,

and from that to read off  $S(E)$  at the same order in  $\hbar$ . This algorithm (which we call the resolvent approach) is in practice intractable after order  $\hbar^2$  because the calculations are too complicated. We explain the resolvent approach in Appendix B.

Our goal, as we said above, is to find a solution to  $\star$  which is useful in practice, i.e. which can realistically be computed for any given particular example. In this thesis, we will derive the following formula:

$$\widehat{B} = f(\widehat{A}) \tag{0.1}$$

$$B = \sum_{\Gamma} \left( \frac{i\hbar}{2} \right)^{E_{\Gamma}} \frac{c_{\Gamma}}{S_{\Gamma}} \lambda_{\Gamma}(A) \frac{f^{(V_{\Gamma})}(A)}{V_{\Gamma}!}$$

The sum is taken over all finite graphs  $\Gamma$  with no isolated vertices. For every such graph  $\Gamma$ ,  $V_{\Gamma}$  is the number of vertices and  $E_{\Gamma}$  is the number of edges.  $\lambda_{\Gamma}(A)$  is a polynomial in the derivatives of  $A$  constructed algorithmically from  $\Gamma$  (see §2.1).  $S_{\Gamma}$  is the order of the symmetry group of  $\Gamma$ .  $c_{\Gamma}$  is a simple integer-valued invariant of  $\Gamma$  (see §2.2.3). The terms through order 4 in  $\hbar$  of (0.1) are shown in Appendix D.

There are two advantages to our method. The first one is that we derive the compact, final result (0.1) whose terms can be explicitly written. This is important, as most of the applications of this formula are in quantum physics, where we would like to perform explicit calculations for a particular given operator. The second advantage is its generality. In the derivation of (0.1) we use:

- Weyl quantization as a bijection between symbols and operators. However, the only thing specific to Weyl quantization that we use is the *star product* (definitions in §1.1). This makes it easy to generalize (0.1) to other quantizations (see §3.1).

- A functional calculus to define a function of an operator  $f(\widehat{A})$  (see §1.2). However, unlike in the resolvent approach, we do not use any particular functional calculus, but just the properties that every functional calculus has. Hence our result is valid for a wider class of functions  $f$  and it generalizes to functions of several variables (see §3.2).

Bohr–Sommerfeld rules are explained in §4.1. There are various other applications of our result:

- *Star exponential.* Omori et al [22] studied the star exponential of quadratic forms, which, although stated differently, is equivalent to studying the symbol of the exponential of an operator. As we explain in §4.2, we believe that our method can help extend their results to star exponential of higher order polynomials.
- *Determinant of certain differential operators* As explained in [19], such determinants naturally arise in quantum field theory at the one loop level. The determinant of an operator can be defined by the property  $\log \det \widehat{A} = \text{trace} \log \widehat{A}$ , which holds in finite dimensional spaces. The trace of the operator  $\widehat{B} = \log \widehat{A}$  can be calculated by integrating its symbol  $B$  in phase space. See §4.3.

The structure of this thesis is as follows.

1. In Chapter 1, we give the background necessary to understand  $\blacklozenge$ . In §1.1 we define quantizations, i.e. correspondences between symbols (smooth functions) and operators, and in particular the Weyl quantization. In §1.2 we define functional calculi, i.e. how to define a function of an operator.

2. Chapter 2 contains the core of this thesis. After introducing graphs and fixing notation, we derive (0.1) and various equivalent formulas.
3. In Chapter 3 we study generalizations of (0.1) to other quantizations and to functions of several variables.
4. In Chapter 4 we study various applications, including Bohr–Sommerfeld quantization rules.

The core of this thesis was published in [10] by *Annales de l’Institut Fourier*.

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Finally, to my parents, to Rebeca, to my friends and relatives in Spain who supported me when I was abandoning them, *gracias*.

# Chapter 1

## Background

Let us recall our problem as was stated in the introduction. Let  $\widehat{A} \in \text{Op}(L^2(\mathbb{R}^N))$  be an operator with symbol  $A \in \mathcal{C}^\infty(T^*\mathbb{R}^N)$  and let  $f$  be a smooth function. Let  $\widehat{B} := f(\widehat{A})$  be another operator with symbol  $B$ . We want to express  $B$  in terms of  $A$  and  $f$ . In this chapter we will give the background necessary to understand this problem. First, in §1.1 we talk about quantizations, i.e. what it means that the function  $A \in \mathcal{C}^\infty(T^*\mathbb{R}^N)$  is the symbol of the operator  $\widehat{A}$ . Then, in §1.2 we talk about the functional calculus, i.e. how to define a function of an operator  $f(\widehat{A})$ .

### 1.1 Quantization

In a few words, a *quantization* is a relation between the classical and quantum description of a physical system. We will first give a heuristic explanation in §1.1.1, and then a definition in §1.1.2. We will mostly use Weyl quantization (§1.1.3), whose main ingredient

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for us is the Moyal product (§1.1.4).

### 1.1.1 A heuristic explanation

The classical and quantum descriptions of a physical system are quite different. In the classical description of a system, the space of states is a Poisson manifold, whereas the quantum state space is a Hilbert space. For a particle in  $N$  dimensions, the Poisson manifold (classical) is  $T^*\mathbb{R}^N$  and the Hilbert space (quantum) is  $L^2(\mathbb{R}^N)$ .

The observables are the physical quantities in which we are interested (e.g. the energy). They are classically described by real-valued smooth functions on the phase space  $\mathcal{C}^\infty(T^*\mathbb{R}^N)$ , which we call *symbols*. In the quantum description they are essentially self-adjoint pseudodifferential operators on the Hilbert space  $L^2(\mathbb{R}^N)$ . (We could discuss quantizations in a more general setup than a particle in  $N$  dimensions, but we will not do so now). See Figure 1.1 for a summary of this comparison between classical and quantum mechanics.

For instance, we have canonical coordinates

$$(x, p) := (x_1, \dots, x_N, p_1, \dots, p_N)$$

on the cotangent bundle  $T^*\mathbb{R}^N$ :  $x_j$  are the coordinates on the base  $\mathbb{R}^N$  and  $p_j$  are the coordinates along the fibers.  $x_j$  and  $p_j$  are elements of  $\mathcal{C}^\infty(T^*\mathbb{R}^N)$  and hence classical observables. We associate to them operators  $\hat{x}_j$  and  $\hat{p}_j$  on  $L^2(\mathbb{R}^N)$  defined by:

$$\begin{aligned}\hat{x}_j[\phi](x) &:= x_j\phi(x) \\ \hat{p}_j[\phi](x) &:= -i\hbar\frac{d\phi}{dx_j}(x)\end{aligned}\tag{1.1}$$

Figure 1.1: Classical vs quantum mechanics.

	Classical	Quantum
Space of states	Poisson manifold $M$	Hilbert space $\mathcal{H}$
Observables  <i>Ex: particle in <math>N</math> dimensions</i>  coordinates on $T^*\mathbb{R}^N \approx \mathbb{R}^{2N}$	<i>Symbols</i> or smooth functions on $M$  $\mathcal{C}^\infty(T^*\mathbb{R}^N)[[\hbar]]$  $x_j \quad j=1,\dots,N$ $p_j \quad j=1,\dots,N$  star product $C = A \star B$	Operators on $\mathcal{H}$  $\text{Op}(L^2(\mathbb{R}^N))[[\hbar]]$  $\hat{x}_j[\phi](x) := x_j\phi(x)$ $\hat{p}_j[\phi](x) := -i\hbar\frac{\partial\phi}{\partial x_j}(x)$  composition of operators $\hat{C} = \hat{A}\hat{B}$
QUANTIZATION	$A \in \mathcal{C}^\infty(T^*\mathbb{R}^N)[[\hbar]]$	$\hat{A} \in \text{Op}(L^2(\mathbb{R}^N))[[\hbar]]$

---

for  $\phi \in L^2(\mathbb{R}^N)$ .

A *quantization* is a suitable extension of this correspondence to a map

$$A \in \mathcal{C}^\infty(T^*\mathbb{R}^N; \mathbb{C}) \mapsto \widehat{A} \in \text{Op}(L^2(\mathbb{R}^N)).$$

What do we mean by suitable? We would like it so satisfy the following properties:

- The correspondence is linear.
- $A$  is real-valued  $\iff \widehat{A}$  is essentially self-adjoint.
- $A$  is positive  $\iff \widehat{A}$  is a positive operator.
- The correspondence is injective.

The correspondence is often only defined on a dense subalgebra. When we restrict the domain and range it becomes a bijection and we can talk about *the* symbol of an operator.

Some of these properties are sometimes relaxed.

Once we have a quantization, we can define an associative operation in  $\mathcal{C}^\infty(T^*\mathbb{R}^N)$ , called the *star product*  $\star$ , that makes the bijection  $A \mapsto \widehat{A}$  into an algebra isomorphism (with respect to composition of operators). In other words,  $C \star D$  is the symbol of the operator  $\widehat{C\widehat{D}}$ .

There is one extra condition, probably the most important:

- *Correspondence principle*: As  $\hbar \mapsto 0$ , the quantum formalism converges to classical formalism.

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To formalize this principle we require

$$\lim_{\hbar \rightarrow 0} \frac{A \star B - B \star A}{\hbar} = i\{A, B\} \quad (1.2)$$

in some topology we do not yet specify.

The mathematical nature of Planck's constant  $\hbar$  is an additional problem. We can treat it in two different ways: as a parameter that takes real values in some interval, or as a formal parameter. They lead to two different ways of making sense of the previous limit, and to two different definitions of quantization, which we discuss in the next subsection.

### 1.1.2 Definitions

We can think of  $\hbar$  as a real parameter that takes values in an interval  $I$  which contains 0 as a limit point. Then we need to consider symbols that depend on  $\hbar$ , i.e.  $\mathcal{C}^\infty(I \times T^*\mathbb{R}^N)$  and similarly for operators. We finally need to choose a topology to make sense of (1.2). We will not follow this *strict quantization* approach here. See [25] for a rigorous definition and examples.

Instead, we will think of  $\hbar$  as a formal parameter and consider all our spaces to consist of formal power series in  $\hbar$ . Thus, the classical observables will be elements of  $\mathcal{C}^\infty(T^*\mathbb{R}^N)[[\hbar]]$ , and the quantum observables will be elements of  $\text{Op}(L^2(\mathbb{R}^N))[[\hbar]]$ . In this approach, we do not need to worry about convergence of the series in  $\hbar$ . It is equivalent to replacing every function that depends on  $\hbar$  by its formal power series expansion, modulo functions that are  $O(\hbar^\infty)$ .

---

**Definition 1.1.** A quantization<sup>1</sup> or symbol correspondence is an injective,  $\mathbb{R}[[\hbar]]$ -linear map

$$A \in \mathcal{C}^\infty(T^*\mathbb{R}^N)[[\hbar]] \mapsto \widehat{A} \in \text{Op}(L^2(\mathbb{R}^N))[[\hbar]]$$

defined on a dense subalgebra of  $\mathcal{C}^\infty(T^*\mathbb{R}^N)[[\hbar]]$  and satisfying (1.1) as well as

$$\widehat{A}^\dagger = \widehat{A^*}, \tag{1.3}$$

where  $A^*$  is the complex conjugate of  $A$ , and

$$\begin{aligned} A \star B &= AB + O(\hbar) \\ A \star B - B \star A &= i\hbar\{A, B\} + O(\hbar^2) \end{aligned} \tag{1.4}$$

(1.3) means that the symbol of the adjoint of an operator is the complex conjugate of the symbol (and hence the correspondence maps real-valued symbols to essentially self-adjoint operators and positive-valued symbols to positive operators). (1.4) mean that *the quantum formalism converges to the classical formalism when  $\hbar \mapsto 0$* .  $\{, \}$  is the Poisson bracket on  $\mathcal{C}^\infty(T^*\mathbb{R}^N)$ .

There are various examples of quantizations in this sense. In this thesis we will mostly use Weyl quantization, which we describe in the next subsection. (The exception is §3.1, where we consider alternative quantizations).

There is still another approach. In Definition 1.1 we start with a symbol correspondence

$$A \in \mathcal{C}^\infty(T^*\mathbb{R}^N)[[\hbar]] \mapsto \widehat{A} \in \text{Op}(L^2(\mathbb{R}^N))[[\hbar]]$$

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<sup>1</sup>This is sometimes called a *formal quantization* to emphasize the difference from a strict quantization.

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and define from it a star product  $\star$  in  $\mathcal{C}^\infty(T^*\mathbb{R}^N)[[\hbar]]$  by

$$\widehat{A \star B} = \widehat{A}\widehat{B}.$$

Since the symbol correspondence is a bijection (when the domain and range are restricted), the star product encodes all the information of the algebra of operators. A *deformation quantization* consists of defining the star product directly in  $\mathcal{C}^\infty(T^*\mathbb{R}^N)[[\hbar]]$  without any reference to operators. More specifically:

**Definition 1.2.** *Let  $M$  be a Poisson manifold. A deformation quantization or star product on  $M$  is an associative,  $\mathbb{R}[[\hbar]]$ -linear product  $\star$  in  $\mathcal{C}^\infty(T^*\mathbb{R}^N)[[\hbar]]$  satisfying (1.4).*

This concept was introduced by Bayen et al in [3]. See also [24] for details and examples.

In §3.1 we will explain how to rephrase the statement of our main problem so that it makes sense in the context of a deformation quantization that might not come from a symbol correspondence.

### 1.1.3 Weyl quantization

Weyl quantization [29] (a.k.a. Weyl–Wigner correspondence) follows from the following idea. We know from (1.1) the operators  $\widehat{x}_j$  and  $\widehat{p}_j$  that correspond to the coordinate functions  $x_j$  and  $p_j$ . We next construct the operator that corresponds to exponentials of linear combinations of them, and finally we use the Fourier transform to build the

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operator for an arbitrary symbol. Specifically, for  $\alpha := (\alpha_1, \dots, \alpha_N) \in \mathbb{R}^N$  let us write

$$\alpha \cdot x = \sum_{j=1}^N \alpha_j x_j.$$

Let  $\alpha, \beta \in \mathbb{R}^N$ . Then,  $\alpha \cdot \hat{x} + \beta \cdot \hat{p}$  is an essentially self-adjoint operator, so that  $e^{i(\alpha \hat{x} + \beta \hat{p})}$  is a well-defined unitary operator. Given a symbol  $A \in \mathcal{C}^\infty(T^*\mathbb{R}^N)$ , let us denote by  $\mathcal{F}[A]$  its Fourier transform, so that

$$A(x, p) = \int \mathcal{F}[A](\alpha, \beta) e^{i(\alpha \cdot x + \beta \cdot p)} d^n \alpha d^n \beta.$$

Then we map the symbol  $A$  to the operator  $\hat{A}$  defined by

$$\hat{A} = \int \mathcal{F}[A](\alpha, \beta) e^{i(\alpha \cdot \hat{x} + \beta \cdot \hat{p})} d^n \alpha d^n \beta.$$

The last integral is taken in the strong topology. Although written for symbols that do not depend on  $\hbar$ , this expression can be extended to all symbols by  $\mathbb{R}[[\hbar]]$ -linearity.

If our symbols are in the Schwartz space of rapidly decreasing functions, then so are their Fourier transforms. Alternatively, we can take a bigger class of symbols, and then the Fourier transforms will be distributions. See [11] for details.

An alternative way of thinking about the Weyl quantization is via the following explicit expression. It produces an operator  $\hat{A}$  from a symbol  $A$  or the symbol from the operator:

$$\begin{aligned} \hat{A}[\phi](x) &= \int \frac{d^n y d^n p}{(2\pi\hbar)^n} e^{i(x-y) \cdot p/\hbar} A\left(\frac{x+y}{2}, p\right) \phi(y) \\ A(x, p) &= \int \frac{d^n s}{(2\pi\hbar)^n} e^{-is \cdot p/\hbar} \langle x + s/2 | \hat{A} | x - s/2 \rangle \end{aligned} \tag{1.5}$$

Again, we refer to [11] for details.

---

In the rest of this thesis, we accept that Weyl quantization is a well defined correspondence between symbols and operators, but we will not need to use its explicit form. We need only the explicit form of the star product, which we discuss in the next subsection.

#### 1.1.4 The Moyal product

Recall that, given a quantization, we define a *star product* in  $\mathcal{C}^\infty(T^*\mathbb{R}^N)[[\hbar]]$  as the operation that makes the bijection  $A \mapsto \widehat{A}$  into an algebra isomorphism. In other words,  $C \star D$  is the symbol of the operator  $\widehat{C}\widehat{D}$ . In the particular case of the Weyl quantization, the star product is called the *Moyal product*. Its explicit form is actually due to Groenewold [12] before Moyal [21]. It can be derived directly from (1.5). If  $C, D$  are symbols in  $\mathcal{C}^\infty(T^*\mathbb{R}^N)$ , then:

$$C \star D = \sum_{k=0}^{\infty} \frac{1}{k!} \left( \frac{i\hbar}{2} \right)^k \{C, D\}_k. \quad (1.6)$$

We need to explain the notation in (1.6). In the natural coordinates  $(x, p)$  on  $T^*\mathbb{R}^N$ , the Poisson bivector field is

$$J = \sum_{j=1}^N (\partial_{x_j} \otimes \partial_{p_j} - \partial_{p_j} \otimes \partial_{x_j}),$$

where  $\partial_q := \frac{\partial}{\partial q}$ . Let us call the coordinates  $(z^1, \dots, z^{2N}) := (x, p)$  and let  $J^{\mu\nu}$  be the coefficients of the Poisson tensor on this chart

$$(J^{\mu\nu}) = \begin{pmatrix} 0 & I_N \\ -I_N & 0 \end{pmatrix},$$

---

where  $I_N$  is the identity  $N \times N$  matrix. Using the Einstein summation criterion (summation over repeated indexes),  $J = J^{\mu\nu} \partial_\mu \otimes \partial_\nu$ . Let us also write

$$C_{,\mu} = \partial_\mu C = \partial_{z^\mu} C = \frac{\partial C}{\partial z^\mu}$$

$$C_{,\mu_1 \dots \mu_k} = \partial_{\mu_1} \dots \partial_{\mu_k} C = \partial_{z^{\mu_1}} \dots \partial_{z^{\mu_k}} C = \frac{\partial^k C}{\partial z^{\mu_1} \dots \partial z^{\mu_k}}$$

Then the Poisson bracket in  $T^*\mathbb{R}^N$  can be written as

$$\{C, D\} = C_{,\mu} J^{\mu\nu} C_{,\nu}.$$

The terms appearing in (1.6) are defined as:

$$\{C, D\}_0 = CD$$

$$\{C, D\}_1 = \{C, D\} = C_{,\mu} J^{\mu\nu} D_{,\nu}$$

$$\{C, D\}_k = C_{,\mu^1 \dots \mu^k} J^{\mu^1 \nu^1} \dots J^{\mu^k \nu^k} D_{,\nu^1 \dots \nu^k}$$

We introduce now some notation that will be more convenient for us than  $\{, \}_k$ , and of which we will make extensive use. Following [5] we use the notation “ $\longrightarrow$ ” for a Poisson tensor in the following way: “ $\longrightarrow$ ” is replaced by  $J^{\mu\nu}$ , the expression at the head of the arrow is acted on by  $\partial_\nu$  and the expression at the tail of the arrow is acted on by  $\partial_\mu$ . For instance

$$C \longrightarrow D = C_{,\mu} J^{\mu\nu} D_{,\nu} = \{C, D\}$$

$$C \Longrightarrow D = C_{,\mu^1 \mu^2} J^{\mu^1 \nu^1} J^{\mu^2 \nu^2} D_{,\nu^1 \nu^2} = \{C, D\}_2$$

$$C \xrightarrow{[k]} D = C_{,\mu^1 \dots \mu^k} J^{\mu^1 \nu^1} \dots J^{\mu^k \nu^k} D_{,\nu^1 \dots \nu^k} = \{C, D\}_k$$

Here,  $\xrightarrow{[k]}$  denotes  $k$  arrows. A more complicated example is

$$C \longrightarrow D \Longrightarrow A = C_{,\mu^1} J^{\mu^1 \nu^1} D_{,\nu^1 \mu^2 \mu^3} J^{\mu^2 \nu^2} J^{\mu^3 \nu^3} A_{,\nu^2 \nu^3} \quad (1.7)$$

---

Since  $J^{\mu\nu}$  is skew-symmetric, inverting an arrow multiplies the expression by  $-1$ :

$$C \longrightarrow D = (-1) C \longleftarrow D$$

With this notation, the Moyal product (1.6) is written:

$$C \star D = \sum_{k=0}^{\infty} \frac{1}{k!} \left( \frac{i\hbar}{2} \right)^k C \overrightarrow{:[k]} D \quad (1.8)$$

The notation is explained in further detail in §2.1. In Appendix A we explain how it makes it simpler to write down expressions and perform certain calculations.

## 1.2 Functional calculus

To make sense of our problem (and to understand (0.1)), we need to define what a function of an operator is. If  $f(y) = y^n$  then  $f(\widehat{A}) = (\widehat{A})^n$ , and similarly we can make sense of  $f(\widehat{A})$  for any polynomial  $f$ . At first sight, there is not a simple way to make sense of  $f(\widehat{A})$  for an arbitrary smooth function  $f$ , and this turns out to be an interesting problem in functional analysis.

**Definition 1.3.** *Let  $\widehat{A}$  be an essentially self-adjoint operator on a Hilbert space. A functional calculus or spectral theorem for  $\widehat{A}$  consists of*

- a (complex) algebra  $\mathcal{B}$  of functions of one variable, and
- a map

$$f \in \mathcal{B} \mapsto f(\widehat{A}) \in \text{Op}(L^2(\mathbb{R}^N)),$$

*satisfying the following properties:*

- 
- $f \mapsto f(\widehat{A})$  is a homomorphism of algebras (with respect to the pointwise product of functions and composition of operators). In particular it is linear and

$$f(\widehat{A})g(\widehat{A}) = (fg)(\widehat{A}).$$

- The identity function is mapped to  $\widehat{A}$ :  $Id(\widehat{A}) = \widehat{A}$ .
- The constant function equal to 1 is mapped to the identity operator:  $1(\widehat{A}) = \widehat{1}$ .
- $f^*(\widehat{A}) = (f(\widehat{A}))^\dagger$ , where  $f^*$  is the complex conjugate of  $f$ .
- If the spectrum of  $\widehat{A}$  does not intersect the support of  $f$ , then  $f(\widehat{A}) = 0$ .

The definition can be extended to operators which are not essentially self-adjoint. Sometimes a continuity condition is also required. Of course, we will only care about functional calculus for operators in  $L^2(\mathbb{R}^N)$  and where the algebra consists of smooth functions  $\mathcal{B} \subseteq \mathcal{C}^\infty(\mathbb{C})$ . See [8] for details on the definition.

There exist various spectral theorems for different algebras  $\mathcal{B}$ . [1] contains a reasonably comprehensive list.

Let us go back to our main problem. Given an operator  $\widehat{A}$  with symbol  $A$  and a smooth function  $f$ , we define the operator  $\widehat{B} := f(\widehat{A})$  with symbol  $B$ . We want to write  $B$  in terms of  $A$  and  $f$ . A priori, the answer could depend on the functional calculus that we are using, i.e. on how we define what  $f(\widehat{A})$  means. In fact, previous approaches to this problem [7, 28] fix one particular functional calculus. We, instead, will not choose any specific functional calculus. We will only assume that the function  $f$  belongs to some algebra  $\mathcal{B}$  for which we have a well-defined functional calculus. We will

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not use its explicit form, but only the properties in Definition 1.3. As a consequence, our result will be valid for a bigger set of functions and will have an easy generalization to functions of several variables (see §3.2).

In Appendix B we will discuss the method used in [7, 28] and will use it to derive an alternative proof of our main result. This will be the only occasion in which we fix an explicit functional calculus.

Finally, notice that we do *not* need a functional calculus to define what we mean by a function of a symbol, since  $f(A) := f \circ A$ .

## Chapter 2

# Main calculations and results

In this section, we will derive (0.1) and various equivalent formulas. By comparison with previous attempts to solve the same problem (see Appendix B), one of our crucial ingredients is the diagrammatic notation first introduced in [5]. This notation allows us to write compact expressions for otherwise long, ugly formulas. In particular we will write formal power series whose terms are labeled by graphs (à la Feynman).

In §2.1, we will describe the families of graphs that we are going to use and fix notation. The core of our calculations is in §2.2 and we finally summarize our results in §2.3.

### 2.1 Notation: Graphs

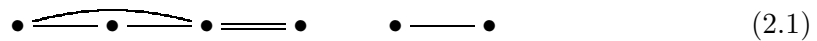
The formulas we are going to derive involve power series whose terms are labeled by graphs. We will use two types of graphs: labeled graphs and unlabeled graphs (which

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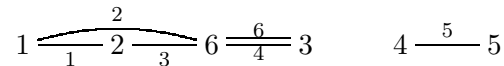
we will simply call graphs).

A *graph* consists of a finite set of vertices and a finite number of edges. Each vertex is represented by a dot. Each edge is represented by a line joining two vertices. Multiple edges joining the same pair of vertices are allowed. A self-edge (an edge from a vertex to itself) is not allowed. A graph does not need to be connected.

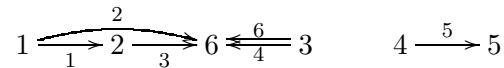
An example of a graph is



A *labeled graph* is a graph in which we have labeled the vertices with the first  $V$  natural numbers  $1, 2, \dots, V$  and the edges with the first  $E$  natural numbers  $1, 2, \dots, E$ . Therefore,  $V$  is the number of vertices and  $E$  is the number of edges. An example is:



Even though a graph as defined above is not oriented, a labeled graph has a natural orientation: every edge is oriented so that the target has a higher label than the source:



All the information in a graph is given by *how many edges there are joining each pair of vertices*. All the information in a labeled graph is given by *which edge joins which pair of vertices*. This leads us to adopt the following formal definitions.

**Definition 2.1.** *Let  $V$  and  $E$  be two non-negative integers. A labeled graph with  $V$*

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vertices and  $E$  edges is a map

$$s : \{1, \dots, E\} \longrightarrow \mathcal{P}_2\{1, \dots, V\},$$

where  $\mathcal{P}_2X$  denotes the set of subsets of  $X$  with 2 elements.

This means simply that the edge  $i$  joins the pair of vertices  $s(i)$ . The group  $S_E$  of permutations of  $E$  letters acts on  $\{1, \dots, E\}$ . The group  $S_V$  of permutations of  $V$  letters acts on  $\{1, \dots, V\}$ , and hence also acts naturally on  $\mathcal{P}_2\{1, \dots, V\}$ . Therefore, the direct product  $S_V \times S_E$  acts on functions  $\{1, \dots, E\} \longrightarrow \mathcal{P}_2\{1, \dots, V\}$ , that is, on the set of labeled graphs with  $V$  vertices and  $E$  edges.

**Definition 2.2.** *An unlabeled graph or simply graph with  $V$  vertices and  $E$  edges is an orbit of this action.*

We will denote a labeled graph by  $\Gamma$  and the corresponding (unlabeled) graph by  $[\Gamma]$ , if we need to distinguish between them. Otherwise, we will abuse notation and denote both simply by  $\Gamma$ .

It is convenient to define now two more concepts that will be needed later. The *order of symmetry* of a labeled graph is the number of permutations of edges and vertices that we can make without changing it. Or, more formally:

**Definition 2.3.** *The order of symmetry  $S_\Gamma$  of a labeled graph  $\Gamma$  is the order of the stabilizer of  $\Gamma$  in the action of  $S_V \times S_E$  on the set of graphs with  $V$  vertices and  $E$  edges. The order of symmetry of an unlabeled graph  $[\Gamma]$  is the order of symmetry of  $\Gamma$ .*

---

Notice that if two labeled graphs  $\Gamma_1$  and  $\Gamma_2$  represent the same unlabeled graph  $[\Gamma_1] = [\Gamma_2]$ , then their stabilizers are conjugate subgroups of  $S_V \times S_E$ , and have the same order. Hence, the order of symmetry of an unlabeled graph is well-defined. See Appendix C for examples.

A labeled graph is *reduced* if it does not have any isolated vertices. Or, more formally:

**Definition 2.4.** *A labeled graph  $s : \{1, \dots, E\} \longrightarrow \mathcal{P}_2\{1, \dots, V\}$  is reduced if every  $i = 1, \dots, V$  is in some element of the image of  $s$  (i.e., “if every vertex is in some edge”). An unlabeled graph  $[\Gamma]$  is reduced if  $\Gamma$  is reduced.*

All the previous examples are reduced. The graph  $\bullet \text{---} \bullet \quad \bullet$  is not reduced.

Given a labeled graph  $\Gamma$  with  $V$  vertices, and given  $V$  symbols  $A_1, \dots, A_V$  we construct a new symbol, called  $\lambda_\Gamma(A_1, \dots, A_V)$ , by replacing the vertices by  $A_1, \dots, A_V$ , and letting every edge represent a Poisson tensor (as explained in §1.1.4). We denote  $\lambda_\Gamma(A, \dots, A)$  simply by  $\lambda_\Gamma(A)$ .

For instance, if  $\Gamma$  is the labeled graph

$$1 \xrightarrow{1} 2 \xrightarrow{\frac{2}{3}} 3,$$

then  $\lambda_\Gamma(C, D, A)$  is the expression in (1.7). And

$$\lambda_\Gamma(A) = A \longrightarrow A \Longrightarrow A = A_{,\mu_1} J^{\mu_1 \nu_1} A_{,\nu_1 \mu_2 \mu_3} J^{\mu_2 \nu_2} J^{\mu_3 \nu_3} A_{,\nu_2 \nu_3}.$$

---

Since changing the direction of one arrow multiplies the expression by  $-1$ ,  $\lambda_{[\Gamma]}$  is defined only up to a sign.

## 2.2 Calculations

We recall our problem. Let us fix an operator  $\widehat{A}$  with symbol  $A$  and a smooth function  $f$ . Let  $\widehat{B} = f(\widehat{A})$  be an operator with symbol  $B$ . In this section we will perform the necessary calculations to obtain various expressions for  $B$  in terms of  $A$  and  $f$ .

The main step is to obtain an expression in terms of graphs for an iterated star product  $C_1 \star \dots \star C_n$  for symbols  $C_i$ . We do this in §2.2.1. Then in §2.2.2 we derive our first expression for  $B$  in terms of  $A$  and  $f$ .

Equation (2.6) at the end of §2.2.2 is a power series whose terms are parametrized by labeled graphs. This is the easiest form of our result to derive, and it is useful for theoretical proofs. However, it is not convenient for explicit calculations when we want to write the first few terms explicitly, as there are many more labeled graphs than unlabeled graphs. In §2.1 we obtain our second expression for  $B$  in terms of  $A$  and  $f$ , (2.10), a series whose terms are parametrized by unlabeled graphs. There is still a third form of our formula, Equation (2.14), whose terms are parametrized by connected graphs. This last form is studied in §2.2.4.

Using (2.10) or (2.14), we have calculated the explicit form of the terms up to order 4 in  $\hbar$  of the symbol  $B$  in terms of  $A$  and  $f$ ; the results are displayed in Appendix D.

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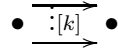
### 2.2.1 The $n$ -th star product.

The main step in the derivation of (0.1) is the following expression for the iterated star product, which generalizes Moyal's formula:

**Lemma 2.5.** *Let  $C_1, \dots, C_n \in \mathcal{C}^\infty(T^*\mathbb{R}^N)$  be symbols. Then*

$$C_1 \star \dots \star C_n = \sum_{k=0}^{\infty} \frac{1}{k!} \left( \frac{i\hbar}{2} \right)^k \sum_{\substack{\text{labeled graphs } \Gamma \\ \text{with } n \text{ vertices} \\ \text{and } k \text{ edges}}} \lambda_\Gamma(C_1, \dots, C_n) \quad (2.2)$$

Notice that for every integer  $k$ , there exists exactly one graph with 2 vertices and  $k$  edges



and there is a unique way to label it. As a consequence, when  $n = 2$ , Lemma 2.5 is exactly the Moyal formula for the star product (1.8):

$$C_1 \star C_2 = \sum_{k=0}^{\infty} \frac{1}{k!} \left( \frac{i\hbar}{2} \right)^k C_1 \begin{array}{c} \xrightarrow{\quad} \\ \text{:}[k] \\ \xrightarrow{\quad} \end{array} C_2$$

As an example, Figure 2.1 shows the first terms of Equation (2.2) when  $n = 3$  and  $C_i = A$  for all  $i$ . Notice how in this figure all graphs have vertices labeled 1, 2, 3 from left to right.

*Proof of lemma 2.5.* We will use induction on  $n$ .

The result is true for  $n = 0, 1, 2$ .

Figure 2.1: Lemma 2.5 when  $n = 3$ .

$$\begin{aligned}
A \star A \star A &= \left( A \quad A \quad A \right) \\
&+ \frac{i\hbar}{2} \left( A \longrightarrow A \quad A \right) + \frac{i\hbar}{2} \left( A \quad A \longrightarrow A \right) \\
&+ \frac{i\hbar}{2} \left( A \overset{\curvearrowright}{\longrightarrow} A \right) + \frac{1}{2!} \left( \frac{i\hbar}{2} \right)^2 \left( A \Longrightarrow A \quad A \right) \\
&+ \frac{1}{2!} \left( \frac{i\hbar}{2} \right)^2 \left( A \quad A \Longrightarrow A \right) + \frac{1}{2!} \left( \frac{i\hbar}{2} \right)^2 \left( A \overset{\curvearrowright}{\Longrightarrow} A \right) \\
&+ \frac{1}{2!} \left( \frac{i\hbar}{2} \right)^2 \left( A \xrightarrow{1} A \xrightarrow{2} A \right) + \frac{1}{2!} \left( \frac{i\hbar}{2} \right)^2 \left( A \xrightarrow{2} A \xrightarrow{1} A \right) \\
&+ \frac{1}{2!} \left( \frac{i\hbar}{2} \right)^2 \left( A \overset{2}{\underset{1}{\longrightarrow}} A \right) + \frac{1}{2!} \left( \frac{i\hbar}{2} \right)^2 \left( A \overset{1}{\underset{2}{\longrightarrow}} A \right) \\
&+ \frac{1}{2!} \left( \frac{i\hbar}{2} \right)^2 \left( A \overset{1}{\underset{A}{\longrightarrow}} A \right) + \frac{1}{2!} \left( \frac{i\hbar}{2} \right)^2 \left( A \overset{2}{\underset{A}{\longrightarrow}} A \right) \\
&+ O(\hbar^3) \\
&= A^3 + \frac{3i\hbar}{2} \left( A \longrightarrow A \right) A + \frac{3}{2} \left( \frac{i\hbar}{2} \right)^2 \left( A \Longrightarrow A \right) A \\
&+ \frac{4-2}{2} \left( \frac{i\hbar}{2} \right)^2 \left( A \longrightarrow A \longleftarrow A \right) + O(\hbar^3)
\end{aligned}$$

---

Inductive step. We use the associativity of the star product.

$$\begin{aligned}
C_1 \star \dots \star C_{n+1} &= (C_1 \star \dots \star C_n) \star C_{n+1} \\
&= \left( \sum_{\substack{\text{labeled} \\ \text{graphs } \Gamma \\ \text{with } n \text{ vertices}}} \frac{1}{E!} \left( \frac{i\hbar}{2} \right)^E \lambda_{\Gamma}(C_1, \dots, C_n) \right) \star C_{n+1} \\
&= \sum_{\substack{\text{labeled} \\ \text{graphs } \Gamma \\ \text{with } n \text{ vertices}}} \sum_{k=0}^{\infty} \frac{1}{E!k!} \left( \frac{i\hbar}{2} \right)^{E+k} \lambda_{\Gamma}(C_1, \dots, C_n) \overrightarrow{:[k]} C_{n+1}
\end{aligned}$$

Applying Lemma A.1 in Appendix A to  $\lambda_{\Gamma}(C_1, \dots, C_n) \overrightarrow{:[k]} C_{n+1}$ , we get a sum over labeled graphs  $\Gamma'$  with  $n+1$  vertices. They are built by starting with a labeled graph  $\Gamma$  with  $n$  vertices (labeled  $1, \dots, n$ ) and  $E$  edges (labeled  $1, \dots, E$ ) and adding the  $(n+1)$ -th vertex and  $k$  edges (labeled  $E+1, \dots, E+k$ ) ending at the  $(n+1)$ -th vertex. The number of edges of  $\Gamma'$  is  $E' = E+k$ . We are not getting all possible labeled graphs with  $n+1$  vertices yet because we are imposing that all the edges ending in the vertex  $n+1$  have the highest labels. For any given graph with  $n+1$  vertices and  $E'$  edges, we need to divide by a factor of  $\binom{E+k}{E}$  in order to account for all ways of relabeling the edges. Fortunately, we can write

$$\frac{1}{E!k!} = \frac{1}{(E+k)!} \binom{E+k}{E},$$

and we get

$$C_1 \star \dots \star C_{n+1} = \sum_{\substack{\text{labeled} \\ \text{graphs } \Gamma' \\ \text{with } n+1 \text{ vertices}}} \frac{1}{E'!} \left( \frac{i\hbar}{2} \right)^{E'} \lambda_{\Gamma'}(C_1, \dots, C_{n+1}).$$

□

---

### 2.2.2 First formula for the symbol of a function of an operator.

We now attack the problem of obtaining the symbol  $B$  of  $\widehat{B} = f(\widehat{A})$  in terms of  $A$  and  $f$ .

We first need the following fact:

**Lemma 2.6.** *Let  $g$  be a smooth function and  $\widehat{C} := g(\widehat{A})$ . Let  $z_0$  be a point in  $T^*\mathbb{R}^N$  and  $a_0 := A(z_0)$ . If  $g$  has a zero of order  $m$  at  $a_0$ , then  $C(z_0) = O(\hbar^{m/2})$ .*

**Note.** Actually, we can do better:  $C(z_0) = O(\hbar^{2m/3})$ . However, we cannot conclude that  $C(z_0) = O(\hbar^m)$  from the hypothesis of Lemma 2.6. As a counterexample, take

$$\begin{aligned} A(x, p) &= x^2 - p, & z_0 &= (1, 1), \\ a_0 = A(z_0) &= 0, & g(y) &= y^3. \end{aligned}$$

Let  $\widehat{C} := g(\widehat{A})$ , so that  $C = A \star A \star A$ . On the one hand,  $a_0$  is a zero of order 3 of  $g$ . On the other hand, substituting

$$A \longrightarrow A \longleftarrow A \quad = \quad A_{,p} A_{,xx} A_{,p} \quad = \quad 2$$

and  $A(z_0) = 0$  into the calculation in Figure 2.1, we get  $C(z_0) = -\hbar^2/2 + O(\hbar^3)$ .

*Proof of Lemma 2.6.* Let us write  $g(y) = g_1(y)(y - a_0)^m$  and let  $\widehat{C}_1 = g_1(\widehat{A})$ . Then

$$\widehat{C} = g(\widehat{A}) = g_1(\widehat{A})(\widehat{A} - a_0)^m$$

and

$$C = C_1 \star (A - a_0)^{*m}. \tag{2.3}$$

---

We now notice that  $(A(z) - a_0)|_{z=z_0} = O(\hbar)$ . When we expand (2.3) using the Moyal formula and evaluate at  $z_0$ , we will get a sum of terms. For the contribution of one of these terms not to be zero, we need all the  $m$  factors  $A(z) - a_0$  to be differentiated at least once. Since each two derivatives come with a factor of  $\hbar$ , all the non-zero terms will be of order at least  $O(\hbar^{m/2})$ .

□

Now to calculate  $B$  we use the following expression [6]:

**Lemma 2.7.** *Let  $z_0 \in T^*\mathbb{R}^N$  and let  $a_0 := A(z_0)$ . Then*

$$B(z_0) = \sum_{k=0}^{\infty} \frac{1}{k!} f^{(k)}(a_0) (A - a_0)^{\star k}(z_0). \quad (2.4)$$

Note that the right hand side of (2.4) is well-defined only at the point  $z_0$  (otherwise there are infinitely many non-zero contributions at each order in  $\hbar$ ).

*Proof.* For every  $m \in \mathbb{N}$ , apply Lemma 2.6 to

$$g(y) := f(y) - \sum_{k=0}^m \frac{1}{k!} f^{(k)}(a_0)(y - a_0)^m.$$

This proves that

$$B(z_0) - \sum_{k=0}^{\infty} \frac{1}{k!} f^{(k)}(a_0) (A - a_0)^{\star k}(z_0) = O(\hbar^{m/2})$$

for all  $m$ . Hence:

$$B(z_0) = \sum_{k=0}^{\infty} \frac{1}{k!} f^{(k)}(a_0) (A - a_0)^{\star k}(z_0) + O(\hbar^{\infty}).$$

□

---

Now we only need to substitute (2.2) into (2.4) to get an expression for  $B$  in terms of graphs:

$$\begin{aligned}
B(z_0) &= \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(A(z_0)) \sum_{k=0}^{\infty} \sum_{\substack{\text{labeled graphs } \Gamma \\ \text{with } n \text{ vertices} \\ \text{and } k \text{ edges}}} \frac{1}{k!} \left(\frac{i\hbar}{2}\right)^k \lambda_{\Gamma}(A - a_0)(z_0) \\
&= \sum_{\substack{\text{labeled} \\ \text{graphs } \Gamma}} \frac{1}{E_{\Gamma}!} \left(\frac{i\hbar}{2}\right)^{E_{\Gamma}} \frac{f^{(V_{\Gamma})}(A(z_0))}{V_{\Gamma}!} \lambda_{\Gamma}(A - a_0)(z_0)
\end{aligned} \tag{2.5}$$

In order to calculate  $\lambda_{\Gamma}(A - a_0)(z_0)$  we need to write the symbol  $A - a_0$  at every vertex of  $\Gamma$ . If a vertex is not isolated, then some derivatives are acting upon that symbol, and we may substitute  $A - a_0$  for  $A$ , since  $a_0$  is a constant. If a vertex is isolated, then it contributes a factor of  $(A - a_0)$ , and  $(A - a_0)(z_0) = 0$ . Hence we only need to consider graphs without isolated vertices, which we called reduced. Putting this all together:

$$B(z_0) = \sum_{\substack{\text{reduced labeled} \\ \text{graphs } \Gamma}} \frac{1}{E_{\Gamma}!} \left(\frac{i\hbar}{2}\right)^{E_{\Gamma}} \frac{f^{(V_{\Gamma})}(A(z_0))}{V_{\Gamma}!} \lambda_{\Gamma}(A)(z_0)$$

And better yet:

$$B = \sum_{\substack{\text{reduced labeled} \\ \text{graphs } \Gamma}} \frac{1}{E_{\Gamma}!} \left(\frac{i\hbar}{2}\right)^{E_{\Gamma}} \frac{f^{(V_{\Gamma})}(A)}{V_{\Gamma}!} \lambda_{\Gamma}(A) \tag{2.6}$$

It is to be noted that the previous equation is not, strictly speaking, a power series expansion in  $\hbar$ , as  $A$  itself depends on  $\hbar$ . However, it is very simple to write  $A = \sum_k \hbar^k A_k$  as a power series in  $\hbar$  and expand (2.6). As a matter of fact, we have an alternative way to write (2.6) with terms parametrized by *graphs with weights* where every term is a monomial in  $\hbar$ . We believe that the approach shown in this thesis is simpler, though.

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Equation (2.6) was easy to derive, and it is useful for proofs and theoretical calculations, as well as to generalize to other quantizations (see §3.1). However, when we want to explicitly write the first few terms, it is not yet our ideal expression. We will now put together the contribution of labeled graphs that differ only in the labels to get a series whose terms are parametrized by unlabeled graphs.

See Appendix B for an alternative derivation of (2.6).

### 2.2.3 Version with non-labeled graphs.

Two labeled graphs which are the same except for the labeling of vertices and edges give the same contribution (up to a sign).

(2.6) can be rewritten as:

$$B = \sum_{\substack{\text{reduced} \\ \text{graphs } [\Gamma]}} \frac{1}{E_\Gamma!} \left(\frac{i\hbar}{2}\right)^{E_\Gamma} \frac{f^{(V_\Gamma)}(A)}{V_\Gamma!} \sum_{\Gamma' \in [\Gamma]} \lambda_{\Gamma'}(A) \quad (2.7)$$

In words, first we sum over all reduced (unlabeled) graphs  $[\Gamma]$ . Then, for each  $[\Gamma]$  we sum over all possible relabelings  $\Gamma'$  of  $\Gamma$ . Remember that  $\lambda_{\Gamma'}$  and  $\lambda_\Gamma$  will be equal up to a sign.

Define

$$c_\Gamma := \sum_{\substack{\Gamma' \text{ is a reordering of} \\ \text{the vertices of } \Gamma}} (-1)^{\# \text{ of arrows inverted going from } \Gamma \text{ to } \Gamma'} \quad (2.8)$$

That is, we start with a labeled graph  $\Gamma$ . Then, we consider the  $V_\Gamma!$  possible ways of numbering the vertices of the graph with  $1, 2, \dots, V_\Gamma$ . For each of them, we orient the arrows so that they all go from the vertex with the lowest label to the vertex with the

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highest label. Then we count these  $V_\Gamma!$  relabelings with signs, depending on the parity of the number of arrows inverted from our original orientation.

We can then write the contribution from (2.7) as

$$\sum_{\Gamma' \in [\Gamma]} \lambda_{\Gamma'}(A) = \frac{E_\Gamma!}{S_\Gamma} c_\Gamma \lambda_\Gamma(A), \quad (2.9)$$

where  $S_\Gamma$  is the order of the symmetry group of the (unlabeled) graph  $[\Gamma]$  (see Definition 2.3). The contribution corresponding to different relabelings of the edges is  $E_\Gamma!$ . The contribution corresponding to different relabelings of the vertices is in  $c_\Gamma$ . And we have to divide by the order of the symmetry group, to account for the situation in which exchanging edges or vertices results in the same labeled graph.

For instance, if  $\Gamma$  is the graph  $\bullet \rightarrow \bullet \rightarrow \bullet$ , then the contribution from renumbering the vertices is:

$$\begin{aligned} c_\Gamma = & \begin{array}{ccc} 1 \rightarrow 2 \rightarrow 3 & 1 \rightarrow 3 \leftarrow 2 & 2 \leftarrow 1 \rightarrow 3 \\ (-1)^0 & + & (-1)^1 & + & (-1)^1 \\ 2 \rightarrow 3 \leftarrow 1 & 3 \leftarrow 1 \rightarrow 2 & 3 \leftarrow 2 \leftarrow 1 \\ + & (-1)^1 & + & (-1)^1 & + & (-1)^2 & = & -2 \end{array} \end{aligned}$$

Finally we just have to substitute (2.9) into (2.7):

$$B = \sum_{\substack{\text{reduced} \\ \text{graphs } [\Gamma]}} \left( \frac{i\hbar}{2} \right)^{E_\Gamma} \frac{c_\Gamma}{S_\Gamma} \frac{f^{(V_\Gamma)}(A)}{V_\Gamma!} \lambda_\Gamma(A) \quad (2.10)$$

Notice how  $c_\Gamma$  and  $\lambda_\Gamma(A)$  are only defined up to a sign for  $[\Gamma]$ . However, those signs cancel in their product  $c_\Gamma \lambda_\Gamma(A)$ , which is well defined.

The explicit calculation of  $c_\Gamma$  for a particular graph is actually very easy. See Appendix C, which includes the value of  $c_\Gamma$  and  $S_\Gamma$  for all reduced, connected graphs

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with 2 or 4 edges. Thanks to Lemma C.1, we only need to consider graphs  $\Gamma$  where every connected component has an even number of edges, since otherwise  $c_\Gamma = 0$ .

#### 2.2.4 Version with connected graphs.

Let us rewrite (2.10) as

$$B = \left[ \sum_{\substack{\text{reduced} \\ \text{graphs } [\Gamma]}} \left( \frac{i\hbar}{2} \right)^{E_\Gamma} \frac{c_\Gamma}{S_\Gamma} \lambda_\Gamma(A) \frac{D^{V_\Gamma}}{V_\Gamma!} \right] f(A), \quad (2.11)$$

where  $D$  is the differential operator which applies to  $f$ .

Expressions like (2.11), a series labeled by a certain family of “pictures”, appear very often in quantum field theory. By a family of pictures we mean a collection of sketches that we draw following certain rules, that we can place next to each other (disjoint union), and such that we can talk about the order of symmetry of each picture. Examples are Feynman diagrams and our collection of graphs. Whenever such expressions arise in quantum field theory, it is standard to reduce all calculations to only connected pictures. This is done usually on a case by case basis. In the following lemma we state the properties that a series labeled by pictures needs to satisfy, so that we can reduce the sum to only connected pictures. We have not found the result stated in this generality in the literature, but the idea behind it is no doubt “in the air”.

**Lemma 2.8.** *Let  $\mathcal{G}$  be the free commutative monoid (i.e., semigroup with identity) generated by the set  $\mathcal{G}_0$ . Let  $S$  be a commutative ring (with multiplicative notation). Let*

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$\mathcal{O} : \mathcal{G} \rightarrow S$  be a map satisfying

$$\mathcal{O}(r_1 x_1 + \dots + r_n x_n) = \frac{1}{r_1! \dots r_n!} (\mathcal{O}(x_1))^{r_1} \dots (\mathcal{O}(x_n))^{r_n} \quad (2.12)$$

for distinct  $x_1, \dots, x_n \in \mathcal{G}$  and  $r_1, \dots, r_n \in \mathbb{N}$ . Then, formally:

$$\sum_{x \in \mathcal{G}} \mathcal{O}(x) = \exp \left[ \sum_{x \in \mathcal{G}_0} \mathcal{O}(x) \right] \quad (2.13)$$

In particular, consider  $\mathcal{G}$  to be a family of pictures closed under disjoint union (that we denote by  $+$ ) and generated by the connected non-empty pictures  $\mathcal{G}_0$ . If we write  $\mathcal{O}(\Gamma) = \frac{\mathcal{M}(\Gamma)}{S_\Gamma}$ , where  $S_\Gamma$  is the order of the symmetry group of the diagram and  $\mathcal{M}$  is a multiplicative function

$$\mathcal{M}(x_1 + x_2) = \mathcal{M}(x_1)\mathcal{M}(x_2) \text{ for all } x_1, x_2 \in \mathcal{G}$$

then  $\mathcal{O}$  satisfies (2.12).

In our case,

$$\mathcal{G} = \text{reduced graphs}$$

$$\mathcal{G}_0 = \text{reduced, connected, non-empty graphs}$$

$$S = \mathcal{C}^\infty(T^*\mathbb{R}^N)$$

$$\mathcal{M}([\Gamma]) = \left( \frac{i\hbar}{2} \right)^{E_\Gamma} c_\Gamma \lambda_\Gamma(A) \frac{D^{V_\Gamma}}{V_\Gamma!}$$

$\mathcal{M}$  is multiplicative from (C.1) in Appendix 2.2

$$\frac{c_{\Gamma_1 + \Gamma_2}}{V_{\Gamma_1 + \Gamma_2}} = \frac{c_{\Gamma_1}}{V_{\Gamma_1}} \cdot \frac{c_{\Gamma_2}}{V_{\Gamma_2}}$$

---

Hence, using (2.13) in (2.11):

$$B = \left[ \exp \sum_{\substack{\text{connected, reduced,} \\ \text{non-empty graphs } [\Gamma]}} \left( \frac{i\hbar}{2} \right)^{E_\Gamma} \frac{c_\Gamma}{S_\Gamma} \lambda_\Gamma(A) \frac{D^{V_\Gamma}}{V_\Gamma!} \right] f(A) \quad (2.14)$$

## 2.3 Summary of results

We have derived three equivalent expressions that solve our problem. Let  $\hat{A}$  be an operator with symbol  $A$  and let  $f$  be a smooth functions. Let  $\hat{B} := f(\hat{A})$  be another operator with symbol  $B$ . Then

$$\begin{aligned} B &= \sum_{\substack{\text{reduced labeled} \\ \text{graphs } \Gamma}} \frac{1}{E_\Gamma!} \left( \frac{i\hbar}{2} \right)^{E_\Gamma} \frac{f^{(V_\Gamma)}(A)}{V_\Gamma!} \lambda_\Gamma(A), \\ B &= \sum_{\substack{\text{reduced} \\ \text{graphs } [\Gamma]}} \left( \frac{i\hbar}{2} \right)^{E_\Gamma} \frac{c_\Gamma}{S_\Gamma} \frac{f^{(V_\Gamma)}(A)}{V_\Gamma!} \lambda_\Gamma(A), \\ B &= \left[ \exp \sum_{\substack{\text{connected, reduced,} \\ \text{non-empty graphs } [\Gamma]}} \left( \frac{i\hbar}{2} \right)^{E_\Gamma} \frac{c_\Gamma}{S_\Gamma} \lambda_\Gamma(A) \frac{D^{V_\Gamma}}{V_\Gamma!} \right] f(A). \end{aligned}$$

The first equation (version with labeled graphs) is the easiest one to derive from scratch. It is useful for theoretical proofs and calculations, but not to calculate explicitly the first few terms in any particular case, since there are too many labeled graphs at every order in  $\hbar$  (i.e., with a fixed number of edges).

The second equation (version with (unlabeled) graphs) is hard to derive directly, but easy to derive from the first one. It is useful to calculate explicitly the first few terms in any particular case, since there are fewer (unlabeled) graphs at every order in  $\hbar$ .

The third formula (version with connected graphs) is only easy to derive from

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the second one. It will be useful for applications in some particular cases (for instance in §4.2).

See Appendix D for an explicit form of  $B$  in terms of  $A$  and  $f$  at order 4 in  $\hbar$ .

## Chapter 3

# Generalizations

As we mentioned in the introduction and explained in Chapter 1, we needed two ingredients to derive our results (and even for the statement of our problem  $\boxtimes$  to make sense):

- A quantization.
- A functional calculus.

We used the Weyl quantization. From it, we derived a form for the Moyal product. The only thing specific to the Weyl quantization that we used in our derivations was the Moyal product. In §3.1 we discuss how to generalize our results to other quantizations, by replacing the Moyal product with a different star product.

We did not use any specific functional calculus. Instead, we assumed that we had a well-defined functional calculus that allows us to define  $f(\widehat{A})$ , and we used only the properties in Definition 1.3. In §3.2 we explain how this allows us to easily extend

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our results to functions of several variables.

### 3.1 Other quantizations

There are other quantizations apart from Weyl quantization, that is, correspondences

$$A \in \mathcal{C}^\infty(T^*\mathbb{R}^N)[[\hbar]] \mapsto \widehat{A} \in \text{Op}(L^2(\mathbb{R}^N))[[\hbar]]$$

between operators and symbols [14]. Assume we want to solve the same problem (i.e. writing the symbol of  $f(\widehat{A})$  in terms of  $A$  and  $f$ ) but with respect to a different quantization. Then we will have a different star product, still defined by  $\widehat{C \star D} := \widehat{C} \widehat{D}$ .

We can try to reproduce all our calculations (§2.2) using this new star product instead of the Moyal product. The explicit form of the Moyal product has been used in two places: to prove lemma 2.6 and to derive an expression for the iterated star product (Equation (2.2) in Lemma 2.5).

Let us consider a general quantization for which the star product that has the form

$$C \star D = \sum_{k=0}^{\infty} \frac{1}{k!} \left( \frac{i\hbar}{2} \right)^k \{C, D\}_k. \quad (3.1)$$

Assume  $(C, D) \mapsto \{C, D\}_k$  is a bidifferential operator of total order  $m_k$  and  $m_0 = 0$ . As long as the sequence  $\{m_k/k \mid k = 1, 2, 3, \dots\}$  is bounded, then Lemma 2.6 is satisfied. Hence, for those star products, we only need to obtain an analogue to Lemma 2.5, that is, an expression for the iterated star product  $C_1 \star \dots \star C_n$  in terms of diagrams. This can often be done by induction if we start by writing the star product of two symbols as a series in terms of diagrams.

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For instance, we can consider *standard order quantization*, which is given by the equation

$$A(x, p) = u_{-p}(x) \widehat{A}[u_p](x),$$

where  $u_p(x) = e^{ip \cdot x/\hbar}$ . From here, the star product has the form (3.1) with  $\{C, D\}_k := \partial_{p_j}^k C \partial_{x^j}^k D$ . Lemma 2.6 still holds and, if we change the meaning of “ $\longrightarrow$ ”, Lemma 2.5 is also true. The simplest way is to use the same definitions we gave in §1.1.4 and §2.1 to construct a polynomial  $\lambda_\Gamma(A)$  from a labeled graph  $\Gamma$ , but using the (non-Poisson) tensor

$$(J^{\mu\nu}) = \begin{pmatrix} 0 & 0 \\ I_N & 0 \end{pmatrix}.$$

With that convention, (2.6) is still valid (except that the notation means something else now!). However, it is no longer true that  $C \longrightarrow D = - (C \longleftarrow D)$ . As a consequence, the versions with unlabeled or connected graphs are messier (although they still exist).

### 3.1.1 Deformation quantization

We could try to ask our main question (what is the symbol of  $f(\widehat{A})$  in terms of  $A$  and  $f$ ?) for a deformation quantization. But first we will need to rephrase it or it will not make sense. As was explained in §1.1.2, a deformation quantization is different from a quantization as we have defined it here. Let us recall:

- A quantization is a symbol correspondence

$$A[[\hbar]] \in \mathcal{C}^\infty(T^*\mathbb{R}^N) \mapsto \widehat{A} \in \text{Op}(L^2(\mathbb{R}^N))[[\hbar]],$$

---

from which we define a star product in  $\mathcal{C}^\infty(T^*\mathbb{R}^N)[[\hbar]]$  by requiring that the map is an algebra homomorphism, i.e.  $\widehat{C \star D} = \widehat{C} \widehat{D}$ .

- A deformation quantization, on the other hand, consists of defining the star product directly in  $\mathcal{C}^\infty(T^*\mathbb{R}^N)[[\hbar]]$  as an associative operation on the set of smooth functions on a Poisson manifold that satisfies certain properties, without any reference whatsoever to operators.

Of course, the problem as stated in the introduction (✖) does not make sense for a deformation quantization that does not come from a correspondence between symbols and operators, as we cannot talk about the symbol of an operator to begin with. However, in certain cases, we can still make sense of the problem in a different way.

One such case is that of star exponentials. (This is explained in more detail in §4.2). Given a symbol  $A \in \mathcal{C}^\infty(T^*\mathbb{R}^N)$ , we can define its *star exponential*  $e_\star^{tA}$  as a smooth family of symbols

$$t \in \mathbb{R} \mapsto e_\star^{tA} \in \mathcal{C}^\infty(T^*\mathbb{R})$$

satisfying the differential equation

$$\begin{aligned} \frac{d}{dt} e_\star^{tA} &= A \star e_\star^{tA}, \\ e_\star^{tA}|_{t=0} &= 1. \end{aligned}$$

Clearly, if the star product comes from a symbol correspondence, then  $e_\star^{tA}$  is the symbol of the operator  $e^{t\widehat{A}}$ , and we can use our formula for the symbol of a function of an operator to calculate the star exponential of  $A$ . However, even if the star product does not come from a symbol correspondence, we can ask how to write  $e_\star^{tA}$  in terms of  $A$ .

---

Once we have calculated the star exponential of  $A$ , we can proceed to arbitrary functions. Let  $\mathcal{F}[f]$  denote the Fourier transform of a function  $f$ , so that

$$f(y) = \int \mathcal{F}[f](t)e^{itx}dt.$$

We define the *star*  $f$  of  $A$  by

$$f_{\star}(A) = \int \mathcal{F}[f](A)e_{\star}^{itA}dt.$$

Again, if the star product comes from a symbol correspondence, then  $\widehat{f_{\star}(A)} = f(\widehat{A})$ . Otherwise, we have extended our original problem  $\blackboxtimes$  to deformation quantizations. And either way we can use the results on this thesis. Notice how the definition of  $f_{\star}(A)$  uses the same idea as the symbol correspondence in Weyl quantization (see 1.1.3).

**Note:** Since we are considering deformation quantization, it is natural to wonder whether we can apply our results in the context of Kontsevich's quantization. In [16], Kontsevich gave a star product that quantizes any Poisson structure on  $\mathbb{R}^N$ . His expression is already a power series in  $\hbar$  whose terms are labeled by a family of diagrams. We can use it to obtain an equivalent of Lemma 2.5 and we can derive, again, the counterparts of Equations (2.6), (2.10) and (2.14). In fact, our set of labeled graphs is a subset of Kontsevich's set of labeled graphs. It is to be noted, though, that working with Kontsevich's star product goes against our original intention. We wanted to write a formula for the symbol of a function of an operator that could be explicitly and easily calculated at any order in  $\hbar$  for any given example. Kontsevich's star product includes a weight  $\omega_{\Gamma}$  associated to every diagram  $\Gamma$  which is, in practice, hard to calculate. (See [15] and [23])

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for some results.) So there is no hope of writing down explicit expressions like those in Appendix D if we use Kontsevich's product.

### 3.2 Functions of several variables

Let  $\widehat{A}_1, \dots, \widehat{A}_n$  be  $n$  commuting operators in  $L^2(\mathbb{R}^N)$  with symbols  $A_1, \dots, A_n$ . Let  $F : \mathbb{R}^n \rightarrow \mathbb{R}$  be a smooth function. We consider the operator  $\widehat{B} = F(\widehat{A}) := F(\widehat{A}_1, \dots, \widehat{A}_n)$  with symbol  $B$ . Can we extend our results to calculate  $B$  in terms of  $A_1, \dots, A_n$  and  $F$ ? The answer is yes. We are still using Weyl quantization and the Moyal product, but we now need a spectral theorem for functions of several variables. Fortunately, such theorems exist and behave equally well. See [1] and the references therein.

Hence, we only need to repeat our calculations, starting from §2.2.2, but with a function of several variables. We obtain a version with labeled graphs (the counterpart of (2.6)):

$$B = \sum_{\substack{\text{reduced labeled} \\ \text{graphs } \Gamma}} \frac{1}{E_\Gamma!} \left( \frac{i\hbar}{2} \right)^{E_\Gamma} \frac{\partial_{i_1} \cdots \partial_{i_{V_\Gamma}} F(A)}{V_\Gamma!} \lambda_\Gamma(A_{i_1}, \dots, A_{i_{V_\Gamma}}),$$

a version with (unlabeled) graphs (the counterpart of (2.10)):

$$B = \sum_{\substack{\text{reduced} \\ \text{graphs } [\Gamma]}} \left( \frac{i\hbar}{2} \right)^{E_\Gamma} \frac{c_\Gamma}{S_\Gamma} \frac{\partial_{i_1} \cdots \partial_{i_{V_\Gamma}} F(A)}{V_\Gamma!} \lambda_\Gamma(A_{i_1}, \dots, A_{i_{V_\Gamma}}), \quad (3.2)$$

and a version with connected graphs (the counterpart of (2.14)):

$$B = \left[ \exp \sum_{\substack{\text{connected, reduced,} \\ \text{non-empty graphs } [\Gamma]}} \left( \frac{i\hbar}{2} \right)^{E_\Gamma} \frac{c_\Gamma}{S_\Gamma} \lambda_\Gamma(A_{i_1}, \dots, A_{i_{V_\Gamma}}) \frac{D_{i_1} \cdots D_{i_{V_\Gamma}}}{V_\Gamma!} \right] F(A),$$

---

where  $D_j F(y) := \frac{\partial F}{\partial y_j}(y)$ . In all the previous equations sum over repeated indices is understood.

For instance the first few terms of (2.10) are

$$B = f(A) - \frac{\hbar^2}{4} \left[ \frac{1}{2} A \Longrightarrow A \frac{f''(A)}{2!} + A \rightarrow A \leftarrow A \frac{f'''(A)}{3!} \right] + O(\hbar^4),$$

and the first few terms of (3.2) are

$$\begin{aligned} B &= F(A) \\ &- \frac{\hbar^2}{4} \left[ \frac{1}{2} A_i \Longrightarrow A_j \frac{\partial_i \partial_j F(A)}{2!} + A_i \rightarrow A_j \leftarrow A_k \frac{\partial_i \partial_j \partial_k F(A)}{3!} \right] \\ &+ O(\hbar^4). \end{aligned}$$

## Chapter 4

# Applications

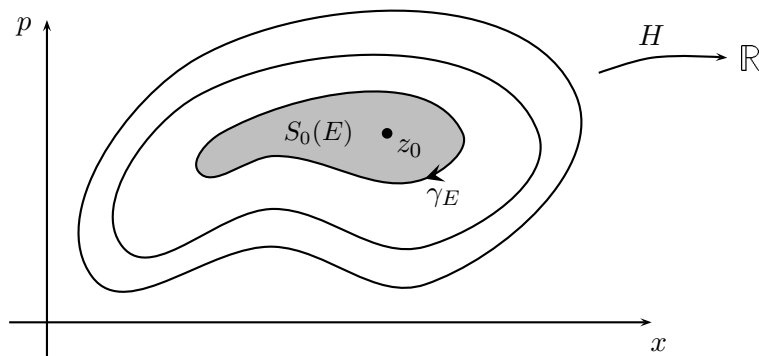
### 4.1 Bohr–Sommerfeld quantization rules

We explain in this section the application that engendered our original interest in this problem.

Let  $\hat{H}$  be an operator with symbol  $H \in C^\infty(T^*\mathbb{R})$ . Bohr–Sommerfeld quantization rules provide a way to asymptotically compute the spectrum of  $\hat{H}$ . Assume for simplicity that  $H$  does not depend on  $\hbar$  (although this requirement can easily be lifted). Assume that  $H$  has a unique minimum  $E_0$  at a point  $z_0 = (x_0, p_0) \in T^*\mathbb{R}$  and that the minimum is regular (i.e, the Hessian is not zero). For any  $E \geq E_0$ , let  $\gamma_E := H^{-1}(E)$  be the level set of  $H$  with value  $E$ . Then, for values of  $E$  close enough to  $E_0$ ,  $\gamma_E$  are simple closed contours around  $z_0$ . In the following,  $E$  close to  $E_0$  will mean *as long as  $\gamma_E$  are simple closed contours around  $z_0$* . See Figure 4.1.

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Figure 4.1: Level sets of  $H$  around a regular minimum.



**Definition 4.1.** For  $E$  close to  $E_0$ , we define the classical action  $S_0(E)$  as the area inside the level set  $\gamma_E$ . Equivalently:

$$S_0(E) = \left| \int_{\gamma_E} p \, dx \right|$$

Then, classical Bohr–Sommerfeld rules say that for values of  $E$  close to  $E_0$ , as a first approximation

$$E \text{ is an eigenvalue of } \hat{H} \iff S_0(E) = 2\pi n\hbar \text{ for some } n \in \mathbb{N}. \quad (4.1)$$

Of course, it remains to describe what “as a first approximation” means. We offer two interpretations.

In §4.1.1 we will describe what we call the *implicit approach*: the classical action is seen as the zeroth order term in  $\hbar$  of the *semiclassical action*  $S(E)$ . Then exact Bohr–Sommerfeld quantization rules are obtained from (4.1) when we replace  $S_0(E)$  with  $S(E)$ . Here we follow [2, 7, 28], although their method is not complete without an algorithm to obtain the symbol of a function of an operator.

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In §4.1.2 we will describe the *explicit approach*: we write  $\widehat{H}$  as a function of an operator whose eigenvalues we know, and read the spectrum from it. Again, (4.1) appears naturally as a low order approximation in  $\hbar$ , and again we require (0.1). We took this approach in [5]. It has various advantages over the previous one: it generalizes to various dimensions, and it allows us to compute both the eigenvalues and the eigenfunctions of  $\widehat{H}$ .

#### 4.1.1 The implicit approach

In [7] Colin de Verdière gives an algorithm which computes the Bohr–Sommerfeld quantization rules to all orders in  $\hbar$  in the one dimensional case  $N = 1$ . His method is inspired by Voros [28] and a similar method previously used by Argyres [2].

**Proposition 4.2.** *Semiclassical Bohr–Sommerfeld Rules.*

*Given the operator  $\widehat{H}$ , there exists a map*

$$S: \mathbb{R} \mapsto S[[\hbar]], \quad S(E) := \sum_{j=0}^{\infty} \hbar^j S_j(E), \quad (4.2)$$

*called the semiclassical action whose lowest order term in  $\hbar$  is the classical action, such that, under certain extra assumptions on the symbol  $H$  (see [7]),*

$$E \text{ is an eigenvalue of } \widehat{H} \iff S(E) = 2\pi n\hbar \text{ for some } n \in \mathbb{N}. \quad (4.3)$$

This should be understood in the following way. Assume we know the form of  $S(E)$  for the operator  $\widehat{H}$  (i.e, we know the semiclassical action to all orders in  $\hbar$ ). Assume also that the eigenvalues  $E$  of  $\widehat{H}$  depend smoothly on  $\hbar$ . Then this method

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allows us to obtain the McLaurin expansion of  $E$  as a power series in  $\hbar$ . First, write formally  $E = \sum \hbar^k E_k$ , then substitute it together with (4.2) into (4.3) to obtain recursive equations for each  $E_k$ . Since (4.3) is an *implicit* equation for  $E$ , we call this the implicit approach.

It remains to calculate the semiclassical action  $S(E)$ . We already gave the value of  $S_0(E)$ . It is also known that  $S_1(E) = \pi$ .

The main result in [7] is the following:

**Theorem 4.3.** *There exists a universal formula for the symbol of a function of an operator of the form*

$$\widehat{B} = f(\widehat{A}),$$

$$B = f(A) + \sum_{j=1}^{\infty} \hbar^j \sum_{l=2}^{L(j)} P_{j,l}(A) \frac{f^{(l-1)}(H)}{(l-1)!},$$

where  $P_{j,l}(A)$  are certain universal polynomials on the derivatives of the symbol  $A$ . From them, we can write the value of the semiclassical action:

$$S_j(E) = \sum_{l=2}^{L(j)} \frac{(-1)^{l-1}}{(l-1)!} \left( \frac{d}{dE} \right)^{l-2} \int_{\gamma_E} P_{j,l}(H(x(t), p(t))) dt,$$

where  $t$  is the parametrization of  $\gamma_E$  by the time evolution

$$dx = H_p dt, \quad dp = -H_x dt.$$

It is to be noted that [7] proves the existence of these universal polynomials  $P_{j,l}$  but does not give their explicit form. Providing them would be equivalent to solving the main problem in this thesis  $\blackstar$  (i.e., deriving (0.1)). Indeed, the algorithm suggested by

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[7] (which we explain in Appendix B) allows us to calculate the terms up to order  $\hbar^2$ , but after that becomes intractable. Hence, without an explicit formula for the symbol of a function of an operator, [7]’s derivation of Bohr–Sommerfeld rules at all orders in  $\hbar$  cannot be used to calculate the eigenvalues of any given operator explicitly.<sup>1</sup>

However, we now have enough tools to explicitly calculate Bohr–Sommerfeld rules to higher orders in  $\hbar$ . Looking back at our result (0.1), we see that  $L_j = 3j/2 + 1$  and the polynomials  $P_{j,l}$  can actually be defined in terms of graphs:

$$P_{j,l}(H) = \sum_{\substack{\text{reduced graphs } \Gamma \\ \text{with } l-1 \text{ vertices} \\ \text{and } j \text{ edges}}} \left(\frac{i}{2}\right)^j \frac{c_\Gamma}{S_\Gamma} \lambda_\Gamma(H),$$

which gives us the following equation for the eigenvalues  $E$  of  $\widehat{H}$ :

$$2\pi(n-1/2)\hbar = S_0(E) + \sum_{\substack{\text{reduced graphs } \Gamma \\ \text{with } E_\Gamma > 0}} \left(\frac{i\hbar}{2}\right)^{E_\Gamma} \frac{(-1)^{V_\Gamma}}{V_\Gamma!} \left(\frac{d}{dE}\right)^{V_\Gamma-1} \frac{c_\Gamma}{S_\Gamma} \int_{\gamma_E} \lambda_\Gamma(H) dt. \quad (4.4)$$

$S_j(E) = 0$  for  $j > 1$  and odd.  $S_2(E)$  is given by the contribution of two graphs, and  $S_4(E)$  is given by the contribution of 15 graphs (see Appendix 2.2). However, there is a trick using Stokes’ theorem that allows us to express the contribution of certain graphs in this expression in terms of others. (This trick is used in [5] and in [7] for  $S_2$ , although without the diagrammatic notation). As a consequence,  $S_2(E)$  can be written in terms of one graph and  $S_4(E)$  can be written in terms of five graphs (those where every vertex has at least two edges). We show the result at order  $\hbar^4$  in (4.5) below.

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<sup>1</sup>Argyres [2] method to calculate the semiclassical action is somewhat different. His algorithm does not require a formula for the symbol of a function of an operator, but just for the symbol of the exponential of an operator. On the other hand, his method is quite less rigorous mathematically.

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Notice how all the integrands in the previous expressions are long polynomials in the derivatives of  $H$ , which would be hard to obtain without the diagrammatic notation. Given a concrete hamiltonian  $H$  we could easily program a computer to write all the terms in (4.4) for that specific operator at higher orders in  $\hbar$ .

$$\begin{aligned}
2\pi(n-1/2)\hbar &= S_0(E) \\
&- \frac{\hbar^2}{4} \left[ \frac{1}{2! \cdot 6} \frac{d}{dE} \int_{\gamma_E} (H \Longrightarrow H) dt \right] \\
&+ \frac{\hbar^4}{16} \left[ \frac{1}{2! \cdot 120} \frac{d}{dE} \int_{\gamma_E} (H \Longtriplearrow H) dt + \frac{1}{4! \cdot 12} \left( \frac{d}{dE} \right)^3 \int_{\gamma_E} (H \Longrightarrow H)^2 dt \right. \\
&\quad - \frac{1}{3! \cdot 15} \left( \frac{d}{dE} \right)^2 \int_{\gamma_E} \begin{array}{c} H \Longrightarrow H \\ \searrow \quad \downarrow \\ \quad \quad H \end{array} dt + \frac{1}{4! \cdot 15} \left( \frac{d}{dE} \right)^3 \int_{\gamma_E} \begin{array}{ccc} H & \longrightarrow & H \\ \uparrow & & \downarrow \\ H & \longleftarrow & H \end{array} dt \\
&\quad \left. - \frac{1}{3! \cdot 12} \left( \frac{d}{dE} \right)^2 \int_{\gamma_E} (H \Longrightarrow H \Longrightarrow H) dt \right] \\
&+ O(\hbar^6)
\end{aligned} \tag{4.5}$$

For the case of a hamiltonian of the form “kinetic plus potential energy”  $H(x, p) = p^2/2m + V(x)$  the contribution of many graphs vanishes, and (4.5) becomes:

$$\begin{aligned}
2\pi(n-1/2)\hbar &= S_0(E) - \frac{\hbar^2}{m} \frac{1}{24} \frac{d}{dE} \int_{\gamma_E} V''(x) dt \\
&+ \frac{\hbar^4}{m^2} \frac{1}{2^7 3^2} \left[ \frac{7}{5} \left( \frac{d}{dE} \right)^3 \int_{\gamma_E} [V''(x)]^2 dt - \left( \frac{d}{dE} \right)^2 \int_{\gamma_E} V^{(4)}(x) dt \right] + O\left(\frac{\hbar^6}{m^3}\right)
\end{aligned}$$

#### 4.1.2 The explicit approach

In [5] we took an approach to Bohr–Sommerfeld rules that uses Weyl quantization more heavily. The basic idea is as follows.

Let  $\widehat{H}$  be an operator in  $L^2(\mathbb{R}^N)$  whose eigenvalues we want to calculate. There

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are very few operators whose eigenvalues we have already calculated exactly. The most important one is probably the hamiltonian of the harmonic oscillator:

$$\widehat{I} = \frac{1}{2}(\widehat{x}^2 + \widehat{p}^2),$$

whose eigenvalues are  $\{(n + 1/2)\hbar \mid n \in \mathbb{N}\}$ . If we could write  $\widehat{H}$  as a function of  $\widehat{I}$ , then we could easily get its spectrum. This is not possible in general. A bit more generally, we can try to find a unitary transformation  $\widehat{U}$  and a smooth function  $f$  such that

$$\widehat{M} := \widehat{U}\widehat{H}\widehat{U}^\dagger = f(\widehat{I}).$$

Since conjugating by a unitary transformation does not change the eigenvalues, this will mean that the eigenvalues of  $\widehat{H}$  are  $\{f((n + 1/2)\hbar) \mid n \in \mathbb{N}\}$ . By way of contrast with (4.3), we call this the *explicit approach*.

The method in [5] consists of manipulating the Weyl symbols to find a unitary transformation  $\widehat{U}$  such that the symbol of the conjugated operator is a function of the symbol of the harmonic oscillator hamiltonian:

$$M = g(I).$$

Then, we need to be able to recover  $f$  from  $g$ , which is exactly our original problem  $\spadesuit$ .

The process is done in consecutive steps, one order of  $\hbar$  at a time. So, we find a function  $g_k$  such that  $M = g_k(I) + O(\hbar^k)$ , then we use (0.1) to get  $f_k$  such that  $\widehat{M} = f_k(\widehat{I}) + O(\hbar^k)$ , and finally the eigenvalues of  $\widehat{H}$  are  $\{f_k((n + 1/2)\hbar + O(\hbar^k)) \mid n \in \mathbb{N}\}$ .

There are various advantages to this approach. Since we know both the eigenvalues and the eigenfunctions of  $\widehat{I}$ , and we obtain an explicit form for the unitary transfor-

---

mation  $\widehat{U}$ , we eventually get both the eigenvalues and the eigenfunctions of  $\widehat{H}$  as formal power series in  $\hbar$ . In addition, and most notably, the method generalizes to various dimensions (see [4]).

Finally, we have to mention that [5] introduces the diagrammatic notation that has been so fundamental in this thesis.

## 4.2 Star-exponential of polynomial forms

Omori et al studied in [22] *evolution equations* and *star exponentials*. This problem is related to finding the symbol of a function of an operator, although their statement of the problem looks different. First, their definition:

**Definition 4.4.** *Let  $A \in C^\infty(T^*\mathbb{R})$  be a symbol. The star exponential  $e_\star^{tA}$  of  $A$  is a smooth family of symbols*

$$t \in \mathbb{R} \mapsto e_\star^{tA} \in C^\infty(T^*\mathbb{R}),$$

*satisfying the differential equation*

$$\begin{aligned} \frac{d}{dt} e_\star^{tA} &= A \star e_\star^{tA}, \\ e_\star^{tA}|_{t=0} &= 1. \end{aligned} \tag{4.6}$$

The solution is unique if it exists.

Notice how this definition is written entirely in terms of symbols, without any reference to operators. However, if we let  $A$  be the symbol of an operator  $\widehat{A}$ , then (4.6)

---

becomes:

$$\begin{aligned}\frac{d}{dt} \widehat{e}_\star^{tA} &= \widehat{A} \widehat{e}_\star^{tA}, \\ \widehat{e}_\star^{tA}|_{t=0} &= 1,\end{aligned}$$

and therefore

$$\widehat{e}_\star^{tA} = e^{t\widehat{A}}.$$

Equivalently

$$B = e_\star^{tA} \iff \widehat{B} = e^{t\widehat{A}}.$$

As a consequence, we can use (0.1) and the equivalent equations to calculate star exponentials. Omori et al [22] consider primarily the star exponential of quadratic symbols. Quadratic symbols simplify our formulas considerably, so they deserve to be treated separately with our approach.

#### 4.2.1 The case of a quadratic symbol

When we restrict to a smaller class of symbols, sometimes the contribution of many graphs vanishes, simplifying our calculations. Quadratic symbols are good examples.

A particular (simple) case of importance consists of taking  $\widehat{A} = \widehat{I}$ , the harmonic oscillator hamiltonian in one dimension. In the standard coordinates  $(z^1, z^2) = (x, p)$  its symbol is  $I = \frac{1}{2}((z^1)^2 + (z^2)^2)$ . This simplifies the calculations because any third derivative vanishes:  $I_{,\mu_1\mu_2\mu_3} = 0$ . The same is true for any quadratic function. Let  $Q_{\mu\nu}$  be a  $2 \times 2$  real symmetric matrix and consider the symbol  $A = \frac{1}{2}z^\mu Q_{\mu\nu} z^\nu$ . Assume that

---

$A$  is the symbol of an operator  $\widehat{A}$ . Then:

$$A_{,\nu} = z^\mu Q_{\mu\nu},$$

$$A_{,\mu\nu} = Q_{\mu\nu},$$

and any third derivative vanishes. As a consequence, we need to consider only graphs where every vertex meets at most two edges. After Lemma C.1 in Appendix B, we only need to consider graphs with an even number of edges. If we also ask them to be connected, reduced and non-empty, there are only two families of such graphs:

$$\begin{array}{l} \Delta_k \quad := \quad \bullet \rightarrow \bullet \rightarrow \dots \rightarrow \bullet \quad (2k \text{ edges}) \quad k \geq 1 \\ \Lambda_k \quad := \quad \bullet \rightarrow \bullet \rightarrow \dots \rightarrow \bullet \quad (2k \text{ edges}) \quad k \geq 1 \\ \qquad \qquad \qquad \uparrow \qquad \qquad \qquad \qquad \qquad \downarrow \\ \qquad \qquad \qquad \bullet \leftarrow \bullet \leftarrow \dots \leftarrow \bullet \end{array}$$

In words,  $\Delta_k$  consists of  $2k + 1$  vertices and  $2k$  edges joined forming a line. Its symmetry group has order 2.  $\Lambda_k$  consists of  $2k$  vertices and  $2k$  edges joined forming a simple cycle. Its symmetry group has order  $4k$ .

The corresponding polynomials in the derivatives of  $A$  can be calculated:

$$\begin{aligned} \lambda_{\Delta_k} &= A_{,\mu_1} J^{\mu_1 \nu_1} A_{,\nu_1 \mu_2} J^{\mu_2 \nu_2} \dots J^{\mu_{2k} \nu_{2k}} A_{,\nu_{2k}} \\ &= z^{\mu_1} ((QJ)^{2k} Q)_{\mu_1 \nu_{2k}} z^{\mu_{2k}} \\ \lambda_{\Lambda_k} &= A_{,\nu_{2k} \mu_1} J^{\mu_1 \nu_1} A_{,\nu_1 \mu_2} J^{\mu_2 \nu_2} \dots J^{\mu_{2k} \nu_{2k}} = \\ &= \text{trace} ((QJ)^{2k}) \end{aligned}$$

Since  $Q$  is symmetric and  $J$  is skew-symmetric, their product  $QJ$  is traceless. Hence the characteristic polynomial of  $QJ$  is  $x^2 + \det(QJ)$ , and  $(QJ)^2 = -\det(QJ) \text{id}$ . Write

---

$\omega^2 := \det(QJ) = \det(Q)$ . Then:

$$\lambda_{\Delta_k} = (-1)^k \omega^{2k} z^\mu Q_{\mu\nu} z^\nu = (-1)^k \omega^{2k} 2A$$

$$\lambda_{\Lambda_k} = (-1)^k \omega^{2k} \text{trace}(\text{id}) = (-1)^k \omega^{2k} 2$$

As for the coefficients  $c_{\Delta_k}$  and  $c_{\Lambda_k}$ , Fact 3 in Appendix C gives us the relation  $c_{\Lambda_k} = -2k c_{\Delta_{k-1}}$ . Let us call  $c_k := (-1)^k c_{\Delta_k}$ .

We now plug all this values in (2.14) to obtain, for a general function  $f$  and a quadratic symbol  $A$ :

$$B = \left( \exp \left[ A \sum_{k=0}^{\infty} \left( \frac{i\hbar}{2} \omega \right)^{2k} c_{k+1} \frac{D^{2k+1}}{(2k+1)!} + \sum_{k=0}^{\infty} \left( \frac{i\hbar}{2} \omega \right)^{2k} c_k \frac{D^{2k}}{(2k)!} \right] \right) f(A) \quad (4.7)$$

We are left with a combinatorics problem: calculate the sequence  $\{c_k\}$ . Fact 3 in Appendix C gives us a recurrence formula:

$$c_k = \sum_{j=0}^{k-1} \binom{2k}{2j+1} c_j c_{k-j-1}, \quad (4.8)$$

$$c_0 = 1.$$

The first few terms are 1, 2, 16, 272, 7936 ... This sequence is called the *Zag numbers* [27].

**Claim.** The Zag numbers appear in the McLaurin expansion of the tangent:

$$\tan x = \sum_{k=0}^{\infty} \frac{c_k}{(2k+1)!} x^{2k+1} \quad (4.9)$$

*Proof.* To prove this, notice that  $\tan x$  is the only odd solution to the differential equation

$$y' = 1 + y^2. \quad (4.10)$$

---

Write a generic solution of the form  $y = f(x) = \sum_{k=0}^{\infty} \frac{\alpha_k}{(2k+1)!} x^{2k+1}$  and substitute it into (4.10). Equating coefficients, we conclude that the sequence  $\alpha_k$  satisfies the same recurrence relation as the sequence  $c_k$  (Equation (4.8)). Hence  $\alpha_k = c_k$ .  $\square$

The Zag numbers can be written in terms of the Bernoulli numbers  $B_n$ :

$$|c_k| = \frac{2^{2k}}{2^{2k} - 1} \frac{|B_{2k}|}{2k}$$

When we use equation (4.9) in (4.7) we obtain a nice, compact expression:

$$\begin{aligned} \widehat{B} &= f(\widehat{A}) \\ B &= \sec \frac{i\hbar\omega D}{2} \exp \left[ \frac{2A}{i\hbar\omega} \tan \frac{i\hbar\omega D}{2} - AD \right] f(A) \end{aligned} \tag{4.11}$$

Remember that  $D$  is the derivative operator that applies to  $f$ .

## 4.2.2 Back to star exponentials

Now we are ready to calculate the star exponential of a quadratic symbol. If we use the function  $f(y) = e^{\varepsilon y}$  in (4.11), then  $D$  acts simply as multiplication by  $\varepsilon$ . In particular, when we consider the time evolution operator:

$$\begin{aligned} \widehat{B} &= e^{-it\widehat{A}/\hbar}, \\ B &= \sec \frac{t\omega}{2} \exp \left[ \frac{2A}{i\hbar\omega} \tan \frac{t\omega}{2}, \right] \end{aligned} \tag{4.12}$$

or equivalently:

$$e_{\star}^{tA} = \operatorname{sech} \frac{t\omega}{2} \exp \left[ \frac{2A}{\hbar\omega} \tanh \frac{t\omega}{2} \right].$$

Equation (4.12) is derived in [22] in a different manner, and appears first in [3] for the case  $\widehat{A} = \widehat{I}$ . A better-known, equivalent expression is the *kernel* of the time evolution

---

operator of the harmonic oscillator, instead of (4.12), the *symbol* of the time evolution operator of the harmonic oscillator. Such kernel is known as the *Mehler kernel* and can be obtained from (4.12) by means of a Fourier transform (see, for instance, [9]).

In a similar manner we can reproduce [22]’s results for star exponentials for other star products by using other quantizations (see §3.1). We believe that the same methods will allow us to calculate star exponentials of higher order polynomials.

### 4.3 Other applications to quantum mechanics.

There are various other applications of (0.1) that appear in quantum mechanics when we are trying to do a calculation with operators using Weyl symbol correspondence.

As an example, let us mention the calculation of determinants of pseudodifferential operators. Such determinants naturally arise in quantum field theory at the one loop level, or in Yang–Mills theory (see, for instance, [19]). If  $M$  is a finite–dimensional matrix, then  $\det e^M = e^{\text{tr } M}$ , where  $\text{tr}$  is the trace. Equivalently

$$\det M = e^{\text{tr}(\log M)}.$$

We use this equation to define the determinant of a pseudodifferential operator  $\widehat{A}$ :<sup>2</sup>

$$\det \widehat{A} := e^{\text{tr}(\log \widehat{A})}. \tag{4.13}$$

Now, Weyl quantization has the property:

$$\text{tr } \widehat{B} = \int_{T^*\mathbb{R}^N} d^N x d^N p B(x, p). \tag{4.14}$$

---

<sup>2</sup>For (4.13) to make sense, we need the operator  $\widehat{A}$  to be of the form “identity + trace class”. Needless to say, this is often not the case in QFT, so we need a “regularization” to redefine its trace.

---

Let us say we want to calculate  $\det \hat{A}$  for a certain operator  $\hat{A}$  to order  $k$  in  $\hbar$ . Let  $\hat{B} := \log \hat{A}$ . Using (0.1), we can write  $B$  in terms of  $A$  to order  $\hbar^k$ . This gives us  $\text{tr} \hat{B}$  using (4.14), and  $\det \hat{A}$  using (4.13).

Equation (4.14) gives us more applications. In *quantum statistical mechanics* (see, for instance, [20]), the partition function corresponding to a hamiltonian  $\hat{H}$  is defined as the trace of the *Boltzmann operator* or *density matrix*:

$$Z(\beta) := \text{tr} e^{-\beta \hat{H}},$$

which again can be written as a power series in  $\hbar$  from the symbol of  $e^{-\beta \hat{H}}$ . Hence we encounter here the symbol of an exponential of an operator. This application was suggested to us by Robert Littlejohn.

Finally, Krivoruchenko and Faessler have applied (0.1) to scattering theory in [18].

## Appendix A

# A lemma for calculations with graphs

The diagrammatic notation introduced in §1.1.4 and §2.1 (originally due to [5]) makes equations and derivations easier to write.

For instance, the skew-symmetry of the Poisson bracket becomes

$$C \longrightarrow D = (-1) C \longleftarrow D. \tag{A.1}$$

As a second example, the identity

$$(CD) \rightarrow E = C(D \rightarrow E) + (C \rightarrow E)D,$$

i.e., that the Poisson bracket is a derivation on each argument (Leibniz rule or product rule), is written as:

$$\{CD, E\} = C\{D, E\} + \{C, E\}D.$$

---

An application of the product rule for ordinary derivatives is

$$\begin{aligned}
(C \rightarrow D) \rightarrow E &= C \rightarrow D \rightarrow E + E \leftarrow C \rightarrow D \\
(C_{,\mu} J^{\mu\nu} D_{,\nu})_{,\alpha} J^{\alpha\beta} E_{,\beta} &= C_{,\mu} J^{\mu\nu} D_{,\nu\alpha} J^{\alpha\beta} E_{,\beta} + C_{,\mu\alpha} J^{\mu\nu} D_{,\nu} J^{\alpha\beta} E_{,\beta}
\end{aligned} \tag{A.2}$$

Notice that (A.2) cannot be written just with Poisson brackets  $\{ , \}$ . If we combine

(A.2) and (A.1) we get a proof of the Jacobi identity:

$$(C \rightarrow D) \rightarrow E + (D \rightarrow E) \rightarrow C + (E \rightarrow C) \rightarrow D = 0$$

The following lemma is a generalization of (A.2) which we use in our derivation in §2.2.1.

**Lemma A.1.** *Let  $\Gamma$  be a labeled graph with  $V$  vertices and  $E$  edges. Let  $D, C_1, \dots, C_V$  be symbols. Then*

$$\lambda_{\Gamma}(C_1, \dots, C_V) \overrightarrow{[k]} D = \sum_{\Gamma'} \lambda_{\Gamma'}(C_1, \dots, C_V, D),$$

where the sum is taken over all labeled graphs  $\Gamma'$  with  $V' = V + 1$  vertices and  $E' = E + k$  edges, which are constructed by putting together

- the labeled graph  $\Gamma$  (conserving its labels),
- an extra vertex labeled by  $V + 1$ ,
- $k$  extra arrows (labeled by  $E + 1, \dots, E + k$ ) starting from the vertices of  $\Gamma$  and ending at the vertex  $V + 1$ .

*Proof.* Write down the definition of both sides in terms of  $J^{\mu\nu}$  and check that they are equal. □

---

For instance:

$$\begin{aligned} & (C \xrightarrow{1} D) \xrightarrow{\quad} E \\ &= C \xrightarrow{1} D \xrightarrow{3} E \quad + \quad C \xrightarrow{1} D \xrightarrow{3} E \\ & \quad + C \xrightarrow{1} D \xrightarrow{3} E \quad + \quad C \xrightarrow{1} D \xrightarrow{2} E \\ &= C \xrightarrow{\quad} D \xrightarrow{\quad} E \quad + \quad C \xrightarrow{\quad} D \xrightarrow{\quad} E \\ & \quad + 2 C \xrightarrow{\quad} D \xrightarrow{\quad} E \end{aligned}$$

## Appendix B

# On Voros and Colin de Verdière's approach

As we mentioned in the introduction and in §4.1, the existence of a universal formula like (0.1) was used by Voros [28] and Colin de Verdière [7] as part of their computation of Bohr–Sommerfeld rules at all orders in  $\hbar$ . While they prove the existence of such a formula, they do not give its explicit form. Instead, a method is suggested that potentially would allow us to calculate the symbol of a function of an operator at any given order in  $\hbar$ , but in practice the calculations are too tedious to be done at order higher than  $\hbar^2$ . In this appendix we will first describe their method, and then use the same idea backwards to check our result (2.6).

---

## B.1 The method of the resolvent

Let  $a \in \mathbb{C}$  and define the resolvent operator  $\widehat{R}_a := (a - \widehat{A})^{-1}$  with symbol  $R_a$ . Then we fix a functional calculus that allows us to write a function of an operator  $f(\widehat{A})$  in terms of the resolvent  $\widehat{R}_a$ . In this way, we can write the symbol of  $f(\widehat{A})$  in terms of the symbol of the resolvent  $R_a$ .

- Colin de Verdière [7] uses Helffer–Sjöstrand’s formula [13]:

$$\widehat{B} = f(\widehat{A}) = -\frac{1}{\pi} \int_{\mathbb{C}} \widehat{R}_z \partial_{\bar{z}} \tilde{f}(z) dx dy.$$

Here  $z = x + iy$ ,  $\tilde{f}$  is an almost analytic extension of  $f$ , and  $\partial_{\bar{z}} = \partial_x + i\partial_y$ . This allows us to write

$$B = -\frac{1}{\pi} \int_{\mathbb{C}} R_z \partial_{\bar{z}} \tilde{f}(z) dx dy. \tag{B.1}$$

- Voros [28] uses Cauchy’s integral formula (see, for instance, [26]):

$$\begin{aligned} \widehat{B} = f(\widehat{A}) &= \int_{\gamma} \frac{da}{2\pi i} f(a) \widehat{R}_a, \\ B &= \int_{\gamma} \frac{da}{2\pi i} f(a) R_a, \end{aligned}$$

for an holomorphic function  $f$ , where  $\gamma$  is a path around the spectrum of  $\widehat{A}$

Either way, finding the symbol of  $f(\widehat{A})$  reduces to finding the symbol of  $\widehat{R}_a$ . In order to do so, we write formally

$$R_a = \sum_{k=0}^{\infty} \left( \frac{i\hbar}{2} \right)^k R_{a(k)}. \tag{B.2}$$

---

We know that  $\widehat{R}_a(a - \widehat{A}) = 1$ . Quantization translates composition of operators into star product, so that

$$R_a \star (a - A) = (a - A) \star R_a = 1. \quad (\text{B.3})$$

Now we substitute (B.2) into (B.3) and use the explicit form of the Moyal product (1.6) to obtain

$$\begin{aligned} 1 = R_a \star (a - A) &= \left[ \sum_{k=0}^{\infty} \left( \frac{i\hbar}{2} \right)^k R_{a(k)} \right] \star (a - A) \\ &= \sum_{k=0}^{\infty} \sum_{m=0}^{\infty} \left( \frac{i\hbar}{2} \right)^{k+m} \frac{1}{m!} R_{a(k)} \overrightarrow{[:m]} (a - A), \end{aligned}$$

which gives us

$$\begin{aligned} 1 &= R_{a(0)}(a - A) \\ 0 &= \sum_{k+m=n} \frac{1}{m!} R_{a(k)} \overrightarrow{[:m]} (a - A) \quad \text{for } n \geq 1. \end{aligned}$$

This was obtained from  $R_a(a - A) = 1$ . When we do the same for  $(a - A)R_a = 1$  and put it together, we get the following recursive relations

$$\begin{aligned} R_{a(0)} &= \frac{1}{a - A}, \\ R_{a(n)} &= 0 \quad \text{for } n \text{ odd}, \\ R_{a(2n)} &= -\frac{1}{a - A} \sum_{m=1}^n \frac{1}{(2m)!} R_{a(2n-2m)} \overrightarrow{[:m]} (a - A) \quad \text{for } n \geq 1. \end{aligned}$$

Although simple, this method quickly proves intractable. Obtaining an explicit form of  $R_{a(4)}$  is already too complex, and we will not find the pattern that (0.1) shows.

---

## B.2 An alternative derivation of (2.6)

We can also use the idea in the method of the resolvent to prove (2.6) in a different way.

If we already have guessed the form of (2.6) and we want to check it, we first do so for the resolvent.

**Claim.** The function

$$h_a(A) = \sum_{\substack{\text{reduced} \\ \text{labeled} \\ \text{graphs } \Gamma}} \frac{1}{E_\Gamma!} \left(\frac{i\hbar}{2}\right)^{E_\Gamma} \frac{\lambda_\Gamma(A)}{(a-A)^{V+1}} \quad (\text{B.4})$$

satisfies  $h_a(A) \star (a - A) = (a - A) \star h_a(A) = 1$ .

The proof is a long combinatorial exercise on calculations with graphs. Therefore

$h_a(A) = R_a$ .

Second, we substitute (B.4) into any of the functional calculi describe in §B.1 to again obtain (2.6).

# Appendix C

## Calculation of $c_\Gamma$ and $S_\Gamma$

Calculating  $c_\Gamma$  is a combinatorial problem. The definition of  $c_\Gamma$ , Equation (2.8), is enough to calculate it. Alternatively, we can use the following five facts. The first three entirely determine the value of  $c_\Gamma$  for any graph  $\Gamma$ , and the five together allow us to obtain quick, recursive rules. An example on how to use them will follow.

1.  $c_\bullet = 1$
2. If  $\Gamma_i \neq \Gamma_j$  for  $i \neq j$ , and  $\Gamma = \Gamma_1 + \dots + \Gamma_n$  is the topological sum, then

$$c_\Gamma = \frac{V_\Gamma!}{V_{\Gamma_1!} \cdots V_{\Gamma_n!}} c_{\Gamma_1} \cdots c_{\Gamma_n}. \quad (\text{C.1})$$

3. If  $p$  is a vertex in  $\Gamma$ , denote by  $\Gamma - p$  the same  $\Gamma$  with the vertex  $p$  and every edge starting or ending at  $p$  erased. For instance:

$$\begin{aligned} \Gamma &= \bullet \longrightarrow p \longrightarrow \bullet \Longrightarrow \bullet, \\ \Gamma - p &= \bullet \qquad \bullet \Longrightarrow \bullet. \end{aligned}$$

---

Then:

$$c_\Gamma = \sum_{\text{vertices } p \text{ in } \Gamma} (-1)^{\# \text{ of arrows starting at } p} c_{\Gamma-p}.$$

*Proof.* Count the possible reorderings of the vertices by choosing first which vertex has label  $V$ . □

4.  $c_\Gamma = 0$  if  $E_\Gamma$  is odd.

This is due to a symmetry property. If we denote by  $\Gamma$  a labeled graph with a numbering of the vertices by  $1, 2, \dots, V$  and by  $i(\Gamma)$  the relabeling of the vertices by the permutation  $\begin{pmatrix} 12 \dots V_\Gamma \\ V_\Gamma \dots 21 \end{pmatrix}$ , then

$$\lambda_{i(\Gamma)} = (-1)^{E_\Gamma} \lambda_\Gamma.$$

And when we sum over reorderings of the vertices:

$$c_\Gamma = (-1)^{E_\Gamma} c_\Gamma.$$

5.  $c_\Gamma$  does not change if we erase two edges with the same endpoints.

For instance

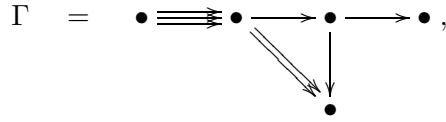
$$c_{1 \rightarrow 2 \rightleftharpoons 3 \rightarrow 4} = c_{1 \rightarrow 2 \quad 3 \rightarrow 4}$$

In particular, putting together Facts 4 and 2 we get:

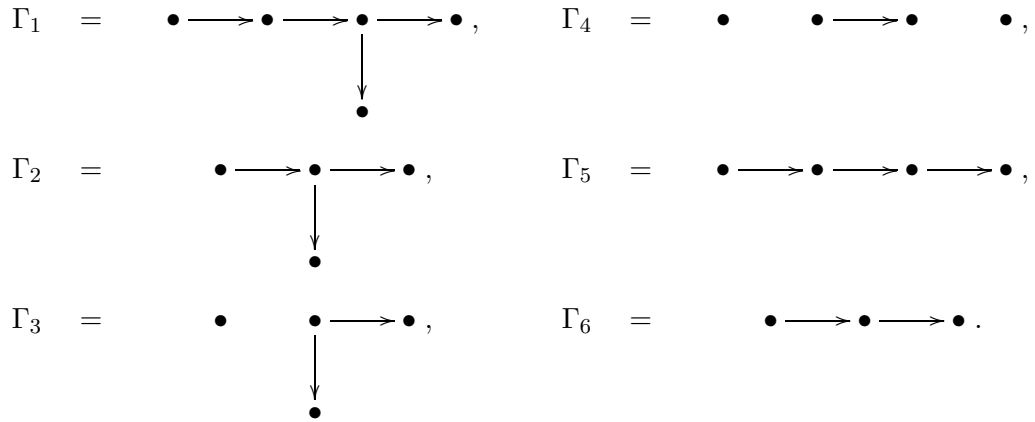
**Lemma C.1.** *If  $\Gamma$  has a connected component with an odd number of edges, then  $c_\Gamma = 0$ .*

---

**Example:** We want to calculate  $c_\Gamma$ , where



Let us consider



$c_\Gamma = c_{\Gamma_1}$  because of Fact 5.

$c_{\Gamma_1} = (-1)^1 c_{\Gamma_2} + (-1)^1 c_{\Gamma_3} + (-1)^2 c_{\Gamma_4} + 2(-1)^0 c_{\Gamma_5}$  because of Fact 3.

$c_{\Gamma_2} = c_{\Gamma_4} = c_{\Gamma_5} = 0$  because of Lemma C.1.

$c_{\Gamma_3} = 4c_\bullet c_{\Gamma_6}$  because of Fact 2.

$c_\bullet = 1$  because of Fact 1.

Continuing with similar calculations we obtain  $c_{\Gamma_6} = -2$ .

Hence  $c_\Gamma = -4 \cdot 1 \cdot (-2) = 8$ .

Figure C.1 shows all the reduced, connected graphs with 2 and 4 edges, and for each of them the value of  $c_\Gamma$  and  $S_\Gamma$ . These results have been independently verified by Krivoruchenko [17] with a MAPLE code.

Figure C.1:  $c_\Gamma$  and  $S_\Gamma$  for reduced, connected graphs  $\Gamma$  with 2 and 4 edges.

$\Gamma$	$E_\Gamma$	$V_\Gamma$	$S_\Gamma$	$c_\Gamma$
	2	2	4	2
	2	3	2	-2
	4	2	48	2
	4	3	6	-2
			8	6
			4	2
	4	4	8	8
			2	0
			4	8
			2	-8
			4	0
	4	5	2	16
			2	-8
			24	-24

## Appendix D

# Symbol of a function of an operator at order 4 in $\hbar$

Using any of the equations derived in §2.2, we write down in Figure D.1 the explicit form of all the terms of the symbol of a function of an operator up to order 4 in  $\hbar$ . The data in Figure C.1 are needed.

Figure D.1: Symbol of a function of an operator at order 4 in  $\hbar$ .

$$\begin{aligned}
 \widehat{B} &= f(\widehat{A}) \\
 B &= f(A) \\
 & - \frac{\hbar^2}{4} \left[ \frac{A \rightleftharpoons A}{2} \frac{f''(A)}{2!} + A \longrightarrow A \longleftarrow A \frac{f'''(A)}{3!} \right] \\
 & + \frac{\hbar^4}{16} \left[ \frac{A \rightleftharpoons A}{24} \frac{f''(A)}{2!} \right. \\
 & \quad + \left( \frac{A \rightleftharpoons A \longleftarrow A}{3} + \frac{1}{2} A \rightleftharpoons A \begin{array}{c} \searrow \\ \downarrow \\ A \end{array} \\
 & \quad + \frac{3}{4} A \rightleftharpoons A \rightleftharpoons A \left. \right) \frac{f'''(A)}{3!} \\
 & \quad + \left( \frac{3}{4} (A \rightleftharpoons A)^2 + \begin{array}{c} A \longrightarrow A \\ \uparrow \qquad \downarrow \\ A \longleftarrow A \end{array} \\
 & \quad + 4 A \rightleftharpoons A \longrightarrow A \longleftarrow A \\
 & \quad + 2 A \rightleftharpoons A \longrightarrow A \begin{array}{c} \downarrow \\ A \end{array} \left. \right) \frac{f^{(4)}(A)}{4!} \\
 & \quad + \left( 8 A \longrightarrow A \longrightarrow A \begin{array}{c} \downarrow \\ A \longleftarrow A \end{array} + A \longrightarrow A \begin{array}{c} \longleftarrow A \\ \uparrow \qquad \swarrow \\ A \qquad A \end{array} \right. \\
 & \quad + 5 (A \rightleftharpoons A) (A \longrightarrow A \longleftarrow A) \\
 & \quad + 4 A \longleftarrow A \longrightarrow A \longrightarrow A \begin{array}{c} \downarrow \\ A \end{array} \left. \right) \frac{f^{(5)}(A)}{5!} \\
 & \quad + 10 (A \longrightarrow A \longleftarrow A)^2 \frac{f^{(6)}(A)}{6!} \left. \right] \\
 & + O(\hbar^6)
 \end{aligned}$$

# Bibliography

- [1] M. Andersson and J. Sjöstrand. Functional calculus for non-commuting operators with real spectra via an iterated Cauchy formula. arXiv:math.SP/0303024, 2003.
- [2] P.N. Argyres. The Bohr–Sommerfeld quantization rule and the Weyl correspondence. *Physics*, 2:131–139, 1965.
- [3] F. Bayen, M. Flato, C. Fronsdal, A. Lichnerowicz, and D. Sternheimer. Deformation theory and quantization I-II. *Ann. Phys.*, 111:61–110, 111–151, 1978.
- [4] M. Cargo, A. Gracia-Saz, and R.G. Littlejohn. Multidimensional quantum normal forms, Moyal star product and torus quantization. arXiv:math-ph/0507032, 2005.
- [5] M. Cargo, A. Gracia-Saz, R.G. Littlejohn, M.W. Reinsch, and P.de M. Rios. Quantum normal forms, Moyal star product and Bohr–Sommerfeld approximation. *J. Phys. A: Math. and Gen.*, 38:1977–2004, 2005. arXiv:math-ph/0409039.
- [6] L. Charles. Berezin–Toeplitz operators, a semi-classical approach. *Commun. Math. Phys.*, 239:1–28, 2003.

- [7] Y. Colin de Verdière. Bohr–Sommerfeld rules to all orders. *Henri Poincaré Acta*, 6:925–936, 2005.
- [8] E.B. Davies. *Spectral theory and differential operators*, volume 42 of *Cambridge studies in advanced mathematics*. Cambridge University Press, 1995.
- [9] I. Davies and A. Truman. Laplace asymptotic expansion of conditional Wiener integrals and generalized Mehler kernel formulas. *Journal of Mathematical Physics*, 11:2059–2070, 1982.
- [10] A. Gracia-Saz. The symbol of a function of a pseudo–differential operator. *Annales de l’Institut Fourier*, 55:2257–2284, 2005. arXiv:math.QA/0411163.
- [11] A. Grigis and J. Sjöstrand. *Microlocal analysis for differential operators*. Lecture Note Series 196. London Mathematical Society, 1994.
- [12] H.J. Groenewold. On the principles of elementary quantum mechanics. *Physica (Amsterdam)*, 12:405–460, 1946.
- [13] B. Helffer and J. Sjöstrand. Équation de Schrödinger avec champ magnétique et équation de Harper. *Springer Lecture Notes in Physics*, 345:118–197, 1989.
- [14] A.C. Hirshfeld and P. Henselder. Deformation quantization in the teaching of quantum mechanics. *Am. J. Physics*, 70:537–547, 2002. arXiv:quant-ph/0208163.
- [15] V. Kathotia. Kontsevich’s universal formula for deformation quantization and

- the Campbell–Baker–Hausdorff formula, I. *Internat. J. Math.*, 11:523–551, 2000. arXiv:math.QA/9811174.
- [16] M. Kontsevich. Deformation quantization of Poisson manifolds I. *Lett Math Phys*, 66:157–216, 2003. arXiv:q-alg/9709040.
- [17] M.I. Krivoruchenko. Private communication, 2006.
- [18] M.I. Krivoruchenko and A. Faessler. Weyl’s symbols of Heisenberg operators of canonical coordinates and momenta as quantum characteristics. arXiv:quant-ph/0604075, 2006.
- [19] J. Loikkanen and C. Paufler. Yang–Mills action from minimally coupled bosons on  $\mathbb{R}^4$  and on the 4D Moyal plane. *J. Math. Phys.*, 46:032301, 2005. arXiv:math-ph/0407039.
- [20] G. Morandi, F. Napoli, and E. Ercolessi. *Statistical mechanics: an intermediate course*. Word Scientific, 2001.
- [21] J.E. Moyal. Quantum mechanics as a statistical theory. *Proc. Cambridge Philos. Soc.*, 45:99–124, 1949.
- [22] H. Omori, Y. Maeda, N. Miyazaki, and A. Yoshioka. Strange phenomena related to ordering problems in quantization. *Journal of Lie theory*, 13:479–508, 2003.
- [23] M. Polyak. Quantization of linear Poisson structures and degrees of maps. *Letters in Mathematical Physics*, 66:15–35, 2003. arXiv:math.GT/0210107.

## Bibliography

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- [24] M.A. Rieffel. Deformation quantization and operator algebras. *Proceedings of symposia in pure mathematics*, 50:411–423, 1990.
- [25] M.A. Rieffel. Quantization and  $C^*$ -algebras. *Contemporary mathematics*, 167:67–97, 1994.
- [26] W. Rudin. *Functional analysis*. International series in pure and applied mathematics. McGraw-Hill, 1991.
- [27] N.J.A. Sloane (editor). The on-line encyclopedia of integer sequences. <http://www.research.att.com/~enjas/sequences/> .
- [28] A. Voros. Asymptotic  $\hbar$ -expansions of stationary quantum states. *Ann. Inst. H. Poincaré Sect. A (N.S.)*, 26:343–403, 1977.
- [29] H. Weyl. Gruppentheorie und Quantenmechanik. *Z. Phys.*, 46:1–46, 1928.