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THE SYMBOL OF A FUNCTION OF A PSEUDO-DIFFERENTIAL OPERATOR

by Alfonso GRACIA-SAZ

1. Introduction.

The goal of this paper is to give a realistically computable formula for the symbol of a function of an operator. 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 (definitions to follow; see §2) of $\widehat{A}$. Let $f : \mathbb{R} \to \mathbb{R}$ be a smooth function and let $\widehat{B} = f(\widehat{A})$ be an operator with symbol B. We want to write B in terms of A. We will derive the formula

$$B = \sum_{\Gamma} \Big(\frac{i\hbar}{2}\Big)^E \frac{c_\Gamma}{S_\Gamma}\, \lambda_\Gamma(A)\, \frac{f^{(V)}(A)}{V!}\,. \tag{1.1}$$

The sum is taken over finite graphs Γ with no isolated vertices. For every such graph Γ:

- 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 Γ (see §3),
- S_Γ is the order of the symmetry group of Γ,
- c_Γ is a simple invariant of Γ (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 a explicit

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spectral theorem that writes $f(\widehat{A})$ in terms of the resolvent.[1] Their method gives a recursive way of obtaining higher order corrections in $\hbar$ but is, in practice, intractable 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 $\log\det\widehat{A} = \operatorname{trace}\log\widehat{A}$, which holds in finite dimensional spaces. Then, the trace of the operator $\widehat{B} = \log\widehat{A}$ can be calculated by integrating its symbol B in phase space. For this to make sense we need the operator $\widehat{A}$ to be of the form "identity + trace class", or we have to use a regularization to redefine it.

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.

[1] In Appendix B we give an alternative derivation of our main result inspired by this approach.

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 $\mathcal{C}^\infty(T^*\mathbb{R}^N)$. In the quantum description they are operators on the Hilbert space $\mathrm{Op}(L^2(\mathbb{R}^N))$. 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. Coordinates x_j and p_j are elements of $\mathcal{C}^\infty(T^*\mathbb{R}^N)$ and hence classical observables. We associate to them operators $\widehat{x}_j$ and $\widehat{p}_j$ on $L^2(\mathbb{R}^N)$ defined by

$$\widehat{x}_j[\phi](x) = x_j\phi(x), \quad \widehat{p}_j[\phi](x) = -i\hbar\,\frac{\mathrm{d}\phi}{\mathrm{d}x_j}(x)$$

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 $\mathcal{C}^\infty(T^*\mathbb{R}^N)[[\hbar]]$ and the quantum observables will be elements of $\mathrm{Op}(L^2(\mathbb{R}^N))[[\hbar]]$.

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

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

In particular the Weyl-Wigner correspondence is defined by:

$$\text{(2.1)} \qquad \begin{cases} \widehat{A}[\phi](x) = \displaystyle\int \frac{\mathrm{d}^n y\,\mathrm{d}^n p}{(2\pi\hbar)^n}\,\mathrm{e}^{i(x-y)\cdot p/\hbar} A\big(\tfrac{1}{2}(x+y),p\big)\phi(y), \\ A(x,p) = \displaystyle\int \frac{\mathrm{d}^n s}{(2\pi\hbar)^n}\,\mathrm{e}^{-is\cdot p/\hbar}\big\langle x+\tfrac{1}{2}s|\widehat{A}|x-\tfrac{1}{2}s\big\rangle. \end{cases}$$

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

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 ($\widehat{C \star D} = \widehat{C}\widehat{D}$) and the explicit form of Weyl quantization (2.1). If C, D are symbols in $\mathcal{C}^\infty(T^*\mathbb{R}^N)$, then

$$C \star D = \sum_{k=0}^{\infty} \frac{1}{k!} \Big(\frac{i\hbar}{2} \Big)^k \{C, D\}_k. \tag{2.2}$$

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 $\partial_q := \partial/\partial q$. Let us call the coordinates $(z^1, \dots, z^{2N}) := (x, p)$ and $J^{\mu\nu}$ 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 Einstein summation criterion (summation over repeated indexes), $J = J^{\mu\nu} \partial_\mu \otimes \partial_\nu$. Let us also write

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

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:

$$\begin{aligned}
\{C,D\}_0 &= CD,\\
\{C,D\}_1 &= \{C,D\} = C_{,\mu}\, J^{\mu\nu}\, D_{,\nu},\\
\{C,D\}_k &= C_{,\mu^1\dots\mu^k}\, J^{\mu^1\nu^1}\cdots J^{\mu^k\nu^k}\, D_{,\nu^1\dots\nu^k}.
\end{aligned}$$

Following [4] we use the notation "$\to$" for a Poisson tensor in the following way: "$\to$" is replaced by $J^{\mu\nu}$, the expression in the head of the arrow is acted on by ∂_ν and the expression in the tail of the arrow is acted on by ∂_μ. For instance

$$\begin{aligned}
C \to D &= C_{,\mu} J^{\mu\nu} D_{,\nu} = \{C,D\},\\
C \rightrightarrows D &= C \xrightarrow[[2]]{} D = C_{,\mu^1\mu^2} J^{\mu^1\nu^1} J^{\mu^2\nu^2} D_{,\nu^1\nu^2} = \{C,D\}_2,\\
C \xrightarrow[[k]]{} D &= C_{,\mu^1\dots\mu^k} J^{\mu^1\nu^1}\cdots J^{\mu^k\nu^k} D_{,\nu^1\dots\nu^k} = \{C,D\}_k.
\end{aligned}$$

Here, $\xrightarrow[[k]]{}$ denotes k arrows:

$$\xrightarrow[[k]]{} = \left.\begin{array}{c}\rightrightarrows\\ \vdots\\ \rightrightarrows\end{array}\right\} \ k \text{ arrows.}$$

The same can be done with more complicated diagrams:

$$\begin{aligned}
C \to D \rightrightarrows A &= C \xrightarrow{J^{\mu_1\nu_1}} D \underset{J^{\mu_3\nu_3}}{\overset{J^{\mu_2\nu_2}}{\rightrightarrows}} A\\
&= C_{,\mu_1}\, J^{\mu_1\nu_1}\, D_{,\nu_1\mu_2\mu_3}\, J^{\mu_2\nu_2}\, J^{\mu_3\nu_3}\, A_{,\nu_2\nu_3}.
\end{aligned} \tag{2.3}$$

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

$$C \to D = (-1)\, C \leftarrow D.$$

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

$$C \star D = \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{i\hbar}{2}\right)^k C \xrightarrow[[k]]{} D. \tag{2.4}$$

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

$$\begin{aligned}
(CD) \to E &= C(D \to E) + (C \to E)D,\\
\{CD,E\} &= C\{D,E\} + \{C,E\}D.
\end{aligned}$$

Another application of the product rule is

$$\begin{cases} (C \to D) \to E = C \to D \to E + E \leftarrow C \to D, \\ (C_{,\mu} J^{\mu\nu} D_{,\nu})_{,\alpha} J^{\alpha\beta} E_{,\beta} = C_{,\mu} J^{\mu\nu} D_{,\nu\alpha} J^{\alpha\beta} E_{,\beta} \\ \qquad\qquad + C_{,\mu\alpha} J^{\mu\nu} D_{,\nu} J^{\alpha\beta} E_{,\beta}. \end{cases} \tag{2.5}$$

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 $f(\widehat{A}) = (\widehat{A})^n$. A spectral theorem extends this definition of $f(\widehat{A})$ to a wider class of functions f. More specifically, let $\mathcal{A}$ be an algebra of smooth functions under pointwise multiplication and let $\widehat{A}$ be an operator. Then a *spectral theorem* is an morphism of algebras

$$f \in \mathcal{A} \longmapsto f(\widehat{A}) \in \mathrm{Op}\big(L^2(\mathbb{R}^N)\big)$$

with certain properties. See [7] for details. There are many spectral theorems (i.e. different algorithms to calculate $f(\widehat{A})$) 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:

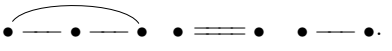
$$f(\widehat{A})g(\widehat{A}) = (fg)(\widehat{A}).$$

3. Graphs.

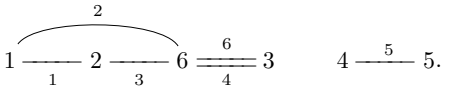
The formulas we are going to derive are power series whose terms are labeled by graphs. We define now the family of graphs that we are going to use and introduce notation.

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.

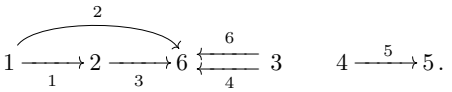
An example of a graph is

(3.1) 

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:



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 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 $\mathcal{P}_2 X$ denotes the set of subsets of X with two 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 $\{1, \ldots, E\} \to \mathcal{P}_2\{1, \ldots, V\}$, 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 Γ 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 Γ.

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_Γ of a labeled graph Γ is the order of the stabilizer of Γ 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 $s:\{1,\dots,E\} \to \mathcal{P}_2\{1,\dots,V\}$ 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").

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

Given a labeled graph Γ 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 substituting the vertices with $A_1,\dots A_V$, and letting every edge represent a Poisson tensor (as explained in §2.2). We denote $\lambda_\Gamma(A,\dots,A)$ simply by $\lambda_\Gamma(A)$.

For instance, if Γ is the labeled graph

$$1 \overset{1}{\text{———}} 2 \overset{2}{\underset{3}{=\!=}} 3$$

then $\lambda_\Gamma(C,D,A)$ is the expression in (2.3). And

$$\begin{aligned}\lambda_\Gamma(A) = A \to A \rightrightarrows A = A \xrightarrow{J^{\mu_1\nu_1}} A \underset{J^{\mu_3\nu_3}}{\overset{J^{\mu_2\nu_2}}{\rightrightarrows}} A \\ = A_{,\mu_1} J^{\mu_1\nu_1} A_{,\nu_1\mu_2\mu_3} J^{\mu_2\nu_2} J^{\mu_3\nu_3} A_{,\nu_2\nu_3}.\end{aligned}$$

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 $\widehat{A}$ 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 of B in terms of A.

The main step is to obtain an expression for an iterated star product $C_1 \star \cdots \star C_n$ for symbols C_i in terms of graphs. We do this in §4.1. Then in §4.2 we derive our first expression for B in terms of A.

Equation (4.4) at the end of §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 explicitely. There are only a few unlabeled graphs, but many labeled graphs. In §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 §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:

LEMMA 4.1. — *Let $C_1, \ldots, C_n \in \mathcal{C}^\infty(T^*\mathbb{R}^N)$ be symbols. Then*

$$C_1 \star \cdots \star C_n = \sum_{k=0}^{\infty} \frac{1}{k!} \Big(\frac{i\hbar}{2}\Big)^k \sum_{\substack{\text{labeled graphs } \Gamma \\ \text{with } n \text{ vertices} \\ \text{and } k \text{ edges}}} \lambda_\Gamma(C_1, \ldots, C_n). \tag{4.1}$$

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 two vertices and k edges.

When $n = 3$, for instance, we get the expression of Figure 1, where 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 $n = 0, 1, 2$.

$$
\begin{aligned}
A\star A\star A = A^3 &+ \frac{i\hbar}{2}(A\to A\quad A) + \frac{i\hbar}{2}(A\quad A\to A)\\
&+ \frac{i\hbar}{2}(\overset{\frown}{A\quad A\quad A}) + \frac{1}{2!}\Big(\frac{i\hbar}{2}\Big)^2(A\rightrightarrows A\quad A)\\
&+ \frac{1}{2!}\Big(\frac{i\hbar}{2}\Big)^2(A\quad A\rightrightarrows A) + \frac{1}{2!}\Big(\frac{i\hbar}{2}\Big)^2(\overset{\frown\frown}{A\quad A\quad A})\\
&+ \frac{1}{2!}\Big(\frac{i\hbar}{2}\Big)^2(A\overset{1}{\longrightarrow}A\overset{2}{\longrightarrow}A) + \frac{1}{2!}\Big(\frac{i\hbar}{2}\Big)^2(A\overset{2}{\longrightarrow}A\overset{1}{\longrightarrow}A)\\
&+ \frac{1}{2!}\Big(\frac{i\hbar}{2}\Big)^2(\overset{\frown}{A\underset{1}{\overset{2}{\longrightarrow}}A\quad A}) + \frac{1}{2!}\Big(\frac{i\hbar}{2}\Big)^2(\overset{\frown}{A\underset{2}{\overset{1}{\longrightarrow}}A\quad A})\\
&+ \frac{1}{2!}\Big(\frac{i\hbar}{2}\Big)^2(\overset{\frown}{A\quad A\underset{1}{\overset{2}{\longrightarrow}}A}) + \frac{1}{2!}\Big(\frac{i\hbar}{2}\Big)^2(\overset{\frown}{A\quad A\underset{2}{\overset{1}{\longrightarrow}}A}) + O(\hbar^3)\\
= A^3 &+ \frac{i\hbar}{2}(A\to A)A + \frac{3}{2}\Big(\frac{i\hbar}{2}\Big)^2(A\rightrightarrows A)A\\
&+ \frac{4-2}{2}\Big(\frac{i\hbar}{2}\Big)^2(A\to A\leftarrow A) + O(\hbar^3).
\end{aligned}
$$

Figure 1. *Illustration of formula* (4.1) *when* $n=3$

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

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

We can apply Lemma A.1 in Appendix A to $\lambda_\Gamma(C_1,\dots,C_n)\overset{\overrightarrow{[k]}}{\longrightarrow}C_{n+1}$ and we will get a sum over labeled graphs Γ' with $n+1$ vertices. They are built by starting with a labeled graph Γ with n vertices (labeled $1,\dots,n$) and E edges (labeled $1,\dots,E$), 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 Γ' 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

$$C_1 \star \cdots \star C_{n+1} = \sum_{\substack{\text{labeled graphs } \Gamma' \\ \text{with } n+1 \text{ vertices}}} \frac{1}{E'!} \Big(\frac{i\hbar}{2}\Big)^{E'} \lambda_{\Gamma'}. \qquad \square$$

4.2. 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. 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*

$$B(z_0) = \sum_{k=0}^{\infty} \frac{1}{k!} f^{(k)}(a_0)(A - a_0)^{\star k}(z_0). \tag{4.2}$$

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 $\widehat{C} := g(\widehat{A})$. Let $a_0 := A(z_0)$. If g has a zero of order m at a_0, then $C(z_0) = O(\hbar^{\frac{1}{2}m})$.*[(2)]

Proof of Lemma 4.3. — 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 $C = C_1 \star (A - a_0)^{*m}$. Since $(A(z) - a_0)|_{z=z_0} = O(\hbar)$, then $C(z_0) = O(\hbar^{\frac{1}{2}m})$. $\square$

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 for all m

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

Now we only need to substitute (4.1) into (4.2) to get an expression for B in terms of graphs:

$$B(z_0) = \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}\big(A(z_0)\big) \sum_{k=0}^{\infty} \sum_{\substack{\text{labeled graphs } \Gamma \\ \text{with } n \text{ vertices} \\ \text{and } k \text{ edges}}} \frac{1}{k!} \Big(\frac{i\hbar}{2}\Big)^k \lambda_\Gamma(A - a_0)(z_0). \tag{4.3}$$

(2) Actually, we can do better: $C(z_0) = O(\hbar^{\frac{2}{3}m})$.

In order to calculate $\lambda_\Gamma(A-a_0)(z_0)$ we need to write the symbol $A-a_0$ at every vertex of Γ. 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:

$$B = \sum_{\substack{\text{reduced labeled}\\ \text{graphs } \Gamma}} \frac{1}{E!}\Big(\frac{i\hbar}{2}\Big)^E \frac{f^{(V)}(A)}{V!}\lambda_\Gamma(A). \tag{4.4}$$

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 (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).

Remark. — Our results (equation (4.4) and the calculations in the next two subsections) bear a similarity with Feynmann diagram expansions in stationary phase method. This is not accidental. We have used the explicit form of the Moyal product (2.2), which is derived from the Weyl-Wigner correspondance (2.1) through a stationary phase expansion. One can actually forget that we know (2.2), and use stationary phase expansion to obtain the iterated star products (Lemma 4.1). That is equivalent to rederiving (2.2) from (2.1).

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).

Equation (4.4) can be rewritten as

$$B = \sum_{\substack{\text{reduced} \\ \text{graphs } [\Gamma]}} \frac{1}{E!} \Big(\frac{i\hbar}{2}\Big)^E \frac{f^{(V)}(A)}{V!} \sum_{\Gamma' \in [\Gamma]} \lambda_{\Gamma'}(A). \tag{4.5}$$

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

Define

$$c_\Gamma = \sum_{\substack{\Gamma' \text{is a reordering of} \\ \text{the vertices of } \Gamma}} (-1)^{\#\text{ of arrows inverted going from } \Gamma \text{ to } \Gamma'}. \tag{4.6}$$

That is, we start with a labeled graph Γ. Then, we consider the $V!$ possible ways of numbering the vertices of the graph with $1, 2, \ldots, V$. 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

$$\sum_{\Gamma' \in [\Gamma]} \lambda_{\Gamma'}(A) = \frac{E!}{S_\Gamma} c_\Gamma \lambda_\Gamma(A) \tag{4.7}$$

where S_Γ 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_Γ. 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 Γ is the graph $\bullet \to \bullet \to \bullet$, then the contribution from renumbering the vertices is

$$\begin{aligned} c_\Gamma &= \overset{1\to2\to3}{(-1)^0} + \overset{1\to3\leftarrow2}{(-1)^1} + \overset{2\leftarrow1\to3}{(-1)^1} + \overset{2\to3\leftarrow1}{(-1)^1} + \overset{3\leftarrow1\to2}{(-1)^1} + \overset{3\leftarrow2\leftarrow1}{(-1)^2} \\ &= -2. \end{aligned}$$

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

$$B = \sum_{\substack{\text{reduced} \\ \text{graphs } [\Gamma]}} \Big(\frac{i\hbar}{2}\Big)^E \frac{c_\Gamma}{S_\Gamma} \frac{f^{(V)}(A)}{V!} \lambda_\Gamma(A). \tag{4.8}$$

Notice how c_Γ 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_Γ for a particular graph is actually very easy. See Appendix C, which includes the value of c_Γ and S_Γ for all reduced, connected graphs with 2 or 4 edges. Thanks to Lemma C.1 we only need to consider graphs Γ 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

$$B = \Big[\sum_{\substack{\text{reduced} \\ \text{graphs } [\Gamma]}} \Big(\frac{i\hbar}{2}\Big)^E \frac{c_\Gamma}{S_\Gamma} \lambda_\Gamma(A) \frac{D^V}{V!} \Big] f(A) \tag{4.9}$$

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

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

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

$$\sum_{x \in \mathcal{G}} \mathcal{O}(x) = \exp\Big[\sum_{x \in \mathcal{G}_0} \mathcal{O}(x) \Big]. \tag{4.11}$$

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_Γ is the order of the symmetry group of the diagram and $\mathcal{M}$ is a multiplicative function

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

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

In our case,

- $\mathcal{G} =$ reduced graphs,
- $\mathcal{G}_0 =$ reduced, connected, non-empty graphs,
- $S = \mathcal{C}^\infty(T^*\mathbb{R}^N)$,
- $\mathcal{M}([\Gamma]) = \left(\frac{1}{2} i\hbar\right)^E c_\Gamma \lambda_\Gamma(A) D^V / V!$.

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

$$\frac{c_\Gamma}{V!} = \frac{c_{\Gamma_1}}{V_1!} \cdots \frac{c_{\Gamma_n}}{V_n!}.$$

Hence, using (4.11) in (4.9):

$$B = \Big[\exp \sum_{\substack{\text{connected} \\ \text{reduced} \\ \text{non-empty graphs } [\Gamma]}} \Big(\frac{i\hbar}{2} \Big)^E \frac{c_\Gamma}{S_\Gamma} \lambda_\Gamma(A) \frac{D^V}{V!} \Big] f(A). \tag{4.12}$$

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 $\widehat{A}_1, \ldots, \widehat{A}_n$ 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 $\widehat{B} = F(\widehat{A}_1, \ldots, \widehat{A}_n)$ 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

$$B = \sum_{\substack{\text{reduced} \\ \text{graphs } [\Gamma]}} \Big(\frac{i\hbar}{2}\Big)^E \frac{c_\Gamma}{S_\Gamma} \frac{\partial_{i_1} \cdots \partial_{i_V} F(A)}{V!} \lambda_\Gamma(A_{i_1}, \ldots, A_{i_V}). \tag{5.1}$$

For instance the first few terms of (4.8) are

$$B = f(A) - \frac{\hbar^2}{4}\Big[\frac{1}{2} A \rightrightarrows A \, \frac{f''(A)}{2!} + A \to A \leftarrow A \frac{f'''(A)}{3!}\Big] + O(\hbar^4)$$

and the first few terms of (5.1) are

$$B = F(A) - \frac{\hbar^2}{4}\Big[\frac{1}{2} A_i \rightrightarrows A_j \, \frac{\partial_i \partial_j F(A)}{2!} + A_i \to A_j \leftarrow A_k \, \frac{\partial_i \partial_j \partial_k F(A)}{3!}\Big] + O(\hbar^4).$$

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, correspondances 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

$$C \star D = \sum_{k=0}^{\infty} \frac{1}{k!} \Big(\frac{i\hbar}{2}\Big)^k \{C, D\}_k. \tag{5.2}$$

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 4.3 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 $C_1 \star \cdots \star C_n$ 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:

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

where $u_p(x) = \mathrm{e}^{ip\cdot x/\hbar}$. In that case, the star product has the form of (5.2) with $\{C, D\}_k := \partial^k_{p_j} C \partial^k_{x^j} D$. Lemma 4.3 still holds and, if we change the meaning of "$\rightarrow$", 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 $\lambda_\Gamma(A)$ from a labeled graph Γ, 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 $C \rightarrow D = -(C \leftarrow D)$. 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 4.1 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 ω_Γ associated to every diagram Γ 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 $\widehat{A} = \widehat{I}$, 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 2×2 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 $\widehat{A}$. Then

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

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:

$$\begin{aligned}
\Delta_k &= \bullet \to \bullet \to \cdots \to \bullet \qquad (2k \text{ edges}, k \geq 1),\\
\Lambda_k &= \begin{array}{ccccccc} \bullet & \to & \bullet & \to & \cdots & \to & \bullet \\ \uparrow & & & & & & \downarrow \\ \bullet & \leftarrow & \bullet & \leftarrow & \cdots & \leftarrow & \bullet \end{array} \qquad (2k \text{ edges}, k \geq 1).
\end{aligned}$$

In words, Δ_k consists of $2k+1$ vertices and $2k$ edges joined forming a line. Its symmetry group has order 2. Λ_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:

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

Since Q is symmetric and J is skew-symmetric, their product QJ is traceless. Hence $(QJ)^2 = -\det(QJ)\,\mathrm{id}$. Write $\omega^2 := \det(QJ) = \det(Q)$. Then

$$\begin{aligned}
\lambda_{\Delta_k} &= (-1)^k \omega^{2k} z^\mu Q_{\mu\nu} z^\nu = (-1)^k \omega^{2k} 2A,\\
\lambda_{\Lambda_k} &= (-1)^k \omega^{2k} \operatorname{trace}(\mathrm{id}) = (-1)^k \omega^{2k} 2.
\end{aligned}$$

As for the coefficients c_{Δ_k} and c_{Λ_k}, Fact 5) in Appendix C gives us the relation $c_{\Lambda_k} = -2k\, c_{\Delta_{k-1}}$.

We now plug all this values in (4.12) to obtain, for a general function f and a quadratic symbol A:

$$\begin{aligned}
B = \Big(\exp\Big[A \sum_{k=0}^{\infty} \Big(\frac{i\hbar}{2}\omega\Big)^{2k} |c_{\Delta_{k+1}}| \frac{D^{2k+1}}{(2k+1)!} \\
+ \sum_{k=0}^{\infty} \Big(\frac{i\hbar}{2}\omega\Big)^{2k} |c_{\Delta_k}| \frac{D^{2k}}{(2k)!}\Big]\Big) f(A).
\end{aligned} \tag{6.1}$$

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

$$c_{\Delta_k} = -\sum_{j=0}^{k-1} \binom{2k}{2j+1} c_{\Delta_j} c_{\Delta_{k-j-1}}. \tag{6.2}$$

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

$$\tan x = \sum_{k=0}^{\infty} \frac{|c_{\Delta_k}|}{(2k+1)!} x^{2k+1}. \tag{6.3}$$

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

$$y' = 1 + y^2. \tag{6.4}$$

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

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:

$$\widehat{B} = f(\widehat{A}), \quad B = \sec \frac{i\hbar\omega D}{2} \exp\Big[\frac{2A}{i\hbar\omega} \tan \frac{i\hbar\omega D}{2} - AD\Big] f(A). \tag{6.5}$$

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

$$\widehat{B} = \mathrm{e}^{-it\widehat{A}/\hbar}, \quad B = \sec \frac{t\omega}{2} \exp\Big[\frac{2A}{i\hbar\omega} \tan \frac{t\omega}{2}\Big]. \tag{6.6}$$

Equation (6.6) is derived in [16] in a different manner, and also 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 (6.6), the *symbol* of the time evolution operator of the harmonic oscillator. Such kernel is known as the *Mehler kernel* and can be obtained from (6.6) by means of a Fourier transform.

7. Application: Bohr-Sommerfeld rules.

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

Colin de Verdière [6] 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 inspried by Voros [19] and a similar method had been previously used by Argyres [2].

Let $\widehat{H}$ 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 $\widehat{H}$. Assume H has a regular minimum at a point. Under certain extra assumptions on the symbol H (see [6]), the eigenvalues of $\widehat{H}$ are given by the solutions E to

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

with $n \in \mathbb{Z}$. To solve the previous equation, write $E = \sum \hbar^k E_k$ 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 $\widehat{H}$.

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

$$S_0(E) = \int_{\gamma_E} p\,\mathrm{d}x, \quad S_1(E) = \pi.$$

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

The main result in [6] is the following:

$$S_j(E) = \sum_{\ell=2}^{L(j)} \frac{(-1)^{\ell-1}}{(\ell-1)!} \Big(\frac{\mathrm{d}}{\mathrm{d}E}\Big)^{\ell-2} \int_{\gamma_E} P_{j,\ell}(x,p)\,\mathrm{d}t,$$

where t is the parametrization of γ_E by the time evolution

$$\mathrm{d}x = H_p\,\mathrm{d}t, \quad \mathrm{d}p = -H_x\,\mathrm{d}t$$

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

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

Looking back at our formula for the symbol for the function of an operator (1.1) and using it for the function $f(y) = (a-y)^{-1}$, we see that $L_j = \frac{3}{2}j + 1$ and the polynomials $P_{j,\ell}$ can actually be defined in terms of graphs:

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

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

$$2\pi\big(n - \tfrac{1}{2}\big)\hbar = S_0(E) + \sum_{\substack{\text{reduced graphs } \Gamma \\ \text{with } E_\Gamma > 0}} \Big(\frac{i\hbar}{2}\Big)^{E_\Gamma} \frac{(-1)^{V_\Gamma}}{V_\Gamma!} \Big(\frac{\mathrm{d}}{\mathrm{d}E}\Big)^{V_\Gamma - 1} \frac{c_\Gamma}{S_\Gamma} \int_{\gamma_E} \lambda_\Gamma(H)\,\mathrm{d}t. \tag{7.2}$$

Here E is an eigenvalue of H, whereas E_Γ is the number of edges of a graph Γ.

One has $S_j(E) = 0$ 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 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 five graphs (those where every vertex has at least two edges):

$$\begin{aligned} 2\pi(n - \tfrac{1}{2})\hbar = S_0(E) \;&- \frac{\hbar^2}{4}\Big[\frac{1}{2!\cdot 6}\,\frac{\mathrm{d}}{\mathrm{d}E}\int_{\gamma_E} (H \rightrightarrows H)\,\mathrm{d}t\Big] \\ &+ \frac{\hbar^4}{16}\Big[\frac{1}{2!\cdot 120}\,\frac{\mathrm{d}}{\mathrm{d}E}\int_{\gamma_E} (H \overrightarrow{\overrightarrow{[4]}} H)\,\mathrm{d}t \\ &+ \frac{1}{4!\cdot 12}\Big(\frac{\mathrm{d}}{\mathrm{d}E}\Big)^3 \int_{\gamma_E} (H \rightrightarrows H)^2\,\mathrm{d}t \\ &- \frac{1}{3!\cdot 15}\Big(\frac{\mathrm{d}}{\mathrm{d}E}\Big)^2 \int_{\gamma_E} \begin{array}{c} H \rightrightarrows H \\ \searrow\ \downarrow \\ \quad H \end{array} \mathrm{d}t \\ &+ \frac{1}{4!\cdot 15}\Big(\frac{\mathrm{d}}{\mathrm{d}E}\Big)^3 \int_{\gamma_E} \begin{array}{c} H \to H \\ \uparrow\ \ \downarrow \\ H \leftarrow H \end{array} \mathrm{d}t \\ &- \frac{1}{3!\cdot 12}\Big(\frac{\mathrm{d}}{\mathrm{d}E}\Big)^2 \int_{\gamma_E} (H \rightrightarrows H \rightrightarrows H)\,\mathrm{d}t\Big] + O(\hbar^6). \end{aligned} \tag{7.3}$$

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:

$$2\pi\big(n - \tfrac{1}{2}\big)\hbar = S_0(E) - \frac{\hbar^2}{m}\,\frac{1}{24}\,\frac{\mathrm{d}}{\mathrm{d}E}\int_{\gamma_E} V''(x)\,\mathrm{d}t + \frac{\hbar^4}{m^2}\,\frac{1}{2^7 3^2}\Big[\frac{7}{5}\Big(\frac{\mathrm{d}}{\mathrm{d}E}\Big)^3\int_{\gamma_E}\big[V''(x)\big]^2\,\mathrm{d}t - \Big(\frac{\mathrm{d}}{\mathrm{d}E}\Big)^2\int_{\gamma_E} V^{(4)}(x)\,\mathrm{d}t\Big] + O\Big(\frac{\hbar^6}{m^3}\Big).$$

The disadvantage of this method is that it does not generalize to the multidimensional case $N > 1$. Cargo & 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.

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A. 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 Γ be a labeled graph with V vertices and E edges.*

Let $D, C_1, \dots, C_V$ be symbols. Then

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

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

- *the labeled graph Γ (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 Γ 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:

$$\begin{aligned}(C \underset{1}{\longrightarrow} D) \overrightarrow{\overrightarrow{}} E &= C \overset{\overset{2}{\curvearrowright}}{\underset{1}{\longrightarrow}} D \overset{3}{\searrow} E + C \underset{1}{\longrightarrow} D \overrightarrow{\overrightarrow{\substack{2\\3}}} E \\ &\quad + C \overset{\overset{2}{\curvearrowright}}{\underset{1}{\longrightarrow}} D \underset{3}{\longrightarrow} E + C \overset{\overset{3}{\curvearrowright}}{\underset{1}{\longrightarrow}} D \underset{2}{\longrightarrow} E \\ &= C \overset{\curvearrowright}{\longrightarrow} D \overset{\curvearrowright}{} E + C \longrightarrow D \overrightarrow{\overrightarrow{}} E + 2\, C \overset{\curvearrowright}{\longrightarrow} D \longrightarrow E.\end{aligned}$$

B. An alternative derivation of (4.4).

As we mentioned in the introduction and in §7, 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 $\widehat{R}_a := (a - \widehat{A})^{-1}$ with symbol R_a. Then we use Helffer-Sjöstrand's formula [10] as a spectral theorem:

$$\widehat{B} = f(\widehat{A}) = -\frac{1}{\pi} \int_{\mathbb{C}} \widehat{R}_z \partial_{\overline{z}} \widetilde{f}(z)\, \mathrm{d}x\, \mathrm{d}y.$$

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

$$B = -\frac{1}{\pi} \int_{\mathbb{C}} R_z \partial_{\overline{z}} \widetilde{f}(z)\, \mathrm{d}x\, \mathrm{d}y. \tag{B.1}$$

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

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

and, since $\widehat{R}_a(a - \widehat{A}) = 1$, 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*

$$h_a(A) = \sum_{\substack{\text{reduced labeled} \\ \text{graphs } \Gamma}} \frac{1}{E!} \Big(\frac{i\hbar}{2} \Big)^E \frac{\lambda_\Gamma(A)}{(a - A)^{V+1}} \tag{B.2}$$

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_Γ and S_Γ.

Calculating c_Γ 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:

$$\widehat{B} = f(\widehat{A}) = \int_\gamma \frac{\mathrm{d}a}{2\pi i} f(a) \widehat{R}_a, \quad B = \int_\gamma \frac{\mathrm{d}a}{2\pi i} f(a) R_a,$$

which will lead to the same results, but it is only valid for analytic functions f. The path γ is around the spectrum of $\widehat{A}$.

FACTS:

1) $c_\bullet = 1$.

2) $c_\Gamma = 0$ *if* E *is odd.*

This is due to a symmetry property. If we denote by Γ *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* $\left(\begin{smallmatrix} 1,2,\dots,V \\ V,\dots,2,1 \end{smallmatrix}\right)$, *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* Γ_i *has* V_i *vertices,* $\Gamma_i \neq \Gamma_j$ *for* $i \neq j$, *and* $\Gamma = \Gamma_1 + \dots + \Gamma_n$ *is the topological sum with* $V = V_1 + \dots + V_n$ *vertices, then*

$$c_\Gamma = \frac{V!}{V_1! \dots V_n!} c_{\Gamma_1} \cdots c_{\Gamma_n}. \tag{C1}$$

4) c_Γ *does not change if we erase two edges with the same endpoints.*

For instance $c_{1\to 2 \rightrightarrows 3\to 4} = c_{1\to 2 \quad 3\to 4}$.

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

$$\begin{aligned} \Gamma &= \bullet \to p \to \bullet \rightrightarrows \bullet, \\ \Gamma - p &= \bullet \qquad\quad \bullet \rightrightarrows \bullet. \end{aligned}$$

Then

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

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

In particular, putting together Facts 2) and 3) we get:

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

The reduced, connected graphs with two and four edges, and for each of them the value of c_Γ and S_Γ are presented Figure 2.

Γ	E	V	S_Γ	c_Γ
	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

Figure 2. *The reduced, connected graphs with two and four edges*

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

Using any of the equations derived in §4, we write down (see Figure 3) 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.

$$
\begin{aligned}
\widehat{B} &= f(\widehat{A}),\\
B &= f(A) - \frac{\hbar^2}{4}\Big[\frac{A \rightrightarrows A}{2}\,\frac{f''(A)}{2!} + A \to A \leftarrow A\frac{f'''(A)}{3!}\Big]\\
&\quad + \frac{\hbar^4}{16}\Big[\frac{A \overset{\overrightarrow{[4]}}{\to} A}{24}\,\frac{f''(A)}{2!}\\
&\quad + \Big(\frac{A \overset{\overrightarrow{[3]}}{\to} A \leftarrow A}{3} + \frac{1}{2}\begin{array}{c} A \rightrightarrows A\\ \searrow\ \downarrow\\ \quad A\end{array} + \frac{3}{4}A \rightrightarrows A \rightrightarrows A\Big)\frac{f'''(A)}{3!}\\
&\quad + \Big(\frac{3}{4}(A \rightrightarrows A)^2 + \begin{array}{c} A \to A\\ \uparrow\quad \downarrow\\ A \leftarrow A\end{array} + 4A \rightrightarrows A \to A \leftarrow A\\
&\qquad\qquad + 2A \rightrightarrows \begin{array}{c} A \to A\\ \downarrow\\ A\end{array}\Big)\frac{f^{(4)}(A)}{4!}\\
&\quad + \Big(8\begin{array}{c} A \to A \to A\\ \quad\downarrow\\ A \leftarrow A\end{array} + \begin{array}{c} A \to A \leftarrow A\\ \uparrow\ \nwarrow\\ A\quad A\end{array}\\
&\qquad + 5(A \rightrightarrows A)(A \to A \leftarrow A)\\
&\qquad\qquad + 4A \leftarrow A \to \begin{array}{c} A \to A\\ \downarrow\\ A\end{array}\Big)\frac{f^{(5)}(A)}{5!}\\
&\quad + 10(A \to A \leftarrow A)^2\frac{f^{(6)}(A)}{6!}\Big] + O(\hbar^6).
\end{aligned}
$$

Figure 3. *Symbol of a function of an operator up to order* 4 *in* $\hbar$

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