The symbol of a function of an operator

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Abstract

We give an explicit formula for the symbol of a function of an operator. Given an operator \( \hat{A} \) on \( L^2(\mathbb{R}^N) \) with symbol \( A \in C^\infty(T^*\mathbb{R}^N) \) and a smooth function \( f \), we obtain the symbol of \( f(\hat{A}) \) in terms of \( A \). As an application, Bohr–Sommerfeld quantization rules are explicitly calculated at order 4 in \( \hbar \).

1 Introduction.

The goal of this paper is to give a realistically computable formula for the symbol of a function of an operator. Let \( \hat{A} \) be an essentially self-adjoint operator in \( L^2(\mathbb{R}^N) \) with symbol \( A \in C^\infty(T^*\mathbb{R}^N) \). Let \( f : \mathbb{R} \to \mathbb{R} \) be an analytic function. Let \( \hat{B} = f(\hat{A}) \) be an operator with symbol \( B \). We want to write \( B \) in terms of \( A \). We will derive the formula:

\[
B = \sum_{\Gamma} \left( \frac{i\hbar}{2} \right)^E \frac{c_{\Gamma}}{S_{\Gamma}} \lambda_{\Gamma}(A) \frac{f^{(V)}(A)}{V!}
\]

The sum is taken over finite graphs \( \Gamma \) with no isolated vertices. For every such graph \( \Gamma \), \( V \) is the number of vertices and \( E \) is the number of edges. \( \lambda_{\Gamma}(A) \) is a polynomial in the derivatives of \( A \) constructed algorithmically from \( \Gamma \) (see §3). \( S_{\Gamma} \) is the order of the symmetry group of \( \Gamma \). \( c_{\Gamma} \) is a simple invariant of \( \Gamma \) (see §4.3). The terms through order 4 in \( \hbar \) of (1.1) are shown in Appendix D.

The existence of a universal equation like (1.1) was used by Voros [19] and Colin de Verdière [6] as part of a calculation to obtain Bohr–Sommerfeld quantization rules at higher orders in \( \hbar \). They derived it by using an explicit spectral theorem that writes \( f(\hat{A}) \) in terms of the resolvent.\(^1\) Their method gives a recursive way of obtaining higher order corrections in \( \hbar \) but is, in practice, intractable

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\(^1\)In Appendix B we give an alternative derivation of our main result inspired by this approach.
after order 2. In contrast, the diagrammatic notation that we use (inspired by [4]) makes it simple to derive all our formulas and to write down explicitly their terms.

For the derivation of (1.1) we need:

- Weyl quantization, i.e., a well defined correspondence between operators and symbols (see §2.1), but we will not use its explicit form.
- The explicit form of the Moyal product (see §2.2).
- A spectral theorem, i.e., a way to define a function of an operator (see §2.3), but we will not use its explicit form.

Before going on, let us mention some possible applications of this calculation:

1. **Bohr–Sommerfeld quantization rules.** This is treated in §7.
2. **Determinant of certain differential operators.** See [14]. Such determinants naturally arise in quantum field theory at the one loop level. The determinant of an operator can be defined with the property \[ \log \det \hat{A} = \text{trace} \log \hat{A}, \] which holds in finite dimensional spaces. Then, the trace of the operator \[ \hat{B} = \log \hat{A} \] can be calculated by means of its symbol \( B \).
3. **Star exponential of quadratic forms.** Omori et al analyzed this problem in [16]. In the case when \( A \) is a quadratic function and \( f \) is an exponential, formula (1.1) simplifies. See §6.

The structure of this paper is as follows. In §2 we explain the necessary background: Weyl quantization, the Moyal product and functions of operators. In §3 we introduce diagrammatic notation that will be used afterwards. §4 is the core of this paper, where we derive (1.1) and other equivalent equations. In §5 we consider generalizations to functions of various variables and to other quantizations. In §6 we study the case of a quadratic symbol, in particular the harmonic oscillator Hamiltonian. This is an example of restricting to a smaller class of symbols \( A \), for which the family of graphs to consider becomes smaller, too, and (1.1) simplifies. §7 explains the application to Bohr–Sommerfeld rules.

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2 Background.

2.1 Weyl quantization.

Weyl quantization [20] (or Weyl–Wigner correspondence) is a way to relate the classical and quantum descriptions of a system. In the classical description of a system, the space of states is a Poisson manifold, whereas the quantum 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 classically described by smooth functions on the phase space \( C^\infty(T^* \mathbb{R}^N) \). In the quantum description they are operators on the Hilbert space \( \text{Op}(L^2(\mathbb{R}^N)) \). For instance, we have canonical coordinates \((x, p) := (x_1, \ldots, x_N, p_1, \ldots, p_N)\) 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 \( C^\infty(T^* \mathbb{R}^N) \) and hence classical observables. We associate to them operators \( \hat{x}_j \) and \( \hat{p}_j \) on \( L^2(\mathbb{R}^N) \) defined by:

\[
\hat{x}_j[\phi](x) = x_j \phi(x)
\]

\[
\hat{p}_j[\phi](x) = -i\hbar \frac{d\phi}{dx_j}(x)
\]

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

Here \( \hbar \) is the Planck constant. We will treat it as a formal parameter and consider that all our spaces are formal power series in \( \hbar \). Thus the classical observables will be elements of \( C^\infty(T^* \mathbb{R}^N)[[\hbar]] \) and the quantum observables will be elements of \( \text{Op}(L^2(\mathbb{R}^N))[[\hbar]] \).

A quantization is an extension of this correspondence to a map

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

In particular the Weyl–Wigner correspondence is defined by:

\[
\hat{A}[\phi](x) = \int \frac{dy dp}{(2\pi \hbar)^n} e^{i(x-y)\cdot p/\hbar} A(x + y/2, p) \phi(y)
\]

\[
A(x, p) = \int \frac{ds}{(2\pi \hbar)^n} e^{-i s \cdot p/\hbar} \langle x + s/2 | \hat{A} | x - s/2 \rangle
\]

In order for it to be a well-defined bijection we need to restrict the domain and consider only a certain family of smooth functions and a certain family of operators. See [8] for details. In §5.2 we consider alternative quantizations.

\( A \) is called the symbol of \( \hat{A} \). Moreover, the space of operators with composition is an algebra. We can define an associative operation in \( C^\infty(T^* \mathbb{R}^N)[[\hbar]] \), called star product \( * \), that makes the bijection \( A \mapsto \hat{A} \) into an algebra isomorphism. In other words, \( C * D \) is the symbol of the operator \( \hat{C} \hat{D} \).
2.2 The Moyal product.

Moyal [15] gave an explicit expression for the star product in the case of the Weyl quantization, called the Moyal product (but actually due to Groenewold [9]). It is derived from the definition of the Moyal product \( \hat{C} \star \hat{D} = \hat{C} \hat{D} \) and the explicit form of Weyl quantization (2.1). If \( C, D \) are symbols in \( C^\infty(T^*\mathbb{R}^N) \), then:

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

(2.2)

We need to explain the notation in (2.2). 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 \((z^1, \ldots, z^{2N}) := (x, p)\) and \( J^{\mu \nu} \) the coefficients of the Poisson tensor on this chart

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

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

\[
C,_{\mu} = \partial_\mu C = \partial_{z^\mu} C = \frac{\partial C}{\partial z^\mu}
\]

\[
C,_{\mu_1 \ldots \mu_k} = \partial_{\mu_1} \ldots \partial_{\mu_k} C = \partial_{z^{\mu_1}} \ldots \partial_{z^{\mu_k}} C = \frac{\partial^k C}{\partial z^{\mu_1} \ldots \partial z^{\mu_k}}
\]

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 (2.2) are defined as:

\[
\{C, D\}_0 = CD
\]

\[
\{C, D\}_1 = \{C, D\} = C,_{\mu} J^{\mu \nu} D,_{\nu}
\]

\[
\{C, D\}_k = C,_{\mu_1 \ldots \mu_k} J^{\mu_1 \nu_1} \ldots J^{\mu_k \nu_k} D,_{\nu_1 \ldots \nu_k}
\]

Following [4] we use the notation “\( \longrightarrow \)” for a Poisson tensor in the following way: “\( \longrightarrow \)” is replaced by \( J^{\mu \nu} \), the expression in the head of the arrow is acted on by \( \partial_\nu \) and the expression in the tail of the arrow is acted on by \( \partial_\mu \). For instance

\[
C \longrightarrow D = C,_{\mu} J^{\mu \nu} D,_{\nu} = \{C, D\}
\]

\[
C \longrightarrow D = C,_{\mu_1} J^{\mu_1 \nu_1} J^{\mu_2 \nu_2} D,_{\nu_1 \nu_2} = \{C, D\}_2
\]

\[
C \longrightarrow D = C,_{\mu_1 \ldots \mu_k} J^{\mu_1 \nu_1} \ldots J^{\mu_k \nu_k} D,_{\nu_1 \ldots \nu_k} = \{C, D\}_k
\]
Here, \( k \) denotes \( k \) arrows. The same can be done with more complicated diagrams:

\[
C \xrightarrow{k} D \xrightarrow{k} A = C \xrightarrow{J_{\mu_1 \nu_1}} D \xrightarrow{J_{\mu_2 \nu_2}} \cdots \xrightarrow{J_{\mu_k \nu_k}} A \quad (2.3)
\]

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

\[
C \xrightarrow{} D = (-1) C \xleftarrow{} D
\]

With this notation, the Moyal product (2.2) is written:

\[
C \star D = \sum_{k=0}^{\infty} \frac{1}{k!} \left( \frac{ih}{2} \right)^k C \xrightarrow{k} D \quad (2.4)
\]

The fact that the Poisson bracket is a derivation on each argument (Leibniz rule or product rule) is written as:

\[
(CD) \rightarrow E = C (D \rightarrow E) + (C \rightarrow E) D
\]

\[\{CD, E\} = C\{D, E\} + \{C, E\} D\]

Another application of the product rule is

\[
(C \rightarrow D) \rightarrow E = C \rightarrow D \rightarrow E + E \xleftarrow{} C \rightarrow D
\]

\[
(C_{\mu} J^{\mu \nu} D_{\nu, \alpha}) \rightarrow E_{\beta} = C_{\mu} J^{\mu \nu} D_{\nu, \alpha} J^{\alpha \beta} E_{\beta} + C_{\mu, \alpha} J^{\mu \nu} D_{\nu, \beta} J^{\alpha \beta} E_{\beta} \quad (2.5)
\]

Notice that (2.5) cannot be written with Poisson brackets \( \{ , \} \).

This notation makes it simpler to write certain calculations. Lemma A.1 in Appendix A is a generalization of (2.5) that will be used in our derivations.

### 2.3 Spectral theorems.

To understand (1.1) we need to define what a function of an operator means. If \( f(y) = y^n \) then \( f(\hat{A}) = (\hat{A})^n \). A spectral theorem extends this definition of \( f(\hat{A}) \) to a wider class of functions \( f \). More specifically, let \( \mathcal{A} \) be an algebra of smooth functions under pointwise multiplication and let \( \hat{A} \) be an operator. Then a spectral theorem is an isomorphism of algebras

\[
f \in \mathcal{A} \mapsto f(\hat{A}) \in \text{Op}(L^2(\mathbb{R}^N))
\]

with certain properties. See [7] for details. There are many spectral theorems (i.e. different algorithms to calculate \( f(\hat{A}) \)) for different algebras \( \mathcal{A} \). See [1] for a complete list of references. We will not use any explicit form of a spectral theorem (with the exception of Appendix B, where we derive an alternative proof of our main result). We just need the fact that a spectral theorem is a morphism of algebras:

\[
f(\hat{A}) g(\hat{A}) = (fg)(\hat{A})
\]
3 Graphs.

The formulas we are going to derive are power series whose terms are labeled by graphs. We define now the family of graphs that we are going to use and introduce notation.

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

\[ \bullet - \bullet - \bullet - \bullet \]

A labeled graph is a graph with in which we have labeled the vertices with the first \( V \) natural numbers \( 1, 2, \ldots, V \) and the edges with the first \( E \) natural numbers \( 1, 2, \ldots, E \). Therefore, \( V \) is the number of vertices and \( E \) is the number of edges. For instance:

\[ 1 \rightarrow 2 \rightarrow 3 \rightarrow 6 \rightarrow 3 \quad 4 \rightarrow 5 \rightarrow 5 \]

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:

\[ 1 \rightarrow 2 \rightarrow 3 \rightarrow 6 \rightarrow 3 \quad 4 \rightarrow 5 \rightarrow 5 \]

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 3.1.** Let \( V \) and \( E \) be two non-negative integers. A labeled graph with \( V \) vertices and \( E \) edges is a map

\[ s : \{1, \ldots, E\} \longrightarrow \mathcal{P}_2\{1, \ldots, V\} \]

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 \( \{1, \ldots, E\} \). The group \( S_V \) of permutations of \( V \) letters acts naturally on \( \mathcal{P}_2\{1, \ldots, V\} \). Hence the direct product \( S_V \times S_E \) acts on functions \( \{1, \ldots, E\} \longrightarrow \mathcal{P}_2\{1, \ldots, V\} \), that is, on the set of labeled graphs with \( V \) vertices and \( E \) edges.

**Definition 3.2.** 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 a graph 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 3.3.** 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.

See Appendix C for examples.

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

**Definition 3.4.** A labeled graph \( s : \{1, \ldots, E\} \rightarrow \mathcal{P}_2\{1, \ldots, V\} \) is reduced if every \( i = 1, \ldots, V \) is in some element of the image of \( s \) (i.e., "if every vertex is in some edge").

Both concepts (order of symmetry of a graph and reduced graph) extend naturally to unlabeled graphs. All the previous examples are reduced. The graph \( \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \) is not reduced.

Given a labeled graph \( \Gamma \) with \( V \) vertices, and given \( V \) symbols \( A_1, \ldots, A_V \) we construct a new symbol, called \( \lambda_\Gamma(A_1, \ldots, A_V) \), by substituting the vertices with \( A_1, \ldots, A_V \), and letting every edge represent a Poisson tensor (as explained in \( \S2.2 \)). We denote \( \lambda_\Gamma(A_1, \ldots, A_V) \) simply by \( \lambda_\Gamma(A) \).

For instance, if \( \Gamma \) is the labeled graph:

\[
1 \quad 1 \quad 2 \quad 2 \quad 3
\]

then \( \lambda_\Gamma(C, D, A) \) is the expression in \( \|3\). And

\[
\lambda_\Gamma(A) = A \rightarrow A \rightarrow A = A_{\mu_1^1\nu_1^1} A_{\nu_1^1\mu_2^2} A_{\mu_2^2\nu_3^3} A_{\nu_3^3\nu_2^2} A_{\nu_2^2\nu_3^3}
\]

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

**4 Main results and calculations.**

We recall our problem. Let us fix an operator \( \hat{A} \) with symbol \( A \) and a smooth function \( f \). Let \( \hat{B} = f(\hat{A}) \) be an operator with symbol \( B \). In this section we will perform the necessary calculations to obtain various expressions of \( B \) in terms of \( A \).
The main step is to obtain an expression for an iterated star product \( C_1 \star \ldots \star C_n \) for symbols \( C_i \) in terms of graphs. We do this in \( \S 4.1 \). Then in \( \S 4.2 \) we derive our first expression for \( B \) in terms of \( A \).

Equation (4.4) at the end of \( \S 4.2 \) 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. There are only a few unlabeled graphs, but many labeled graphs. In \( \S 4.3 \) we obtain our second expression for \( B \) in terms of \( A \), (4.8), a series whose terms are parametrized by unlabeled graphs. There is still a third form of our formula, Equation (4.12), whose terms are parametrized by connected graphs. This last form is studied in \( \S 4.4 \).

Using either of these equations, we have included in Appendix D the explicit form of the terms up to order 4 in \( \hbar \) of the symbol \( B \) in terms of \( A \).

4.1 The \( n \)-th star product.

The main step in the derivation of (1.1) is the following expression for the iterated star product, which generalizes Moyal’s formula:

\[ C_1 \star \cdots \star C_n = \sum_{k=0}^{\infty} \frac{1}{k!} \left( \frac{i\hbar}{2} \right)^k \sum_{\text{labeled graphs } \Gamma \text{ with } n \text{ vertices and } k \text{ edges}} \lambda_{\Gamma}(C_1, \ldots, C_n) \quad (4.1) \]

Note that when \( n = 2 \), the previous lemma is exactly the Moyal formula for the star product (2.4). For every \( k \), there is only one labeled graph with 2 vertices and \( k \) edges.
When \( n = 3 \), for instance:

\[
A \ast A \ast A = A^3 + \frac{i\hbar}{2} \left( A \rightarrow A \rightarrow A \right) + \frac{i\hbar}{2} \left( A \rightarrow A \rightarrow A \right) + \frac{i\hbar}{2} \left( A \rightarrow A \rightarrow A \right) + \frac{1}{2!} \left( \frac{i\hbar}{2} \right)^2 \left( A \rightarrow A \rightarrow A \right) + \frac{1}{2!} \left( \frac{i\hbar}{2} \right)^2 \left( A \rightarrow A \rightarrow A \right) + \frac{1}{2!} \left( \frac{i\hbar}{2} \right)^2 \left( A \rightarrow A \rightarrow A \right) + \frac{1}{2!} \left( \frac{i\hbar}{2} \right)^2 \left( A \rightarrow A \rightarrow A \right) + \frac{1}{2!} \left( \frac{i\hbar}{2} \right)^2 \left( A \rightarrow A \rightarrow A \right) + \frac{1}{2!} \left( \frac{i\hbar}{2} \right)^2 \left( A \rightarrow A \rightarrow A \right) + \frac{1}{2!} \left( \frac{i\hbar}{2} \right)^2 \left( A \rightarrow A \rightarrow A \right) + \frac{1}{2!} \left( \frac{i\hbar}{2} \right)^2 \left( A \rightarrow A \rightarrow A \right) + O(\hbar^3)
\]

In the previous expression, the vertices are labeled from left to right 1, 2, 3 in all graphs.

**Proof of lemma 4.1**

We will use induction on \( n \).

The result is true for \( n = 0, 1, 2 \).

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

\[
C_1 \ast \ldots \ast C_{n+1} = (C_1 \ast \ldots \ast C_n) \ast C_{n+1}
\]

\[
= \sum_{\text{labeled graphs } \Gamma \text{ with } n \text{ vertices}} \frac{1}{E!} \left( \frac{i\hbar}{2} \right)^E \lambda_\Gamma(C_1, \ldots, C_n) \ast C_{n+1}
\]

\[
= \sum_{\text{labeled graphs } \Gamma' \text{ with } n \text{ vertices}} \sum_{k=0}^{\infty} \frac{1}{E!k!} \left( \frac{i\hbar}{2} \right)^{E+k} \lambda_{\Gamma'}(C_1, \ldots, C_n) \ast_{k} C_{n+1}
\]

We can apply lemma A.1 in Appendix A to \( \lambda_{\Gamma'}(C_1, \ldots, C_n) \ast_{k} C_{n+1} \) and we will 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, \ldots, \( n \)) and
edges (labeled \(1, \ldots, E\)), adding the \((n + 1)\)-th vertex and \(k\) edges (labeled \(E + 1, \ldots, E + k\)) ending at the \((n + 1)\)-th vertex. The number of edges of \(\Gamma'\) is \(E' = E + k\). If we want to account for all possible labeled graphs 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

\[
C_1 \ast \ldots \ast C_{n+1} = \sum_{\text{labeled graphs } \Gamma'} \frac{1}{E'!} \left( \frac{i\hbar}{2} \right)^E' \lambda_{\Gamma'}
\]

4.2 First formula for the symbol of a function of an operator.

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

To calculate \(B\) we use the following expression \[5\]:

**Lemma 4.2.** Let \(z_0 \in T^*\mathbb{R}^N\) and let \(a_0 := A(z_0)\). Then

\[
B(z_0) = \sum_{k=0}^{\infty} \frac{1}{k!} f^{(k)}(a_0) \left( A - a_0 \right)^*k (z_0)
\]

(4.2)

Note that the right hand side of \(4.2\) is well–defined only at the point \(z_0\). To prove it, we need the following fact:

**Lemma 4.3.** Let \(g\) be a smooth function and \(\hat{C} := g(\hat{A})\). Let \(a_0 := A(z_0)\). If \(g\) has a zero of order \(m\) at \(a_0\), then \(C(z_0) = O(h^{m/2})\).\[2\]

**Proof of lemma 4.3** Let us write \(g(y) = g_1(y)(y - a_0)^m\) and let \(\hat{C}_1 = g_1(\hat{A})\). Then \(\hat{C} = g(\hat{A}) = g_1(\hat{A}) (\hat{A} - a_0)^m\) and \(C = C_1 \ast (A - a_0)^*m\). Since \((A(z) - a_0)|_{z=z_0} = O(h)\), then \(C(z_0) = O(h^{m/2})\).\[\Box\]

**Proof of lemma 4.2** For every \(m\), apply lemma 4.3 with

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

This proves that

\[
B(z_0) = \sum_{k=0}^{\infty} \frac{1}{k!} f^{(k)}(a_0) \left( A - a_0 \right)^*k (z_0) = O(h^{m/2})
\]

for all \(m\).\[\Box\]

\[2\]Actually, we can do better: \(C(z_0) = O(h^{2m/3})\).
Now we only need to substitute $4.1$ into $4.2$ to get an expression for $B$ in terms of graphs:

$$B(z_0) = \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(A(z_0)) \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{ih}{2}\right)^k \lambda_\Gamma(A - a_0)(z_0)$$

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 $A - a_0$ with $A$, 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:

$$B = \sum_{\text{reduced labeled graphs } \Gamma} \frac{1}{E!} \left(\frac{ih}{2}\right)^E \frac{f^{(V)}(A)}{V!} \lambda_\Gamma(A)$$

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 $A = \sum_k h^k A_k$ as a power series in $\hbar$ and expand $4.4$. As a matter of fact, we have an alternative way to write $4.4$ with terms parametrized by graphs with weights where every term is a monomial in $\hbar$. We believe that the approach shown in this paper is simpler, though, and clearly illustrates the method.

Equation $4.4$ was easy to derive, and it is useful for proofs and theoretical calculations, as well as to generalize to other quantizations (see §5.2). However, when we want to explicitly write the first few terms of it, this is not yet our ideal expression. We can put together the contribution of labeled graphs that differ only in the labels to get a series whose terms are parametrized by unlabeled graphs. We will do it next.

See Appendix B for an alternative derivation of $4.4$.

### 4.3 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).

$4.4$ can be rewritten as:

$$B = \sum_{\text{reduced graphs } \Gamma} \lambda_{\Gamma'}(A)\ \text{with } \Gamma' \in [\Gamma]$$

In words, we need to sum $\lambda_{\Gamma'}$ when $\Gamma'$ runs through all possible relabelings of $\Gamma$. Remember that $\lambda_{\Gamma'}$ and $\lambda_\Gamma$ will be equal up to a sign.

Define

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

$$11$$
That is, we start with a labeled graph $\Gamma$. Then, we consider the $V!$ possible ways of numbering the vertices of the graph with $1, 2, \cdots, V$. 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 highest label. Then we count these $V!$ relabelings with a sign, depending on the parity of the number of arrows inverted from our original orientation.

We can then write the contribution from (4.5) as:

$$\sum_{\Gamma' \in [\Gamma]} \lambda_{\Gamma'}(A) = \frac{E!}{S_{\Gamma}} c_{\Gamma} \lambda_{\Gamma}(A)$$

(4.7)

where $S_{\Gamma}$ is the order of the symmetry group of the (unlabeled) graph $[\Gamma]$ (see Definition 3.3). The contribution corresponding to different relabelings of the edges is $E!$. 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:

$$c_{\Gamma} = (-1)^0 + (-1)^1 + (-1)^1 + (-1)^1 + (-1)^1 + (-1)^1 + (-1)^2 = -2$$

Finally we just have to substitute (4.7) into (4.5):

$$B = \sum_{\text{reduced graphs } [\Gamma]} \left( \frac{i\hbar}{2} \right)^E \frac{c_{\Gamma}}{S_{\Gamma}} f(V)(A) \frac{D^V}{V!} \lambda_{\Gamma}(A)$$

(4.8)

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 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 $c_{\Gamma} = 0$.

### 4.4 Version with connected graphs.

Let us rewrite (4.8) as:

$$B = \sum_{\text{reduced graphs } [\Gamma]} \left( \frac{i\hbar}{2} \right)^E \frac{c_{\Gamma}}{S_{\Gamma}} \lambda_{\Gamma}(A) \frac{D^V}{V!} \lambda_{\Gamma}(A)$$

(4.9)
where $D$ is the differential operator which applies to $f$.

Whenever we have an expression like (4.9), a series labeled by a certain family of diagrams, it is standard to reduce all calculations to only connected diagrams. Let’s generalize.

Let $\mathcal{G}$ be the free commutative monoid generated by the set $\mathcal{G}_0$. Let $S$ be a commutative ring (with multiplicative notation). Let $\mathcal{O} : \mathcal{G} \rightarrow S$ be a map satisfying

$$\mathcal{O}(r_1 x_1 + \cdots + r_n x_n) = \frac{1}{r_1! \cdots r_n!} (\mathcal{O}(x_1))^{r_1} \cdots (\mathcal{O}(x_n))^{r_n}$$  \hspace{1cm} (4.10)

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

$$\sum_{x \in \mathcal{G}} \mathcal{O}(x) = \exp \left[ \sum_{x \in \mathcal{G}_0} \mathcal{O}(x) \right]$$  \hspace{1cm} (4.11)

In particular, consider $\mathcal{G}$ to be a family of diagrams closed under topological sum and generated by the connected non-empty diagrams $\mathcal{G}_0$. If we write $\mathcal{O}(\Gamma) = \mathcal{M}(\Gamma) S^{\Gamma}$, where $S^{\Gamma}$ is the order of the symmetry group of the diagram and $\mathcal{M}$ is a multiplicative function

$$\mathcal{M}(x_1 + x_2) = \mathcal{M}(x_1) \mathcal{M}(x_2)$$

for all $x_1, x_2 \in \mathcal{G}$

then $\mathcal{O}$ satisfies (4.10).

In our case,

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

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

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

$\mathcal{M}(\Gamma) = \left( \frac{i\hbar}{2} \right)^E c_\Gamma \lambda_\Gamma(A) \frac{D^V}{V!}$

$\mathcal{M}$ is multiplicative from (4.11) in Appendix C

Hence, using (4.11) in (4.9):

$$B = \left[ \exp \sum_{\text{connected, reduced, non-empty graphs } \Gamma} \left( \frac{i\hbar}{2} \right)^E \frac{c_\Gamma}{S_\Gamma} \lambda_\Gamma(A) \frac{D^V}{V!} \right] f(A)$$  \hspace{1cm} (4.12)

5 Generalizations.

As we mentioned in the introduction, we needed three things to derive our results:
• Weyl quantization.
• The Moyal product.
• A spectral theorem.

Of these, we only used the explicit form of the Moyal product. Actually, the form of the Moyal product is calculated from the form of the Weyl quantization. We discuss now how to generalize to functions of various variables and other quantizations.

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

Hence, we only need to repeat our calculations, starting from §4.2 but with a function of a several variables. The counterpart of (4.8) is

$$B = \sum_{\text{reduced graphs } [\Gamma]} \left( \frac{i\hbar}{2} \right)^E \frac{1}{S_{\Gamma}} \frac{\partial_{i_1} \cdots \partial_{i_v} F(A)}{V!} \lambda_{\Gamma}(A_{i_1}, \ldots, A_{i_v})$$  (5.1)

For instance the first few terms of (4.8) are

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

and the first few terms of (5.1) are

$$B = F(A) - \frac{\hbar^2}{4} \left[ \frac{1}{2} A_i \quad \frac{\partial_i \partial_j F(A)}{2!} + A_i \rightarrow A_j \leftrightarrow A_k \quad \frac{\partial_i \partial_j \partial_k F(A)}{3!} \right] + O(\hbar^4)$$

There are also the obvious versions with labeled or connected graphs.

5.2 Other quantizations.
There are other quantizations apart from Weyl quantization, that is, correspondences between operators and symbols [11]. If we want to use them, then we have a different star product instead of the Moyal product. The explicit form of the Moyal product has been used in two places: to prove lemma 4.3 and to derive an expression for the iterated star product (lemma 4.1).
Let us consider a generic star product that has the form

\[ C \star D = \sum_{k=0}^{\infty} \frac{1}{k!} \left( \frac{i\hbar}{2} \right)^{k} \{C, D\}_{k} \tag{5.2} \]

As long as \((C, D) \mapsto \{C, D\}_{k}\) is a bidifferential operator of order \(m_{k}\) and \(\lim_{k \to \infty} m_{k} = \infty\), then lemma \(1.20\) is satisfied. Hence, for those star products, we only need to obtain an analogue to lemma \(4.1\) that is, an expression for the iterated star product \(C_{1} \star \ldots \star C_{n}\) 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.

For instance, we can consider standard order quantization:

\[ A(x, p) = u_{p}(x)\hat{A}[u_{p}](x) \]

where \(u_{p}(x) = e^{ip \cdot x/\hbar}\). In that case, the star product has the form of (5.2) with \(\{C, D\}_{k} := \partial_{p}^{k} C \partial_{x}^{k} D\). Lemma \(4.3\) still holds and, if we change the meaning of “\(\mapsto\)”, lemma \(4.1\) is also true. The simplest way is to use the same definitions we gave in §2.2 and §3 to construct a polynomial \(\lambda_{\Gamma}(\hat{A})\) 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, (4.4) is still valid. However, it is no longer true that \(C \mapsto D = - C \leftarrow D\). As a consequence, the versions with unlabeled or connected graphs are messier (although they still exist).

In [13], 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 \(1.2\) and we can derive, again, the counterparts of Equations (4.4), (4.8), and (4.12). In fact, our set of labeled graphs is a subset of Kontsevich’s set of labeled graphs. It is to be noted, though, that Kontsevich’s star product includes a weight \(\omega_{\Gamma}\) associated to every diagram \(\Gamma\) which is, in practice, hard to calculate. (See [12] and [17] for some results.)

6 The case of a quadratic symbol.

When we restrict to a smaller class of symbols, it is possible that the contribution of many graphs vanishes, simplifying our calculations. As an example, we study here quadratic symbols.

A particular (simple) case of importance consists of taking \(\hat{A} = \hat{I}\), the harmonic oscillator hamiltonian in 1 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 $A$ is the symbol of an operator $\hat{A}$. Then:

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

and any third derivative vanishes. As a consequence, we only need to consider graphs where every vertex has at most two edges. After lemma C.1 in Appendix C, 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:

$$\Delta_k = \bullet \rightarrow \bullet \rightarrow \cdots \rightarrow \bullet \quad (2k \text{ edges}) \quad k \geq 1$$
$$\Lambda_k = \bullet \rightarrow \bullet \rightarrow \cdots \rightarrow \bullet \quad (2k \text{ edges}) \quad k \geq 1$$

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:

$$\lambda_{\Delta_k} = A_{,\mu_1} J_{\mu_1\nu_1} A_{,\mu_2} J_{\mu_2\nu_2} \cdots J_{\mu_{2k}\nu_{2k}} A_{,\nu_{2k}}$$
$$\lambda_{\Lambda_k} = A_{,\nu_{2k}\mu_1} J_{\mu_1\nu_1} A_{,\mu_2} J_{\mu_2\nu_2} \cdots J_{\mu_{2k}\nu_{2k}} = \text{trace}((QJ)^{2k})$$

Since $Q$ is symmetric and $J$ is skew-symmetric, their product $QJ$ is traceless. Hence $(QJ)^2 = -\det(QJ)\text{id}$. 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 5 in Appendix C gives us the relation $c_{\Lambda_k} = -2k c_{\Delta_{k-1}}$.

We now plug all these values in (6.1) to obtain, for a general function $f$ and a quadratic symbol $A$:

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

(6.1)

We are left with a combinatorics problem: the sequence $\{c_{\Delta_k}\}$. Fact 5 in Appendix C gives us a recurrence formula:

$$c_{\Delta_k} = -\sum_{j=0}^{k-1} \left( \frac{2k}{2j+1} \right) c_{\Delta_j} c_{\Delta_k-j-1}$$

(6.2)
The sequence is alternating in sign, and the first few absolute values are 1, 2, 16, 272, 7936 . . . This sequence is called the Zag numbers \[18\] and they appear in the McLaurin expansion of the tangent:

\[
\tan x = \sum_{k=0}^{\infty} \frac{|c_{\Delta k}|}{(2k+1)!} x^{2k+1}
\]  

(6.3)

To prove this, notice that tan \(x\) is the only odd solution to the differential equation

\[
y' = 1 + y^2
\]  

(6.4)

Write a generic solution of the form \(y = f(x) = \sum_{k=0}^{\infty} \frac{a_k}{(2k+1)!} x^{2k+1}\) and substitute it into (6.4). Equating coefficients, we conclude that the sequence \(a_k\) satisfies the same recurrence relation as the sequence \(c_{\Delta k}\) (Equation (6.2)). Hence \(a_k = |c_{\Delta k}|\).

The Zag numbers can be written in terms of the Bernoulli numbers \(B_n\):

\[
|c_{\Delta k}| = \frac{2^{2k}}{2^{2k} - 1} \frac{|B_{2k}|}{2k}
\]

When we use equation (6.3) in (6.1) we obtain a nice, compact expression:

\[
\hat{B} = f(\hat{A})
\]

\[
B = \sec \frac{i\hbar \omega D}{2} \exp \left[ \frac{2A}{i\hbar \omega} \tan \frac{i\hbar \omega D}{2} - AD \right] f(A)
\]  

(6.5)

Remember that \(D\) is the derivative operator that applies to \(f\). If we also take the function \(f(y) = e^{\epsilon y}\), then \(D\) acts simply as multiplication by \(\epsilon\). In particular, when we consider the time evolution operator:

\[
\hat{B} = e^{-it\hat{A}/\hbar}
\]

\[
B = \sec \frac{t\omega}{2} \exp \left[ \frac{2A}{i\hbar \omega} \tan \frac{t\omega}{2} \right]
\]  

(6.6)

Equation (6.6) is derived in [16] derived in a different manner. For the case \(\hat{A} = \hat{I}\), it is a well known formula. (See, for instance, [3].)

7 Application: Bohr–Sommerfeld rules.

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

In [6], Colin de Verdiére 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 [19] and a similar method had been previously used by Argyres [2].
Let $\hat{H}$ be an operator with symbol $H \in C^\infty(\mathbb{T}^*\mathbb{R})$. Bohr–Sommerfeld quantization rules provide a way to asymptotically compute the spectrum of $\hat{H}$. Assume $H$ has a regular minimum at a point. Under certain extra assumptions on the symbol $H$ (see [6]), the eigenvalues of $\hat{H}$ are given by the solutions $E$ to

$$2\pi n\hbar = S(E) = \sum_{j=0}^{\infty} h^j S_j(E)$$  \hspace{1cm} (7.1)$$

with $n \in \mathbb{Z}$. To solve the previous equation, write $E = \sum h^k E_k$ as a power series in $\hbar$ and substitute it into (7.1) to obtain recursive expressions for each $E_k$. This requires knowing the form of $S(E)$, called the semiclassical action, for the hamiltonian $\hat{H}$.

Let us consider for simplicity the case where the symbol $H$ does not depend on $\hbar$. It is known that at lowest orders in $\hbar$:

$$S_0(E) = \int_{\gamma_E} p \, dx , \quad S_1(E) = \pi$$

$\gamma_E$ denotes the level set $H^{-1}(E)$ around the minimum of $H$ and $(x, p)$ are the natural coordinates in $\mathbb{T}^*\mathbb{R}$.

The main result in [6] is the following:

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

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

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

and $P_{j,l}$ are universal polynomials in the derivatives of $H$ defined by the symbol $R_a$ of the resolvent $\hat{R}_a = (a - \hat{A})^{-1}$:

$$R_a = \frac{1}{a - H} + \sum_{j=1}^{\infty} \frac{1}{(a - H)^j} \sum_{l=2}^{L(j)} \frac{P_{j,l}(H)}{(a - H)^l}$$

Looking back at our formula for the symbol for the function of an operator and using it for the function $f(y) = (a - y)^{-1}$, we see that $L_j = 3j/2 + 1$ and the polynomials $P_{j,l}$ can actually be defined in terms of graphs:

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

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

$$2\pi(n - 1/2)\hbar = S_0(E) + \sum_{\text{reduced graphs } \Gamma \text{ with } E_{\Gamma} > 0} \left( \frac{i\hbar}{2} \right)^{E_{\Gamma}} \frac{(-1)^{V_{\Gamma}}}{V_{\Gamma}^!} \left( \frac{d}{dE} \right)^{V_{\Gamma} - 1} \frac{c_{\Gamma}}{S_{\Gamma}} \int_{\gamma_E} \lambda_{\Gamma}(H) \, dt$$  \hspace{1cm} (7.2)$$

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Here $E$ is an eigenvalue of $H$, whereas $E_{\Gamma}$ is the number of edges of a graph $\Gamma$.

$S_j(E) = 0$ for $j > 1$ and odd. $S_2(E)$ is given by the contribution of 2 graphs, and $S_4(E)$ is given by the contribution of 15 graphs (see Appendix C).

However, there is a trick using Stokes’ theorem that allow us to express the contribution of certain graphs in this expression in terms of others. (This trick is used in [4] and in [6] for $S_2$, although without the diagrammatic notation.) As a consequence, $S_2(E)$ can be written in terms of 1 graph and $S_4(E)$ can be written in terms of 5 graphs (those where every vertex has at least two edges):

\[
2\pi(n - 1/2)\hbar = S_0(E) - \frac{\hbar^2}{4} \left[ \frac{1}{2!} \cdot 6 \frac{d}{dE} \int_{\gamma_E} (H \rightarrow H) \, dt \right] \\
+ \frac{\hbar^4}{16} \left[ \frac{1}{2!} \cdot 120 \frac{d}{dE} \int_{\gamma_E} (H \rightarrow H) \, dt + \frac{1}{4!} \cdot 12 \left( \frac{d}{dE} \right)^3 \int_{\gamma_E} (H \rightarrow H)^2 \, dt \\
- \frac{1}{3!} \cdot 15 \left( \frac{d}{dE} \right)^2 \int_{\gamma_E} H \rightarrow H \, dt + \frac{1}{4!} \cdot 15 \left( \frac{d}{dE} \right)^3 \int_{\gamma_E} H \rightarrow H \, dt \\
- \frac{1}{3!} \cdot 12 \left( \frac{d}{dE} \right)^2 \int_{\gamma_E} (H \rightarrow H \rightarrow H) \, dt \right] \\
+ O(\hbar^6)
\]  

(7.3)

All the integrands in the previous expressions are long polynomials in the derivatives of $H$. The expression 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 (7.2) for that specific operator at higher orders in $\hbar$.

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 (7.3) becomes:

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

The disadvantage of this method is that it does not generalize to the multidimensional case $N > 1$. Cargo et al [4] approached this problem in a totally different way to obtain a result valid in all dimensions. The symbol of a function of an operator plays a role in their derivation, too.
A lemma for calculations with graphs.

The diagramatic notation introduced in §3 makes equations and derivations easier to write. The following lemma is needed in some of those derivations:

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

$$\lambda_\Gamma(C_1, \ldots, C_V) \xrightarrow{k} D = \sum_{\Gamma'} \lambda_{\Gamma'}(C_1, \ldots, C_V, D)$$

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 $E + 1, \ldots, E + k$) 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:

$$(C \xrightarrow{D} D) \xrightarrow{E}$$

$$= C \xrightarrow{1} 2 \xrightarrow{D} 3 \xrightarrow{E} + C \xrightarrow{1} D \xrightarrow{2} 3 \xrightarrow{E}$$

$$+ C \xrightarrow{1} D \xrightarrow{3} 2 \xrightarrow{E} + C \xrightarrow{1} D \xrightarrow{3} E$$

$$= C \xrightarrow{1} D \xrightarrow{E} + C \xrightarrow{1} D \xrightarrow{E}$$

$$+ 2 C \xrightarrow{1} D \xrightarrow{E}$$

B An alternative derivation of (4.4).

As we mentioned in the introduction and in [14] the existence of a universal formula like (1.1) was used by Voros [19] and Colin de Verdière [6] (and, indirectly, by Argyres [2]). They start by writing a smooth function of an operator in terms of the resolvent. Let $a \in \mathbb{C}$ and define the resolvent operator $\hat{R}_a := (a - \hat{A})^{-1}$ with symbol $R_a$. Then we use Helffer–Sjöstrand’s formula [10] as a spectral theorem:

$$\hat{B} = f(\hat{A}) = -\frac{1}{\pi} \int_{\mathbb{C}} \hat{R}_z \partial_z \bar{f}(z) \, dx dy$$

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

$$B = -\frac{1}{\pi} \int_C R_z \partial_\Sigma \tilde{f}(z) \, dx dy$$  \hspace{1cm} (B.1)$$

Hence, finding the symbol of $f(\hat{A})$ reduces to finding the symbol of $\hat{R}_a$.\(^3\) In order to do so, we may write

$$R_a = \sum_{k=0}^\infty R_{a(k)} h^k$$

and, since $\hat{R}_a(a - \hat{A}) = 1$, substitute it into

$$R_a \star (a - A) = (a - A) \star R_a = 1$$

to obtain recursively the value of each $R_{a(k)}$. Although simple, this method quickly proves intractable. The calculations at order 4 are already too complex and we will not find the pattern that (1.1) shows.

But we can also use this idea to prove (4.4) in a different way. First, we prove it for the function $f(y) = (a - y)^{-1}$:

**Claim.** The function

$$h_a(A) = \sum_{\text{reduced labeled graphs } \Gamma} \frac{1}{E!} \left( \frac{i\hbar}{2} \right)^E \frac{\lambda_\Gamma(A)}{(a - A)^{E+1}}$$ \hspace{1cm} (B.2)$$

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 can substitute (B.2) into (B.1) to obtain again (4.4).

**C Calculation of $c_\Gamma$ and $S_\Gamma$.**

Calculating $c_\Gamma$ is a combinatorial problem. The following five facts give quick, recursive rules for it:

\(^3\)We could also use Cauchy’s integration formula as a spectral theorem:

$$\hat{B} = f(\hat{A}) = \int_\gamma \frac{da}{2\pi i} f(a) \hat{R}_a$$

$$B = \int_\gamma \frac{da}{2\pi i} f(a) R_a$$

which will lead to the same results, but it is only valid for analytic functions $f$. $\gamma$ is a path around the spectrum of $A$.\(\square\)
Facts:

1. $c_* = 1$

2. $c_\Gamma = 0$ if $E$ is odd.
   
   This is due to a symmetry property. If we denote by $\Gamma$ a labeled graph with a numbering of the vertices by $1, 2, \cdots V$ and by $i(\Gamma)$ the relabeling of the vertices by the permutation $(12 \cdots V)$, then
   
   $$\lambda_i(\Gamma) = (-1)^E \lambda_\Gamma$$

   And when we sum over reorderings of the vertices:

   $$c_\Gamma = (-1)^E c_\Gamma$$

3. If $\Gamma_i$ has $V_i$ vertices, $\Gamma_i \neq \Gamma_j$ for $i \neq j$, and $\Gamma = \Gamma_1 + \cdots + \Gamma_n$ is the topological sum with $V = V_1 + \cdots + V_n$ vertices, then

   $$c_\Gamma = \frac{V!}{V_1! \cdots V_n!} c_{\Gamma_1} \cdots c_{\Gamma_n} \quad (C.1)$$

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

   $$c_{1 \rightarrow 2 \rightarrow 3 \rightarrow 4} = c_{1 \rightarrow 2} \cdot 3 \rightarrow 4$$

5. 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:

   $$\Gamma = \bullet \quad p \quad \bullet \quad \bullet$$

   $$\Gamma - p = \bullet \quad \bullet \quad \bullet$$

   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 $V$. \hfill \square

In particular, putting together facts 2 and 3 we get:

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

These are the reduced, connected graphs with 2 and 4 edges, and for each of them the value of $c_\Gamma$ and $S_\Gamma$: 

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D  Symbol of a function of an operator at order 4 in \( \hbar \).

Using any of the equations derived in \( \S \) we write down 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 the table in Appendix C are needed.
\[ \hat{B} = f(\hat{A}) \]
\[ B = f(A) \]
\[ - \frac{\hbar^2}{4} \left[ \frac{A \rightarrow A A}{2} \frac{f''(A)}{2!} + A \rightarrow A \leftarrow A \left( f''(A) \right) \frac{3!}{3!} \right] \]
\[ + \frac{\hbar^4}{16} \left[ \frac{A \rightarrow A A}{24} \frac{f''(A)}{2!} + \left( \frac{A \rightarrow A A}{3} \right) \frac{f''(A)}{3!} \right. \]
\[ \left. + \frac{3}{4} A \rightarrow A \rightarrow A \right] \frac{f''(A)}{3!} \]
\[ + \left( \frac{3}{4} (A \rightarrow A)^2 \right) + \left( \frac{3}{4} (A \rightarrow A)^2 \right) + A \rightarrow A \rightarrow A \rightarrow A \]
\[ + 2 A \rightarrow A \rightarrow A \left( \frac{f^{(4)}(A)}{4!} \right) \]
\[ + \left( 8 A \rightarrow A \rightarrow A \rightarrow A \right) + A \rightarrow A \left( \frac{f^{(5)}(A)}{5!} \right) \]
\[ + 10 (A \rightarrow A \rightarrow A)^2 \left( \frac{f^{(6)}(A)}{6!} \right) \]
\[ + O(\hbar^6) \]
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